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Radiation for the Analysis of Molecular Structures with Non-Crystalline Symmetry: Modelling and Representation Theoretic Design

Dominik Jüstel

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Vorsitzender:		Univ.-Prof. Dr. Martin Brokate
Prüfer der Dissertation:	1.	Univ.-Prof. Gero Friesecke, Ph. D.
	2.	Univ.-Prof. Dr. Rupert Lasser
	3.	Prof. Richard D. James, Ph. D. University of Minnesota, Minneapolis, USA (schriftliche Beurteilung)

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Dedicated to my late mother

Abstract

X-ray crystallography is the main tool for the structural analysis of molecules today. In this dissertation, an extension of the principles of this method to a general class of highly symmetric structures is studied by introducing a criterion for the design of suitable radiation. The solutions to these design equations are explicitly determined for a class of nanotube-like structures. Under certain conditions, a generalization of the von Laue condition of X-ray crystallography can be formulated. Tools include harmonic analysis and representation theory.

Zusammenfassung

Die Röntgenstrukturanalyse ist heutzutage die zentrale Methode zur Bestimmung der Struktur von Molekülen. Die vorliegende Arbeit behandelt die Verallgemeinerung der Prinzipien, die dieser Methode zugrunde liegen, auf eine allgemeine Klasse von hochgradig symmetrischen Strukturen. Ein theoretisches Kriterium für das Design strukturadaptierter elektromagnetischer Strahlung wird formuliert und für eine Klasse von Strukturen explizit gelöst. Unter bestimmten Bedingungen kann die von-Laue-Bedingung der Kristallstrukturanalyse verallgemeinert werden. Dabei werden Methoden der harmonischen Analysis sowie der Darstellungstheorie verwendet.

Contents

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Introduction

X-ray Crystallography. Before the invention of X-ray crystallography, structural analysis of molecular structures at the atomic scale was limited to theoretical considerations. This situation changed dramatically, when in 1912, Max von Laue, Walter Friedrich and Paul Knippig first demonstrated the diffraction of X-rays by crystals [FKL12] in Wilhelm Röntgen's laboratory in Munich [Ewa62]. Von Laue's team was awarded the 1914 Nobel Prize for Physics for this discovery. Not only did their experiment clarify the nature of electromagnetic radiation, it also was quickly realized that the highly structured diffraction patterns bear the possibility to reconstruct the atomic structure of a crystal.

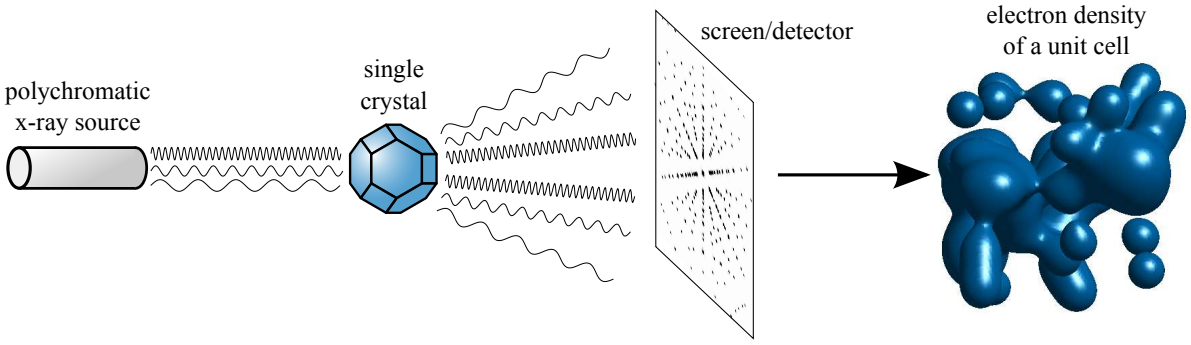


FIGURE 0.1. Visualization of the classic von Laue method of X-ray Crystallography. Polychromatic X-rays are diffracted by a single crystal, resulting in a structured peak pattern on a screen. The electron density of a unit cell of the crystal can be recovered (up to the phase problem) from the measured intensity of the outgoing radiation.

When measuring the intensity of the scattered radiation, a part of the information contained in the field is lost. This problem is called the phase problem and makes the reconstruction a mathematically challenging task.

William Lawrence Bragg and his father William Henry Bragg solved the first simple crystal structures in the following years [Bra13], earning them the 1915 Nobel Prize for Physics for their contributions. The list of Nobel laureates related to X-ray crystallography is long. Most notably, Herbert Hauptman and Jerome Karle won the 1985 Nobel Prize for Chemistry for their mathematical work on the phase problem [HK53] that led

to the reconstruction of more complex structures and made X-ray crystallography the central tool for the structural analysis of biomolecules, and Dan Shechtman won the 2011 Nobel Prize for Chemistry for his discovery of quasicrystals [SBGC84] that was motivated by X-ray diffraction data. This illustrates the significance of X-ray crystallography for the natural sciences.

The major drawback of X-ray crystallography is its exclusive applicability to crystal structures. Because of this restriction, a lot of effort is put in the crystallization of structures that naturally do not form crystals [GEA11]. A method to analyze the structure of macromolecules without the need to crystallize them is therefore of great interest.

Coherent Diffraction Imaging. In 1999, the possibility of the extension of X-ray diffraction methods for the analysis of non-crystalline samples was first demonstrated by Jianwei (John) Miao et al. [MCKS99]. The method is based on an observation made by David Sayre [Say52-2].

Coherent Diffraction Imaging (CDI) uses highly brilliant third generation X-ray sources to illuminate a general sample. The continuous diffraction pattern is then used to reconstruct a projection of the sample. The time gap between the idea and its realization has two reasons – the need of high-quality sources and detectors on the one hand, and for algorithms and computational power to solve the corresponding high-dimensional phase problem for reconstruction on the other hand.

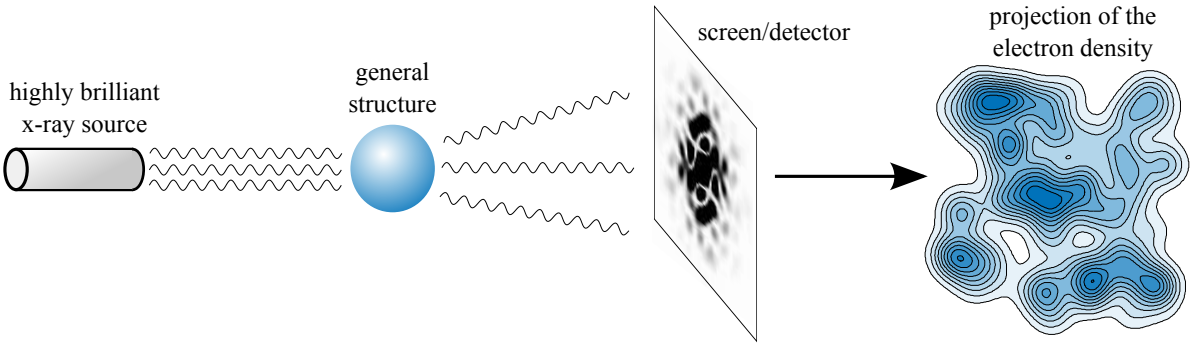


FIGURE 0.2. Visualization of Coherent Diffraction Imaging. Monochromatic X-rays are diffracted by a specimen. A projection of the electron density of the sample can be recovered (up to the phase problem) from the measured intensity of the outgoing radiation.

Even though CDI is a very promising method, it currently only achieves a resolution of a few nanometers and is hence not useful for the analysis of molecular structures. The resolution of the reconstruction depends on the quality of the source and the resolution of the detector, as well as on the energy of the used radiation. For the analysis of

biomolecules, this last point is crucial, because at high energies the specimen is destroyed. Methods like femtosecond diffractive imaging [CEA06] try to avoid the destruction of the specimen by a short exposure time. Many other methods related to CDI were proposed, e.g. Ptychography [TEA08], Fresnel coherent diffractive imaging [WEA06] or massively parallel X-ray holography [MEA08], just to name a few.

All these methods have one thing in common. They do not use any structural information, even though, many interesting structures in biology and nanotechnology are highly symmetric. The idea of this dissertation is to exploit these symmetries by designing new kinds of radiation for the analysis of molecular structures.

The von Laue Condition and Radiation Design. X-ray Crystallography achieves atomic resolution for crystals with a few hundred atoms per unit cell with little technical requirements [US99]. For simple crystals, atoms can even be resolved using a simple X-ray tube. The reason for this superiority in resolution is of theoretical nature and lies in the intimate relationship between the periodic structure of a crystal and the translation invariance of plane wave radiation. It leads to constructive interference of the outgoing waves in a discrete set of directions and, more importantly, to destructive interference else. As a consequence, on a screen in the far-field, a highly structured peak pattern is produced by the outgoing radiation (see Figure 0.1). This pattern allows direct reconstruction of the translational symmetries of the crystal – a fact that is mathematically expressed by the von Laue condition.

This idea, that plane waves are the right choice for the analysis of crystals because of the relationship of the symmetries of radiation and structure, is the starting point for the theory developed in this dissertation.

When assuming that the structure under consideration is highly symmetric without necessarily being a crystal, a natural question to ask is the following. Is there a certain kind of electromagnetic radiation that reflects the symmetries of the structure in the same way as plane waves do for crystals? And if there is, can we somehow reconstruct the symmetries and/or the structure of the sample from the diffraction patterns? This problem is called radiation design.

Time-Harmonic Maxwell Equations. To solve the design problem, the first thing is to understand what is meant by 'radiation'. Mathematically, we look for solutions to Maxwell's equations. These equations describe the behavior of electromagnetic fields in the presence of electric charge and current densities. An important property of plane waves is their periodicity in time that leads to harmonic oscillations of an illuminated charge density. We keep this favorable property by considering time-harmonic solutions

to Maxwell's equations as our radiation space. This natural choice reduces the design problem to the spatial part of the electromagnetic field.

A central contribution of this dissertation is a mathematical model of the scattering of time-harmonic radiation. The resulting formula for the outgoing field was derived in collaboration with Gero Friesecke and Richard D. James. Applying this formula to the case of plane waves being scattered by a crystal, the theory behind X-ray crystallography and CDI is recovered.

Objective Structures. The natural generalization of crystal structures was studied by Richard D. James in [Jam06]. Objective structures are molecular structures with the property that every atom 'sees' the same atomic environment. This kind of objectivity gives these highly symmetric structures their name. Realizations of objective structures are found in many areas of science. In nanotechnology, graphene, carbon nanotubes, and fullerenes like the buckyball are examples. Qualitatively, also biological structures like DNA or α-helices in proteins can be viewed as objective structures.

Rephrasing the definition in a group theoretic way makes objective structures accessible to mathematical theory. The translation group that defines the symmetries of crystal structures is generalized to the Euclidean group of isometries of three-dimensional space. This group, for example, also contains rotations, reflections, and screw displacements that appear as symmetries of objective structures.

The Design Equations. Knowing the radiation space and a class of structures to consider, we need a design criterion that relates the symmetries of structure and radiation. The classic case of plane waves and crystals guides the way. The plane waves can be characterized as the eigenfunctions of the translation group in our radiation space. At the same time, the class of crystal structures is characterized as the objective structures that are generated by a discrete closed subgroup of the translation group.

The generalization is now straightforward. Take an abelian closed subgroup G of the Euclidean group that plays the role of the translation group. This group is called the design group. It defines the structures to consider as the objective structures generated by a discrete closed subgroup of G and the radiation to use as the eigenfunctions of the action of G on our radiation space. This design criterion is summarized in the design equations. These need to be solved to find radiation that induces resonant oscillations of the molecules of the analyzed structure.

Nanotubes and Twisted Waves. A central example, that is worked out in detail, is the design group that consists of all rotations and screw displacements about, and all translations along a fixed axis. The corresponding structures are called nanotube

structures. A carbon nanotube is an example of such a structure when considered as an objective structure with a molecule that consists of two atoms.

The design equations are solved explicitly and define an interesting form of radiation. We call the solutions twisted waves as they propagate helically in space and share many properties of plane waves. The scattering of these waves by nanotube structures results in a diffraction pattern on a screen that does not directly allow reconstruction of the symmetries of the structure. However, when measuring the outgoing intensity in axis direction as a function of the radiation parameters, we find a twisted von Laue condition. The symmetries can directly be recovered, while the reconstruction of the charge density reduces to a scalar phase problem.

A Generalized von Laue Condition. The treatment of the general case needs some preliminary work. We coarsly classify the abelian design groups and find that most groups are either combinations of a translation or a nanotube group with a compact group, or are themselves compact.

When considering discrete or one-dimensional design groups, the solution spaces of the design equations are very big, making it necessary to select a subset that still makes reconstruction possible. The observation that twisted waves are projections of plane waves onto invariant subspaces of the radiation space motivates the definition of symmetry-adapted waves. Two mathematical tools that are introduced to study these waves are the Wigner projections and a generalization of the Zak transform.

The scattering of symmetry-adapted waves by the corresponding class of objective structures is related to an integral transform of the charge density. We call this transform the wave transform. It plays the role that the Fourier transform plays in the classic case.

Its scalar counterpart – the scalar wave transform – is of mathematical interest in its own right. It yields a symmetry-frequency decomposition of a function and has many nice properties.

The main theorem is a generalized von Laue condition. If the orthogonal part of the design group fixes an axis, the intensity measurements in axis direction allow direct symmetry reconstruction. In this case, the reconstruction of the charge density reduces to a phase problem for the scalar wave transform.

Many ideas can be generalized to non-abelian compact groups. However, a von Laue condition cannot be formulated.

Reader's Guide. Part 1 that treats the classic theory is written in a less formal style as it is intended as an introduction to the different topics surrounding the problem of reconstruction from diffraction patterns. Some basic concepts, notations and results from

Fourier analysis, Maxwell's equations, and Crystallography are included as Appendices at the end of the text. For a detailed treatment of X-ray physics, Crystallography, and reconstruction algorithms, we refer to [AM11], [GEA11], and [Thi07].

The fist part ends with an example that motivates the need for new kinds of radiation by illustrating the problems that arise when the symmetries of structure and radiation are not related.

Part 2 starts with the formulation of the design problem that is based on a model of the scattering of time-harmonic radiation. The design criterion that relates the symmetries of strucure and radiation is then solved explicitly for a special class of structures. This part of the dissertation (Chapters 3 and 4) is joint work with Gero Friesecke and Richard D. James.

From a more abstract point of view, the ideas are then generalized to classes of structures that are defined via abelian or compact isometry groups. The treatment uses methods from harmonic analysis and representation theory.

To improve the readability of the text, an index of the used notation with short explanations is added at the very end.

Part 1

Analysis of Molecular Structures by Plane Wave Diffraction

The standard method for the analysis of molecular structures today is the reconstruction from X-ray diffraction patterns. The discovery of the highly structured diffraction of plane waves by crystals that resulted in the development of X-ray crystallography depended on the following two facts.

First, plane waves appear naturally as the far-field limit of spherical waves that are generated by oscillating charges. So, a simple X-ray tube essentially produces plane waves. Second, most solids form crystals, making these structures available for experiments.

The relationship between the symmetries of radiation and structure leads to a highly structured and sharply peaked diffraction pattern. The crucial observation is the following. It is possible to directly reconstruct symmetry information from the structure of this diffraction pattern. In addition, the intensity of the peaks is related to the Fourier transform of the electron density in a unit cell of the crystal. This fact makes reconstruction of the electron density possible in many cases and led to the development of generalizations of X-ray crystallography to general non-crystalline structures. By illuminating an arbitrary sample with highly brilliant X-rays, the projection of the electron density in propagation direction can be reconstructed from intensity measurements in the far field.

Before we begin to generalize the methods for the analysis of molecular structures by plane wave radiation, we need to understand the mathematical theory behind these methods and work out the reasons for their success. This is the main goal of this first part.

However, it is not a mere summary of the existing theory, but contains some new results and insights. In particular, the theory of X-ray crystallography and CDI is inferred from a general result on the scattering of time-harmonic radiation that will be derived in Chapter 3. To gain a qualitative understanding of the diffraction patterns, the information that is contained in the different features of the patterns is analyzed.

The inverse scattering problem of reconstructing a structure from its diffraction pattern is in general not uniquely solvable. Since only the intensity is measured, the phase information of the outgoing radiation is lost. Without any additional assumptions, there is no hope of finding the right phases. The fact that in many situations the problem is solvable when restricting to non-negative or compactly supported structures is still not fully understood. We make some progress in this area by identifying different reasons for non-uniqueness of the solution and giving some mathematical insight on the constraints that are mainly used.

Finally, the standard algorithms for phase retrieval are presented. Simple algorithms like the Gerchberg-Saxton scheme that iteratively enforces the right intensity on the Fourier side and non-negativity and/or support constraints on the direct side have been

greatly improved to more sophisticated projection-based algorithms and gradient flow methods.

This first part will be followed by a central example that motivates the need of a different kind of radiation than plane waves, as it shows that a mismatch of the symmetries of radiation and structure results in an extension of the phase problem to structural information while at the same time making phase retrieval much harder by greatly enlarging the dimension of the reconstruction problem.

CHAPTER 1

Scattering of Plane Waves

The interaction of electromagnetic fields and electric charges is classically described by Maxwell's equations and the Lorentz force. Consequently, the scattering of plane waves by a charge density is analyzed in this framework. The line of thought in this chapter is as follows.

First, plane waves are introduced as solutions of the homogeneous Maxwell equations, i.e. when no charge or current is present. Properties like frequency, wavelength, phase, polarization and intensity of a plane wave are defined and justify the usual intuitive understanding of plane waves.

Next, when an electric charge distribution is present, it feels the Lorentz force that is exerted by a plane wave. The non-transient solution of this periodic forcing is an oscillating charge that itself produces an electromagnetic field as dictated by Maxwell's equations. These are solved by the Liénard-Wiechert potentials. In an appropriate limit, we obtain a formula for the electromagnetic field resulting from the scattering event. A rigorous derivation of this scattering formula will be given in Chapter 3 for general time-harmonic radiation. The resulting outgoing field is a modulated spherical wave with the same frequency as the incoming wave (elastic scattering) and an intensity that is up to a constant and dependencies on distance and direction the absolute value squared of the Fourier transform of the charge density evaluated at a certain point.

When the analyzed structure is a crystal, the reconstruction of structural information from the diffraction pattern is called X-ray Crystallography. In this case, the diffraction pattern consists of sharp peaks whose location contains information on the translational symmetries of the crystal. This fact is mathematically expressed by the von Laue condition that can be directly inferred from the scattering formula by applying it to a model for the electron density of a perfect crystal. Additional information on the structure is contained in other features of the pattern. The peak intensities encode the electron density in a unit cell, while the peak shape results from the shape of the crystal sample.

When dealing with non-crystalline structures, the diffraction pattern of a plane wave is not as structured as in the crystalline case but still contains a lot of information on the structure. Using the scattering formula, we show that locally the intensity on a screen is the absolute value squared of the Fourier transform of a projection of the charge density.

This result is the mathematical justification of Coherent Diffraction Imaging and related methods.

1. Plane Wave Radiation

The material presented in this section is standard textbook material from classic electrodynamics (see e.g. [Jac98, Gri99]). For the convenience of the reader and for later reference we give a short review.

The first step towards understanding the scattering of plane waves by a general electron density, is to understand plane waves themselves.

The electric field $\mathbf{E}$ of a plane wave at a point $\mathbf{x} \in \mathbb{R}^3$ and a time $t \in \mathbb{R}$ is described by the formula

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{n} \cos(\mathbf{k} \cdot \mathbf{x} - \omega t + \zeta), \tag{1.1}$$

with amplitude $\mathbf{n} \in \mathbb{R}^3$, wave vector $\mathbf{k} \in \mathbb{R}^3$, angular frequency $\omega > 0$ and phase angle $\zeta \in [0, \pi)$, that satisfy $|\mathbf{k}|^2 = \frac{\omega^2}{c^2}$ and $\mathbf{k} \cdot \mathbf{n} = 0$ with c denoting speed of light. More precisely, $\mathbf{E}$ is the special case of a linearly polarized plane wave. We will shortly see what that means.

First, we have a look at some important properties of plane waves. Like all electromagnetic fields, plane waves are solutions to Maxwell's equations – a set of coupled partial differential equations that describe the dependence of the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$ on present charges, currents and on each other (see also Appendix B). Denoting the electric charge density by ρ_{el} and the current density by $\mathbf{J}_{\text{el}}$, Maxwell's equations in SI units are

$$\operatorname{div} \mathbf{E} = \tfrac{1}{\varepsilon_0} \rho_{\text{el}}, \tag{M1}$$

$$\operatorname{div} \mathbf{B} = 0, \tag{M2}$$

$$\operatorname{curl} \mathbf{E} = -\partial_t \mathbf{B}, \tag{M3}$$

$$\operatorname{curl} \mathbf{B} = \mu_0(\mathbf{J}_{\text{el}} + \varepsilon_0 \partial_t \mathbf{E}), , \tag{M4}$$

where ε_0 and μ_0 are the electric and magnetic constants, respectively (see [Jac98]). We call the pair $(\mathbf{E}, \mathbf{B})$ the electromagnetic field.

The electric field (1.1) of a linearly polarized plane wave together with the magnetic field $\mathbf{B}$, given by

$$\mathbf{B}(\mathbf{x}, t) = \frac{\mathbf{k} \times \mathbf{n}}{\omega} \cos(\mathbf{k} \cdot \mathbf{x} - \omega t + \zeta) \tag{1.2}$$

at a point $\mathbf{x} \in \mathbb{R}^3$ and a time $t \in \mathbb{R}$, are easily seen to solve Maxwell's equations without charge and current, i.e. for $\rho_{\text{el}} = 0$ and $\mathbf{J}_{\text{el}} = 0$. We call this special case the homogeneous Maxwell equations.

The relations between $\mathbf{k}$, $\mathbf{n}$ and ω follow directly from Maxwell's equations: Applying (M1) to $\mathbf{E}$ shows that $\mathbf{k} \cdot \mathbf{n} = 0$, meaning that the field is perpendicular to its propagation direction. Waves of this kind are called transverse waves (in contrast to longitudinal waves, e.g. sound waves). Analogously, (M2) says that the magnetic field $\mathbf{B}$ is a transverse wave, which is in addition perpendicular to the electric field by (M3) (see Figure 1.1).

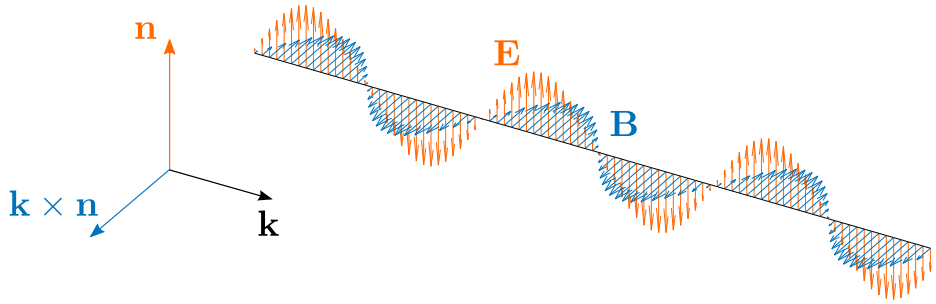


FIGURE 1.1. Visualization of plane wave radiation. The electric field and the (normalized) magnetic field of a linearly polarized plane wave are plotted along a line in $\mathbf{k}$-direction.

The relation $|\mathbf{k}|^2 = \frac{\omega^2}{c^2}$ between the wave vector and the angular frequency relates the spatial shape and the time evolution of the wave. Defining the wave length $\lambda := \frac{2\pi}{|\mathbf{k}|}$ that describes the spatial periodicity of the wave in $\mathbf{k}$-direction, and the frequency $f_0 := \frac{|\omega|}{2\pi}$, describing the time-periodicity of the wave, the relation can be restated as

$$\lambda = \frac{c}{f_0}, \tag{1.3}$$

saying that high-frequency electromagnetic waves have a short wavelength and vice versa. This relation can directly be inferred from the homogeneous wave equations for $\mathbf{E}$ and $\mathbf{B}$:

$$\left(\Delta - \frac{1}{c^2}\partial_t^2\right)\mathbf{E} = 0, \qquad \left(\Delta - \frac{1}{c^2}\partial_t^2\right)\mathbf{B} = 0. \tag{1.4}$$

These equations are derived from Maxwell's equations as follows:

$$\partial_t^2 \mathbf{E} \overset{\text{(M4)}}{=} c^2 \operatorname{curl} \partial_t \mathbf{B} \overset{\text{(M3)}}{=} -c^2 \operatorname{curl}(\operatorname{curl} \mathbf{E}) = -c^2(\nabla(\operatorname{div} \mathbf{E}) - \Delta \mathbf{E}) \overset{\text{(M1)}}{=} c^2 \Delta \mathbf{E},$$

$$\partial_t^2 \mathbf{B} \overset{\text{(M3)}}{=} -\operatorname{curl} \partial_t \mathbf{E} \overset{\text{(M4)}}{=} -c^2 \operatorname{curl}(\operatorname{curl} \mathbf{B}) = -c^2(\nabla(\operatorname{div} \mathbf{B}) - \Delta \mathbf{B}) \overset{\text{(M2)}}{=} c^2 \Delta \mathbf{B}.$$

Usually, Maxwell's equations are solved assuming that the electric and magnetic fields are complex vector fields, since many calculations are much easier in the complex number field. The physical fields are then taken as the real parts of the complex fields (Note that

by linearity, the real part is again a solution.). To simplify notation, we will write $\widetilde{\mathbf{E}}$ and $\widetilde{\mathbf{B}}$ for the complex solutions and define

$$\mathbf{E} := \mathrm{Re}(\widetilde{\mathbf{E}}), \quad \mathbf{B} := \mathrm{Re}(\widetilde{\mathbf{B}}). \tag{1.5}$$

The general complex form of a plane wave is given by the vector fields

$$\widetilde{\mathbf{E}}(\mathbf{x},t) = \mathbf{n}e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}, \quad \widetilde{\mathbf{B}}(\mathbf{x},t) = \frac{\mathbf{k}\times\mathbf{n}}{\omega}e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}, \quad \mathbf{x}\in\mathbb{R}^3,\ t\in\mathbb{R}, \tag{1.6}$$

with $\mathbf{k}\in\mathbb{R}^3$, $\omega\in\mathbb{R}$ and $\mathbf{n}\in\mathbb{C}^3$ that satisfy $\mathbf{k}\cdot\mathbf{n}=0$ and $|\mathbf{k}|^2=\frac{\omega^2}{c^2}$. Again, these fields are easily seen to solve the homogeneous Maxwell equations.

To make the real parts of these solutions easier to interpret, one usually writes the vector $\mathbf{n}\in\mathbb{C}^3$ – called complex amplitude of the wave – in a different way. Letting $\mathbf{n}\cdot\mathbf{n}=|\mathbf{n}\cdot\mathbf{n}|e^{2i\zeta}$ with $\zeta\in[0,\pi)$, and $\mathbf{n}=e^{i\zeta}(\mathbf{n}_1-i\mathbf{n}_2)$ with $\mathbf{n}_1,\mathbf{n}_2\in\mathbb{R}^3$, we immediately get $\mathbf{n}\cdot\mathbf{n}=e^{2i\zeta}(\mathbf{n}_1\cdot\mathbf{n}_1-2i\mathbf{n}_1\cdot\mathbf{n}_2-\mathbf{n}_2\cdot\mathbf{n}_2)$ and thus $\mathbf{n}_1\cdot\mathbf{n}_2=0$. Consequently, the general form of a real plane wave can be written as follows:

$$\begin{aligned}\mathbf{E}(\mathbf{x},t) &= \mathbf{n}_1\cos(\mathbf{k}\cdot\mathbf{x}-\omega t+\zeta)+\mathbf{n}_2\sin(\mathbf{k}\cdot\mathbf{x}-\omega t+\zeta),\\ \mathbf{B}(\mathbf{x},t) &= \frac{\mathbf{k}\times\mathbf{n}_1}{\omega}\cos(\mathbf{k}\cdot\mathbf{x}-\omega t+\zeta)+\frac{\mathbf{k}\times\mathbf{n}_2}{\omega}\sin(\mathbf{k}\cdot\mathbf{x}-\omega t+\zeta)\end{aligned} \tag{1.7}$$

at a point $\mathbf{x}\in\mathbb{R}^3$ and a time $t\in\mathbb{R}$ with real vectors $\mathbf{n}_1,\mathbf{n}_2\in\mathbb{R}^3$ that are orthogonal.

Since, for fixed $\mathbf{x}$, the field vectors in (1.7) describe an ellipse about $\mathbf{x}$ when moving forward in time, these general plane waves are called elliptically polarized. There are two important special cases of elliptic polarization:

- linear polarization for $\mathbf{n}_2=0$, and
- spherical polarization for $|\mathbf{n}_1|=|\mathbf{n}_2|$.

The different kinds of polarization are visualized in Figure 1.2.

Next, we want to investigate the radiation properties of electromagnetic plane waves. Radiation in general is a process of energy transfer. In our particular case, the electromagnetic energy density u is defined as

$$u(\mathbf{x},t) := \frac{1}{2}\left(\varepsilon_0|\mathbf{E}(\mathbf{x},t)|^2+\frac{1}{\mu_0}|\mathbf{B}(\mathbf{x},t)|^2\right), \quad \mathbf{x}\in\mathbb{R}^3,\ t\in\mathbb{R}. \tag{1.8}$$

The directional energy flux density is described by the so-called Poynting vector $\mathbf{S}$ that is defined as

$$\mathbf{S}(\mathbf{x},t) := \frac{1}{\mu_0}\mathbf{E}(\mathbf{x},t)\times\mathbf{B}(\mathbf{x},t), \quad \mathbf{x}\in\mathbb{R}^3,\ t\in\mathbb{R}. \tag{1.9}$$

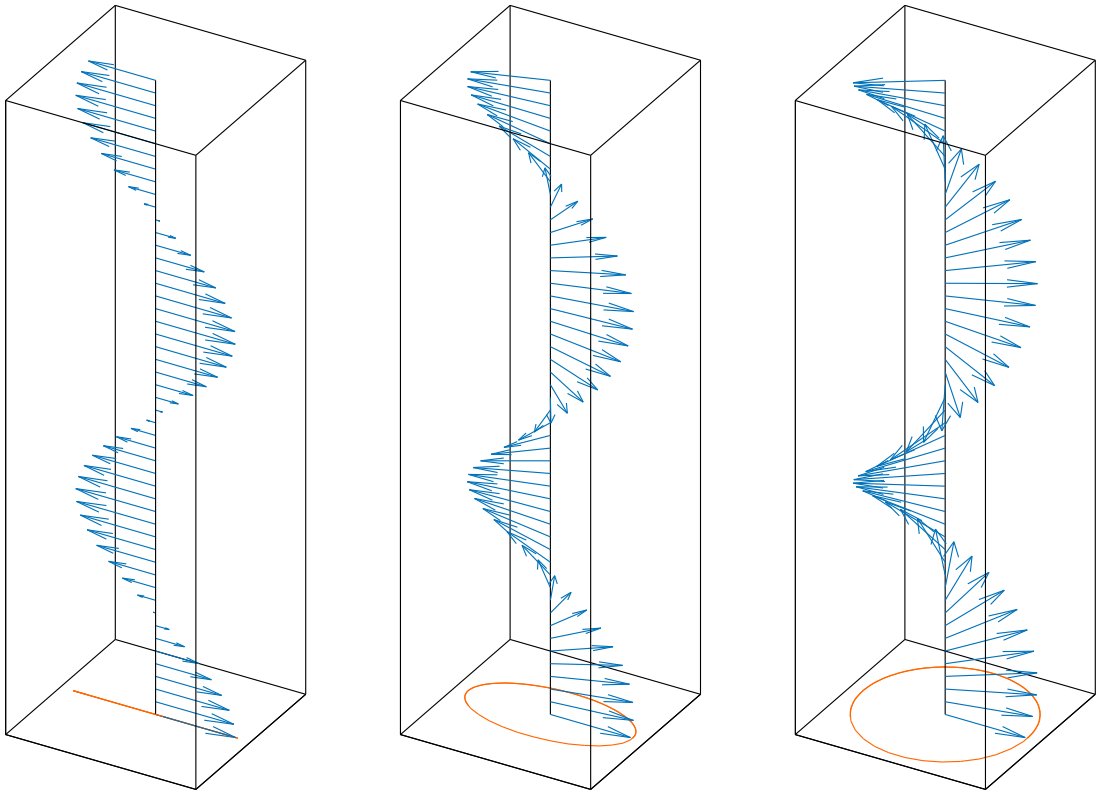


FIGURE 1.2. Visualization of the polarization of plane wave radiation. The field vector of a linearly polarized, an elliptically polarized, and a spherically polarized plane wave (from left to right) is plotted along a line in $\mathbf{k}$-direction. On the bottom the shape that the tips of the field vectors describe is shown.

For plane wave radiation, traveling with the speed of light c in direction $\frac{\mathbf{k}}{|\mathbf{k}|}$, this can be seen to be equivalent to the conventional definition of directional energy flux density:

$$\mathbf{S}(\mathbf{x},t) = c\varepsilon_0|\mathbf{E}(\mathbf{x},t)|^2\frac{\mathbf{k}}{|\mathbf{k}|} = c\frac{\mathbf{k}}{|\mathbf{k}|}u(\mathbf{x},t),$$

where we used that $c^2 = \frac{1}{\varepsilon_0\mu_0}$ and $|\mathbf{B}| = \frac{1}{c}|\mathbf{E}|$ what can be seen from (1.6) and yields $u(\mathbf{x},t) = \varepsilon_0|\mathbf{E}(\mathbf{x},t)|^2$ for $\mathbf{x}\in\mathbb{R}^3$ and $t\in\mathbb{R}$.

The quantity that is usually measured in diffraction experiments is the intensity I of an electromagnetic field. Intensity is the power transferred per unit area. At a point $\mathbf{x}\in\mathbb{R}^3$ it is defined as the time average of the magnitude of the Poynting vector $\mathbf{S}$ (see [Gri99]):

$$\mathrm{I}(\mathbf{x}) := \lim_{T\to\infty}\frac{1}{T}\int_{-T/2}^{T/2}|\mathbf{S}(\mathbf{x},t)|\mathrm{d}t. \tag{1.10}$$

For a plane wave, the intensity can be determined by averaging over one time period. Since the averages of $\cos^2$ and $\sin^2$ are equal to $\frac{1}{2}$ and $\mathbf{n}_1 \cdot \mathbf{n}_2 = 0$, we get

$$\mathrm{I}(\mathbf{x}) = \frac{c\varepsilon_0}{2}\left(|\mathbf{n}_1|^2 + |\mathbf{n}_2|^2\right) = \frac{c\varepsilon_0}{2}|\mathbf{n}|^2. \tag{1.11}$$

I.e., the intensity of a plane wave is essentially the absolute value squared of its complex amplitude.

Since plane waves are central objects throughout the text, we introduce a short notation. For $\mathbf{k} \in \mathbb{R}^3$, we set

$$\mathbf{E}_{\mathbf{k}}(\mathbf{x}) := \mathbf{n}e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{for some } \mathbf{n} \in \mathbf{k}^{\perp} \setminus \{0\} \text{ and all } \mathbf{x} \in \mathbb{R}^3, \tag{1.12}$$

suppressing the dependence on $\mathbf{n}$, since the complex amplitude will play a minor role. We also introduce the notation

$$e_{\mathbf{k}} := e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \mathbf{x} \in \mathbb{R}^3, \tag{1.13}$$

for the scalar counterparts.

At times, we will need families of plane waves $\{\mathbf{E}_{\mathbf{k}}\}_{\mathbf{k}\in K}$, $\{e_{\mathbf{k}}\}_{\mathbf{k}\in K}$, for some set $K \subseteq \mathbb{R}^3$. Then, as the complex amplitude depends on the wave vector, we write $\mathbf{E}_{\mathbf{k}}(\mathbf{x}) = \mathbf{n}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}$, $\mathbf{k} \in K$, for the single plane waves. We also introduce the notations $\mathbf{E}_{\omega,\mathbf{k}_0} := \mathbf{E}_{\mathbf{k}}$ and $e_{\omega,\mathbf{k}_0} := e_{\mathbf{k}}$ to emphasize the dependence on the two parameters frequency and propagation direction $\mathbf{k}_0 := \frac{\mathbf{k}}{|\mathbf{k}|}$.

2. Scattering of Plane Waves

Our goal in this section is to determine the electromagnetic field that results from the interaction of plane wave radiation with an electric charge density ρ_{el}. Mathematically minded readers that are not interested in the physical origin of the expressions can take Definition 1.2 as a starting point.

When a charge density ρ_{el} is illuminated by plane wave radiation $(\mathbf{E}, \mathbf{B})$ as in (1.7), it feels a force – the so-called Lorentz force $\mathbf{F}_{\mathrm{L}}$ – that is given by

$$\mathbf{F}_{\mathrm{L}} := \rho_{\mathrm{el}}\mathbf{E} + \mathbf{J}_{\mathrm{el}} \times \mathbf{B}, \tag{1.14}$$

and starts moving according to Newtonian mechanics. At the same time, a moving charge density influences the electromagnetic field as dictated by Maxwell's equations.

Let $\mathbf{n} \in \mathbb{R}^3$ be the complex amplitude of the linearly polarized plane wave

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{n}\cos(\mathbf{k} \cdot \mathbf{x} - \omega t)$$

with $\mathbf{n}\cdot\mathbf{k}=0$ and $|\mathbf{k}|^2=\frac{\omega^2}{c^2}$. We start by considering a point charge $\rho_{\mathrm{el}}(\mathbf{x},t):=e_{\mathrm{el}}\delta_{\mathbf{r}(t)}(\mathbf{x})$ at a point $\mathbf{y}_0\in\mathbb{R}^3$ with electric charge e_{el} moving in $\mathbf{n}$-direction, i.e. $\mathbf{r}(t)=\mathbf{y}_0+\xi_{\mathbf{y}_0}(t)\mathbf{n}$. The current density is then given as $\mathbf{J}_{\mathrm{el}}(\mathbf{x},t)=e_{\mathrm{el}}\delta_{\mathbf{r}(t)}(\mathbf{x})\partial_t\mathbf{r}(t)=e_{\mathrm{el}}\delta_{\mathbf{r}(t)}(\mathbf{x})\partial_t\xi_{\mathbf{y}_0}(t)\mathbf{n}$. Consequently, using (1.7), the Lorentz force exerted on the point charge at $\mathbf{r}(t)$ is

$$\begin{aligned}\mathbf{F}_{\mathrm{L}}(\mathbf{r}(t),t)&=e_{\mathrm{el}}\mathbf{n}\cos(\mathbf{k}\cdot\mathbf{r}(t)-\omega t)+e_{\mathrm{el}}\partial_t\xi_{\mathbf{y}_0}(t)\mathbf{n}\times\frac{\mathbf{k}\times\mathbf{n}}{\omega}\cos(\mathbf{k}\cdot\mathbf{r}(t)-\omega t)\\&=e_{\mathrm{el}}\left(\mathbf{n}+\frac{\partial_t\xi_{\mathbf{y}_0}(t)}{c}\frac{\mathbf{k}}{|\mathbf{k}|}\right)\cos(\mathbf{k}\cdot\mathbf{y}_0-\omega t),\end{aligned}$$

where we used that $\mathbf{k}\cdot\mathbf{n}=0$.

Assuming that the velocity $\partial_t\xi_{\mathbf{y}_0}(t)$ of the charge is non-relativistic, i.e. $\partial_t\xi_{\mathbf{y}_0}(t)\ll c$, we neglect the contribution of the magnetic field. When $m_{\mathrm{el}}\delta_{\mathbf{r}(t)}(\mathbf{x})$ is the mass density, Newton's second law $\mathbf{F}_{\mathrm{L}}(\mathbf{r}(t),t)=m_{\mathrm{el}}\partial_t^2\mathbf{r}(t)$ reads

$$e_{\mathrm{el}}\mathbf{n}\cos(\mathbf{k}\cdot\mathbf{y}_0-\omega t)=m_{\mathrm{el}}\mathbf{n}\partial_t^2\xi_{\mathbf{y}_0}(t),$$

yielding the non-transient solution

$$\xi_{\mathbf{y}_0}(t)=-\frac{e_{\mathrm{el}}}{m_{\mathrm{el}}\omega^2}\cos(\mathbf{k}\cdot\mathbf{y}_0-\omega t).$$

This results in the following charge and current densities:

$$\rho_{\mathrm{el}}(\mathbf{x},t)=e_{\mathrm{el}}\delta_{\mathbf{r}(t)}(\mathbf{x}),\quad \mathbf{J}_{\mathrm{el}}(\mathbf{x},t)=-\frac{e_{\mathrm{el}}}{m_{\mathrm{el}}\omega}\sin(\mathbf{k}\cdot\mathbf{y}_0-\omega t)\mathbf{n}\delta_{\mathbf{r}(t)}(\mathbf{x}),$$

with $\mathbf{r}(t)=\mathbf{y}_0+\frac{e_{\mathrm{el}}}{m_{\mathrm{el}}\omega^2}\cos(\mathbf{k}\cdot\mathbf{y}_0-\omega t)\mathbf{n}$.

As we don't want to investigate the scattering of point charges, but of general charge densities, we now consider ρ_{el} to be a function supported on a compact set $\Omega\subset\mathbb{R}^3$. The main assumption we make for the following is that the density oscillates in phase when illuminated by plane wave radiation, i.e.

$$\rho_{\mathrm{el}}(\mathbf{x}+\xi_{\mathbf{x}}(t),t)=\rho_{\mathrm{el}}(\mathbf{x},0).$$

Maxwell's equations (M1)-(M4) can be solved in terms of potentials (for details see Appendix B). We define the vector potential $\mathbf{A}_{\mathrm{el}}$ and the scalar potential φ_{el} via

$$\mathbf{B}=\operatorname{curl}\mathbf{A}_{\mathrm{el}},\quad \mathbf{E}+\partial_t\mathbf{A}_{\mathrm{el}}=-\nabla\varphi_{\mathrm{el}},$$

using that $\mathbf{B}$ is divergence-free and $\mathbf{E}+\partial_t\mathbf{A}_{\mathrm{el}}$ is curl-free under suitable regularity assumptions on $\mathbf{E}$ and $\mathbf{B}$. In addition, we have some freedom in the choice of the potentials and can impose the additional condition

$$\operatorname{div}\mathbf{A}_{\mathrm{el}}+\frac{1}{c^2}\partial_t\varphi_{\mathrm{el}}=0, \tag{1.15}$$

which is called Lorenz gauge condition. Maxwell's equations then reduce to a set of inhomogeneous wave equations

$$-\Delta\varphi_{\mathrm{el}} + \frac{1}{c^2}\partial_t^2\varphi_{\mathrm{el}} = \frac{1}{\varepsilon_0}\rho_{\mathrm{el}}, \quad -\Delta\mathbf{A}_{\mathrm{el}} + \frac{1}{c^2}\partial_t^2\mathbf{A}_{\mathrm{el}} = \mu_0\mathbf{J}_{\mathrm{el}}.$$

A particular solution of these equations are the retarded potentials:

$$\begin{aligned}\varphi_{\mathrm{el}}(\mathbf{x},t) &= \frac{1}{4\pi\varepsilon_0}\int_{\mathbb{R}^3}\frac{\rho_{\mathrm{el}}\left(\mathbf{y}, t-\frac{|\mathbf{x}-\mathbf{y}|}{c}\right)}{|\mathbf{x}-\mathbf{y}|}\mathrm{d}\mathbf{y},\\ \mathbf{A}_{\mathrm{el}}(\mathbf{x},t) &= \frac{\mu_0}{4\pi}\int_{\mathbb{R}^3}\frac{\mathbf{J}_{\mathrm{el}}\left(\mathbf{y}, t-\frac{|\mathbf{x}-\mathbf{y}|}{c}\right)}{|\mathbf{x}-\mathbf{y}|}\mathrm{d}\mathbf{y}.\end{aligned} \tag{1.16}$$

In an appropriate regime that will be defined in Chapter 3 in a more general setting, these potentials result in an approximation of the electric field $\mathbf{E} = -\partial_t\mathbf{A}_{\mathrm{el}} - \nabla\varphi_{\mathrm{el}}$ given by

$$\begin{aligned}\mathbf{E}(\mathbf{x},t) =& c_{\mathrm{el}}\frac{\mathrm{P}((\mathbf{x}-\mathbf{y}_c)^\perp)\mathbf{n}}{|\mathbf{x}-\mathbf{y}_c|}\\ &\times\int_\Omega \cos\left(-\frac{\omega}{c}\left(\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\cdot\mathbf{y} + \omega\left(\frac{(\mathbf{x}-\mathbf{y}_c)\cdot\mathbf{x}}{c|\mathbf{x}-\mathbf{y}_c|}-t\right)\right)\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y},\end{aligned}$$

where $c_{\mathrm{el}} := -\frac{e_{\mathrm{el}}^2}{4\pi\varepsilon_0 m_{\mathrm{el}}c^2}$ is the scattering constant, $\mathbf{y}_c \in \Omega$ is a typical point in the sample (e.g. the center of mass) and $\mathrm{P}(\mathbf{x}^\perp) := \left(\mathbf{I} - \frac{\mathbf{x}}{|\mathbf{x}|}\otimes\frac{\mathbf{x}}{|\mathbf{x}|}\right)$ is the projection onto the orthogonal complement of a vector $\mathbf{x}\in\mathbb{R}^3$.

Since the dependence on the point $\mathbf{y}_c$ is not important for our considerations, we choose $\mathbf{y}_c = 0$ as a natural choice of origin to get the final version of the outgoing electromagnetic field which will be subsequently called the scattering formula

$$\mathbf{E}(\mathbf{x},t) = c_{\mathrm{el}}\frac{\mathrm{P}(\mathbf{x}^\perp)\mathbf{n}}{|\mathbf{x}|}\int_\Omega\cos\left(-\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\cdot\mathbf{y}+\omega\left(\frac{|\mathbf{x}|}{c}-t\right)\right)\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y}. \tag{1.17}$$

The analog approximation of the magnetic field $\mathbf{B} = \operatorname{curl}\mathbf{A}_{\mathrm{el}}$ is given by

$$\mathbf{B}(\mathbf{x},t) = \frac{c_{\mathrm{el}}}{c}\frac{\mathbf{x}\times\mathbf{n}}{|\mathbf{x}|^2}\int_\Omega\cos\left(-\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\cdot\mathbf{y}+\omega\left(\frac{|\mathbf{x}|}{c}-t\right)\right)\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y}. \tag{1.18}$$

A short calculation shows that

$$\mathrm{P}(\mathbf{x}^\perp)\mathbf{n}\times\left(\frac{\mathbf{x}}{|\mathbf{x}|}\times\mathbf{n}\right) = |\mathbf{n}|^2\sin^2(\sphericalangle(\mathbf{x},\mathbf{n}))\frac{\mathbf{x}}{|\mathbf{x}|},$$

where $\sphericalangle(\mathbf{x},\mathbf{n})$ is the angle between the outgoing direction and the field vector.

By equation (1.9), the Poynting vector $\mathbf{S}$ of the field $(\mathbf{E}, \mathbf{B})$ is thus given by

$$\begin{aligned}\mathbf{S}(\mathbf{x}, t) =& c_{\mathrm{el}}^2 \frac{c\varepsilon_0 |\mathbf{n}|^2}{|\mathbf{x}|^2} \sin^2(\sphericalangle(\mathbf{x}, \mathbf{n})) \frac{\mathbf{x}}{|\mathbf{x}|} \\ &\times \left(\int_\Omega \cos\left(-\frac{\omega}{c} \left(\frac{\mathbf{x}}{|\mathbf{x}|} - \frac{\mathbf{k}}{|\mathbf{k}|} \right) \cdot \mathbf{y} + \omega \left(\frac{|\mathbf{x}|}{c} - t \right) \right) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right)^2 .\end{aligned}$$

To determine the intensity I via equation (1.10), we use the following lemma.

Lemma 1.1 (Intensity of the Scattered Field). *Let* $\mathbf{F} \in C_b(\mathbb{R}^3; \mathbb{C}^3)$, $\rho_{\mathrm{el}} \in \mathcal{S}(\mathbb{R}^3)$, $\rho_{\mathrm{el}} \geq 0$, *and* $\omega > 0$. *Then*

$$\lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} \left| \int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y}) e^{-i\omega t}) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right|^2 \mathrm{d}t = \frac{1}{2} \left| \int_\Omega \mathbf{F}(\mathbf{y}) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right|^2 . \tag{1.19}$$

Proof. We first expand the integrand:

$$\begin{aligned}&\left| \int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y}) e^{-i\omega t}) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right|^2 \\ &= \left(\int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y})) \cos(\omega t) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} + \int_\Omega \mathrm{Im}(\mathbf{F}(\mathbf{y})) \sin(\omega t) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right)^2 \\ &= \cos^2(\omega t) \left(\int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y})) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right)^2 + \sin^2(\omega t) \left(\int_\Omega \mathrm{Im}(\mathbf{F}(\mathbf{y})) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right)^2 \\ &\quad + 2\cos(\omega t) \sin(\omega t) \int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y})) \rho_{\mathrm{el}} \mathrm{d}\mathbf{y} \int_\Omega \mathrm{Im}(\mathbf{F}(\mathbf{y})) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y}.\end{aligned}$$

Now, we can evaluate the time integrals

$$\lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} \cos^2(\omega t) \mathrm{d}t = \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} \sin^2(\omega t) \mathrm{d}t = \frac{\omega}{2\pi} \int_{-\pi/\omega}^{\pi/\omega} \sin^2(\omega t) \mathrm{d}t = \frac{1}{2}$$

and

$$\lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} \cos(\omega t) \sin(\omega t) \mathrm{d}t = \frac{\omega}{2\pi} \int_{-\pi/\omega}^{\pi/\omega} \cos(\omega t) \sin(\omega t) \mathrm{d}t = 0.$$

Consequently,

$$\begin{aligned}&\lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} \left| \int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y}) e^{-i\omega t}) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right|^2 \mathrm{d}t \\ &= \frac{1}{2} \left(\int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y})) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right)^2 + \frac{1}{2} \left(\int_\Omega \mathrm{Im}(\mathbf{F}(\mathbf{y})) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right)^2 = \frac{1}{2} \left| \int_\Omega \mathbf{F}(\mathbf{y}) \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right|^2 ,\end{aligned}$$

where we used the linearity of the integral and the fact that $|z|^2 = \mathrm{Re}(z)^2 + \mathrm{Im}(z)^2$ for $z \in \mathbb{C}$. □

Now, setting $\mathbf{F}(\mathbf{y}) := \frac{\mathbf{x}}{|\mathbf{x}|} e^{i\left(-\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\cdot\mathbf{y}+\frac{\omega|\mathbf{x}|}{c}\right)}$, $\mathbf{y}\in\mathbb{R}^3$, we can determine the intensity I from equation (1.10) using Lemma 1.1.

$$\begin{aligned}
\mathrm{I}(\mathbf{x}) &= c_{\mathrm{el}}^2 \frac{c\varepsilon_0|\mathbf{n}|^2}{|\mathbf{x}|^2}\sin^2(\sphericalangle(\mathbf{x},\mathbf{n}))\lim_{T\to\infty}\frac{1}{T}\int_{-T/2}^{T/2}\left|\int_\Omega \mathrm{Re}(\mathbf{F}(\mathbf{y})e^{-i\omega t})\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y}\right|^2\mathrm{d}t\\
&= c_{\mathrm{el}}^2 \frac{c\varepsilon_0|\mathbf{n}|^2}{|\mathbf{x}|^2}\sin^2(\sphericalangle(\mathbf{x},\mathbf{n}))\frac{1}{2}\left|\int_\Omega \mathbf{F}(\mathbf{y})\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y}\right|^2\\
&= c_{\mathrm{el}}^2 \frac{c\varepsilon_0|\mathbf{n}|^2}{2|\mathbf{x}|^2}\sin^2(\sphericalangle(\mathbf{x},\mathbf{n}))\left|\int_\Omega e^{-i\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\cdot\mathbf{y}}\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y}\right|^2
\end{aligned}$$

The term $\sin^2(\sphericalangle(\mathbf{x},\mathbf{n}))|\mathbf{n}|^2$ can be reformulated as the absolute value squared of the vector $\mathrm{P}(\mathbf{x}^\perp)\mathbf{n}$, while the integral is recognized as the Fourier transform of the charge density ρ_{el} evaluated at the point $\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)$. So, our final result for the intensity of the outgoing radiation is the following special case of equation (3.28).

$$\mathrm{I}(\mathbf{x}) = c_{\mathrm{el}}^2\frac{c\varepsilon_0}{2|\mathbf{x}|^2}\left|\mathrm{P}(\mathbf{x}^\perp)\mathbf{n}\widehat{\rho_{\mathrm{el}}}\left(\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\right)\right|^2, \tag{1.20}$$

at a point $\mathbf{x}\in\mathbb{R}^3$ and a time $t>0$.

This formula shows the relationship between the scattering of plane waves and the Fourier transform. The fact that only the absolute value squared of the Fourier transform of the charge density is given by the intensity of the outgoing radiation is known as the phase problem. We loose the phase of the complex function $\widehat{\rho_{\mathrm{el}}}$, which makes it hard to reconstruct the density. The phase problem and algorithms for reconstruction will be discussed in the next chapter.

From now on, we are done with physical considerations and take equations (1.17), (1.18), and (1.20) as a starting point for subsequent mathematical analysis. We summarize our results in the following

Definition 1.2 (Plane Wave Scattering Data). *For given vectors $\mathbf{k}\in\mathbb{R}^3$ (wave vector), $\mathbf{n}\in\mathbf{k}^\perp$ (complex amplitude), and a given function $\rho_{\mathrm{el}}\in C_c(\mathbb{R}^3)$ (charge density), the integrals* (1.17), (1.18), *and* (1.20) *are called the outgoing electric field, outgoing magnetic field, and scattering intensity, respectively.*

It is convenient to work with the square root of the intensity. We call this quantity the scattering amplitude $\mathrm{A} := \mathrm{I}^{1/2}$. For the scattering of a plane wave, A is given by

$$\mathrm{A}(\mathbf{x}) = c_{\mathrm{el}}\left(\frac{c\varepsilon_0}{2|\mathbf{x}|^2}\right)^{1/2}\left|\mathrm{P}(\mathbf{x}^\perp)\mathbf{n}\widehat{\rho_{\mathrm{el}}}\left(\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\right)\right|. \tag{1.21}$$

Mathematically, the scattering amplitude has the advantage that it can be extended to more general models for the electron density. When assuming that the electron density

is an infinite sum of delta distributions as is usually done in X-ray Crystallography, the intensity might not be well-defined as the square of a tempered distribution. The scattering amplitude, instead, is in this case a well-defined tempered distribution again. We use this property of the scattering amplitude to formulate the von Laue condition in the next section.

3. X-ray Crystallography

When plane wave radiation is scattered by a crystal, a highly structured peak pattern emerges on a screen in the far-field. This fact was first observed in 1912 by Max von Laue and his team [FKL12]. We will explain in this section why this is the case by modeling the electron density of a crystal and applying the formula for the scattering amplitude (1.21) we inferred in the last section. The crystallographic terminology that is used in this section is explained in Appendix C.

3.1. Von Laue Condition and Bragg's Law. We assume that the electron density ρ_{el} of a crystal sample shares the symmetry of the crystal. Moreover, the density shall be smooth and well-localized.

The translational symmetries of a crystal lattice are described by a Bravais lattice (see Definition C.1). Given an invertible matrix $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \in \mathrm{GL}(3, \mathbb{R})$, a Bravais lattice $\mathcal{B} \subset \mathbb{R}^3$ is defined as the set

$$\mathcal{B} := \mathbf{A}\mathbb{Z}^3.$$

It is the set of points of the form $j\mathbf{a}_1 + k\mathbf{a}_2 + \ell\mathbf{a}_3$, $j, k, \ell \in \mathbb{Z}$, that form a lattice in $\mathbb{R}^3$. Now, given a finite set $\mathbf{M} \subset \mathbb{R}^3$, a crystal lattice $\mathcal{L} \subset \mathbb{R}^3$ is defined as a set of the form

$$\mathcal{L} := \mathcal{B} + \mathbf{M}.$$

Translating the set $\mathbf{M}$ by the elements of the Bravais lattice $\mathcal{B}$, we obtain a model for the atom positions in a periodic crystal structure.

When $\mathcal{B} = \mathbf{A}\mathbb{Z}^3 \subset \mathbb{R}^3$, $\mathbf{A} \in \mathrm{GL}(3, \mathbb{R})$, is a three-dimensional Bravais lattice that generates our crystal, consider the following model for its electron density

$$\rho_{\text{el}} := (\delta_{\mathcal{B}} \cdot \mathbf{1}_{\Omega}) * \varphi, \tag{1.22}$$

where $\delta_{\mathcal{B}} = \sum_{\mathbf{b} \in \mathcal{B}} \delta_{\mathbf{b}} \in \mathcal{S}'(\mathbb{R}^3)$ is the tempered distribution associated to $\mathcal{B}$, $\Omega \subset \mathbb{R}^3$ is a compact set and $\varphi \in \mathcal{S}(\mathbb{R}^3)$ is a Schwartz function. This model is a finite section of a $\mathcal{B}$-periodic function.

The function φ is a model for the electron density in one single unit cell, while the multiplication with $\mathbf{1}_{\Omega}$ selects the finitely many unit cells that are contained in Ω (see Figure (1.3)). The restriction of $\delta_{\mathcal{B}}$ to Ω is obviously a compactly supported distribution.

Since the convolution of a compactly supported distribution with a Schwartz function is again a Schwartz function, we see that $\rho_{\mathrm{el}} \in \mathcal{S}(\mathbb{R}^3)$ is a smooth and well-localized function.

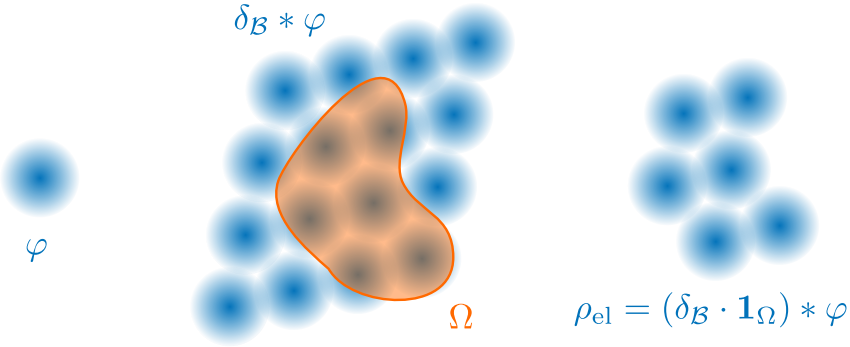


FIGURE 1.3. A model for the electron density ρ_{el} of a two-dimensional crystal. The function φ is a model for the electron density of the atoms in one unit cell. The compact set Ω selects finitely many of these unit cells.

When a plane wave is scattered by the charge density ρ_{el}, we can use equation (1.20) to determine the intensity of the outgoing radiation. The central term in this formula is the Fourier transform of the electron density. Using the convolution theorem (Theorem A.3) in both directions and the generalized Poisson summation formula (Theorem C.2), we get

$$\widehat{\rho_{\mathrm{el}}} = \mathcal{F}((\delta_{\mathcal{B}} \cdot \mathbf{1}_\Omega) * \varphi) = \frac{1}{\mathrm{V}_{\mathcal{B}}} (\delta_{\mathcal{B}^\perp} * \widehat{\mathbf{1}}_\Omega) \cdot \widehat{\varphi}, \tag{1.23}$$

where $\mathrm{V}_{\mathcal{B}} := |\det(\mathbf{A})|$, and $\mathcal{B}^\perp$ is the reciprocal lattice of $\mathcal{B}$, that is defined as

$$\mathcal{B}^\perp := \{\mathbf{k} \in \mathbb{R}^3.\ \mathbf{k} \cdot \mathbf{b} \in 2\pi\mathbb{Z} \text{ for all } \mathbf{b} \in \mathcal{B}\} = 2\pi \mathbf{A}^{-T} \mathbb{Z}^3.$$

We introduce the notation $\mathbf{A}^\perp := 2\pi\mathbf{A}^{-T}$ for the generator matrix of the reciprocal lattice.

In the case of a perfect crystal, i.e. $\rho_{\mathrm{el}} = \delta_{\mathcal{B}} * \varphi$, we recover the von Laue condition. Even though the formula for the scattering amplitude (1.21) is not applicable in this case, the result can be seen as an approximation of the case of a single crystal with a diameter that is large compared to the size of a unit cell.

Theorem 1.3 (von Laue Condition). *The scattering amplitude* A *defined in formula* (1.21) *(physically arising from scattering a plane wave* $\mathbf{E}(\mathbf{x}, t) = \mathbf{n} \cos(\mathbf{k} \cdot \mathbf{x} - \omega t)$, $\mathbf{n}, \mathbf{k} \in \mathbb{R}^3$, $\mathbf{n} \cdot \mathbf{k} = 0$, $\omega = c|\mathbf{k}|$*), in the case* $\rho_{\mathrm{el}} = \delta_{\mathcal{B}} * \varphi$ *for a Bravais lattice* $\mathcal{B}$ *and a Schwartz function* $\varphi \in \mathcal{S}(\mathbb{R}^3)$*, satisfies*

$$\mathrm{A}(\mathbf{x}) = (2\pi)^3 c_{\mathrm{el}} \left(\frac{c\varepsilon}{2|\mathbf{x}|^2} \right)^{1/2} |\mathrm{P}(\mathbf{x}^\perp)\mathbf{n}| \, (\delta_{\mathcal{B}^\perp} \cdot |\widehat{\varphi}|) \left(\frac{\omega}{c} \left(\frac{\mathbf{x}}{|\mathbf{x}|} - \frac{\mathbf{k}}{|\mathbf{k}|} \right) \right), \tag{1.24}$$

for $\mathbf{x} \in \mathbb{R}^3$ *and* $t > 0$.

I.e. constructive interference occurs if and only if $\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)$ *is a reciprocal lattice vector.*

Remark 1.4 (Bragg's Law). *The von Laue condition is often expressed differently in form of Bragg's law. Consider the angle* θ *defined by*

$$\left|\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right| = 2\sin\theta.$$

It is half the angle between incoming direction $\frac{\mathbf{k}}{|\mathbf{k}|}$ *and outgoing direction* $\frac{\mathbf{x}}{|\mathbf{x}|}$ *(see Figure (1.4)). Now, when* $\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)$ *is an arbitrary reciprocal lattice vector, it can be written in the form* $j\mathbf{k}_\iota$, $j\in\mathbb{N}$, $\iota\in\mathbb{Z}^3$, $\gcd(\iota_1,\iota_2,\iota_3)=1$, *where* $\mathbf{k}_\iota = \mathbf{A}^\perp\iota$. *The vector* ι *is called the Miller index of the family* $\mathbb{N}\mathbf{k}_\iota$ *of reciprocal lattice vectors. As shown in Appendix C, we know that* $|\mathbf{k}_\iota| = \frac{2\pi}{\lambda_\iota}$, *where* λ_ι *is the distance of neighboring lattice planes with Miller index* ι. *Consequently,*

$$2\sin\theta = \left|\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right| = \frac{c}{\omega}\left|\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\right| = \frac{c}{\omega}|j\mathbf{k}_\iota| = \frac{c}{\omega}j\frac{2\pi}{\lambda_\iota}.$$

Since $\frac{c}{\omega}=\frac{\lambda}{2\pi}$, *where* λ *is the wavelength of the incoming radiation, we conclude that*

$$2\lambda_\iota\sin\theta = j\lambda, \quad j\in\mathbb{N}, \tag{1.25}$$

what is known as Bragg's law.

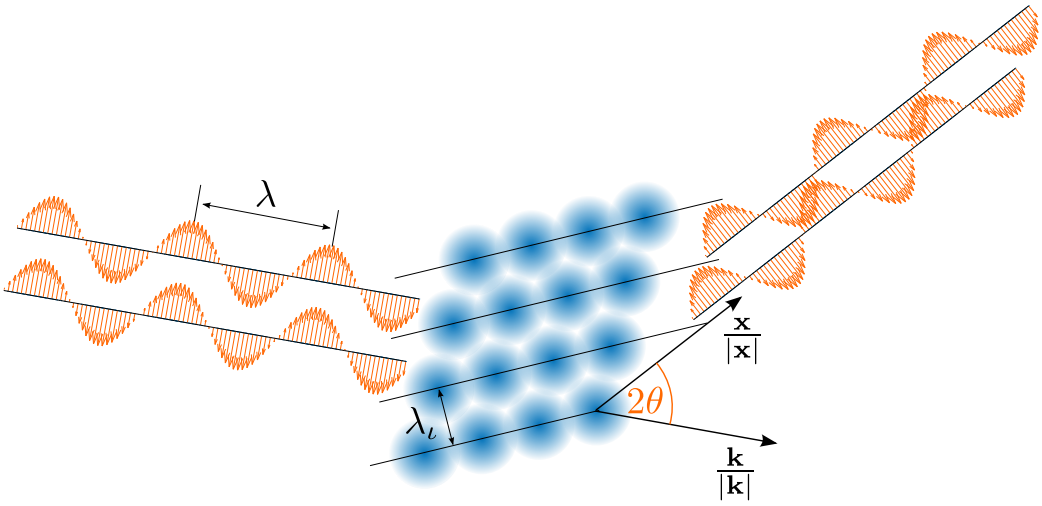


FIGURE 1.4. Visualization of Bragg's law. Plane waves that are 'reflected' at neighboring lattices planes need to have a wavelength that satisfies Bragg's law, i.e. $\lambda_\iota\sin\theta = j\lambda$ for some $j\in\mathbb{N}$, to achieve constructive interference in $\mathbf{x}$-direction. In the depicted example, Bragg's law is not satisfied – the outgoing waves almost cancel.

It gives a geometric interpretation of the scattering event. When the incoming waves are 'reflected' at neighboring lattice planes, the waves going out from two atoms in these planes need to have a relative phase shift that is a multiple of its wavelength to achieve constructive interference.

Formula (1.24) does not only describe the location of the peaks on a screen, it also shows that the scattering amplitude at a peak is essentially the absolute value of the Fourier transform of the function φ. This fact makes it possible to reconstruct the density within a unit cell up to the phase problem.

3.2. Reconstruction of the Translational Symmetries. First, we show how to reconstruct the translational symmetries of ρ_{el} from the peak locations. If we know the incoming direction $\frac{\mathbf{k}}{|\mathbf{k}|}$ and the angular frequency ω of the incoming plane wave, a peak in outgoing direction $\frac{\mathbf{x}}{|\mathbf{x}|}$ means that the vector $\mathbf{b}'$ given by $\mathbf{b}' := \frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|} - \frac{\mathbf{k}}{|\mathbf{k}|}\right)$ is an element of the reciprocal lattice $\mathcal{B}^\perp$. Collecting the peaks in different directions and for different frequencies, we can eventually determine the reciprocal lattice. The lattice $\mathcal{B}$ that describes the translational invariances of ρ_{el} can be recovered by the observation that the reciprocal lattice of the reciprocal lattice is the original lattice:

$$(\mathcal{B}^\perp)^\perp = 2\pi(2\pi\mathbf{A}^{-T})^{-T}\mathbb{Z}^3 = 2\pi\left(\frac{1}{2\pi}\mathbf{A}\right)\mathbb{Z}^3 = \mathbf{A}\mathbb{Z}^3 = \mathcal{B}.$$

When polychromatic radiation is used and the intensity of the outgoing radiation is measured on a flat screen in the far-field, a highly structured peak pattern – called a Laue photograph – is observed (see Figure (1.5)). Even though, the scattering formula is not applicable, it is experimentally confirmed that this pattern is a superposition of the patterns for the single plane waves.

To determine the symmetries from a Laue photograph, an additional step is necessary. The procedure of determining the frequency of the plane wave that produced a specific peak in a Laue photograph is called indexing. This name comes from the fact that the Miller index of the corresponding reciprocal lattice vector is identified. In view of Bragg's law (1.25), the peak with Miller index $\iota \in \mathbb{Z}^3$ results from the waves that are reflected at the family of lattice planes with Miller index ι. In particular, because of peak overlap, not all values of $|\widehat{\varphi}|$ are accessible from a Laue photograph.

This short discussion shows that a Laue photograph can be used to identify the symmetries, but is not the best choice for the reconstruction of ρ_{el}.

A very clever way to collect data for the analysis of crystal structure is the rotating crystal method. Using monochromatic radiation with a fixed frequency ω, the resulting peaks can directly be indexed. Instead of changing the frequency or changing the incoming

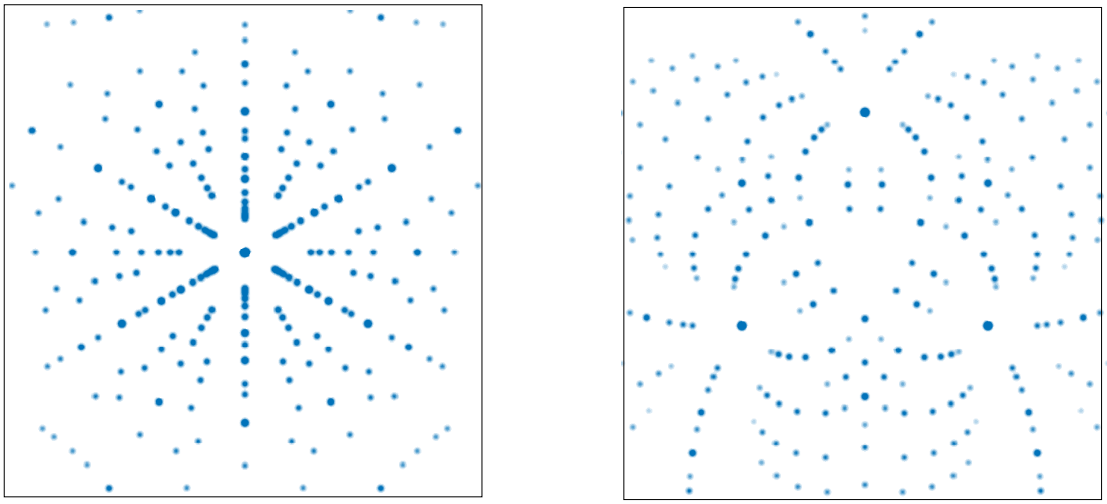


FIGURE 1.5. Simulated Laue photograph of an fcc-lattice along a 3-fold axis. The left figure shows the forward, the right shows the backscattering pattern.

direction $\frac{\mathbf{k}}{|\mathbf{k}|}$, the crystal is rotated. This is equivalent to rotating the argument of the electron density what again is equivalent to rotating the argument of its Fourier transform. So, fixing $\mathbf{k}$ and ω, we vary $\frac{\mathbf{x}}{|\mathbf{x}|}$ and rotate $\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|} - \frac{\mathbf{k}}{|\mathbf{k}|}\right)$. Like that, we reach every reciprocal lattice vector $\mathbf{b}' \in \mathcal{B}^\perp$ that satisfies $|\mathbf{b}'| \leq 2\frac{\omega}{c}$. The used frequency thus determines the resolution of the reconstruction. Different measurement techniques will be shortly discussed in Chapter 3, Section 2.2, from a more abstract point of view.

3.3. The Phase Problem for the Electron Density. Measuring the peak intensities, we have access to the data

$$\{|\widehat{\varphi}(\mathbf{b}')|\}_{\mathbf{b}'\in\mathcal{B}^\perp}\,.$$

Now, the inverse Fourier transform of the distribution $\delta_{\mathcal{B}} \cdot |\widehat{\varphi}| \cdot e^{i\zeta}$ is a $\mathcal{B}$-invariant periodic function for every choice of the phase function $\zeta : \mathbb{R}^3 \to \mathbb{R}$ by the Poisson summation formula. This shows that instead of φ, we can reconstruct the content of a unit cell of the crystal from this data (this is the same effect as in music technology when undersampling an audio file, see [Fri07]).

Indexing the peaks, we get the reciprocal lattice $\mathcal{B}^\perp$ and choose a generator matrix $\mathbf{A}^\perp \in \mathrm{GL}(3,\mathbb{R})$, s.t. $\mathcal{B}^\perp = \mathbf{A}^\perp\mathbb{Z}^3$. Defining $\mathbf{A} := (\mathbf{A}^\perp)^\perp$, we have $\mathcal{B} = \mathbf{A}\mathbb{Z}^3$ as we saw above. Now, consider the canonical unit cell $\mathrm{U}_{\mathcal{B}}^{\mathbf{A}} := \mathbf{A}[0,1)^3$ of $\mathcal{B}$ with respect to $\mathbf{A}$.

Then, when $\rho_{\mathrm{el}} = \delta_{\mathcal{B}} * \varphi$, the electron density can be rewritten as

$$\rho_{\mathrm{el}} = \delta_{\mathcal{B}} * \left((\delta_{\mathcal{B}} * \varphi)|_{\mathrm{U}_{\mathcal{B}}^{\mathbf{A}}} \right) = \delta_{\mathcal{B}} * \varphi_{\mathcal{B}}^{\mathbf{A}},$$

where $\varphi_{\mathcal{B}}^{\mathbf{A}} := (\delta_{\mathcal{B}} * \varphi)|_{\mathrm{U}_{\mathcal{B}}^{\mathbf{A}}}$ will be called the canonical unit cell density. We immediately see that

$$|\widehat{\rho_{\mathrm{el}}}| = \frac{(2\pi)^3}{\mathrm{V}_{\mathcal{B}}} \delta_{\mathcal{B}^\perp} \cdot |\widehat{\varphi_{\mathcal{B}}^{\mathbf{A}}}|.$$

In words, the scattering amplitude at the peaks is essentially the absolute value of the Fourier coefficients of the canonical unit cell density. Here, we run into the so-called phase problem. By taking the absolute value, we loose the phase information. Finding the right phases to get back $\varphi_{\mathcal{B}}^{\mathbf{A}}$ via an inverse Fourier transform is called phase retrieval. The next chapter is devoted to these topics.

In our model density (1.22) we had an additional term that determined the support Ω from the crystal sample. If you want to determine Ω from the diffraction pattern, the term to consider in formula (1.23) for the Fourier transform of the electron density is the Fourier transform of the characteristic function $\widehat{\mathbf{1}_\Omega}$. This factor essentially determines the shape of the peaks. We do not directly see what information on the support is contained in the shape of the peaks on a flat screen. The answer to this question is given in the following section on Coherent Diffraction Imaging.

4. Coherent Diffraction Imaging

A method for the analysis of arbitrary samples was first demonstrated in 1999 (see [MCKS99]). Coherent Diffraction Imaging uses highly brilliant third generation X-ray sources to generate diffraction patterns from which a projection of the sample can be reconstructed. It is not obvious that the diffraction pattern contains the necessary information. Using the formula for the scattering intensity (1.20), we proof the following

Corollary 1.5 (Coherent Diffraction Imaging). *Let $\rho_{\mathrm{el}} \in \mathcal{S}(\mathbb{R}^3)$ (electron density) and $\mathbf{x} = D\frac{\mathbf{k}}{|\mathbf{k}|} + \mathbf{x}_0$ with $D > 0$, $\mathbf{k} \in \mathbb{R}^3$ and $\mathbf{x}_0 \in \mathbf{k}^\perp$ (point on the screen). The scattering intensity* I *defined in formula* (1.20) *satisfies*

$$\mathrm{I}(\mathbf{x}) = c_{\mathrm{el}}^2 \frac{c\varepsilon_0}{2} \frac{|\mathbf{n}|^2}{D^2} \left| \widehat{\mathrm{p}_{\mathbf{k}}\rho_{\mathrm{el}}} \left(\frac{\omega \mathbf{x}_0}{cD} \right) \right|^2 + O\left(\frac{|\mathbf{x}_0|^2}{D^2} \right) \quad \text{as } D \to \infty, \tag{1.26}$$

where $\mathrm{p}_{\mathbf{k}}\varphi(\mathbf{x}_0) := \int_{-\infty}^{\infty} \varphi(\mathbf{x}_0 + r\mathbf{k}/|\mathbf{k}|)\mathrm{d}r$ *for* $\mathbf{x}_0 \in \mathbf{k}^\perp$ *and* $\varphi \in \mathcal{S}(\mathbb{R}^3)$ *is the projection operator along* $\mathbf{k}$.

Proof.

We evaluate the intensity of the scattered radiation (1.20) at the point $\mathbf{x} = D\frac{\mathbf{k}}{|\mathbf{k}|} + \mathbf{x}_0$.

The sine-term can be written as follows:

$$\begin{aligned}\sin^2(\sphericalangle(\mathbf{x},\mathbf{n})) &= 1-\cos^2(\sphericalangle(\mathbf{x},\mathbf{n})) = 1-\frac{(\mathbf{x}\cdot\mathbf{n})^2}{|\mathbf{x}|^2|\mathbf{n}|^2}\\ &= 1-\frac{(\mathbf{x}_0\cdot\mathbf{n})^2}{D^2\left(1+\frac{|\mathbf{x}_0|^2}{D^2}\right)|\mathbf{n}|^2} = 1+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right),\end{aligned}$$

where we used that $\mathbf{n}\cdot\mathbf{k}=0$ and $|\mathbf{x}|^2 = D^2+|\mathbf{x}_0|^2$. By Talyor expansion, we find that

$$|\mathbf{x}|^{-2} = D^{-2}\left(1+\frac{|\mathbf{x}_0|^2}{D^2}\right)^{-1} = D^{-2}\left(1+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\right).$$

For the argument of the Fourier transform, we get

$$\begin{aligned}\frac{\omega}{c}\left(\frac{\mathbf{x}}{|\mathbf{x}|}-\frac{\mathbf{k}}{|\mathbf{k}|}\right) &= \frac{\omega}{c}\left(\frac{D\frac{\mathbf{k}}{|\mathbf{k}|}+\mathbf{x}_0}{\sqrt{D^2+|\mathbf{x}_0|^2}}-\frac{\mathbf{k}}{|\mathbf{k}|}\right)\\ &= \frac{\omega}{c}\left(\mathbf{x}_0\frac{1}{D\sqrt{1+\frac{|\mathbf{x}_0|^2}{D^2}}}+\frac{\mathbf{k}}{|\mathbf{k}|}\left(\frac{1}{\sqrt{1+\frac{|\mathbf{x}_0|^2}{D^2}}}-1\right)\right)\\ &= \frac{\omega}{c}\left(\mathbf{x}_0\left(\frac{1}{D}+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\right)+\frac{\mathbf{k}}{|\mathbf{k}|}O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\right) = \frac{\omega\mathbf{x}_0}{cD}+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\end{aligned}$$

again by Taylor expansion of the respective terms.

So, with (1.20), we have

$$\mathrm{I}(\mathbf{x}) = c_{\mathrm{el}}^2\frac{c\varepsilon_0}{2}|\mathbf{n}|^2\left(\frac{1}{D^2}+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\right)\left|\widehat{\rho_{\mathrm{el}}}\left(\frac{\omega\mathbf{x}_0}{cD}+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\right)\right|^2.$$

With $e^{-iO\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)} = 1+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)$ and ρ_{el} being a Schwartz function, we get

$$\widehat{\rho_{\mathrm{el}}}(\mathbf{y})\left(\frac{\omega\mathbf{x}_0}{cD}+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\right) = \widehat{\rho_{\mathrm{el}}}\left(\frac{\omega\mathbf{x}_0}{cD}\right)+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right).$$

Now, introducing the slice operator $\mathrm{s}_{\mathbf{k}}:\mathcal{S}(\mathbb{R}^3)\to\mathcal{S}(\mathbf{k}^\perp)$, $\mathrm{s}_{\mathbf{k}}\varphi(\mathbf{x}_0) := \varphi(\mathbf{x}_0)$ for $\mathbf{x}_0\in\mathbf{k}^\perp$, we can use the projection-slice theorem (Theorem A.14), that says $\widehat{\mathrm{p}_{\mathbf{k}}\varphi} = \mathrm{s}_{\mathbf{k}}\widehat{\varphi}$. We get

$$\begin{aligned}\mathrm{I}(\mathbf{x}) &= c_{\mathrm{el}}^2\frac{c\varepsilon_0}{2}\frac{|\mathbf{n}|^2}{D^2}\left|\mathrm{s}_{\mathbf{k}}\widehat{\rho_{\mathrm{el}}}\left(\frac{\omega\mathbf{x}_0}{cD}\right)\right|^2+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right)\\ &= c_{\mathrm{el}}^2\frac{c\varepsilon_0}{2}\frac{|\mathbf{n}|^2}{D^2}\left|\widehat{\mathrm{p}_{\mathbf{k}}\rho_{\mathrm{el}}}\left(\frac{\omega\mathbf{x}_0}{cD}\right)\right|^2+O\left(\frac{|\mathbf{x}_0|^2}{D^2}\right).\end{aligned}$$

□

This corollary tells us that on a flat screen in the far-field we get the absolute value squared of the two-dimensional Fourier transform of the projection of ρ_{el} along the propagation direction of the plane wave. The frequency and the distance of the screen appear as scaling parameters. To reconstruct the projection of the sample, one again has to solve a phase problem – this time in two dimensions. How can we determine $\mathrm{p}_{\mathbf{k}}\rho_{\text{el}}$, given $|\widehat{\mathrm{p}_{\mathbf{k}}\rho_{\text{el}}}|$?

In the last section, we saw that we can reconstruct the full three-dimensional electron density in a unit cell of a crystal sample from plane wave diffraction data, when we solve the phase problem. In Coherent Diffraction Imaging, the three-dimensional electron density is not accessible from one single diffraction pattern. But, since we saw in the above proof that we get the absolute values of a slice of the three-dimensional Fourier transform, we could in principle determine the full Fourier modulus by rotating the sample and collecting all the diffraction patterns. This is an example of a tomographic reconstruction.

A Laue photograph can also be understood from the CDI point of view. The forward diffraction pattern is a superposition of slices through the reciprocal lattice, where each slice is scaled by the corresponding frequency.

We also get an answer to the question, what information is contained in the shape of a Bragg peak. It is essentially the modulus of the Fourier transform of the projection of the support of the sample. This idea has been used to reconstruct the shape of nanocrystals in [REA01].

In the following chapter, we discuss the phase problem and introduce some state-of-the-art algorithms for phase retrieval.

CHAPTER 2

Reconstruction from Intensity Measurements

Now, that we have solved the direct problem and know the outgoing radiation of our diffraction experiment, we will investigate the inverse problem. How can we reconstruct the charge density from intensity measurements in the far-field?

As we can only measure the intensity, part of the information that is carried by the field is lost. By formula (1.20), we only have access to the absolute value squared of the Fourier transform of the density, while the phase information is lost.

It is easily seen that the reconstruction problem is in general ill-posed, since any choice of phase yields a reconstruction that could be the solution. However, we can utilize additional information on the structure. A first try is to analyze the problem in a space of non-negative functions, since the electron density ρ_{el} is non-negative. Additionally, we know that the structure has compact support what might be useful information as well.

As turns out, with these assumptions, one can get reasonable results in many situations. However, we will present examples of non-negative compactly supported smooth functions that share the same Fourier modulus, showing that one still needs to be careful when interpreting the results.

We give some mathematical insight on the non-negativity constraint. Up to modulations (or equivalently translations of the structure) there is no manipulation of the phases, s.t. for any non-negative function the corresponding reconstruction is again a non-negative Schwartz function.

When considering the inverse problem in X-ray crystallography, one comes across a different flavor of the phase problem. Usually, the crystal is assumed to be perfect, i.e. that it extends infinitely in space. To reconstruct the content of a translational unit cell from the Fourier coefficient modulus, we do not have a support constraint at hand and run into the following problem. When the density is not only non-negative, but greater than an $\varepsilon > 0$, we find a whole neighborhood of solutions by a continuity argument. Because of this fact, the assumption that molecular structures are atomistic – meaning that the electron density consists of peaks at the atom positions – is usually made. When the goal is to locate the atoms, this might give reasonable results, but it is not clear that it can be used to find an approximation for the electron density.

In the second part of this chapter, we present a few standard algorithms for phase retrieval. Some of them can be motivated from a variational point of view, while others have counterparts in the field of convex optimization. Numerical examples show that a simple iterative scheme as the Gerchberg-Saxton algorithm often runs into areas where stagnation of the approximation error occurs, while more involved projection-based algorithms like Fienup's hybrid input-output algorithm or Elser's difference-map algorithm converge much faster.

1. The Phase Problem

As we have seen in the previous chapter, the task of reconstructing a structure from its diffraction pattern can be essentially reduced to the problem of finding the electron density $\rho_{\mathrm{el}} \in \mathcal{S}(\mathbb{R}^3)$ from its Fourier modulus $|\widehat{\rho_{\mathrm{el}}}|$. The loss of the phase of $\widehat{\rho_{\mathrm{el}}}$ causes the reconstruction problem to be ill-posed. In general, there is no unique solution – a fact that is known as the phase problem.

It is easily seen that, when only assuming that ρ_{el} is a Schwartz function, there are many possible solutions to the phase problem. Take any measurable function $\zeta : \mathbb{R}^3 \to \mathbb{R}$, s.t. $|\widehat{\rho_{\mathrm{el}}}|e^{i\zeta}$ is a Schwartz function and define the function

$$\rho_\zeta := \mathcal{F}^{-1}(|\widehat{\rho_{\mathrm{el}}}|e^{i\zeta}) \in \mathcal{S}(\mathbb{R}^3).$$

We find that

$$|\widehat{\rho_\zeta}| = \left||\widehat{\rho_{\mathrm{el}}}|e^{i\zeta}\right| = |\widehat{\rho_{\mathrm{el}}}|,$$

s.t. ρ_ζ solves the phase problem for every such ζ. There are many such functions. For example, when ζ_{el} is the phase of $\widehat{\rho_{\mathrm{el}}}$, i.e. $\widehat{\rho_{\mathrm{el}}} = |\widehat{\rho_{\mathrm{el}}}|e^{i\zeta_{\mathrm{el}}}$, and ζ_0 is a tempered function, then $\zeta := \zeta_{\mathrm{el}} + \zeta_0$ satisfies the condition.

Consequently, we need additional information on the function ρ_{el} to reduce the number of solutions. Choosing the space of real Schwartz functions doesn't help, since for a function ρ_{el} to be real is equivalent to satisfying $\widehat{\rho_{\mathrm{el}}} = \overline{\widehat{\rho_{\mathrm{el}-}}}$, where $\rho_{\mathrm{el}-}(\mathbf{x}) := \rho_{\mathrm{el}}(-\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}$. So, again choosing a measurable function $\zeta : \mathbb{R}^3 \to \mathbb{R}^3$, s.t. $|\widehat{\rho_{\mathrm{el}}}|e^{i\zeta}$ is a Schwartz function and additionally satisfying $\zeta_- = -\zeta$, we get

$$\overline{\widehat{\rho_{\zeta-}}} = \overline{|\widehat{\rho_{\mathrm{el}-}}|e^{i\zeta-}} = |\widehat{\rho_{\mathrm{el}}}|\overline{e^{-i\zeta}} = |\widehat{\rho_{\mathrm{el}}}|e^{i\zeta} = \widehat{\rho_\zeta},$$

s.t. the real Schwartz function ρ_ζ solves the phase problem.

As an electron density is naturally non-negative, and a physical sample is finite in size, we consider the two subsets of the space of Schwartz functions

$$\mathcal{S}^{\geq 0}(\mathbb{R}^3) := \{\varphi \in \mathcal{S}(\mathbb{R}^3).\ \varphi \geq 0\},$$
$$\mathcal{S}_\Omega(\mathbb{R}^3) := \{\varphi \in \mathcal{S}(\mathbb{R}^3).\ \mathrm{supp}(\varphi) \subseteq \Omega\},\ \Omega \subset \mathbb{R}^3 \text{ compact.}$$

Note that $\mathcal{S}_\Omega(\mathbb{R}^3)$ is a subspace of $\mathcal{S}(\mathbb{R}^3)$, while $\mathcal{S}^{\geq 0}$ is not. As turns out, these sets do the trick in many cases. Before we turn to these constraints, we consider some special choices of ζ.

When ζ_{el} is the phase of $\widehat{\rho_{\mathrm{el}}}$, i.e. $\widehat{\rho_{\mathrm{el}}} = |\widehat{\rho_{\mathrm{el}}}|e^{i\zeta_{\mathrm{el}}}$, and we choose $\zeta(\mathbf{x}) := \zeta_{\mathrm{el}}(\mathbf{x}) + \mathbf{y}\cdot\mathbf{x}$ for some $\mathbf{y} \in \mathbb{R}^3$ and all $\mathbf{x} \in \mathbb{R}^3$, we get

$$\rho_\zeta(\mathbf{x}) = \mathcal{F}^{-1}(|\widehat{\rho_{\mathrm{el}}}|e^{i\zeta}) = \mathcal{F}^{-1}(|\widehat{\rho_{\mathrm{el}}}|e^{i\zeta_{\mathrm{el}}}e^{i\mathbf{y}\cdot\mathbf{x}}) = \mathcal{F}^{-1}(e^{i\mathbf{y}\cdot\mathbf{x}}\widehat{\rho_{\mathrm{el}}}) = \rho_{\mathrm{el}}(\mathbf{x}+\mathbf{y}),$$

where we used the translation-modulation duality (A.5).

So, this special choice of ζ gives just a translate of the original function. The set $\mathcal{S}^{\geq 0}(\mathbb{R}^3)$ is closed w.r.t. translations, s.t. this ambiguity will stay for the non-negativity constraint. However, as we are interested in the structure and not the exact position of ρ_{el}, this is not a problem for structure analysis.

Another special choice of ζ is $\zeta = -\zeta_{\mathrm{el}}$, s.t.

$$\rho_\zeta = \mathcal{F}^{-1}(|\widehat{\rho_{\mathrm{el}}}|e^{-i\zeta_{\mathrm{el}}}) = \mathcal{F}^{-1}(\overline{|\widehat{\rho_{\mathrm{el}}}|e^{i\zeta_{\mathrm{el}}}}) = \mathcal{F}^{-1}(\overline{\widehat{\rho_{\mathrm{el}}}}) = \overline{\mathcal{F}^{-1}(\widehat{\rho_{\mathrm{el}}})_-} = \overline{\rho_{\mathrm{el}}}_-.$$

Again, this is not a problem for structure determination, if one is not interested in orientation. For complex functions, one further trivial solution to the phase problem is the multiplication by a complex number of absolute value one – a global phase.

In summary, what we can hope for, is to reconstruct ρ_{el} up to translations and inversion when ρ_{el} is real, and up to translations, inversion plus complex conjugation and a global phase when it is complex.

1.1. The General Phase Problem. We introduce a notion that specifies if a given constraint set is strong enough, in the sense that one cannot directly give multiple solutions for every set of measurements, as we saw is possible in the space of (real) Schwartz functions.

Consider the following operators on a set of functions $\mathrm{F}(\mathbb{R}^3) \subseteq \mathcal{S}'(\mathbb{R}^3)$:

$$\mathrm{M}_\zeta\varphi := \mathcal{F}^{-1}(e^{i\zeta}\widehat{\varphi}), \quad \varphi \in \mathrm{F}(\mathbb{R}^3),$$

for measurable functions $\zeta : \mathbb{R}^3 \to \mathbb{R}$, s.t. $\mathrm{M}_\zeta\varphi$ is again a function in $\mathrm{F}(\mathbb{R}^3)$. Then

$$|\widehat{\mathrm{M}_\zeta\varphi}| = |e^{i\zeta}\widehat{\varphi}| = |\widehat{\varphi}|.$$

So, this family of operators specifies the operations on the phases of the Fourier transform that solve the phase problem for every function in $\mathrm{F}(\mathbb{R}^3)$. In this sense, they define a general phase problem in the set $\mathrm{F}(\mathbb{R}^3)$. For example, we saw that for the choice $\mathrm{F}(\mathbb{R}^3) = \mathcal{S}(\mathbb{R}^3)$, every real tempered function $\zeta \in \mathcal{T}(\mathbb{R}^3)$ yields an operator M_ζ s.t. $\mathrm{M}_\zeta\varphi \in \mathcal{S}(\mathbb{R}^3)$ for all $\varphi \in \mathcal{S}(\mathbb{R}^3)$.

The global phase and the translations are operations on the phases of this kind. They correspond to ζ being an affine linear form, i.e. $\zeta = \langle \mathbf{y}, \cdot\rangle + a$ for some $\mathbf{y} \in \mathbb{R}^3$ and an $a \in \mathbb{R}$. We call the space of affine linear forms $\mathrm{Aff}(\mathbb{R}^3, \mathbb{R})$. The inversion (plus conjugation), however, depends on ρ_{el} (via ζ_{el}) and is therefore not a general phase problem in our sense.

Introducing the set $\mathrm{Z}(\mathrm{F}(\mathbb{R}^3))$ of phase functions that produce a phase problem of this general kind,

$$\mathrm{Z}(\mathrm{F}(\mathbb{R}^3)) := \{\zeta : \mathbb{R}^3 \to \mathbb{R} \text{ measurable. } \mathrm{M}_\zeta\varphi \in \mathrm{F}(\mathbb{R}^3) \text{ for all } \varphi \in \mathrm{F}(\mathbb{R}^3)\},$$

and noting that it is a group with respect to addition, we make the following definition

Definition 2.1 (General phase problem). *Let $\mathrm{F}(\mathbb{R}^3) \subset \mathcal{S}'(\mathbb{R}^3)$ be a set of functions. We say that there is no general phase problem in $\mathrm{F}(\mathbb{R}^3)$, if $\mathrm{Z}(\mathrm{F}(\mathbb{R}^3))$ is a subgroup of the group of affine linear forms $\mathrm{Aff}(\mathbb{R}^3, \mathbb{R})$. If this is not the case, we say that there is a general phase problem in $\mathrm{F}(\mathbb{R}^3)$.*

We already showed that there is a general phase problem in the space of (real) Schwartz functions.

For the choice $\mathrm{F}(\mathbb{R}^3) = \mathcal{S}^{\geq 0}(\mathbb{R}^3)$, we show that there is no general phase problem.

Proposition 2.2 (No General Phase Problem in $\mathcal{S}^{\geq 0}(\mathbb{R}^3)$). *There is no general phase problem in $\mathcal{S}^{\geq 0}(\mathbb{R}^3)$. In particular,*

$$\mathrm{Z}(\mathcal{S}^{\geq 0}(\mathbb{R}^3)) = \{\zeta : \ \mathbf{x} \mapsto \ \langle \mathbf{y}, \mathbf{x}\rangle \text{ for some } \mathbf{y} \in \mathbb{R}^3\}.$$

Proof. We introduce the set $\mathrm{K}(\mathrm{F}(\mathbb{R}^3)) := \{\mathrm{K}_\zeta := \mathcal{F}^{-1}(e^{i\zeta}).\ \zeta \in \mathrm{Z}(\mathrm{F}(\mathbb{R}^3))\} \subset \mathcal{S}'(\mathbb{R}^3)$. Obviously, the group $(\mathrm{K}(\mathrm{F}(\mathbb{R}^3)), *)$ is isomorphic to $(\mathrm{Z}(\mathrm{F}(\mathbb{R}^3)), +)$. Now, we show that $\mathrm{K}(\mathcal{S}^{\geq 0}(\mathbb{R}^3)) = \{\delta_{\mathbf{y}}.\ \mathbf{y} \in \mathbb{R}^3\}$ what is equivalent to the statement of the proposition.

First, we show that

$$\mathrm{K}_\zeta \in \mathrm{K}(\mathcal{S}^{\geq 0}(\mathbb{R}^3)) \Rightarrow \mathrm{K}_\zeta \geq 0. \qquad (*)$$

Assume that $\mathrm{K}_\zeta \not\geq 0$, i.e. there is a $\psi \in \mathcal{S}^{\geq 0}(\mathbb{R}^3)$, s.t. $\mathrm{K}_\zeta(\psi) < 0$ (note that K_ζ is a tempered distribution). When $\mathrm{G}_\varepsilon(\mathbf{x}) := \frac{1}{(2\pi\varepsilon^2)^{3/2}} e^{-|\mathbf{x}|^2/2\varepsilon^2}$, $\mathbf{x} \in \mathbb{R}^3$ is the Gaussian with

standard deviation $\varepsilon > 0$, we conclude that by continuity of K_ζ, for ε small enough

$$\mathrm{M}_\zeta\psi_-(\mathrm{G}_\varepsilon) = (\mathrm{K}_\zeta * \psi_-)(\mathrm{G}_\varepsilon) = \mathrm{K}_\zeta(\psi * \mathrm{G}_\varepsilon) < 0,$$

where we interpreted $\mathrm{M}_\zeta\psi_-$ as tempered distribution and used that $\psi * \mathrm{G}_\varepsilon \to \psi$ in $\mathcal{S}^{\geq 0}(\mathbb{R}^3)$ for $\varepsilon \to 0$. Thus $\mathrm{M}_\zeta\psi_- \not\geq 0$ and therefore $\mathrm{M}_\zeta\psi_- \notin \mathcal{S}^{\geq 0}(\mathbb{R}^3)$, showing $(*)$.

So, assuming $\mathrm{K}_\zeta \in \mathrm{K}(\mathcal{S}^{\geq 0}(\mathbb{R}^3))$, we know that $\mathrm{K}_\zeta \geq 0$ and $|\widehat{\mathrm{K}_\zeta}| = |e^{i\zeta}| = 1$ and have to show that $\mathrm{K}_\zeta = \delta_{\mathbf{y}}$ for some $\mathbf{y} \in \mathbb{R}^3$.

Now, since $\mathrm{K}_\zeta \geq 0$, we know that K_ζ is actually a measure (Proposition A.15). In addition, $|\widehat{\mathrm{K}_\zeta}| = 1$, so K_ζ is a probability measure.

Using the convolution theorem (Corollary A.11), we get

$$1 = |\widehat{\mathrm{K}_\zeta}|^2 = \widehat{\mathrm{K}_\zeta} \cdot \overline{\widehat{\mathrm{K}_\zeta}} = \mathcal{F}(\mathrm{K}_\zeta * \overline{\mathrm{K}_\zeta}_-) = \mathcal{F}(\mathrm{K}_\zeta * \mathrm{K}_{\zeta\,-}),$$

so that by an inverse Fourier transform, we get

$$\mathrm{K}_\zeta * \mathrm{K}_{\zeta\,-} = \delta_0.$$

Now, for the support of the convolution of two probability measures μ and ν, we know that

$$\mathrm{supp}(\mu * \nu) = \mathrm{supp}(\mu) + \mathrm{supp}(\nu).$$

In our case, we get

$$\{0\} = \mathrm{supp}(\mathrm{K}_\zeta * (\mathrm{K}_\zeta)_-) = \mathrm{supp}(\mathrm{K}_\zeta) + \mathrm{supp}(\mathrm{K}_{\zeta\,-}) = \mathrm{supp}(\mathrm{K}_\zeta) - \mathrm{supp}(\mathrm{K}_\zeta),$$

where we used that $\mathrm{supp}(T_-) = -\mathrm{supp}(T)$. Assuming that $|\mathrm{supp}(\mathrm{K}_\zeta)| \geq 2$, we get that

$$1 = |\{0\}| = |\mathrm{supp}(\mathrm{K}_\zeta) - \mathrm{supp}(\mathrm{K}_\zeta)| \geq 2,$$

what is a contradiction and shows that $|\mathrm{supp}(\mathrm{K}_\zeta)| = 1$.

But the only probability measures supported on a single point are the measures $\delta_{\mathbf{y}}$ for $\mathbf{y} \in \mathbb{R}^3$. □

Note, that this result can be extended to the n-dimensional case with the exact same proof.

This proposition shows that it is not totally meaningless to try to solve the phase problem in the set $\mathcal{S}^{\geq 0}(\mathbb{R}^3)$.

To make use of the support constraint, we need to find an explicit compact set $\Omega \subset \mathbb{R}^3$, s.t. $\mathrm{supp}(\varphi) \subseteq \Omega$, given the Fourier modulus of a Schwartz function φ that is compactly supported. Calculating the inverse Fourier transform of $|\widehat{\varphi}|^2$, we get the autocorrelation function (Corollary A.12):

$$\mathcal{F}^{-1}(|\widehat{\varphi}|^2) = \varphi * \overline{\varphi}_-.$$

Now,

$$\operatorname{supp}(\varphi * \overline{\varphi}_-) = \operatorname{supp}(\varphi) + \operatorname{supp}(\overline{\varphi}_-) = \operatorname{supp}(\varphi) - \operatorname{supp}(\varphi),$$

which is a compact set when $\operatorname{supp}(\varphi)$ is compact.

Hence, defining $\Omega := \operatorname{supp}(\mathcal{F}^{-1}(|\widehat{\varphi}|^2))$, we get $\operatorname{supp}(\varphi) \subseteq \Omega$, so $\varphi \in \mathcal{S}_\Omega(\mathbb{R}^3)$. Better estimates for the support of a function given its autocorrelation support are for example given in [CFT90].

As a corollary, we get

Corollary 2.3 (No General Phase Problem in $\mathcal{S}_\Omega^{\geq 0}(\mathbb{R}^3)$). *Let $\Omega \subset \mathbb{R}^3$ be a compact set such that there is a function $\varphi \in \mathcal{S}(\mathbb{R}^3)$ with $\operatorname{supp}(\varphi) = \Omega$ and*

$$\mathcal{S}_\Omega^{\geq 0}(\mathbb{R}^3) := \{\varphi \in \mathcal{S}(\mathbb{R}^3).\ \varphi \geq 0,\ \operatorname{supp}(\varphi) \subseteq \Omega\}.$$

There is no general phase problem in $\mathcal{S}_\Omega^{\geq 0}(\mathbb{R}^3)$. In particular, $\mathrm{Z}(\mathcal{S}_\Omega^{\geq 0}(\mathbb{R}^3))$ is trivial.

Proof. That $\mathrm{Z}(\mathcal{S}_\Omega^{\geq 0}(\mathbb{R}^3)) \leq \{\zeta :\ \mathbf{x} \mapsto \langle \mathbf{y}, \mathbf{x}\rangle \text{ for some } \mathbf{y} \in \mathbb{R}^3\}$ follows from Proposition 2.2. Now, as there is a Schwartz function φ with support $\operatorname{supp}(\varphi) = \Omega$, we find that for $\zeta(\mathbf{x}) := \langle \mathbf{y}, \mathbf{x}\rangle$ for some $\mathbf{y} \in \mathbb{R}^3$ and all $\mathbf{x} \in \mathbb{R}^3$,

$$\mathrm{M}_\zeta \varphi(\mathbf{x}) = \varphi(\mathbf{x} + \mathbf{y}).$$

So, when $\mathbf{y} \neq 0$, $\operatorname{supp}(\mathrm{M}_\zeta \varphi) = \Omega + \mathbf{y} \not\subseteq \Omega$, showing that $\mathrm{Z}(\mathrm{F}(\mathbb{R}^3))$ is trivial. □

1.2. The Phase Problem in 1D and its Consequences. Even though these results show that it is not entirely hopeless to try to solve the phase problem in the respective spaces, we did not get an answer to the question if there is a phase problem for a given function.

This question has been investigated by different authors starting with [BS79]. There, distributions on $\mathbb{R}$ of the form

$$T = \sum_{j=0}^{N} a_j \delta_{j\Delta\mathbf{x}} \in \mathcal{S}'(\mathbb{R}), \quad N \in \mathbb{N},\ a_j > 0, j \in \{0, \ldots, N\},\ \Delta\mathbf{x} > 0,$$

are considered. T can be seen as as approximation of the electron density of a one-dimensional atomic structure or as sampling of a continuous electron density. Since the functions $T * \varphi$ are elements of $\mathcal{S}^{\geq 0}(\mathbb{R})$ for all $\varphi \in \mathcal{S}^{\geq 0}(\mathbb{R})$, and $|\widehat{T * \varphi}| = |\widehat{T}||\widehat{\varphi}|$, these distributions are also relevant for the case of smooth functions.

The main result of [BS79] is the construction of all solutions to the phase problem of the same form as T, i.e. all distributions $\widetilde{T}$ of the form $\widetilde{T} = \sum_{j=0}^{N} \widetilde{a}_j \delta j\Delta\mathbf{x}$ that satisfy $|\widehat{\widetilde{T}}| = |\widehat{T}|$. The construction is the following:

First, a polynomial p_T is constructed that is related to the Fourier modulus $|\widehat{T}|$. Let

$$p_T(z) := \sum_{j=0}^{N} a_j z^j.$$

Then, setting $z_k := e^{-ik\Delta x}$ for $k \in \mathbb{R}$, we get $|\widehat{T}(k)| = |p_T(z_k)|$.

Now, writing $p_T(z) = a_N \prod_{j=1}^{N}(z - z_j)$ for $z_j \in \mathbb{C}$, $j = 1, \ldots, N$, using the fundamental theorem of algebra, we define another function Q_T that is related to the squared Fourier modulus:

$$Q_T(z) := |p_T(z)p_T(z^{-1})z^N| = a_N a_0 \prod_{j=1}^{N} |z - z_j||z - z_j^{-1}|.$$

Because $p_T(z^{-1})z^N$ is the polynomial that you get by reversing the order of the coefficients of p_T, we immediately get that

$$Q_T(z_k) = |\widehat{T}(k)|^2.$$

Now choosing $\widetilde{z}_j \in \{z_j, z_j^{-1}\}$, $j = 1, \ldots, N$, we define the polynomial

$$p_{\widetilde{T}}(z) := \sqrt{\frac{a_N a_0}{\prod_{j=1}^{N} |\widetilde{z}_j|}} \prod_{j=1}^{N} (z - \widetilde{z}_j).$$

Considering the distribution $\widetilde{T}$ associated to $p_{\widetilde{T}}$, i.e. choosing the coefficients $\widetilde{a}_j$ as the respective coefficients of $p_{\widetilde{T}}$, we see that

$$Q_T = Q_{\widetilde{T}},$$

and hence $|\widehat{\widetilde{T}}| = |\widehat{T}|$.

The simplest non-trivial example of this phase problem is the distribution

$$T_1 := 4\delta_0 + 4\delta_1 + \delta_2.$$

We get $p_{T_1}(z) = (z + 2)^2$ and $Q_{T_1} = 4(z + 2)^2(z + 1/2)^2$. Choosing $\widetilde{z}_1 = 2$ and $\widetilde{z}_2 = \frac{1}{2}$, we define the distribution T_2 by the polynomial

$$p_{T_2}(z) = 2(z + 2)(z + 1/2) = 2z^2 + 5z + 2,$$

so, $T_2 = 2\delta_0 + 5\delta_1 + 2\delta_2$. The two distributions T_1 and T_2 then have identical Fourier modulus, what can also be seen by direct calculation:

$$|\widehat{T_1}|^2 = |\widehat{T_2}|^2 = 33 + 40\cos(k) + 8\cos(2k).$$

As we saw above, choosing a function $\varphi \in \mathcal{S}^{\geq 0}(\mathbb{R})$, we also get $|\widehat{T_1 * \varphi}| = |\widehat{T_2 * \varphi}|$.

The construction can also be used to construct examples in higher dimensions by forming tensor products. Define

$$T_{ij} := (T_i * \varphi) \otimes (T_j * \varphi) \in \mathcal{S}(\mathbb{R}^2),\ i, j = 1, 2, i \geq j.$$

Then, for $k = (k_1, k_2) \in \mathbb{R}^2$

$$\begin{aligned} |\widehat{T_{ij}}(k)|^2 &= |\widehat{T_i * \varphi}(k_1) \cdot \widehat{T_j * \varphi}(k_2)|^2 = |\widehat{T}_i(k_1)\widehat{\varphi}(k_1)\widehat{T}_j(k_2)\widehat{\varphi}(k_2)|^2 \\ &= |\widehat{T}_i(k_1)|^2 |\widehat{\varphi}(k_1)|^2 |\widehat{T}_j(k_2)|^2 |\widehat{\varphi}(k_2)|^2, \end{aligned}$$

so, $|\widehat{T_{ij}}| = |\widehat{T_{i'j'}}|$ for any choice of i, j, i', j'. These three functions are shown in Figure 2.1 for φ being a Gaussian. Choosing $\varphi \in \mathcal{S}^{\geq 0}$ with compact support instead, this yields an example fot the phase problem in the set $\mathcal{S}^{\geq 0}_{\Omega}$, when choosing Ω appropriately.

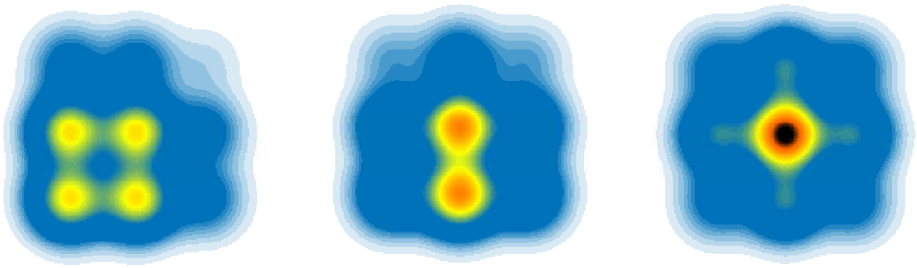


FIGURE 2.1. The three functions T_{11}, T_{12}, and T_{22} for φ being a Gaussian. These functions share the exact same Fourier modulus. This is an example for the phase problem in $\mathcal{S}^{\geq 0}(\mathbb{R}^2)$.

The construction of Bruck and Sodin has been generalized to investigate the phase problem in higher dimension in [Hay82]. The author comes to the conclusion that the phase problem is not as severe as in one dimension, since the polynomials that can be factored as above are a null set in the space of all polynomials. In this sense, there seems to be almost no phase problem in higher dimensions. However, this is a very weak statement, since a null set can be dense, making the reconstruction problem unstable. In addition, the set of electron densities of molecular structures is not a random set and could intersect this null set non-trivially. We will see, that the phase problem is far from being harmless when considering a special class of periodic functions.

1.3. The Phase Problem for Periodic Functions. First, we go back to Proposition 2.2. The functions $e^{i\zeta}$, $\zeta : \mathbb{R}^3 \to \mathbb{R}$ measurable, can be identified with functionals L_ζ on the space of finite complex measures $\mathrm{M}^1(\mathbb{R}^3)$:

$$L_\zeta \mu := \int_{\mathbb{R}^3} e^{i\zeta} \mathrm{d}\mu, \quad \mu \in \mathrm{M}^1(\mathbb{R}^3).$$

The tempered distribution $\mathrm{K}_\zeta := \mathcal{F}^{-1}(e^{i\zeta})$ can thus be extended to a functional on the space of Fourier transforms of finite complex measures $\mathcal{F}\mathrm{M}^1(\mathbb{R}^3)$ by

$$\mathrm{K}_\zeta \widehat{\mu} := L_\zeta \mathcal{F}^{-1}\widehat{\mu} = L_\zeta \mu, \quad \mu \in \mathrm{M}^1(\mathbb{R}^3).$$

With this construction, the proof of Proposition 2.2 with $\mathcal{S}^{\geq 0}(\mathbb{R}^3)$ replaced by $\mathcal{F}\mathrm{M}^1_{\geq 0}(\mathbb{R}^3)$ gives

Corollary 2.4 (No General Phase Problem in $\mathcal{F}\mathrm{M}^1_{\geq 0}(\mathbb{R}^3)$). *Let*

$$\mathcal{F}\mathrm{M}^1_{\geq 0}(\mathbb{R}^3) := \{\varphi \in \mathcal{F}\mathrm{M}^1(\mathbb{R}^3).\ \varphi \geq 0\}.$$

There is no general phase problem in $\mathcal{F}\mathrm{M}^1_{\geq 0}(\mathbb{R}^3)$. In particular,

$$Z(\mathcal{F}\mathrm{M}^1_{\geq 0}(\mathbb{R}^3)) = \{\zeta :\ \mathbf{x} \mapsto \langle \mathbf{y}, \mathbf{x}\rangle \text{ for some } \mathbf{y} \in \mathbb{R}^3\}.$$

Now, Fourier transforms of finite measures are bounded continuous functions. In particular, choosing a non-negative function $\varphi \in \mathcal{S}^{\geq 0}(\mathbb{R}^3)$, define the bounded continuous function

$$\rho_{\mathrm{el}} := \delta_{\mathcal{B}} * \varphi,$$

where $\mathcal{B} \subset \mathbb{R}^3$ is a Bravais lattice. Then we know that

$$\widehat{\rho_{\mathrm{el}}} = \frac{(2\pi)^3}{\mathrm{V}_{\mathcal{B}}} \delta_{\mathcal{B}^\perp} \cdot \widehat{\varphi}.$$

Now, since $\delta_{\mathcal{B}^\perp}$ is a tempered distributionand and $\widehat{\varphi} \in \mathcal{S}(\mathbb{R}^3)$,

$$\widehat{\rho_{\mathrm{el}}}(\mathbb{R}^3) = \frac{(2\pi)^3}{\mathrm{V}_{\mathcal{B}}} \sum_{\mathbf{b} \in \mathcal{B}^\perp} \widehat{\varphi}(\mathbf{b}) = \frac{(2\pi)^3}{\mathrm{V}_{\mathcal{B}}} \delta_{\mathcal{B}^\perp}(\widehat{\varphi}) < \infty.$$

Consequently, $\widehat{\rho_{\mathrm{el}}} \in M^1(\mathbb{R}^3)$ and $\rho_{\mathrm{el}} \in \mathcal{F}\mathrm{M}^1_{\geq 0}(\mathbb{R}^3)$. This means, that our model densities from Chapter 1, Section 3, fall into this class of functions. Consequently, Corollary 2.4 says that it is not absolutely hopeless to try to solve the phase problem.

However, we come across a different flavor of the phase problem due to the continuity of the phase transformations M_ζ. Consider the following set of functions:

$$\mathcal{F}\mathrm{M}^1_\varepsilon(\mathbb{R}^3) := \{\varphi \in \mathcal{F}\mathrm{M}^1(\mathbb{R}^3).\ \varphi \geq \varepsilon\}, \quad \varepsilon > 0.$$

Then choosing the phase function ζ s.t. $\|\zeta\|_\infty \leq \delta$ for some $\delta > 0$, we get for $\varphi \in \mathcal{F}\mathrm{M}^1_\varepsilon(\mathbb{R}^3)$:

$$\begin{aligned}|\mathrm{M}_\zeta\varphi(\mathbf{x}) - \varphi(\mathbf{x})| &= |\mathcal{F}^{-1}(e^{i\zeta}\widehat{\varphi})(\mathbf{x}) - \mathcal{F}^{-1}\widehat{\varphi}| = |\mathcal{F}^{-1}(\widehat{\varphi}(e^{i\zeta}-1))(\mathbf{x})| \\ &= \frac{1}{(2\pi)^3}\left|\int_{\mathbb{R}^3} \underbrace{(e^{i\zeta(\mathbf{k})}-1)}_{=2ie^{i\zeta(\mathbf{k})/2}\sin(\zeta(\mathbf{k})/2)} e^{i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}(\mathbf{k})\right| \\ &\leq \frac{2}{(2\pi)^3}\int_{\mathbb{R}^3} |\sin(\zeta(\mathbf{k})/2)|\mathrm{d}|\widehat{\varphi}|(\mathbf{k}) \leq \frac{\delta}{(2\pi)^3}\|\widehat{\varphi}\|_{M^1(\mathbb{R}^3)} < \infty,\end{aligned}$$

where we used $|\sin(\mathbf{x})| \leq |\mathbf{x}|$. So, whenever $\delta \leq \frac{(2\pi)^3\varepsilon}{\|\widehat{\varphi}\|_{M^1(\mathbb{R}^3)}}$, then $\mathrm{M}_\zeta \in \mathcal{F}\mathrm{M}^1_{\geq 0}(\mathbb{R}^3)$. In other words, when the electron density in the unit cell of a crystal is greater than an $\varepsilon > 0$, then there is a whole neighborhood of solutions to the phase problem. This seems to be one of the reasons that in X-ray Crystallography, in contrast to Coherent Diffraction Imaging, additional constraints are needed to solve the phase problem uniquely.

Usually, the electron density of a crystal is highly concentrated at the atom positions. So, it is natural to try to find the solution to a given phase problem that is most concentrated in some sense. The corresponding constraint is usually called atomicity. In its most restrictive form it says that the density consists of non-overlapping equal atoms, i.e.

$$\varphi(\mathbf{x}) = \delta_{\mathbf{M}^{\mathbf{A}}_{\mathcal{B}}} * \varphi_{\mathrm{a}}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3,$$

where $\mathbf{M}^{\mathbf{A}}_{\mathcal{B}} \subset \mathbb{R}^3$ is a finite set and $\varphi_{\mathrm{a}} \in \mathcal{S}(\mathbb{R}^3)$ satisfies

$$\mathrm{supp}(\varphi_{\mathrm{a}}(\cdot - \mathbf{y})) \cap \mathrm{supp}(\varphi_{\mathrm{a}}(\cdot - \mathbf{y}')) = \emptyset \quad \text{for all } \mathbf{y}, \mathbf{y}' \in \mathcal{B} + \mathbf{M}^{\mathbf{A}}_{\mathcal{B}},\ \mathbf{y} \neq \mathbf{y}'.$$

A crucial observation was made by D. Sayre in [Say52-1], where he found an invariance property of the considered structures. Since the atoms do not overlap, we have

$$\rho^2_{\mathrm{el}} = \delta_{\mathcal{L}} * \varphi^2_{\mathrm{a}}, \quad \text{where } \mathcal{L} := \mathcal{B} + \mathbf{M}^{\mathbf{A}}_{\mathcal{B}}.$$

Defining the function

$$\varphi_{\mathrm{Sayre}}(\mathbf{x}) := \mathcal{F}^{-1}\left(\frac{\widehat{\varphi_{\mathrm{a}}}}{\widehat{\varphi^2_{\mathrm{a}}}}\mathbf{1}_{\{\widehat{\varphi^2_{\mathrm{a}}}\neq 0\}}\right)(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3,$$

the density satisfies the so-called Sayre equation (compare the account in [Els03]):

$$\rho_{\mathrm{el}} = \varphi_{\mathrm{Sayre}} * \rho^2_{\mathrm{el}}. \tag{2.1}$$

This equation is closely related to the development of the tangent formula of J. Karle and H. Hauptman that were awarded the 1985 Nobel prize in chemistry for their so-called direct methods for solving crystal structures [HK53]. These methods were refined over the years (e.g. [CW55, Gia76, US99]) and are still in use today.

A different idea for the solution of the phase problem in X-ray crystallography is to simply measure the phases experimentally. In [Wol09,Wol10] a method is proposed but, to the knowledge of the author, hasn't been successfully realized for determining the phases in X-ray diffraction experiments.

2. Phase Retrieval

In the last section, we saw that given the Fourier modulus $|\widehat{\rho_{\mathrm{el}}}|$ of a function ρ_{el}, one can only reconstruct the original function up to the phase problem. However, for data coming from experiments, it is often possible to uniquely solve the phase problem.

In this section, therefore, we suppose that the phase problem is solvable and ask the question how to find a solution explicitly. This problem is known as phase retrieval.

Suppose that the electron density $\rho_{\mathrm{el}} \in \mathcal{S}^{\geq 0}(\mathbb{R}^n)$ of the structure is non-negative and compactly supported, and that the absolute value squared of the Fourier transform of ρ_{el} that we extracted from intensity measurements is I. In the previous chapter, we saw that when defining

$$\Omega := \mathrm{supp}(\mathcal{F}^{-1}\mathrm{I}),$$

or have any other support constraint at hand, then we know that $\rho_{\mathrm{el}} \in \mathcal{S}^{\geq 0}_{\Omega}(\mathbb{R}^n)$. Therefore, we have three constraints any solution must fulfill:

(i) $|\widehat{\rho_{\mathrm{el}}}|^2 = \mathrm{I}$,
(ii) $\rho_{\mathrm{el}} \geq 0$,
(iii) $\mathrm{supp}(\rho_{\mathrm{el}}) \subseteq \Omega$.

We shortly discuss a few algorithms for phase retrieval that use these constraints without going into details concerning convergence results. Instead, to get a feeling for the performance of the algorithms, we provide a numerical example at the end of the section.

2.1. The Error-Reduction Algorithm. A very simple algorithm was origined by Gerchberg and Saxton [GS72] and is called Gerchberg-Saxton algorithm or error-reduction algorithm. In its basic form, it only cares about the constrainsts (i) and (ii) and works as follows. Start with a random choice ζ_0 for the phase function that satisfies $(\zeta_0)_- = -\zeta_0$ to get a real inverse Fourier transform and set

$$\widetilde{\rho_0} := \mathcal{F}^{-1}(\sqrt{I}e^{i\zeta_0}).$$

This first guess perfectly satisfies condition (i), but most certainly is not non-negative. So, one defines

$$\rho_1 := \widetilde{\rho_0} \cdot \mathbf{1}_{\{\widetilde{\rho_0} \geq 0\}}.$$

Now, ρ_1 satisfies (ii), but in general not (i). Consequently, one starts another iteration by writing $\widehat{\rho_1} = |\widehat{\rho_1}|e^{i\zeta_1}$ (note that ζ_1 is not unique – we will come to that later) and setting

$$\widetilde{\rho_1} := \mathcal{F}^{-1}(\sqrt{I}e^{i\zeta_1}) \text{ and } \rho_2 := \widetilde{\rho_1} \cdot \mathbf{1}_{\{\widetilde{\rho_1} \geq 0\}}.$$

The error-reduction algorithm thus woks as follows. For $j \in \mathbb{N}$ repeat the two steps

$$\widetilde{\rho_j} := \mathcal{F}^{-1}(\sqrt{I}e^{i\zeta_j}), \tag{ER1}$$

$$\rho_{j+1} := \widetilde{\rho_j} \cdot \mathbf{1}_{\{\widetilde{\rho_j} > 0\}}, \tag{ER2}$$

until the algorithm converges in some sense.

It is not obvious that ρ_{n+1} should be a better guess than ρ_n. But in fact it is. This can be seen as follows (see [Fie82]).

Define the following two quantities to track the progress of the iteration:

$$\mathrm{e}_j := \|\rho_{j+1} - \widetilde{\rho_j}\|_2, \quad \widehat{\mathrm{e}}_j := \|\widehat{\rho_j} - \widehat{\widetilde{\rho_j}}\|_2.$$

Note, that $\widehat{\mathrm{e}}_j = \||\widehat{\rho_j}| - \sqrt{\mathrm{I}}\|_2$, because $\widehat{\rho_j}$ and $\widehat{\widetilde{\rho_j}}$ share the same phases as can be seen from the definition of $\widetilde{\rho_j}$. So $\widehat{\mathrm{e}}_j$ gives the L^2-distance of our guess ρ_j from being a solution.

We will show that $\widehat{\mathrm{e}}_{j+1} \leq (2\pi)^{n/2}\mathrm{e}_j \leq \widehat{\mathrm{e}}_j$. Hence, the errors are non-increasing, justifying the name error-reduction algorithm.

First, we note that for all $\mathbf{x}, \mathbf{k} \in \mathbb{R}^n$

$$|\rho_{j+1}(\mathbf{x}) - \widetilde{\rho_j}(\mathbf{x})| = \min\{|a - \widetilde{\rho_j}(\mathbf{x})|.\ a \geq 0\},$$
$$|\widehat{\rho_{j+1}}(\mathbf{k}) - \widehat{\widetilde{\rho_{j+1}}}(\mathbf{k})| = \min\{|\widehat{\rho_{j+1}}(\mathbf{k}) - b|.\ b \in \mathbb{C},\ |b| = \sqrt{\mathrm{I}(\mathbf{k})}\}.$$

The first equation is true, because the non-negative number that is closest to a negative number is zero and ρ_{j+1} is zero where $\widetilde{\rho_j}$ is negative and equal else. The second equation is true, because the complex number with given absolute value that is closest to another complex number is the one with identical phase and $\widehat{\rho_j}$ and $\widehat{\widetilde{\rho_j}}$ have identical phases. In particular, we have for all $\mathbf{x}, \mathbf{k} \in \mathbb{R}^n$:

$$|\rho_{j+1}(\mathbf{x}) - \widetilde{\rho_j}(\mathbf{x})| \leq |\rho_j(\mathbf{x}) - \widetilde{\rho_j}(\mathbf{x})|,$$
$$|\widehat{\rho_{j+1}}(\mathbf{k}) - \widehat{\widetilde{\rho_{j+1}}}(\mathbf{k})| \leq |\widehat{\rho_{j+1}}(\mathbf{k}) - \widehat{\widetilde{\rho_j}}(\mathbf{k})|.$$

Thus, using the Plancherel formula, we get

$$\widehat{\mathrm{e}_{j+1}}^2 = \|\widehat{\rho_{j+1}} - \widehat{\widetilde{\rho_{j+1}}}\|_2^2 \leq \|\widehat{\rho_{j+1}} - \widehat{\widetilde{\rho_j}}\|_2^2 = (2\pi)^n\|\rho_{j+1} - \widetilde{\rho_j}\|_2^2$$
$$= (2\pi)^n\mathrm{e}_j^2 \leq (2\pi)^n\|\rho_j - \widetilde{\rho_j}\|_2^2 = \|\widehat{\rho_j} - \widehat{\widetilde{\rho_j}}\|_2^2 = \widehat{\mathrm{e}_j}^2.$$

We can use the exact same proof, when instead of our definition of ρ_{j+1}, we set

$$\rho_{j+1} := \widetilde{\rho_j} \cdot \mathbf{1}_{\{\widetilde{\rho_j} \geq 0\} \cap \Omega},$$

meaning that we also include the support constraint (iii).

Although the error-reduction algorithm decreases the error, it has a serious problem. In most cases, the error stagnates and stays at the same level for long periods of time. When getting closer to a solution, the stagnation times increase, making the algorithms very slow. In Figure 2.2, an example for the progress of the error-reduction algorithm is shown.

2.2. Gradient Flow Methods. A different view on the error-reduction algorithm is given in [Fie82]. There it is shown that the error-reduction algorithm can also be seen as a steepest descent algorithm for the functional $\widehat{\mathrm{e}}^2(\rho) := \frac{1}{2}\left\| |\widehat{\rho}| - \sqrt{\mathrm{I}} \right\|_2^2$ with a certain step size and an additional step to satisfy (ii). This is seen as follows. We calculate the L^2-gradient of $\widehat{\mathrm{e}}^2$. Let $\psi \in L^2(\mathbb{R}^n)$, then

$$\begin{aligned}\langle \nabla \widehat{\mathrm{e}}^2(\rho), \psi \rangle &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0} \widehat{\mathrm{e}}^2(\rho + \varepsilon\psi) = \int_{\mathbb{R}^n} (|\widehat{\rho}| - \sqrt{\mathrm{I}}) \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0} |\widehat{\rho + \varepsilon\psi}| \mathrm{d}\mathcal{L}^n \\ &= \int_{\{\widehat{\rho}\neq 0\}} (|\widehat{\rho}| - \sqrt{\mathrm{I}}) \frac{\widehat{\rho}}{|\widehat{\rho}|} \widehat{\psi} \mathrm{d}\mathcal{L}^n = \int_{\{\widehat{\rho}\neq 0\}} \left(\widehat{\rho} - \frac{\widehat{\rho}}{|\widehat{\rho}|}\sqrt{\mathrm{I}} \right) \widehat{\psi} \mathrm{d}\mathcal{L}^n.\end{aligned}$$

Writing $\widehat{\rho} = |\widehat{\rho}| e^{i\zeta(\widehat{\rho})}$, using the Plancherel formula and setting $\widetilde{\rho} := \mathcal{F}^{-1}(\sqrt{\mathrm{I}} e^{i\zeta(\widehat{\rho})})$, we get

$$\langle \nabla \widehat{\mathrm{e}}^2(\rho), \psi \rangle = (2\pi)^n \int_{\{\widehat{\rho}\neq 0\}} (\rho - \mathcal{F}^{-1}(\sqrt{\mathrm{I}} e^{i\zeta(\widehat{\rho})})) \psi \mathrm{d}\mathcal{L}^n = (2\pi)^n \int_{\{\widehat{\rho}\neq 0\}} (\rho - \widetilde{\rho}) \psi \mathrm{d}\mathcal{L}^n.$$

So, $\nabla \widehat{\mathrm{e}}^2(\rho) = (2\pi)^n (\rho - \widetilde{\rho})$, giving the steepest-descent algorithm

$$\rho_{j+1} := \rho_j - h \nabla \widehat{\mathrm{e}}^2(\rho_j) = \rho_j - (2\pi)^n h (\rho_j - \widetilde{\rho_j})$$

with stepsize $h > 0$. The particular choice $h = (2\pi)^{-n}$ results in the first step of the error-reduction algorithm.

In [Fie82], the non-negativity step is added to get the full error-reduction step, showing that this algorithm can be seen as a projected gradient method. We will show that this part of the algorithm can also be viewed as a steepest-descent step for a different functional. Define

$$e_{\geq 0}^2(\rho) := \frac{1}{2} \| \mathbf{1}_{\{\rho<0\}} \rho \|_2^2 = \frac{1}{2} \left\| \frac{1}{2}(|\rho| - \rho) \right\|_2^2.$$

Then for all $\psi \in L^2(\mathbb{R}^n)$

$$\begin{aligned}\langle \nabla e^2_{\geq 0}(\rho), \psi\rangle &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\big|_{\varepsilon=0} e^2_{\geq 0}(\rho+\varepsilon\psi) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\big|_{\varepsilon=0}\frac{1}{2}\int_{\mathbb{R}^n}\frac{1}{4}(|\rho+\varepsilon\psi| - (\rho+\varepsilon\psi))^2 \mathrm{d}\mathcal{L}^n \\ &= \frac{1}{4}\int_{\mathbb{R}^n}(|\rho|-\rho)\left(\frac{\rho}{|\rho|}-1\right)\psi \mathrm{d}\mathcal{L}^n = \frac{1}{4}\int_{\mathbb{R}^n} 2(\rho-|\rho|)\psi \mathrm{d}\mathcal{L}^n = \int_{\{\rho<0\}}\rho\psi \mathrm{d}\mathcal{L}^n.\end{aligned}$$

So, $\nabla e^2_{\geq 0} = \mathbf{1}_{\{\rho<0\}}\rho$. The non-negativity step can thus be written as a steepest descent step with respect to $e^2_{\geq 0}$ with step size $h = 1$:

$$\rho_j := \widetilde{\rho_{j-1}} - \nabla e^2_{\geq 0}(\widetilde{\rho_{j-1}}), \quad j \in \mathbb{N}.$$

Hence, the error-reduction algorithm can be seen as alternating between two different steepest-descent algorithms.

Of course, one could define different functionals that combine different constraints to get new gradient based methods.

Before we introduce further algorithms, we reformulate the phase problem as set intersection problem and the error-reduction algorithms in terms of projections onto sets (see [BCL02]).

2.3. Phase Retrieval as Set Intersection Problem. As we assumed that the electron density ρ_{el} is a Schwartz function, we can identify the different constraints with the corresponding subsets of $\mathcal{S}(\mathbb{R}^n)$. We already did that for the non-negativity constraint and the support constraint by defining the set $\mathcal{S}^{\geq 0}(\mathbb{R}^n)$, $\mathcal{S}_\Omega(\mathbb{R}^n)$ and $\mathcal{S}^{\geq 0}_\Omega(\mathbb{R}^n)$. Analogously, one can define

$$\mathcal{S}_{\mathrm{I}}(\mathbb{R}^n) := \{\varphi \in \mathcal{S}(\mathbb{R}^n).\ |\widehat{\varphi}|^2 = \mathrm{I}\},$$

where I is the square of the Fourier modulus obtained from our intensity measurements. The phase problem associated to I can then be reformulated as the question, if there is an element in the intersection $\mathcal{S}^{\geq}_\Omega(\mathbb{R}^n) \cap \mathcal{S}_{\mathrm{I}}(\mathbb{R}^n)$.

For the moment, we will change the setting a bit by considering $\rho_{\mathrm{el}} \in L^2(\mathbb{R}^n)$ to have Hilbert space methods at hand. We introduce the sets $L^2_{\geq 0}(\mathbb{R}^n)$, $L^2_\Omega(\mathbb{R}^n)$, and $L^2_{\mathrm{I}}(\mathbb{R}^n)$ as the analogs of the respective subsets of Schwartz space, where the properties are defined in the L^2-sense.

The set $L^2_\Omega(\mathbb{R}^n)$ is a closed subspace of $L^2(\mathbb{R}^n)$ and hence a closed convex set. $L^2_{\geq}(\mathbb{R}^n)$ is also a closed convex set, but not a subspace, whereas $L^2_{\mathrm{I}}(\mathbb{R}^n)$ is closed but not convex. The non-convexity of $L^2_{\mathrm{I}}(\mathbb{R}^n)$ makes phase retrieval such a hard problem.

Now, defining the operators

$$\begin{aligned}
\mathrm{p}_{\geq 0} &: L^2(\mathbb{R}^n) \to L^2_{\geq 0}(\mathbb{R}^n),\ f \mapsto \mathbf{1}_{f\geq 0} f,\\
\mathrm{p}_{\Omega} &: L^2(\mathbb{R}^n) \to L^2_{\Omega}(\mathbb{R}^n),\ f \mapsto \mathbf{1}_{\Omega} f,\\
\mathrm{p}_{\mathrm{I}} &: L^2(\mathbb{R}^n) \to L^2_{\mathrm{I}}(\mathbb{R}^n),\ f \mapsto \mathcal{F}^{-1}\left(\sqrt{\mathrm{I}}\left(\mathbf{1}_{\{|\widehat{f}|>0\}}\frac{\widehat{f}}{|\widehat{f}|} + \mathbf{1}_{\{|\widehat{f}|=0\}}\right)\right),
\end{aligned}$$

we find that $\mathrm{p}_{\geq 0}$ and p_{Ω} are the projections on the respective closed convex sets. For p_{I}, there is no unique projection (as we already noted earlier), so we made a choice by setting the phase to zero at the points where $\widehat{f}$ vanishes.

Now, we can reformulate the error-reduction algorithm in its original form as

$$\rho_{j+1} := \mathrm{p}_{\geq 0} \circ \mathrm{p}_{\mathrm{I}}(\rho_j), \quad j \in \mathbb{N}. \tag{ER}$$

In convex optimization, an algorithm of this form is called alternating projection method or projection onto convex sets (POCS). Thus, it is a non-convex version of POCS.

Some relations between algorithms in convex optimization and phase retrieval algorithms have been studied in [BCL02]. Here, we use the language of convex optimization for a clear formulation of some of the known phase retrival algorithms.

Some important algorithms – called input-output algorithms were introduced by Fienup in [Fie82]. We only introduce the most important of these algortihms, since the others are not a great improvement of the ER algorithm. We also only formulate it for the combined projection $\mathrm{p}_{\Omega} \circ \mathrm{p}_{\geq 0}$, but could also use only the non-negativity constraint instead.

Fienup's hybrid input-output alogirthm (HIO, [Fie82]) does not stagnate as much as the previous algorithms and converges quite quickly to regions of reasonable approximations of the solution. Even though it sometimes does not minimize the error as effectively as the ER algorithms, a visual inspection often shows qualitatively good results. It is for that reason that in praxis, after using the HIO algorithm, one usually adds some error-reduction steps. The algorithm has been shown to be related to a Douglas-Rachford algorithm when one of the constraint sets is a subspace (see [BCL02]). For a parameter h, a step of this algortihm works as follows:

$$\rho_{j+1} := ((1+h)\mathrm{p}_{\Omega} \circ \mathrm{p}_{\geq 0} \circ \mathrm{p}_{\mathrm{I}} - \mathrm{p}_{\Omega} \circ \mathrm{p}_{\geq 0} - h\mathrm{p}_{\mathrm{I}} + \mathrm{id})\rho_j, \quad j \in \mathbb{N}. \tag{HIO}$$

We remark that, as noted in [Els03], there are two versions of the HIO algorithm. For our combined constraint, Fienup's original version (see [Fie82]) uses the non-negativity constraint always w.r.t. $\mathrm{p}_{\mathrm{I}}\rho_j$, i.e. $\psi \mapsto \mathbf{1}_{\{\mathrm{p}_{\mathrm{I}}\rho_j \geq 0\}}\psi$. Instead, Elser (see [Els03]) uses the variant that we introduced above.

Finally, we consider a general framework called difference-map that was introduced in [Els03]. This class of algorithms is based on two projections p_1 and p_2 and has the form

$$\rho_{j+1} := \rho_j + h(\mathrm{p}_1 \circ f_1 - \mathrm{p}_2 \circ f_2)\rho_j,$$

where h is a parameter and $f_1, f_2 : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ are two maps that need to be specified. A reasonable choice of the f_i, $i = 1, 2$ is the following

$$f_i(\rho) := (1 - \gamma_i)\mathrm{p}_i\rho - \gamma_i\rho, \quad i = 1, 2,$$

with parameters γ_1 and γ_2.

Choosing the projections $\mathrm{p}_1 := \mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0}$ and $\mathrm{p}_2 := \mathrm{p}_\mathrm{I}$, and the parameters $\gamma_1 := -1$ and $\gamma_2 := h^{-1}$, we get Elser's version of the HIO algorithm as a special case of the difference map.

In [Els03] the local convergence properties of the difference-map with the above f_i is optimized. The result is an algorithm that in our special case reads:

$$\rho_{j+1} := \rho_j - \mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0}\left((h-1)\mathrm{p}_\mathrm{I} + \mathrm{id}\right)\rho_j + \mathrm{p}_\mathrm{I}\left((h+1)\mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0} - \mathrm{id}\right)\rho_j, \quad j \in \mathbb{N}. \tag{DM}$$

Note, that choosing a negative h results in exchanging the two projections.

This algorithm which we will call difference-map algorithm (DM), outperforms the other algorithms most of the time.

2.4. Comparison of Performance. The performance of the following three algorithms is shown in Figures 2.2 and 2.3. They are the error-reduction algorithm (ER) for the combined projection $\mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0}$, Elser's version of the hybrid input-output algorithm (HIO) for $h = 1$, and the difference-map algorithm (DM) for $h = 1$.

$$\rho_{j+1} := \mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0} \circ \mathrm{p}_\mathrm{I}\rho_j, \tag{ER}$$

$$\rho_{j+1} := (2\mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0} \circ \mathrm{p}_\mathrm{I} - \mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0} - \mathrm{p}_\mathrm{I} + \mathrm{id})\rho_j, \tag{HIO}$$

$$\rho_{j+1} := \rho_j - \mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0}\rho_j + \mathrm{p}_\mathrm{I}\left(2\mathrm{p}_\Omega \circ \mathrm{p}_{\geq 0} - \mathrm{id}\right)\rho_j. \tag{DM}$$

We generated a test set of uniformly distributed Gaussian atoms with uniformly distributed standard deviations and amplitudes that are clustered near the origin and simulated 500 steps of the respective algorithms.The results are shown in Figure 2.3.

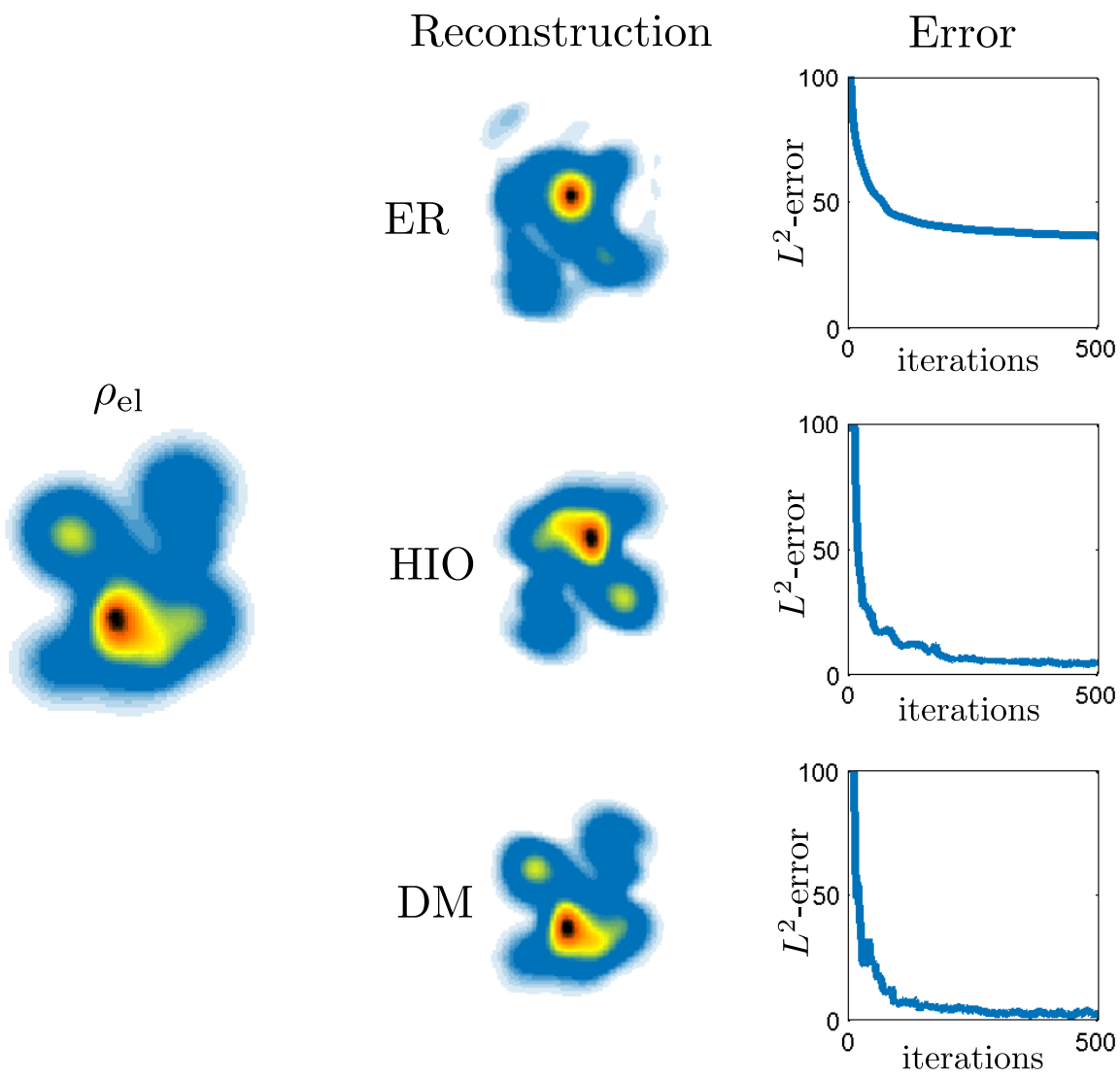


FIGURE 2.2. Typical reconstruction of a two-dimensional function ρ_{el} by the three algorithms (ER), (HIO), and (DM). The reconstructions by (ER) and (HIO) show the inversion ambiguity.

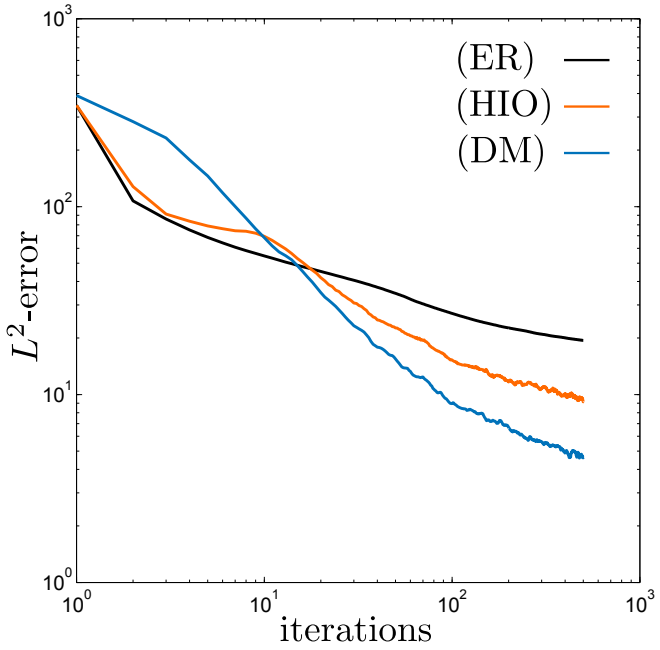


FIGURE 2.3. Loglog-plot of the mean value of the L^2-error of 100 reconstructions by the phase retrieval algorithms (ER), (HIO), and (DM). The test densities were randomly generated sums of scaled Gaussians. A typical density and its reconstructions are shown in Figure 2.2

Motivating Example: A Nanotube

After having studied the scattering of plane waves and the reconstruction of molecular structures from far-field intensity measurements in the first part, we want to develop new kinds of radiation that are specifically designed for the analysis of a more general class of molecular structures than crystals.

Before doing that, an example of a structure that is just as simple as a crystal, but with different symmetries will show that a mismatch in the symmetries of the structure and the radiation causes severe problems for reconstruction.

Given an integer $n \in \mathbb{N}$, a real number $\tau \neq 0$, and an angle $\vartheta \in \mathbb{T}$, we consider the two isometries

$$h := (\mathbf{R}_\vartheta | \tau \mathbf{e}), \quad g := (\mathbf{R}_{2\pi/n} | 0),$$

where $\mathbf{e} \in \mathbb{S}^2$ is a unit vector, $\mathbf{R}_\mu$ is the rotation about the axis $\mathbb{R}\mathbf{e}$ by the angle $\mu \in \mathbb{T}$, and $(\mathbf{Q}|\mathbf{c})$, $\mathbf{Q} \in \mathrm{O}(3)$, $\mathbf{c} \in \mathbb{R}^3$, is the isometry of $\mathbb{R}^3$ defined by

$$(\mathbf{Q}|\mathbf{c})\mathbf{x} := \mathbf{Q}\mathbf{x} + \mathbf{c}, \quad \mathbf{x} \in \mathbb{R}^3. \tag{2.2}$$

The group of all isometries of $\mathbb{R}^3$ is called the Euclidean group $\mathrm{E}(3)$. The natural action of an isometry $(\mathbf{Q}|\mathbf{c}) \in \mathrm{E}(3)$ on the function ρ_{el} is given by

$$((\mathbf{Q}|\mathbf{c})\rho_{\mathrm{el}})(\mathbf{x}) := \rho_{\mathrm{el}}((\mathbf{Q}|\mathbf{c})^{-1}\mathbf{x}) = \rho_{\mathrm{el}}(\mathbf{Q}^{-1}(\mathbf{x} - \mathbf{c})).$$

Now, we define the group $H_\mathcal{N}$ that is generated by these two isometries

$$H_\mathcal{N} := \{h^j g^k.\ j, k \in \mathbb{Z}\}$$

and the structure

$$\mathcal{N} := H_\mathcal{N} \mathbf{M}_\mathcal{N} \subset \mathbb{R}^3,$$

where $\mathbf{M}_\mathcal{N} \subset \mathbb{R}^3$ is a finite set. $\mathcal{N}$ is the orbit of the set $\mathbf{M}_\mathcal{N}$ under the group $H_\mathcal{N}$. Instead of translating the molecule $\mathbf{M}_\mathcal{N}$ to form a crystal, we rotate about and translate along $\mathbb{R}\mathbf{e}$ to form a nanotube (see Figure 2.4).

Again, we put the details of the unit cell into a Schwartz function $\varphi \in \mathcal{S}^{\geq 0}(\mathbb{R}^3)$ and define the model of our non-crystalline electron density by

$$\rho_{\mathrm{el}}(\mathbf{x}) := \sum_{h \in H_\mathcal{N}} \varphi(h^{-1}\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3.$$

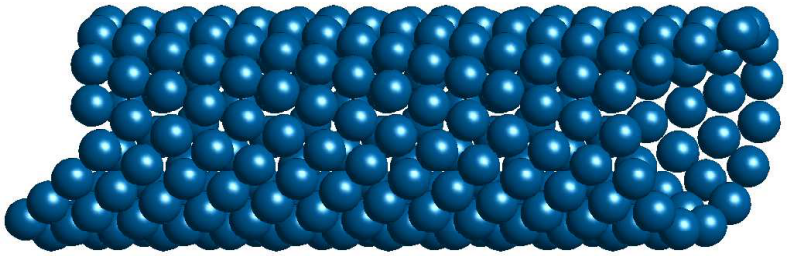


FIGURE 2.4. A nanotube structure like $\mathcal{N}$.

This function is obviously invariant with respect to the action of $H_{\mathcal{N}}$, i.e. $(h\rho_{\mathrm{el}}) = \rho_{\mathrm{el}}$ for all $h \in H_{\mathcal{N}}$.

To understand the Fourier transform of ρ_{el}, we observe the following. Define the rotation $\mathbf{Q} := \mathbf{R}_{(j\vartheta+2\pi k/n)}$, $j, k \in \mathbb{Z}$, and the translation $\mathbf{c} := j\tau\mathbf{e}$. Then we know that $(\mathbf{Q}|\mathbf{c}) \in H_{\mathcal{N}}$. Now, rotating the Fourier transform with $\mathbf{Q}$ yields

$$\begin{aligned}(\mathbf{Q}\widehat{\rho_{\mathrm{el}}})(\mathbf{k}) = \widehat{\rho_{\mathrm{el}}}(\mathbf{Q}^{-1}\mathbf{k}) &= \int_{\mathbb{R}^3} e^{-i\mathbf{Q}^{-1}\mathbf{k}\cdot\mathbf{x}}\rho_{\mathrm{el}}(\mathbf{x})\mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} e^{-i\mathbf{k}\cdot\mathbf{Q}\mathbf{x}}\rho_{\mathrm{el}}(\mathbf{x})\mathrm{d}\mathbf{x} \\ &= \int_{\mathbb{R}^3} e^{-i\mathbf{k}\cdot\mathbf{x}}\rho_{\mathrm{el}}(\mathbf{Q}^{-1}\mathbf{x})\mathrm{d}\mathbf{x} = \widehat{\mathbf{Q}\rho_{\mathrm{el}}}(\mathbf{k}),\end{aligned}$$

where we used that $\mathbf{Q}$ is an orthogonal transformation and the invariance of the Lebesgue measure with respect to isometries.

Since, ρ_{el} is $H_{\mathcal{N}}$ invariant, we find that

$$\begin{aligned}(\mathbf{Q}\rho_{\mathrm{el}})(\mathbf{x}) = \rho_{\mathrm{el}}(\mathbf{Q}^{-1}\mathbf{x}) &= \rho_{\mathrm{el}}(\mathbf{Q}^{-1}((\mathbf{x}+\mathbf{c})-\mathbf{c})) = \rho_{\mathrm{el}}((\mathbf{Q}|\mathbf{c})^{-1}(\mathbf{x}+\mathbf{c})) \\ &= \rho_{\mathrm{el}}(\mathbf{x}+\mathbf{c}).\end{aligned}$$

Finally, the translation-modulation duality yields

$$(\mathbf{Q}\widehat{\rho_{\mathrm{el}}})(\mathbf{k}) = \widehat{\mathbf{Q}\rho_{\mathrm{el}}}(\mathbf{k}) = \widehat{\rho_{\mathrm{el}}(\cdot+\mathbf{c})}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{c}}\widehat{\rho_{\mathrm{el}}}(\mathbf{k}).$$

Thus a rotation of the Fourier transform by $\mathbf{Q}$ is equivalent to a modulation by $e^{-i\mathbf{k}\cdot\mathbf{c}}$. For the Fourier modulus this means that

$$|\mathbf{Q}\widehat{\rho_{\mathrm{el}}}| = |\widehat{\rho_{\mathrm{el}}}|.$$

The Fourier modulus is invariant with respect to every transformation $\mathbf{Q}$ that appears as the orthogonal part of an element of $H_{\mathcal{N}}$. Obviously, these transformations form a subgroup of O(3). This group is called the isogonal point group $\mathrm{Iso}_{H_{\mathcal{N}}}$ of $H_{\mathcal{N}}$:

$$\mathrm{Iso}_{H_{\mathcal{N}}} := \{\mathbf{Q} \in \mathrm{O}(3).\ (\mathbf{Q}|\mathbf{c}) \in H_{\mathcal{N}} \text{ for some } \mathbf{c} \in \mathbb{R}^3\}.$$

As we didn't use the special structure of $H_{\mathcal{N}}$, and every isometry is of the form (2.2) by the Mazur-Ulam theorem (see [Vai03]), we just proved the following proposition.

Proposition 2.5 (Isogonal Invariance of the Fourier Modulus). *Let H be an isometry group and $\rho_{\mathrm{el}} := \sum_{h\in H} h\varphi$ for some $\varphi \in \mathcal{S}(\mathbb{R}^3)$. The Fourier modulus of ρ_{el} is invariant w.r.t. the isogonal point group Iso_H of H:*

$$|\mathbf{Q}\widehat{\rho_{\mathrm{el}}}| = |\widehat{\rho_{\mathrm{el}}}| \quad \textit{for all} \quad \mathbf{Q} \in \mathrm{Iso}_H.$$

When $\vartheta \notin 2\pi\mathbb{Q}$, the situation is especially bad. The set $\vartheta\mathbb{Z} \mod 2\pi$ is then dense in $\mathbb{T}$. Thus, the isogonal point group is a dense subset of all rotations about the axis $\mathbb{R}\mathbf{e}$. Because $|\widehat{\rho_{\mathrm{el}}}|$ is continuous, Proposition 2.5 shows that $|\widehat{\rho_{\mathrm{el}}}|$ has full rotational symmetry. In addition, the group $H_{\mathcal{N}}$ does not contain any translations in this case, because

$$h^j g^k = (\mathbf{I}|\mathbf{c}) \quad \Leftrightarrow \quad j\vartheta 2\pi k/n \mod 2\pi = 0.$$

This only happens, when $j = 0$ and $k \in n\mathbb{Z}$, i.e. when $h^j g^k = \mathrm{id}_{\mathbb{R}^3}$. Consequently, the structure has no translational invariance at all.

In summary, $|\widehat{\rho_{\mathrm{el}}}|$ does not reveal any symmetry of the structure, except its axis.

So, it turns out that the phase problem extends to symmetry information when the symmetries of radiation and structure are not related in a suitable way. For our crystal model, the Fourier modulus is supported on a lattice, effectively reducing the phase problem to a discrete set while ensuring that for any guess of the phases, the resulting structure has the right translational symmetry. This largely simplifies phase retrieval.

For the model of the tube structure, in turn, the Fourier modulus only tells that the structure is axial in some sense and doesn't have translational symmetry. But instead of a highly symmetric discrete structure, it could also be a fully rotationally invariant structure. In particular, the order n of the rotational symmetry of ρ_{el} doesn't influence the rotational symmetry of $|\widehat{\rho_{\mathrm{el}}}|$ when $\vartheta \notin 2\pi\mathbb{Q}$. The Fourier modulus is not supported on a discrete set, largely increasing the dimension of the phase problem.

The only thing we can do to improve the situation for structures that are not crystalline but still highly structured as the tube considered above is to use different radiation than plane waves. The goal of part two is to design new forms of radiation in a way that reveals structural information directly.

Part 2

Radiation Design for Non-Crystalline Structures

Having understood the methods for the analysis of molecular structures by X-ray diffraction, we can turn our attention to the main topic of this dissertation – the design of new forms of radiation suited for the high-resolution analysis of symmetric molecular structures that are not necessarily crystals.

The need for such new kinds of radiation is motivated in the example following Part 1. Even though, in principle, one could reconstruct any structure from its Fourier modulus up to the phase problem, there are two difficulties when trying to analyze non-crystalline structures with plane wave radiation.

First, modern techniques for the analysis of general structures, like Coherent Diffraction Imaging only achieve a resolution of a few nanometers. This is mainly due to technical reasons: the quality of the X-ray beams and the resolution of the detectors does not yet allow reconstructions at the atomic scale.

X-ray Crystallography on the other hand achieves atomic resolution for a moderate number of atoms in the unit cell with less technical requirements. The reason for this superior resolution lies in the translational invariance of both plane waves and crystals. The central result of this relationship is the von Laue condition (Theorem 1.3) that makes direct reconstruction of symmetry information possible.

As we have seen in the motivating example, an incompatibility of the symmetries of the radiation and the structure leads to an extension of the phase problem to structural information. Thus, the goal must be to find some kind of von Laue condition for non-crystalline structures by designing radiation that reflects the symmetries of the structure in the same way as plane waves do for crystals. This program will be carried out in the following chapters.

First, we need to become clear about the radiation space – the space of solution of Maxwell's equations – in which to formulate a design criterion. A natural choice is the space of time-harmonic solutions of the homogeneous Maxwell equations. These share the property of plane waves to induce harmonic oscillations of a charge density.

We determine the outgoing field that is produced when a charge density is illuminated by time-harmonic radiation by solving Maxwell's equations via the Liénard-Wiechert potentials. In the regime of small oscillations, the formula for the outgoing radiation is closely related to the Fourier transform, motivating the notion Fourier radiation.

Interpreting Fourier radiation as an integral transform of the electron density, we consider the general reconstruction problem – how can the density be reconstructed from intensity measurements? Unlike for plane waves, this in not just a scalar phase problem. In addition to the phase, orientational information is lost in the measurement process.

Guided by the classic case, we formulate the corresponding design problem as follows. Given a class of molecular structures, how to choose the incoming radiation, s.t. the intensity of the outgoing Fourier radiation develops characteristic peaks as either the observation point or the radiation parameters are varied?

We introduce a family of molecular structures that are highly symmetric without necessarily being a crystal. So-called objective structures are the natural generalization of crystal structures: they are the orbits of a finite number of atoms under a discrete closed subgroup of the euclidean group E(3) of isometries of $\mathbb{R}^3$. Prominent examples of objective structures are graphene, carbon nanotubes and the buckball, as well as some secondary and quaternary protein structures or tail and capsids of certain viruses [Jam06].

Just as the plane waves are the eigenfunctions of the translation group, we consider time-harmonic radiation that is an eigenfunction of a general closed isometry group G – these are our design equations. The group G is called the design group, as it defines at the same time the radiation and the class of structures that can be analyzed, namely, the objective structures that are generated by a discrete closed subgroup of G.

As a first and central example, nanotube structures like the one in the motivating example are analyzed. The corresponding design group is the group $C_{\mathbf{e}}$ of all rotations and screw displacements about and all translation along an axis $\mathbb{R}\mathbf{e}$, $\mathbf{e} \in \mathbb{S}^2$. The solutions are explicitly determined and turn out to share many properties of plane waves. We call these solutions twisted waves, as they propagate helically in space. The reconstruction problem is shown to reduce to a scalar phase problem, while the symmetries can be directly reconstructed from intensity measurements in axis direction while varying the radiation parameters. This result generalizes the von Laue condition, showing the potential of twisted waves for the analysis of chiral structures.

Next, we move on to the general case. Introducing two mathematical tools – the Wigner projections and the Zak transform, we find a generalization of plane and twisted waves – so-called symmetry-adapted waves. While for compact abelian design groups, these are defined in a straight-forward manner, we need some structure theory to define the symmetry-adapted waves for general abelian isometry groups in a rather ad hoc manner.

The scattering intensity of symmetry-adapted waves is closely related to the integral transform of the density with the symmetry-adapted waves being the integral kernel. We call this transform the wave transform. It maps a charge density to a function on the radiation parameter space that can be interpreted as a frequency-symmetry decomposition.

Its scalar counterpart – the scalar wave transform – is the generalization of the Fourier transform and the scalar transform appearing in the reconstruction problem for nanotube structures.

The main theorem is the generalized von Laue condition for abelian design groups. If the isogonal point group of the design group is axial, the reconstruction problem reduces to a phase problem for the scalar wave transform. The symmetries of the analyzed structure can directly be reconstructed from the support of the radiation transform in parameter space. The classic phase retrieval algorithms can be adapted to the situation.

Finally, we try to generalize this result to compact (non-abelian) design groups. The theory for the scalar wave transform is analog to the abelian case, while the vector-valued theory does not allow for a generalized von Laue condition.

CHAPTER 3

Radiation Design

The content of this chapter is based on joint work which will appear in [FJJ-1, FJJ-2]. We will formulate the problem of radiation design and provide a design criterion for its solution.

Since the object we want to design is an electromagnetic field, the first thing we need to specify is a space of solutions to Maxwell's equations that suitably generalizes plane wave radiation. As we want to keep the capability to induce oscillations of the charge density, we consider the time-harmonic Maxwell equations. Its solutions are seen to be superpositions of plane waves of a fixed frequency. The space of bounded solutions of the time-harmonic Maxwell equations is our choice for the radiation space to work in.

Since the classical theory of the scattering of radiation by matter is not explained very detailed in textbooks, we give a derivation of the full vector valued scattering formula for time-harmonic radiation. It sheds some light on the simplifications that are usually made. Calculating the outgoing field from the Liénard-Wiechert potentials and considering the regime of small oscillations, we find an expression fot the scattering intensity. As the scattered field has the form of a Fourier integral, we name it Fourier radiation.

Having chosen the radiation space we work in and understood the scattering of its elements, we take a different point of view. We interpret the essential part of the Fourier radiation formula as an integral transform of the charge density. This radiation transform allows to formulate the general reconstruction problem given the intensities of the outgoing field in different directions and for varying radiation parameters. We also loosely formulate the design problem by orienting ourselves at the crystalline case: How do we need to choose the radiation for a given class of molecular structures to achieve characteristic peaks as either the outgoing direction or the radiation parameters are varied?

To answer this question, we analyze the relationship between the invariances of plane waves and the symmetries of crystals. The central observation is the following: the plane waves are exactly the simultaneous eigenfunctions of the action of the translation group on the radiation space.

To follow this idea, we need to find a class of molecular structures that generalize crystal structures in the right way. Crystals are generated by discrete closed subgrouops of the translation group. Similarly, so-called objective structures are generated by discrete

closed isometry groups. We give a short introduction to this class of molecular structures that is in detail discussed in [Jam06]. Realizations of objective structures can be frequently found in nanotechnology and biology. Examples are graphene, carbon nanotubes, fullerenes like the buckyball, capsids and tails of certain viruses and some secondary and quaternary protein structures.

Then we have everything in place to formulate a design criterion. Given a closed abelian subgroup G of E(3) playing the role of the translation group, we define the class of structures we want to anlayze as the objective structures that are generated by a discrete closed subgroup of G. To reflect the symmetries of these structures in the right way, the radiation needs to be an eigenfunction of the action of G on our radiation space. This approach seems promising, as the characters of the group G appear naturally in the design equations, giving hope that one might end up with Fourier transform information.

1. Scattering of Time-Harmonic Radiation

This section is the basis of the theory developed in this dissertation. Its main result is a formula for the electromagnetic field that results from the interaction of time-harmonic radiation with a charge density. The special case for plane wave radiation was already used in Chapter 1 to derive the classical theory.

1.1. Time-Harmonic Radiation. The first question we have to address is how to generalize plane wave radiation. We have to define an appropriate space of solutions to Maxwell's equations to work with.

As we have seen in Chapter 1, plane waves are particular solutions to the homogeneous Maxwell equations. So, a natural space to work in, is the space of all solutions to these equations. However, we want to keep the property of plane wave radiation to induce oscillations of the charge density. We do this by setting the time-dependent part of the radiation to $e^{-i\omega t}$ for some angular frequency $\omega > 0$. The result are the time-harmonic Maxwell equations:

Proposition 3.1 (Time-Harmonic Maxwell Equations). *Let* $\mathbf{E}_0$, $\mathbf{B}_0 \in \mathcal{S}'(\mathbb{R}^3)$, *and* $\omega > 0$. *Then the tempered distributions*

$$\widetilde{\mathbf{E}}(t) := \mathbf{E}_0 e^{-i\omega t} \quad \textit{and} \quad \widetilde{\mathbf{B}}(t) := \mathbf{B}_0 e^{-i\omega t}$$

solve the homogeneous Maxwell equations if and only if $\mathbf{E}_0$ *and* $\mathbf{B}_0$ *satisfy the following equations.*

$$\Delta \mathbf{E}_0 = -\frac{\omega^2}{c^2}\mathbf{E}_0, \tag{T1}$$

$$\operatorname{div} \mathbf{E}_0 = 0, \tag{T2}$$

$$\mathbf{B}_0 = -\frac{i}{\omega}\operatorname{curl} \mathbf{E}_0. \tag{T3}$$

In particular, the Fourier transforms $\widehat{\mathbf{E}_0}$ *and* $\widehat{\mathbf{B}_0}$ *are supported on a subset of the set* $\left\{(\mathbf{k},\omega) \in \mathbb{R}^4.\ |\mathbf{k}|^2 = \frac{\omega^2}{c^2}\right\}$. *The spatial parts* $\mathbf{E}_0$ *and* $\mathbf{B}_0$ *are tempered vector fields.*

Proof. We need to check that the three equations (T1)-(T3) are equivalent to Maxwell's equations (M1)-(M4) for the given fields and $\rho_{\text{el}} = 0$, $\mathbf{J}_{\text{el}} = 0$.

Plugging $\widetilde{\mathbf{E}}$ and $\widetilde{\mathbf{B}}$ into (M1)-(M4) yields

$$\operatorname{div} \mathbf{E}_0 e^{-i\omega t} = 0, \tag{M1}$$

$$\operatorname{div} \mathbf{B}_0 e^{-i\omega t} = 0, \tag{M2}$$

$$\operatorname{curl} \mathbf{E}_0 e^{-i\omega t} = i\omega \mathbf{B}_0 e^{-i\omega t}, \tag{M3}$$

$$\operatorname{curl} \mathbf{B}_0 e^{-i\omega t} = -i\omega\varepsilon_0\mu_0 \mathbf{E}_0 e^{-i\omega t}. \tag{M4}$$

This shows that (M1) and (M3) are equivalent to (T2) and (T3), respectively. Now, note that (T1) is equivalent to the wave equation (1.4) for $\widetilde{\mathbf{E}}$. As (1.4) was inferred from the homogeneous Maxwell equations, we have already shown that (M1)-(M4) imply (T1)-(T3).

We still have to derive (M2) and (M4) from the time-harmonic equations. Calculating the divergence of (T3) yields (M2), using $\operatorname{div}\operatorname{curl} = 0$, while (M4) is obtained as follows.

$$\begin{aligned}\operatorname{curl} \mathbf{B}_0 &\overset{\text{(T3)}}{=} -\frac{i}{\omega}\operatorname{curl}(\operatorname{curl} \mathbf{E}_0) = -\frac{i}{\omega}(\nabla(\operatorname{div} \mathbf{E}_0) - \Delta \mathbf{E}_0) \overset{\text{(T2)}}{=} \frac{i}{\omega}\Delta \mathbf{E}_0 \\ &\overset{\text{(T1)}}{=} \frac{i}{\omega}\left(-\frac{\omega^2}{c^2}\mathbf{E}_0\right) = -i\omega\varepsilon_0\mu_0 \mathbf{E}_0,\end{aligned}$$

where we used that $c^{-2} = \varepsilon_0\mu_0$.

Next, we show that $\operatorname{supp}(\widehat{\mathbf{E}_0}), \operatorname{supp}(\widehat{\mathbf{B}_0}) \subseteq \left\{(\mathbf{k},\omega) \in \mathbb{R}^4.\ |\mathbf{k}|^2 = \frac{\omega^2}{c^2}\right\}$. Applying a Fourier transform to (T1) yields

$$\left(|\mathbf{k}|^2 - \frac{\omega^2}{c^2}\right)\widehat{\mathbf{E}_0} = 0. \tag{$*$}$$

Now, assume that there is a $(\mathbf{k}_0,\omega_0) \in \operatorname{supp}(\widehat{\mathbf{E}_0})$ with $|\mathbf{k}_0|^2 \neq \frac{\omega_0^2}{c^2}$. Let $U \subset \mathbb{R}^4$ be an open neighborhood of $(\mathbf{k}_0,\omega_0)$ with $d(U, \frac{\omega}{c}\mathbb{S}^2) > 0$. By the definition of the support of

a tempered distribution, there is a Schwartz function $\varphi_0 \in \mathcal{S}(U)$ with $\widehat{\mathbf{E}_0}(\varphi_0) \neq 0$. The function $f : (\mathbf{k}, \omega) \mapsto \left(|\mathbf{k}|^2 - \frac{\omega^2}{c^2}\right)^{-1}$ is bounded and C^∞ on $\overline{U}$. Thus $f\varphi_0 \in \mathcal{S}(U)$ and consequently

$$0 \overset{(*)}{=} (f^{-1}\widehat{\mathbf{E}_0})(f\varphi_0) = \widehat{\mathbf{E}_0}(\varphi_0),$$

in contradiction to the assumption that $(\mathbf{k}_0, \omega_0) \in \operatorname{supp}(\widehat{\mathbf{E}_0})$. This argument shows that $\operatorname{supp}(\widehat{\mathbf{E}_0}) \subseteq \left\{(\mathbf{k}, \omega) \in \mathbb{R}^4.\ |\mathbf{k}|^2 = \frac{\omega^2}{c^2}\right\}$. Applying the Fourier transform to (T3) yields $\widehat{\mathbf{B}_0} = -\frac{i}{\omega}(-i\mathbf{k} \times \widehat{\mathbf{E}_0})$, implying that $\operatorname{supp}(\widehat{\mathbf{B}_0}) = \operatorname{supp}(\widehat{\mathbf{E}_0}) \subseteq \left\{(\mathbf{k}, \omega) \in \mathbb{R}^4.\ |\mathbf{k}|^2 = \frac{\omega^2}{c^2}\right\}$.

Finally, since we have in particular shown that $\widehat{\mathbf{E}_0}$ and $\widehat{\mathbf{B}_0}$ are compactly supported distributions, the inverse Fourier transform of $\mathbf{E}_0$ is given by the tempered function

$$\mathcal{F}^{-1}\widehat{\mathbf{E}_0}(\mathbf{x}) := (2\pi)^{-4}\widehat{\mathbf{E}_0}(e_{\mathbf{x}}) = \mathbf{E}_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3.$$

That $\mathbf{B}_0$ is a tempered function follows analogously. □

In other words, a time-harmonic electric field is a divergence-free eigenfunction of the vector Laplacian, while the magnetic field is given as a constant multiple of its curl via the third equation of the above proposition.

Based on this proposition, we define the radiation space we will work with in the following chapters. Besides time-harmonicity, we ask for boundedness of the fields.

Definition 3.2 (Time-harmonic radiation). *The space* R_b^ω *of time-harmonic radiations is defined as*

$$\mathrm{R}_b^\omega := \left\{\mathbf{E}_0 : \mathbb{R}^3 \to \mathbb{C}^3,\ \textit{bounded measurable.}\ \Delta\mathbf{E}_0 = -\frac{\omega^2}{c^2}\mathbf{E}_0,\ \operatorname{div}\mathbf{E}_0 = 0\right\}.$$

The elements of R_b^ω *are called time-harmonic radiations.*

Note that we reduced the radiation to the spatial part of the electric field. We will at times also call the full electric field $\mathbf{E}_0 e^{-i\omega t}$ (or the full electromagnetic field) time-harmonic radiation, but this shouldn't lead to confusion.

In Proposition 3.1 we already saw that the elements of R_b^ω are not only measurable, but even tempered functions.

We introduce the natural generalization of the complex amplitude of a plane wave. Assuming that a time-harmonic radiation $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ has a Fourier transform $\widehat{\mathbf{E}_0}$ that is a finite complex measure on the set $\left\{(\mathbf{k}, \omega) \in \mathbb{R}^4.\ |\mathbf{k}|^2 = \frac{\omega^2}{c^2}\right\}$, we can write $\mathbf{E}_0$ as an integral. Note that

$$\left\{(\mathbf{k}, \omega) \in \mathbb{R}^4.\ |\mathbf{k}|^2 = \frac{\omega^2}{c^2}\right\} = \left\{(\mathbf{k}, c|\mathbf{k}|) \in \mathbb{R}^4.\ \mathbf{k} \in \frac{\omega}{c}\mathbb{S}^2\right\}.$$

So, for $\mathbf{x} \in \mathbb{R}^3$

$$\mathbf{E}_0(\mathbf{x}) = (2\pi)^{-4}\widehat{\mathbf{E}_0}(e_{\mathbf{x}}) = (2\pi)^{-4}\int_{\frac{\omega}{c}\mathbb{S}^2} e^{i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\widehat{\mathbf{E}_0}(\mathbf{k}, c|\mathbf{k}|). \tag{3.1}$$

Defining the complex vector measure $\mathbf{n}$ on $\frac{\omega}{c}\mathbb{S}^2$ by $A \mapsto (2\pi)^4\widehat{\mathbf{E}_0}(A, \{c|a|.\ a \in A\})$, we get

$$\mathbf{E}_0(\mathbf{x}) = \int_{\frac{\omega}{c}\mathbb{S}^2} e^{i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\mathbf{n}(\mathbf{k}) = \mathbf{n}(e^{i\mathbf{k}\cdot\mathbf{n}}).$$

So, the electric field is a superposition of plane waves with wave vectors $\mathbf{k} \in \frac{\omega}{c}\mathbb{S}^2$ and complex amplitudes $\mathbf{n}(\mathbf{k})$. Thus the natural generalization of the complex amplitude of a plane wave is the distribution $\mathbf{n} := (2\pi)^4\widehat{\mathbf{E}_0}$ interpreted as distribution on $\frac{\omega}{c}\mathbb{S}^2$.

1.2. Modelling X-ray Diffraction Patterns. X-ray diffraction patterns arise from four basic physical processes, all of which need to be considered to obtain a predictive mathematical model: a suitable electromagnetic wave is turned on and sent towards a stationary electronic charge distribution; the incoming field induces an oscillatory motion of the charges; this motion produces electromagnetic radiation; the intensity of the outgoing radiation is measured by a detector. In the following subsections, we deal in turn with each process. Depending on the approximations made, one arrives in a natural way at three models of increasing simplicity but decreasing accuracy which we term *Maxwell radiation*, *dipole radiation* and *Fourier radiation*.

Mathematically, each model may be viewed as an input-output map

$$\begin{array}{c}\text{incoming electromagnetic field}\\ \text{stationary electronic charge distribution}\end{array} \longrightarrow \text{(intensity of) outgoing radiation.}$$

It solves the 'direct' problem of predicting the diffraction pattern of a known structure for given incoming field. Once such a map is available, one can address 'inverse' problems where the diffraction pattern is known but the structure unknown, or begin to tackle our ultimate goal – to contemplate novel forms of incoming fields adapted to the structures one seeks to analyze.

We note that our most accurate model already involves substantial approximations, including treating the electron motion induced by the incoming field classically instead of quantum mechanically. A detailed account of the difficulties that arise when modelling charged particles is given in [Spo04]. Nevertheless, even our least accurate model predicts experimentally observed X-ray patterns with remarkable precision; see Figure 1.5.

We begin by assuming that the incoming radiation is *time-harmonic*, i.e. a solution to Maxwell's equations of form

$$\mathbf{E}(\mathbf{x},t) = \mathbf{E}_0(\mathbf{x})e^{-i\omega t}. \tag{3.2}$$

The associated magnetic field is given by $\mathbf{B}_0(\mathbf{x})e^{-i\omega t}$, $\mathbf{B}_0 = -(i/\omega)\mathrm{curl}\mathbf{E}_0$. Prototypical are plane waves,

$$\mathbf{E}(\mathbf{x},t) = \alpha\mathbf{n}e^{i(\mathbf{k}_0\cdot\mathbf{x}-\omega t)} \tag{3.3}$$

where $\alpha \geq 0$ is the amplitude and $|\mathbf{n}| = 1$. Mathematically, $\mathbf{n}$ is allowed to be complex. This solves Maxwell's equations with no charge or current sources ($\mathbf{J} = \rho = 0$) provided $\mathbf{k}_0 \cdot \mathbf{n} = 0$ and $\omega^2 = c^2|\mathbf{k}_0|^2$ and the corresponding magnetic field is

$$\mathbf{B}(\mathbf{x},t) = \frac{\alpha}{c}\frac{\mathbf{k}_0}{|\mathbf{k}_0|} \times \mathbf{n}e^{i(\mathbf{k}_0\cdot\mathbf{x}-\omega t)}. \tag{3.4}$$

The more general form (3.2) is important when scattering from non-crystalline structures is under consideration.

1.3. Oscillation of a single electron. Now assume that there is a single electron present of mass m and charge e. It feels a force $e(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ (electric force plus Lorentz force), where $\mathbf{v}$ is the electron velocity. We treat the electron classically, so its motion satisfies

$$m\ddot{\mathbf{q}}(t) = e\Big(\mathbf{E}_0(\mathbf{q}(t)) + \dot{\mathbf{q}}(t) \times \mathbf{B}_0(\mathbf{q}(t))\Big)e^{-i\omega t}, \tag{3.5}$$

where we used the notation $\dot{f} := \partial_t f$ for more transparency.

A simplified model which still captures the essential physics is obtained by three assumptions: (i) transient solutions to (3.5) can be ignored; (ii) the magnetic contribution to the force can be dropped; (iii) the position dependence of the field term $\mathbf{E}_0(\mathbf{q}(t))$ can be neglected. This leads to the equation

$$m\ddot{\mathbf{q}}(t) = e\mathbf{E}_0(\mathbf{q}_0)e^{-i\omega t}, \tag{3.6}$$

where $\mathbf{q}_0$ is the expected electron position in the absence of incoming radiation. Assumption (i) is empirical, and we are not aware of attempts to justify it theoretically. A theoretical analysis would be highly desirable but lies beyond our scope. Assumption (ii) relies on the fact that in X-ray structure determination, the induced electron motion is much slower than the speed of light,

$$\frac{|\mathbf{v}|}{c} = \frac{|\dot{\mathbf{q}}|}{c} \ll 1 \tag{3.7}$$

(note the extra factor $1/c$ in front of the magnetic field (3.4)). Finally, assumption (iii) (neglecting the position dependence of the field term) is justified provided the maximum

electron displacement is much smaller than the spatial wavelength λ_0 of the incoming radiation,

$$(\Delta q)_{max} \ll \lambda_0 = \frac{2\pi}{|\mathbf{k}_0|} = 2\pi\,\frac{c}{\omega}. \tag{3.8}$$

Both (3.7) and (3.8) place indirect limitations on the field strength. To understand these limitations, we estimate v/c and $(\Delta q)_{max}$ via the unique nontransient solution of (3.6),

$$\mathbf{q}(t) = \mathbf{q}_0 - \frac{e}{m\omega^2}\mathbf{E}_0(\mathbf{q}_0)e^{-i\omega t}.$$

It follows that $v = (e/m\omega)|\mathbf{E}_0|$ and $(\Delta q)_{max} = |\mathbf{q}(t) - \mathbf{q}_0| = (e/m\omega^2)|\mathbf{E}_0|$, whence both (3.7) and (3.8) lead, interestingly, to the *same* restriction

$$|\mathbf{E}_0| \ll \frac{c\,m\,\omega}{e}. \tag{3.9}$$

To summarize: the model (3.6) relies on the semi-empirical assumption of a non-transient electron response and the moderate field strength condition (3.9).

1.4. Field produced by the electron. The moving electron is a source of charge and current and therefore produces a field. This field solves Maxwell's equations with

$$\rho(\mathbf{x},t) = e\delta_{\mathbf{q}(t)}(\mathbf{x}), \quad \mathbf{J}(\mathbf{x},t) = e\delta_{\mathbf{q}(t)}(\mathbf{x})\dot{\mathbf{q}}(t). \tag{3.10}$$

Note that the source terms satisfies charge conservation in the sense of distributions.

This problem can be solved using vector potentials. The solution is well known and goes back to Liénard and Wiechert. Since we are not aware of a mathematially satisfactory derivation in the literature, we give our own derivation here.

Put $\mathbf{B} = \mathrm{curl}\mathbf{A}$ to solve the second of Maxwell's equations; the third then becomes $\mathrm{curl}(\dot{\mathbf{A}}+\mathbf{E}) = 0$, which implies that $\mathbf{E} = -\dot{\mathbf{A}} - \nabla\varphi$. Using the freedom of gauge invariance (e.g., $\mathbf{A} \to \mathbf{A} + \nabla\psi$), we require that

$$c^2\mathrm{div}\mathbf{A} + \dot{\varphi} = 0. \tag{3.11}$$

(This Lorenz gauge condition, named after Ludvik Lorenz not Hendrik Lorentz, has the geometric meaning that the four-potential in SI units, obtained by setting $A_0 = \varphi/c$, is divergence-free in space-time, with respect to the coordinates $x_0 = ct, x_1, x_2, x_3$.) Then, using $\mathrm{curl}\,\mathrm{curl} = \nabla\mathrm{div} - \Delta$, we have that the first and third Maxwell's equations become sourced wave equations:

$$\frac{1}{c^2}\ddot{\mathbf{A}} - \Delta\mathbf{A} = \mu_0\mathbf{J}, \quad \frac{1}{c^2}\ddot{\varphi} - \Delta\varphi = \frac{1}{\varepsilon_0}\rho. \tag{3.12}$$

Note that (3.11) together with the second of (3.12) and $\mathbf{E} = -\dot{\mathbf{A}} - \nabla\varphi$ gives charge conservation. For smooth, as well as distributional, solutions, (3.11) and (3.12) imply Maxwell's equations.

A particular solution of (3.11) and (3.12) is given by the follwing "retarded potentials" which involve the time $\tau_{\mathbf{x},\mathbf{x}'}(t) = t - |\mathbf{x}-\mathbf{x}'|/c$ at which an electromagnetic signal must have emanated from $\mathbf{x}'$ in order to arrive at $\mathbf{x}$ at time t:

$$\begin{aligned}\mathbf{A}(\mathbf{x},t) &= \frac{\mu_0}{4\pi}\int_{\mathbb{R}^3}\frac{\mathbf{J}(\mathbf{x}',\tau_{\mathbf{x},\mathbf{x}'}(t))}{|\mathbf{x}-\mathbf{x}'|}\mathrm{d}\mathbf{x}',\\ \varphi(\mathbf{x},t) &= \frac{1}{4\pi\varepsilon_0}\int_{\mathbb{R}^3}\frac{\rho(\mathbf{x}',\tau_{\mathbf{x},\mathbf{x}'}(t))}{|\mathbf{x}-\mathbf{x}'|}\mathrm{d}\mathbf{x}'.\end{aligned} \tag{3.13}$$

Uniqueness of time-harmonic solutions to Maxwell's equations is, for example, studied in [BCX12].

Substituting (3.10) into (3.13), one gets

$$\begin{aligned}\mathbf{A}(\mathbf{x},t) &= \frac{e\mu_0}{4\pi}\int_{\mathbb{R}^3}\frac{\dot{\mathbf{q}}(\tau_{\mathbf{x},\mathbf{x}'}(t))}{|\mathbf{x}-\mathbf{x}'|}\delta(\mathbf{x}'-\mathbf{q}(\tau_{\mathbf{x},\mathbf{x}'}(t)))\,\mathrm{d}\mathbf{x}',\\ \varphi(\mathbf{x},t) &= \frac{e}{4\pi\varepsilon_0}\int_{\mathbb{R}^3}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\delta(\mathbf{x}'-\mathbf{q}(\tau_{\mathbf{x},\mathbf{x}'}(t)))\,\mathrm{d}\mathbf{x}'.\end{aligned} \tag{3.14}$$

It is not trivial to evaluate the integrals on the right hand side. The first step is to introduce the concept of retarded time.

Definition 3.3 (Retarded Time). *Assume we are given the position of a moving particle as a function of time, denoted* $\mathbf{q}(t)$ *(*$t \in \mathbb{R}$*). The retarded time* $\tau_{\mathbf{x}}(t)$ *is the time at which the particle must have sent out a signal if this signal reaches point* $\mathbf{x}$ *at time* t*. (See Figure 3.1.) That is to say it is the solution to the nonlinear equation*

$$\tau = t - |\mathbf{x}-\mathbf{q}(\tau)|/c. \tag{3.15}$$

The retarded time is well defined because of:

Lemma 3.4. *If* $\mathbf{q}$ *is continuously differentiable and moves slower than the speed of light,* $s := \sup_{t\in\mathbb{R}}|\dot{\mathbf{q}}(t)| < c$*, then for each* $\mathbf{x}\in\mathbb{R}^3$ *and each* $t\in\mathbb{R}$*, eq. (3.15) possesses a unique solution* $\tau = \tau_x(t)$*.*

Proof. One way to see this is to appeal to Banach's fixed point theorem: the iteration

$$\tau_{\mathbf{x}}^{(n+1)}(t) = t - |\mathbf{x}-\tau_{\mathbf{x}}^{(n)}(t)|/c =: F(\tau_{\mathbf{x}}^{(n)}(t))$$

satisfies $|\tau_{\mathbf{x}}^{(n+1)} - \tau_{\mathbf{x}}^{(n)}| \le \frac{1}{c}|\mathbf{q}(\tau_{\mathbf{x}}^{(n)}) - \mathbf{q}(\tau_{\mathbf{x}}^{(n-1)})| \le (s/c)|\tau_{\mathbf{x}}^{(n)} - \tau_{\mathbf{x}}^{(n-1)}|$, so F is a contraction due to the assumption $s/c < 1$, and hence possesses a unique fixed point. □

To carry out the integration in (3.14) over $\mathbf{x}'$ we need a further lemma to deal with the difficulty that the integration variable appears nonlinearly inside the delta function. This difficulty appears to be a source of considerable confusion in the literature.

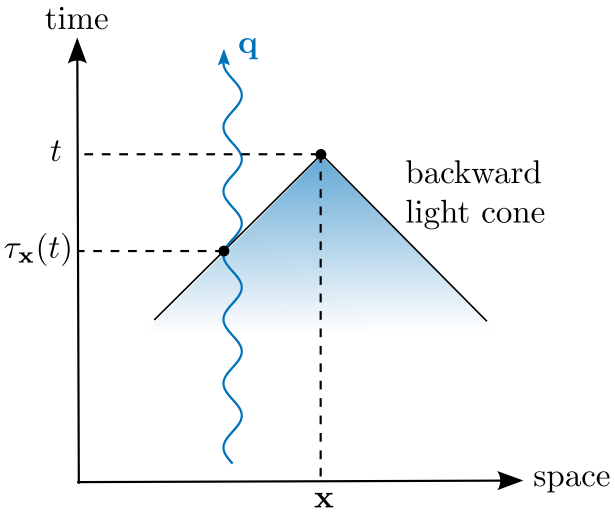


FIGURE 3.1. Geometric meaning of retarded time. The condition that the particle moves slower than the speed of light means geometrically that the slope of the particle trajectory $\mathbf{q}$ is always steeper than that of the backward light cone $\{(\mathbf{x}', t') \ : \ |\mathbf{x}' - \mathbf{x}| = c|t' - t|,\ t' \le t\}$, leading to a unique intersection point.

Lemma 3.5 (Chain rule for the delta function). *If* $\mathbf{f} : \mathbb{R}^d \to \mathbb{R}^d$ *is continuously differentiable and satisfies*
(i) $\mathbf{f}(\mathbf{x}_0) = 0$
(ii) $\mathbf{f}(\mathbf{x}') \neq 0$ *for* $\mathbf{x}' \neq \mathbf{x}_0$
(iii) $\det D\mathbf{f}(\mathbf{x}_0) \neq 0$,
then $\delta(\mathbf{f}(\mathbf{x}')) = \frac{1}{|\det D\mathbf{f}(\mathbf{x}_0)|}\delta(\mathbf{x}' - \mathbf{x}_0)$.

Here the composition $\delta(\mathbf{f}(\mathbf{x}'))$ is rigorously defined as follows: approximate $\delta(\mathbf{x})$ by $g_\varepsilon(\mathbf{x}) = (1/\varepsilon^d)g(\mathbf{x}/\varepsilon)$, where $g : \mathbb{R}^d \to \mathbb{R}$ is nonnegative, smooth, zero outside $|\mathbf{x}| \le 1$, $\int g = 1$. Define $\delta(\mathbf{f}(\mathbf{x}))$ as the limit of $g_\varepsilon(\mathbf{f}(\mathbf{x}))$ in the sense that

$$\int \delta(\mathbf{f}(\mathbf{x}))\,\varphi(\mathbf{x})\,d\mathbf{x} = \lim_{\varepsilon\to 0}\int g_\varepsilon(\mathbf{f}(\mathbf{x}))\,\varphi(\mathbf{x})\,d\mathbf{x} \text{ for all continuous, compactly supported } \varphi$$

(mathematically, $\delta \circ \mathbf{f}$ is the weak* limit in the sense of Radon measures of $g_\varepsilon \circ \mathbf{f}$). The argument below shows that the limit exists and is given by the expression in the lemma, and in particular does not depend on the choice of the approximating functions g_ε.

Proof. By the implicit function theorem, under the assumptions of the lemma $\mathbf{f}$ is a diffeomorphism from a neighbourhood U of $\mathbf{x}_0$ to a neighbourhood V of 0. Moreover $\mathbf{f}(\mathbf{x})$ is bounded away from zero in $(\operatorname{supp}\varphi)\backslash U$ and so for sufficiently small ε, $g_\varepsilon(\mathbf{f}(\mathbf{x}))$ vanishes

in this region. Using the transformation of variables $\mathbf{y} = \mathbf{f}(\mathbf{x})$, $\mathrm{d}\mathbf{y} = |\det D\mathbf{f}(\mathbf{x})|\,\mathrm{d}\mathbf{x}$ gives

$$\begin{aligned}\int_{\mathbb{R}^d} g_\varepsilon(\mathbf{f}(\mathbf{x}))\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x} &= \int_U g_\varepsilon(\mathbf{f}(\mathbf{x}))\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_V g_\varepsilon(\mathbf{y})\varphi(\mathbf{f}^{-1}(\mathbf{y}))\frac{1}{|\det D\mathbf{f}(\mathbf{f}^{-1}(\mathbf{y}))|}\mathrm{d}\mathbf{y} \\ &\longrightarrow \varphi(\mathbf{f}^{-1}(0))\frac{1}{|\det D\mathbf{f}(\mathbf{f}^{-1}(0))|} = \frac{\varphi(\mathbf{x}_0)}{|\det D\mathbf{f}(\mathbf{x}_0)|} \text{ as } \varepsilon \longrightarrow 0,\end{aligned}$$

as was to be shown. □

To apply the lemma to the integrals in (3.14) we fix $\mathbf{x}$ and t and let $\mathbf{f}$ be the map which appears inside the delta function,

$$\mathbf{f}(\mathbf{x}') = \mathbf{x}' - \mathbf{q}(\tau_{\mathbf{x},\mathbf{x}'}(t)) = \mathbf{x}' - \mathbf{q}(t - |\mathbf{x} - \mathbf{x}'|/c). \tag{3.16}$$

This map is zero at the point $\mathbf{x}' = \mathbf{q}(\tau_{\mathbf{x}}(t)) =: \mathbf{x}_0$ (i.e., at the particle position at the retarded time), since at this point the argument of $\mathbf{q}$ in (3.16) is equal to $\tau_{\mathbf{x}}(t)$ so that the right hand side becomes $\mathbf{q}(\tau_{\mathbf{x}}(t)) - \mathbf{q}(\tau_{\mathbf{x}}(t)) = 0$. Next we need to determine the value of the Jacobian determinant of $\mathbf{f}$ at $\mathbf{x}_0$. Differentiating (3.16) with respect to $\mathbf{x}'$ gives

$$D\mathbf{f}(\mathbf{x}') = I - \dot{\mathbf{q}}(t - |\mathbf{x} - \mathbf{x}'|/c) \otimes (-\nabla_{\mathbf{x}'}\frac{|\mathbf{x} - \mathbf{x}'|}{c}) = I - \frac{\dot{\mathbf{q}}(t - |\mathbf{x} - \mathbf{x}'|/c)}{c} \otimes \frac{\mathbf{x} - \mathbf{x}'}{|\mathbf{x} - \mathbf{x}'|},$$

where for any $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$, $\mathbf{a} \otimes \mathbf{b}$ denotes the 3×3 matrix $A = \mathbf{a}\mathbf{b}^T$. To simplify this expression, it is useful to introduce

$$\begin{aligned}\mathbf{v}(\tau) &= \dot{\mathbf{q}}(\tau) \text{ (velocity of particle at time } \tau), \\ \mathbf{n}(\mathbf{x}, \tau) &= \frac{\mathbf{x} - \mathbf{q}(\tau)}{|\mathbf{x} - \mathbf{q}(\tau)|} \text{ (direction from particle at time } \tau).\end{aligned} \tag{3.17}$$

Hence $D\mathbf{f}(\mathbf{x}_0) = I - \frac{\mathbf{v}(\tau)}{c} \otimes \mathbf{n}(\mathbf{x}, \tau)|_{\tau=\tau_{\mathbf{x}}(t)}$. Now $D\mathbf{f}(\mathbf{x}_0)$ has a double eigenvalue 1, corresponding to eigenvectors orthogonal to $\mathbf{n}$, and a single eigenvalue $1 - \frac{\mathbf{v}}{c} \cdot \mathbf{n}$, corresponding to the eigenvector $\mathbf{v}$. It follows that

$$\det D\mathbf{f}(\mathbf{x}_0) = 1 - \frac{\mathbf{v}(\tau)}{c} \cdot \mathbf{n}(\mathbf{x}, \tau)\Big|_{\tau=\tau_{\mathbf{x}}(t)}.$$

Applying Lemma 3.5 to the integrals (3.14) yields

$$\begin{aligned}\mathbf{A}(\mathbf{x}, t) &= \frac{e\mu_0}{4\pi} \frac{1}{1 - \frac{\mathbf{v}(\tau)}{c} \cdot \mathbf{n}(\mathbf{x}, \tau)} \frac{\mathbf{v}(\tau)}{|\mathbf{x} - \mathbf{q}(\tau)|}\Big|_{\tau=\tau_{\mathbf{x}}(t)}, \\ \varphi(\mathbf{x}, t) &= \frac{e}{4\pi\varepsilon_0} \frac{1}{1 - \frac{\mathbf{v}(\tau)}{c} \cdot \mathbf{n}(\mathbf{x}, \tau)} \frac{1}{|\mathbf{x} - \mathbf{q}(\tau)|}\Big|_{\tau=\tau_{\mathbf{x}}(t)}\end{aligned} \tag{3.18}$$

These expressions are called Liénard-Wiechert potentials, and are solutions to equations (3.10), (3.11), (3.12). We remark that the Jacobian factor $1/(1 - \mathbf{v}/c)$ which emerged here from the chain rule for the delta function can be interpreted physically as a relativistic

length change factor of the charge distribution when viewed from a distant point $\mathbf{x}$. To understand the presence of this factor despite the source being a point charge, it is essential that the two operations of integration over $\mathbf{x}'$ and sending the width of the charge distribution to zero are carried out in the correct order, namely integration *before* sending the width to zero. This order arises naturally in the derivation of Lemma 3.5, and is also respected in discussions in the physics literature which obtain (3.18) from the principle of relativistic length contraction, such as [Fey64]).

To obtain the electromagnetic fields $\mathbf{E}$ and $\mathbf{B}$, we need various derivatives associated with the retarded time.

Lemma 3.6. *For a given particle motion* $\mathbf{q}$ *as in Lemma 3.4, let* $\mathbf{v}$, $\mathbf{n}$ *be as defined in* (3.17)*. We have*

(i) (time derivative of retarded time) $\dot{\tau_{\mathbf{x}}}(t) = \frac{1}{1-\frac{\mathbf{v}(\tau)}{c}\cdot\mathbf{n}(\mathbf{x},\tau)}\Big|_{\tau=\tau_{\mathbf{x}}(t)}$

(ii) (space derivative of retarded time) $\nabla_{\mathbf{x}}\tau_{\mathbf{x}}(t) = -\frac{1}{c}\frac{\mathbf{n}}{1-\frac{\mathbf{v}(\tau)}{c}\cdot\mathbf{n}(\mathbf{x},\tau)}\Big|_{\tau=\tau_{\mathbf{x}}(t)}$

(iii) (time derivative of retarded distance) $\frac{\partial}{\partial t}|\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))| = -\frac{\mathbf{v}(\tau)\cdot\mathbf{n}(\mathbf{x},\tau)}{1-\frac{\mathbf{v}(\tau)}{c}}\Big|_{\tau=\tau_{\mathbf{x}}(t)}$

(iv) (space derivative of retarded distance) $\nabla_{\mathbf{x}}|\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))| = \frac{\mathbf{n}}{1-\frac{\mathbf{v}(\tau)}{c}\cdot\mathbf{n}(\mathbf{x},\tau)}\Big|_{\tau=\tau_{\mathbf{x}}(t)}$.

Proof (i): Differentiating (3.15) with respect to t yields

$$\dot{\tau_{\mathbf{x}}}(t) = 1 - \frac{1}{c}\Big\langle \frac{\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))}{|\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))|}, -\dot{\mathbf{q}}(\tau_{\mathbf{x}}(t))\dot{\tau_{\mathbf{x}}}(t)\Big\rangle = 1 + \dot{\tau_{\mathbf{x}}}(t)\Big\langle \mathbf{n}(\mathbf{x},\tau), \frac{\mathbf{v}(\tau))}{c}\Big\rangle\Big|_{\tau=\tau_{\mathbf{x}}(t)}.$$

Solving for $\tau_{\mathbf{x}}(t)$ yields (i).

(ii): Let $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ be some orthonormal basis of $\mathbb{R}^3$, and denote the associated components of any vector $\mathbf{a}$ by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. Differentiating (3.15) with respect to any component $\mathbf{x}_i$ of $\mathbf{x}$ yields

$$\frac{\partial\tau_{\mathbf{x}}}{\partial\mathbf{x}_i}(t) = -\frac{1}{c}\frac{\partial}{\partial\mathbf{x}_i}|\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))|. \tag{3.19}$$

Carrying out the differentiation on the right explicitly gives

$$\begin{aligned}\frac{\partial}{\partial\mathbf{x}_i}|\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))| &= \frac{\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))}{|\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))|}\cdot\Big(\mathbf{e}_i - \dot{\mathbf{q}}(\tau_{\mathbf{x}}(t))\frac{\partial\tau_{\mathbf{x}}}{\partial\mathbf{x}_i}(t)\Big)\\ &= \mathbf{n}_i(\mathbf{x},\tau_{\mathbf{x}}(t)) - \mathbf{n}(\mathbf{x},\tau)\cdot\dot{\mathbf{q}}(\tau)\Big|_{\tau=\tau_{\mathbf{x}}(t)}\cdot\frac{\partial\tau_{\mathbf{x}}}{\partial\mathbf{x}_i}(t).\end{aligned}$$

Substituting into (3.19) and solving for $\frac{\partial\tau_{\mathbf{x}}}{\partial\mathbf{x}_i}(t)$ yields

$$\frac{\partial\tau_{\mathbf{x}}}{\partial\mathbf{x}_i}(t) = -\frac{1}{c}\frac{\mathbf{n}_i(\mathbf{x},\tau)}{1-\mathbf{n}(\mathbf{x},\tau)\cdot\frac{\mathbf{v}(\mathbf{x},\tau)}{c}}\Big|_{\tau=\tau_{\mathbf{x}}(t)}.$$

(iii): This follows from the fact that $\frac{\partial}{\partial t}|\mathbf{x}-\mathbf{q}(\tau_{\mathbf{x}}(t))| = \frac{\partial}{\partial t}c(t-\tau_{\mathbf{x}}(t))$ and (i).

(iv): This is immediate from (ii) and the fact that $\nabla\tau_{\mathbf{x}}(t) = -(1/c)\nabla|\mathbf{x} - \mathbf{q}(\tau_{\mathbf{x}}(t))|$ by (3.19).

We are finally in a position to derive the electric and magnetic fields ensuing from the potentials (3.18), via $\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}$, $\mathbf{B} = \operatorname{curl}\mathbf{A}$. Armed with Lemma 3.6, we can compute the required derivatives explicitly and find after some calculation, abbreviating $\boldsymbol{\beta}(\tau) = \mathbf{v}(\tau)/c$ (relative particle velocity with respect to the speed of light), $\mathbf{n} = \mathbf{n}(\mathbf{x}, \tau)$, and dropping the argument τ from $\mathbf{q}$, $\ddot{\mathbf{q}}$, $\boldsymbol{\beta}$

$$\begin{aligned}\mathbf{E}(\mathbf{x},t) &= \frac{e}{4\pi\varepsilon_0}\,\frac{1}{(1-\boldsymbol{\beta}\cdot\mathbf{n})^3}\left(\frac{\mathbf{n}\times[(\mathbf{n}-\boldsymbol{\beta})\times\frac{\ddot{\mathbf{q}}}{c^2}]}{|\mathbf{x}-\mathbf{q}|} + (1-|\boldsymbol{\beta}|^2)\frac{\mathbf{n}-\boldsymbol{\beta}}{|\mathbf{x}-\mathbf{q}|^2}\right)\Big|_{\tau=\tau_{\mathbf{x}}(t)} \\ \mathbf{B}(\mathbf{x},t) &= \frac{1}{c}\mathbf{n}(\mathbf{x},\tau_{\mathbf{x}}(t))\times\mathbf{E}(\mathbf{x},t). \end{aligned} \tag{3.20}$$

These fields solve Maxwell's equations with charge and current given by (3.10); we therefore call them Maxwell radiation.

A simplified model for the fields (3.20) is obtained via the same simplifying assumptions discussed in the previous section. We assume that the particle motion is much slower than the speed of light, eq. (3.7), and the maximum electron displacement is much smaller than the wavelength of the incoming radiation, (3.8). Hence the $\boldsymbol{\beta}$ terms can be dropped and the vector $\mathbf{n}(\mathbf{x}, \tau_{\mathbf{x}}(t))$ can be replaced by the fixed direction vector

$$\mathbf{n}_0 = \frac{\mathbf{x}-\mathbf{q}_0}{|\mathbf{x}-\mathbf{q}_0|}.$$

Moreover by the identity for iterated vector products that $\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b})$,

$$\mathbf{n}_0\times(\mathbf{n}_0\times\ddot{\mathbf{q}}) = -(I - \mathbf{n}_0\otimes\mathbf{n}_0)\ddot{\mathbf{q}}.$$

Thus expression (3.20) for the electric field reduces to

$$\mathbf{E}(\mathbf{x},t) = \frac{e}{4\pi\varepsilon_0}\left(-(I-\mathbf{n}_0\otimes\mathbf{n}_0)\frac{\ddot{\mathbf{q}}(\tau_{\mathbf{x}}(t))/c^2}{|\mathbf{x}-\mathbf{q}_0|} + \frac{\mathbf{x}-\mathbf{q}_0}{|\mathbf{x}-\mathbf{q}_0|^3}\right).$$

Approximating the retarded time $\tau_{\mathbf{x}}(t)$ which appears inside $\ddot{\mathbf{q}}$ is a little more tricky. Clearly

$$\tau_{\mathbf{x}}(t) = t - \frac{|\mathbf{x}-\mathbf{q}_0|}{c} + O\left(\frac{(\Delta q)_{max}}{c}\right), \tag{3.21}$$

but the admissibility of dropping the error term depends on the timescales on which $\ddot{\mathbf{q}}$ is varying. We therefore confine ourselves to the case when the particle motion is governed by eq. (3.6). In this case the retarded time enters only through the phase factor $e^{-i\omega\tau_{\mathbf{x}}(t)}$. Hence dropping the error term in (3.21) is admissible provided

$$(\Delta q)_{max}\cdot\frac{\omega}{c} \ll 2\pi. \tag{3.22}$$

Remarkably, due to the relation $\omega/c = 2\pi/\lambda_0$ between frequency and spatial wavelength of the incoming time-harmonic radiation, this is precisely equivalent to the assumption we already made in (3.8) that the particle displacement is much smaller than the wavelength of the incoming radiation. Thus expression (3.20) finally simplifies to

$$\mathbf{E}(\mathbf{x},t) = \frac{e}{4\pi\varepsilon_0}\left(-(I-\mathbf{n}_0\otimes\mathbf{n}_0)\frac{\ddot{\mathbf{q}}(t-|\mathbf{x}-\mathbf{q}_0|/c)/c^2}{|\mathbf{x}-\mathbf{q}_0|}+\frac{\mathbf{x}-\mathbf{q}_0}{|\mathbf{x}-\mathbf{q}_0|^3}\right). \tag{3.23}$$

The first term is a kind of dipole radiation, and is absent when the charged particle is not moving. It is similar to the typical starting point in books on X-ray analysis. The second term is the usual static Coulomb field produced by a charged particle at position $\mathbf{q}_0$.

When the particle motion is driven by an incoming field of form (3.2), combining (3.23), (3.6) gives

$$\mathbf{E}(\mathbf{x},t) = \frac{e}{4\pi\varepsilon_0}\left(-(I-\mathbf{n}_0\otimes\mathbf{n}_0)\frac{e\mathbf{E}_0(\mathbf{q}_0)}{mc^2|\mathbf{x}-\mathbf{q}_0|}e^{-i\omega(t-|\mathbf{x}-\mathbf{q}_0|/c)}+\frac{\mathbf{x}-\mathbf{q}_0}{|\mathbf{x}-\mathbf{q}_0|^3}\right). \tag{3.24}$$

Note that after the approximations made, the particle trajectory has been eliminated and the field produced by the electron has been expressed directly in terms of the expected initial electron position $\mathbf{q}_0$ and the incoming field $\mathbf{E}_{in}(\mathbf{q}_0,\tau) = \mathbf{E}_0(\mathbf{q}_0)e^{-i\omega\tau}$ at that position at the approximate retarded time $\tau = t - |\mathbf{x}-\mathbf{q}_0|/c$.

1.5. Field produced by a charge density. Assume now that instead of a single electron, a whole molecule is present. The molecule consists of electrons and atomic nuclei, and can be described by an electron density and a density of nuclei. The field produced by the electron density is a superposition of the field given above for one electron. An analogous field is produced by the atomic nuclei. For each individual atom, the total electronic charge and the total nuclear charge are equal and opposite, whence the second, electrostatic, part in (3.24) almost completely cancels outside the region where electronic and nuclear charge are localized. On the other hand, the first term in (3.24) contains the inverse mass of the particle as a prefactor. Hence the first term does not cancel; instead the term coming from the nuclei can be neglected, due to the much heavier nuclear mass.

These considerations lead to the following expression for the outgoing radiation. Let $\rho_{\mathrm{el}}(\mathbf{y})$ be the number of electrons per unit volume at $\mathbf{y}$. Suppose the illuminated region is Ω. Then the outgoing radiation at a point $\mathbf{x}$ outside Ω is, by simple superposition of the first term of (3.24),

$$\mathbf{E}(\mathbf{x},t) = -\frac{e^2}{4\pi\varepsilon_0 mc^2}\int_\Omega\left(\mathbf{I}-\frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|}\otimes\frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|}\right)\frac{\mathbf{E}_0(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,\rho_{\mathrm{el}}(\mathbf{y})\,e^{-i\omega(t-|\mathbf{x}-\mathbf{y}|/c)}\,\mathrm{d}\mathbf{y}. \tag{3.25}$$

As in Chapter 1, we introduce the scattering constant $c_{\mathrm{el}} := -\frac{e^2}{4\pi\varepsilon_0 mc^2}$ and the projection $\mathrm{P}((\mathbf{x}-\mathbf{y})^\perp) := \mathbf{I} - \frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|} \otimes \frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|}$, and remove the time-dependence from the integral. Then

$$\mathbf{E}(\mathbf{x},t) = c_{\mathrm{el}} e^{-i\omega t} \int_\Omega \frac{\mathrm{P}((\mathbf{x}-\mathbf{y})^\perp)}{|\mathbf{x}-\mathbf{y}|} \mathbf{E}_0(\mathbf{y}) e^{i\frac{\omega}{c}|\mathbf{x}-\mathbf{y}|} \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y}.$$

At this point, we want to exploit the fact that $\mathrm{dia}(\Omega) \ll |\mathbf{x}-\mathbf{y}|$ for $\mathbf{y} \in \Omega$. We directly see that in the term $\frac{\mathrm{P}((\mathbf{x}-\mathbf{y})^\perp)}{|\mathbf{x}-\mathbf{y}|}$, we can replace $\mathbf{y}$ by an arbitrary point $\mathbf{y}_c \in \Omega$ and remove the resulting term from the integral.

We linearize the exponential term. Writing

$$\frac{\omega}{c}|\mathbf{x}-\mathbf{y}| = \frac{\omega}{c}\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\cdot(\mathbf{x}-\mathbf{y}) + \frac{\omega}{c}\left(\frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|} - \frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\right)\cdot(\mathbf{x}-\mathbf{y}),$$

we need the second term to vanish. Taylor expansion in $\mathbf{y}$ at $\mathbf{y}_c$ yields

$$\begin{aligned}
&\frac{\omega}{c}\left(\frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|} - \frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\right)\cdot(\mathbf{x}-\mathbf{y}) \\
&\approx 0 + 0 + \frac{\omega}{2c}(\mathbf{y}-\mathbf{y}_c)^T \left(\frac{1}{|\mathbf{x}-\mathbf{y}_c|}\left(\mathbf{I} - \frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\otimes\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\right)\right)(\mathbf{y}-\mathbf{y}_c) \\
&\approx \frac{\mathrm{dia}(\Omega)^2|\mathbf{k}|}{2|\mathbf{x}-\mathbf{y}_c|} \approx \frac{\mathrm{dia}(\Omega)^2|\mathbf{k}|}{2d(\mathbf{x},\Omega)} = \frac{1}{2}\mathrm{F}(\mathbf{x};\mathbf{k},\Omega),
\end{aligned}$$

where in the last two approximations, we again used that $|\mathbf{x}-\mathbf{y}| \ll 1$ for $\mathbf{y} \in \Omega$. The quantity $\mathrm{F}(\mathbf{x};\mathbf{k},\Omega)$ is called Fresnel number and relates the wavelength, the diameter of the sample and the distance of the obsevation point. The right limit to consider is $\mathrm{F}(\mathbf{x};\mathbf{k},\Omega) \to 0$ which is know as far-field or Fraunhofer approximation. In fact, this approximation should more precisely be called a linear phase approximation.

The final version of the outgoing electromagnetic field which will be subsequently called Fourier radiation, as it actually is a Fourier integral, is

$$\mathbf{E}(\mathbf{x},t) = c_{\mathrm{el}} e^{i\frac{\omega}{c}\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\cdot\mathbf{x} - i\omega t} \frac{\mathrm{P}((\mathbf{x}-\mathbf{y}_c)^\perp)}{|\mathbf{x}-\mathbf{y}_c|} \int_\Omega \mathbf{E}_0(\mathbf{y}) e^{-i\frac{\omega}{c}\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\cdot\mathbf{y}} \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y}, \tag{3.26}$$

$$\mathbf{B}(\mathbf{x},t) = \frac{c_{\mathrm{el}}}{c} e^{i\frac{\omega}{c}\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\cdot\mathbf{x} - i\omega t} \frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|^2} \times \int_\Omega \mathbf{E}_0(\mathbf{y}) e^{-i\frac{\omega}{c}\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\cdot\mathbf{y}} \rho_{\mathrm{el}}(\mathbf{y}) \mathrm{d}\mathbf{y}. \tag{3.27}$$

As we did for plane wave radiation, we calculate the intensity of Fourier radiation. Denote the integral in (3.26) and (3.27) by $\mathbf{F}$. Then a short calculation shows that

$$\mathrm{P}((\mathbf{x}-\mathbf{y}_c)^\perp)\mathbf{F} \times \left(\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|} \times \mathbf{F}\right) = \sin^2(\sphericalangle(\mathbf{x}-\mathbf{y}_c,\mathbf{F}))\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}|\mathbf{F}|^2,$$

where $\sphericalangle(\mathbf{x}-\mathbf{y}_c,\mathbf{F})$ is the angle between the outgoing direction and $\mathbf{F}$. Again, we write $\sin^2(\sphericalangle(\mathbf{x}-\mathbf{y}_c,\mathbf{F})|\mathbf{F}|^2 = |\mathrm{P}((\mathbf{x}-\mathbf{y}_c)^\perp)\mathbf{F}|^2$.

By equation (1.9), the Poynting vector $\mathbf{S}$ of the field $(\mathbf{E}, \mathbf{B})$ is thus given by

$$\mathbf{S}(\mathbf{x}, t) = c_{\text{el}}^2 \frac{c\varepsilon_0}{|\mathbf{x} - \mathbf{y}_c|^2} |\mathrm{P}((\mathbf{x} - \mathbf{y}_c)^\perp)\mathbf{F}|^2 \frac{\mathbf{x} - \mathbf{y}_c}{|\mathbf{x} - \mathbf{y}_c|}$$

To determine the intensity I via equation (1.10), we use Lemma 1.1 to find

$$\mathrm{I}(\mathbf{x}) = c_{\text{el}}^2 \frac{c\varepsilon_0}{2|\mathbf{x} - \mathbf{y}_c|^2} \left| \mathrm{P}((\mathbf{x} - \mathbf{y}_c)^\perp) \int_\Omega \mathbf{E}_0(\mathbf{y}) e^{-i\frac{\omega}{c}\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\cdot\mathbf{y}} \rho_{\text{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right|^2, \tag{3.28}$$

We summarize our results in the following

Definition 3.7 (Fourier Radiation Data). *For a given time-harmonic radiation* $\mathbf{E}_0 \in \mathrm{R}_b^\omega$*, and a given function* $\rho_{\text{el}} \in C_c(\mathbb{R}^3)$ *(charge density), the integrals* (3.26), (3.27), *and* (3.28) *are called Fourier radiation and Fourier radiation intensity, respectively.*

Again, we introduce the scattering amplitude $\mathrm{A} := \mathrm{I}^{1/2}$. For Fourier radiation, A is given by

$$\mathrm{A}(\mathbf{x}) = c_{\text{el}} \left(\frac{c\varepsilon_0}{2|\mathbf{x} - \mathbf{y}_c|^2} \right)^{1/2} \left| \mathrm{P}((\mathbf{x} - \mathbf{y}_c)^\perp) \int_\Omega \mathbf{E}_0(\mathbf{y}) e^{-i\frac{\omega}{c}\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}\cdot\mathbf{y}} \rho_{\text{el}}(\mathbf{y}) \mathrm{d}\mathbf{y} \right|. \tag{3.29}$$

2. Reconstruction and Design

In the previous section we modeled the radiation that results from the interaction of time-harmonic radiation with a charge density and introduced an approximate expression – so-called Fourier radiation. Having solved the direct problem, we turn our attention to the inverse problem of determining the charge density from measurements of Fourier radiation intensity.

For this purpose, we look at Fourier radiation in a different light. The essential part of the formula can be seen as an integral transform that depends on the incoming radiation and maps the charge density to a vector-valued function on the 2-sphere. We call this integral the radiation transform of the density with respect to the incoming radiation. The intensity of the outgoing radiation is essentially the absolute value squared of a projection of the radiation transform.

To gain more flexibility for reconstruction, we consider multi-parameter families of radiation. A family of plane waves, for example, can be parametrized by its wave vectors. The reconstruction problem is then formulated as the recovery of the charge density from the intensity of the outgoing radiation with respect to the family of incoming radiation. This problem is in general ill-posed due to the information loss resulting from the reduction of a complex vectorial quantity to a non-negative scalar quantity.

Given a family of structures (e.g. crystals), it is then natural to ask how to choose the radiation family to reconstruct these structures in an optimal manner.

2.1. The Outgoing Radiation as an Integral Transform. The Fourier radiation approximation of the outgoing field resulting from the interaction of a charge density $\rho_{\text{el}} \in L^1(\mathbb{R}^3)$ and an incoming time-harmonic field $\mathbf{E}_0 \in \mathrm{R}_b^\omega$, $\omega > 0$, is given in formula (3.28). The essential part of the expression is the integral term that determines the amount of constructive/destructive interference of the outgoing waves at a point on the screen. We interpret this term as an integral transform that depends on the incoming field $\mathbf{E}_0$ and maps the charge density ρ_{el} to a vector field. This transform will be called the radiation transform of ρ_{el} with respect to $\mathbf{E}_0$ and is defined as follows:

Definition 3.8 (Radiation Transform). *Let $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ be time-harmonic radiation with frequency $\omega > 0$ (see Definition 3.2) and $\rho_{\text{el}} \in L^1(\mathbb{R}^3)$. The radiation transform $\mathcal{R}[\mathbf{E}_0]\rho_{\text{el}}$ of ρ_{el} with respect to $\mathbf{E}_0$ is defined as*

$$\mathcal{R}[\mathbf{E}_0]\rho_{\text{el}}(\mathbf{s}_0) := \int_{\mathbb{R}^3} e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{y}}\mathbf{E}_0(\mathbf{y})\rho_{\text{el}}(\mathbf{y})\mathrm{d}\mathbf{y}, \quad \mathbf{s}_0 \in \mathbb{S}^2. \tag{3.30}$$

As the integral in (3.28) only depends on the outgoing direction $\frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|} \in \mathbb{S}^2$, we define the transform $\mathcal{R}[\mathbf{E}_0]\rho_{\text{el}}$ as a vector-valued function on the unit sphere $\mathbb{S}^2$ as is usually done for outgoing fields or intensities in scattering theory.

The following lemma collects some basic properties of the radiation transform of integrable functions:

Lemma 3.9 (Properties of the Radiation Transform on $L^1(\mathbb{R}^3)$). *Let $\omega > 0$ and $\mathbf{E}_0 \in \mathrm{R}_b^\omega$. The radiation transform associated to $\mathbf{E}_0$ maps integrable functions $\rho_{\text{el}} \in L^1(\mathbb{R}^3)$ ("charge densities") to continuous vector-valued functions on $\mathbb{S}^2$ ("radiation fields"). The operator $\mathcal{R}[\mathbf{E}_0] : L^1(\mathbb{R}^3) \to C(\mathbb{S}^2, \mathbb{C}^3)$ is bounded and linear. It satisfies the following transformation law under $\mathrm{E}(3)$. When $(\mathbf{Q}|\mathbf{c}) \in \mathrm{E}(3)$, then*

$$\mathcal{R}[(\mathbf{Q}|\mathbf{c})\mathbf{E}_0]\rho_{\text{el}}(\mathbf{s}_0) = e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{c}}\mathbf{Q}\mathcal{R}[\mathbf{E}_0]((\mathbf{Q}|\mathbf{c})^{-1}\rho_{\text{el}})(\mathbf{Q}^{-1}\mathbf{s}_0) \tag{3.31}$$

for all $\mathbf{s}_0 \in \mathbb{S}^2$.

Proof. Observing that the radiation transform is a Fourier integral

$$\mathcal{R}[\mathbf{E}_0]\rho_{\text{el}}(\mathbf{s}_0) = \mathcal{F}(\mathbf{E}_0\rho_{\text{el}})\left(\frac{\omega}{c}\mathbf{s}_0\right),$$

we directly see that the operator $\mathcal{R}[\mathbf{E}_0]$ is linear and bounded. Since $\mathbf{E}_0\rho_{\text{el}}$ is an L^1-vector field, we know that its Fourier transform $\mathcal{F}(\mathbf{E}_0\rho_{\text{el}})$ is continuous. Then $\mathcal{R}[\mathbf{E}_0]\rho_{\text{el}}$ is also continuous, as it is the restriction of $\mathcal{F}(\mathbf{E}_0\rho_{\text{el}})$ to the set $\frac{\omega}{c}\mathbb{S}^2$.

For $(\mathbf{Q}|\mathbf{c}) \in \mathrm{E}(3)$ and $\mathbf{s}_0 \in \mathbb{S}^2$, we get

$$\begin{aligned}\mathcal{R}[(\mathbf{Q}|\mathbf{c})\mathbf{E}_0]\rho_{\mathrm{el}}(\mathbf{s}_0) &= \int_{\mathbb{R}^3} e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{y}}\mathbf{Q}\mathbf{E}_0(\mathbf{Q}^{-1}(\mathbf{y}-\mathbf{c}))\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y}\\ &= \mathbf{Q}\int_{\mathbb{R}^3} e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot(\mathbf{Q}|\mathbf{c})\mathbf{y}}\mathbf{E}_0(\mathbf{y})\rho_{\mathrm{el}}((\mathbf{Q}|\mathbf{c})\mathbf{y})\mathrm{d}\mathbf{y}\\ &= e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{c}}\mathbf{Q}\int_{\mathbb{R}^3} e^{-i\frac{\omega}{c}\mathbf{Q}^{-1}\mathbf{s}_0\cdot\mathbf{y}}\mathbf{E}_0(\mathbf{y})\rho_{\mathrm{el}}((\mathbf{Q}|\mathbf{c})\mathbf{y})\mathrm{d}\mathbf{y}\\ &= e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{c}}\mathbf{Q}\mathcal{R}[\mathbf{E}_0]((\mathbf{Q}|\mathbf{c})^{-1}\rho_{\mathrm{el}})(\mathbf{Q}^{-1}\mathbf{s}_0).\end{aligned}$$

□

Remark 3.10. *The restriction of the radiation transform to integrable functions is not necessary. It can be extended to tempered measures via the formulation as a Fourier transform. This extension maps to the space of vector-valued distributions on* $\mathbb{S}^2$.

In the special case that the incoming radiation is a plane wave $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) := \mathbf{n}e^{i\frac{\omega}{c}\mathbf{k}_0\cdot\mathbf{x}}$, $\mathbf{x} \in \mathbb{R}^3$, with frequency $\omega > 0$, $\mathbf{k}_0 \in \mathbb{S}^2$ and $\mathbf{n}\cdot\mathbf{k}_0 = 0$, according to (1.17), the radiation transform is up to a constant vector the Fourier transform of the charge density ρ_{el} evaluated at a certain point:

$$\mathcal{R}[\mathbf{E}_{\omega,\mathbf{k}_0}]\rho_{\mathrm{el}}(\mathbf{s}_0) = \mathbf{n}\widehat{\rho_{\mathrm{el}}}\left(\frac{\omega}{c}(\mathbf{s}_0-\mathbf{k}_0)\right), \quad \mathbf{s}_0 \in \mathbb{S}^2. \tag{3.32}$$

A variation of the incoming direction $\mathbf{k}_0$ can be realized via a rotation of the incoming field. For $\mathbf{Q} \in \mathrm{SO}(3)$ we get:

$$(\mathbf{Q}\mathbf{E}_{\omega,\mathbf{k}_0})(\mathbf{x}) = \mathbf{Q}\mathbf{n}e^{i\mathbf{k}_0\cdot\mathbf{Q}^{-1}\mathbf{x}} = \mathbf{Q}\mathbf{n}e^{i\mathbf{Q}\mathbf{k}_0\cdot\mathbf{x}} = \mathbf{Q}\mathbf{E}_{\omega,\mathbf{Q}\mathbf{k}_0}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3.$$

Using lemma 3.9, we infer

$$\mathcal{R}[\mathbf{Q}\mathbf{E}_{\omega,\mathbf{Q}\mathbf{k}_0}]\rho_{\mathrm{el}}(\mathbf{s}_0) = \mathbf{Q}\mathcal{R}[\mathbf{E}_{\omega,\mathbf{k}_0}](\mathbf{Q}^{-1}\rho_{\mathrm{el}})(\mathbf{Q}^{-1}\mathbf{s}_0), \quad \mathbf{s}_0 \in \mathbb{S}^2. \tag{3.33}$$

Thus, instead of varying the incoming direction, one can rotate the sample and adjust the observation point. This fact is exploited in the rotating crystal method and the powder method of X-ray crystallography.

2.2. Reconstruction Problem and Design Problem. The information contained in the outgoing radiation for one single incoming field is in general not enough to successfully reconstruct a three-dimensional density. To overcome this problem, parameters of the incoming radiation are varied to collect additional information and thereby make reconstruction possible. These radiation parameters could for example be the frequency or incoming angle of a plane wave or the relative orientation and relative phase of multiple incoming plane waves.

We introduce a radiation parameter set $\mathcal{P}$ that parametrizes a family of time-harmonic radiation:

$$\{\mathbf{E}_{\omega,p}\}_{(\omega,p)\in\mathcal{P}}, \quad \text{where } \mathbf{E}_{\omega,p} \in \mathrm{R}_b^\omega \text{ for } \omega \in [0,\infty). \tag{3.34}$$

We can, for example, parametrize a family of plane wave radiations $\{\mathbf{E}_{\omega,\mathbf{k}_0}\}_{(\omega,\mathbf{k}_0)\in\mathcal{P}}$ with the parameter set $\mathcal{P} := [0,\infty)\times\mathbb{S}^2$ by setting $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) := \mathbf{n}(\mathbf{k}_0)e^{i\frac{\omega}{c}\mathbf{k}_0\cdot\mathbf{x}}$ for $\mathbf{x}\in\mathbb{R}^3$, where the vectors $\mathbf{n}(\mathbf{k}_0)$ satisfy $\mathbf{n}(\mathbf{k}_0)\cdot\mathbf{k}_0 = 0$ for $\mathbf{k}_0\in\mathbb{S}^2$. The additional freedom in $\mathbf{n}(\mathbf{k}_0)$, i.e. in amplitude and polarization of the waves, plays a minor role for reconstruction as can be seen from (3.32).

Assume that we have a family of time-harmonic radiation $\{\mathbf{E}_{\omega,p}\}_{(\omega,p)\in\mathcal{P}}$ with radiation parameter set $\mathcal{P}$ and want to reconstruct the charge density ρ_{el} from intensity measurements. Formula (3.28) yields the following relation between the measured intensities and the radiation transform:

$$\mathrm{I}(\mathbf{x}) = c_{\mathrm{el}}^2\frac{c\varepsilon_0}{2|\mathbf{s}_0|^2}\left|\mathrm{P}(\mathbf{s}_0^\perp)\mathcal{R}[\mathbf{E}_{\omega,p}]\rho_{\mathrm{el}}(\mathbf{s}_0)\right|^2, \tag{3.35}$$

where $\mathbf{s}_0 := \frac{\mathbf{x}-\mathbf{y}_c}{|\mathbf{x}-\mathbf{y}_c|}$ is the outgoing direction.

So, we essentially measure the absolute value squared of a projection of the radiation transform. It might not be possible to measure the intensity in every outgoing direction $\mathbf{s}_0$. Reasons for missing data could for example be the experimental setup (e.g. a beam stop) or the resolution of the detector that only allows a certain spatial sampling rate. We model these cases by introducing an observation parameter set $\mathcal{O}\subset\mathbb{S}^2$ that contains the directions in which measurements are available.

The general reconstruction problem can now be formulated as follows:

Reconstruction Problem:

Given a parameter family $\{\mathbf{E}_{\omega,p}\}_{(\omega,p)\in\mathcal{P}}$ of time-harmonic radiation with radiation parameter set $\mathcal{P}$ and an observation parameter set $\mathcal{O}\subset\mathbb{S}^2$, reconstruct the charge density ρ_{el} from the data set

$$\left\{\left|\mathrm{P}(\mathbf{s}_0^\perp)\mathcal{R}[\mathbf{E}_{\omega,p}]\rho_{\mathrm{el}}(\mathbf{s}_0)\right|^2\right\}_{(\omega,p)\in\mathcal{P},\mathbf{s}_0\in\mathcal{O}}. \tag{3.36}$$

Assume that we want to reconstruct a charge density ρ_{el} from measurements with respect to the family $\{\mathbf{E}_{\omega,\mathbf{k}_0}\}_{(\omega,\mathbf{k}_0)\in\mathcal{P}}$ of plane waves $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) = \mathbf{n}(\mathbf{k}_0)e^{i\frac{\omega}{c}\mathbf{k}_0\cdot\mathbf{x}}$, $\mathbf{x}\in\mathbb{R}^3$, with radiation parameter set $\mathcal{P} = [0,\infty)\times\mathbb{S}^2$. With the full observation parameter set $\mathcal{O} = \mathbb{S}^2$, the reconstruction problem is to find ρ_{el}, given the data

$$\left\{|\mathbf{n}(\mathbf{k})|^2\sin^2(\sphericalangle(\mathbf{n}(\mathbf{k}),\mathbf{s}_0))\left|\widehat{\rho_{\mathrm{el}}}\left(\frac{\omega}{c}(\mathbf{s}_0-\mathbf{k}_0)\right)\right|^2\right\}_{(\omega,\mathbf{k}_0)\in\mathcal{P},\mathbf{s}_0\in\mathcal{O}}.$$

Since this data set determines all values of the function $|\widehat{\rho_{\mathrm{el}}}|^2$, the reconstruction problem reduces to a scalar phase retrieval problem. Note that the data is redundant. Choosing one single incoming direction $\mathbf{k}_0$ or one single observation point $\mathbf{s}_0$ and varying the other parameters, the data set still determines $|\widehat{\rho_{\mathrm{el}}}|^2$ at every point in $\mathbb{R}^3$. This redundancy gives some flexibility in the measurement techniques that can be used for structure determination (see the list below).

Remark 3.11. *Since the radiation transform $\mathcal{R}[\mathbf{E}_{\omega,p}]\rho_{\mathrm{el}}$ is a vector field, reconstruction will in general not reduce to a scalar phase problem. Instead, the information that is lost by projecting the radiation transform perpendicular to the outgoing direction and then taking the absolute value of this vectorial quantity needs to be reconstructed as well.*

We enumerate the most common measurement techniques for reconstruction from plane wave diffraction, focusing on the subsets of the parameter sets $\mathcal{P} = [0,\infty) \times \mathbb{S}^2$ and $\mathcal{O} = \mathbb{S}^2$ that are used.

- **Laue method:** Fixing an incoming direction $\mathbf{k}_0 \in S^2$, a polychromatic ("white") X-ray source is used to obtain the highly structured diffraction pattern of a crystal on a screen in propagation direction ("forward scattering") or in the opposite direction ("backscattering") (see Figure 1.5). The parameter sets are

  $$\mathcal{P} = [0,\infty) \times \{\mathbf{k}_0\}, \quad \text{and } \mathcal{O} = \mathbb{S}^2.$$

  By using a polychromatic source, the measurements of all the frequencies are made at the same time. Because of peak overlaps, the density cannot be reconstructed with this method. However, the symmetries can be determined, as we already saw in Chapter 1.
- **Rotating crystal method:** Monochromatic X-rays with frequency $\omega_0 \in [0,\infty)$ illuminate a crystal sample that is rotated while the intensity is measured at the screen. As seen in (3.33), rotating the sample is equivalent to changing the incoming direction, so the parameter sets are

  $$\mathcal{P} = \{\omega_0\} \times \mathbb{S}^2, \quad \text{and } \mathcal{O} = \mathbb{S}^2.$$

  With these sets, it is easily checked, that the argument $\frac{\omega_0}{c}(\mathbf{s}_0 - \mathbf{k}_0)$ of the Fourier transform attains all values in $B_{2\omega_0/c}(0)$. So, the used frequency ω_0 determines the resolution of the reconstruction.
- **Powder method (Debye-Scherrer):** When instead of a single crystal, crystal powder is analyzed with monochromatic X-rays of frequency $\omega_0 \in [0,\infty)$, a ring pattern emerges on the screen. This is due to the different orientations of the crystal grains in the powder. Lemma 3.9 tells us that the diffraction pattern is a

superposition of the diffraction patterns for the different incoming directions that correspond to these orientations. Because of the redundancy of the pattern, it is enough to measure the intensity on a (half) great circle through the incoming direction $\mathbf{k}_0$. The result is a so-called 2θ-plot, where 2θ is the angle between incoming and outgoing direction. The corresponding parameter sets are

$$\mathcal{P} = \{\omega_0\} \times \mathbb{S}^2, \quad \text{and } \mathcal{O} = \mathbb{S}^2 \cap E,$$

where $E \subset \mathbb{R}^3$ is a two-dimensional subspace of $\mathbb{R}^3$ that contains $\mathbf{k}_0$. The 2θ-plot does not contain enough information for reconstruction of ρ_{el}, but is a clever way to determine the Bravais class and the lattice parameters of a crystal.

- **Coherent Diffraction Imaging (CDI):** Highly brilliant X-rays of frequency $\omega_0 \in [0, \infty)$ coming from a fixed direction $\mathbf{k}_0$ illuminate a sample that is not necessarily a crystal. The diffraction pattern is then not concentrated in peaks but continuous. As detectors are restricted to a specific spatial sampling rate, a discrete subset D of the full observation parameter set is selected:

  $$\mathcal{P} = \{\omega_0\} \times \{\mathbf{k}_0\}, \quad \text{and } \mathcal{O} = D \subset \mathbb{S}^2, \quad D \text{ discrete.}$$

  Knowing a compact support constraint, a projection of the structure (see Corollary 1.5) can in principle be reconstructed by invoking the Shannon sampling theorem [Say52-2]. It has been shown in [MSC98, Mil96] that with a certain amount of oversampling, the phase problem can be solved successfully in many cases. When collecting the measurements for all incoming directions (or equivalently, all orientations of the sample), the three-dimensional structure can be tomographically reconstructed.
- **Variation of Radiation Parameters:** In theory, it would also be possible to fix an outgoing direction $\mathbf{s}_0 \in \mathbb{S}^2$ and to only vary the radiation parameters ω and $\mathbf{k}_0$. The corresponding parameter sets are

  $$\mathcal{P} = [0, \infty) \times \mathbb{S}^2, \quad \text{and } \mathcal{O} = \{\mathbf{s}_0\}.$$

  As already mentioned above, these parameter sets are sufficient to reconstruct ρ_{el} up to the phase problem, as the function $|\widehat{\rho_{\text{el}}}|^2$ is known everywhere. We will come across this theoretical way of reconstruction again in Chapters 4 and 6.

The family of plane waves is naturally parametrized by its wave vectors, i.e. by the corresponding radiation parameter set $\mathcal{P} = [0, \infty) \times \mathbb{S}^2$. But how does this family stand out among the many possible families of time-harmonic radiation?

For the class of crystal structures, the usage of plane waves leads to particularly nice diffraction patterns. The highly structured peak patterns have the following favorable features:

- The characteristic locations of the peaks make a direct reconstruction of symmetry information possible without having to solve a phase problem. This is due to the von Laue condition 1.24 that relates the translational symmetries of the crystal to the peak locations.
- The huge amount of destructive interference singles out a discrete set of observation points, thereby reducing the dimension of the reconstruction problem severely.
- The concentration of the intensity to sharp peaks makes the use of highly brilliant sources unnecessary.

Taking these features as a guideline, we formulate the following general radiation design problem for a given class of molecular structures.

The Design Problem

For a given class of molecular structures $\mathcal{S}$, find a family $\{\mathbf{E}_{\omega,p}\}_{(\omega,p)\in\mathcal{P}}$ of time-harmonic radiation with parameter set $\mathcal{P}$ and an observation parameter set $\mathcal{O}\subset\mathbb{S}^2$, s.t. for every structure $\rho_{\mathrm{el}}\in\mathcal{S}$, the data set $\left\{\left|\mathrm{P}(\mathbf{s}_0^\perp)\mathcal{R}[\mathbf{E}_{\omega,p}]\rho_{\mathrm{el}}(\mathbf{s}_0)\right|^2\right\}_{(\omega,p)\in\mathcal{P},\mathbf{s}_0\in\mathcal{O}}$ develops sharp characteristic peaks as either the observation point $\mathbf{s}_0$ or the radiation parameters (ω,p) are varied.

In the following, we formulate a mathematically precise design criterion for certain classes of highly symmetric structures that are not necessarily crystalline. The plane waves turn out to be the solutions of this criterion when choosing the class of crystal structures.

3. The Design Equations for Abelian Design Groups

3.1. Plane Waves as Solutions to a Design Criterion. We have a second look at plane waves. Why exactly are they the right radiation to use for the analysis of crystals?

The answer lies in the derivation of the von Laue condition (1.24), where we used the generalized Poisson summation formula for a Bravais lattice $\mathcal{B}$,

$$\widehat{\delta_{\mathcal{B}}}=\frac{(2\pi)^3}{\mathrm{V}_{\mathcal{B}}}\delta_{\mathcal{B}^\perp},$$

to get the result. The plane waves appear in this formula in their scalar form as the building blocks of the Fourier transform on Schwartz space $\mathcal{S}(\mathbb{R}^3)$. Qualitatively, the above equation can be written as

$$\lim_{R\to\infty} \sum_{\mathbf{b}\in\mathcal{B},|\mathbf{b}|<R} e^{-i\mathbf{k}\cdot\mathbf{b}} = \begin{cases} 0, & \mathbf{k}\notin\mathcal{B}^\perp, \\ +\infty, & \mathbf{k}\in\mathcal{B}^\perp, \end{cases}, \quad \mathbf{k}\in\mathbb{R}^3. \tag{3.37}$$

When $\mathbf{k}\in\mathcal{B}^\perp$, i.e. $\mathbf{k}\cdot\mathbf{b}\in 2\pi\mathbb{Z}$ for all $\mathbf{b}\in\mathcal{B}$, all the terms on the left hand side become 1 and add up constructively to produce a peak. This is due to the translational invariance of the complex exponentials. Defining the translation operators $\mathrm{T}_{\mathbf{y}}f(\mathbf{x}) := f(\mathbf{x}-\mathbf{y})$ for a continuous function f on $\mathbb{R}^3$ and $\mathbf{x},\mathbf{y}\in\mathbb{R}^3$, and and usual writing $e_{\mathbf{k}}(\mathbf{x}) := e^{i\mathbf{k}\cdot\mathbf{x}}$, $\mathbf{x}\in\mathbb{R}^3$, we get

$$\mathrm{T}_{\mathbf{y}}e_{\mathbf{k}}(\mathbf{x}) = e^{-i\mathbf{k}\cdot\mathbf{y}}e_{\mathbf{k}}(\mathbf{x}).$$

In particular,

$$\mathrm{T}_{\mathbf{b}}e_{\mathbf{k}} = e_{\mathbf{k}} \text{ for all } \mathbf{b}\in\mathcal{B}, \ \mathbf{k}\in\mathcal{B}^\perp.$$

This justifies an alternative definition of the reciprocal lattice that puts more emphasis on this fact:

$$\mathcal{B}^\perp = \{\mathbf{k}\in\mathbb{R}^n.\ \mathrm{T}_{\mathbf{b}}e_{\mathbf{k}} = e_{\mathbf{k}} \text{ for all } \mathbf{b}\in\mathcal{B}\}. \tag{3.38}$$

So, the scalar plane waves are simultaneous eigenfunctions of the group of translation operators – called the translation group. The ones with wave vector in the reciprocal lattice $\mathcal{B}^\perp$ are exactly the ones that are invariant w.r.t. to the operators associated to $\mathcal{B}$.

In fact, this property characterizes the plane waves – not only in the scalar case.

Proposition 3.12 (Characterization of Plane Waves). *Let $\omega > 0$. The plane waves*

$$\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) := \mathbf{n}e^{i\frac{\omega}{c}\mathbf{k}_0\cdot\mathbf{x}}, \ \ \mathbf{k}_0\in\mathbb{S}^2, \ \mathbf{n}\in\mathbb{C}^3, \ \mathbf{k}_0\cdot\mathbf{n}=0, \ \mathbf{x}\in\mathbb{R}^3,$$

are exactly the eigenfunctions of the translation group in the space R_b^ω of time-harmonic radiation, i.e. the bounded measurable vector fields satisfying

(i) $\Delta\mathbf{E}_{\omega,\mathbf{k}_0} = -\dfrac{\omega^2}{c^2}\mathbf{E}_{\omega,\mathbf{k}_0}$,

(ii) $\operatorname{div}\mathbf{E}_{\omega,\mathbf{k}_0} = 0$,

(iii) $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}-\mathbf{y}) = \chi(\mathbf{y})\mathbf{E}_{\omega,\mathbf{k}_0}$ *for all* $\mathbf{x},\mathbf{y}\in\mathbb{R}^3$ *and some* $\chi(\mathbf{y})\in\mathbb{C}$.

Proof. Assume that a vector field $\mathbf{E}_0\in C_b(\mathbb{R}^3,\mathbb{C}^3)$ satisfies (i)-(iii).

Since $\mathbf{E}_0$ is bounded and continuous, the left hand side of (iii) is bounded and continuous with respect to $\mathbf{y}$. But then the same must be true for the right hand side, showing

that $\chi \in C_b(\mathbb{R}^3, \mathbb{C})$. For $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^3$ and $\mathbf{x} \in \mathbb{R}^3$, we get

$$\chi(\mathbf{y}_1 + \mathbf{y}_2)\mathbf{E}_0(\mathbf{x}) \overset{\text{(iii)}}{=} \mathbf{E}_0(\mathbf{x} - (\mathbf{y}_1 + \mathbf{y}_2) = \mathbf{E}_0((\mathbf{x} - \mathbf{y}_1) - \mathbf{y}_2) \overset{\text{(iii)}}{=} \chi(\mathbf{y}_1)\chi(\mathbf{y}_2)\mathbf{E}_0(\mathbf{x}).$$

This shows that the function $\chi : \mathbb{R}^3 \to \mathbb{C}$ is a bounded continuous group homomorphism from $(\mathbb{R}^3, +)$ to $(\mathbb{C} \setminus \{0\}, \cdot)$ when $\mathbf{E}_0 \neq 0$ (else there is nothing to show). Such functions are called characters of the group $(\mathbb{R}^3, +)$. The characters of $\mathbb{R}^3$ are well-known to be of the form $\chi(\mathbf{y}) = e^{i\mathbf{k}\cdot\mathbf{y}}$ for some $\mathbf{k} \in \mathbb{R}^3$.

Thus, we get for $\mathbf{x} \in \mathbb{R}^3$

$$\mathbf{E}_0(\mathbf{x}) = \mathbf{E}_0(0 - (-\mathbf{x})) \overset{\text{(iii)}}{=} \chi(-\mathbf{x})\mathbf{E}_0(0) = e^{-i\mathbf{k}\cdot\mathbf{x}}\mathbf{E}_0(0).$$

Setting $\mathbf{n} := \mathbf{E}_0(0)$, the vector field $\mathbf{E}_0$ already is of the right form $\mathbf{E}_0(\mathbf{x}) = \mathbf{n}e^{-i\mathbf{k}\cdot\mathbf{x}}$.

The vector Helmholtz equation (i) yields

$$\Delta\mathbf{E}_0 = -|\mathbf{k}|^2\mathbf{E}_0 \overset{\text{(i)}}{=} -\frac{\omega^2}{c^2}\mathbf{E}_0,$$

showing that $\mathbf{k} \in \frac{\omega}{c}\mathbb{S}^2$, while from (ii)

$$\operatorname{div}\mathbf{E}_0 = -i\mathbf{k} \cdot \mathbf{E}_0(\mathbf{x}) = -i\mathbf{k} \cdot \mathbf{n}e^{-i\mathbf{k}\cdot\mathbf{x}} \overset{\text{(ii)}}{=} 0,$$

we get that $\mathbf{k} \cdot \mathbf{n} = 0$. □

So, being an eigenfunction of a group of symmetries turns out to be the right design criterion in this case. The appearance of the characters when considering the eigenvalues as functions on the group brings the Fourier transform into play. This will be an important feature in the general case as well.

Before we generalize this criterion, we introduce a class of molecular structures that generalizes crystal structures in a natural way.

3.2. Objective Structures. In [Jam06], R. D. James introduced a notion describing a special class of molecular structures – so-called objective structures. In words, every atom of such a structure has the same atomic environment in the following sense. When you locate yourself at one of the atoms, you can not decide at which specific atom of the structure you are, because at every other atom you can orient yourself in a way that you see exactly the same environment. This kind of objectivity gives these structures their name.

Even from this vague description one can already see that Bravais lattices are an example for objective structures. At two different atoms looking in the same direction, you cannot decide where you are. This is just a different way of saying that a crystal is invariant with respect to the respective translation. Objective structures as a generalization

can be invariant with respect to more general transformations. Before we analyze which these are, we give the precise definition from [Jam06].

Definition 3.13 (Objective Structure).
A discrete closed set $\mathcal{S} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \subset \mathbb{R}^3, N \in \mathbb{N} \cup \{\infty\}$, *is called an objective atomic structure, if there is a set of orthogonal transformations* $\{\mathbf{Q}_1, \dots, \mathbf{Q}_N\} \in \mathrm{O}(3)$, *s. t.*

$$\mathcal{S} = \{\mathbf{x}_j + \mathbf{Q}_j(\mathbf{x}_k - \mathbf{x}_1).\ k = 1, \dots, N\}\ \forall j = 1, \dots, N.$$

A discrete closed set $\mathcal{S} = \{\mathbf{x}_{j,k}.\ j = 1, \dots, N, k = 1, \dots, M\} \subset \mathbb{R}^3, N \in \mathbb{N} \cup \{\infty\}, M \in \mathbb{N}$, *is called an objective molecular structure, if there is a set of orthogonal transformations* $\{\mathbf{Q}_{j,k}.\ j = 1, \dots, N, k = 1, \dots, M\} \subset \mathrm{O}(3)$, *s. t. for all* j, k

$$\mathcal{S} = \{\mathbf{x}_{j,k} + \mathbf{Q}_{j,k}(\mathbf{x}_{n,m} - \mathbf{x}_{1,k}).\ n = 1, \dots, N,\ m = 1, \dots, M\}.$$

Since every objective atomic structure is a objective molecular structure with $M = 1$, we will in the following always refer to objective molecular structures just as objective structures.

Consider $\mathcal{S} \subset \mathbb{R}^3$ to be an objective structure. Then the mappings

$$\psi_{j,k} :\ \mathbb{R}^3 \to \mathbb{R}^3,\ \mathbf{x} \mapsto \mathbf{x}_{j,k} + \mathbf{Q}_{j,k}(\mathbf{x} - \mathbf{x}_{1,k}),$$

keep the structure fixed for $j = 1, \dots, N,\ k = 1, \dots, M$. So, defining the group $H_{\mathcal{S}}$ generated by these mappings

$$H_{\mathcal{S}} := \langle \psi_{j,k}.\ j = 1, \dots, N,\ k = 1, \dots, M \rangle,$$

we find that $\mathcal{S}$ is invariant with respect to this group:

$$\mathcal{S} = H_{\mathcal{S}}\mathcal{S}.$$

Moreover, since $\psi_{j,k}(\mathbf{x}_{1,k}) = \mathbf{x}_{j,k}$, defining $\mathbf{M}_{\mathcal{S}} := \{\mathbf{x}_{1,k}.\ k = 1, \dots, M\}$, we get the whole group as the orbit of $\mathbf{M}_{\mathcal{S}}$ under $H_{\mathcal{S}}$:

$$\mathcal{S} = H_{\mathcal{S}}\mathbf{M}_{\mathcal{S}}.$$

The mappings $\psi_{j,k}$ belong to a special class of transformations of $\mathbb{R}^3$: they are isometries, i.e. $\|\mathbf{x} - \mathbf{y}\| = \|\psi_{j,k}(\mathbf{x}) - \psi_{j,k}(\mathbf{y})\|$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, what is obviously true as $\mathbf{Q}_{j,k} \in \mathrm{O}(3)$. The group $\mathrm{E}(3)$ of isometries of $\mathbb{R}^3$ is called Euclidean group. So, what we have seen so far is that every objective structure is the orbit of a finite molecule under an isometry group, i.e. a subgroup of $\mathrm{E}(3)$.

In fact, objective structures can be characterized as orbits of finite sets in the following way

Proposition 3.14 (Objective Structures as Orbits). *A subset of* $\mathbb{R}^3$ *is an objective structures if and only if it is the orbit of a finite set under a discrete closed isometry group.*

Proof. For $\mathbf{x} \in \mathbb{R}^3$ consider the mapping $f_{\mathbf{x}} :\ \mathrm{E}(3) \to \mathbb{R}^3,\ h \mapsto h(\mathbf{x})$. $f_{\mathbf{x}}$ is obviously continuous. Since $f_{\mathbf{x}}(H_{\mathcal{S}}) = H_{\mathcal{S}}\mathbf{x}$ and $H_{\mathcal{S}}\mathbf{x}$ is closed, because it is an atomic objective structure, we see that $H_{\mathcal{S}}$ as the preimage of a closed set under a continuous map is closed. Since $H_{\mathcal{S}}$ is obviously discrete, we already have shown that every objective structure is the orbit of a finite set under a discrete closed isometry group – namely $\mathcal{S} = H_{\mathcal{S}}\mathbf{M}_{\mathcal{S}}$.

So, it remains to show that the orbit of any finite set $\mathbf{M}$ under a discrete closed subgroup H of $\mathrm{E}(3)$ is an objective structure.

Let $\mathcal{S} := H\mathbf{M}$. By the Mazur-Ulam theorem (see [Vai03]), every isometry $h \in H$ has the form

$$h(\mathbf{x}) = \mathbf{Q}\mathbf{x} + \mathbf{c}, \quad \text{for some } \mathbf{Q} \in \mathrm{O}(3),\ \mathbf{c} \in \mathbb{R}^3.$$

Usually the element h is then written in the form $h = (\mathbf{Q}|\mathbf{c})$ as in (2.2).

The set $\mathcal{S}$ can be written as

$$\mathcal{S} = \{h(\mathbf{m}).\ h \in H,\ \mathbf{m} \in \mathbf{M}\} = \{\mathbf{Q}\mathbf{m} + \mathbf{c}.\ (\mathbf{Q}|\mathbf{c}) \in H,\ \mathbf{m} \in \mathbf{M}\}.$$

Now, let $|\mathbf{M}| = M \in \mathbb{N}$ and $|H| = N \in \mathbb{N} \cup \infty$. Then we can enumerate the elements

$$\mathbf{M} = \{\mathbf{x}_{1,k}.\ k = 1, \dots, M\} \ \text{ and } \ H_{\mathcal{S}} = \{h_j.\ j = 1, \dots, N\}.$$

Setting $\mathbf{x}_{j,k} := h_j(\mathbf{x}_{1,k})$, we get

$$\mathcal{S} = \{\mathbf{x}_{j,k}.\ j = 1, \dots, N,\ k = 1, \dots, M\}.$$

Writing $h_j = (\mathbf{Q}_j|\mathbf{c}_j)$ for some $\mathbf{Q}_j \in \mathrm{O}(3)$, $\mathbf{c}_j \in \mathbb{R}^3$, $j = 1, \dots, N$, we find that the translational part is given by $\mathbf{c}_j = \mathbf{x}_{j,k} - \mathbf{Q}_j\mathbf{x}_{1,k}$ from the definition of $\mathbf{x}_{j,k}$. Setting $\mathbf{Q}_{j,k} := \mathbf{Q}_j$ for $j = 1, \dots, N$, $k = 1, \dots, M$, we get

$$h_j(\mathbf{x}) = \mathbf{x}_{j,k} + \mathbf{Q}_{j,k}(\mathbf{x} - \mathbf{x}_{1,k}) = \psi_{j,k}(\mathbf{x}).$$

Consequently, $\psi_{j,k}\mathcal{S} = \mathcal{S}$ for all $j \in \{1, \dots, N\}$ and $k \in \{1, \dots, M\}$, showing that $\mathcal{S}$ is an objective structure. □

The proof shows that in the above definition of an objective structure, indexing the orthogonal transformations only by j would not change the class of structures defined.

As we already mentioned above, crystals are objective structures. When $\mathcal{L} = \mathcal{B}_{\mathcal{L}} + \mathbf{M}_{\mathcal{L}}^{\mathbf{A}}$, $\mathcal{B}_{\mathcal{L}} = \mathbf{A}\mathbb{Z}^3$, $\mathbf{A} \in \mathrm{GL}(3, \mathbb{R})$, $\mathbf{M}_{\mathcal{L}}^{\mathbf{A}} \subset \mathbb{R}^3$ finite, is a crystal lattice, consider the group

$$H_{\mathcal{L}} := \{(\mathbf{I}|\mathbf{b}).\ \mathbf{b} \in \mathcal{B}_{\mathcal{L}}\}$$

of translations associated to $\mathcal{B}_{\mathcal{L}}$. Then, obviously,

$$\mathcal{L} = H_{\mathcal{L}}\mathbf{M}_{\mathcal{L}}^{\mathbf{A}},$$

giving a characterization as in Lemma 3.14.

We give some further examples of objective structures.

Given $\mathbf{A} \in \mathrm{Mat}(3,3;\mathbb{R})$ with $\mathrm{rk}(\mathbf{A}) < 3$, and a finite set $\mathbf{M} \subset \mathbb{R}^3$, we set

$$\mathcal{S} := \mathbf{A}\mathbb{Z}^3 + \mathbf{M}.$$

This structure is a $\mathrm{rk}(\mathbf{A})$-dimensional crystal. Again, setting $H_{\mathcal{S}} := (\mathbf{I}|\mathbf{A}\mathbb{Z}^3)$, we get $\mathcal{S} = H_{\mathcal{S}}\mathbf{M}$.

These translational structures are already quite general, as it can be shown that the groups $(\mathbf{I}|\mathbf{A}\mathbb{Z}^3)$ are exactly the discrete closed subgroups of the full translation group.

Let's reconsider the structure from the motivating example. The group $H_{\mathcal{N}}$ considered there is a discrete closed isometry group. So, the nanotube structure $\mathcal{N}$ is an objective structure.

Given a unit vector $\mathbf{e} \in \mathbb{R}^3$, we define the group

$$C_{\mathbf{e}} := \{(\mathbf{R}_{\vartheta}|\tau\mathbf{e}).\ \vartheta \in \mathbb{T},\ \tau \in \mathbb{R}\} \tag{3.39}$$

of all rotations and screw displacements about and all translations along the axis $\mathbb{R}\mathbf{e}$. Then every closed discrete subgroup of $C_{\mathbf{e}}$ has the form of $H_{\mathcal{N}}$ (see Lemma 5.2), i.e. it is generated by a rotation (which might be the identity) and a screw displacement (which might be the identity or a translation). We call the objective structures that are generated by an infinite closed subgroup of $C_{\mathbf{e}}$ for some unit vector $\mathbf{e}$ nanotube structures. We will analyze these structures in more detail in the next chapter.

Another possible choice for $H_{\mathcal{S}}$ is to take a discrete closed subgroup of $\mathrm{O}(3)$ to generate a finite structure. For example the choice $H_{\mathcal{S}} = \{(\mathbf{R}_{2\pi j/n}|0).\ j = 1,\dots,n\}$ leads to structures that are n-fold rotationally invariant.

Figure 3.2 shows some examples of objective structures.

3.3. The Design Equations. In the last three sections we set the grounds for formulating a design criterion. We have decided which kind of radiation we want to use and which class of structures we want to analyze. Even more, we already found a criterion that identifies the plane waves as the right choice of radiation to analyze crystals.

The plane waves with frequency $\omega > 0$ are the eigenfunctions of the full translation group in the space R_b^{ω} of time-harmonic radiation, while crystal lattices are the orbits of finite sets under a discrete closed subgroup of the translation group. So, the translation

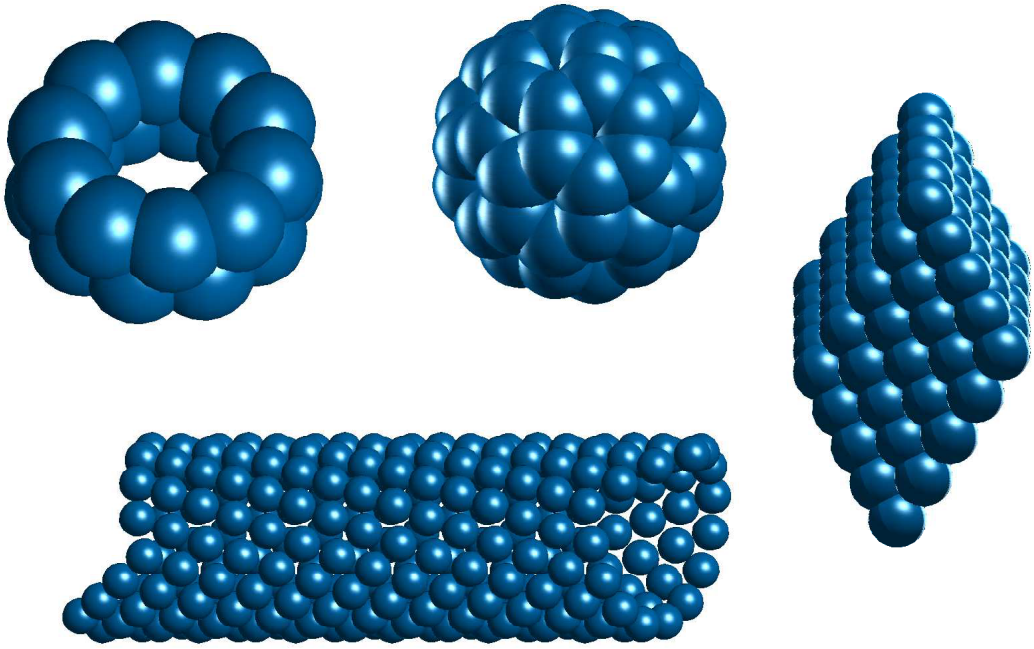


FIGURE 3.2. Examples of objective structures. Shown is a ring structure with an improper rotation symmetry, an icosahedral structure like the buckyball, a finite sample of crystal structure and a nanotube-like structure.

group is the object that defines the radiation to use and the class of structures to analyze with this radiation at the same time.

In the following, we will start from a general closed isometry group $G \leq \mathrm{E}(3)$, that defines the class of structures and the corresponding space of radiations. We call this group the design group.

The natural action of the group $\mathrm{E}(3)$ on the space $L^\infty(\mathbb{R}^3;\mathbb{C}^3)$ of L^∞-vector fields is the following. Let $\mathbf{E}_0 \in L^\infty(\mathbb{R}^3;\mathbb{C}^3)$ and $(\mathbf{Q}|\mathbf{c}) \in \mathrm{E}(3)$. Then for $\mathbf{x} \in \mathbb{R}^3$,

$$(\mathbf{Q}|\mathbf{c})\mathbf{E}_0(\mathbf{x}) := \mathbf{Q}\mathbf{E}_0(\mathbf{Q}^T(\mathbf{x}-\mathbf{c})).$$

Note, that $\mathbf{Q}^T(\cdot - \mathbf{c}) = (\mathbf{Q}|\mathbf{c})^{-1}$.

First, we consider the case that the design group G is a closed abelian subgroup of $\mathrm{E}(3)$. We formulate the design criterion analogous to the case when G is the translation group.

Definition 3.15 (Design Equations – Abelian Design Group). *Let G be a closed abelian subgroup of* $\mathrm{E}(3)$*. A vector field* $\mathbf{E}_0 \in L^\infty(\mathbb{R}^3;\mathbb{C}^3)$ *solves the design equations for G when it satisfies*

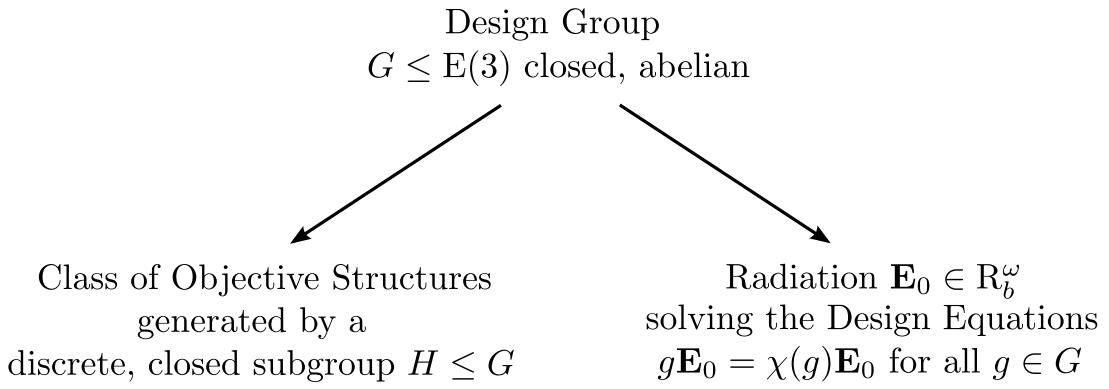
(i) $\Delta \mathbf{E}_0 = -\dfrac{\omega^2}{c^2}\mathbf{E}_0$, *for some* $\omega > 0$,

(ii) $\operatorname{div} \mathbf{E}_0 = 0$,

(iii) $g\mathbf{E}_0 = \chi(g)\mathbf{E}_0$ *for some* $\chi(g) \in \mathbb{C}$ *and all* $g \in G$.

We denote the space of time-harmonic radiation with frequency ω that satisfies the design equations for G with $\mathrm{R}_b^\omega(G)$.

The relation between the design group G, the class of objective structure it defines and the radiation that solves the Design Equations is summarized in the following diagram:



We will solve these equations for a special choice of G in the next chapter. For the moment, we show some similarities to the crystalline case that give hope that the choice of criterion might be the right thing. However, it has to be noted that we are far from done, since, even if we have solved the equations, it is not clear what information is contained in the intensity of the outgoing raditation in the far-field and if we can reconstruct a structure of the corresponding class.

In the proof of Proposition 3.12 we first showed that the eigenvalue χ as a function on the group is actually a character. We can do the same in the general abelian case:

Lemma 3.16 (Character Lemma). *Let* $G \leq \mathrm{E}(3)$ *be a closed abelian isometry group. The function* $\chi : G \to \mathbb{C}$ *from* (iii) *in Definition 3.15 is a character of the group G.*

Proof. Boundedness and continuity of χ are a direct consequence of the same properties for $\mathbf{E}_0$.

χ is a group homomorphism from G to $\mathbb{C}^*$, as for all $g_1, g_2 \in G$:

$$\chi(g_1 g_2)\mathbf{E}_0 \overset{\text{(iii)}}{=} (g_1 g_2)\mathbf{E}_0 = g_1(g_2\mathbf{E}_0) \overset{\text{(iii)}}{=} \chi(g_1)\chi(g_2)\mathbf{E}_0.$$

So, χ is a character of G. □

This Lemma shows that the Fourier transform on the group G will play an important role in the following chapters.

It also gives some additional structure to the space R_b^ω. Every element of this space solves the eigenfunction equation for a specific character χ of G. We define the subspace

$$\mathrm{R}_b^{\omega,\chi}(G) := \{\mathbf{E}_0 \in \mathrm{R}_b^\omega.\ g\mathbf{E}_0 = \chi(g)\mathbf{E}_0\}, \quad \chi \in \widehat{G}.$$

So, we get the identity

$$\mathrm{R}_b^\omega(G) = \bigcup_{\chi \in \widehat{G}} \mathrm{R}_b^{\omega,\chi}(G).$$

The radiation we design, will thus have at least two parameters – the frequency $\omega > 0$ and the character $\chi \in \widehat{G}$ that describes its transformation under G. Considering the crystalline case, i.e. $G = \mathbb{R}^3$ the translation group, we know that the characters are $\chi^{(\mathbf{k})} = e_{\mathbf{k}}$, while ω fixes the absolute value of $\mathbf{k}$ by $|\mathbf{k}| = \frac{\omega}{c}$. We write $\mathrm{R}_b^{\omega,\mathbf{k}}$ for the corresponding radiation space, and can restate our findings of Proposition 3.12 as

$$\mathrm{R}_b^{\omega,\mathbf{k}}(\mathbb{R}^3) = \{\mathbf{n}e_{\mathbf{k}}.\ \mathbf{n} \in \mathbb{C}^3,\ \mathbf{k}\cdot\mathbf{n} = 0\}.$$

This space is consequently isomorphic to the space of three-dimensional complex vectors that are perpendicular to $\mathbf{k}$, which is a 5-dimensional linear space.

In this case, we also found that given a Bravais lattice $\mathcal{B}$, the reciprocal lattice $\mathcal{B}^\perp$ consisted of the wave vectors, s.t. the corresponding character is invariant w.r.t. $\mathcal{B}$. In particular, identifying the wave vectors with the corresponding character, the reciprocal lattice can be identified with a subgroup of the dual group. Being invariant with respect to $\mathcal{B}$ can also be expressed as being equal to one on $\mathcal{B}$. In the theory of locally compact abelian groups, this construction is known as the orthogonal group (see [Rei68] or [Fol95]). It is defined as follows.

Definition 3.17 (Orthogonal group). *Let G be a locally compact abelian group with dual group $\widehat{G}$ and H a closed subgroup of G. Then the orthogonal group $H_G^\perp$ of H with respect to G is defined as*

$$H_G^\perp := \{\chi \in \widehat{G}.\ \chi \downarrow_H^G \equiv 1\}.$$

When G is the translation group and $H_{\mathcal{L}}$ is the group of translations associated to a crystal lattice $\mathcal{L}$, we find that the mapping

$$\mathcal{B}_{\mathcal{L}}^{\perp} \to H_{\mathcal{L}}^{\perp},\ \mathbf{k} \mapsto \chi^{(\mathbf{k})},$$

is a group isomorphism.

3.4. Example: Two-Dimensional Crystals. As a preliminary example, we want to consider the case of a two-dimensional crystal. So, let $\mathbf{A} \in \mathrm{Mat}(3,3;\mathbb{R})$, $\mathrm{rk}(\mathbf{A}) = 2$, and define the discrete closed group $H_{\mathcal{L}} = (\mathbf{I}|\mathbf{A}\mathbb{Z}^3)$. Let $\mathbf{e}_3 \in \mathbb{S}^2$ with $\mathbf{A}\mathbf{e}_3 = 0$ be a normal to the plane $\mathbf{A}\mathbb{R}^3$. We consider the closed subgroup $G_{\mathcal{L}} = (\mathbf{I}|\mathbf{A}\mathbb{R}^3)$ of $\mathrm{E}(3)$. Then every discrete closed subgroup H of $G_{\mathcal{L}}$ has the form $H = (\mathbf{I}|\widetilde{\mathbf{A}}\mathbb{Z}^3)$ for some $\widetilde{\mathbf{A}} \in \mathrm{Mat}(3,3;\mathbb{R})$ with $\mathrm{rk}(\widetilde{\mathbf{A}}) \leq 2$ and $\widetilde{\mathbf{A}}\mathbf{e}_3 = 0$. So the class of objective structures that we consider are crystals of dimension ≤ 2 that lie in the plane $\mathbf{A}\mathbb{R}^3$.

Let $\{\mathbf{e}_1, \mathbf{e}_2\}$ be an orthonormal basis of $\mathbf{A}\mathbb{R}^3 = \mathbf{e}_3^{\perp}$, s.t. $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ form an orthonormal basis of $\mathbb{R}^3$. The characters of $G_{\mathcal{L}}$ are found via the isomorphism

$$\varphi :\ G_{\mathcal{L}} \to \mathbb{R}^2,\ (\mathbf{I}|y_1\mathbf{e}_1 + y_2\mathbf{e}_2) \mapsto (y_1, y_2).$$

Now, the characters of $\mathbb{R}^2$ are

$$\chi_{\mathbb{R}^2}^{(k_1,k_2)}(y_1, y_2) := e^{i(k_1y_1+k_2y_2)},\ (y_1, y_2) \in \mathbb{R}^2,\ (k_1, k_2) \in \mathbb{R}^2 \cong \widehat{\mathbb{R}^2},$$

yielding the characters of $G_{\mathcal{L}}$

$$\chi_{G_{\mathcal{L}}}^{(k_1,k_2)} := \chi_{\mathbb{R}^2}^{(k_1,k_2)} \circ \varphi.$$

The design equations for $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,(k_1,k_2)}$ are thus

(i) $\Delta\mathbf{E}_0 = -\dfrac{\omega^2}{c^2}\mathbf{E}_0$,

(ii) $\operatorname{div}\mathbf{E}_0 = 0$,

(iii) $\mathbf{E}_0(\mathbf{x} - (y_1\mathbf{e}_1 + y_2\mathbf{e}_2)) = \chi_{\mathbb{R}^2}^{(k_1,k_2)}(y_1, y_2)\mathbf{E}_0(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$, $(y_1, y_2) \in \mathbb{R}^2$.

As in the three-dimensional case, we use equation (iii) to determine $\mathbf{E}_0$ on the orbits of $G_{\mathcal{L}}$. For every $\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3 \in \mathbb{R}^3$:

$$\mathbf{E}_0(\mathbf{x}) = \mathbf{E}_0(x_3\mathbf{e}_3 - (-x_1\mathbf{e}_1 - x_2\mathbf{e}_2)) \overset{\text{(iii)}}{=} e^{-i(k_1x_1+k_2x_2)}\mathbf{E}_0(x_3\mathbf{e}_3).$$

Unlike in the three-dimensional case, we still have to determine the function $\mathbf{E}_0(\cdot\mathbf{e}_3)$ from (i) and (ii).

The vector Helmholtz equation (i) simplifies to the ordinary differential equation

$$\frac{\partial^2}{\partial x_3^2}\mathbf{E}_0(x_3\mathbf{e}_3) = -\left(\frac{\omega^2}{c^2} - (k_1^2 + k_2^2)\right)\mathbf{E}_0(x_3\mathbf{e}_3),$$

yielding the solution

$$\mathbf{E}(x_3\mathbf{e}_3) = e^{\pm i\sqrt{\frac{\omega^2}{c^2}-(k_1^2+k_2^2)}x_3}\mathbf{n}, \quad \mathbf{n} \in \mathbb{C}^3.$$

Since the solutions need to be bounded, we have to make the additional restriction $\sqrt{k_1^2+k_2^2} \leq \frac{\omega}{c}$. Setting $k_3 := \mp\sqrt{\frac{\omega^2}{c^2}-(k_1^2+k_2^2)}$, and $\mathbf{k} := (k_1, k_2, k_3)$, we find that $|\mathbf{k}|^2 = \frac{\omega^2}{c^2}$ and get

$$\mathbf{E}_0(\mathbf{x}) = \mathbf{n}e^{-i\mathbf{k}\cdot\mathbf{x}}.$$

As in the three-dimensional case, we get from (ii) that $\mathbf{k}\cdot\mathbf{n} = 0$. Thus, the solutions to the design equations are again the plane waves.

Now, assuming that we analyze our objective structure that is generated by the group $H_{\mathcal{L}} = (\mathbf{I}|\mathbf{A}\mathbb{Z}^3)$, we want to find the wave vectors that lead to resonance of all its unit cells. The orthogonal group $H_{\mathcal{L}}^{\perp}$ of $H_{\mathcal{L}}$ is given by

$$\begin{aligned} H_{\mathcal{L}}^{\perp} &= \{\chi \in \widehat{G_{\mathcal{L}}}.\ \chi \downarrow_{H_{\mathcal{L}}}^{G_{\mathcal{L}}} \equiv 1\} \\ &\cong \{(k_1,k_2) \in \mathbb{R}^2.\ e^{i(k_1x_1+k_2x_2)} = 1 \text{ for all } (x_1,x_2) \in \mathbf{A}\mathbb{Z}^3\} \\ &= \{(k_1,k_2) \in \mathbb{R}^2.\ k_1x_2 + k_2x_2 \in 2\pi\mathbb{Z} \text{ for all } (x_1,x_2) \in \mathbf{A}\mathbb{Z}^3\}. \end{aligned}$$

So, it consists of all vectors of the two-dimensional reciprocal lattice of $\mathbf{A}\mathbb{Z}^3$. Note that, as there is no condition on k_3, the Fourier transform of the structure is supported on the lines $k_1\mathbf{e}_1 + k_2\mathbf{e}_2 + \mathbb{R}\mathbf{e}_3$, $\chi_{G_{\mathcal{L}}}^{(k_1,k_2)} \in H_{\mathcal{L}}^{\perp}$. These lines can thus be seen as the reciprocal structure of a two-dimensional crystal.

There is an implication for reconstruction. The Fourier transform is supported on a lattice in k_1 and k_2, giving a two-dimensional crystallographic reconstruction problem. In the third dimension, however, it is supported continuously, yielding a one-dimensional CDI reconstruction problem. Thus this problem is an intermediate case.

In the next chapter we will consider a special abelian closed subgroup of E(3) that defines a novel form of radiation.

CHAPTER 4

Nanotube Structures and Twisted Waves

Like Chapter 3, this chapter is part of joint work which will appear in [FJJ-1, FJJ-2].

The class of nanotube structures is the class of objective structures that are generated by a discrete closed subgroup of screw displacements about an axis $\mathbb{R}\mathbf{e}$, $e \in \mathbb{S}^2$. Prominent examples of nanotube structures are carbon nanotubes.

Choosing the design group $C_{\mathbf{e}} = \{(\mathbf{R}_\vartheta|\tau\mathbf{e}).\ \vartheta \in \mathbb{T},\ \tau \in \mathbb{R}\}$, the design equations can be explicitly solved, leading to electromagnetic fields that propagate helically in space. They share many properties with plane waves and will be called twisted waves.

When these twisted waves are scattered by a nanotube structure, the outgoing intensity does not reveal symmetry information by a simple geometric relationship between incoming and outgoing radiation as in the case of plane waves scattered by crystals. However, when considering the outgoing intensity in axis direction as a function of the radiation parameters, we find the analog of the von Laue condition.

In addition, the reconstruction problem reduces to a scalar phase problem. Instead of the Fourier transform, the corresponding scalar transform is a combination of Fourier and Hankel transforms that is related to the expansion in cylindrical harmonics.

1. Solution of the Design Equations – Twisted Waves

1.1. Twisted Waves. The first non-crystalline class of objective structures that we want to consider in detail is the class of nanotube structures that we already introduced in the last chapter. Given a unit vector $\mathbf{e} \in \mathbb{S}^2$ these are generated by an infinite discrete closed subgroup of the group $C_{\mathbf{e}}$ that is defined as

$$C_{\mathbf{e}} := \{(\mathbf{R}_\vartheta|\tau\mathbf{e}).\ \vartheta \in \mathbb{T},\ \tau \in \mathbb{R}\}.$$

By lemma 3.16, the function $\chi : C_{\mathbf{e}} \to \mathbb{C}$ appearing in the design equations is a character of the group $C_{\mathbf{e}}$. We find these characters via the following isomorphism between $C_{\mathbf{e}}$ and the group $\mathbb{T} \times \mathbb{R}$:

$$\iota :\ C_{\mathbf{e}} \to \mathbb{T} \times \mathbb{R},\ (\mathbf{R}_\vartheta|\tau\mathbf{e}) \mapsto (\vartheta, \tau).$$

The dual group of $\mathbb{T}\times\mathbb{R}$ is

$$\widehat{\mathbb{T}\times\mathbb{R}} = \widehat{\mathbb{T}}\times\widehat{\mathbb{R}} = \{\chi^{(\alpha,\widehat{z})}_{\mathbb{T}\times\mathbb{R}} : \mathbb{T}\times\mathbb{R}\to\mathbb{C},\ (\vartheta,\tau)\mapsto e^{i(\alpha\vartheta+\widehat{z}\tau)},\ \alpha\in\mathbb{Z},\ \widehat{z}\in\mathbb{R}\}.$$

Thus, the characters of $C_{\mathbf{e}}$ are given by

$$\chi^{(\alpha,\widehat{z})}_{C_{\mathbf{e}}}((\mathbf{R}_\vartheta|\tau\mathbf{e})) := \chi^{(\alpha,\widehat{z})}_{\mathbb{T}\times\mathbb{R}}\circ\iota((\mathbf{R}_\vartheta|\tau\mathbf{e})) = e^{i(\alpha\vartheta+\widehat{z}\tau)}.$$

The Fourier transform on $C_{\mathbf{e}}$ turns out to be a Fourier series in the angle ϑ and a Fourier transform in τ.

The elements of the spaces $\mathrm{R}^{\omega,(\alpha,\widehat{z})}_b(C_{\mathbf{e}})$ are given in the following theorem. They are waves propagating helically in space that share many properties with plane waves. We call these solutions of the design equations twisted waves.

Theorem 4.1 (Twisted Waves). *Let $\mathbf{e}\in\mathbb{S}^2$ be a unit vector, $\omega>0$, and $\mathbf{E}_0\in\mathrm{R}^\omega_b$ be an eigenfunction of the action of $C_{\mathbf{e}}$ on R^ω_b, i.e. $\mathbf{E}_0$ solves the following equations:*

(i) $\Delta\mathbf{E}_0 = -\dfrac{\omega^2}{c^2}\mathbf{E}_0$,

(ii) $\operatorname{div}\mathbf{E}_0 = 0$,

(iii) $\mathbf{R}_\vartheta\mathbf{E}_0(\mathbf{R}_{-\vartheta}(\mathbf{x}-\tau\mathbf{e})) = \chi(\vartheta,\tau)\mathbf{E}_0(\mathbf{x})$
for all $\mathbf{x}\in\mathbb{R}^3$, $(\vartheta,\tau)\in\mathbb{T}\times\mathbb{R}$ and some $\chi(\vartheta,\tau)\in\mathbb{C}$.

When $\mathbf{E}_0\neq 0$, there are $\alpha\in\mathbb{Z}$ and $\widehat{z}\in\mathbb{R}$, $|\widehat{z}|\le\frac{\omega}{c}$, s.t.

$$\mathbf{E}_0(\mathbf{x}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}}\mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0 e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi},\quad \mathbf{x}\in\mathbb{R}^3, \tag{4.1}$$

where $\mathbf{k}_0 := (0,\widehat{r},\widehat{z})^T$, $\mathbf{n}_0\in\mathbf{k}_0^\perp$, $\widehat{r} := \sqrt{\frac{\omega^2}{c^2}-\widehat{z}^2}$.

Given an orthonormal basis $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}\}$ of $\mathbb{R}^3$, these solutions are explicitly expressed in cylindrical coordinates $\mathbf{x} = \xi_{\mathbf{e}}(r,\varphi,z) = r\cos(\varphi)\mathbf{e}_1 + r\sin(\varphi)\mathbf{e}_2 + z\mathbf{e}$ about $\mathbf{e}$ as follows:

$$\mathbf{E}_0(r,\varphi,z) = \mathbf{N}\begin{pmatrix} J_{\alpha-1}(\widehat{r}r)e^{i\varphi}\\ J_{\alpha+1}(\widehat{r}r)e^{-i\varphi}\\ J_\alpha(\widehat{r}r)\end{pmatrix} e^{-i(\alpha\varphi+\widehat{z}z)},\quad r\in[0,\infty),\ \varphi\in\mathbb{T},\ z\in\mathbb{R}, \tag{4.2}$$

where $\mathbf{N} = \mathbf{U}\mathrm{diag}(\mathbf{c})$ for some $\mathbf{c}\in\mathbb{C}^3$ that satisfies $\frac{\widehat{r}}{\sqrt{2}}(\mathbf{c}_1+\mathbf{c}_2)+\widehat{z}\mathbf{c}_3 = 0$, and $\mathbf{U}$ is the unitary matrix $\mathbf{U} := \frac{1}{\sqrt{2}}\begin{pmatrix} i & -i & \\ 1 & 1 & \\ & & \sqrt{2}\end{pmatrix}\in\mathrm{U}(3)$.

The vectors $\mathbf{c}$ and $\mathbf{n}_0$ are related by $\mathbf{n}_0 = \mathbf{U}\mathbf{c}$.

Proof. By Lemma 3.16 there are $(\alpha,\widehat{z})\in\mathbb{Z}\times\mathbb{R}$, s.t. $\chi = \chi^{(\alpha,\widehat{z})}_{C_{\mathbf{e}}}\in\widehat{C_{\mathbf{e}}}$.

Step 1: Exploiting the design equations (iii)

First, we rewrite (iii) in cylindrical coordinates $\mathbf{x} = \xi_{\mathbf{e}}(r, \varphi, z)$. These coordinates are the natural choice when dealing with the action of the group $C_{\mathbf{e}}$ on $\mathbb{R}^3$ as the coordinate surfaces for fixed r are $C_{\mathbf{e}}$-invariant while the r-coordinate parametrizes the space of orbits. The action simplifies to $(\mathbf{R}_\vartheta|\tau\mathbf{e})\xi_{\mathbf{e}}(r, \varphi, z) = \xi_{\mathbf{e}}(r, \varphi + \vartheta, z + \tau)$. Let $\widetilde{\mathbf{E}_0} := \mathbf{E}_0 \circ \xi_{\mathbf{e}}$, then (iii) reads

$$\mathbf{R}_\vartheta \widetilde{\mathbf{E}_0}(r, \varphi - \vartheta, z - \tau) = e^{i(\alpha\vartheta + \widehat{z}\tau)} \widetilde{\mathbf{E}_0}(r, \varphi, z).$$

Thus, we find that at $\mathbf{x} = \xi_{\mathbf{e}}(r, 0, 0)$, and for $(\vartheta, \tau) = (\varphi, z)$ we get the equation $\mathbf{R}_\varphi \widetilde{\mathbf{E}_0}(r, 0, 0) = e^{i(\alpha\varphi + \widehat{z}z)} \widetilde{\mathbf{E}_0}(r, \varphi, z)$, yielding

$$\widetilde{\mathbf{E}_0}(r, \varphi, z) = e^{-i(\alpha\varphi + \widehat{z}z)} \mathbf{R}_\varphi \widetilde{\mathbf{E}_0}(r, 0, 0). \tag{1}$$

Note that the φ- and z-dependence of $\widetilde{\mathbf{E}_0}$ is fully determined by (iii) as a consequence of the transitivity of the group action on the coordinate surfaces. The dependence on r will be determined in the next step via the Helmholtz equation (i).

Step 2: Solution of the vector Helmholtz equation (i)

We first simultaneously diagonalize the matrices $\mathbf{R}_\varphi$, $\varphi \in \mathbb{T}$, by conjugating with a unitary matrix $\mathbf{U} \in \mathrm{U}(3)$, which is possible because these matrices form an abelian group.

$$\mathbf{R}_\varphi = \mathbf{U} \begin{pmatrix} e^{i\varphi} & & \\ & e^{-i\varphi} & \\ & & 1 \end{pmatrix} \mathbf{U}^{-1}, \qquad \text{where } \mathbf{U} := \frac{1}{\sqrt{2}} \begin{pmatrix} i & -i & \\ 1 & 1 & \\ & & \sqrt{2} \end{pmatrix} \in \mathrm{U}(3).$$

Equation (1) then becomes

$$\mathbf{U}^{-1} \widetilde{\mathbf{E}_0}(r, \varphi, z) = e^{-i(\alpha\varphi + \widehat{z}z)} \begin{pmatrix} e^{i\varphi} & & \\ & e^{-i\varphi} & \\ & & 1 \end{pmatrix} \mathbf{U}^{-1} \widetilde{\mathbf{E}_0}(r, 0, 0). \tag{2}$$

Setting $\mathbf{E}_{\mathbf{U}}(r) := \mathbf{U}^{-1} \widetilde{\mathbf{E}_0}(r, 0, 0)$, $r > 0$, and using the fact that the vector Laplacian and the multiplication by $\mathbf{U}$ commute, the vector Helmholtz equation reduces to the three scalar equations

$$\Delta e^{-i((\alpha + \sigma_j)\varphi + \widehat{z}z)} \mathbf{E}_{\mathbf{U},j}(r) = -\frac{\omega^2}{c^2} \mathbf{E}_{\mathbf{U},j}(r), \quad \text{where } \sigma := (-1, 1, 0)^T, \quad j = 1, 2, 3.$$

The vector σ encodes the shift in the parameter α in the respective components that results from the additional factors in the diagonal matrix.

The Laplacian in cylindrical coordinates is given by $(\xi_{\mathbf{e}})_* \Delta = \frac{1}{r}\partial_r(r\partial_r) + \frac{1}{r^2}\partial_\varphi^2 + \partial_z^2$, giving the following ordinary differential equations for the components of $\mathbf{E}_{\mathbf{U}}$:

$$\left(\partial_r^2 + \frac{1}{r}\partial_r + \left(\left(\frac{\omega^2}{c^2} - \widehat{z}^2 \right) - \frac{(\alpha + \sigma_j)^2}{r^2} \right) \right) \mathbf{E}_{\mathbf{U},j}(r) = 0, \qquad j = 1, 2, 3.$$

These are rescaled versions of Bessel differential equations. Setting $\widehat{r} := \sqrt{\frac{\omega^2}{c^2} - \widehat{z}^2}$, we find that there is no non-trivial bounded solution to these equations when $|\widehat{z}| > \frac{\omega}{c}$, since then $\widehat{r}$ is purely imaginary and the solutions are the unbounded modified Bessel functions. In case $\widehat{r}$ is real, the bounded solutions are

$$\mathbf{E}_{\mathbf{U},j}(r) = \mathbf{c}_j J_{\alpha+\sigma_j}(\widehat{r}r), \quad \text{where } \mathbf{c}_j \in \mathbb{C}, \quad j = 1, 2, 3,$$

and J_α, $\alpha \in \mathbb{Z}$, is the Bessel function of the first kind of order α. The Bessel functions of the second kind that also solve the equations for real $\widehat{r}$ are unbounded. With (2), we arrive at

$$\widetilde{\mathbf{E}_0}(r, \varphi, z) = \mathbf{U}\mathrm{diag}(\mathbf{c}) \begin{pmatrix} J_{\alpha-1}(\widehat{r}r)e^{i\varphi} \\ J_{\alpha+1}(\widehat{r}r)e^{-i\varphi} \\ J_\alpha(\widehat{r}r) \end{pmatrix} e^{-i(\alpha\varphi+\widehat{z}z)}, \tag{3}$$

where $\mathrm{diag}(\mathbf{c})$ is the diagonal matrix with the components of $\mathbf{c}$ on the diagonal.

We still have to determine the vector $\mathbf{c}$ from the divergence condition (ii) and derive the Fourier representation (4.1). We first move to the Fourier side.

Step 3: Switch to the Fourier side

We take a closer look at the function $\xi_{\mathbf{e}}(r, \varphi, z) \mapsto J_\alpha(\widehat{r}r)e^{-i(\alpha\varphi+\widehat{z}z)}$ using the Bessel integral

$$J_\alpha(\widehat{r}r) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(\alpha\widehat{\varphi} - \widehat{r}r\sin(\widehat{\varphi}))}\mathrm{d}\widehat{\varphi}.$$

We find

$$\begin{aligned} J_\alpha(\widehat{r}r)e^{-i(\alpha\varphi+\widehat{z}z)} &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(\alpha(\widehat{\varphi}-\varphi) - \widehat{r}r\sin(\widehat{\varphi})+\widehat{z}z)}\mathrm{d}\widehat{\varphi} = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(\alpha\widehat{\varphi} - \widehat{r}r\sin(\widehat{\varphi}+\varphi)+\widehat{z}z)}\mathrm{d}\widehat{\varphi} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(\alpha\widehat{\varphi} - \widehat{r}r(\sin(\widehat{\varphi})\cos(\varphi)+\cos(\widehat{\varphi})\sin(\varphi))+\widehat{z}z)}\mathrm{d}\widehat{\varphi} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}} e^{-i\begin{pmatrix}\widehat{r}\sin(\widehat{\varphi})\\ \widehat{r}\cos(\widehat{\varphi})\\ \widehat{z}\end{pmatrix}\cdot\begin{pmatrix}r\cos(\varphi)\\ r\sin(\varphi)\\ z\end{pmatrix}}\mathrm{d}\widehat{\varphi} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}} e^{-i\mathbf{R}_{-\widehat{\varphi}}\begin{pmatrix}0\\ \widehat{r}\\ \widehat{z}\end{pmatrix}\cdot\xi_{\mathbf{e}}(r,\varphi,z)}\mathrm{d}\widehat{\varphi}, \end{aligned}$$

where we translated the integrand without shifting the domain of integration using the 2π-periodicity of the integrand in the second equality and used the angle sum formula for the sine in the third equality. We decomposed the function into scalar plane waves and motivated the notation $\widehat{z}$ and $\widehat{r}$ for the parameters, as they are the $\mathbf{e}$-component and

the cylindrical radius of the wave vectors, respectively. Using this representation for the components of the vector field $\mathbf{E}_0$ and setting $\mathbf{k}_0 := (0, \widehat{r}, \widehat{z})^T$, we get

$$\begin{aligned}\mathbf{E}_0(\mathbf{x}) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathbf{U}\mathrm{diag}(\mathbf{c}) \begin{pmatrix} e^{i(\alpha-1)\widehat{\varphi}} \\ e^{i(\alpha+1)\widehat{\varphi}} \\ e^{i\alpha\widehat{\varphi}} \end{pmatrix} e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}} \underbrace{\mathbf{U}\begin{pmatrix} e^{-i\widehat{\varphi}} & & \\ & e^{i\widehat{\varphi}} & \\ & & 1 \end{pmatrix}}_{=\mathbf{R}_{-\widehat{\varphi}}\mathbf{U}} \mathbf{c} e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi} \\ &\overset{\mathbf{n}_0:=\mathbf{U}\mathbf{c}}{=} \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}}\mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0 e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}\end{aligned}$$

what is the Fourier representation (4.1). It remains to find the condition on $\mathbf{n}_0$ that guarantees that $\mathbf{E}_0$ is divergence-free. Via $\mathbf{n}_0 = \mathbf{U}\mathbf{c}$, we then get the respective condition on $\mathbf{c}$.

Step 4: The divergence condition (ii)

The divergence condition (ii) for the Fourier representation is

$$0 = \mathrm{div}\,\mathbf{E}_0(\mathbf{x}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}}(-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0 \cdot \mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0) e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}.$$

This is satisfied, if and only if

$$\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0 \cdot \mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0 = 0 \quad \Leftrightarrow \quad \mathbf{k}_0 \cdot \mathbf{n}_0 = 0.$$

For $\mathbf{c}$, this means

$$0 = \mathbf{k}_0 \cdot \mathbf{n}_0 = \mathbf{k}_0 \cdot \mathbf{U}\mathbf{c} = \mathbf{U}^T\mathbf{k}_0 \cdot \mathbf{c} = \frac{\widehat{r}}{\sqrt{2}}(\mathbf{c}_1 + \mathbf{c}_2) + \widehat{z}\mathbf{c}_3.$$

Setting $\mathbf{N} := \mathbf{U}\mathrm{diag}(\mathbf{c})$, we get the explicit representation (4.2) from (3). □

We will rewrite the Fourier representation (4.1) in a more abstract way. Define a manifold $M \subset \frac{\omega}{c}\mathbb{S}^2$ and a parametrization ψ by

$$M := \left\{\mathbf{k} \in \frac{\omega}{c}\mathbb{S}^2.\ \mathbf{k}\cdot\mathbf{e} = \widehat{z}\right\}, \quad \psi:\ [-\pi,\pi) \to M,\ \widehat{\varphi} \mapsto \mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0.$$

With the following vector field $\mathbf{n}$ on M

$$\mathbf{n}:\ M \to \mathbb{R}^3,\ \mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0 \mapsto \frac{1}{2\pi\widehat{r}} e^{i\alpha\widehat{\varphi}}\mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0,$$

the Fourier representation (4.1) of $\mathbf{E}_0$ can be written as follows:

$$\mathbf{E}_0(\mathbf{x}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}}\mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0 e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi} = \int_{\psi^{-1}(M)} \widehat{r}\mathbf{n}\circ\psi(\widehat{\varphi})e^{-i\psi(\widehat{\varphi})\cdot\mathbf{x}}\mathrm{d}\mathcal{H}^1(\widehat{\varphi})$$
$$= \int_M \widehat{r}\mathbf{n}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}(\psi_*\mathcal{H}^1)(\mathbf{k}) = \int_M \mathbf{n}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\mathcal{H}^1(\mathbf{k}),$$

noting that the pushforward measure $\psi_*\mathcal{H}^1$ satisfies $(\psi_*\mathcal{H}^1)(A) = \mathcal{H}^1(\psi^{-1}(A)) = \frac{1}{\widehat{r}}\mathcal{H}^1(A)$ for measurable sets A, since M is a circle with radius $\widehat{r}$. Thus, a twisted wave is the Fourier transform of the singular complex vector measure $\mathbf{n}\mathrm{d}\mathcal{H}^1$ on M.

The same construction shows that the scalar function $\xi_{\mathbf{e}}(r,\varphi,z) \mapsto J_\alpha(\widehat{r}r)e^{-i(\alpha\varphi+\widehat{z}z)}$ is the Fourier transform of the singular complex measure $\frac{1}{2\pi\widehat{r}}e^{i\alpha\psi^{-1}(\mathbf{k})}\mathrm{d}\mathcal{H}^1(\mathbf{k})$ on M.

The field $\mathbf{E}_0$ can thus be seen as a superposition of plane waves with wave vectors on M, which is a ring about $\mathbb{R}\mathbf{e}$, with a relative phase shift that depends on the parameter $\alpha \in \mathbb{Z}$. This view of the representation (4.1) is visualized in Figure 4.1. The explicit representation (4.2) shows that this superposition yields a field that is essentially a plane wave in φ and z with different radial dependencies in every component.

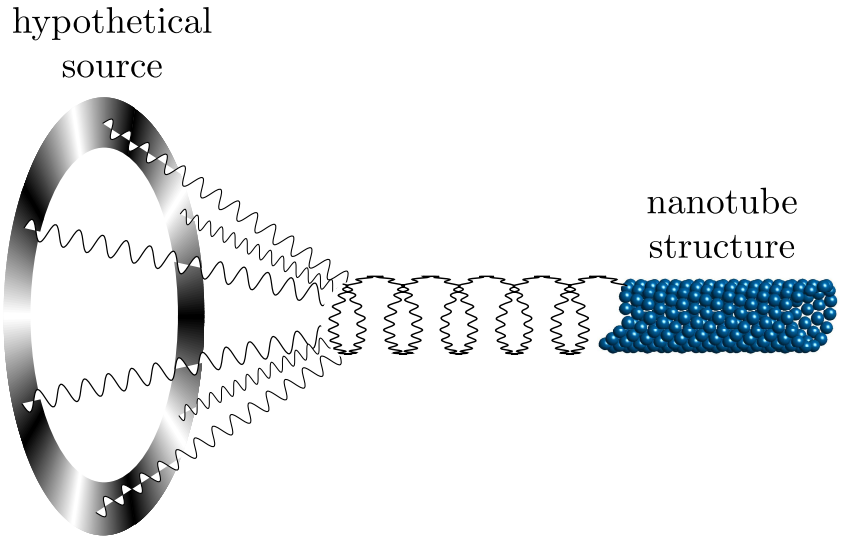


FIGURE 4.1. Visualization of a hypothetical source of twisted waves according to (4.1). Plane waves of a fixed frequency with wave vectors that enclose a fixed angle with the axis of the structure superimpose to generate a twisted wave, if their phases are aligned in the right way. The shading of the ring on the left indicates the relative phases.

Since twisted waves will be important when considering a general class of non-compact design groups, we introduce a special notation. Let $\mathbf{k} \in \mathbb{R}^3$ and $\alpha \in \mathbb{Z}$. Then we define

$$\mathbf{E}_{\mathbf{k}}^{(\alpha)}(\mathbf{x}) := \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\alpha\widehat{\varphi}}\mathbf{R}_{\widehat{\varphi}}\mathbf{n}e^{i\mathbf{R}_{\widehat{\varphi}}\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}, \quad \mathbf{x}\in\mathbb{R}^3, \tag{4.3}$$

for some $\mathbf{n} \in \mathbf{k}^\perp$. We also write

$$e_{\mathbf{k}}^{(\alpha)}(\mathbf{x}) := \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-i\alpha\widehat{\varphi}} e^{i\mathbf{R}_{\widehat{\varphi}}\mathbf{k}\cdot\mathbf{x}} \mathrm{d}\widehat{\varphi}, \quad \mathbf{x} \in \mathbb{R}^3, \tag{4.4}$$

for the scalar twisted waves.

1.2. Properties of Twisted Waves. We will go a bit further into detail concerning the vector $\mathbf{n}_0 \in \mathbf{k}_0^\perp$. The space $\mathbf{k}_0^\perp$ is parametrization of the space $\mathrm{R}_b^{\omega,(\alpha,\widehat{z})}(C_{\mathbf{e}})$, showing that as for plane waves, these spaces are five-dimensional. We can write

$$\mathbf{n}_0 = e^{i\zeta}(\mathbf{n}_1 - i\mathbf{n}_2) \quad \text{with } \mathbf{n}_1, \mathbf{n}_2 \in \mathbb{R}^3, \quad \mathbf{n}_1 \cdot \mathbf{n}_2 = 0.$$

Then, we say that $\mathbf{E}_0$ is linearly polarized when $\mathbf{n}_2 = 0$, spherically polarized when $|\mathbf{n}_1| = |\mathbf{n}_2|$, and elliptically polarized else. So, polarization is a global property of a twisted wave.

Let's consider a linearly polarized twisted wave $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,(\alpha,\widehat{z})}$. Then

$$\mathbf{n}_0 = e^{i\zeta}\mathbf{n}_1 = e^{i\zeta}|\mathbf{n}_1|\frac{\mathbf{n}_1}{|\mathbf{n}_1|}.$$

Choosing an orthonormal basis $\{\mathbf{b}_1, \mathbf{b}_2\}$ of $\mathbf{k}^\perp$, we can define the angle $\eta \in \mathbb{T}$ by

$$\frac{\mathbf{n}_1}{|\mathbf{n}_1|} = \cos(\eta)\mathbf{b}_1 + \sin(\eta)\mathbf{b}_2.$$

η is called polarization angle of the linearly polarized twisted wave $\mathbf{E}_0$.

Making the choice $\mathbf{b}_1 = \frac{c}{\omega}(0, \widehat{z}, -\widehat{r})^T$ and $\mathbf{b}_2 = (1, 0, 0)^T$, we can determine the vector $\mathbf{c}$ from the explicit representation (4.2) of $\mathbf{E}_0$ via the relation $\mathbf{n}_0 = \mathbf{U}\mathbf{c}$. Solving for $\mathbf{c}$, we get

$$\begin{aligned}\mathbf{c} = \mathbf{U}^{-1}\mathbf{n}_0 &= e^{i\zeta}|\mathbf{n}_1|\left(\mathbf{U}^{-1}\mathbf{b}_1\cos(\eta) + \mathbf{U}^{-1}\mathbf{b}_2\sin(\eta)\right) \\ &= e^{i\zeta}|\mathbf{n}_1|\frac{c}{\sqrt{2}\omega}\begin{pmatrix} \widehat{z}\cos(\eta) - i\frac{\omega}{c}\sin(\eta) \\ \widehat{z}\cos(\eta) + i\frac{\omega}{c}\sin(\eta) \\ -\sqrt{2}\widehat{r}\cos(\eta)\end{pmatrix}.\end{aligned}$$

Setting $c(\eta) := \frac{\widehat{z}}{\sqrt{2}}\cos(\eta) + i\frac{\omega}{\sqrt{2}c}\sin(\eta)$, we get

$$\mathbf{c} = e^{i\zeta}|\mathbf{n}_1|\frac{c}{\omega}\begin{pmatrix} c(\eta) \\ \overline{c(\eta)} \\ -\widehat{r}\cos(\eta)\end{pmatrix}.$$

Now, we can rewrite the matrix $\mathbf{N} = \mathbf{U}\mathrm{diag}(\mathbf{c})$ from (4.2) in terms of the polarization angle. We define the matrix $\mathbf{N}(\eta) := (e^{i\zeta}|\mathbf{n}_1|)^{-1}\mathbf{N}$, which evaluates to

$$\mathbf{N}(\eta) = \frac{c}{\omega}\begin{pmatrix} i\frac{c(\eta)}{\sqrt{2}} & -i\frac{\overline{c(\eta)}}{\sqrt{2}} & 0 \\ \frac{c(\eta)}{\sqrt{2}} & \frac{\overline{c(\eta)}}{\sqrt{2}} & 0 \\ 0 & 0 & -\widehat{r}\cos(\eta) \end{pmatrix}. \tag{4.5}$$

We call this matrix the polarization matrix of the twisted wave $\mathbf{E}_0$. The representation of linearly polarized twisted waves with respect to the polarization angle is given by the following corollary.

Corollary 4.2 (Linearly Polarized Twisted Waves).
Let $\mathbf{E}_0 \in \mathrm{R}_b^{(\alpha,\widehat{z})}(C_\mathbf{e})$, $|\widehat{z}| \leq \frac{\omega}{c}$. When $\mathbf{E}_0$ is linearly polarized, it can up to a multiplicative constant be written as

$$\mathbf{E}_0(r,\varphi,z) = \mathbf{N}(\eta)\begin{pmatrix} J_{\alpha-1}(\widehat{r}r)e^{i\varphi} \\ J_{\alpha+1}(\widehat{r}r)e^{-i\varphi} \\ J_\alpha(\widehat{r}r) \end{pmatrix} e^{-i(\alpha\varphi+\widehat{z}z)}, \quad \eta \in \mathbb{T}. \tag{4.6}$$

The corresponding spatial part of the electromagnetic field is then given as

$$\mathbf{B}_0(r,\varphi,z) = -c^{-1}\mathbf{N}\left(\eta+\frac{\pi}{2}\right)\begin{pmatrix} J_{\alpha-1}(\widehat{r}r)e^{i\varphi} \\ J_{\alpha+1}(\widehat{r}r)e^{-i\varphi} \\ J_\alpha(\widehat{r}r) \end{pmatrix} e^{-i(\alpha\varphi+\widehat{z}z)}, \quad \eta \in \mathbb{T}. \tag{4.7}$$

Proof. Let $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,(\alpha,\widehat{z})}(C_\mathbf{e})$ be linearly polarized. By Theorem 4.1, up to a multiplicative constant,

$$\mathbf{E}_0(\mathbf{x}) = \int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}}\mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0 e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi},$$

with $\mathbf{k}_0 = (0,\widehat{r},\widehat{z})^T$ and $\mathbf{n}_0 \in \mathbf{k}_0^\perp$. The spatial part $\mathbf{B}_0$ of the corresponding magnetic field is given by

$$\mathbf{B}_0(\mathbf{x}) = -\frac{1}{\omega}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}}\mathbf{R}_{-\widehat{\varphi}}(\mathbf{k}_0\times\mathbf{n}_0)e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}.$$

As above, as $\mathbf{E}_0$ is linearly polarized, we write $\mathbf{n}_0 = e^{i\zeta}|\mathbf{n}_1|\frac{c}{\omega}(\frac{\omega}{c}\sin(\eta),\widehat{z}\cos(\eta),-\widehat{r}\cos(\eta))^T$ for $\eta \in \mathbb{T}$. Thus,

$$\begin{aligned}\frac{1}{\omega}\mathbf{k}_0\times\mathbf{n}_0 &= e^{i\zeta}|\mathbf{n}_1|\frac{c}{\omega^2}\begin{pmatrix} \widehat{r}^2\cos(\eta)+\widehat{z}^2\cos(\eta) \\ -\frac{\omega\widehat{z}}{c}\sin(\eta) \\ \frac{\omega\widehat{r}}{c}\sin(\eta)\end{pmatrix} = e^{i\zeta}|\mathbf{n}_1|\frac{1}{\omega}\begin{pmatrix} \frac{\omega}{c}\cos(\eta) \\ -\widehat{z}\sin(\eta) \\ \widehat{r}\sin(\eta)\end{pmatrix} \\ &= e^{i\zeta}|\mathbf{n}_1|\frac{1}{\omega}\begin{pmatrix} \frac{\omega}{c}\sin(\eta+\pi/2) \\ \widehat{z}\cos(\eta+\pi/2) \\ -\widehat{r}\cos(\eta+\pi/2)\end{pmatrix}.\end{aligned}$$

As this expression has the same form as $\mathbf{n}_0$ in the derivation of the representation (4.6) of $\mathbf{E}_0$ with polarization angle $\eta + \pi/2$ and a multiplicative constant c^{-1}, we get the representation (4.7) of $\mathbf{B}_0$ analogously. □

The representation of a linearly polarized twisted wave we just derived can be used to calculate the Poynting vector

$$\mathbf{S}(\mathbf{x}, t) = \frac{1}{\mu_0} \mathrm{Re}(\mathbf{E}_0(\mathbf{x}) e^{-i\omega t}) \times \mathrm{Re}(\mathbf{B}_0(\mathbf{x}) e^{-i\omega t}).$$

Proposition 4.3 (Poynting Vector of Twisted Waves). *The Poynting vector* $\mathbf{S}$ *of the electromagnetic field* $(\mathbf{E}_0 e^{-i\omega t}, \mathbf{B}_0 e^{-i\omega t})$*,* $t > 0$*, with* $\mathbf{E}_0, \mathbf{B}_0$ *as in Corollary 4.2 is given by*

$$\mathbf{S}(r, \varphi, z, t) = -\frac{1}{2\omega\mu_0} \begin{pmatrix} \widehat{r}(C_{\alpha-1} + C_{\alpha+1}) C_\alpha \\ \widehat{r}(S_{\alpha-1} - S_{\alpha+1}) C_\alpha \\ \frac{\widehat{z}}{2}((C_{\alpha-1} + C_{\alpha+1})^2 + (S_{\alpha-1} - S_{\alpha+1})^2) \end{pmatrix}, \tag{4.8}$$

where $S_\alpha := J_\alpha(\widehat{r}r) \sin(\alpha\varphi + \widehat{z}z - \omega t)$*, and* $C_\alpha := J_\alpha(\widehat{r}r) \cos(\alpha\varphi + \widehat{z}z - \omega t)$*.*

Proof. The real parts of $\mathbf{E}_0(\mathbf{x}) e^{-i\omega t}$ and $\mathbf{B}_0(\mathbf{x}) e^{-i\omega t}$ are

$$\mathrm{Re}(\mathbf{E}_0(\mathbf{x}) e^{-i\omega t}) = \mathrm{Re}(\mathbf{N}(\eta)) \begin{pmatrix} C_{\alpha-1} \\ C_{\alpha+1} \\ C_\alpha \end{pmatrix} + \mathrm{Im}(\mathbf{N}(\eta)) \begin{pmatrix} S_{\alpha-1} \\ S_{\alpha+1} \\ S_\alpha \end{pmatrix},$$

$$\mathrm{Re}(\mathbf{B}_0(\mathbf{x}) e^{-i\omega t}) = -c^{-1} \mathrm{Re}(\mathbf{N}(\eta + \pi/2)) \begin{pmatrix} C_{\alpha-1} \\ C_{\alpha+1} \\ C_\alpha \end{pmatrix} - c^{-1} \mathrm{Im}(\mathbf{N}(\eta + \pi/2)) \begin{pmatrix} S_{\alpha-1} \\ S_{\alpha+1} \\ S_\alpha \end{pmatrix}.$$

To determine $\mathbf{S}$, we need to evaluate the four cross products between the different summands. The ones between the real parts and the imaginary parts yield

$$-c^{-1} \mathrm{Re}(\mathbf{N}(\eta)) \begin{pmatrix} C_{\alpha-1} \\ C_{\alpha+1} \\ C_\alpha \end{pmatrix} \times \mathrm{Re}(\mathbf{N}(\eta + \pi/2)) \begin{pmatrix} C_{\alpha-1} \\ C_{\alpha+1} \\ C_\alpha \end{pmatrix} = -\frac{1}{2\omega} \begin{pmatrix} \widehat{r}(C_{\alpha-1} + C_{\alpha+1}) C_\alpha \\ 0 \\ \frac{\widehat{z}}{2}(C_{\alpha-1} + C_{\alpha+1})^2 \end{pmatrix},$$

$$-c^{-1} \mathrm{Im}(\mathbf{N}(\eta)) \begin{pmatrix} S_{\alpha-1} \\ S_{\alpha+1} \\ S_\alpha \end{pmatrix} \times \mathrm{Im}(\mathbf{N}(\eta + \pi/2)) \begin{pmatrix} S_{\alpha-1} \\ S_{\alpha+1} \\ S_\alpha \end{pmatrix} = -\frac{1}{2\omega} \begin{pmatrix} 0 \\ 0 \\ \frac{\widehat{z}}{2}(S_{\alpha-1} - S_{\alpha+1})^2 \end{pmatrix}.$$

The sum of the mixed products simplifies to

$$
\begin{aligned}
&-c^{-1}\mathrm{Re}(\mathbf{N}(\eta))\begin{pmatrix} C_{\alpha-1}\\ C_{\alpha+1}\\ C_\alpha\end{pmatrix}\times \mathrm{Im}(\mathbf{N}(\eta+\pi/2))\begin{pmatrix} S_{\alpha-1}\\ S_{\alpha+1}\\ S_\alpha\end{pmatrix}\\
&-c^{-1}\mathrm{Im}(\mathbf{N}(\eta))\begin{pmatrix} S_{\alpha-1}\\ S_{\alpha+1}\\ S_\alpha\end{pmatrix}\times \mathrm{Re}(\mathbf{N}(\eta+\pi/2))\begin{pmatrix} C_{\alpha-1}\\ C_{\alpha+1}\\ C_\alpha\end{pmatrix}=-\frac{1}{2\omega}\begin{pmatrix} 0\\ \widehat{r}(S_{\alpha-1}-S_{\alpha+1})C_\alpha\\ 0\end{pmatrix}.
\end{aligned}
$$

Summing these terms yields the Poynting vector (4.8). □

Note that, since an elliptically polarized twisted wave $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,(\alpha,\widehat{z})}$ can be written as $\mathbf{E}_0 = \mathbf{E}_1 - i\mathbf{E}_2$, where $\mathbf{E}_1$ and $\mathbf{E}_2$ are linearly polarized twisted waves that differ only in amplitude and polarization, the formula for the Poynting vector (that does not depend on the polarization angle) is also right in the general case.

From this representation of the Poynting vector, we can not directly see the energy flow. However, at certain radii, we can determine the streamlines of the Poynting vector, revealing a helical energy flow.

Corollary 4.4 (Streamlines of the Poynting Vector). *Let $r_j \geq 0$ be the radius at which the Bessel function $J_\alpha(\widehat{r}\cdot)$ attains its j-th extremum. The Poynting vector $\mathbf{S}$ of a linearly polarized twisted wave given in Corollary 4.3 at these radii simplifies to*

$$
\mathbf{S}(r_j,\varphi,z,t) = -\frac{\alpha}{\omega\mu_0 r_j^2}C_\alpha^2\begin{pmatrix} r_j\cos(\varphi)\\ -r_j\sin(\varphi)\\ \frac{\alpha\widehat{z}}{\widehat{r}^2}\end{pmatrix},\quad j\in\mathbb{N}, \tag{4.9}
$$

where $C_\alpha := J_\alpha(\widehat{r}r_j)\cos(\alpha\varphi+\widehat{z}z-\omega t)$.

In particular, the streamlines $\gamma_{\mathbf{S}}$ of the Poynting vector at these radii through $r_j\mathbf{e}_1$ are given by

$$
\gamma_{\mathbf{S}}(s) = \begin{pmatrix} r_j\sin(s)\\ r_j\cos(s)\\ \frac{\alpha\widehat{z}}{\widehat{r}^2}s\end{pmatrix}.
$$

The electric field has the form

$$
\mathrm{Re}(\mathbf{E}_0(r_j,\varphi,z)e^{-i\omega t}) = \frac{c}{\omega}C_\alpha\mathbf{R}_\varphi\begin{pmatrix} \widehat{z}\frac{\alpha}{\widehat{r}r_j}\cos(\eta)\\ -\frac{\omega\alpha}{c\widehat{r}r_j}\sin(\eta)\\ -\widehat{r}\cos(\eta)\end{pmatrix} \tag{4.10}
$$

Along the streamlines at r_j, the electromagnetic field has the wavelength

$$\lambda_j = 2\pi \frac{c^2\sqrt{r_j^2\widehat{r}^4 + \alpha^2\widehat{z}^2}}{\alpha\omega^2}.$$

Proof. The Bessel functions obey the identity

$$\frac{\mathrm{d}}{\mathrm{d}r}J_\alpha(\widehat{r}r) = \frac{\widehat{r}}{2}(J_{\alpha-1}(\widehat{r}r) - J_{\alpha+1}(\widehat{r}r)),$$

such that at the extrema of $J_\alpha(\widehat{r}\cdot)$, we know that $J_{\alpha-1}(\widehat{r}r_j) = J_{\alpha+1}(\widehat{r}r_j)$. By the further identity

$$\frac{\alpha}{r}J_\alpha(\widehat{r}r) = \frac{\widehat{r}}{2}(J_{\alpha-1}(\widehat{r}r) + J_{\alpha+1}(\widehat{r}r)),$$

we get that

$$J_{\alpha-1}(\widehat{r}r_j) = J_{\alpha+1}(\widehat{r}r_j) = \frac{\alpha}{\widehat{r}r_j}J_\alpha(\widehat{r}r_j).$$

The two terms $(C_{\alpha-1} + C_{\alpha+1})$ and $(S_{\alpha-1} - S_{\alpha+1})$ thus simplify as follows:

$$\begin{aligned} C_{\alpha-1} + C_{\alpha+1} &= \frac{\alpha}{\widehat{r}r_j}J_\alpha(\widehat{r}r_j)(\cos((\alpha-1)\varphi + \widehat{z}z - \omega t) + \cos((\alpha+1)\varphi + \widehat{z}z - \omega t)) \\ &= 2\frac{\alpha}{\widehat{r}r_j}J_\alpha(\widehat{r}r_j)\cos(\alpha\varphi + \widehat{z}z - \omega t)\cos(\varphi) = 2\frac{\alpha}{\widehat{r}r_j}C_\alpha\cos(\varphi), \end{aligned}$$

$$\begin{aligned} S_{\alpha-1} - S_{\alpha+1} &= \frac{\alpha}{\widehat{r}r_j}J_\alpha(\widehat{r}r_j)(\sin((\alpha-1)\varphi + \widehat{z}z - \omega t) - \sin((\alpha+1)\varphi + \widehat{z}z - \omega t)) \\ &= -2\frac{\alpha}{\widehat{r}r_j}J_\alpha(\widehat{r}r_j)\cos(\alpha\varphi + \widehat{z}z - \omega t)\sin(\varphi) = -2\frac{\alpha}{\widehat{r}r_j}C_\alpha\sin(\varphi), \end{aligned}$$

where we used the angle sum and difference identities for the sine and cosine functions with argument $(\alpha\varphi + \widehat{z}z - \omega t) \pm \varphi$.

The Poynting vector (4.8) at r_j thus is

$$\mathbf{S}(r_j,\varphi,z,t) = -\frac{1}{2\omega\mu_0}\begin{pmatrix} 2\frac{\alpha}{r_j}C_\alpha^2\cos(\varphi) \\ -2\frac{\alpha}{r_j}C_\alpha^2\sin(\varphi) \\ \widehat{z}\frac{\alpha^2}{\widehat{r}^2r_j^2}C_\alpha^2(\sin(\varphi)^2 + \cos(\varphi)^2) \end{pmatrix} = -\frac{\alpha}{\omega\mu_0 r_j^2}C_\alpha^2\begin{pmatrix} r_j\cos(\varphi) \\ -r_j\sin(\varphi) \\ \frac{\alpha\widehat{z}}{\widehat{r}^2} \end{pmatrix}$$

A streamline $\gamma_{\mathbf{S}} : \mathbb{R} \to \mathbb{R}^3$ is defined by the condition $\gamma_{\mathbf{S}}' \times (\mathbf{S} \circ \gamma_{\mathbf{S}}) = 0$. The streamline given above obviously satisfies this condition.

By direct calculation, using the special form of the terms $C_{\alpha\pm1}$ and $S_{\alpha\pm1}$, one arrives at the simplified form of the electric field at the radii r_j.

To find the wavelengths λ_j, we parametrize $\gamma_{\mathbf{S}}$ by arc length.

Let $\widetilde{\gamma_{\mathbf{S}}}(s) := (r_j \sin(bs), r_j \cos(bs), \frac{\alpha\widehat{z}}{\widehat{r}^2} bs)^T$ for $b \in \mathbb{R}$. We determine b via $|\widetilde{\gamma_{\mathbf{S}}}'|^2 = 1$. For $s \in \mathbb{R}$:

$$|\widetilde{\gamma_{\mathbf{S}}}'(s)|^2 = \left| \begin{pmatrix} br_j \cos(bs) \\ -br_j \sin(bs) \\ \frac{\alpha\widehat{z}}{\widehat{r}^2} b \end{pmatrix} \right|^2 = b^2 r_j^2 + b^2 \frac{\alpha^2 \widehat{z}^2}{\widehat{r}^4}.$$

So, $b = \frac{1}{\sqrt{r_j^2 + \frac{\alpha^2\widehat{z}^2}{\widehat{r}^4}}}$. Now, setting $\mathbf{v}(\eta) := (\widehat{z}\frac{\alpha}{\widehat{r}r_j}\cos(\eta), -\frac{\omega\alpha}{c\widehat{r}r_j}\sin(\eta), -\widehat{r}\cos(\eta))^T$ the electric field on $\widetilde{\gamma_{\mathbf{S}}}$ is

$$\mathrm{Re}(\mathbf{E}_0 \circ \widetilde{\gamma_S}(s) e^{-i\omega t}) = \frac{c}{\omega} J_\alpha(\widehat{r}r) \cos(\alpha b s + \widehat{z}\frac{\alpha\widehat{z}}{\widehat{r}^2} bs - \omega t) \mathbf{R}_\varphi \mathbf{v}(\eta).$$

So, we get the wavelength by

$$\alpha b \lambda_j + \frac{\alpha\widehat{z}^2}{\widehat{r}^2} b\lambda_j = 2\pi \Leftrightarrow \lambda_j = 2\pi \frac{c^2\sqrt{r_j^2\widehat{r}^4 + \alpha^2\widehat{z}^2}}{\alpha\omega^2}.$$

□

Note that for $\alpha \gg 1$, the first maximum of $J_\alpha(\widehat{r}\cdot)$ is approximately at $r_1 \approx \frac{\alpha}{\widehat{r}}$, s.t. the wavelength is $\lambda_1 \approx \frac{2\pi c}{\omega}$. This agrees with the relation between frequency and wavelength of a plane wave given in (1.3).

Using this result, we can visualize a twisted wave by plotting the fields along the streamline at the radius r_1 as is shown in Figure 4.2.

Our discussion of the properties of twisted waves shows that in many aspects they behave like plane waves just that they are propagating helically in space.

2. Scattering of Twisted Waves – the Twisted von Laue condition

2.1. Scattering of Twisted Waves. In the last section, we found the solutions to the design equations for nanotube structures. We called them twisted waves in analogy to plane waves, since they behave like that: they are waves propagating helically in space.

In this section, we will investigate the scattering of twisted waves by nanotube structures with our goal in mind: to find a generalized von Laue condition that enables us to reconstruct the symmetries of the structure directly, and to formulate the analog of the phase problem that has to be solved to reconstruct the electron density within a unit cell.

First, we draw some comparisons between crystal structures and cylindrical structures. Let $H_{\mathcal{C}}$ be a discrete closed subgroup of $C_{\mathbf{e}}$, $\mathbf{e} \in \mathbb{S}^2$, and let $\mathcal{C} = H_{\mathcal{C}}\mathbf{M}_{\mathcal{C}}$, $\mathbf{M}_{\mathcal{C}} \subset \mathbb{R}^3$ finite, be a nanotube structure. Then there are $n \in \mathbb{N}$, $\vartheta \in \mathbb{T}$, and $\tau \in \mathbb{R}$, $\tau \neq 0$, s.t. $\mathcal{C}$ is generated by the two isometries

$$h = (\mathbf{R}_\vartheta | \tau\mathbf{e}), \quad g = (\mathbf{R}_{2\pi/n} | 0),$$

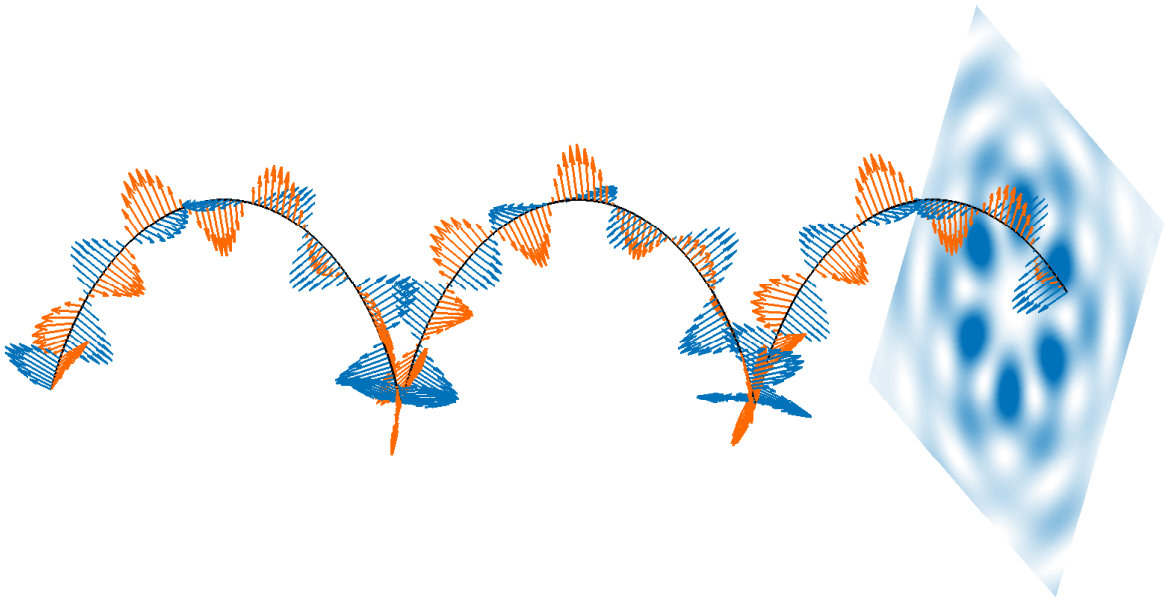


FIGURE 4.2. A twisted wave for $\alpha = 3$, $\widehat{z} = 4$, and $\omega/c = 6$, plotted along the streamline of the Poynting vector at the radius r_1. The pattern on the right is a slice through the absolute value of the Poynting vector.

i.e.

$$H_{\mathcal{C}} = \{h^j g^k.\ j,k \in \mathbb{Z}\}.$$

This will be shown in Lemma 5.2. Just as in the crystalline case, we can define a unit cell of the structure as follows. Define the set $H \setminus \mathbb{R}^3$ of orbits of $H_{\mathcal{C}}$ by

$$H \setminus \mathbb{R}^3 := \{H\mathbf{x}.\ \mathbf{x} \in \mathbb{R}^3\}.$$

Then a unit cell of the structure $\mathcal{C}$ is a set of representatives of the orbits. Again, we can define a canonical unit cell $\mathrm{U}_{\mathcal{C}}$ by

$$\mathrm{U}_{\mathcal{C}} := \{(\mathbf{R}_{\lambda_1\vartheta+\lambda_2 2\pi/n}|\lambda_1\tau\mathbf{e})(r,0,0)^T.\ \lambda_1,\lambda_2 \in [0,1),\ r \in [0,\infty)\}.$$

Just as for a crystal, we scale the action of the group $H_{\mathcal{C}}$ by scalars between 0 and 1, while we have an additional degree of freedom in $r \geq 0$. This quantity parametrizes the orbits $C_{\mathbf{e}} \setminus \mathbb{R}^3$ of the group $C_{\mathbf{e}}$ and is thus in analogy to the additional dimension in the case of a two-dimensional crystal in three-dimensional space considered in the last section.

Nanotube structures are particularly easy to describe in cylindrical coordinates about the axis $\mathbf{e}$. The structure $\mathcal{C}$ can be written as

$$\mathcal{S} = \bigcup_{\mathbf{m}\in\mathbf{M}_{\mathcal{C}}} \{\xi(r_{\mathbf{m}}, \varphi_{\mathbf{m}} + \varphi, z_{\mathbf{m}} + z).\ (\varphi,z) \in \mathbf{C}\mathbb{Z}^2\}, \quad \text{where } \mathbf{C} = \begin{pmatrix} \vartheta & \tau \\ 2\pi/n & 0 \end{pmatrix},$$

and $\mathbf{m} = \xi_{\mathbf{e}}(r_{\mathbf{m}}, \varphi_{\mathbf{m}}, z_{\mathbf{m}})$ for $\mathbf{m} \in \mathbf{M}_{\mathcal{C}}$. So, a nanotube structure is crystalline in the two parameters φ and z. We call $\mathbf{C}$ the generator matrix of $\mathcal{C}$. The unit cell can then alternatively be seen as

$$\mathrm{U}_{\mathcal{C}} = \{\xi_{\mathbf{e}}(r, \varphi, z).\ r \in [0, \infty),\ (\varphi, z) \in \mathbf{C}[0, 1)^2\}.$$

Next, we model the electron density ρ_{el} of $\mathcal{C}$. We put the details of the molecule $\mathbf{M}$ into the Schwartz function $\varphi \in \mathcal{S}(\mathbb{R}^3)$ that describes the electron density in a unit cell. We define the electron density

$$\rho_{\mathrm{el}} := \sum_{h \in H_{\mathcal{C}}} (h\varphi). \tag{4.11}$$

To derive a generalization of the von Laue condition, we again made the assumption of a infinite (perfect) structure. In this case, we can – as we did for a crystal – define the canonical unit cell density $\varphi_{\mathcal{C}}$ by

$$\varphi_{\mathcal{C}} := \left(\sum_{h \in H_{\mathcal{C}}} (h\varphi) \right) \big|_{\mathrm{U}_{\mathcal{C}}}.$$

Then our model can be written as

$$\rho_{\mathrm{el}} = \sum_{h \in H_{\mathcal{C}}} (h\varphi_{\mathcal{C}}).$$

Now, let $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,(\alpha,\widehat{z})}$, $|\widehat{z}| \leq \frac{\omega}{c}$, be a twisted wave

$$\mathbf{E}_0(r, \varphi, z) = \mathbf{N} \begin{pmatrix} J_{\alpha-1}(\widehat{r}r)e^{i\varphi} \\ J_{\alpha+1}(\widehat{r}r)e^{-i\varphi} \\ J_{\alpha}(\widehat{r}r) \end{pmatrix} e^{-i(\alpha\varphi + \widehat{z}z)}.$$

The scattering of the incoming electromagnetic field $\widetilde{\mathbf{E}_{\mathrm{in}}}(\mathbf{x}, t) := \mathbf{E}_0(\mathbf{x})e^{-i\omega t}$, $\mathbf{x} \in \mathbb{R}^3$, $t > 0$, by the nanotube structure $\mathcal{C}$ is given by the following theorem.

Theorem 4.5 (Scattering of Twisted Waves). *Let* $\mathbf{s}_0 := \mathbf{R}_\mu(0, \sin(\nu), \cos(\nu))^T$ *(outgoing direction) in spherical coordinates* $\mu \in \mathbb{T}$, $\nu \in [0, \pi]$. *Let* $\mathbf{E}_0$ *be a twisted wave with parameters* $\widehat{r}$ *and* $\widehat{z}$ *as in Theorem 4.1 and* $\rho_{\mathrm{el}} := \sum_{h \in H_{\mathcal{C}}} (h\varphi_{\mathcal{C}})$ *a model for the electron density of a cylindrical objective structure. The radiation transform* $\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}$ *of*

ρ_{el} at $\mathbf{s}_0$ is given by

$$\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}(\mathbf{s}_0) = \frac{2\pi}{|\det(\mathbf{C})|}\mathbf{N}\sum_{\mathbf{c}'\in 2\pi\mathbf{C}^{-T}\mathbb{Z}^2}\delta_{\mathbf{c}'_2}\left(\widehat{z}+\frac{\omega}{c}\cos(\nu)\right)$$
$$\times\int_{[0,\infty)\times\mathbf{C}[0,1)^2}\varphi_{\mathcal{C}}(r,\varphi,z)\begin{pmatrix}\widehat{f}_{\mathbf{c}'_1}(\alpha-1)J_{\alpha-1}(\widehat{r}r)e^{i\varphi}\\ \widehat{f}_{\mathbf{c}'_1}(\alpha+1)J_{\alpha+1}(\widehat{r}r)e^{-i\varphi}\\ \widehat{f}_{\mathbf{c}'_1}(\alpha)J_{\alpha}(\widehat{r}r)\end{pmatrix}e^{-i(\alpha\varphi+(\widehat{z}+\frac{\omega}{c}\cos(\nu))z)}r\mathrm{d}(r,\varphi,z),$$

where $\widehat{f}_{\mathbf{c}'_1}(\alpha) := e^{-i(\mathbf{c}'_1-\alpha)(\varphi-\mu)}J_{\mathbf{c}'_1-\alpha}\left(\frac{\omega}{c}\sin(\nu)r\right)$.

Proof. We start by decomposing the radiation transform integral into integrals over the unit cells of the action of $H_{\mathcal{C}}$.

$$\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}(\mathbf{s}_0) = \int_{\mathbb{R}^3}\mathbf{E}_0(\mathbf{y})e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{y}}\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y} = \int_{\mathrm{U}_{\mathcal{C}}}\sum_{h\in H_{\mathcal{C}}}\mathbf{E}_0(h\mathbf{u})e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot h\mathbf{u}}\rho_{\mathrm{el}}(h\mathbf{u})\mathrm{d}\mathbf{u}.$$

Now for $h=(\mathbf{R}_\eta|\lambda\mathbf{e})\in H_{\mathcal{C}}$, we know from the design equations, that

$$\begin{aligned}\mathbf{E}_0(h\mathbf{u}) &= \mathbf{E}_0((\mathbf{R}_\eta|\lambda\mathbf{e})\mathbf{u}) = \mathbf{R}_\eta\mathbf{R}_{-\eta}\mathbf{E}_0((\mathbf{R}_\eta|\lambda\mathbf{e})\mathbf{u})\\ &= \mathbf{R}_\eta(\mathbf{R}_\eta|\lambda\mathbf{e})^{-1}\mathbf{E}_0(\mathbf{u}) = \mathbf{R}_\eta e^{-i(\alpha\eta+\widehat{z}\lambda)}\mathbf{E}_0(\mathbf{u}).\end{aligned}$$

Since we also know that ρ_{el} is invariant with respect to the action of $H_{\mathcal{C}}$, we find that $\rho_{\mathrm{el}}(h\mathbf{u})=\varphi_{\mathcal{C}}(\mathbf{u})$ for all $h\in H_{\mathcal{C}}$ and all $\mathbf{u}\in\mathrm{U}_{\mathcal{C}}$. Plugging these two equalities into our radiation transform and diagonalizing the matrices $\mathbf{R}_\eta$ by conjugation with a unitary matrix $\mathbf{U}\in\mathrm{U}(3)$ as given in Theorem 4.1, we get

$$\begin{aligned}\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}(\mathbf{s}_0) &= \int_{\mathrm{U}_{\mathcal{C}}}\sum_{(\mathbf{R}_\eta|\lambda\mathbf{e})\in H_{\mathcal{C}}}\mathbf{R}_\eta e^{-i(\alpha\eta+\widehat{z}\lambda)}\mathbf{E}_0(\mathbf{u})e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot(\mathbf{R}_\eta|\lambda\mathbf{e})\mathbf{u}}\varphi_{\mathcal{C}}(\mathbf{u})\mathrm{d}\mathbf{u}\\ &= \int_{\mathrm{U}_{\mathcal{C}}}\varphi_{\mathcal{C}}(\mathbf{u})\mathbf{U}\underbrace{\sum_{(\mathbf{R}_\eta|\lambda\mathbf{e})\in H_{\mathcal{C}}}\begin{pmatrix}e^{i\eta}&&\\&e^{-i\eta}&\\&&1\end{pmatrix}e^{-i(\alpha\eta+\widehat{z}\lambda)}e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot(\mathbf{R}_\eta|\lambda\mathbf{e})\mathbf{u}}}_{=:\mathbf{T}}\mathbf{U}^{-1}\mathbf{E}_0(\mathbf{u})\mathrm{d}\mathbf{u}.\end{aligned}$$

Next, we calculate the diagonal entries of the matrix valued sum $\mathbf{T}$.

Setting $\sigma := (-1,1,0)^T$, these are

$$\mathbf{T}_{jj} = \sum_{(\mathbf{R}_\eta|\lambda\mathbf{e})\in H_{\mathcal{C}}}e^{-i((\alpha+\sigma_j)\eta+\widehat{z}\lambda)}e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot(\mathbf{R}_\eta|\lambda\mathbf{e})\mathbf{u}},\quad j=1,2,3.$$

Now, writing $\mathbf{u} = \xi_{\mathbf{e}}(r, \varphi, z)$ in cylindrical coordinates about $\mathbf{e}$ and identifying $H_{\mathcal{C}}$ with $\mathbf{C}\mathbb{Z}^2$ as above, we have

$$\mathbf{T}_{jj} = \sum_{(\eta,\lambda)\in\mathbf{C}\mathbb{Z}^2} e^{-i((\alpha+\sigma_j)\eta+\widehat{z}\lambda)} e^{-i\frac{\omega}{c}\mathbf{R}_\mu \begin{pmatrix} 0 \\ \sin(\nu) \\ \cos(\nu) \end{pmatrix} \cdot \begin{pmatrix} r\cos(\varphi+\xi) \\ r\sin(\varphi+\xi) \\ z+\lambda \end{pmatrix}}.$$

In the exponent, we get

$$\mathbf{R}_\mu \begin{pmatrix} 0 \\ \sin(\nu) \\ \cos(\nu) \end{pmatrix} \cdot \begin{pmatrix} r\cos(\varphi+\xi) \\ r\sin(\varphi+\xi) \\ z+\lambda \end{pmatrix} = r\sin(\nu)\sin(\varphi+\xi-\mu) + \cos(\nu)(z+\lambda),$$

using the angle difference formula for the sine.

Now, defining the function f on $\mathbb{T}$ by $f(\eta) := e^{-i\frac{\omega}{c}(r\sin(\nu)\sin(\varphi+\eta-\mu)}, \quad \eta \in \mathbb{T}$, we find that

$$\mathbf{T}_{jj} = e^{-i\frac{\omega}{c}\cos(\nu)z} \sum_{(\eta,\lambda)\in\mathbf{C}\mathbb{Z}^2} e^{-i((\alpha+\sigma_j)\eta+(\widehat{z}+\frac{\omega}{c}\cos(\nu))\lambda)} f(\eta).$$

The sum can be interpreted as a Fourier transform of the tempered distribution $\delta_{\mathbf{C}\mathbb{Z}^2} \cdot (f \otimes 1)$ on $\mathbb{T}\times\mathbb{R}$, evaluated at $(\alpha+\sigma_j, \widehat{z}+\frac{\omega}{c}\cos(\nu))$. We use the convolution theorem, the generalized Poisson summation formula and the rule for the Fourier transform of tensor products to get

$$\begin{aligned}
\mathbf{T}_{jj} &= e^{-i\frac{\omega}{c}\cos(\nu)z}\mathcal{F}(\delta_{\mathbf{C}\mathbb{Z}^2}\cdot(f\otimes 1))(\alpha+\sigma_j, \widehat{z}+\frac{\omega}{c}\cos(\nu)) \\
&= e^{-i\frac{\omega}{c}\cos(\nu)z}(2\pi)^{-2}\widehat{\delta_{\mathbf{C}\mathbb{Z}^2}} * (\widehat{f}\otimes\widehat{1}))(\alpha+\sigma_j, \widehat{z}+\frac{\omega}{c}\cos(\nu)) \\
&= e^{-i\frac{\omega}{c}\cos(\nu)z}|\det(\mathbf{C})|^{-1}\delta_{2\pi\mathbf{C}^{-T}\mathbb{Z}^2} * (\widehat{f}\otimes(2\pi\delta_0))(\alpha+\sigma_j, \widehat{z}+\frac{\omega}{c}\cos(\nu)).
\end{aligned}$$

Eventually, we determine the Fourier transform of the function f. f is 2π-periodic, so its Fourier transform for integer arguments is up to a scalar given by its Fourier coefficients

$$\begin{aligned}
\widehat{f}(\alpha) &= \int_{-\pi}^{\pi} f(\eta)e^{-i\alpha\eta}\mathrm{d}\eta = e^{i\alpha(\varphi-\mu)}\int_{-\pi}^{\pi} e^{-i\frac{\omega}{c}\sin(\nu)r\sin(\eta)}e^{-i\alpha\eta}\mathrm{d}\eta \\
&= e^{i\alpha(\varphi-\mu)}J_{-\alpha}\left(\frac{\omega}{c}\sin(\nu)r\right), \quad \alpha\in\mathbb{Z},
\end{aligned}$$

where we used the integral representation of the Bessel function of the first kind. So,

$$\mathbf{T}_{jj} = \frac{2\pi e^{-i\frac{\omega}{c}\cos(\nu)z}}{|\det(\mathbf{C})|} \sum_{\mathbf{c}'\in 2\pi\mathbf{C}^{-T}\mathbb{Z}^2} \underbrace{e^{-i(\mathbf{c}'_1-(\alpha+\sigma_j))(\varphi-\mu)}J_{\mathbf{c}'_1-(\alpha+\sigma_j)}\left(\frac{\omega}{c}\sin(\nu)r\right)}_{=:\widehat{f}_{\mathbf{c}'_1}(\alpha+\sigma_j)} \delta_{\mathbf{c}'_2}\left(\widehat{z}+\frac{\omega}{c}\cos(\nu)\right)$$

Now, we collect our results. Since $\mathbf{N} = \mathbf{U}\mathrm{diag}(\mathbf{c})$, with $\mathbf{c}$ from Theorem 4.1, we find that

$$\mathbf{UTU}^{-1}\mathbf{N} = \mathbf{UTU}^{-1}\mathbf{U}\mathrm{diag}(\mathbf{c}) = \mathbf{UT}\mathrm{diag}(\mathbf{c}) = \mathbf{U}\mathrm{diag}(\mathbf{c})\mathbf{T} = \mathbf{NT},$$

where we used that the diagonal matrices $\mathbf{T}$ and $\mathrm{diag}(\mathbf{c})$ commute.

Thus, writing the integral over $\mathrm{U}_{\mathcal{C}}$ in cylindrical coordinates

$$\begin{aligned}
\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}(\mathbf{s}_0) &= \int_{[0,\infty)\times\mathbf{C}[0,1)^2} \varphi_{\mathcal{C}}(r,\varphi,z)\mathbf{UTU}^{-1}\mathbf{E}_0(r,\varphi,z) r\mathrm{d}(r,\varphi,z) \\
&= \frac{2\pi}{|\det(\mathbf{C})|}\mathbf{N}\int_{[0,\infty)\times\mathbf{C}[0,1)^2} \varphi_{\mathcal{C}}(r,\varphi,z) \sum_{\mathbf{c}'\in 2\pi\mathbf{C}^{-T}\mathbb{Z}^2} e^{-i\frac{\omega}{c}\cos(\nu)z}\delta_{\mathbf{c}'_2}\left(\widehat{z}+\frac{\omega}{c}\cos(\nu)\right) \\
&\times \begin{pmatrix} \widehat{f}_{\mathbf{c}'_1}(\alpha-1)J_{\alpha-1}(\widehat{r}r)e^{i\varphi} \\ \widehat{f}_{\mathbf{c}'_1}(\alpha+1)J_{\alpha+1}(\widehat{r}r)e^{-i\varphi} \\ \widehat{f}_{\mathbf{c}'_1}(\alpha)J_{\alpha}(\widehat{r}r) \end{pmatrix} e^{-i(\alpha\varphi+\widehat{z}z)} r\mathrm{d}(r,\varphi,z) \\
&= \frac{2\pi}{|\det(\mathbf{C})|}\mathbf{N}\sum_{\mathbf{c}'\in 2\pi\mathbf{C}^{-T}\mathbb{Z}^2} \delta_{\mathbf{c}'_2}\left(\widehat{z}+\frac{\omega}{c}\cos(\nu)\right) \\
&\times \int_{[0,\infty)\times\mathbf{C}[0,1)^2} \varphi_{\mathcal{C}}(r,\varphi,z) \begin{pmatrix} \widehat{f}_{\mathbf{c}'_1}(\alpha-1)J_{\alpha-1}(\widehat{r}r)e^{i\varphi} \\ \widehat{f}_{\mathbf{c}'_1}(\alpha+1)J_{\alpha+1}(\widehat{r}r)e^{-i\varphi} \\ \widehat{f}_{\mathbf{c}'_1}(\alpha)J_{\alpha}(\widehat{r}r) \end{pmatrix} e^{-i(\alpha\varphi+(\widehat{z}+\frac{\omega}{c}\cos(\nu))z)} r\mathrm{d}(r,\varphi,z).
\end{aligned}$$

□

Even though the formula we just derived looks quite complicated, it has the main features we were looking for. With respect to $\widehat{z}$ it behaves just as in the crystalline case. When $\widehat{z}$ is the second component of a vector in $2\pi\mathbf{C}^{-T}\mathbb{Z}^2$, we get the Fourier transform with respect to z shifted by $\frac{\omega}{c}\cos(\nu)$. If it is not the second component of a reciprocal lattice vector, the whole expression becomes zero. However, with respect to α, we do not have this nice structure. The formula is a sum over the reciprocal lattice but the transform of the canonical unit cell density is not just a Fourier transform with respect to φ. Instead, the contributions of the different α-values in $2\pi\mathbf{C}^{-T}\mathbb{Z}^2$ mix, and it is not directly visible how to separate them.

2.2. The Twisted von Laue Condition. When looking closely, at a certain point $\mathbf{s}_0$ (remember that $\mathbf{s}_0 = \mathbf{R}_\mu(0,\sin(\nu),\cos(\nu))^T$), the formula simplifies dramatically. Setting $\nu = 0$, i.e. $\mathbf{s}_0 = \mathbf{e}$, we see that

$$e^{-i(\mathbf{c}'_1-(\alpha+\sigma_j))(\varphi-\mu)}J_{\mathbf{c}'_1-(\alpha+\sigma_j)}\left(\frac{\omega}{c}\sin(0)r\right) = \delta_{\mathbf{c}'_1,\alpha+\sigma_j}.$$

The result is a von Laue condition for twisted waves:

Corollary 4.6 (Twisted von Laue Condition). *In axial direction* $\mathbf{s}_0 = \mathbf{e}$*, the radiation transform in Theorem 4.5 for a linearly polarized twisted wave with polarization angle* $\eta \in \mathbb{T}$ *simplifies to*

$$\mathrm{P}(\mathbf{e}^\perp)\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}(\mathbf{e}) = \frac{2\pi}{|\det(\mathbf{C})|}\mathbf{N}(\eta)\sum_{\mathbf{c}'\in 2\pi\mathbf{C}^{-T}\mathbb{Z}^2}\begin{pmatrix}\delta_{\mathbf{c}'+(1,0)}\\ \delta_{\mathbf{c}'-(1,0)}\\ 0\end{pmatrix}\left(\alpha, \widehat{z}+\frac{\omega}{c}\right)$$
$$\times\int_{[0,\infty)\times\mathbf{C}[0,1)^2}\varphi_{\mathcal{C}}(r,\varphi,z)J_{\mathbf{c}'_1}(\widehat{r}r)e^{-i\left(\mathbf{c}'_1\varphi+\mathbf{c}'_2 z\right)}r\mathrm{d}(r,\varphi,z).$$

In particular, the Fourier radiation intensity I *at* $\mathbf{x} = D\mathbf{e}$ *is given by*

$$\mathrm{I}(D\mathbf{e}) = c_{\mathrm{el}}^2\frac{c\varepsilon_0}{2}\frac{(2\pi)^2}{|\det(\mathbf{C})|^2D^2}\left(\frac{c^2\widehat{z}^2}{\omega^2}\cos^2(\eta)+\sin^2(\eta)\right) \tag{4.12}$$
$$\times\sum_{\mathbf{c}'\in 2\pi\mathbf{C}^{-T}\mathbb{Z}^2}\delta_{\mathbf{c}'\pm(1,0)}\left(\alpha,\widehat{z}+\frac{\omega}{c}\right)\left|\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi_{\mathcal{C}}\left(\omega,\mathbf{c}'\right)\right|^2, \tag{4.13}$$

where $\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi$ *denotes the scalar transform*

$$\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi(\omega,\mathbf{c}') := \int_{[0,\infty)\times\mathbf{C}[0,1)^2}\varphi(r,\varphi,z)J_{\mathbf{c}'_1}\left(\sqrt{\frac{\omega^2}{c^2}-\widehat{z}^2}r\right)e^{-i\left(\mathbf{c}'_1\varphi+\mathbf{c}'_2 z\right)}r\mathrm{d}(r,\varphi,z).$$

For unpolarized incoming radiation, the η*-dependent factor reduces to* $\frac{1}{2}\left(\frac{c^2\widehat{z}^2}{\omega^2}+1\right)$.

Proof. The simplified form of the radiation transform follows directly by setting $\nu = 0$ in Theorem 4.5.

The intensity is inferred from (3.28). The field vector of the outgoing radiation is one of the first two columns of $\mathbf{N}(\eta)$, depending on whether $\alpha \in 2\pi\mathbf{C}^{-T}\mathbb{Z}^2 \pm 1$. These are perpendicular to $\mathbf{s}_0 = \mathbf{e}$. Moreover, the two columns have the same absolute value squared:

$$|(\mathbf{N}(\eta)_{i,j})_i|^2 = \frac{c^2}{\omega^2}|c(\eta)|^2 = \frac{1}{2}\left(\frac{c^2\widehat{z}^2}{\omega^2}\cos^2(\eta)+\sin^2(\eta)\right),\quad j=1,2.$$

When the incoming radiation is unpolarized, averaging over $\eta \in \mathbb{T}$ yields the simplified factor. □

This corollary makes it in principle possible to reconstruct ρ_{el} from the intensity measurements in the far-field at the specific point $\mathbf{x} = D\mathbf{e}$ on the symmetry axis, given the transform $\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi_{\mathcal{C}}$ is invertible and the phase problem can be solved. In fact, this transformation is a combination of a Fourier transform, a Fourier series and a Hankel transform and is thus invertible. Where this transform comes from will be seen in Chapter 6.

2.3. Reconstruction of a Nanotube. We demonstrate the twisted von Laue condition by analyzing a nanotube structure as given in the motivating example. There we saw, that with plane wave radiation we cannot make any useful statement about the symmetries of the structure from the diffraction patterns.

Comparing with the measurement techniques for plane wave radiation that were discussed in Chapter 3, we see that fixing the outgoing direction of our measurements, we use the method of variation of radiation parameters. As the plane waves were parametrized by its wave vectors, we parametrize a family of twisted waves by its parameters $(\omega, \alpha, \widehat{z})$:

$$\left\{\mathbf{E}^{(\alpha)}_{\mathbf{k}(\omega,\widehat{z})}\right\}_{(\omega,\alpha,\widehat{z})\in\mathcal{P}}, \quad \mathcal{P} := [0,\infty)\times\mathbb{Z}\times\mathbb{R},$$

where $\mathbf{k}(\omega,\widehat{z}) := (0,\widehat{r},\widehat{z})^T$, $\widehat{r} := \sqrt{\frac{\omega^2}{c^2} - \widehat{z}^2}$ and $|\widehat{z}| \leq \omega$. The observation parameter set is chosen as $\mathcal{O} := \{\mathbf{e}\}$.

The structure we want to analyze with this radiation family is shown in Figure 4.3. It is a nanotube structure with a molecule that consists of 16 atoms and has no rotational symmetry. Since the structure has translational symmetry, it would also be possible to analyze it with plane wave radiation. However, the translational unit cell contains 2336 atoms – a phase problem that cannot be solved from a realistic data set without additional knowledge about the structure.

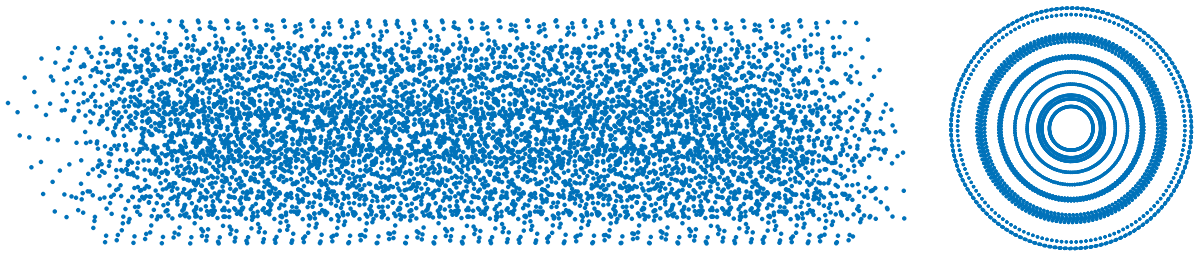


FIGURE 4.3. Side and front view of a nanotube structure with a 16-atom molecule. The sample consists of 6832 atoms, i.e. 427 nanotube unit cells. It also has translational symmetry. The translational unit cell contains 2336 atoms.

As a model for the electron density ρ_{el}, we consider equal Gaussians at the atom positions. Corollary 4.6 tells us, that the scattering amplitude in direction $\mathbf{e}$ considered as a function of the radiation parameters is supported in the set

$$[0,\infty)\times(\mathbf{C}^{\perp}\mathbb{Z}^3 \pm (1,0)^T).$$

The double peak pattern in $(\alpha,\widehat{z})$ is shown in Figure 4.4. The intensity at each of the two peaks at $(\omega, \alpha\pm 1, \widehat{z}+\frac{\omega}{c})$ is equal to a multiple of $\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi_{\mathcal{C}}(\omega,\alpha,\widehat{z})$. So, the reconstruction

problem is to find the canonical unit cell density $\varphi_{\mathcal{C}}$ given the data

$$\left\{\left|\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}(\omega,\alpha,\widehat{z})\right|\right\}, \quad \text{for } (\omega,\alpha,\widehat{z}) \in [0,\infty)\times \mathbf{C}^{\perp}. \tag{4.14}$$

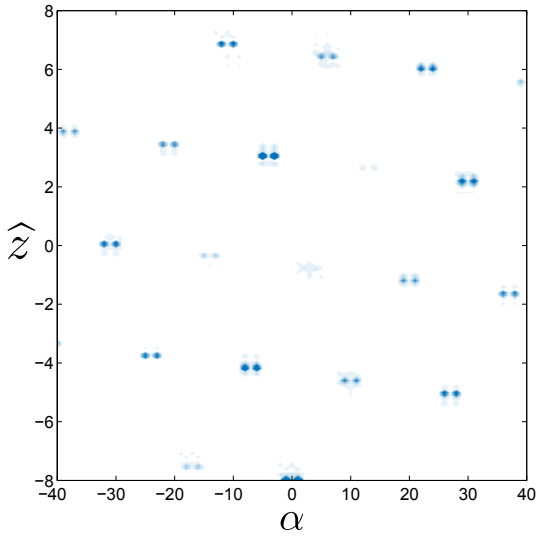


FIGURE 4.4. The scattering amplitude in direction $\mathbf{e}$ for $\frac{\omega}{c} = 8$, plotted in dependence on α and $\widehat{z}$. The double peak pattern predicted by Corollary 4.6 is clearly visible. Note also the shift in $\widehat{z}$. The origin of the reciprocal lattice is shifted to $\alpha = 0$, $\widehat{z} = -8 = -\frac{\omega}{c}$.

From the support, we can directly reconstruct the group $H_{\mathcal{C}}$ as the reciprocal lattice of $\mathbf{C}^{\perp}\mathbb{Z}^3$. This gives us the unit cell $\mathrm{U}_{\mathcal{C}}$ of the structure.

We formulate this scalar phase problem as a set intersection problem as in Chapter 2. First, we define the space of Schwartz functions on the unit cell $\mathrm{U}_{\mathcal{C}}$ as

$$\mathcal{S}(\mathrm{U}_{\mathcal{C}}) := \left\{\varphi : \mathrm{U}_{\mathcal{C}} \to \mathbb{C}.\ \sum_{h\in H_{\mathcal{C}}} (h\varphi) \in C^{\infty}(\mathbb{R}^3),\ r \mapsto r^{\beta}\varphi(r,\varphi,z) \in L^{\infty} \text{ for } \beta \in \mathbb{N}\right\}.$$

Then, consider the following subsets of $\mathcal{S}(\mathrm{U}_{\mathcal{C}})$:

$$\mathcal{S}^{\geq 0}(\mathrm{U}_{\mathcal{C}}) := \{\varphi \in \mathcal{S}(\mathrm{U}_{\mathcal{C}}).\ \varphi \geq 0\},$$
$$\mathcal{S}_{\mathrm{A}}(\mathrm{U}_{\mathcal{C}}) := \{\varphi \in \mathcal{S}(\mathrm{U}_{\mathcal{C}}).\ |\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi| = A\},$$

where $A := |\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi_{\mathcal{C}}|$ is the data. Then the phase retrieval problem is to find an element of the set $\mathcal{S}^{\geq 0}(\mathrm{U}_{\mathcal{C}}) \cap \mathcal{S}_{\mathrm{A}}(\mathrm{U}_{\mathcal{C}})$.

Defining the projections

$$\begin{aligned} \mathrm{p}_{\geq 0} &: \mathcal{S}(\mathrm{U}_{\mathcal{C}}) \to \mathcal{S}^{\geq 0}(\mathrm{U}_{\mathcal{C}}),\ \varphi \mapsto \varphi \cdot \mathbf{1}_{\{\varphi \geq 0\}}, \\ \mathrm{p}_{\mathrm{A}} &: \mathcal{S}(\mathrm{U}_{\mathcal{C}}) \to \mathcal{S}_{\mathrm{A}}(\mathrm{U}_{\mathcal{C}}),\ \varphi \mapsto \mathcal{W}^{-1}_{C_{\mathbf{e}}/H_{\mathcal{C}}} \left(\mathrm{A}(e^{i\zeta_\varphi}\mathbf{1}_{\{\varphi \neq 0\}} + \mathbf{1}_{\{\varphi = 0\}})\right), \end{aligned}$$

where ζ_φ is the phase function of $\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi$, i.e. $\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi = |\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi|e^{i\zeta_\varphi}$.

Using these projections, we can generalize the phase retrieval algorithms we introduced in Chapter 2. To reconstruct the considered structure, we use the following difference map algorithm

$$\varphi_{n+1} := \varphi_n - \mathrm{p}_{\geq 0}\varphi_n + \mathrm{p}_{\mathrm{A}}(2\mathrm{p}_{\geq 0} - \mathrm{id})\varphi_n, \quad n \in \mathbb{N}, \tag{DM$_{\mathcal{C}}$}$$

where we choose φ_0 with an arbitrary initial phase function ζ_0, i.e. $\varphi_0 := \mathcal{W}^{-1}_{C_{\mathbf{e}}/H_{\mathcal{C}}}(\mathrm{A}e^{i\zeta_0})$.

The reconstruction of a radial slice of 3×3 unit cells is shown in Figure 4.5. It is close to the original up to an inversion. This is due to the inversion ambiguity we found in our discussion of the phase problem in Chapter 1. The transform $\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}$ is a Fourier transform in $(\alpha, \widehat{z})$, resulting in this possibility. It is an inversion in the cylindrical coordinates (φ, z). Now, $\xi_{\mathbf{e}}(r, -\varphi, -z) = (r\cos(-\varphi), r\sin(-\varphi), -z)^T = (r\cos(\varphi), -\sin(\varphi), -z)^T$, showing that this is a rotation by 180° about an axis perpendicular to $\mathbf{e}$.

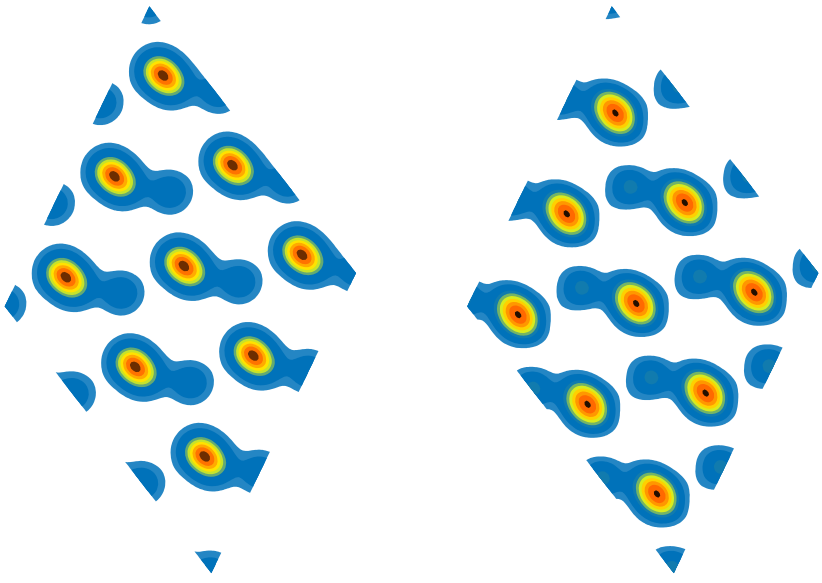


FIGURE 4.5. Reconstruction of a radial slice of 3×3 nanotube unit cells by the difference map algorithm (DM$_{\mathcal{C}}$). The original density is shown on the left. The reconstruction on the right is very close to the original density up to an inversion. This shows the analog of the inversion ambiguity of classical phase retrieval.

The interesting part of the reconstruction is the radial direction. In this direction, the transform $\mathcal{W}_{C_\mathbf{e}/H_\mathcal{C}}$ is a Hankel transform of order α. Because the Bessel functions are real functions, the phase problem in this dimension is actually only a sign problem. In Figure 4.6, the radial distribution φ_r of the reconstructed function is plotted against the original. This quantity is defined as follows

$$\varphi_r(r) := \int_{\mathbf{C}^\perp[0,1)^2} \varphi_\mathcal{C}(r,\varphi,z)\mathrm{d}(\varphi,z). \tag{4.15}$$

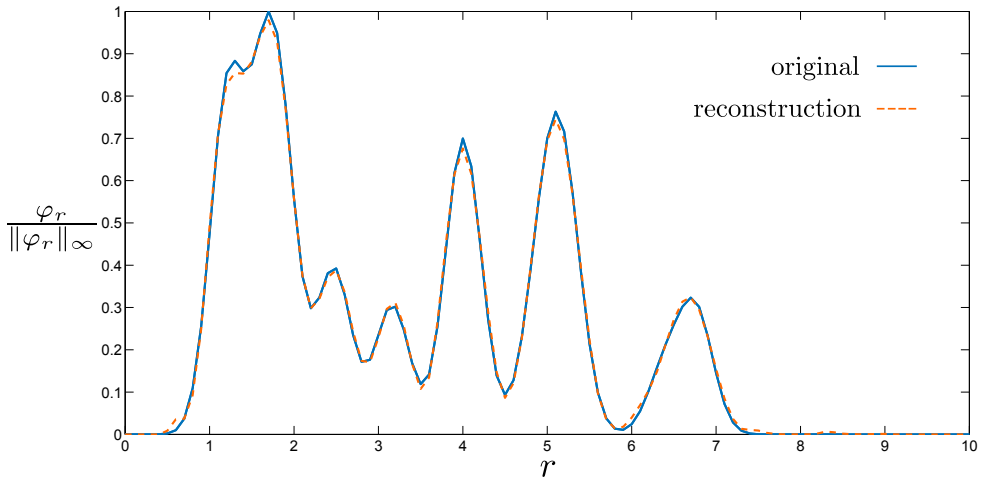


FIGURE 4.6. Reconstruction of the average radial distribution φ_r given in (4.15).

The reconstruction is in good agreement with the original, showing that the difference map algorithm can also be used for nanotube phase problems.

This example also shows the potential of twisted wave diffraction for the analysis of nanotube structures that cannot be analyzed with plane waves.

CHAPTER 5

Symmetry-Adapted Waves

Having successfully solved the design equations for nanotube structures in Chapter 4, we solve the case of general abelian design groups next. The main idea is to utilize, and adapt to our context, tools from representation theory which appear to go back to E. Wigner [Wig31] in the context of quantum mechanics.

First, we study the structure of abelian design groups. By utilizing the structure theory for compactly generated groups, we coarsly classify these groups in Proposition 5.3. It turns out that closed abelian isometry groups are either compact, of nanotube type, or belong to a quite general class of translational structures. To keep the account transparent, we focus on a subset of the translational class, noting that the remaining cases are of minor interest and can be worked out similarly.

The structure of the radiation spaces $\mathrm{R}_b^{\omega,\chi}(G)$ for an abelian design group G and $\chi \in \widehat{G}$ is analyzed next. For this purpose, we introduce the Wigner projections (see [Wig31]) for compact abelian design groups K. These map time-harmonic radiation to the invariant subspaces $\mathrm{R}_b^{\omega,\chi}(K)$, resulting in Proposition 5.4 that gives a direct sum decomposition of R_b^{ω} with respect to K. Since the spaces $\mathrm{R}_b^{\omega,\chi}(K)$ can be quite big for small groups K, we identify an important subset that will turn out to be the right choice for structure analysis – the symmetry-adapted waves.

For non-compact design groups, the Wigner projections cannot be defined in the same way as in the compact case. Therefore, we introduce a tool we call the Zak transform as it is a generalization of the classic Zak transform (see [Zak67]). This transform allows to decompose time-harmonic radiation into its invariant parts in a distributional sense. Even though we cannot give a decomposition of R_b^{ω}, we are able to define the symmetry-adapted waves for abelian design groups using the Zak transform. They turn out to be variants of plane waves, twisted waves and compact symmetry-adapted waves (Proposition 5.13).

1. The Structure of Abelian Design Groups

To design radiation for abelian design groups, we first need to understand these groups, i.e. closed abelian isometry groups. First, we use a structure theorem for compactly generated locally compact abelian groups to decompose the design group into a direct product of simple factors. This decomposition enables us to give a coarse classification of

abelian design groups. We use this classification later to define the central objects – the symmetry-adapted waves – for general abelian design groups.

Lemma 5.1 (Structure of Abelian Design Groups). *An abelian design group* $G \leq$
$frac\omega c$ *can be decomposed as follows:*

$$G = K \times \prod_{j=1}^{n} R_j \times \prod_{k=1}^{m} Z_k, \tag{5.1}$$

where $n, m \in \mathbb{N}$, $R_j \cong \mathbb{R}$, $j = 1, \dots, n$, $Z_k \cong \mathbb{Z}$, $k = 1, \dots, m$, *and* $K \leq \mathrm{E}(3)$ *is a closed compact abelian group.*

Moreover, the groups R_j, $j = 1, \dots, n$, *are of one of the following forms*

(R1) $R_j = \{(\mathbf{I}|\tau a\mathbf{e}).\ a \in \mathbb{R}\}$,
with $\mathbf{e} \in \mathbb{S}^2$, $\tau \neq 0$.

(R2) $R_j = (\mathbf{I}|\mathbf{c}_0)\{(\mathbf{R}_{\lambda a}|\tau a\mathbf{e}).\ a \in \mathbb{R}\}(\mathbf{I}|-\mathbf{c}_0)$,
with $\mathbf{e} \in \mathbb{S}^2$, $\lambda, \tau \neq 0$, $\mathbf{c}_0 \in \mathbf{e}^{\perp}$.

The groups Z_k, $k = 1, \dots, m$, *are of one of the following forms:*

(Z1) $Z_k = \{(\mathbf{I}|\tau j\mathbf{e}).\ j \in \mathbb{Z}\}$,
with $\mathbf{e} \in \mathbb{S}^2$, $\tau \neq 0$.

(Z2) $Z_k = (\mathbf{I}|\mathbf{c}_0)\{(\mathbf{R}_{\lambda j}|\tau j\mathbf{e}).\ j \in \mathbb{Z}\}(\mathbf{I}|-\mathbf{c}_0)$
with $\mathbf{e} \in \mathbb{S}^2$, $\lambda, \tau \neq 0$, $\mathbf{c}_0 \in \mathbf{e}^{\perp}$.

(Z3) $Z_k = (\mathbf{I}|\mathbf{c}_0)\{((\mathbf{I} - 2\mathbf{e}_{\perp} \otimes \mathbf{e}_{\perp})^j|\tau j\mathbf{e}).\ j \in \mathbb{Z}\}(\mathbf{I}|-\mathbf{c}_0)$
with $\mathbf{e}, \mathbf{e}_{\perp} \in \mathbb{S}^2$, $\mathbf{e} \cdot \mathbf{e}_{\perp} = 0$, $\tau \neq 0$, $\mathbf{c}_0 \in \mathbb{R}\mathbf{e}_{\perp}$.

Proof. The group E(3) is a compactly generated locally compact group (generated by the set $\{(\mathbf{Q}|\mathbf{c}).\ \mathbf{Q} \in \mathrm{O}(3),\ |\mathbf{c}| \leq 1\}$, for example). Thus, every abelian subgroup is as well compactly generated.

By the structure theorem for compactly generated locally compact abelian groups (see [Rei68], 2.9 (i), p. 97), the design group G is isomorphic to a direct product of simpler groups as follows

$$G \cong \widetilde{K} \times \mathbb{R}^n \times \mathbb{Z}^m, \quad n, m \in \mathbb{N},\ \widetilde{K} \text{ closed compact abelian.} \tag{5.2}$$

Given an isomorphism $\iota : G \to \widetilde{K} \times \mathbb{R}^n \times \mathbb{Z}^m$, we set

$$R_j := \iota^{-1}(\{e_{\widetilde{K}}\} \times (\underbrace{0, \dots, 0}_{j-1}, \mathbb{R}, 0, \dots, 0) \times \{0\}^m),\ j = 1, \dots, n,$$
$$Z_k := \iota^{-1}(\{e_{\widetilde{K}}\} \times \{0\}^n \times (\underbrace{0, \dots, 0}_{k-1}, \mathbb{R}, 0, \dots, 0)),\ k = 1, \dots, m,$$
$$K := \iota^{-1}(\widetilde{K} \times \{0\}^{n+m}),$$

where $e_{\widetilde{K}}$ is the neutral element of $\widetilde{K}$. These definitions yield

$$G = \iota^{-1}(\widetilde{K} \times \mathbb{R}^n \times \mathbb{Z}^m) = K \times \prod_{j=1}^{n} R_j \times \prod_{k=1}^{m} Z_k$$

with $R_j \cong \mathbb{R}$, $j = 1, \dots, n$, $Z_k \cong \mathbb{Z}$, $k = 1, \dots, m$ and $K \leq \mathrm{E}(3)$ closed compact abelian.

Let $1 \leq j \leq n$ and $\iota_j : \mathbb{R} \to R_j$ be an isomorphism. Then there are continuous functions $\mathbf{Q} : \mathbb{R} \to \mathrm{O}(3)$ and $\mathbf{c} : \mathbb{R} \to \mathbb{R}^3$, s.t. $\iota_j(a) = (\mathbf{Q}(a)|\mathbf{c}(a))$ for all $a \in \mathbb{R}$. So,

$$\begin{aligned}(\mathbf{Q}(a+b)|\mathbf{c}(a+b)) &= \iota_j(a+b) = \iota_j(a)\iota_j(b)\\ &= (\mathbf{Q}(a)\mathbf{Q}(b)|\mathbf{Q}(a)\mathbf{c}(b) + \mathbf{c}(a))\\ &= (\mathbf{Q}(b)\mathbf{Q}(a)|\mathbf{Q}(b)\mathbf{c}(a) + \mathbf{c}(b))\end{aligned}$$

for all $a, b \in \mathbb{R}$, using commutativity of R_j for the last equation.

In particular, we get $\mathbf{Q}(a+b) = \mathbf{Q}(a)\mathbf{Q}(b)$ for $a, b \in \mathbb{R}$. So, $\mathbf{Q} : \mathbb{R} \to \mathrm{O}(3)$ is a real (orthogonal) representation of the group $\mathbb{R}$ on $\mathbb{R}^3$. Consequently, there is a $\lambda \in \mathbb{R}$ and an $\mathbf{e} \in \mathbb{S}^2$, s.t. $\mathbf{Q}(a) = \mathbf{R}_{\lambda a}$ for $a \in \mathbb{R}$, where as usual, $\mathbf{R}_{\lambda a}$ is the rotation about the axis $\mathbb{R}\mathbf{e}$ by the angle λa.

We decompose $\mathbf{c} : \mathbb{R} \to \mathbb{R}^3$ orthogonally w.r.t. the axis $\mathbf{e}$: $\mathbf{c}(a) = \mathbf{c}_{\mathbf{e}}(a) + \mathbf{c}_{\perp}(a)$, where $\mathbf{c}_{\mathbf{e}}(a) \in \mathbb{R}\mathbf{e}$ and $\mathbf{c}_{\perp}(a) \in \mathbf{e}^{\perp}$ for all $a \in \mathbb{R}$. Then, in the translation component of $\iota_j(a+b)$ we find that

$$\mathbf{c}(a+b) = \mathbf{Q}(a)\mathbf{c}(b) + \mathbf{c}(a) = \mathbf{Q}(b)\mathbf{c}(a) + \mathbf{c}(b)$$

for $a, b \in \mathbb{R}$. Using $\mathbf{Q}(a) = \mathbf{R}_{\lambda a}$, the decomposition of $\mathbf{c}$ and the fact that $\mathbf{R}_{\lambda a}\mathbf{c}_{\mathbf{e}}(a) = \mathbf{c}_{\mathbf{e}}(a)$ for $a \in \mathbb{R}$, we find that this is true if and only if

$$\begin{aligned}&\mathbf{c}_{\mathbf{e}}(a+b) = \mathbf{c}_{\mathbf{e}}(a) + \mathbf{c}_{\mathbf{e}}(b), \quad \text{and}\\ &\mathbf{c}_{\perp}(a+b) = \mathbf{R}_{\lambda a}\mathbf{c}_{\perp}(b) + \mathbf{c}_{\perp}(a) = \mathbf{R}_{\lambda b}\mathbf{c}_{\perp}(a) + \mathbf{c}_{\perp}(b)\end{aligned}$$

for all $a, b \in \mathbb{R}$. The first equation says that $\mathbf{c}_{\mathbf{e}} : \mathbb{R} \to \mathbb{R}\mathbf{e}$ is linear (using continuity), so there is a $\tau \in \mathbb{R}$, s.t. $\mathbf{c}_{\mathbf{e}}(a) = \tau a\mathbf{e}$ for $a \in \mathbb{R}$. From the second equations, we get $(I - \mathbf{R}_{\lambda a})\mathbf{c}_{\perp}(a) = (I - \mathbf{R}_{\lambda b})\mathbf{c}_{\perp}(b)$. We need to distinguish two cases.

When $\lambda = 0$, we get $\mathbf{c}_\perp(a+b) = \mathbf{c}_\perp(a) + \mathbf{c}_\perp(b)$. So, together with the form of $\mathbf{c}_\mathbf{e}$, it follows that there is a $\tau \in \mathbb{R}$ and an $\mathbf{e} \in \mathbb{S}^2$, s.t. $\mathbf{c}(a) = a\tau\mathbf{e}$. Since ι_j is injective, we need $\tau \neq 0$. This yields the case (R1).

When $\lambda \neq 0$, we can determine $\mathbf{c}_\perp$ with the following trick. At the point $b = \frac{\pi}{\lambda}$, we find $\mathbf{Q}(\frac{\pi}{\lambda}) = \mathbf{R}_\pi = -\mathrm{id}_{\mathbf{e}^\perp}$. So, for all $a \in \mathbb{R}$:

$$(\mathbf{I} - \mathbf{R}_{\lambda a})\mathbf{c}_\perp\left(\frac{\pi}{\lambda}\right) = 2\mathbf{c}_\perp(a).$$

So, $\mathbf{c}_\perp(a) = \frac{1}{2}(\mathbf{I} - \mathbf{R}_{\lambda a})\mathbf{c}_\perp(\frac{\pi}{\lambda})$. When setting $\mathbf{c}_0 := \frac{1}{2}\mathbf{c}_\perp(\frac{\pi}{\lambda})$, we get by direct calculation that for $a \in \mathbb{R}$

$$(\mathbf{Q}(a)|\mathbf{c}(a)) = (\mathbf{I}|\mathbf{c}_0)(\mathbf{R}_{\lambda a}|\tau a\mathbf{e})(\mathbf{I}| - \mathbf{c}_0).$$

Injectivity of ι_j again yields the restriction $\tau \neq 0$. Thus, we established (R2).

The special form of the factors $Z_k \cong \mathbb{Z}$, $k = 1, \ldots, m$, is easier to proof. Let $1 \leq k \leq m$ and $\tilde{\iota}_k : \mathbb{Z} \to Z_k$ be an isomorphism. Then

$$\tilde{\iota}_k(j) = \tilde{\iota}_k(1)^j \quad \text{for all } j \in \mathbb{Z}.$$

So, it suffices to determine $\tilde{\iota}_k(1)$. Since $\tilde{\iota}_k$ is injective, the element $\tilde{\iota}_k(1)$ is of infinite order. This restricts to the following three cases. $\tilde{\iota}(1)$ is either a translation, a screw displacement or a glide reflection (see [DEJ]). Closedness of Z_k excludes the additional cases of $\tilde{\iota}_k(1)$ being a rotation or improper rotation by an angle that is not in $2\pi\mathbb{Q}$.

In the first case, $\tilde{\iota}(1) = (\mathbf{I}|\mathbf{c})$ for some $\mathbf{c} \neq 0$. This is case (Z1), choosing $\mathbf{e} = \mathbf{c}/|\mathbf{c}|$ and $\tau = |\mathbf{c}| \neq 0$.

In the second case, $\tilde{\iota}(1) = (\mathbf{Q}|\mathbf{c})$ with $\det \mathbf{Q} = 1$ and $\mathbf{c} \cdot \mathbf{e} \neq 0$, where $\mathbf{e} \in \mathbb{S}^2$ is on the axis of $\mathbf{Q}$. This yields case (Z2) analog to the similar representation of the factors isomorphic to $\mathbb{R}$.

Finally, when $\tilde{\iota}(1)$ is a glide reflection, there is a $\mathbf{e}_\perp \in \mathbb{S}^2$ and a $\mathbf{c} \in \mathbb{R}^3 \setminus \{0\}$ with $\mathbf{c}$ not parallel to $\mathbf{e}_\perp$, s.t. $\tilde{\iota}(1) = (\mathbf{I} - 2\mathbf{e}_\perp \otimes \mathbf{e}_\perp|\mathbf{c})$. Decomposing $\mathbf{c} = \mathbf{c}_\perp + \widetilde{\mathbf{c}}$ with $\mathbf{c}_\perp \in \mathbb{R}\mathbf{e}_\perp$ and $\widetilde{\mathbf{c}} \cdot \mathbf{e}_\perp = 0$, and setting $\mathbf{c}_0 := \frac{1}{2}\mathbf{c}_\perp$, we find by direct calculation that

$$(\mathbf{Q}|\mathbf{c}) = (\mathbf{I}|\mathbf{c}_0)(\mathbf{I} - 2\mathbf{e}_\perp \otimes \mathbf{e}_\perp|\widetilde{\mathbf{c}})(\mathbf{I}| - \mathbf{c}_0).$$

Setting $\tau := |\widetilde{\mathbf{c}}|$ and $\mathbf{e} := \widetilde{\mathbf{c}}/\tau$, this is case (Z3) and completes the proof. □

This lemma shows that the non-compact factors of the group G are either continuous groups of translations or screw displacements or discrete groups that are generated by a translation, a screw displacement or a glide reflection.

We want to give a more detailed classification of abelian design groups. For this purpose, we first proof the following lemma which was already used in Chapter 4 to write nanotube structures in their canonical form.

Lemma 5.2 (Closed Subgroups of $C_{\mathbf{e}}$). *Every closed subgroup G of $C_{\mathbf{e}}$, $e \in \mathbb{S}^2$, is of the form*

$$G = K \times S, \tag{5.3}$$

where K is a subgroup of the group $R_{\mathbf{e}}$ of all rotations about $\mathbb{R}\mathbf{e}$ and S is either trivial or isomorphic to $\mathbb{R}$ or $\mathbb{Z}$ and consists of translations or screw displacements.

Proof. Since $G \leq C_{\mathbf{e}}$, there are sets $T \subseteq \mathbb{T}$ and $R \subseteq \mathbb{R}$, s.t.

$$G = \{(\mathbf{Q}_G(a)|\mathbf{c}_G(a)).\ a \in T \times R\}.$$

Let $K := \{(\mathbf{Q}_G(a)|\mathbf{c}_G(a)).\ \mathbf{c}_G(a) = 0\}$. Obviously, K is a subgroup of G as well as of $R_{\mathbf{e}}$. When $K = G$, then we are done.

When there is an element in G with non-trivial translational part, using Lemma 5.1, we get that $G = K \times S$, where S is a direct product of isometry groups with at least one non-compact factor.

We will show that $S \cong \mathbb{R}$ or $S \cong \mathbb{Z}$. The result is then a consequence of Lemma 5.1.

First, assume that S is not discrete. Then it has a subgroup isomorphic to $\mathbb{R}$ by Lemma 5.1 that is of the form

$$R = \{(\mathbf{R}_{\lambda a}|\tau a\mathbf{e}).\ a \in \mathbb{R}\},\ \lambda \in \mathbb{R},\ \tau \neq 0,\ \mathbf{e} \in \mathbb{S}^2.$$

If S contains a further element $g = (\mathbf{R}_\mu|\delta\mathbf{e}) \notin R$, then $\delta \neq 0$, because else $g \in K$. Then for all $a \in \mathbb{R}$

$$\begin{aligned}(\mathbf{R}_{\lambda a}|\tau a\mathbf{e})(\mathbf{R}_\mu|\delta\mathbf{e}) &= (\mathbf{R}_{\lambda a+\mu}|(\tau a+\delta)\mathbf{e})\\ &= (\mathbf{R}_{\mu-\lambda\delta/\tau}|0)(\mathbf{R}_{\lambda(a+\delta/\tau)}|\tau(a+\delta/\tau)\mathbf{e}) \in S.\end{aligned}$$

So, $(\mathbf{R}_{\mu-\lambda\delta/\tau}|0) \in S$, hence $\mu = \lambda\delta/\tau$. But then $g = (\mathbf{R}_{\lambda\delta/\tau}|\tau\delta/\tau\mathbf{e}) \in R$ in contradiction to $g \notin R$. This shows that $S \cong \mathbb{R}$ if it is not discrete.

So, assume that S is discrete. Let $g = (\mathbf{R}_\lambda|\tau\mathbf{e}) \in S$ be an element with $\tau > 0$ minimal, i.e. for all $g' = (\mathbf{R}_{\lambda'}|\tau'\mathbf{e}) \in S$ we have $|\tau'| \geq \tau$.

We show that $S = \{g^j.\ j \in \mathbb{Z}\}$. Assume there is a $h = (\mathbf{R}_\mu|\delta\mathbf{e}) \in S \setminus \{g^j.\ j \in \mathbb{Z}\}$. Then for all $j \in \mathbb{Z}$

$$\begin{aligned}(\mathbf{R}_\mu|\delta\mathbf{e})(\mathbf{R}_{j\lambda}|j\tau\mathbf{e}) &= (\mathbf{R}_{j\lambda+\mu}|(j\tau+\delta)\mathbf{e})\\ &= (\mathbf{R}_{\mu-\lambda\delta/\tau}|0)(\mathbf{R}_{\lambda(j+\delta/\tau)}|\tau(j+\delta/\tau)\mathbf{e}) \in S.\end{aligned}$$

Again, $\mu = \lambda\delta/\tau$ follows, s.t. $h = (\mathbf{R}_{\lambda\delta/\tau}|\delta\mathbf{e})$.

When $\delta = j\tau$ for some $j \in \mathbb{Z}$ then $h \in S$ in contradiction to our selection of h.

So, $\delta \notin \mathbb{Z}\tau$. Let $k := \lfloor \delta/\tau \rfloor$, then

$$hg^{-k} = (\mathbf{R}_{\lambda\delta/\tau}|\delta\mathbf{e})(\mathbf{R}_{-k\lambda}| - k\tau\mathbf{e}) = (\mathbf{R}_{\lambda\delta/\tau - k\lambda}|(\delta - k\tau)\mathbf{e}) \in S.$$

But $\delta - k\tau < \tau$ in contradiction to the minimality of τ. So $S \cong \mathbb{Z}$ in this case.

Lemma 5.1 yields the desired form of the factor S. □

We use this lemma to refine the structure of closed abelian isometry groups. The following proposition coarsly classifies these groups into three classes.

Proposition 5.3 (Coarse Classification of Abelian Design Groups). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group. Then G can be written in one of the following forms:*

(1) $G = K \times \prod_{j=1}^{n} R_j \times \prod_{k=1}^{m} Z_k$,
where $R_j \cong \mathbb{R}$, $j = 1, \ldots, n$, and $Z_k \cong \mathbb{Z}$, $k = 1, \ldots, m$, $n + m \leq 3$, are either translation groups, glide reflection groups or screw displacement groups with isogonal point group of order 2, and K is closed and compact.

(2) $G = K \times S$,
where $S \cong \mathbb{R}$ or $S \cong \mathbb{Z}$ is a screw displacement group with order greater than 2, and K is closed and compact.

(3) $G = K$,
where K is closed and compact.

Proof. We compose G as in Lemma 5.1:

$$G = K_0 \times \prod_{j=1}^{n} R_j \times \prod_{k=1}^{m} Z_k, \qquad (*)$$

where $R_j \cong \mathbb{R}$, $j = 1, \ldots, n$, $Z_k \cong \mathbb{Z}$, $k = 1, \ldots, m$, K_0 compact, are closed isometry groups.

Now, assume that G is not of type (1) or (3). Then one of the non-compact factors of G in $(*)$ is a group of screw displacements about an axis $\mathbb{R}\mathbf{e}$, $\mathbf{e} \in \mathbb{S}^2$. We call this factor S_0. In addition, the isogoal point group Iso_{S_0} of S_0 is of order greater or equal than 3.

When $A \leq \mathrm{E}(3)$ is another non-compact factor of G, then every element $(\mathbf{Q}_A|\mathbf{c}_A) \in A$ needs to commute with every element $(\mathbf{Q}_S|\mathbf{c}_S) \in S_0$, i.e.

$$(\mathbf{Q}_A\mathbf{Q}_S|\mathbf{Q}_A\mathbf{c}_S + \mathbf{c}_A) = (\mathbf{Q}_S\mathbf{Q}_A|\mathbf{Q}_S\mathbf{c}_A + \mathbf{c}_S). \qquad (**)$$

We set the origin, s.t. $(\mathbf{Q}_S|\mathbf{c}_S) = (\mathbf{R}_\lambda|\tau_S\mathbf{e})$ for some $\lambda, \tau_S \in \mathbb{R}$ and consider the different possibilities for the factor A:

- If A is a group of translations, i.e. $\mathbf{Q}_A = \mathbf{I}$ for all elements of A, then $(**)$ says that $(\mathbf{Q}_S|\mathbf{c}_S + \mathbf{c}_A) = (\mathbf{Q}_S|\mathbf{Q}_S\mathbf{c}_A + \mathbf{c}_S)$, showing that $\mathbf{Q}_S\mathbf{c}_A = \mathbf{c}_A$. So, every translation in A is of the form $(\mathbf{Q}_A|\mathbf{c}_A) = (\mathbf{I}|\tau_A\mathbf{e})$ for some $\tau_A \in \mathbb{R}$, i.e. all translational factors of G share the axis of S_0.
- If A is a group generated by a glide reflection

$$(\mathbf{Q}_A|\mathbf{c}_A) = (\mathbf{I} - 2\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp|2\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp\mathbf{c}_0 + \tau_A\widetilde{\mathbf{e}}),$$

$\tau_A \neq 0$, $\widetilde{\mathbf{e}}, \widetilde{\mathbf{e}}_\perp \in \mathbb{S}^2$, $\widetilde{\mathbf{e}}_\perp \cdot \widetilde{\mathbf{e}} = 0$, $\mathbf{c}_0 \in \mathbb{R}^3$. Then the orthogonal part of $(**)$ yields

$$(\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp)\mathbf{Q}_S = \mathbf{Q}_S(\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp). \qquad (***)$$

In particular, applying this to the vector $\widetilde{\mathbf{e}}$, we get

$$(\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp)\mathbf{Q}_S\widetilde{\mathbf{e}} = \mathbf{Q}_S(\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp)\widetilde{\mathbf{e}} = 0.$$

Consequently, $\mathbf{Q}_S\widetilde{\mathbf{e}} \in \widetilde{\mathbf{e}}_\perp^\perp$, showing that either $\mathbf{e} = \pm\widetilde{\mathbf{e}}$ or $\mathbf{e} = \pm\widetilde{\mathbf{e}}_\perp$.

In the first case, there is a $(\mathbf{Q}_S|\mathbf{c}_S) \in S_0$, s.t. $\mathbf{Q}_S(\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp)\widetilde{\mathbf{e}}_\perp = \mathbf{Q}_S\widetilde{\mathbf{e}}_\perp \notin \mathbf{R}\widetilde{\mathbf{e}}_\perp$, because Iso_{S_0} is of order ≥ 3. So, we can decompose $\mathbf{Q}_S\widetilde{\mathbf{e}}_\perp = \mathbf{v}_\perp + \mathbf{v}$, $\mathbf{v}_\perp \in \mathbb{R}\widetilde{\mathbf{e}}_\perp$, $\mathbf{v} \cdot \widetilde{\mathbf{e}}_\perp = 0$, $\mathbf{v} \neq 0$. But then $(\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp)\mathbf{Q}_S\widetilde{\mathbf{e}}_\perp = (\widetilde{\mathbf{e}}_\perp \otimes \widetilde{\mathbf{e}}_\perp)(\mathbf{v}_\perp + \mathbf{v}) = \mathbf{v}_\perp$ in contradiction to $(***)$.

In the second case, comparing the translational parts of $(**)$, we find that $(\mathbf{R}_\lambda - \mathbf{I})\tau_A\widetilde{\mathbf{e}} = -2\tau_S\mathbf{e}$. Since $\mathbf{e} \neq 0$, this is true if and only if $\mathbf{R}_\lambda\widetilde{\mathbf{e}} = -\widetilde{\mathbf{e}}$ for all elements of S_0, what contradicts $\mathbf{e} = \pm\widetilde{\mathbf{e}}_\perp$. So, G has no glide reflection factors.
- If A is a group of screw displacements, then Iso_A needs to be an abelian subgroup of the group of rotations about the axis $\mathbf{e}$, because these are the only elements of SO(3) that commute with Iso_{S_0}. So, every screw discplacement factor shares the axis of S_0.

In addition, when the elements of A are of the form $(\mathbf{I}|\mathbf{c}_0)(\mathbf{R}_\mu|\delta\mathbf{e})(\mathbf{I}|-\mathbf{c}_0)$, then a comparison of the translational parts shows that $\mathbf{c}_0 \in \mathbb{R}\mathbf{e}$.

In summary, we have shown that all the factors R_j, $j = 1, \ldots, n$, Z_k, $k = 1, \ldots, m$, are groups of translations along or screw displacements about $\mathbb{R}\mathbf{e}$. This shows that

$$\prod_{j=1}^{n} R_j \times \prod_{k=1}^{m} Z_k \leq C_{\mathbf{e}}.$$

By Lemma 5.2, we get that $\prod_{j=1}^{n} R_j \times \prod_{k=1}^{m} Z_k = \widetilde{K} \times S$ for some closed compact $\widetilde{K}$ and a group of screw displacements S. Defining $K := K_0 \times \widetilde{K}$, we get $G = K \times S$. □

Proposition 5.3 shows that abelian design groups are either compact, of nanotube type or belong to class (1) which are essentially translational groups. This last class can have

non-compact factors that are either generated by glide reflections or screw displacements by 180°. These additional non-compact symmetries are of minor interest, because they have translational subgroups of order 2. Because of that we will in the following focus on the subset of class (1) with all non-compact factors being translation groups. This will keep the presentation more transparent.

2. Wigner-Projections and the Zak Transform

To find a general method for the construction of solutions to the design equations, we have a second look at the Fourier representation (4.1) of twisted waves

$$\mathbf{E}_0(\mathbf{x}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\alpha\widehat{\varphi}}\mathbf{R}_{-\widehat{\varphi}}\mathbf{n}_0 e^{-i\mathbf{R}_{-\widehat{\varphi}}\mathbf{k}_0\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}, \quad \mathbf{k}_0 = (0,\widehat{r},\widehat{z})^T,\ \mathbf{n}_0 \in \mathbf{k}_0^{\perp}.$$

Interpreting the complex exponential as a conjugated character $e^{i\alpha\widehat{\varphi}} = \overline{\chi_{\mathbb{T}}^{(-\alpha)}(\widehat{\varphi})}$ of $\mathbb{T}$ and the rest of the integrand as the action of $\mathbb{T}$ on the plane wave $\mathbf{E}_{\omega,\mathbf{k}_0} = \mathbf{n}_0 e^{-i\mathbf{k}_0\cdot}$ via the representation $\widehat{\varphi} \mapsto \mathbf{R}_{-\widehat{\varphi}}$, $\widehat{\varphi} \in \mathbb{T}$, we can write the integral as follows:

$$\mathbf{E}_0(\mathbf{x}) = \int_{\mathbb{T}} \overline{\chi_{\mathbb{T}}^{(-\alpha)}(\widehat{\varphi})}(\mathbf{R}_{-\widehat{\varphi}}\mathbf{E}_{\omega,\mathbf{k}_0})(\mathbf{x})\mathrm{d}\mu_{\mathbb{T}}(\widehat{\varphi}), \tag{5.4}$$

where $\mathrm{d}\mu_{\mathbb{T}}(\widehat{\varphi}) := \frac{1}{2\pi}\mathrm{d}\widehat{\varphi}$ is the normalized Haar measure on the torus group $\mathbb{T}$.

Now, consider the operator

$$P_{\mathbb{T}}^{(\alpha)} :\ \mathrm{R}_b^{\omega} \to \mathrm{R}_b^{\omega},\ \mathbf{E} \mapsto P_{\mathbb{T}}^{(\alpha)}\mathbf{E} := \int_{\mathbb{T}} \overline{\chi_{\mathbb{T}}^{(\alpha)}(\widehat{\varphi})}(\mathbf{R}_{\widehat{\varphi}}\mathbf{E})\,\mathrm{d}\mu_{\mathbb{T}}(\widehat{\varphi}).$$

It maps to the space of time-harmonic radiation R_b^{ω}, because the time-harmonic Maxwell equations are linear and invariant with respect to isometries. This operator is a so-called Wigner-projection or symmetry-projection operator. We will see that these operators provide a method to characterize the invariant spaces $\mathrm{R}_b^{\omega,\chi}(K)$ for compact isometry groups K and $\chi \in \widehat{K}$. They were first introduced and studied by Eugene Wigner (see [Wig31]) for applications in quantum mechanics.

Before studying these operators in detail, we come back to our twisted wave $\mathbf{E}_0$. We ask ourselves what happened to the projection with respect to the translational part of the group $C_{\mathbf{e}}$. We know that $C_{\mathbf{e}} \cong \mathbb{T}\times\mathbb{R}$, s.t. for the corresponding symmetry-projection

operator, written as operator-valued integral,

$$\begin{aligned} P_{C_{\mathbf{e}}}^{(\alpha,\widehat{z})} &= \int_{C_{\mathbf{e}}} \overline{\chi_{C_{\mathbf{e}}}^{(\alpha,\widehat{z})}(g)} g \,\mathrm{d}\mu_{C_{\mathbf{e}}}(g) \\ &= \int_{\mathbb{T}\times\mathbb{R}} \overline{\chi_{\mathbb{T}\times\mathbb{R}}^{(\alpha,\widehat{z})}(g_1,g_2)}(g_1,g_2)\,\mathrm{d}\mu_{\mathbb{T}\times\mathbb{R}}(g_1,g_2) \\ &= \int_{\mathbb{T}}\int_{\mathbb{R}} \overline{\chi_{\mathbb{T}}^{(\alpha)}(g_1)\chi_{\mathbb{R}}^{(\widehat{z})}(g_2)} g_1\circ g_2 \,\mathrm{d}\mu_{\mathbb{R}}(g_2)\,\mathrm{d}\mu_{\mathbb{T}}(g_1) \\ &= P_{\mathbb{T}}^{(\alpha)}\circ P_{\mathbb{R}}^{(\widehat{z})}, \end{aligned}$$

where the Haar measure of $C_{\mathbf{e}}$ is normalized, s.t. $\mu_{C_{\mathbf{e}}} = \mu_{\mathbb{T}} \otimes \mu_{\mathbb{R}}$.

Note that the projection with respect to $\mathbb{R}$ acting by translations along the axis is in the above integral formulation only defined for nice functions (e.g. Schwartz or compactly supported). In particular, the projection $P_{\mathbb{R}}^{(\widehat{z})}\mathbf{E}_{\omega,\mathbf{k}_0}$ cannot be defined in this way, because the integral diverges.

However, we can reformulate the projection in a way that allows a generalization of the concept. Consider once again the projection with respect to $\mathbb{T}$ acting by rotations about the axis $\mathbb{R}\mathbf{e}$. We write $\mathcal{F}_{\mathbb{T}}$ for the Fourier transform on $\mathbb{T}$, i.e. mapping a function $f \in L^1(\mathbb{T})$ to its Fourier coefficients considered as a function on the dual group that is isomorphic to $\mathbb{Z}$:

$$\mathcal{F}_{\mathbb{T}} f :\ \mathbb{Z} \to \mathbb{C},\ k \mapsto \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ikx} f(x)\mathrm{d}x.$$

Now, consider the bounded continuous function

$$\mathbf{E}_{\mathbf{x}} :\ \mathbb{T} \to \mathbb{C}^3,\ \widehat{\varphi} \mapsto (\mathbf{R}_{\widehat{\varphi}}\mathbf{E}_{\omega,\mathbf{k}_0})(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3.$$

Then we recognize the projection in (5.4) as a Fourier transform on the group $\mathbb{T}$ evaluated at the integer $-\alpha \in \mathbb{Z}$:

$$\mathbf{E}_0(\mathbf{x}) = \mathcal{F}_{\mathbb{T}}\mathbf{E}_{\mathbf{x}}(-\alpha).$$

This idea can now be generalized to the group $\mathbb{R}$ acting by translations. Defining the function

$$\mathbf{E}_{\mathbf{x}} :\ \mathbb{R} \to \mathbb{C}^3,\ y \mapsto \mathbf{E}(\mathbf{x} - y\mathbf{e}),$$

we would like to write the projection operator via the Fourier transform of $\mathbf{E}_{\mathbf{x}}$ in the distributional sense: $\widehat{\mathbf{E}_{\mathbf{x}}} \in \mathcal{S}'(\mathbb{R})^3$. Now, the projection of $\mathbf{E}$ with respect to the character $\chi^{(\widehat{z})}$ of $\mathbb{R}$ would be the evaluation of $\widehat{\mathbf{E}_{\mathbf{x}}}$ at $\widehat{z}$. Of course, it is not clear that this evaluation can be defined in some sense, as distributions are not defined pointwise.

Following this strategy for the plane wave $\mathbf{E}_{\omega,\mathbf{k}_0}$, we find for all $\varphi \in \mathcal{S}(\mathbb{R}^3)$:

$$\begin{aligned}\widehat{\mathbf{E}_{\mathbf{x}}\varphi} = \mathbf{E}_{\mathbf{x}}\widehat{\varphi} &= \int_{\mathbb{R}} \mathbf{E}_{\mathbf{x}}(y)\widehat{\varphi}(y)\mathrm{d}y = \mathbf{n}\int_{\mathbb{R}} e^{-i\mathbf{k}(\mathbf{x}-y\mathbf{e})}\widehat{\varphi}(y)\mathrm{d}y \\ &= \mathbf{n}e^{-i\mathbf{k}\cdot\mathbf{x}}\int_{\mathbb{R}} e^{iy\mathbf{k}\cdot\mathbf{e}}\widehat{\varphi}(y)\mathrm{d}y = \mathbf{n}e^{-i\mathbf{k}\cdot\mathbf{x}}\widehat{\widehat{\varphi}}(-\mathbf{k}\cdot\mathbf{e}) = 2\pi\mathbf{E}_{\omega,\mathbf{k}_0}\varphi(\mathbf{k}\cdot\mathbf{e}).\end{aligned}$$

So, $\widehat{\mathbf{E}_{\mathbf{x}}} = 2\pi\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\delta_{\mathbf{k}\cdot\mathbf{e}}$, where the 2π come from our non-unitary definition of the Fourier transform. The projection of $\mathbf{E}_{\omega,\mathbf{k}_0}$ with respect to $\chi^{(\widehat{z})}$ is then naturally defined as

$$P_{\mathbb{R}}^{(\widehat{z})}\mathbf{E}_{\omega,\mathbf{k}_0} := (2\pi)^{-1}\widehat{\mathbf{E}_{\mathbf{x}}}(\mathbf{1}_{\{\widehat{z}\}}) = \begin{cases}\mathbf{E}_{\omega,\mathbf{k}_0}, & \mathbf{k}\cdot\mathbf{e} = \widehat{z}, \\ 0, & \text{else.}\end{cases} \tag{5.5}$$

In summary, we can then say that

$$P_{C_{\mathbf{e}}}^{(-\alpha,\widehat{z})}\mathbf{E}_{\omega,\mathbf{k}_0} = P_{\mathbb{T}}^{(-\alpha)} \circ P_{\mathbb{R}}^{(\widehat{z})}\mathbf{E}_{\omega,\mathbf{k}_0} = P_{\mathbb{T}}^{(-\alpha)}\mathbf{E}_{\omega,\mathbf{k}_0} = \mathbf{E}_0.$$

So, twisted waves are projections of plane waves with respect to the design group $C_{\mathbf{e}}$. We will call these functions symmetry-adapted waves in the general case.

In the following, we discuss symmetry-projection operators for general closed abelian design groups G. For non-compact groups we have to formalize the idea used above to define the projection in a meaningful way. The main tool we will introduce is a generalization of the Zak transform.

2.1. Compact Abelian Design Groups. Let $K \leq \mathrm{O}(3)$ be a compact abelian design group. Given time-harmonic radiation $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ and a character $\chi \in \widehat{K}$, the symmetry-projection $P_K^\chi\mathbf{E}_0$ is defined by the integral

$$P_K^\chi\mathbf{E}_0(\mathbf{x}) := \int_K \overline{\chi(g)}(g\mathbf{E}_0)(\mathbf{x})\mathrm{d}\mu_K(g) \quad \text{for } \mathbf{x} \in \mathbb{R}^3,$$

where μ_K is the normalized Haar measure of K. As K is compact, the Haar measure is finite (see [Rei68], 3.1. (iv), p. 56), s.t. the function $P_K^\chi\mathbf{E}_0$ is bounded and continuous.

The projection operators can be used to characterize the solutions to the design equations for compact design groups as shown in the following statement.

Proposition 5.4 (Decomposition of R_b^ω – Compact Abelian Design Groups). *Let $K \leq \mathrm{O}(3)$ be a compact abelian design group. The operators P_K^χ, $\chi \in \widehat{K}$, are projections and map to the space $\mathrm{R}_b^{\omega,\chi}(K)$ of solutions to the design equations. In particular,*

$$\mathrm{R}_b^{\omega,\chi}(K) = P_K^\chi\mathrm{R}_b^\omega, \quad \textit{and} \quad \mathrm{R}_b^\omega = \bigoplus_{\chi\in\widehat{K}} \mathrm{R}_b^{\omega,\chi}(K).$$

Proof. We first show that for every $\mathbf{E}_0 \in \mathrm{R}_b^\omega$, the projection $P_K^\chi\mathbf{E}_0$ is an element of $\mathrm{R}_b^{\omega,\chi}(K)$, i.e. satisfies the design equations. The invariance of the time-harmonic Maxwell

equations with respect to isometries together with the fact that $P_K^\chi \mathbf{E}_0$ is bounded and continuous, shows that $P_K^\chi \mathbf{E}_0 \in \mathrm{R}_b^\omega$. That $P_K^\chi \mathbf{E}_0$ is an eigenfunction of the action of K follows with the translation invariance of the Haar measure. Let $h \in K$, then for $\mathbf{x} \in \mathbb{R}^3$:

$$\begin{aligned} hP_K^\chi \mathbf{E}_0(\mathbf{x}) &= \int_K \overline{\chi(g)}(hg\mathbf{E}_0)(\mathbf{x})\mathrm{d}\mu_K(g) = \int_K \overline{\chi(h^{-1}g)}(g\mathbf{E}_0)(\mathbf{x})\mathrm{d}\mu_K(g) \\ &= \overline{\chi(h^{-1})} \int_K \overline{\chi(g)}(g\mathbf{E}_0)(\mathbf{x})\mathrm{d}\mu_K(g) = \chi(h) P_K^\chi \mathbf{E}_0(\mathbf{x}). \end{aligned}$$

So, $P_K^\chi \mathbf{E}_0 \in \mathrm{R}_b^{\omega,\chi}(K)$.

Using this invariance and the normalization of the Haar measure, we can proof that P_K^χ is a projection. For $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,\chi}(K)$:

$$\begin{aligned} P_K^\chi \mathbf{E}_0(\mathbf{x}) &= \int_K \overline{\chi(g)}(g\mathbf{E}_0)(\mathbf{x})\mathrm{d}\mu_K(g) = \int_K \overline{\chi(g)}\chi(g)\mathbf{E}_0(\mathbf{x})\mathrm{d}\mu_K(g) \\ &= \int_K \mathrm{d}\mu_K(g)\mathbf{E}_0(\mathbf{x}) = \mathbf{E}_0(\mathbf{x}). \end{aligned}$$

From $P_K^\chi \mathbf{E}_0 \in \mathrm{R}_b^{\omega,\chi}(K)$ for all $\mathbf{E}_0 \in \mathrm{R}_b^\omega$, we get $P_K^\chi \mathrm{R}_b^\omega \subseteq \mathrm{R}_b^{\omega,\chi}(K)$, while from $P_K^\chi \mathbf{E}_0 = \mathbf{E}_0$ for all $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,\chi}(K)$, we get $P_K^{\omega,\chi}(K) \subseteq P_K^\chi \mathrm{R}_b^\omega$. So, in summary, $P_K^\chi \mathrm{R}_b^\omega = \mathrm{R}_b^{\omega,\chi}(K)$.

Finally, the Schur orthogonality relations show that the space R_b^ω is the direct sum of the invariant subspaces. Let $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,\chi}(K)$ and $\chi' \in \widehat{K}$ another character of K. Then with the same calculation as above

$$\begin{aligned} P_K^{\chi'} \mathbf{E}_0(\mathbf{x}) &= \int_K \overline{\chi'(g)}(g\mathbf{E}_0)(\mathbf{x})\mathrm{d}\mu_K(g) = \int_K \overline{\chi'(g)}\chi(g)\mathbf{E}_0(\mathbf{x})\mathrm{d}\mu_K(g) \\ &= \int_K \overline{\chi'(g)}\chi(g)\mathrm{d}\mu_K(g)\mathbf{E}_0(\mathbf{x}) = \delta_{\chi',\chi}\mathbf{E}_0(\mathbf{x}). \end{aligned}$$

□

As a result of this proposition, we get a symmetry decomposition of time-harmonic radiation $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ as follows:

$$P_K \mathbf{E}_0 : \ \widehat{K} \to \mathrm{R}_b^\omega, \ \chi \mapsto P_K^\chi \mathbf{E}_0.$$

The orthogonality relations for the dual group show that reconstruction of $\mathbf{E}_0$ from $P_K \mathbf{E}_0$ can be achieved by simple superposition:

$$\mathbf{E}_0 = \sum_{\chi \in \widehat{K}} P_K^\chi \mathbf{E}_0.$$

Even though this statement describes all solutions of the design equations, it doesn't give the final answer to the question which radiation to use for the analysis of the respective class of objective structures.

Consider the case of $\mathbb{T}$ acting via the representation $\widehat{\varphi} \mapsto \mathbf{R}_{\widehat{\varphi}}$, $\widehat{\varphi} \in \mathbb{T}$, by rotations about an axis $\mathbb{R}\mathbf{e}$, $\mathbf{e} \in \mathbb{S}^2$. Proposition 5.4 says that $\mathrm{R}_b^{\omega,\alpha}(\mathbb{T}) = P_{\mathbb{T}}^{(\alpha)} \mathrm{R}_b^\omega$ for all $\alpha \in \mathbb{Z}$. In particular, this space is very big, as every time-harmonic radiation $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ with a complex amplitude distribution $\mathbf{n}$ supported on the half circle that is the intersection of $\frac{\omega}{c}\mathbb{S}^2$ with a half plane bordered by the axis yields a different symmetry-adapted radiation. Consequently, there are at least as many elements as there are finite measures on an interval.

To design a reasonable method for structure analysis, we need to select a small set of radiation that is sufficient for reconstruction. The following elements of $\mathrm{R}_b^{\omega,\chi}(K)$ will turn out to be the right choice for our purposes.

Definition 5.5 (Symmetry-Adapted Waves – Compact Abelian Design Group). *Let $K \leq \mathrm{O}(3)$ be a compact abelian design group and $\chi \in \widehat{K}$. We define the symmetry-adapted waves $\mathbf{E}_{\omega,\mathbf{k}_0,\chi}$ with wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$ as follows:*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\chi} := P_K^\chi \mathbf{E}_{\omega,\mathbf{k}_0}. \tag{5.6}$$

The corresponding scalar symmetry-adapted wave is

$$e_{\omega,\mathbf{k}_0,\chi} := P_K^\chi e_{\omega,\mathbf{k}_0}. \tag{5.7}$$

The definition of the symmetry-adpated waves is very natural. It combines the structure of the underlying space $\mathbb{R}^3$ with the structure of the group K that acts on $\mathbb{R}^3$. We can already anticipate that these functions will be a complete set in appropriate function spaces while at the same time being invariant with respect to K.

Before we can define the symmetry-adapted waves for general abelian design groups, we need to understand how to generalize the projection operators to this case. For this purpose we take a different point of view on projections by introducing a transform that is closely related to the projection operators – the Zak transform.

Definition 5.6 (Zak transform on R_b^ω – compact abelian design group). *Let $K \leq \mathrm{O}(3)$ be a compact closed abelian isometry group and $\mathbf{E}_0 \in \mathrm{R}_b^\omega$. The Zak transform $\mathcal{Z}_K \mathbf{E}_0$ of $\mathbf{E}_0$ with respect to K is defined as*

$$\mathcal{Z}_K \mathbf{E}_0(\mathbf{x}, \chi) := \mathcal{F}_K \mathbf{E}_\mathbf{x}(\chi) \quad \text{for } \mathbf{x} \in \mathbb{R}^3,\ \chi \in \widehat{K}, \tag{5.8}$$

where the function $\mathbf{E}_\mathbf{x} : K \to \mathbb{C}^3$ is defined as

$$\mathbf{E}_\mathbf{x}(g) := (g\mathbf{E}_0)(\mathbf{x}) \quad \text{for } g \in K.$$

We call this transform the Zak transform, as it is a generalization of the classic Zak transform that was first in detail studied by J. Zak in [Zak67] (see Remark 6.2). We summarize some properties in the following lemma.

Lemma 5.7 (Properties of the Zak Transform on R_b^ω – Compact Abelian Design Group). *The Zak transform maps time-harmonic radiation to bounded continuous functions from $\mathbb{R}^3 \times \widehat{K}$ to $\mathbb{C}^3$. In particular,*

$$\mathcal{Z}_K \mathbf{E}_0(\mathbf{x}, \chi) = P_K^\chi \mathbf{E}_0(\mathbf{x}) \quad \text{for } \mathbf{x} \in \mathbb{R}^3,\ \chi \in \widehat{K}. \tag{5.9}$$

The inverse Zak transform $\mathcal{Z}_K^{-1}$ is defined as

$$\mathcal{Z}_K^{-1} f(\mathbf{x}) := \sum_{\chi \in \widehat{K}} f(\mathbf{x}, \chi) = \mathcal{F}_K^{-1} f(\mathbf{x}, \mathrm{id}_{\mathbb{R}^3}), \quad \text{for } \mathbf{x} \in \mathbb{R}^3, \tag{5.10}$$

for all functions $f : \mathbb{R}^3 \times \widehat{K} \to \mathbb{C}^3$, s.t. $f(\mathbf{x}, \cdot)$ is l^1 for all $\mathbf{x} \in \mathbb{R}^3$. It satisfies

$$\mathcal{Z}_K^{-1} \mathcal{Z}_K = \mathrm{id}_{\mathrm{R}_b^\omega}.$$

Proof. The identity (5.9) follows directly from the definitions of the Zak transform and the Fourier transform. For $\mathbf{E}_0 \in \mathrm{R}_b^\omega$, $\mathbf{x} \in \mathbb{R}^3$ and $\chi \in \widehat{K}$:

$$\begin{aligned} \mathcal{Z}_K \mathbf{E}_0(\mathbf{x}, \chi) = \mathcal{F}_K \mathbf{E}_\mathbf{x}(\chi) &= \int_K \overline{\chi(g)} \mathbf{E}_\mathbf{x}(g) \mathrm{d}\mu_K(g) \\ &= \int_K \overline{\chi(g)} (g\mathbf{E}_0)(\mathbf{x}) \mathrm{d}\mu_K(g) = P_K^\chi \mathbf{E}_0(\mathbf{x}). \end{aligned}$$

The inversion formula is a direct consequence of the Fourier inversion formula on K. For $\mathbf{E}_0 \in \mathrm{R}_b^\omega$, $\mathbf{x} \in \mathbb{R}^3$:

$$\mathcal{Z}_K^{-1} \mathcal{Z}_K \mathbf{E}_0(\mathbf{x}) = \mathcal{F}_K^{-1}(\mathcal{F}_K \mathbf{E}_\mathbf{x})(\mathrm{id}_{\mathbb{R}^3}) = \mathbf{E}_\mathbf{x}(\mathrm{id}_{\mathbb{R}^3}) = \mathbf{E}_0(\mathbf{x}).$$

□

The Zak transform is a space-symmetry decomposition of a function and can also be defined similarly for non-compact abelian groups.

2.2. Abelian Design Groups. For the non-compact factors, the symmetry-projection cannot be defined as an integral, as this integral diverges in general. Instead, we generalize the Zak transform.

For an extension of the Zak transform to non-compact design groups, one has to overcome the difficulty that the radiations $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ are not necessarily in $L^1(\mathbb{R}^3; \mathbb{C}^3)$, s.t. the functions $\mathbf{E}_\mathbf{x}$ are in general not in $L^1(G; \mathbb{C}^3)$. However, since these functions are bounded and continuous, the task is to extend the Fourier transform on G to this space of functions. To avoid the technicalities that come along with the introduction of the

Schwartz-Bruhat spaces of smooth rapidly decaying functions on locally compact abelian groups (see [Osb75]), we make a minimal extension that is tailored to our needs.

Definition 5.8 (Fourier transform on $C_b(G;\mathbb{C}^3)$). *Let $G \leq \mathrm{E}(3)$ be an abelian closed isometry group, and $\mathbf{E} \in C_b(G;\mathbb{C}^3)$. We define the Fourier transform $\mathcal{F}_G$ on $C_b(G;\mathbb{C}^3)$ as a linear operator on the space $\mathcal{F}M^1(G)$ of Fourier transforms of finite complex measures on G. The mapping $\mathcal{F}_G\mathbf{E} : \mathcal{F}M^1(G) \to \mathbb{C}^3$ is defined by*

$$(\mathcal{F}_G\mathbf{E})\psi := \int_G \mathbf{E}(g)\mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) \quad \text{for } \psi \in \mathcal{F}M^1(G). \tag{5.11}$$

The corresponding inverse Fourier transform $\mathcal{F}_G^{-1}$ is given by

$$(\mathcal{F}_G^{-1}\mathbf{F})\psi := \mathbf{F}(\mathcal{F}_{\widehat{G}}^{-1}\psi) \quad \text{for } \psi \in M^1(G), \tag{5.12}$$

where $\mathbf{F} \in \mathcal{F}C_b(G;\mathbb{C}^3)$.

This definition inherits all the nice properties of the Fourier transform on L^1-functions in the same way as the Fourier transform of tempered distribution on $\mathbb{R}^n$. These properties will be discussed when they are explicitly needed.

With this definition, we can introduce the generalized Zak transform for general abelian design groups.

Definition 5.9 (Zak transform on R_b^ω – abelian design group). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group and $\mathbf{E}_0 \in \mathrm{R}_b^\omega$. The Zak transform $\mathcal{Z}_G\mathbf{E}_0$ of $\mathbf{E}_0$ with respect to G is defined as*

$$\mathcal{Z}_G\mathbf{E}_0(\mathbf{x},\psi) := (\mathcal{F}_G\mathbf{E}_\mathbf{x})(\psi) \quad \text{for } \mathbf{x} \in \mathbb{R}^3,\ \psi \in \mathcal{F}M^1(G), \tag{5.13}$$

where the function $\mathbf{E}_\mathbf{x} : G \to \mathbb{C}^3$ is defined as

$$\mathbf{E}_\mathbf{x}(g) := (g\mathbf{E})(\mathbf{x}) \quad \text{for } g \in G.$$

Unlike in the compact case, the Zak transform cannot be used in general to define projection operators, because it cannot be pointwise evaluated (note that δ_χ, $\chi \in \widehat{G}$, is not in $\mathcal{F}M^1(G)$). When $\psi_\chi \in \mathcal{F}L^1(\widehat{G})$ is concentrated around a character $\chi \in \widehat{G}$, the function $\mathbf{x} \mapsto \mathcal{Z}_G(\mathbf{x},\psi_\chi)$ is in some sense 'almost invariant'.

We summarize some properties of the Zak transform in the following lemma.

Lemma 5.10 (Properties of the Zak Transform on R_b^ω – Abelian Design Group). *For $\psi \in \mathcal{F}M^1(G)$, the operator P_G^ψ on R_b^ω, defined by*

$$P_G^\psi\mathbf{E}_0(\mathbf{x}) := \mathcal{Z}_G\mathbf{E}_0(\mathbf{x},\psi) \quad \text{for } \mathbf{E}_0 \in \mathrm{R}_b^\omega,\ \mathbf{x} \in \mathbb{R}^3, \tag{5.14}$$

maps to R_b^ω. *When* $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,\chi}(G)$, $\chi \in \widehat{G}$, *then*

$$\mathcal{Z}_G \mathbf{E}_0(\mathbf{x}, \psi) = \psi(\chi)\mathbf{E}_0(\mathbf{x}). \tag{5.15}$$

The inverse Zak transform $\mathcal{Z}_G^{-1}$ *is given by*

$$\mathcal{Z}_G^{-1} f(\mathbf{x}) := f(\mathbf{x}, \mathbf{1}_{\widehat{G}}) = \mathcal{F}_G^{-1} f(\mathbf{x}, \delta_{\mathrm{id}_{\mathbb{R}^3}}).$$

It satisfies $\mathcal{Z}_G^{-1}\mathcal{Z}_G = \mathrm{id}_{\mathrm{R}_b^\omega}$.

Proof. Let $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ and $\psi \in \mathcal{F}M^1(G)$. Then $P_G^\psi \mathbf{E}_0$ is continuous, because of the continuity of $\mathbf{E}_0$ and of $\mathcal{F}_G$. It is also bounded, as

$$\begin{aligned}\|P_G^\psi \mathbf{E}_0\|_\infty &= \sup_{\mathbf{x}\in\mathbb{R}^3} |\mathcal{F}_G \mathbf{E}_\mathbf{x}(\psi)| = \sup_{\mathbf{x}\in\mathbb{R}^3} \left| \int_G (g\mathbf{E}_0)(\mathbf{x}) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) \right| \\ &\leq \int_G |(g\mathbf{E}_0)(\mathbf{x})| \mathrm{d}|\mathcal{F}_{\widehat{G}}\psi|(g) \leq \|\mathbf{E}_0\|_\infty \cdot \|\mathcal{F}_{\widehat{G}}\psi\|_{M^1(G)} < \infty.\end{aligned}$$

Linearity and invariance with respect to isometries of the time-harmonic Maxwell equations implies that $P_G^\psi \mathbf{E}_0 \in \mathrm{R}_b^\omega$.

Now, let $\mathbf{E}_0 \in \mathrm{R}_b^{\omega,\chi}(G)$ for some $\chi \in \widehat{G}$. Then

$$\begin{aligned}\mathcal{Z}_G \mathbf{E}_0(\mathbf{x}, \psi) = \mathcal{F}_G \mathbf{E}_\mathbf{x}(\psi) &= \int_G (g\mathbf{E}_0)(\mathbf{x}) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) \\ &= \int_G \chi(g)\mathbf{E}_0(\mathbf{x}) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) = \int_G \chi(g) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g)\mathbf{E}_0(\mathbf{x}) \\ &= \psi(\chi)\mathbf{E}_0(\mathbf{x}),\end{aligned}$$

using the invariance of $\mathbf{E}_0$ and the Fourier inversion formula on $M^1(G)$.

Finally, for $\mathbf{E}_0 \in \mathrm{R}_b^\omega$:

$$\begin{aligned}\mathcal{Z}_G^{-1}\mathcal{Z}_G \mathbf{E}_0(\mathbf{x}) &= \mathcal{Z}_G \mathbf{E}_0(\mathbf{x}, \mathbf{1}_{\widehat{G}}) = \mathcal{F}_G \mathbf{E}_\mathbf{x}(\mathbf{1}_{\widehat{G}}) \\ &= \mathbf{E}_\mathbf{x}(\mathcal{F}_{\widehat{G}}(\mathbf{1}_{\widehat{G}})) = \mathbf{E}_\mathbf{x}(\delta_{\mathrm{id}_{\mathbb{R}^3}}) = \mathbf{E}_0(\mathbf{x}).\end{aligned}$$

□

We will use the Zak transform to define symmetry-adapted waves with respect to abelian design groups in the next section.

3. Symmetry-Adapted Waves for Abelian Design Groups

To define symmetry-adapted waves for abelian design groups, we want to utilize Proposition 5.3 in the following way. We first determine the symmetry-adapted waves for the single factors of the decomposition using the Zak transform and then make an iterative construction to generalize the definition to general abelian design groups.

Even though this method is very ad hoc, once we have done the work, we can use this explicit construction to easily determine the symmetry-adapted waves for concrete examples.

We start with the non-compact factors of an abelian isometry groups by computing the Zak transform of plane waves with respect to these groups.

Lemma 5.11 (Zak Transform of Plane Waves).
Let the groups $R = \{(\mathbf{Q}_R(a)|\mathbf{c}_R(a)).\ a \in \mathbb{R}\} \leq \mathrm{E}(3)$ *be closed and isomorphic to* $\mathbb{R}$*, and* $Z = \{(\mathbf{Q}_Z(j)|\mathbf{c}_Z(j)).\ j \in \mathbb{Z}\} \leq \mathrm{E}(3)$ *be closed and isomorphic to* $\mathbb{Z}$*, respectively, and let* $\mathbf{E}_{\omega,\mathbf{k}_0} = \mathbf{n}e^{i\mathbf{k}\cdot}$*,* $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$*, be a plane wave.*

The Zak transforms of the plane waves $\mathbf{E}_{\omega,\mathbf{k}_0}$ *with repsect to* R *and* Z *at* $\mathbf{x} \in \mathbb{R}^3$ *and* $\psi \in \mathcal{F}M^1(\mathbb{R}^3)$ *are given by*

(1) *When* R *is a group of translations, i.e.* $\mathbf{Q}_R(a) = \mathbf{I}$*,* $\mathbf{c}_R(a) = \tau a\mathbf{e}$ *for some* $\tau \neq 0$*,* $\mathbf{e} \in \mathbb{S}^2$ *and all* $a \in \mathbb{R}$*, then*

$$\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) = 2\pi\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\psi(-\tau\mathbf{k}\cdot\mathbf{e}).$$

(2) *When* R *is a group of screw displacements, i.e.* $\mathbf{Q}_R(a) = \mathbf{R}_{\lambda a}$ *and* $\mathbf{c}_R(a) = \tau a\mathbf{e}$ *for some* $\lambda, \tau \neq 0$*,* $\mathbf{e} \in \mathbb{S}^2$ *and all* $a \in \mathbb{R}$*, then*

$$\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) = 2\pi\sum_{\ell\in\mathbb{Z}}\mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}(\mathbf{x})\psi(\lambda\ell - \tau\mathbf{k}\cdot\mathbf{e}).$$

(3) *When* Z *is a group of translations, i.e.* $\mathbf{Q}_Z(j) = \mathbf{I}$ *and* $\mathbf{c}_Z(j) = \tau j\mathbf{e}$ *for some* $\tau \neq 0$*,* $\mathbf{e} \in \mathbb{S}^2$ *and all* $j \in \mathbb{Z}$*, then*

$$\mathcal{Z}_Z\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) = 2\pi\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\sum_{m\in2\pi\mathbb{Z}}\psi(m - \tau\mathbf{k}\cdot\mathbf{e}).$$

(4) *When* Z *is a group of screw displacements, i.e.* $\mathbf{Q}_Z(j) = \mathbf{R}_{\lambda j}$ *and* $\mathbf{c}_Z(j) = \tau j\mathbf{e}$ *for some* $\lambda, \tau \neq 0$*,* $\mathbf{e} \in \mathbb{S}^2$ *and all* $j \in \mathbb{Z}$*, then*

$$\mathcal{Z}_Z\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) = 2\pi\sum_{\ell\in\mathbb{Z}}\mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}(\mathbf{x})\sum_{m\in2\pi\mathbb{Z}}\psi(m + \lambda\ell - \tau\mathbf{k}\cdot\mathbf{e}).$$

(5) *When* Z *is a group of glide reflections, i.e.* $\mathbf{Q}_Z(1) = \mathbf{I} - 2\mathbf{e}\otimes\mathbf{e}$*,* $\mathbf{c}_Z(1) = \tau\mathbf{c}_\perp$ *for some* $\mathbf{e} \in \mathbb{S}^2$*,* $\tau \neq 0$ *and* $\mathbf{c}_\perp \in \mathbf{e}^\perp \cap \mathbb{S}^2$*, then, when defining* $\widetilde{\mathbf{n}} := \mathbf{Q}_Z(1)\mathbf{n}$ *and* $\widetilde{\mathbf{k}_0} := \mathbf{Q}_Z(1)\mathbf{k}_0$*,*

$$\begin{aligned}\mathcal{Z}_Z\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) =& \frac{2\pi}{2}\sum_{m\in2\pi\mathbb{Z}}(\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) + \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}(\mathbf{x}))\psi(m - \tau\mathbf{k}\cdot\mathbf{c}_\perp)\\ &+ (\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) - \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}(\mathbf{x}))\psi(m + \tau\mathbf{k}\cdot\mathbf{c}_\perp).\end{aligned}$$

Proof. In the case that R is a group of translations, i.e. $\mathbf{Q}_R(a) = \mathbf{I}$, $\mathbf{c}_R(a) = \tau a\mathbf{e}$ for some $\tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$ and all $a \in \mathbb{R}$, for $\psi \in \mathcal{F}M^1(\mathbb{R})$:

$$\begin{aligned}\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) &= \int_{\mathbb{R}} \mathbf{n}e^{i\mathbf{k}\cdot(\mathbf{x}-\tau a\mathbf{e})}\mathrm{d}\mathcal{F}_{\widehat{\mathbb{R}}}\psi(a) = \mathbf{n}e^{i\mathbf{k}\cdot\mathbf{x}}\int_{\mathbb{R}} e^{-ia\tau\mathbf{k}\cdot\mathbf{e}}\mathrm{d}\widehat{\psi}(a)\\ &= \mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\widehat{\widehat{\psi}}(\tau\mathbf{k}\cdot\mathbf{e}) = 2\pi\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\psi(-\tau\mathbf{k}\cdot\mathbf{e}).\end{aligned}$$

When R is a group of screw displacements, i.e. $\mathbf{Q}_R(a) = \mathbf{R}_{\lambda a}$ and $\mathbf{c}_R(a) = \tau a\mathbf{e}$ for some $\lambda, \tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$ and all $a \in \mathbb{R}$, for every $\psi \in \mathcal{F}M^1(\mathbb{R})$, we get

$$\begin{aligned}\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) &= \int_{\mathbb{R}} \mathbf{R}_{\lambda a}\mathbf{n}e^{i\mathbf{k}\cdot\mathbf{R}_{-\lambda a}(\mathbf{x}-\tau a\mathbf{e})}\mathrm{d}\widehat{\psi}(a)\\ &= \mathbf{U}\underbrace{\int_{\mathbb{R}} \begin{pmatrix} e^{i\lambda a} & & \\ & e^{-i\lambda a} & \\ & & 1\end{pmatrix} e^{i\mathbf{k}\cdot(\mathbf{R}_{-\lambda a}\mathbf{x}-\tau a\mathbf{e})}\mathrm{d}\widehat{\psi}(a)}_{=:\mathbf{S}}\,\mathbf{U}^{-1}\mathbf{n},\end{aligned}$$

where $\mathbf{U} \in \mathrm{U}(3)$ is the unitary matrix that simultaneously diagonalizes the matrices $\mathbf{R}_{\lambda a}$ in the given way. Writing $\mathbf{x} = \xi_{\mathbf{e}}(r,\varphi,z)$ and $\mathbf{k} = \xi_{\mathbf{e}}(\widehat{r},\widehat{\varphi},\widehat{z})$ in cylindrical coordinates about $\mathbb{R}\mathbf{e}$, we can use the angle difference formula of the cosine to write the exponent of the exponential as follows:

$$\begin{aligned}\mathbf{k}\cdot(\mathbf{R}_{-\lambda a}\mathbf{x}-\tau a\mathbf{e}) &= \widehat{r}r(\cos(\widehat{\varphi})\cos(\varphi-\lambda a)+\sin(\widehat{\varphi})\sin(\varphi-\lambda a)) + \widehat{z}(z-\tau a)\\ &= \widehat{r}r\cos(\widehat{\varphi}-\varphi+\lambda a)+\widehat{z}(z-\tau a).\end{aligned}$$

Now, setting $\sigma := (-1,1,0)^T$, we can write the diagonal elements of the matrix-valued integral $\mathbf{S}$ as follows:

$$\begin{aligned}\mathbf{S}_{kk} &= e^{i\widehat{z}z}\int_{\mathbb{R}} e^{-i\tau\widehat{z}}e^{ia\sigma_k\lambda}e^{i\widehat{r}r\cos(\widehat{\varphi}-\varphi+\lambda a)}\mathrm{d}\widehat{\psi}(a)\\ &= e^{i\widehat{z}z}\mathcal{F}(e^{i\sigma_k\lambda}e^{i\widehat{r}r\cos(\widehat{\varphi}-\varphi+\lambda\cdot)}\widehat{\psi})(\tau\widehat{z})\\ &= e^{i\widehat{z}z}\mathcal{F}(e^{i\sigma_k\lambda}e^{i\widehat{r}r\cos(\widehat{\varphi}-\varphi+\lambda\cdot)}) * (2\pi\psi_-)(\tau\widehat{z})\\ &= e^{i\widehat{z}z}\sum_{\ell\in\lambda\mathbb{Z}}\int_{-\pi}^{\pi} e^{-ia\ell/\lambda}e^{i\sigma_k a}e^{i\widehat{r}r\cos(\widehat{\varphi}-\varphi+a)}\mathrm{d}a\,\delta_l * \psi_-(\tau\widehat{z})\\ &= \sum_{\ell\in\lambda\mathbb{Z}}\int_{-\pi}^{\pi} e^{-ia\ell/\lambda}e^{i\sigma_k a}e^{i\mathbf{k}\cdot\mathbf{R}_{-a}\mathbf{x}}\mathrm{d}a\,\psi(\ell-\tau\mathbf{k}\cdot\mathbf{e}),\end{aligned}$$

where we used the convolution theorem, the formula for the double Fourier transform and the Fourier transform of a periodic function.

So,

$$\begin{aligned}\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) &= \sum_{\ell\in\lambda\mathbb{Z}}\int_{-\pi}^{\pi} e^{-ia\ell}\mathbf{U}\begin{pmatrix} e^{ia} & & \\ & e^{-ia} & \\ & & 1\end{pmatrix}\mathbf{U}^{-1}\mathbf{n}e^{i\mathbf{R}_a\mathbf{k}\cdot\mathbf{x}}\mathrm{d}a\,\psi(\ell-\tau\mathbf{k}\cdot\mathbf{e})\\ &= \sum_{\ell\in\lambda\mathbb{Z}}\int_{-\pi}^{\pi} e^{-ia\ell}\mathbf{R}_a\mathbf{n}e^{i\mathbf{R}_a\mathbf{k}\cdot\mathbf{x}}\mathrm{d}a\,\psi(\ell-\tau\mathbf{k}\cdot\mathbf{e}).\end{aligned}$$

Comparing with formula (4.3), we find

$$\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) = 2\pi\sum_{\ell\in\lambda\mathbb{Z}}\mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}(\mathbf{x})\psi(\ell-\tau\mathbf{k}\cdot\mathbf{e}).$$

Next, we consider the discrete case that Z is a group of translations, i.e. $\mathbf{Q}_Z(j)=\mathbf{I}$ and $\mathbf{c}_Z(j)=\tau j\mathbf{e}$ for some $\tau\neq 0$, $\mathbf{e}\in\mathbb{S}^2$ and all $j\in\mathbb{Z}$. We see that this is a discretization of the continuous case. We extend the function $\mathbf{E}_\mathbf{x}: j\mapsto(\mathbf{Q}_Z(j)|\mathbf{c}(j))\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})$ to $\mathbb{R}$ by setting $\mathbf{Q}_Z(a):=\mathbf{I}$ and $\mathbf{c}_Z(a)=\tau a\mathbf{e}$ for $a\in\mathbb{R}$. Now, using the theory of tempered distributions on $\mathbb{R}$ and the convolution theorem, we find that for a Schwartz function $\psi\in\mathcal{S}(\mathbb{R})$

$$\mathcal{F}_\mathbb{R}(\delta_\mathbb{Z}\cdot\mathbf{E}_\mathbf{x})\psi = \delta_{2\pi\mathbb{Z}}*\mathcal{Z}_R\mathbf{E}_0(\mathbf{x},\psi),$$

for all $\mathbf{E}_0\in\mathrm{R}_b^\omega$, $\mathbf{x}\in\mathbb{R}^3$, where $\mathbf{E}_\mathbf{x}$ is the extended function considered above and the convolution is with respect to the second argument. Then the Zak transform $\mathcal{Z}_Z\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\cdot)$ is the restriction of this function to $\mathcal{F}M^1(\mathbb{T})$. For $\mathcal{F}M^1(\mathbb{T})$ we get:

$$\begin{aligned}\delta_{2\pi\mathbb{Z}}*\mathcal{Z}_R\mathbf{E}_0(\mathbf{x},\psi) &= 2\pi\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})(\delta_{2\pi\mathbb{Z}}*\delta_{-\tau\mathbf{k}\cdot\mathbf{e}})\psi\\ &= 2\pi\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\sum_{m\in 2\pi\mathbb{Z}}\psi(m-\tau\mathbf{k}\cdot\mathbf{e}).\end{aligned}$$

The same trick works for the discrete group Z generated by a screw displacement, i.e. $\mathbf{Q}_Z(j)=\mathbf{R}_{\lambda j}$ and $\mathbf{c}_Z(j)=\tau j\mathbf{e}$ for some $\lambda,\tau\neq 0$, $\mathbf{e}\in\mathbb{S}^2$ and all $j\in\mathbb{Z}$. With the same notation as for the translations, we get

$$\begin{aligned}\delta_{2\pi\mathbb{Z}}*\mathcal{Z}_R\mathbf{E}_0(\mathbf{x},\psi) &= 2\pi\sum_{\ell\in\lambda\mathbb{Z}}\mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}(\mathbf{x})\delta_{2\pi\mathbb{Z}}*\delta_{\ell-\tau\mathbf{k}\cdot\mathbf{e}}\\ &= 2\pi\sum_{\ell\in\lambda\mathbb{Z}}\mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}(\mathbf{x})\sum_{m\in 2\pi\mathbb{Z}}\delta_{m+\ell-\tau\mathbf{k}\cdot\mathbf{e}}.\end{aligned}$$

Finally, we treat the case that the group Z is generated by $\mathbf{Q}_Z(1)=\mathbf{I}-2\mathbf{e}\otimes\mathbf{e}$, $\mathbf{c}_Z(1)=\tau\mathbf{c}_\perp$ for some $\mathbf{e}\in\mathbb{S}^2$, $\tau\neq 0$ and $\mathbf{c}_\perp\in\mathbf{e}^\perp\cap\mathbb{S}^2$. It can be reduced to the case of two discrete groups generated by translations as follows. Define $\widetilde{\mathbf{n}}:=(\mathbf{I}-2\mathbf{e}\otimes\mathbf{e})\mathbf{n}$ and $\widetilde{\mathbf{k}}:=(\mathbf{I}-2\mathbf{e}\otimes\mathbf{e})\mathbf{k}$.

Then for all $\psi \in \mathcal{F}M^1(\mathbb{T})$:

$$\begin{aligned}
\mathcal{Z}_Z \mathbf{E}_{\omega,\mathbf{k}_0} &== \sum_{j\in\mathbb{Z}} (\mathbf{I} - 2\mathbf{e}\otimes\mathbf{e})^j \mathbf{n} e^{i\mathbf{k}\cdot(\mathbf{I}-2\mathbf{e}\otimes\mathbf{e})(\mathbf{x}-\tau j\mathbf{c}_\perp)} \mathcal{F}_{\widehat{G}}\psi(j) \\
&= \sum_{j\in 2\mathbb{Z}} \mathbf{n} e^{i\mathbf{k}\cdot(\mathbf{x}-\tau j\mathbf{c}_\perp)} \widehat{\psi}(j) + \sum_{j\in 2\mathbb{Z}+1} \widetilde{\mathbf{n}} e^{i\widetilde{\mathbf{k}}\cdot(\mathbf{x}-\tau j\mathbf{c}_\perp)} \widehat{\psi}(j) \\
&= \mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) \sum_{j\in 2\mathbb{Z}} e^{-i\tau\mathbf{k}\cdot\mathbf{c}_\perp j} \widehat{\psi}(j) + \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}(\mathbf{x}) \sum_{j\in 2\mathbb{Z}+1} e^{-i\tau\widetilde{\mathbf{k}}\cdot\mathbf{c}_\perp j} \widehat{\psi}(j) \\
&= \mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) \sum_{m\in 2\pi\mathbb{Z}} \frac{2\pi}{2} (\psi(m - \tau\mathbf{k}\cdot\mathbf{c}_\perp) + \psi(m + \tau\mathbf{k}\cdot\mathbf{c}_\perp)) \\
&+ \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}(\mathbf{x}) \sum_{m\in 2\pi\mathbb{Z}} \frac{2\pi}{2} (\psi(m - \tau\mathbf{k}\cdot\mathbf{c}_\perp) - \psi(m + \tau\mathbf{k}\cdot\mathbf{c}_\perp))
\end{aligned}$$

So,

$$\mathcal{Z}_Z \mathbf{E}_{\omega,\mathbf{k}_0} = \frac{2\pi}{2} \sum_{m\in 2\pi\mathbb{Z}} (\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) + \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}(\mathbf{x}))\delta_{m-\tau\mathbf{k}\cdot\mathbf{c}_\perp} + (\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) - \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}(\mathbf{x}))\delta_{m+\tau\mathbf{k}\cdot\mathbf{c}_\perp}.$$

□

This lemma shows in particular, that the distributions $\mathcal{Z}_R \mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\cdot)$ and $\mathcal{Z}_Z \mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\cdot)$ are point measures on $\mathbb{R}$ and $\mathbb{T}$, respectively, in all the cases. This means that we can define symmetry-adapted waves with respect to the non-compact factors as follows

Definition 5.12 (Symmetry-Adapted Waves – Non-Compact Factors). *Let $R \cong \mathbb{R}$ and $Z \cong \mathbb{Z}$ be closed abelian isometry groups and $\mathbf{E}_{\omega,\mathbf{k}_0}$ be a plane wave with frequency $\omega > 0$ and wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$. We define the symmetry-adapted waves with respect to R and Z pointwise at $\mathbf{x} \in \mathbb{R}^3$ by*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\alpha}(\mathbf{x}) := (2\pi)^{-1} \mathcal{Z}_R \mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}, \mathbf{1}_{\{\alpha\}}), \quad \alpha \in \mathbb{R}, \tag{5.16}$$

$$\mathbf{E}_{\omega,\mathbf{k}_0,\beta}(\mathbf{x}) := (2\pi)^{-1} \mathcal{Z}_Z \mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}, \mathbf{1}_{\{\beta\}}), \quad \beta \in \mathbb{T}. \tag{5.17}$$

We define the operators $P_R^{(\alpha)}$ and $P_Z^{(\beta)}$ on the space of time harmonic radiation that is a finite sum of plane waves as follows. Let $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ be given by $\mathbf{E}_0 = \sum_{j=1}^n \mathbf{E}_{\omega,\mathbf{k}_j}$ with $\mathbf{k}_j \in \mathbb{S}^2$, $j = 1,\dots,n$. Then we define $P_R^{(\alpha)}\mathbf{E}_0$ and $P_Z^{(\beta)}\mathbf{E}_0$ by

$$P_R^{(\alpha)}\mathbf{E}_0 := \sum_{j=1}^n \mathbf{E}_{\omega,\mathbf{k}_j,\alpha}, \quad P_Z^{(\beta)}\mathbf{E}_0 := \sum_{j=1}^n \mathbf{E}_{\omega,\mathbf{k}_j,\beta}.$$

We still have to check that these functions are elements of the corresponding spaces $\mathrm{R}_b^{\omega,\alpha}(R)$ and $\mathrm{R}_b^{\omega,\beta}(Z)$. We do this by explicitly writing down the functions.

Proposition 5.13 (Symmetry-Adapted Waves). *Let $R \cong \mathbb{R}$ and $Z \cong \mathbb{Z}$ be closed abelian isometry groups and $\mathbf{E}_{\omega,\mathbf{k}_0}$ be a plane wave with frequency $\omega > 0$ and wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$. For $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{T}$, the non-trivial symmetry-adapted waves with respect to R and Z are explicitly given as follows.*

(1) *When R is a group of translations, i.e. $\mathbf{Q}_R(a) = \mathbf{I}$, $\mathbf{c}_R(a) = \tau a\mathbf{e}$ for some $\tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$ and all $a \in \mathbb{R}$, then*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\alpha} = \mathbf{E}_{\omega,\mathbf{k}_0}, \quad \alpha = -\tau\mathbf{k}\cdot\mathbf{e}.$$

(2) *When R is a group of screw displacements, i.e. $\mathbf{Q}_R(a) = \mathbf{R}_{\lambda a}$ and $\mathbf{c}_R(a) = \tau a\mathbf{e}$ for some $\lambda, \tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$ and all $a \in \mathbb{R}$, then*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\alpha} = \mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}, \quad \ell := \frac{\alpha + \tau\mathbf{k}\cdot\mathbf{e}}{\lambda} \in \mathbb{Z}.$$

(3) *When Z is a group of translations, i.e. $\mathbf{Q}_Z(j) = \mathbf{I}$ and $\mathbf{c}_Z(j) = \tau j\mathbf{e}$ for some $\tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$ and all $j \in \mathbb{Z}$, then*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\beta} = \mathbf{E}_{\omega,\mathbf{k}_0} \quad \beta = -\tau\mathbf{k}\cdot\mathbf{e} \mod 2\pi.$$

(4) *When Z is a group of screw displacements, i.e. $\mathbf{Q}_Z(j) = \mathbf{R}_{\lambda j}$ and $\mathbf{c}_Z(j) = \tau j\mathbf{e}$ for some $\lambda, \tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$ and all $j \in \mathbb{Z}$, then*
   (a) *when $\beta + \tau\mathbf{k}\cdot\mathbf{e} \neq 0 \mod 2\pi$, then*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\beta} = \mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}, \quad \ell := \frac{\beta + \tau\mathbf{k}\cdot\mathbf{e}}{\lambda} \mod 2\pi \in \mathbb{Z}.$$

   (b) *when $\beta + \tau\mathbf{k}\cdot\mathbf{e} = 0 \mod 2\pi$, then*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\beta} = \frac{1}{\lambda q}\mathbf{E}_{\omega,\mathbf{k}_0}, \quad \lambda = 2\pi\frac{p}{q}, p \in \mathbb{Z}\setminus\{0\}, q \in \mathbb{N}.$$

(5) *When Z is a group of glide reflections, i.e. $\mathbf{Q}_Z(1) = \mathbf{I} - 2\mathbf{e}\otimes\mathbf{e}$, $\mathbf{c}_Z(1) = \tau\mathbf{c}_\perp$ for some $\mathbf{e} \in \mathbb{S}^2$, $\tau \neq 0$ and $\mathbf{c}_\perp \in \mathbf{e}^\perp \cap \mathbb{S}^2$, then, when defining $\widetilde{\mathbf{n}} := \mathbf{Q}_Z(1)\mathbf{n}$ and $\widetilde{\mathbf{k}_0} := \mathbf{Q}_Z(1)\mathbf{k}_0$,*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\beta} = \begin{cases} \frac{1}{2}(\mathbf{E}_{\omega,\mathbf{k}_0} + \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}), & \beta = -\tau\mathbf{k}\cdot\mathbf{c}_\perp \mod 2\pi,\ \tau\mathbf{k}\cdot\mathbf{c}_\perp \notin \pi\mathbb{Z}, \\ \frac{1}{2}(\mathbf{E}_{\omega,\mathbf{k}_0} - \mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}), & \beta = \tau\mathbf{k}\cdot\mathbf{c}_\perp \mod 2\pi,\ \tau\mathbf{k}\cdot\mathbf{c}_\perp \notin \pi\mathbb{Z}, \\ \mathbf{E}_{\omega,\mathbf{k}_0}, & \beta = \tau\mathbf{k}\cdot\mathbf{c}_\perp \mod 2\pi, \tau\mathbf{k}\cdot\mathbf{c}_\perp \in \pi\mathbb{Z} \end{cases}.$$

In particular, $\mathbf{E}_{\omega,\mathbf{k}_0,\alpha} \in \mathrm{R}_b^{\omega,\alpha}(R)$ and $\mathbf{E}_{\omega,\mathbf{k}_0,\beta} \in \mathrm{R}_b^{\omega,\beta}(Z)$ in all the cases.

Proof. As in all the cases, the functions are plane waves, twisted waves or sums of two plane waves, they are obviously elements of R_b^ω. The proper invariance is shown as

follows. For $\psi \in \mathcal{F}M^1(\mathbb{R})$ and $b \in \mathbb{R}$ we get

$$\begin{aligned}(\mathbf{Q}_R(b)|\mathbf{c}_R(b))\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\psi) &= (\mathbf{Q}_R(b)|\mathbf{c}_R(b))\int_{\mathbb{R}}(\mathbf{Q}_R(a)|\mathbf{c}_R(a))\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\mathrm{d}\widehat{\psi}(a)\\ &= \int_{\mathbb{R}}(\mathbf{Q}_R(a+b)|\mathbf{c}_R(a+b))\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\mathrm{d}\widehat{\psi}(a)\\ &= \int_{\mathbb{R}}(\mathbf{Q}_R(a)|\mathbf{c}_R(a))\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\mathrm{d}\widehat{\psi}(a-b)\\ &= \int_{\mathbb{R}}(\mathbf{Q}_R(a)|\mathbf{c}_R(a))\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})\mathrm{d}\widehat{e^{ib\cdot}\psi}(a)\\ &= \mathbf{E}_{\mathbf{x}}(\widehat{e^{ib\cdot}\psi}) = (e^{ib\cdot}\cdot\widehat{\mathbf{E}_{\mathbf{x}}})\psi,\end{aligned}$$

where $\mathbf{E}_{\mathbf{x}}(a) = (\mathbf{Q}_R(a)|\mathbf{c}_R(a))\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^3$, $a \in \mathbb{R}$.

Thus, for $\alpha \in \mathbb{R}$,

$$\begin{aligned}(\mathbf{Q}_R(b)|\mathbf{c}_R(b))\mathbf{E}_{\omega,\mathbf{k}_0,\alpha} &= (\mathbf{Q}_R(b)|\mathbf{c}_R(b))\mathcal{Z}_R\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\mathbf{1}_{\{\alpha\}})\\ &= (e^{ib\cdot}\cdot\widehat{\mathbf{E}_{\mathbf{x}}})(\mathbf{1}_{\{\alpha\}}) = e^{ib\alpha}\mathbf{E}_{\omega,\mathbf{k}_0,\alpha}(\mathbf{x}).\end{aligned}$$

For Z the invariance follows analogously.

The explicit formulas in cases (1)-(3) and (4a) follow directly from Lemma 5.11 by evaluating at $\mathbf{1}_{\{\alpha\}}$ and $\mathbf{1}_{\{\beta\}}$, respectively.

In case (4b), when $\beta + \tau\mathbf{k}\cdot\mathbf{e} = 0 \mod 2\pi$, say $\alpha + \tau\mathbf{k}\cdot\mathbf{e} = 2\pi\ell$, $\ell \in \mathbb{Z}$, then the equation $\lambda n + 2\pi(m-\ell) = 0$ has to be solved for $(n,m) \in \mathbb{Z}^2$. Let $m' := m - \ell$, then $m' = -\frac{\lambda}{2\pi}n$, s.t. this equation has no solution for $\lambda \notin 2\pi\mathbb{Q}$. When $\lambda = 2\pi\frac{p}{q}$, $p \in \mathbb{Z}\setminus\{0\}$, $q \in \mathbb{N}$, then $(n, -\frac{p}{q}n)$, $n \in q\mathbb{Z}$, are all solutions. Thus, in 'physics notation':

$$\begin{aligned}\mathcal{Z}_Z\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x},\mathbf{1}_{\{\beta\}}) &= 2\pi\sum_{\ell\in\lambda q\mathbb{Z}}\mathbf{E}^{(\ell)}_{\omega,\mathbf{k}_0}(\mathbf{x}) = 2\pi\sum_{\ell\in\lambda q\mathbb{Z}}\int_{-\pi}^{\pi}e^{-ia\ell}\mathbf{R}_a\mathbf{n}e^{i\mathbf{R}_a\mathbf{k}\cdot\mathbf{x}}\mathrm{d}a\\ &= 2\pi\int_{-\pi}^{\pi}\sum_{\ell\in\lambda q\mathbb{Z}}e^{-ia\ell}\mathbf{R}_a\mathbf{n}e^{i\mathbf{R}_a\mathbf{k}\cdot\mathbf{x}}\mathrm{d}a = 2\pi\int_{-\pi}^{\pi}\delta(a\lambda q)\mathbf{R}_a\mathbf{n}e^{i\mathbf{R}_a\mathbf{k}\cdot\mathbf{x}}\mathrm{d}a\\ &= \frac{2\pi}{\lambda q}\mathbf{n}e^{i\mathbf{k}\cdot\mathbf{x}} = \frac{2\pi}{\lambda q}\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}).\end{aligned}$$

In case (5), the third row results from the fact that when $\beta = \tau\mathbf{k}\cdot\mathbf{c}_\perp \in \pi\mathbb{Z}$, then $\beta \in 2\pi\mathbb{Z} + \tau\mathbf{k}\cdot\mathbf{c}_\perp$ and $\beta \in 2\pi\mathbb{Z} - \tau\mathbf{k}\cdot\mathbf{c}_\perp$, s.t. the $\mathbf{E}_{\omega,\widetilde{\mathbf{k}_0}}$-terms cancel while the others sum to $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x})$. □

As a corollary, we get the scalar symmetry-adapted waves for the single non-compact factors by replacing $\mathbf{E}_{\omega,\mathbf{k}_0}$ by $e_{\omega,\mathbf{k}_0}$ with the appropriate action of E(3). In particular, the

scalar twisted waves $e^{(\ell)}_{\omega,\mathbf{k}_0}$ are given in cylindrical coordinates $\mathbf{x} = \xi_{\mathbf{e}}(r,\varphi,z)$ by

$$e^{(\ell)}_{\omega,\mathbf{k}_0}(r,\varphi,z) = J_\ell(\widehat{r}r)e^{-i(\ell(\varphi+\varphi_0)+\widehat{z}z)}, \quad \text{where } \mathbf{k}_0 = \mathbf{R}_{\varphi_0}(0,\widehat{r},\widehat{z})^T. \tag{5.18}$$

The scalar versions of the projections with respect to a glide reflection can also be given more explicitly. Decomposing the wave vector $\mathbf{k} = \mathbf{k}_\perp + \mathbf{k}_\mathbf{e}$ with $\mathbf{k}_\perp \cdot \mathbf{e} = 0$ and $\mathbf{k}_\mathbf{e} \in \mathbb{R}\mathbf{e}$, we find that

$$e_{\omega,\mathbf{k}_0,\beta}(\mathbf{x}) = \begin{cases} e^{i\mathbf{k}_\perp\cdot\mathbf{x}}\cos(\mathbf{k}_\mathbf{e}\cdot\mathbf{x}), & \beta = -\tau\mathbf{k}\cdot\mathbf{c}_\perp \mod 2\pi,\ \tau\mathbf{k}\cdot\mathbf{c}_\perp \notin \pi\mathbb{Z}, \\ ie^{i\mathbf{k}_\perp\cdot\mathbf{x}}\sin(\mathbf{k}_\mathbf{e}\cdot\mathbf{x}), & \beta = \tau\mathbf{k}\cdot\mathbf{c}_\perp \mod 2\pi,\ \tau\mathbf{k}\cdot\mathbf{c}_\perp \notin \pi\mathbb{Z}, \\ e_{\omega,\mathbf{k}_0}(\mathbf{x}), & \beta = \tau\mathbf{k}\cdot\mathbf{c}_\perp \mod 2\pi,\ \tau\mathbf{k}\cdot\mathbf{c}_\perp \in \pi\mathbb{Z}. \end{cases} \tag{5.19}$$

Having explicitly determined the symmetry-adapted waves for the single factors of an abelian design group, we can gather our results to treat the general case.

First, we determine the characters of an abelian design group G. Let

$$G = K \times \prod_{j=1}^{n} R_j \times \prod_{k=1}^{m} Z_k \cong K \times \mathbb{R}^n \times \mathbb{Z}^m$$

be the decomposition of G according to Lemma 5.1, i.e. K is compact, $R_j \cong \mathbb{R}$ for $j = 1,\dots,n$, and $Z_k \cong \mathbb{Z}$, $k = 1,\dots,m$. Let $\iota : G \to K \times \mathbb{R}^n \times \mathbb{Z}^m$ be an isomorphism. The characters of G are then given by

$$\chi_G^{(\chi_K,\alpha,\beta)}(g) = \chi^{(\chi_K,\alpha,\beta)}(\iota(g)) := \chi_K(k)e^{i(\alpha\cdot\mathbf{a}+\beta\cdot\mathbf{b})},$$

for some $(\chi_K,\alpha,\beta) \in \widehat{K} \times \mathbb{R}^n \times \mathbb{T}^m$, where $\iota(g) = (k,\mathbf{a},\mathbf{b}) \in K \times \mathbb{R}^n \times \mathbb{Z}^m$. We define the symmetry-adapted waves for the following three classes of abelian design groups.

Definition 5.14 (Symmetry-Adapted Waves – Abelian Design Group). *Let $G \leq \mathrm{E}(3)$ be an abelian design group. The symmetry-adapted waves with wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$, $\mathbf{k}_0 \in \mathbb{S}^2$, $\omega > 0$, are defined as follows.*

(1) *When $G = K \times \prod_{j=1}^n R_j \times \prod_{k=1}^m Z_k$, where K is compact, and the group $T := \prod_{j=1}^n R_j \times \prod_{k=1}^m Z_k$ is a translation group, then for $\chi_G = \chi^{(\chi_K,\alpha,\beta)} \circ \iota \in \widehat{G}$ with $(\chi_K,\alpha,\beta) \in \widehat{K} \times \mathbb{R}^n \times \mathbb{T}^m$,*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\chi_G} := P_K^{\chi_K} \circ P_{R_1}^{(\alpha_1)} \circ \cdots \circ P_{R_n}^{(\alpha_n)} \circ P_{Z_1}^{(\beta_1)} \circ \cdots \circ P_{Z_m}^{(\beta_m)} \mathbf{E}_{\omega,\mathbf{k}_0}.$$

(2) *When $G = K \times S$ with K compact, $S \cong \mathbb{R}$ or $S \cong \mathbb{Z}$ a group of screw displacements and $\chi_G = \chi^{(\chi_K,\alpha)} \circ \iota \in \widehat{G}$ with $(\chi_K,\alpha) \in \widehat{K} \times \mathbb{R}$ or $(\chi_K,\alpha) \in \widehat{K} \times \mathbb{Z}$, then*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\chi_G} := P_K^{\chi_K} \circ P_S^{(\alpha)} \mathbf{E}_{\omega,\mathbf{k}_0}.$$

(3) *When $G = K$ compact and $\chi_K \in \widehat{K}$ then*

$$\mathbf{E}_{\omega,\mathbf{k}_0,\chi_K} := P_K^{\chi_K} \mathbf{E}_{\omega,\mathbf{k}_0}.$$

That these symmetry-adapted waves are well-defined can be seen as follows. The operators $P_{Z_k}^{(\beta_k)}$ and $P_{R_j}^{(\alpha_j)}$ in case (1) map plane waves to plane waves by Definition 5.12 and Proposition 5.13. The operator $P_S^{(\alpha)}$ in case (2) maps a plane wave to a twisted wave by Proposition 5.13, again. Finally, the operator $P_K^{\chi_K}$ maps from R_b^ω to R_b^ω by Proposition 5.4. So, $\mathbf{E}_{\omega,\mathbf{k}_0,\chi_G} \in \mathrm{R}_b^\omega$. The right transformation under group action follows from the facts that the single operators map to the respective spaces of invariant functions and that the group is abelian.

Before we study the usage of symmetry-adapted waves for the analysis of molecular structures, we determine the set of symmetry-adapted waves for some specific abelian design groups.

3.1. Examples: Symmetry-Adapted Waves. Let $G = T = \{(\mathbf{I}|\mathbf{c}).\ \mathbf{c} \in \mathbb{R}^3\}$ be the translation group. It is isomorphic to $\mathbb{R}^3$, s.t. the symmetry-adapted waves are projections with respect to three groups that are isomorphic to $\mathbb{R}$. Let $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ be an orthonormal basis of $\mathbb{R}^3$, then T can be written as the direct product $T = \prod_{j=1}^3 R_j$, where $R_j := \{(\mathbf{I}|a\mathbf{e}_j).\ a \in \mathbb{R}\}$, $j = 1, 2, 3$.

According to Proposition 5.13, when $\chi^{(\alpha_j)}((\mathbf{I}|a\mathbf{e}_j)) := e^{i\alpha_j a}$, $\alpha_j, a \in \mathbb{R}$, is a character of R_j and $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$ for some $\omega > 0$ and $\mathbf{k}_0 \in \mathbb{S}^2$, then $\mathbf{E}_{\omega,\mathbf{k}_0,\alpha_1} = \mathbf{E}_{\omega,\mathbf{k}_0}$ if and only if $\mathbf{k}_j := \mathbf{k} \cdot \mathbf{e}_j = -\alpha_j$.

Thus, the symmetry adapted plane waves are given by

$$\mathbf{E}_{\omega,\mathbf{k}_0,-\mathbf{k}}(\mathbf{x}) = \mathbf{n} e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{for } \mathbf{x} \in \mathbb{R}^3.$$

For every character $\chi^{(\alpha)}$ of $\mathbb{R}^3$ the corresponding non-trivial symmetry-adapted waves are the ones with wavevector $\mathbf{k} = -\alpha \in \mathbb{R}^3$.

The radiation family that our design suggests to use for the analysis of structures that are generated by discrete closed subgroups of T, namely crystal structures, is the family of plane waves. We already got that result from the design equation, as we did for the case of degenerated two-dimensional crystal structures.

For the group $R = \{(\mathbf{I}|a\mathbf{e}).\ a \in \mathbb{R}\} \cong \mathbb{R}$ of translations along an axis in direction $\mathbf{e} \in \mathbb{S}^2$, the corresponding structures are the degenerated case of one-dimensional crystal structures. The design equations for this group yield a very large set of solutions. We determine the set of symmetry-adapted waves for this case. By Proposition 5.13, given a character $\chi^{(\alpha)}((\mathbf{I}|a\mathbf{e})) = e^{i\alpha a}$, $a \in \mathbb{R}$, the wave vectors of the non-trivial symmetry-adapted waves satisfy $\mathbf{k} \cdot \mathbf{e} = -\alpha$. These are the wave vectors in the plane $-\alpha\mathbf{e} + \mathbf{e}^\perp$. The

union of all these planes is again the whole space $\mathbb{R}^3$, s.t. the symmetry-adapted waves turn out to be once again the family of plane waves.

Let's consider a discrete translation group $B = \{(\mathbf{I}|\mathbf{b}).\ \mathbf{b} \in \mathcal{B}\}$, where $\mathcal{B} = \mathbf{A}\mathbb{Z}^3$ is a Bravais lattice generated by $\mathbf{A} \in \mathrm{GL}(3,\mathbb{R})$. The dual group $\widehat{B}$ is parametrized by a unit cell of the reciprocal lattice $\mathcal{B}^\perp$. Let $\mathbf{A}^\perp := 2\pi\mathbf{A}^{-T}$ be the generator of the reciprocal lattice, then the corresponding canonical unit cell of $\mathcal{B}^\perp$ is given by

$$\mathrm{U}_{\mathcal{B}^\perp} := \mathbf{A}^\perp[0,1)^3.$$

The characters are thus of the form

$$\chi^{(\mathbf{b}')}((\mathbf{I}|\mathbf{b})) = e^{i\mathbf{b}'\cdot\mathbf{b}}, \quad \mathbf{b}' \in \mathrm{U}_{\mathcal{B}^\perp},\ \mathbf{b} \in \mathcal{B}.$$

Consequently, the symmetry-adapted waves $\mathbf{E}_{\omega,\mathbf{k}_0,\mathbf{b}'}$ are the plane waves with wave vector $\mathbf{k} \in -\mathrm{U}_{\mathcal{B}^\perp}$. Of course, one could also parametrize the dual group with $-\mathrm{U}_{\mathcal{B}^\perp}$ and end up with the wave vectors $\mathbf{k} \in \mathrm{U}_{\mathcal{B}^\perp}$.

In the case that the design group is the trivial group, describing the class of structures that have no symmetry at all, the symmetry-adapted waves are also the plane waves. In this sense, CDI is the right choice for the analysis of arbitrary structures according to our design.

Another very degenerate case is the case of the compact group $\mathbb{T}$ acting by rotations about an axis $\mathbb{R}\mathbf{e}$, $\mathbf{e} \in \mathbb{S}^2$. The characters are of the form $\chi^{(\alpha)}(\mathbf{R}_{\widehat{\varphi}}) = e^{i\alpha\widehat{\varphi}}$, $\widehat{\varphi} \in \mathbb{T}$, $\alpha \in \mathbb{Z}$. We already discussed that the solution space of the design equations is too big for structure analysis. The symmetry-adapted waves give the right choice of invariant fields. They can be determined via the projection operators:

$$\mathbf{E}_{\omega,\mathbf{k}_0,\alpha}(\mathbf{x}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\alpha\widehat{\varphi}}\mathbf{R}_{\widehat{\varphi}}\mathbf{n}e^{i\mathbf{k}\cdot\mathbf{R}_{-\widehat{\varphi}}\mathbf{x}}\mathrm{d}\widehat{\varphi}.$$

These are exactly the twisted waves, $\mathbf{E}_{\omega,\mathbf{k}_0,\alpha} = \mathbf{E}^{(\alpha)}_{\omega,\mathbf{k}_0}$.

A new kind of radiation are the symmetry-adapted waves with respect to a finite rotation group. Let $C_n := \{(\mathbf{R}_{2\pi j/n}|0).\ j = 0,\dots,n-1\}$ be the n-fold rotation group about the axis $\mathbb{R}\mathbf{e}$. The characters are given by $\chi^{(\alpha)}(\mathbf{R}_{2\pi j/n}) = e^{2\pi i\alpha j/n}$, $\alpha = 0,\dots,n-1$. Again, as the group is compact, the symmetry-adapted waves are given by the projections

$$\mathbf{E}_{\omega,\mathbf{k}_0,\alpha}(\mathbf{x}) = \frac{1}{n}\sum_{j=1}^{n} e^{2\pi i\alpha j/n}\mathbf{R}_{2\pi j/n}\mathbf{n}e^{i\mathbf{k}\cdot\mathbf{R}_{-2\pi j/n}\mathbf{x}}, \quad \mathbf{x} \in \mathbb{R}^3. \tag{5.20}$$

We call these waves n-twisted waves. A cross-section of the absolute value of a 5-twisted wave perpendicular to the axis reveals a quasi-crystalline pattern (see Figure 5.1). This is due to the fact that the Fourier transform of this wave has by construction a 5-fold axis

and is discrete. It might be possible to exploit this relationship between the symmetries of n-fold waves and quasicrystals.

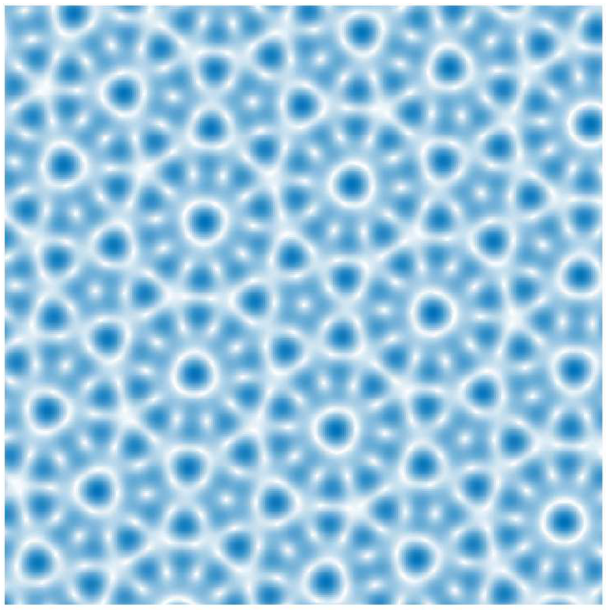


FIGURE 5.1. A slice through the absolute value of a 5-twisted wave showing its quasicrystalline nature.

The n-fold twisted waves might also be useful for the analysis of nanotube structures with a finite isogonal point group. By simple plane wave radiation, the order n of the isogonal point group can be determined. Consequently, the order of the rotational symmetry of the structure divides n making the n-fold twisted waves a possible radiation family for analysis. These waves might be easier to produce than twisted waves as only n single plane waves have to be phase aligned.

CHAPTER 6

Radiation Design for Abelian Design Groups

In this central chapter, we will investigate the scattering of symmetry-adapted waves by invariant structures for abelian design groups.

First, we need to understand the relation between symmetry-adapted waves and the charge density. For this purpose, we introduce the generalized Zak transform on our model space $\mathcal{S}(\mathbb{R}^3)$. This transform has applications in quantum mechanics and signal processing in its classic form (see [Zak67, Kut02]). It carries the structure of the design group to the function space, making it possible to transfer results on the group structure, like the Poisson summation formula, to the space of charge densities.

We find that we can decompose the charge density into scalar symmetry-adapted waves. This motivates the introduction of the scalar wave transform – the integral transform of the density with the scalar symmetry-adapted waves being the integral kernel. This transform is a function on the space of radiation parameters , which are $(\omega, \mathbf{k}_0, \chi) \in (0, \infty) \times \mathbb{S}^2 \times \widehat{G}$, and is closely related to the Fourier transform on $\mathbb{R}^3$ and the Zak transform with respect to the design group G. The scalar wave transform will turn out to be the generalization of the scalar transforms that appear in the phase retrieval problem for plane waves and twisted waves.

When a function is invariant with respect to a discrete closed subgroup of the design group, the scalar wave transform is supported on the orthogonal group. This fact is central for the derivation of the generalized von Laue condition.

We lift the scalar theory to the vector-valued case by introducing the vector-valued wave transform that is seen to be closely related to the radiation transform with respect to symmetry-adapted waves. We show that this transform is invertible and infer the central result. If the isogonal point group of the design group fixes a non-trivial vector, then the symmetry can be reconstructed directly from intensity measurements, and the reconstruction problem reduces to a scalar phase problem. This is the generalized von Laue condition for abelian design groups and generalizes the classical as well as the twisted von Laue condition.

Finally, the phase retrieval problem for the inferred scalar phase problem is discussed shortly. The standard algorithms can be adapted to the general case in a straight-forward manner. Because of the close relation of the wave transform to the Fourier transforms on

$\mathbb{R}^3$ and G, the algorithms can be implemented in an efficient way using the Fast Fourier Transform.

1. The Scalar Wave Transform

In this section, we analyze the space of charge densities with respect to the action of the design group G. As a model space, we consider the space $\mathcal{S}(\mathbb{R}^3)$ of Schwartz functions. The restriction to non-negative functions is not necessary at this point – it will become important when we consider the phase retrieval problem later.

1.1. Zak Transform and Wigner Projections. We consider an abelian design group $G \leq \mathrm{E}(3)$. The natural action of $\mathrm{E}(3)$ on the space $\mathcal{S}(\mathbb{R}^3)$ is

$$(gf)\mathbf{x} := f(g^{-1}\mathbf{x}), \quad \text{for } f \in \mathcal{S}(\mathbb{R}^3),\ \mathbf{x} \in \mathbb{R}^3,\ g \in \mathrm{E}(3).$$

The Zak transform and the Wigner projections with respect to this action are then as usual defined as

Definition 6.1 (Zak Transform and Wigner Projections on $\mathcal{S}(\mathbb{R}^3)$ – abelian design group). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group, and $f \in \mathcal{S}(\mathbb{R}^3)$. The Zak transform $\mathcal{Z}_G f$ of f with respect to G is defined as*

$$\mathcal{Z}_G f(\mathbf{x}, \chi) := \mathcal{F}_G f_{\mathbf{x}}(\chi), \quad \textit{for } \mathbf{x} \in \mathbb{R}^3,\ \chi \in \widehat{G}. \tag{6.1}$$

Given $\chi \in \widehat{G}$, the projection operator P_G^χ is defined as

$$P_G^\chi f(\mathbf{x}) := \mathcal{Z}_G f(\mathbf{x}, \chi) \quad \textit{for } \mathbf{x} \in \mathbb{R}^3. \tag{6.2}$$

Remark 6.2 (Classic Zak transform). *The classic Zak transform (see [Zak67]) is the special case of the non-compact abelian group $a\mathbb{Z}$ acting on $\mathbb{R}$ by translations. The dual group of $a\mathbb{Z}$ is the torus group $a^{-1}\mathbb{T}$, s.t. the Zak transform $\mathcal{Z}_a$ of a function $f \in \mathcal{S}(\mathbb{R})$, for example, is (up to sign and normalization conventions) given by*

$$\mathcal{Z}_a f(x, \omega) := \mathcal{F}_{\mathbb{Z}} f_x(\omega) = \sum_{j \in \mathbb{Z}} f(x - aj) e^{-iaj\omega}. \tag{6.3}$$

The Zak transform has been successfully applied in quantum mechanics and signal processing. It has also been generalized to the action of a lattice on a quite general class of locally compact groups in [Kut02].

We summarize some properties of the Zak transform in the following lemma.

Lemma 6.3 (Properties of the Zak Transform on $\mathcal{S}(\mathbb{R}^3)$). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group. For all $\chi \in \widehat{G}$, the Wigner projection $P_G^\chi f$ of a function*

$f \in \mathcal{S}(\mathbb{R}^3)$ is a tempered function that satisfies

$$gP_G^\chi f = \chi(g) P_G^\chi f \quad \textit{for all } g \in G. \tag{6.4}$$

The inverse Zak transform is given by

$$\mathcal{Z}_G^{-1} F(\mathbf{x}) := \mathcal{F}_G^{-1} F(\mathbf{x}, \mathrm{id}_{\mathbb{R}^3}), \quad \mathbf{x} \in \mathbb{R}^3, \tag{6.5}$$

for $F : \mathbb{R}^3 \times \widehat{G} \to \mathbb{C}$ with $\chi \mapsto F(\mathbf{x}, \chi) \in \mathcal{F}L^1(G)$ for all $\mathbf{x} \in \mathbb{R}^3$.

When $G = K$ is compact, then

$$P_K^\chi \mathcal{S}(\mathbb{R}^3) \subseteq \mathcal{S}(\mathbb{R}^3), \quad \textit{and} \quad \mathcal{S}(\mathbb{R}^3) = \bigoplus_{\chi \in \widehat{G}} P_K^\chi \mathcal{S}(\mathbb{R}^3). \tag{6.6}$$

In this case, the Zak transform commutes with the Fourier transform on $\mathbb{R}^3$, i.e.

$$\mathcal{Z}_K \circ \mathcal{F} = \mathcal{F} \circ \mathcal{Z}_K.$$

Proof. The form of the inverse Zak transform follows immediately from the definition of the Zak transform.

Given a function $f \in \mathcal{S}(\mathbb{R}^3)$ and a character $\chi \in \widehat{G}$, the projection $P_G^\chi f$ is bounded and continuous, since the function $f_{\mathbf{x}} : G \to \mathbb{C}$ is integrable. In addition, all derivatives of $P_G^\chi f$ are bounded, because we can exchange the order of differentiation and projection via dominated convergence. The boundedness follows then from the fact that the derivative of f is again a Schwartz function.

The action of G on $P_G^\chi f$ yields

$$gP_G^\chi f(\mathbf{x}) = \int_G \overline{\chi(h)}((gh)f)(\mathbf{x}) \mathrm{d}\mu_G(h) = \int_G \overline{\chi(g^{-1}h)}(hf)(\mathbf{x}) \mathrm{d}\mu_G(h) = \chi(g) P_G^\chi f(\mathbf{x}).$$

When $G = K$ is compact, the Wigner projection of a Schwartz function is a compact integral of Schwartz functions and hence again a Schwartz function. The invariance property plus the orthogonality relations of the characters yields the direct sum decomposition just as for R_b^ω in Proposition 5.4.

That for compact design group, the Zak transform commutes with the Fourier transform on $\mathbb{R}^3$ uses the fact that $K \leq \mathrm{O}(3)$.

$$\begin{aligned}
\widehat{P_K^\chi f}(\mathbf{k}) &= \int_{\mathbb{R}^3} e^{-i\mathbf{k}\cdot\mathbf{x}} \int_K \overline{\chi(g)} f(g^{-1}\mathbf{x}) \mathrm{d}\mu_K(g) \mathrm{d}\mathbf{x} \\
&= \int_K \overline{\chi(g)} \int_{\mathbb{R}^3} e^{-i\mathbf{k}\cdot\mathbf{x}} f(g^{-1}\mathbf{x}) \mathrm{d}\mathbf{x} \mathrm{d}\mu_K(g) \\
&= \int_K \overline{\chi(g)} \int_{\mathbb{R}^3} e^{-ig^{-1}\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) \mathrm{d}\mathbf{x} \mathrm{d}\mu_K(g) = P_K^\chi \widehat{f}(\mathbf{k}).
\end{aligned}$$

□

The Zak transform carries the structure of the group G to a function space. This is best seen by the following important proposition that shows that the Zak transform of invariant functions is of a very special form.

For this purpose, we need to generalize the Zak transform using the generalization of the Fourier transform on G to bounded continuous function in Definition 5.8. For $f \in C_b(G)$, we define

$$\mathcal{Z}_G f(\mathbf{x}, \psi) := \mathcal{F}_G f_{\mathbf{x}}(\psi), \quad \text{for all } \psi \in \mathcal{F}M^1(G). \tag{6.7}$$

We can then show the following:

Proposition 6.4 (Zak Transform of Invariant Functions). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group and $H \leq G$ a discrete closed subgroup of G. When f is an H-invariant function, s.t. $f_{\mathbf{x}}$ is compactly supported on a fundamental domain of H, then*

$$\mathcal{Z}_G f(\mathbf{x}, \chi) = \mathcal{Z}_{G/H} f(\mathbf{x}, \chi \downarrow^G_{G/H}) \delta_{H_G^\perp}(\chi) \tag{6.8}$$

in the distributional sense.

Proof. We use the Poisson summation formula for locally compact abelian groups (see [Fol95], Theorem 4.42, or [Rei68], Ch. 5, 5.). Choose a fundamental domain of H and identify it with G/H. Let $\psi \in \mathcal{F}M^1(G)$ and $\mathbf{x} \in \mathbb{R}^3$. Then

$$\begin{aligned}
\mathcal{Z}_G f(\mathbf{x}, \psi) = \mathcal{F}_G f_{\mathbf{x}}(\psi) &= \int_G f_{\mathbf{x}}(g) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) = \int_G \sum_{h \in H} f_{\mathbf{x}}\big|_{G/H}(hg) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) \\
&\overset{\text{Poisson}}{=} \int_G \int_{H_G^\perp} \mathcal{F}_G f_{\mathbf{x}}\big|_{G/H}(\chi)\chi(g) \mathrm{d}\mu_{H_G^\perp}(\chi) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) \\
&= \int_{H_G^\perp} \mathcal{Z}_{G/H} f(\mathbf{x}, \chi \downarrow^G_{G/H}) \int_G \chi(g) \mathrm{d}\mathcal{F}_{\widehat{G}}\psi(g) \mathrm{d}\mu_{H_G^\perp}(\chi) \\
&= \int_{H_G^\perp} \mathcal{Z}_{G/H} f(\mathbf{x}, \chi \downarrow^G_{G/H}) \psi(\mathbf{x}) \mathrm{d}\mu_{H_G^\perp}(\chi),
\end{aligned}$$

where we used the Fourier inversion formula on $M^1(G)$. □

Proposition 6.4 shows that the Zak transform has the potential to induce resonance of the unit cells of an invariant structure. Consequently, for radiation design we need to implement the Zak transform via an integral transform. We introduce and study the natural choice for such a transform, next.

1.2. The Scalar Wave Transform. Lemma 6.3 tells us how to decompose a Schwartz function into invariant functions. But what we really want, is to decompose it into scalar versions of time-harmonic radiation that are invariant. The Fourier transform is the natural representation of a function in terms of 'scalar radiation'. For compact design groups

K, we can make this radiation invariant using Proposition 5.4. We decompose the scalar plane waves into its invariant components.

Let $f \in \mathcal{S}(\mathbb{R}^3)$, and $e_{\omega,\mathbf{k}_0}(\mathbf{x}) := e^{i\mathbf{k}\cdot\mathbf{x}}$, $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$, the scalar plane waves. Then we can decompose $e_{\omega,\mathbf{k}_0}$ into its invariant components, which are the scalar symmetry-adapted waves: $e_{\omega,\mathbf{k}_0,\chi} := P_K^\chi(e_{\omega,\mathbf{k}_0}) \in C_b(\mathbb{R}^3)$:

$$e_{\omega,\mathbf{k}_0} = \sum_{\chi\in\widehat{K}} e_{\omega,\mathbf{k}_0,\chi}.$$

Then, Fourier-expanding f, we get

$$f(\mathbf{x}) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e_{\omega,\mathbf{k}_0}(\mathbf{x})\widehat{f}(\mathbf{k})\mathrm{d}\mathbf{k} = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\sum_{\chi\in\widehat{K}} e_{\omega,\mathbf{k}_0,\chi}(\mathbf{x})\widehat{f}(\mathbf{k})\mathrm{d}\mathbf{k}. \tag{6.9}$$

In view of this decomposition, we introduce the following transform that will turn out to be the natural choice for the analysis of invariant structures.

Definition 6.5 (Scalar Wave Transform). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group and $f \in \mathcal{S}(\mathbb{R}^3)$. We define the scalar wave transform $\mathcal{W}_G f$ of f with respect to G by*

$$\mathcal{W}_G f(\mathbf{k},\chi) := \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0,\chi}(\mathbf{x})} f(\mathbf{x})\mathrm{d}\mathbf{x}, \tag{6.10}$$

where $e_{\omega,\mathbf{k}_0,\chi} := P_G^\chi e_{\omega,\mathbf{k}_0}$ is a scalar symmetry-adapted wave with wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$.

For compact design groups, the relation to the Zak and the Fourier transform is given in the following lemma. We also find the inverse scalar wave transform.

Lemma 6.6 (Properties of the Scalar Wave Transform – Compact Abelian Design Group). *Let $K \leq \mathrm{O}(3)$ be a compact abelian design group. The wave transform satisfies*

$$\mathcal{W}_K f = \mathcal{Z}_K \widehat{f} = \mathcal{F}\mathcal{Z}_K f \quad \text{for } f \in \mathcal{S}(\mathbb{R}^3). \tag{6.11}$$

In particular, the inverse wave transform $\mathcal{W}_K^{-1}$ is given by

$$\mathcal{W}_K^{-1} F := \mathcal{F}^{-1} \circ \mathcal{Z}_K^{-1} F = \mathcal{Z}_K^{-1} \circ \mathcal{F} F, \tag{6.12}$$

for functions $F : \mathbb{R}^3 \times \widehat{K} \to \mathbb{C}$, that lie in the image of $\mathcal{S}(\mathbb{R}^3)$ under $\mathcal{W}_K$.

Proof. Let $f \in \mathcal{S}(\mathbb{R}^3)$, $\mathbf{k} \in \mathbb{R}^3$ and $\chi \in \widehat{K}$. Then

$$\begin{aligned}\mathcal{W}_K f(\mathbf{k},\chi) &= \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0,\chi}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3}\int_K \chi(g) e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_K(g) f(\mathbf{x})\mathrm{d}\mathbf{x} \\ &= \int_K \chi(g) \int_{\mathbb{R}^3} e^{-ig\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mu_K(g) = \int_K \chi(g)\widehat{f}(g\mathbf{k})\mathrm{d}\mu_K(g) \\ &= \int_K \chi(g^{-1})\widehat{f}(g^{-1}\mathbf{k})\mathrm{d}\mu_K(g) = P_K^\chi \widehat{f}(\mathbf{k}) = \mathcal{Z}_K \widehat{f}(\mathbf{k},\chi),\end{aligned}$$

where we used Fubini, the fact that K is a group of orthogonal transformations and the inversion invariance of the Haar measure of a compact group. Now, in Lemma 6.3 we showed that for compact groups the Fourier transform and the Zak transform commute, showing that $\mathcal{W}_K = \mathcal{F}\mathcal{Z}_K$. The forms of the inverse transform follows immediately. □

For non-compact abelian design groups, the situation is a bit tricky, as we introduced the wave transform via the symmetry-adapted waves. The ad hoc construction of those does not allow a direct generalization of Lemma 6.6. Instead, we can show the invertibility of the scalar wave transform by reducing it to a scalar wave transfrom for a compact design group. We again do this only for the classes of design groups from Definition 5.14. We start by considering two examples.

Let $G = R \cong \mathbb{R}$ be a group of translations along an axis $\mathbb{R}\mathbf{e}$, $\mathbf{e} \in \mathbb{S}^2$. Then the group elements are given by $R = \{(\mathbf{I}|\tau a\mathbf{e}).\ a \in \mathbb{R}\}$ for some $\tau \neq 0$. The dual group $\widehat{R}$ of R is given by $\widehat{R} = \{\chi^{(\alpha)}.\ \alpha \in \mathbb{R}\}$, $\chi^{(\alpha)}(a) = e^{i\alpha a}$, $\alpha, a \in \mathbb{R}$. Now, consider the mapping

$$\varphi_R :\ \mathbb{R}^3 \to \widehat{R},\ \mathbf{k} \mapsto \chi^{(-\tau\mathbf{k}\cdot\mathbf{e})}.$$

This mapping is obviously surjective, since $\varphi_R^{-1}(\{\chi^{(\alpha)}\}) = \{\mathbf{k} \in \mathbb{R}^3.\ \mathbf{k}\cdot\mathbf{e} = -\alpha/\tau\}$ is a plane in $\mathbb{R}^3$ for every $\alpha \in \mathbb{R}$. Now, for $f \in \mathcal{S}(\mathbb{R}^3)$

$$\mathcal{W}_R f(\mathbf{k},\varphi_R(\mathbf{k})) = \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0,\varphi(\mathbf{k})}(\mathbf{x})} f(\mathbf{x})\mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0}(\mathbf{x})} f(\mathbf{x})\mathrm{d}\mathbf{x} = \widehat{f}(\mathbf{k}),$$

since $e_{\omega,\mathbf{k}_0,\varphi(\mathbf{k})} = e_{\omega,\mathbf{k}_0}$ when $\varphi_R(\mathbf{k}) = \chi^{(-\tau\mathbf{k}\cdot\mathbf{e})}$ by Proposition 5.13. So, the wave transform $\mathcal{W}_R f$ restricted to its support $\mathrm{supp}(\mathcal{W}_R f) \subseteq \{(\mathbf{k},\chi^{(\alpha)}) \in \mathbb{R}^3 \times \widehat{R}.\ \alpha = -\tau\mathbf{k}\cdot\mathbf{e}\}$ is nothing but the Fourier transform of f.

A similar argument works for a screw displacement group $G = S \cong \mathbb{R}$, given by $S = \{(\mathbf{R}_{\lambda a}|\tau a\mathbf{e}).\ a \in \mathbb{R}\}$, where $\lambda, \tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$. The dual group is then again given by $\widehat{S} = \{\chi^{(\alpha)}.\ \alpha \in \mathbb{R}\}$. We consider the mapping

$$\varphi_S :\ [0,\infty) \times \mathbb{Z} \times \mathbb{R} \to \mathbb{R}^3 \times \widehat{S},\ (\omega,\alpha,\widehat{z}) \mapsto (\mathbf{k}(\omega,\widehat{z}), \chi^{(\lambda\alpha - \tau\widehat{r})}),$$

where $\mathbf{k}(\omega, \widehat{z}) = (0, \widehat{z}, \widehat{r})^T$, $\widehat{r} := \sqrt{\frac{\omega^2}{c^2} - \widehat{z}^2}$. Then again by Proposition 5.13, we find that for $f \in \mathcal{S}(\mathbb{R}^3)$

$$\mathcal{W}_S f(\varphi_S(\omega, \alpha, \widehat{z})) = \int_{\mathbb{R}^3} \overline{e^{(\alpha)}_{\omega, \mathbf{k}_0(\omega,\widehat{z})}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x},$$

where $\mathbf{k}_0(\omega, \widehat{z}) := \frac{c}{\omega}\mathbf{k}(\omega, \widehat{z})$. So, the scalar wave transform $\mathcal{W}_S$ reduces to the twisted wave transform treated in Chapter 4.

This relation to the cases of plane and twisted waves can be generalized to our classes of design groups as follows.

Lemma 6.7 (The Scalar Wave Transform for Abelian Design Groups). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group.*

(1) *When $G = K \times T$, where K is compact and $T := \prod_{j=1}^n R_j \times \prod_{k=1}^m Z_k$ is a translation group with $R_j \cong \mathbb{R}$, $j = 1, \ldots, n$, and $Z_K \cong \mathbb{Z}$, $k = 1, \ldots, m$, then there is a function $\varphi_T : \mathbb{R}^3 \to \widehat{T}$, s.t. for $f \in \mathcal{S}(\mathbb{R}^3)$*

$$\mathcal{W}_G f(\mathbf{k}, (\chi_K, \varphi_T(\mathbf{k}))) = \mathcal{W}_K f(\mathbf{k}, \chi_K).$$

(2) *When $G = K \times S$ where K is compact and $S \cong \mathbb{R}$ or $S \cong \mathbb{Z}$ is a screw displacement group, then there is a function $\varphi_S : \mathbb{R}^3 \times \mathbb{Z} \to \widehat{S}$, s.t.*

$$\mathcal{W}_G f(\mathbf{k}, (\chi_K, \varphi_S(\mathbf{k}, \alpha))) = \mathcal{W}_{K\times\mathbb{T}} f(\mathbf{k}, \chi_K \cdot \chi^{(\alpha)}_{\mathbb{T}}).$$

Proof. In case (1), we consider the mapping

$$\varphi_T : \ \mathbb{R}^3 \to \widehat{T}, \ \mathbf{k} \mapsto (-\tau_1 \mathbf{k} \cdot \mathbf{e}_1, \ldots, -\tau_n \mathbf{k} \cdot \mathbf{e}_n, \widetilde{\tau}_1 \mathbf{k} \cdot \widetilde{\mathbf{e}}_1, \ldots, -\widetilde{\tau}_m \mathbf{k} \cdot \widetilde{\mathbf{e}}_m),$$

where $R_j = \{(\mathbf{I}|\tau_j a \mathbf{e}_j).\ a \in \mathbb{R}\}$, $\tau_j \neq 0$, $\mathbf{e}_j \in \mathbb{S}^2$, $j = 1, \ldots, n$, and $Z_k = \{(\mathbf{I}|\widetilde{\tau}_k j \widetilde{\mathbf{e}}_k).\ j \in \mathbb{Z}\}$, $\widetilde{\tau}_k \neq 0$, $\widetilde{\mathbf{e}}_k \in \mathbb{S}^2$, $k = 1, \ldots, m$.

Then for $\mathcal{S}(\mathbb{R}^3)$, we get

$$\mathcal{W}_T f(\mathbf{k}, \varphi_T(\mathbf{k})) = \widehat{f}(\mathbf{k})$$

using Proposition 5.13. Now, when $(\chi_K, \chi_T) \in \widehat{G} = \widehat{K} \times \widehat{T}$, then

$$\begin{aligned}\mathcal{W}_G f(\mathbf{k}, (\chi_K, \chi_T)) &= \int_{\mathbb{R}^3} \overline{P_K^{\chi_K} e_{\omega, \mathbf{k}_0, \chi_T}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} \\ &= \int_{\mathbb{R}^3} \int_K \chi_K(g) \overline{g e_{\omega, \mathbf{k}_0, \chi_T}(\mathbf{x})} \mathrm{d}\mu_K(g) f(\mathbf{x}) \mathrm{d}\mathbf{x}.\end{aligned}$$

Thus, when $\chi_T = \varphi_T(\mathbf{k})$, then

$$\begin{aligned}\mathcal{W}_G f(\mathbf{k}, (\chi_K, \varphi_T(\mathbf{k}))) &= \int_{\mathbb{R}^3} \int_K \chi_K(g) e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_K(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\ &= \int_{\mathbb{R}^3} \overline{e_{\omega, \mathbf{k}_0, \chi_K}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} = \mathcal{W}_K f(\mathbf{k}, \chi_K).\end{aligned}$$

In case (2), we consider the case $S \cong \mathbb{Z}$, because part of the case $S \cong \mathbb{R}$ was already treated above. Let $S = \{(\mathbf{R}_{\lambda j}|\tau j\mathbf{e}).\ j \in \mathbb{Z}\}$, $\lambda, \tau \neq 0$, $\mathbf{e} \in \mathbb{S}^2$. Then consider the mapping

$$\varphi_S :\ \mathbb{R}^3 \times \mathbb{Z} \to \widehat{S},\ (\mathbf{k}, \alpha) \mapsto \chi^{(\beta)},$$

where $\beta := \lambda\alpha - \tau\mathbf{k}\cdot\mathbf{e} \mod 2\pi$. Then by Proposition 5.13, we get that the scalar wave transform is given by $\mathcal{W}_S f(\varphi_S(\alpha, \widehat{z})) = \int_{\mathbb{R}^3} \overline{e^{(\alpha)}_{\omega,\mathbf{k}_0}(\mathbf{x})} f(\mathbf{x})\mathrm{d}\mathbf{x}$ just as in the case $S \cong \mathbb{R}$.

Now, $e^{(\alpha)}_{\omega,\mathbf{k}_0} = P^{(\alpha)}_{\mathbb{T}} e_{\omega,\mathbf{k}_0}$, where $\mathbb{T}$ acts via $\widehat{\varphi} \mapsto \mathbf{R}_{\widehat{\varphi}}$. Thus, for $\chi_K \in \widehat{K}$ and $f \in \mathcal{S}(\mathbb{R}^3)$

$$\begin{aligned}\mathcal{W}_G f(\mathbf{k}, (\chi_K, \varphi_S(\mathbf{k}, \alpha))) &= \int_{\mathbb{R}^3} \overline{P^{\chi_K}_K e^{(\alpha)}_{\omega,\mathbf{k}_0}(\mathbf{x})} f(\mathbf{x})\mathrm{d}\mathbf{x} \\ &= \int_{\mathbb{R}^3} \overline{P^{\chi_K}_K P^{(\alpha)}_{\mathbb{T}} e_{\omega,\mathbf{k}_0}(\mathbf{x})} f(\mathbf{x})\mathrm{d}\mathbf{x} = \mathcal{W}_{K\times\mathbb{T}} f(\mathbf{k}, \chi_K \cdot \chi^{(\alpha)}_{\mathbb{T}}).\end{aligned}$$

□

Thus, the treatment of the scalar wave transform for the considered classes reduces to the compact case. The construction can, of course, be also applied to different non-compact design groups. When the group is the product of a compact group K and a glide reflection group, for example, the corresponding compact group the scalar wave transform reduces to will be of the form $K \times \mathbb{Z}_2$, where $\mathbb{Z}_2$ acts by reflection.

As a corollary of Lemma 6.7, we immediately get the inverse transform for the non-compact cases considered there by using Lemma 6.6.

1.3. Generalized Translation Operators. Before we address the wave transform of invariant functions, we shortly discuss a different topic. Since we found that the plane waves and the twisted waves are the solutions to the design equations for the corresponding design groups, we ask ourselves, if we can motivate the symmetry-adapted waves in a similar way. For compact design groups, this is possible.

As elements of the invariant spaces $P^{\chi}_K \mathcal{S}(\mathbb{R}^3)$, the symmetry-adapted scalar plane waves $e_{\omega,\mathbf{k}_0,\chi}$ are simultaneous eigenfunctions of the group action. In fact they can be seen to be a complete set of simultaneous eigenfunctions of operators that are very natural in this context – the so-called generalized translation operators $T^K_{\mathbf{y}}$, $\mathbf{y} \in \mathbb{R}^3$. They are defined as follows:

$$T^K_{\mathbf{y}} f(\mathbf{x}) := \int_K f(\mathbf{x} - g^{-1}\mathbf{y})\mathrm{d}\mu_K(g) \quad \text{for } f \in C_b(\mathbb{R}^3),\ \mathbf{x} \in \mathbb{R}^3. \tag{6.13}$$

We can proof the following:

Proposition 6.8 (Generalized Translation Operators). *The generalized translation operators $T^K_{\mathbf{y}}$, $\mathbf{y} \in \mathbb{R}^3$ map bounded continuous functions to bounded continuous functions.*

Moreover, when $f \in C_b^\chi(\mathbb{R}^3) := P_K^\chi C_b(\mathbb{R}^3)$, $\chi \in \widehat{K}$, *then*

$$T_{\mathbf{y}}^K f = P_K^\chi f(\cdot - \mathbf{y}). \tag{6.14}$$

In particular, $T_{\mathbf{y}}^K C_b^\chi(\mathbb{R}^3) \subset C_b^\chi(\mathbb{R}^3)$.

The symmetry-adapted waves $e_{\omega,\mathbf{k}_0,\chi} \in C_b^\chi(\mathbb{R}^3)$, $\omega > 0$, $\mathbf{k}_0 \in \mathbb{S}^2$, *are simultaneous eigenfunctions of the generalized translation operators. In particular,*

$$T_{\mathbf{y}}^K e_{\omega,\mathbf{k}_0,\chi} = e_{\omega,\mathbf{k}_0,1}(\mathbf{y}) e_{\omega,\mathbf{k}_0,\chi} \quad \textit{for all } \mathbf{y} \in \mathbb{R}^3. \tag{6.15}$$

Proof. The generalized translation of a C_b-function is an integral of C_b-functions over a compact set and hence again bounded and continuous.

When $f \in C_b^\chi(\mathbb{R}^3)$ for some $\chi \in \widehat{K}$, then for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$:

$$\begin{aligned} T_{\mathbf{y}}^K f(\mathbf{x}) &= \int_K f(\mathbf{x} - g^{-1}\mathbf{y}) \mathrm{d}\mu_K(g) = \int_K f(g^{-1}(g\mathbf{x} - \mathbf{y})) \mathrm{d}\mu_K(g) \\ &= \int_K \chi(g) f(g\mathbf{x} - \mathbf{y}) \mathrm{d}\mu_K(g) = \int_K \overline{\chi(g)} f(g^{-1}\mathbf{x} - \mathbf{y}) \mathrm{d}\mu_K(g) \\ &= (P_K^\chi f(\cdot - \mathbf{y}))(\mathbf{x}), \end{aligned}$$

where we used the eigenfunction property of f and the inversion-invariance of the Haar measure.

Hence, $T_{\mathbf{y}}^K = P_K^\chi f(\cdot - \mathbf{y}) \in C_b^\chi(\mathbb{R}^3)$, showing that $C_b^\chi(\mathbb{R}^3)$ is closed under generalized translations.

Now, let $e_{\omega,\mathbf{k}_0,\chi}$ be a symmetry-adapted wave, then

$$\begin{aligned} T_{\mathbf{y}}^K e_{\omega,\mathbf{k}_0,\chi}(\mathbf{x}) &= \int_K e_{\omega,\mathbf{k}_0,\chi}(\mathbf{x} - g^{-1}\mathbf{y}) \mathrm{d}\mu_K(g) \\ &= \int_K \int_K \overline{\chi(h)} e^{i\mathbf{k}\cdot h^{-1}(\mathbf{x} - g^{-1}\mathbf{y})} \mathrm{d}\mu_K(h) \mathrm{d}\mu_K(g) \\ &= \int_K \int_K e^{i\mathbf{k}\cdot(gh)^{-1}\mathbf{y}} \mathrm{d}\mu_K(g) \overline{\chi(h)} e^{i\mathbf{k}\cdot h^{-1}\mathbf{x}} \mathrm{d}\mu_K(h) \\ &= \int_K e^{i\mathbf{k}\cdot g'^{-1}\mathbf{y}} \mathrm{d}\mu_K(g') \int_K \overline{\chi(h)} e^{i\mathbf{k}\cdot h^{-1}\mathbf{x}} \mathrm{d}\mu_K(h) \\ &= e_{\omega,\mathbf{k}_0,1}(\mathbf{y}) e_{\omega,\mathbf{k}_0,\chi}(\mathbf{x}), \end{aligned}$$

where we used Fubini, and the translation invariance of the Haar measure. □

So, for the compact case, we can formulate design equations for the symmetry-adapted waves. For non-compact groups, the generalized translation operators can not be defined as above, because, again, the integrals would diverge. It might be possible to define these operators via the constructions we used above to generalize the Zak transform, but we

will not follow this idea here. Instead, we shortly remark on a special structure that is related to generalized translation operators.

Remark 6.9 (Orbit Hypergroups).
The space of K-invariant L^1-functions $L^{1,1}_K(\mathbb{R}^3) := P^1_K L^1(\mathbb{R}^3)$ has a special structure. The invariant functions are determined by their values on the orbits of the group K.

Let $\mathcal{K} := \{K\mathbf{x}.\ \mathbf{x} \in \mathbb{R}^3\}$, then the space $L^{1,1}_K(\mathbb{R}^3)$ is isometrically isomorphic to the space $L^1(\mathcal{K}, \mathrm{d}\mu_{\mathcal{K}})$ where $\mu_{\mathcal{K}}$ is the projection of the Lebesgue measure to $\mathcal{K}$, i.e. $\int_{\mathcal{K}} f(K\mathbf{x})\mathrm{d}\mu_{\mathcal{K}}(K\mathbf{x}) = \int_{\mathbb{R}^3} f(\mathbf{x})\mathrm{d}\mathbf{x}$.

Defining the convolution $f *_K g$ of two functions $f, g \in L^1(\mathcal{K}, \mathrm{d}\mu_{\mathcal{K}})$ by

$$f *_K g(\mathbf{x}) := \int_{\mathcal{K}} T^K_{\mathbf{y}} f(\mathbf{x}) g(\mathbf{y}) \mathrm{d}\mu_{\mathcal{K}}(\mathbf{y}) \quad \text{for } \mathbf{x}, \mathbf{y} \in \mathcal{K},$$

and extending it to the space $M^1(\mathcal{K})$ of finite measures on $\mathcal{K}$, we can identify the points of $\mathcal{K}$ with the corresponding Dirac deltas and define the convolution on $\mathcal{K}$ by

$$\mathbf{x} *_K \mathbf{y} := \delta_{\mathbf{x}} *_K \delta_{\mathbf{y}}.$$

With the involution $\widetilde{\ }: \mathcal{K} \to \mathcal{K},\ \mathbf{x} \mapsto \widetilde{\mathbf{x}} := -\mathbf{x}$, the triple $(\mathcal{K}, *_K, \widetilde{\ })$ is a so-called hypergroup. This special kind of a hypergroup is known as an orbit hypergroup and can more generally be defined for the action of a compact automorphism group on a locally compact group (see [Jew75, Rau05]).

Proposition 6.8 shows, that the symmetry-adapted waves $e_{\omega,\mathbf{k}_0,1}$ satisfy the functional equation

$$T^K_{\mathbf{y}} e_{\omega,\mathbf{k}_0,1}(\mathbf{x}) = e_{\omega,\mathbf{k}_0,1}(\mathbf{y}) \cdot e_{\omega,\mathbf{k}_0,1}(\mathbf{x}), \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^3.$$

They also satisfy $e_{\omega,\mathbf{k}_0,1}(\widetilde{\mathbf{x}}) = \overline{e_{\omega,\mathbf{k}_0,1}(\mathbf{x})}$, showing that they are (hermitian) characters of the hypergroup, i.e. bounded continuous hypergroup homomorphisms from $\mathcal{K}$ to $\mathbb{C}^*$. The calculation can be generalized to a compact automorphism group acting on a locally compact abelian group, giving a natural method to identify hypergroup characters as symmetry-adapted characters.

The decomposition of a K-invariant function into symmetry-adapted waves is the Fourier decomposition with respect to this hypergroup, while the wave transform restricted to the K-invariant functions is the hypergroup Fourier transform.

See [BH94] and the forthcoming monograph [Las] for more information on hypergroups.

1.4. Scalar Wave Transform of Invariant Functions. To show the potential of symmetry-adapted waves for the analysis of objective structures, we consider a function f to be invariant with respect to a discrete closed subgroup H of the abelian design group G. Using Proposition 6.4, we show that the wave transform of f is supported on the

orthogonal group of H analog to the Fourier transform of a function that is invariant with respect to a Bravais lattice that is supported on the reciprocal lattice.

For this purpose, we have to generalize the scalar wave transform to bounded continuous functions. Having defined the Zak transform for bounded continuous functions in (6.7), we can define the analog of the symmetry-adapted waves as $e_{\omega,\mathbf{k}_0,\psi} := \mathcal{Z}_G e_{\omega,\mathbf{k}_0}(\cdot,\psi)$, where $\psi \in \mathcal{F}M^1(G)$.

The corresponding wave transform on $\mathcal{S}(\mathbb{R}^3)$ looks as follows:

Definition 6.10 (Distributional Scalar Wave Transform). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group and $f \in \mathcal{S}(\mathbb{R}^3)$. We define the distributional scalar wave transform $\mathcal{W}_G f$ of f with repsect to G by*

$$\mathcal{W}_G f(\mathbf{k},\psi) := \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0,\psi}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x}, \quad \mathbf{k} \in \mathbb{R}^3,\ \psi \in \mathcal{F}M^1(\mathbb{R}^3), \tag{6.16}$$

where $e_{\omega,\mathbf{k}_0,\psi} := \mathcal{Z}_G e_{\omega,\mathbf{k}_0}(\cdot,\psi)$, and $e_{\omega,\mathbf{k}_0}(\mathbf{x}) := e^{i\mathbf{k}\cdot\mathbf{x}}$, $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$.

We will drop the 'distributional' and just call this transform the wave transform, because it is clear from the context which transform we talk about.

As in the compact case, this transform is closely related to the Zak transform.

Lemma 6.11 (Properties of the Scalar Wave Transform). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group. For $\mathbf{k} \in \mathbb{R}^3$ and $\psi \in \mathcal{F}M^1(G)$, the scalar wave transform satisfies:*

$$\mathcal{W}_G f(\mathbf{k},\psi) = \mathcal{F}\mathcal{Z}_G f(\mathbf{k},\overline{\psi}) \quad \text{for } f \in \mathcal{S}(\mathbb{R}^3). \tag{6.17}$$

In particular, the inverse wave transform $\mathcal{W}_G^{-1}$ is given by

$$\mathcal{W}_G^{-1} F := \mathcal{Z}_G^{-1} \circ \mathcal{F}^{-1} F(\cdot,\dot{-}) \tag{6.18}$$

for functions $F : \mathbb{R}^3 \times \widehat{G} \to \mathbb{C}$, that lie in the image of $\mathcal{S}(\mathbb{R}^3)$ under $\mathcal{W}_G$.

Proof. Let $f \in \mathcal{S}(\mathbb{R}^3)$, $\mathbf{k} \in \mathbb{R}^3$ and $\psi \in \mathcal{F}M^1(\mathbb{R}^3)$. Then

$$\begin{aligned}
\mathcal{W}_G f(\mathbf{k},\psi) &= \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0,\psi}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \overline{P_G^\chi e_{\omega,\mathbf{k}_0}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^3} \int_G e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\overline{\mathcal{F}_{\widehat{G}}\psi}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \int_G e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\mathcal{F}_{\widehat{G}}\overline{\psi}(g^{-1}) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^3} \int_G e^{-i\mathbf{k}\cdot g\mathbf{x}} \mathrm{d}\mathcal{F}_{\widehat{G}}\overline{\psi}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} = \int_G \int_{\mathbb{R}^3} e^{-i\mathbf{k}\cdot g\mathbf{x}} f(\mathbf{x}) \mathrm{d}\mathbf{x} \mathrm{d}\mathcal{F}_{\widehat{G}}\overline{\psi}(g) \\
&= \int_G \int_{\mathbb{R}^3} e^{-i\mathbf{k}\cdot\mathbf{x}} f(g^{-1}\mathbf{x}) \mathrm{d}\mathbf{x} \mathrm{d}\mathcal{F}_{\widehat{G}}\overline{\psi}(g) = \int_{\mathbb{R}^3} e^{-i\mathbf{k}\cdot\mathbf{x}} \int_G f(g^{-1}\mathbf{x}) \mathrm{d}\mathcal{F}_{\widehat{G}}\overline{\psi}(g) \\
&= \mathcal{F}\mathcal{Z}_G f(\mathbf{k},\overline{\psi}),
\end{aligned}$$

where we used the generalization of the rule $\overline{\mathcal{F}_G f(g)} = \mathcal{F}_G \overline{f}(g^{-1})$ to measures, the invariance of the Lebesgue measure with repsect to isometries and Fubini twice.

The formula for the inverse transform follows immediately. □

In a final step, we can generalize the scalar wave transform to bounded continuous functions. Note that for $f \in C_b(\mathbb{R}^3)$ and $\psi \in \mathcal{F}M^1(G)$, the function $\mathbf{x} \mapsto \mathcal{Z}_G f(\mathbf{x}, \psi)$ is again bounded and continuous. So, we can define

$$\mathcal{W}_G f := \mathcal{F}\mathcal{Z}_K f(\cdot, \overline{\psi}) \tag{6.19}$$

in a distributional sense.

With this definition, we can study the scalar wave transform of invariant functions.

Proposition 6.12 (Scalar Wave Transform of Invariant Functions). *Let $G \leq \mathrm{E}(3)$ be a a closed compact abelian isometry group and H a discrete closed subgroup of G. The scalar wave transform of an H-invariant function f, s.t. $f_{\mathbf{x}}$ is compactly supported on a fundamental domain of H, is given by*

$$\mathcal{W}_G f(\mathbf{k}, \chi) = \mathcal{W}_{G/H} f(\mathbf{k}, \chi \downarrow^G_{G/H}) \delta_{H_G^\perp}(\chi), \tag{6.20}$$

for all $\mathbf{k} \in \mathbb{R}^3$, $\chi \in \widehat{G}$.

Proof. Let $f \in C_b(\mathbb{R}^3)$ be an H-invariant function, s.t. $f_{\mathbf{x}}$ is compactly supported on a fundamental domain of H. Then for $\mathbf{k} \in \mathbb{R}^3$ and $\psi \in \mathcal{F}M^1(G)$, using Proposition 6.4,

$$\mathcal{W}_G f(\mathbf{k}, \psi) = \mathcal{F}\mathcal{Z}_G f(\mathbf{k}, \overline{\psi}) = \mathcal{F}\mathcal{Z}_{G/H} f(\mathbf{k}, \overline{\psi}\big|_{G/H}) \delta_{H_G^\perp}(\overline{\psi}) = \mathcal{W}_{G/H} f(\mathbf{k}, \overline{\psi}\big|_{G/H}) \delta_{H_G^\perp}(\overline{\psi}).$$

□

So, the scalar wave transform is the integral transform that implements the Zak transfrom we were looking for.

As a corollary, we get the following. The subgroup H can be recovered from the scalar wave transform.

Corollary 6.13 (Reconstruction of Symmetry). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group and f invariant with respect to a discrete closed subgroup H of G, s.t. f is not invariant with respect to any group H' that lies in between G and H, i.e. $G \leq H' < H$. Then H can be reconstructed from $\mathcal{W}_G f$ as follows:*

$$H = \{g \in G.\ \chi(g) = 1 \text{ for all } \chi \in \mathrm{supp}(\mathcal{W}_G f)\}. \tag{6.21}$$

Proof. Identifying the double dual $\widehat{\widehat{G}}$ with G itself by Pontryagin duality (see [Fol95], Theorem 4.31), and noting that $\mathrm{supp}(\mathcal{W}_G f) = H_G^\perp$ by Proposition 6.12, we find that

$$\{g \in G.\ \chi(g) = 1 \text{ for all } \chi \in \mathrm{supp}(\mathcal{W}_G f)\} = (H_G^\perp)^\perp_{\widehat{G}}.$$

Now, the orthogonal group of the orthogonal group (as subgroup of G) is the original group itself – $(H_G^\perp)_{\widehat{G}}^\perp = H$ – when H is closed (see [Fol95], Proposition 4.38, p. 104). □

Proposition 6.12 and Corollary 6.13 formulate a kind of scalar generalized von Laue condition – or better – a Poisson summation formula for group actions. From the scalar wave transform of an invariant function, the symmetry can be reconstructed from the support.

In the following section, we lift the scalar theory we developed to the vector-valued case and relate it to the radiation transform to formulate a generalized von Laue condition.

2. The Generalized von Laue Condition

Finally, we will gather all our results to derive the generalized von Laue condition. We introduce the vector-valued wave transform and relate it to both the scalar wave transform and the radiation transform, showing that it is the link between the decomposition of the charge density and the outgoing field of the diffraction experiment.

Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group. We work in the distributional setting. For this purpose, we introduce

$$\mathbf{E}_{\omega,\mathbf{k}_0,\psi}(\mathbf{x}) := \mathcal{F}_G \mathbf{E}_{\mathbf{x}}(\psi), \quad \text{for } \psi \in \mathcal{F}M^1(G), \tag{6.22}$$

where $\mathbf{E}_{\mathbf{x}}(g) := (g\mathbf{E}_{\mathbf{k}})(\mathbf{x})$. Then we define the wave transform as follows.

Definition 6.14 (Wave Transform). *Let $G \leq \mathrm{E}(3)$ be a closed abelian isometry group. The wave transform $\boldsymbol{\mathcal{W}}_G f$ of a function $f \in \mathcal{S}(\mathbb{R}^3)$ is defined as*

$$\boldsymbol{\mathcal{W}}_G f(\mathbf{k}, \psi) := \int_{\mathbb{R}^3} \overline{\mathbf{E}_{\omega,\mathbf{k}_0,\psi}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} \quad \textit{for } \mathbf{k} \in \mathbb{R}^3,\ \chi \in \widehat{G}, \quad \textit{for } \mathbf{k} \in \mathbb{R}^3,\ \psi \in \mathcal{F}M^1(G), \tag{6.23}$$

where $\{\mathbf{E}_{\omega,\mathbf{k}_0}\}_{(\omega,\mathbf{k}_0)\in[0,\infty)\times\mathbb{S}^2}$ is a family of plane waves, i.e. $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) = \mathbf{n}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}$ for some $\mathbf{n}(\mathbf{k}) \in \mathbf{k}^\perp$, where $\mathbf{k} := \frac{\omega}{c}\mathbf{k}_0$, and all $\mathbf{x} \in \mathbb{R}^3$.

An immediate question is, whether this vector-valued wave transform is invertible. The answer is affirmative, as its values determine the corresponding scalar wave transform. In the following proofs, we will wirte the group Fourier transform $\mathcal{F}_G$ as an integral, always keeping in mind that the distributional Fourier transform on $\mathcal{F}M^1(G)$ is meant.

Lemma 6.15 (Invertibility of the Wave Transform). *Let $G \leq \mathrm{E}(3)$ be a closed compact abelian isometry group and $\{\mathbf{E}_{\omega,\mathbf{k}_0}\}_{(\omega,\mathbf{k}_0)\in[0,\infty)\times\mathbb{S}^2}$ a family of plane waves given by $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) = \mathbf{n}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}$, $\mathbf{n}(\mathbf{k}) \neq 0$. The associated wave transform $\boldsymbol{\mathcal{W}}_G f$ of a function $f \in \mathcal{S}(\mathbb{R}^3)$ is related to the scalar wave transform $\mathcal{W}_G f$ as follows. There is a unitary*

matrix $\mathbf{U} \in \mathrm{U}(3)$*, s.t. when setting*

$$\mathbf{v}(\mathbf{k},\chi) := \mathbf{U}^{-1}\boldsymbol{\mathcal{W}}_G f(\mathbf{k},\chi), \quad \textit{and} \quad \widetilde{\mathbf{n}}(\mathbf{k}) := \mathbf{U}^{-1}\overline{\mathbf{n}(\mathbf{k})},$$

for $\mathbf{k} \in \mathbb{R}^3$ *and* $\chi \in \widehat{G}$*, we have*

$$\mathbf{v}_j(\mathbf{k},\chi) = \mathcal{W}_G f(\mathbf{k}, \chi\cdot\chi_j)\widetilde{\mathbf{n}}_j(\mathbf{k}) \tag{6.24}$$

for some $\chi_j \in \widehat{K}$*,* $j = 1,2,3$*, and all* $\mathbf{k} \in \mathbb{R}^3$*,* $\chi \in \widehat{G}$*.*

In particular, the wave transform $\boldsymbol{\mathcal{W}}_G$ *is invertible.*

Proof. We write the symmetry adapted plane waves as integrals, keeping in mind that we mean the distributional Fourier transform. For $\mathbf{k} \in \mathbb{R}^3$ and $\chi \in \widehat{K}$:

$$\begin{aligned}\boldsymbol{\mathcal{W}}_G f(\mathbf{k},\chi) &= \int_{\mathbb{R}^3} \overline{\mathbf{E}_{\omega,\mathbf{k}_0,\chi}(\mathbf{x})} f(\mathbf{x})\mathrm{d}\mathbf{x} = \int_{\mathbb{R}}\int_G \chi(\mathbf{Q})\overline{\mathbf{Q}\mathbf{n}(\mathbf{k})} e^{-i\mathbf{k}\cdot\mathbf{Q}^{-1}\mathbf{x}}\mathrm{d}\mu_G(\mathbf{Q}) f(\mathbf{x})\mathrm{d}\mathbf{x}\\ &= \mathbf{U}\int_{\mathbb{R}^3}\int_G \chi(\mathbf{Q})\mathrm{diag}(\chi_1(\mathbf{Q}),\chi_2(\mathbf{Q}),\chi_3(\mathbf{Q}))e^{-i\mathbf{k}\cdot\mathbf{Q}^{-1}\mathbf{x}}\mathrm{d}\mu_G(\mathbf{Q}) f(\mathbf{x})\mathrm{d}\mathbf{x}\mathbf{U}^{-1}\overline{\mathbf{n}(\mathbf{k})},\end{aligned}$$

where $\mathbf{U} \in \mathrm{U}(3)$ is a unitary matrix that simultaneously diagonalizes the matrices $\mathbf{Q}$ in G and $\chi_j \in \widehat{G}$, $j = 1,2,3$, are the characters of G with

$$\mathbf{Q} = \mathbf{U}\mathrm{diag}(\chi_1(\mathbf{Q}),\chi_2(\mathbf{Q}),\chi_3(\mathbf{Q}))\mathbf{U}^{-1}.$$

The integral is matrix-valued with diagonal-entries $\mathbf{T}_{jj}$, $j = 1,2,3$ given by

$$\begin{aligned}\mathbf{T}_{jj} &= \int_{\mathbb{R}^3}\int_G \chi(\mathbf{Q})\chi_j(\mathbf{Q}) e^{-i\mathbf{k}\cdot\mathbf{Q}^{-1}\mathbf{x}}\mathrm{d}\mu_G(\mathbf{Q}) f(\mathbf{x})\mathrm{d}\mathbf{x}\\ &= \int_{\mathbb{R}^3}\int_G (\chi\cdot\chi_j)(\mathbf{Q}) e^{-i\mathbf{k}\cdot\mathbf{Q}^{-1}\mathbf{x}}\mathrm{d}\mu_G(\mathbf{Q}) f(\mathbf{x})\mathrm{d}\mathbf{x} = \mathcal{W}_G f(\mathbf{k},\chi\cdot\chi_j).\end{aligned}$$

In particular,

$$\mathbf{v}_j(\mathbf{k},\chi) = (\mathbf{U}^{-1}\boldsymbol{\mathcal{W}}_G f)_j(\mathbf{k},\chi) = \mathbf{T}_{jj}\widetilde{\mathbf{n}}_j(\mathbf{k}) = \mathcal{W}_G f(\mathbf{k},\chi\cdot\chi_j)\widetilde{\mathbf{n}}_j(\mathbf{k}).$$

Since $\mathbf{n}(\mathbf{k}) \neq 0$ for all $\mathbf{k} \in \mathbb{R}^3$ and $\mathbf{U}$ is unitary, we get $\widetilde{\mathbf{n}}(\mathbf{k}) \neq 0$. Consequently, for every $\mathbf{k} \in \mathbb{R}^3$ there is a $j \in \{1,2,3\}$ s.t. $\widetilde{\mathbf{n}}_j(\mathbf{k}) \neq 0$. Thus, all values of the scalar wave transform are accessible, and it can be inverted by the inverse scalar wave transform given in Lemma 6.11. □

The character χ_j, $j = 1,2,3$, appearing in Lemma 6.15 are the irreducible components of the representation of the isogonal point group of G on $\mathbb{R}^3$ that acts on the field vector. In the case of twisted waves, these components lead to the double peak pattern in parameter space by translation in Fourier space (see Figure 4.4). The same happens in the general case. We proof the vector analog of Proposition 6.12 concerning the wave transform of functions that are H-invariant.

Corollary 6.16 (Wave Transform of Invariant Functions). *Let $G \leq \mathrm{E}(3)$ be a compact abelian closed isometry group and H a discrete closed subgroup of G. The wave transform of an H-invariant function f is given by*

$$\boldsymbol{\mathcal{W}}_G f(\mathbf{k},\chi) = \mathbf{U}\left(\mathcal{W}_{G/H} f(\mathbf{k},(\chi\cdot\chi_j)\downarrow^G_{G/H})\delta_{H^\perp_G\chi_j^{-1}}(\chi)\widetilde{\mathbf{n}}_j(\mathbf{k})\right)_{j=1,2,3}, \tag{6.25}$$

where $\widetilde{\mathbf{n}}(\mathbf{k}) := \mathbf{U}^{-1}\overline{\mathbf{n}(\mathbf{k})}$ and $\mathbf{n}(\mathbf{k})$ is the complex amplitude of the symmetry-adapted wave with wave vector $\mathbf{k}$, $\mathbf{U}\in\mathrm{U}(3)$, and χ_j, $j=1,2,3$ are the irreducible components of the representation of the isogonal point group on $\mathbb{R}^3$.

Proof. By Lemma 6.15, we know that for $j=1,2,3$,

$$(\mathbf{U}^{-1}\boldsymbol{\mathcal{W}}_G f(\mathbf{k},\chi))_j = \mathcal{W}_G f(\mathbf{k},\chi\cdot\chi_j)\widetilde{\mathbf{n}}_j(\mathbf{k}).$$

Now, Proposition 6.12 says that $\mathcal{W}_G f(\mathbf{k},\chi\cdot\chi_j) = \mathcal{W}_{G/H} f(\mathbf{k},(\chi\cdot\chi_j)\downarrow^G_{G/H})\delta_{H^\perp_G}(\chi\cdot\chi_j)$. Since $\delta_{H^\perp_G}(\chi\cdot\chi_j) = \delta_{H^\perp_G\chi_j^{-1}}(\chi)$, we get the desired result. □

This lemma has an immediate consequence for the radiation transform associated to a family of symmetry-adapted waves with respect to a compact abelian design group. This is seen from the relationship between the radiation transform with respect to symmetry-adapted waves and the wave transform. When $\rho_{\mathrm{el}}\in\mathcal{S}(\mathbb{R}^3)$ is the charge density of a molecular structure, then

$$\mathcal{R}[\mathbf{E}_{\omega,\mathbf{k}_0,\psi}]\rho_{\mathrm{el}}(\mathbf{s}_0) = \boldsymbol{\mathcal{W}}_G\left(e^{i\frac{\omega}{c}\mathbf{s}_0\cdot}\rho_{\mathrm{el}}\right)(\mathbf{k},\psi), \tag{6.26}$$

for $\mathbf{s}_0\in\mathbb{S}^2$, $\mathbf{k}\in\mathbb{R}^3$, and $\psi\in\mathcal{F}M^1(G)$.

We can use the last corollary to formulate the main theorem – the generalized von Laue Condition.

Theorem 6.17 (Generalized von Laue Condition). *Let $G\leq\mathrm{E}(3)$ be a compact abelian closed isometry group, H a discrete closed subgroup of G, and $\{\mathbf{E}_{\omega,\mathbf{k}_0,\chi}\}_{(\omega,\mathbf{k}_0,\chi)\in\mathcal{P}}$ a family of symmetry-adapted waves with respect to G with the full radiation parameter set $\mathcal{P}=[0,\infty)\times\mathbb{S}^2\times\widehat{G}$.*

When there is an $\mathbf{s}_0\in\mathbb{S}^2$ that is Iso_H-invariant, then

$$\mathcal{R}[\mathbf{E}_{\omega,\mathbf{k}_0,\chi}]\rho_{\mathrm{el}}(\mathbf{s}_0) = \mathbf{U}\left(\mathcal{W}_{G/H}(e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot}\rho_{\mathrm{el}})(\mathbf{k},(\chi\cdot\chi_j)\downarrow^G_{G/H})\delta_{H^\perp_G\chi_j^{-1}}(\chi)\widetilde{\mathbf{n}}_j(\mathbf{k})\right)_{j=1,2,3}, \tag{6.27}$$

where $\widetilde{\mathbf{n}}(\mathbf{k}) := \mathbf{U}^{-1}\overline{\mathbf{n}(\mathbf{k})}$ and $\mathbf{n}(\mathbf{k})$ is the complex amplitude of the symmetry-adapted wave with wave vector $\mathbf{k}$ and $\mathbf{U}\in\mathrm{U}(3)$, and χ_j, $j=1,2,3$ are the irreducible components of the representation of the isogonal point group on $\mathbb{R}^3$.

In particular, the data set

$$\left\{\left|\mathrm{P}(\mathbf{s}_0^\perp)\mathcal{R}[\mathbf{E}_{\omega,\mathbf{k}_0,\chi}]\rho_{\mathrm{el}}(\mathbf{s}_0)\right|^2\right\}_{(\omega,\mathbf{k}_0,\chi)\in\mathcal{P}}$$

is supported on a subset of $[0,\infty)\times\mathbb{S}^2\times\bigcup_{j=1}^3 H_G^\perp\chi_j^{-1}\subset\mathcal{P}$.

When $\mathbf{s}_0$ *is* Iso_G*-invariant, the reconstruction problem reduces to a scalar phase problem. In particular, the data makes the following values accessible:*

$$\left\{\left|\mathcal{W}_{G/H}\rho_{\mathrm{el}}\left(\frac{\omega}{c}(\mathbf{k}_0+\mathbf{s}_0),\chi\right)\right|^2\right\},\quad (\omega,\mathbf{k}_0,\chi)\in[0,\infty)\times\mathbb{S}^2\times\widehat{G/H}.$$

When ρ_{el} *is real, the values for negative first argument, i.e.* $\left|\mathcal{W}_{G/H}\rho_{\mathrm{el}}\left(-\frac{\omega}{c}(\mathbf{k}_0+\mathbf{s}_0),\chi\right)\right|^2$ *are also accessible.*

Proof. Equation (6.27) is a direct consequence of Corollary 6.16 and the Iso_H-invariance of $\mathbf{s}_0$. The restricted support of the data set follows immediately.

Since the dual group of G/H is the orthogonal group $H_G^\perp$ restricted to G/H (see [Rei68], Ch. 4, 2.8, (i)), we have access to the values

$$\left|\mathcal{W}_{G/H}(e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot}\rho_{\mathrm{el}})\,(\mathbf{k},\chi)\right|^2$$

for $\mathbf{k}\in\mathbb{R}^3$ and $\chi\in H_G^\perp\big|_{G/H}=\widehat{G/H}$. Now, for $\mathbf{k}\in\mathbb{R}^3$ and $\chi\in\widehat{G/H}$,

$$\begin{aligned}
\mathcal{W}_{G/H}(e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot}\rho_{\mathrm{el}})(\mathbf{k},\chi) &= \int_{\mathbb{R}^3}\int_{G/H}\chi(g)e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}}\mathrm{d}\mu_{G/H}(g)e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{x}}\rho_{\mathrm{el}}(\mathbf{x})\mathrm{d}\mathbf{x}\\
&= \int_{G/H}\chi(g)\int_{\mathbb{R}^3}e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}}e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{x}}\rho_{\mathrm{el}}(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mu_{G/H}(g)\\
&= \int_{G/H}\chi(g)\int_{\mathbb{R}^3}e^{-i((g\mathbf{k}+\frac{\omega}{c}\mathbf{s}_0)\cdot\mathbf{x}}\rho_{\mathrm{el}}(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mu_{G/H}(g)\\
&= \int_{G/H}\chi(g)\int_{\mathbb{R}^3}e^{-i\frac{\omega}{c}(\mathbf{k}_0+\mathbf{s}_0)\cdot g^{-1}\mathbf{x}}\rho_{\mathrm{el}}(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mu_{G/H}(g)\\
&= \int_{\mathbb{R}^3}\int_{G/H}\chi(g)e^{-i\frac{\omega}{c}(\mathbf{k}_0+\mathbf{s}_0)\cdot g^{-1}\mathbf{x}}\mathrm{d}\mu_{G/H}(g)\rho_{\mathrm{el}}(\mathbf{x})\mathrm{d}\mathbf{x}\\
&= \mathcal{W}_{G/H}\rho_{\mathrm{el}}\left(\frac{\omega}{c}(\mathbf{k}_0+\mathbf{s}_0),\chi\right),
\end{aligned}$$

using the G-invariance of $\mathbf{s}_0$.

When ρ_{el} is real, the accessibility of the values for negative first argument follows from the identity

$$\mathcal{W}_{G/H}\rho_{\mathrm{el}}(-\mathbf{k},\chi)=\overline{\mathcal{W}_{G/H}\overline{\rho_{\mathrm{el}}}(\mathbf{k},\overline{\chi})}$$

and the closedness of $\widehat{G/H}$ with respect to conjugation. □

So, for the related diffraction experiment, this means that constructive interference in axis direction occurs if and only if the character, the radiation is adapted to, lies in the orthogonal group of its symmetry group.

Let's have a second look at twisted waves and nanotube structures. In Theorem 4.6, we reduced the reconstruction problem to a phase problem for a function we called $\mathcal{W}_{C_{\mathbf{e}}/H_{\mathcal{C}}}\varphi_{\mathcal{C}}$. This was a slight abuse of notation, because the arguments of this function were the radiation parameters $(\omega, \alpha, \widehat{z} + \frac{\omega}{c})$ instead of the corresponding wave vector and character. Introducing the mapping $\kappa : [0, \infty) \times \mathbb{Z} \times \mathbb{R} \to \mathbb{R}^3 \times \widehat{C_{\mathbf{e}}}$ by

$$\kappa(\omega, \alpha, \widehat{z}) := (\mathbf{k}(\omega, \widehat{z}), \chi^{(\alpha, \widehat{z})}), \tag{6.28}$$

we find that

$$\kappa\left(\omega, \alpha, \widehat{z} + \frac{\omega}{c}\right) = \left(\mathbf{k}\left(\omega, \widehat{z} + \frac{\omega}{c}\right), \chi^{(\alpha, \widehat{z} + \frac{\omega}{c})}\right) = \left(\frac{\omega}{c}\left(\mathbf{k}_0(\omega, \widehat{z}) + \mathbf{e}\right), \chi^{(\alpha, \widehat{z} + \frac{\omega}{c})}\right),$$

showing that Corollary 4.6 is an instance of Theorem 6.17.

In the classic case of X-ray crystallography, the scalar wave transform reduces to the Fourier transform. In Theorem 1.3, we saw that the accessible data is $\left|\widehat{\rho_{\text{el}}}\left(\frac{\omega}{c}(\mathbf{s}_0 - \mathbf{k}_0)\right)\right|$. The different sign of $\mathbf{k}_0$ results from our definition of the wave transform via the conjugated symmetry-adapted waves. In the classic case, we started with a plane wave $\mathbf{E}_{\mathbf{k}}$ instead of $\overline{\mathbf{E}_{\mathbf{k}}} = \mathbf{E}_{-\mathbf{k}}$.

3. Phase Retrieval

We shortly consider generalizations of the phase retrieval algorithms introduced in Chapter 2. To use Theorem 6.17, we consider an abelian design group G, such that there is a vector $\mathbf{s}_0 \in \mathbb{S}^2$ with $g\mathbf{s}_0 = \mathbf{s}_0$ for all $g \in \text{Iso}_G$, and a charge density $\rho_{\text{el}} \in \mathcal{S}^{\geq 0}(\mathbb{R}^3)$ that is invariant with respect to a discrete closed subgroup H of G. Furthermore, assume that we know the intensity of the outgoing radiation in $\mathbf{s}_0$-direction that results from the scattering of symmetry-adapted waves on the whole parameter space $[0, \infty) \times \mathbb{S}^2 \times \widehat{G}$.

In the case of twisted waves (see Chapter 4), we found an explicit version of scalar the wave transform what made it easy to formulate phase retrieval algorithms. In the general case, we make the following observation.

The scalar wave transform is the Fourier transform of the Zak transform according to Lemma 6.11, and the Zak transform itself is a group Fourier transform. So, given a function $\rho_{\text{el}} \in \mathcal{S}(\mathbb{R}^3)$, and an abelian design group $G \leq \text{E}(3)$, we define the function

$$\rho_G : \ \mathbb{R}^3 \times G \to \mathbb{C}, \ (\mathbf{x}, g) \mapsto (g\rho_{\text{el}})(\mathbf{x}) = \rho_{\text{el}}(g^{-1}\mathbf{x}). \tag{6.29}$$

Then the scalar wave transform of ρ_{el} can be written as

$$\mathcal{W}_G f(\mathbf{k}, \chi) = \mathcal{F}_{\mathbb{R}^3 \times G}\rho_G(\mathbf{k}, \chi), \tag{6.30}$$

where $\chi \in \widehat{G}$ and the character $e_{\mathbf{k}}$ of $\mathbb{R}^3$ is identified with its wave vector $\mathbf{k}$.

So, the scalar wave and inverse scalar wave transform can be implemented as a Fourier transform on the group $\mathbb{R}^3 \times G$, using the FFT algorithm.

There is one problem with this approach. The functions on $\mathbb{R}^3 \times G$ are a much bigger class then the functions f on $\mathbb{R}^3 \times G$ that satisfy $f(h^{-1}\mathbf{x}, g) = f(\mathbf{x}, hg)$ for $h \in G$. These functions are determined by its values on the set $\mathbb{R}^3/G \times G$, because $f(g\mathbf{x}, e_G) = f(\mathbf{x}, g)$ for all $g \in G$, $\mathbf{x} \in \mathbb{R}^3$, where e_G is the neutral element of G. Of course, they are also determined by the values for $(\mathbf{x}, g) \in \mathbb{R}^3 \times \{e_G\}$.

From Theorem 6.17, we know that the outgoing intensity in $\mathbf{s}_0$ direction is supported on a superposition of two translated versions of $H_G^\perp$. Using Corollary 6.13, we can determine H from this pattern. Then, we know that ρ_G is determined by its values at the points $(\mathbf{x}, g) \in \mathbb{R}^3/H \times \{e_G\}$, or equivalently for $(\mathbf{x}, g) \in \mathbb{R}^3/G \times G/H$. In the case of twisted waves, i.e. for $G = C_{\mathbf{e}}$, the set $\mathbb{R}^3/C_{\mathbf{e}}$ is parametrized by the radial variable $r \in [0, \infty)$, while $C_{\mathbf{e}}/H$ is the unit cell on a cylindrical surface.

So, by restricting the reconstruction to $\mathbb{R}^3/G \times G/H$ or equivalently, by imposing the corresponding symmetries, we can formulate generalization of the phase retrieval algorithms of Chapter 2.

Define the space of functions on $\mathbb{R}^3/G \times G/H$ that are Schwartz functions when extended to $\mathbb{R}^3$ by

$$\mathcal{S}(\mathbb{R}^3/G \times G/H) := \left\{ \varphi : \mathbb{R}^3/G \times G/H \to \mathbb{C}. \ \left(g^{-1}\mathbf{x} \mapsto \sum_{h \in H} \varphi(\mathbf{x}, hg) \right) \in \mathcal{S}(\mathbb{R}^3) \right\}.$$

Again, we consider the following subsets of $\mathcal{S}(\mathbb{R}^3/G \times G/H)$:

$$\mathcal{S}^{\geq 0}(\mathbb{R}^3/G \times G/H) := \{\varphi \in \mathcal{S}(\mathbb{R}^3/G \times G/H). \ \varphi \geq 0\},$$
$$\mathcal{S}_{\mathrm{A}}(\mathbb{R}^3/G \times G/H) := \{\varphi \in \mathcal{S}(\mathbb{R}^3/G \times G/H). \ |\mathcal{W}_{G/H}\varphi| = \mathrm{A}\},$$

where $\mathcal{W}_{G/H}\varphi$ is defined as the application of $\mathcal{W}_{G/H}$ to the function on $\mathbb{R}^3$ that corresponds to φ, and A is the given data.

The projections to formulate the algorithms are

$$\mathrm{p}_{\geq 0} : \mathcal{S}(\mathbb{R}^3/G \times G/H) \to \mathcal{S}^{\geq 0}(\mathbb{R}^3/G \times G/H), \ \varphi \mapsto \varphi \cdot \mathbf{1}_{\{\varphi \geq 0\}},$$
$$\mathrm{p}_{\mathrm{A}} : \mathcal{S}(\mathbb{R}^3/G \times G/H) \to \mathcal{S}_{\mathrm{A}}(\mathbb{R}^3/G \times G/H), \ \varphi \mapsto \mathcal{W}_{G/H}^{-1}(\mathrm{A}(e^{i\zeta_\varphi}\mathbf{1}_{\{\varphi \neq 0\}} + \mathbf{1}_{\{\varphi = 0\}})),$$

where ζ_φ is the phase function of $\mathcal{W}_{G/H}\varphi$. The corresponding difference map algorithms would be

$$\varphi_{n+1} := \varphi_n - \mathrm{p}_{\geq 0}\varphi_n + \mathrm{p}_{\mathrm{A}}(2\mathrm{p}_{\geq 0} - \mathrm{id})\varphi_n, \quad n \in \mathbb{N}., \tag{$\mathrm{DM}_{G/H}$}$$

where φ_0 is chosen with an arbitrary initial phase function ζ_0, i.e. $\varphi_0 := \mathcal{W}_{G/H}^{-1}(\mathrm{A}e^{i\zeta_0})$.

CHAPTER 7

Radiation Design for Compact Design Groups

Having identified the abelian design groups that lead to a generalized von Laue condition (Theorem 6.17), we consider the non-abelian case, next. Since a Fourier tranform analog is only available for compact groups K, we restrict ourselves to this case.

First, we give a short summary of harmonic analysis on compact groups to introduce the central objects and notations. We then need to generalize the design equations to the non-abelian case. Eigenvalues of the action are one-dimensional unitary irreducible representations of K and thus carry only information about the center of K. The right non-abelian analog of being an eigenfunction is belonging to an irreducible K-invariant subspace of the radiation space. These functions transform via irreducible representations of K under the group action, and these representations define the Fourier transform on K.

The transforms introduced in Chapter 6 can be generalized to the compact case in two different ways. The characters of the irreducible representations of the group are a basis for the space of class functions on K, while the matrix coefficients span the whole $L^2(K)$. Both viewpoints lead to a decomposition of functions on $\mathbb{R}^3$ via the action of the group. We introduce the Zak and wave transform related to the character decomposition and call the matrix coefficient versions the refined Zak transform and refined wave transform, respectively.

For simplicity, the special case of finite groups is treated in detail. An analog to the Poisson summation formula is available – the so-called Frobenius reciprocity theorem (which can also be generalized to general compact groups, see [Fol95], Theorem 6.10). We can identify a generalization of the orthogonal group and generalize the theory for the scalar wave transform.

For the vector-valued case things are more complicated. The action on the field vector does not simply lead to multiple translated versions of the orthogonal structure as in the abelian case. Instead, the resonances mix in a way that doesn't allow to reconstruct the symmetries. Consequently, a generalized von Laue condition cannot be formulated. However, we can give a result on the support of the wave transform that could be useful for some special compact design groups.

1. The Design Equations – Characters and Matrix Coefficients

The design equations introduced in Chapter 3, are intrinsically abelian. In particular, when a bounded continuous function $f \in C_b(\mathbb{R}^3)$ is a simultaneous eigenfunction of an action of a group G, it satisfies

$$(gh)f = \chi(g)(hf) = \chi(g)\chi(h)f = \chi(h)\chi(g)f = \chi(h)(gf) = (hg)f,$$

where $g, h \in G$ and $\chi : G \to \mathbb{C}$ is the eigenvalue considered as a function on G. So, even though the group is non-abelian, the action on a simultaneous eigenfunction is abelian in the sense that $(gh)f = (hg)f$, $g, h \in G$. The reason is that the function χ is scalar and thus maps the group to an abelian structure. Consequently, it cannot capture the non-abelian features of the group G.

The right framework for harmonic analysis on non-abelian groups is representation theory. We will restrict ourselves to compact groups, i.e. in our case subgroups K of the orthogonal group $\mathrm{O}(3)$, as in this case the Peter-Weyl theorem provides us with a Fourier theory for these groups (see e.g. [Fol95] Ch. 5, or [SD80], Ch. IV).

We give a short summary of harmonic analysis on compact groups.

1.1. Harmonic Analysis on Compact Groups. To generalize the design equations to non-abelian compact groups, we reverse the argument of Lemma 3.16 and start from the non-abelian analog of the characters of an abelian group – the unitary irreducible representations. It can be shown (e.g. [Fol95], Theorem 5.2) that all irreducible representations of a compact group K are finite dimensional. The set of equivalence classes of unitary irreducible representations of K is called the dual of K and is denoted by $\widehat{K}$ like the dual group of an abelian group:

$$\widehat{K} := \{[\sigma].\ \sigma \text{ unitary irreducible representation of } K\}, \tag{7.1}$$

where $[\sigma]$ denotes the unitary equivalence class of σ. Unlike for abelian groups, the dual of a non-abelian group is itself not a group. However, it still carries a lot of information on K.

Given an element $\sigma \in \widehat{K}$ (we will use this as short notation for 'a representative of an element of the dual'), $\sigma : K \to H_\sigma$, where H_σ a Hilbert space of dimension $d_\sigma \in \mathbb{N}$, we define two important related objects. The character χ_σ of the representation σ is defined as the mapping

$$\chi_\sigma(g) := \mathrm{tr}(\sigma(g)), \quad g \in K, \tag{7.2}$$

while the matrix coefficients $\sigma_{j,k}$, $j, k = 1, \ldots, d_\sigma$, of σ are given by

$$\sigma_{j,k}(g) := \langle \sigma(g)\mathbf{h}_k, \mathbf{h}_j \rangle_{H_\sigma}, \tag{7.3}$$

where $\{\mathbf{h}_1, \ldots, \mathbf{h}_{d_\sigma}\}$ is a basis of H_σ and $\langle \cdot, \cdot \rangle_{H_\sigma}$ denotes the scalar product on H_σ.

With the scalar product on $L^2(K)$

$$\langle f_1, f_2 \rangle_{L^2(K)} := \int_K f_1(g)\overline{f_2(g)}\mathrm{d}\mu_K(g)$$

for $f_1, f_2 \in L^2(K)$, the characters as well as the normalized matrix coefficients obey orthogonality relations. When $\sigma, \sigma' \in \widehat{K}$ are representations of dimensions d and d', respectively, then

$$\langle \chi_\sigma, \chi_{\sigma'} \rangle_{L^2(K)} = \delta_{\sigma,\sigma'}, \tag{7.4}$$

$$\langle \sqrt{d}\sigma_{j,k}, \sqrt{d'}\sigma'_{j',k'} \rangle_{L^2(K)} = \delta_{\sigma,\sigma'}\delta_{j,j'}\delta_{k,k'}, \tag{7.5}$$

for $j, k = 1, \ldots, d$ and $j', k' = 1, \ldots, d'$.

The set of normalized matrix coefficients of all elements of $\widehat{K}$ is an orthonormal basis of the space $L^2(K)$ with the corresponding Fourier transform $\mathcal{F}_K$ on $L^2(K)$ given by

$$\mathcal{F}_K f(\sigma_{j,k}) := \int_K \overline{\sigma_{j,k}(g)} f(g)\mathrm{d}\mu_K(g), \quad j, k = 1, \ldots, d_\sigma. \tag{7.6}$$

Note, that in this Formula, the Fourier transform depends on the choice of the basis as we defined it via the matrix coefficients. The basis independent definition of the Fourier transform is the family of operators $\{\mathcal{F}_K f(\sigma)\}_{\sigma \in \widehat{K}}$. Our formulation is then the representation of $\mathcal{F}_K f$ in our basis, i.e. $\mathcal{F}_K f(\sigma)_{j,k} = \mathcal{F}_K f(\sigma)_{j,k}$.

Given a family of operators $\{F(\sigma)\}_{\sigma \in \widehat{K}}$ in the image of $\mathcal{F}_K$, we define its inverse Fourier transform $\mathcal{F}_K^{-1} F$ by

$$\mathcal{F}_K^{-1} := \sum_{\sigma \in \widehat{K}} d_\sigma \mathrm{tr}(\sigma(g)^* F(g)).$$

This sum converges in the L^2-sense.

We can also introduce a Fourier transform on the subspace of $L^2(K)$ consisting of all functions that are constant on conjugacy classes

$$L^2_{\mathrm{class}}(K) := \{f \in L^2(K).\ f(h^{-1}gh) = f(g) \text{ for all } g, h \in K\}.$$

These functions are called class functions (or central functions). The characters χ_σ, $\sigma \in \widehat{K}$, are not only class functions, they form an orthonormal basis of $L^2_{\mathrm{class}}(K)$. The corresponding decomposition of a class function $f \in L^2_{\mathrm{class}}(K)$ is its Fourier transform $\mathcal{F}_{K,\mathrm{class}}$ that is given by

$$\mathcal{F}_{K,\mathrm{class}} f(\sigma) := \int_K \overline{\chi_\sigma}(g) f(g)\mathrm{d}\mu_K(g)$$

with the corresponding inverse transform

$$\mathcal{F}^{-1}_{K,\text{class}} F(\sigma) := \sum_{\sigma \in \widehat{K}} \chi_\sigma(g) F(\sigma)$$

for functions $F : \widehat{K} \to \mathbb{C}$ that lie in the image of $\mathcal{F}_{K,\text{class}}$.

Remark 7.1 (Class Hypergroup and Character Hypergroup). *As already noted, the dual $\widehat{K}$ of a non-abelian compact group is not a group itself. However, the set of characters of a finite group has the algebraic structure of a hypergroup (see [Wil97]).*

First, consider the conjugacy classes of K as elements of the group algebra $\mathbb{C}K$. When $C_j \subset K$, $j = 1, \dots, n$ are the conjugacy classes of K, i.e. $C_j = \{h^{-1} g_j h.\ h \in K\}$ for some $g_j \in G$, $j = 1, \dots, n$, then we define

$$c_j := \frac{1}{|C_j|} \sum_{g \in C_j} g \in \mathbb{C}K,\ j = 1, \dots, n.$$

The set $\mathcal{K} := \{c_1, \dots, c_n\}$ is a hypergroup – the so-called class hypergroup of K. The convolution operation of the hypergroup is given by the product of conjugacy classes

$$c_j * c_k := c_j c_k = \sum_{\ell=1}^{n} a_{j,k}(\ell) c_\ell,\ j, k = 1, \dots, n,$$

for some coefficients $a_{j,k}(\ell) \in \mathbb{N}$, while the involution is given by $\widetilde{c_j} := \frac{1}{|C_j|} \sum_{g \in C_j} g^{-1}$.

Now, the characters χ_σ, $\sigma \in \widehat{K}$ can be identified with functions on $\mathcal{K}$ by setting $\chi_\sigma(c_j) := \chi_\sigma(g_j)$ for some $g_j \in C_j$. This definition is independent of the choice of the element g_j as characters are constant on conjugacy classes. It can now be shown that the set $\widehat{\mathcal{K}} := \{X_\sigma := \chi_\sigma / d_\sigma.\ \sigma \in \widehat{K}\}$ of normalized characters satisfies

$$X_\sigma(c_j) X_\sigma(c_k) = \sum_{\ell=1}^{n} a_{j,k}(\ell) X_\sigma(c_\ell),$$

showing that they are hypergroup characters. The normalized characters form themselves a hypergroup with a convolution that is again given by the expansion of the product:

$$X_j * X_k := X_j X_k = \sum_{\ell=1}^{n} b_{j,k}(\ell) X_\ell,$$

and involution $\widetilde{X}_j := \overline{X_j}$. This hypergroup can be shown to be the dual hypergroup of the class hypergroup.

1.2. Wigner Projections and the Design Equations. Both structures introduced in the last subsection can be utilized for decomposition of functions. Consider a bounded continuous function $f \in C_b(\mathbb{R}^3)$ and the natural action $(gf)(\mathbf{x}) = f(g^{-1}\mathbf{x})$,

$g \in^K$, $\mathbf{x} \in \mathbb{R}^3$. We define the Wigner projection operators (compare [Wig31])

$$P_K^{\chi_\sigma} f(\mathbf{x}) := \int_K \overline{\chi_\sigma(g)}(gf)(\mathbf{x})\mathrm{d}\mu_K(g), \tag{7.7}$$

$$P_K^{\sigma,j,k} f(\mathbf{x}) := \int_K \overline{\sigma_{j,k}(g)}(gf)(\mathbf{x})\mathrm{d}\mu_K(g). \tag{7.8}$$

We write $P_K^{\sigma,j} := P_K^{\sigma,j,j}$ to simplify notation. We also introduce the matrix valued projection P_K^σ by

$$P_K^\sigma f(\mathbf{x}) := \int_K \sigma(g)^*(gf)(\mathbf{x})\mathrm{d}\mu_K(g). \tag{7.9}$$

This will simplify notation later.

For finite groups, a function $f \in C_b(\mathbb{R}^3)$ can be reconstructed from its projections by

$$f = \frac{1}{|K|}\sum_{\sigma\in\widehat{K}} P_K^{\chi_\sigma} f = \frac{1}{|K|}\sum_{\sigma\in\widehat{K}}\sum_{j=1}^{d_\sigma} P_K^{\sigma,j} f. \tag{7.10}$$

Usig the column orthogonality relations $\sum_{\sigma\in\widehat{K}} \chi_\sigma(g) = |K|\delta_{g,e_K}$ where e_K is the neutral element of K, we can see this as follows:

$$\begin{aligned}
\frac{1}{|K|}\sum_{\sigma\in\widehat{K}}\sum_{j=1}^{d_\sigma} P_K^{\sigma,j} f(\mathbf{x}) &= \frac{1}{|K|}\sum_{\sigma\in\widehat{K}}\sum_{j=1}^{d_\sigma}\int_K \overline{\sigma_{j,j}(g)}(gf)(\mathbf{x})\mathrm{d}\mu_K(g) \\
&= \frac{1}{|K|}\sum_{\sigma\in\widehat{K}}\int_K \underbrace{\left(\sum_{j=1}^{d_\sigma}\overline{\sigma_{j,j}(g)}\right)}_{=\overline{\chi_\sigma(g)}}(gf)(\mathbf{x})\mathrm{d}\mu_K(g) \\
&= \frac{1}{|K|}\sum_{\sigma\in\widehat{K}} P_K^{\chi_\sigma} f(\mathbf{x}) = \frac{1}{|K|}\int_K \underbrace{\left(\sum_{\sigma\in\widehat{K}}\overline{\chi_\sigma(g)}\right)}_{=|K|\delta_{g,e_K}}(gf)(\mathbf{x})\mathrm{d}\mu_K(g) \\
&= f(\mathbf{x}).
\end{aligned}$$

The transformation properties of the projections $P_K^{\chi_\sigma} f$ and $P_K^{\sigma,j} f$ are the non-abelian analog of being an eigenfunction. They are derived from the transformation properties of characters and matrix coefficients. Let $\sigma \in \widehat{K}$, $\chi_\sigma = \mathrm{tr}(\sigma)$, and $g, h \in K$, then

$$\begin{aligned}
h\chi_\sigma(g) = \chi_\sigma(h^{-1}g) &= \mathrm{tr}(\sigma(h^{-1}g)) = \mathrm{tr}(\sigma(h^{-1})\sigma(g)) \\
&= \mathrm{tr}(\sigma(h)^*\sigma(g)) = \sum_{j,k=1}^{d_\sigma}\overline{\sigma_{j,k}(h)}\sigma_{j,k}(g),
\end{aligned}$$

and

$$h\sigma_{j,k}(g) = \sigma_{j,k}(h^{-1}g) = \langle \sigma(h^{-1}g)\mathbf{h}_k, \mathbf{h}_j\rangle_{H_\sigma} = \langle \sigma(g)\mathbf{h}_k, \sigma(h)\mathbf{h}_j\rangle$$
$$= \sum_{\ell=1}^{d_\sigma} \overline{\sigma_{\ell,j}(h)}\sigma_{\ell,k}(g).$$

Consequently, for $f \in C_b(\mathbb{R}^3)$

$$hP_K^{\chi_\sigma} f = \sum_{j,k=1}^{d_\sigma} \sigma_{j,k}(h) P_K^{\sigma,j,k} f = \operatorname{tr}(\sigma(h) P_K^\sigma f), \tag{7.11}$$

$$hP_K^{\sigma,j} f = \sum_{\ell=1}^{d_\sigma} \sigma_{\ell,j}(h) P_K^{\sigma,\ell,j} f = (\sigma(h) P_K^\sigma f)_{j,j}. \tag{7.12}$$

We define the invariant subspaces of the space $C_b(\mathbb{R}^3)$ as follows

$$C_b^{\chi_\sigma}(\mathbb{R}^3) := \{f \in C_b(\mathbb{R}^3).\ gf = \operatorname{tr}(\sigma(g)P_K^\sigma f) \text{ for all } g \in K\},$$
$$C_b^{\sigma,j}(\mathbb{R}^3) := \{f \in C_b(\mathbb{R}^3).\ gf = (\sigma(g)P_K^\sigma f)_{j,j} \text{ for all } g \in K\}.$$

Then we can summarize our findings as follows

$$C_b(\mathbb{R}^3) = \bigoplus_{\sigma\in\widehat{K}} C_b^{\chi_\sigma}(\mathbb{R}^3) = \bigoplus_{\sigma\in\widehat{K}} \bigoplus_{j=1}^{d_\sigma} C_b^{\sigma,j}(\mathbb{R}^3).$$

This decomposition can, of course, also be applied to the space of vector valued functions $C_b(\mathbb{R}^3;\mathbb{C}^3)$ and our radiation spaces R_b^ω. To use our notation in this case, we formally introduce matrices with vector entries. Define

$$P_K^\sigma \mathbf{E}(\mathbf{x}) :\ \{1,\dots,d_\sigma\}^2 \to \mathbb{C}^3,\ (j,k) \mapsto \int_K \overline{\sigma_{k,j}(g)}(g\mathbf{E})(\mathbf{x})\mathrm{d}\mu_K(g).$$

In an analog manner, we define the multiplication of a matrix with $P_K^\sigma\mathbf{E}$, the trace and the component function. Then we can decompose the radiation spaces R_b^ω as follows

$$\mathrm{R}_b^\omega = \bigoplus_{\sigma\in\widehat{K}} \mathrm{R}_b^{\omega,\chi_\sigma}(K) = \bigoplus_{\sigma\in\widehat{K}} \bigoplus_{j=1}^{d_\sigma} \mathrm{R}_b^{\omega,\sigma,j}(K), \tag{7.13}$$

where

$$\mathrm{R}_b^{\omega,\chi_\sigma}(K) := \{\mathbf{E}_0 \in \mathrm{R}_b^\omega.\ g\mathbf{E}_0 = \operatorname{tr}(\sigma(g)P_K^\sigma\mathbf{E}_0) \text{ for all } g \in K\},$$
$$\mathrm{R}_b^{\omega,\sigma,j}(K) := \{\mathbf{E}_0 \in \mathrm{R}_b^\omega.\ g\mathbf{E}_0 = (\sigma(g)P_K^\sigma\mathbf{E}_0)_{j,j} \text{ for all } g \in K\}.$$

The design equation for compact isometry groups can now be stated as follows

Definition 7.2 (Design Equations – Compact Groups). *Let $K \leq \mathrm{O}(3)$ be a compact isometry group. A time-harmonic radiation $\mathbf{E}_0 \in \mathrm{R}_b^\omega$ with frequency $\omega > 0$ is said to satisfy the design equations for K when it belongs to the invariant subspace $\mathrm{R}_b^{\omega,\chi_\sigma}(K)$ for some $\sigma \in \widehat{K}$, i.e. when it satisfies the equations*

(i) $\Delta \mathbf{E}_0 = -\dfrac{\omega^2}{c^2}\mathbf{E}_0$,

(ii) $\operatorname{div} \mathbf{E}_0 = 0$,

(iii) $g\mathbf{E}_0 = \operatorname{tr}(\sigma(g) P_K^\sigma \mathbf{E}_0)$ *for all* $g \in G$.

When $\mathbf{E}_0$ additionally satisfies

(iv) $g\mathbf{E}_0 = (\sigma(g) P_K^\sigma \mathbf{E}_0)_{j,j}$ *for some* $j \in \{1, \ldots, d_\sigma\}$ *and all* $g \in G$,

i.e. when it is an element of one of the spaces $\mathrm{R}_b^{\omega,\sigma,j}(K)$, then $\mathbf{E}_0$ is said to satisfy the refined design equations.

2. The Wave Transform

As we did for abelian groups before, we define the Zak transform, the symmetry-adapted waves, and the (scalar) wave transform. All these objects come in two flavours – with respect to the characters or the matrix coefficients.

Definition 7.3 (Zak transform). *Let $K \leq \mathrm{O}(3)$ be a compact isometry group and $f \in \mathcal{S}(\mathbb{R}^3)$. We define the Zak transform and the refined Zak transform by*

$$\mathcal{Z}_K^{\mathrm{class}} f(\mathbf{x}, \sigma) := \mathcal{F}_K^{\mathrm{class}} f_{\mathbf{x}}(\sigma) = P_K^{\chi_\sigma} f(\mathbf{x}), \tag{7.14}$$

$$\mathcal{Z}_K f(\mathbf{x}, \sigma) := \mathcal{F}_K f_{\mathbf{x}}(\sigma) = P_K^{\sigma,j} f(\mathbf{x}), \tag{7.15}$$

where $f_{\mathbf{x}}(g) := (gf)(\mathbf{x})$, $g \in G$.

The corresponding inverse Zak transforms are given by

$$(\mathcal{Z}_K^{\mathrm{class}})^{-1} F_{\mathrm{class}}(\mathbf{x}) := (\mathcal{F}_K^{\mathrm{class}})^{-1} F_{\mathrm{class}}(\mathbf{x}, \mathrm{id}_K), \quad \mathcal{Z}_K^{-1} F(\mathbf{x}) := \mathcal{F}_K^{-1} F(\mathbf{x}, \mathrm{id}_K), \tag{7.16}$$

where F_{class} and F are elements of the image of $\mathcal{S}(\mathbb{R}^3)$ under $\mathcal{Z}_K^{\mathrm{class}}$ and $\mathcal{Z}_K$, respectively.

To define the wave transform, we introduce the symmetry-adapted waves. As the space of bounded continuous functions is closed with respect to projections onto irreducible subspaces of compact groups, these are again bounded and continuous functions. Let $e_{\omega,\mathbf{k}_0}(\mathbf{x}) := e^{i\mathbf{k}\cdot\mathbf{x}}$ and $\mathbf{E}_{\omega,\mathbf{k}_0}(\mathbf{x}) := \mathbf{n} e^{i\mathbf{k}\cdot\mathbf{x}}$ for all $\mathbf{x} \in \mathbb{R}^3$, where $\omega > 0$ and $\mathbf{k} := \frac{\omega}{c}\mathbf{k}_0$, $\mathbf{n} \in \mathbf{k}^\perp$.

We set

$$\mathbf{E}_{\omega,\mathbf{k}_0,\chi_\sigma} := P_K^{\chi_\sigma}\mathbf{E}_{\omega,\mathbf{k}_0} \in \mathrm{R}_b^{\omega,\chi_\sigma}(K), \quad e_{\omega,\mathbf{k}_0,\chi_\sigma} := P_K^{\chi_\sigma} e_{\omega,\mathbf{k}_0} \in C_b^{\chi_\sigma}(\mathbb{R}^3),$$
$$\mathbf{E}_{\omega,\mathbf{k}_0,\sigma,j} := P_K^{\sigma,j}\mathbf{E}_{\omega,\mathbf{k}_0} \in \mathrm{R}_b^{\omega,\sigma,j}(K), \quad e_{\omega,\mathbf{k}_0,\sigma,j} := P_K^{\sigma,j} e_{\omega,\mathbf{k}_0} \in C_b^{\sigma,j}(\mathbb{R}^3).$$

The wave transform and scalar wave transform on $\mathcal{S}(\mathbb{R}^3)$ are then defined as follows.

Definition 7.4 (Wave Transform – Compact Design Group). *Let $K \leq \mathrm{O}(3)$ be a closed compact isometry group. The scalar wave transform $\mathcal{W}_K^{\mathrm{class}} f$ and refined scalar wave transform $\mathcal{W}_K f$ of a function $f \in \mathcal{S}(\mathbb{R}^3)$ are defined as follows.*

$$\mathcal{W}_K^{\mathrm{class}} f(\mathbf{k},\sigma) := \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0,\chi_\sigma}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{7.17}$$

$$\mathcal{W}_K f(\mathbf{k},\sigma) := \int_{\mathbb{R}^3} \overline{e_{\omega,\mathbf{k}_0,\sigma,j}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x}. \tag{7.18}$$

The corresponding vector-valued wave transforms $\boldsymbol{\mathcal{W}}_K^{\mathrm{class}} f$ and $\boldsymbol{\mathcal{W}}_K f$ are given by

$$\boldsymbol{\mathcal{W}}_K^{\mathrm{class}} f(\mathbf{k},\sigma) := \int_{\mathbb{R}^3} \overline{\mathbf{E}_{\omega,\mathbf{k}_0,\chi_\sigma}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{7.19}$$

$$\boldsymbol{\mathcal{W}}_K f(\mathbf{k},\sigma) := \int_{\mathbb{R}^3} \overline{\mathbf{E}_{\omega,\mathbf{k}_0,\sigma,j}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x}. \tag{7.20}$$

These wave transforms share the properties of their abelian counterparts.

Lemma 7.5. *Let $K \leq \mathrm{O}(3)$ ba a closed compact isometry group. The scalar wave transforms satisfy*

$$\mathcal{W}_K^{\mathrm{class}} = \mathcal{Z}_K^{\mathrm{class}} \circ \mathcal{F} = \mathcal{F} \circ \mathcal{Z}_K^{\mathrm{class}}, \tag{7.21}$$

$$\mathcal{W}_K = \mathcal{Z}_K \circ \mathcal{F} = \mathcal{F} \circ \mathcal{Z}_K. \tag{7.22}$$

Consequently, the inverse transforms are given by

$$(\mathcal{W}_K^{\mathrm{class}})^{-1} := (\mathcal{Z}_K^{\mathrm{class}})^{-1} \circ \mathcal{F}^{-1}, \quad \mathcal{W}_K^{-1} := \mathcal{Z}_K^{-1} \circ \mathcal{F}^{-1}. \tag{7.23}$$

Proof. The proofs are identical to the respective proofs for abelian compact groups in Lemma 6.6. □

Up to this point, everything works out exactly as in the abelian compact case. This changes when we consider the scalar wave transform of functions that are invariant with respect to a discrete closed (i.e. finite) subgroup H of the design group K. In the abelian case, the scalar wave transform with respect to K reduced to the scalar wave transform with respect to the subgroup K/H supported on the orthogonal group $H_K^\perp$ of H, which is a subgroup of the dual group $\widehat{K}$. For compact groups, neither the quotient K/H nor the dual $\widehat{K}$ is a group in general.

If we start from a finite group K and the subgroup H is a normal subgroup, i.e. the quotient K/H is a group, we can get a similar result as in the abelian case.

We first need to define the analog of the orthogonal group $H_K^\perp$. Just like $H_K^\perp$ is the set of all characters that are trivial when restricted to H in the abelian case, we define the orthogonal set of a normal subgroup H with respect to K by

$$H_K^\perp := \{\sigma \in \widehat{K}.\ \mathrm{mult}(1, \sigma \downarrow_H^K) \geq 1\}. \tag{7.24}$$

The multiplicity $\mathrm{mult}(\sigma, \sigma')$ of a unitary irreducible representation σ in an arbitrary unitary representation σ' is defined as

$$\mathrm{mult}(\sigma, \sigma') := \langle \chi_\sigma, \chi_{\sigma'} \rangle_{L^2(K)}.$$

The formulation via multiplicities is necessary, because the restriction of an irreducible representation to a subgroup need not be irreducible. So $H_K^\perp$ is the set of unitary irreducible representations of K that contain at least one copy of the trivial representation when restricted to H. For abelian groups this construction reduces to the orthogonal group. To the knowledge of the author, this construction for non-abelian hasn't been considered before.

In the abelian case, we cited a result that says that the restrictions of the elements of $H_K^\perp$ to K/H form the dual $\widehat{K/H}$. A similar identification is possible in the finite case.

Lemma 7.6 (Dual of K/H). *Let $K \leq \mathrm{O}(3)$ be a finite isometry group and H a normal subgroup of K. Then*

$$\widehat{K/H} = \{\sigma \downarrow_{K/H}^K .\ \sigma \in H_K^\perp\}. \tag{7.25}$$

Proof. First, we construct elements of $H_K^\perp$ explicitly from the elements of $\widehat{K/H}$. Let $\widetilde{\sigma} \in \widehat{K/H}$. We lift $\widetilde{\sigma}$ to a representation σ of K by setting

$$\sigma(g) := \widetilde{\sigma}(g'H), \quad \text{for } g \in g'H,\ g' \in G.$$

Then, obviously, $\sigma(h) = \widetilde{\sigma}(H) = 1$ for all $h \in H$, so, $\sigma \downarrow_H^K = 1$. Moreover, we know that $\mathrm{mult}(1, \sigma \downarrow_H^K) = d_\sigma$.

The representation σ is irreducible, since

$$\begin{aligned}
\langle \chi_\sigma, \chi_\sigma \rangle_{L^2(K)} &= \frac{1}{|K|} \sum_{g \in K} \overline{\chi_\sigma(g)} \chi_\sigma(g) = \frac{1}{|K|} \sum_{g'H \in K/H} \sum_{h \in H} \overline{\chi_\sigma(g'h)} \chi_\sigma(g'h) \\
&= \frac{|H|}{|K|} \sum_{g'H \in K/H} \overline{\chi_\sigma(g')} \chi_\sigma(g') = \frac{1}{|K/H|} \sum_{g' \in K/H} \overline{\chi_{\widetilde{\sigma}}(g')} \chi_{\widetilde{\sigma}} \\
&= \langle \chi_{\widetilde{\sigma}}, \chi_{\widetilde{\sigma}} \rangle_{L^2(K/H)} = 1.
\end{aligned}$$

So, $\sigma \in H_K^\perp$ and $\sigma \downarrow_{K/H}^K = \widetilde{\sigma} \in \widehat{K/H}$, i.e.

$$\widehat{K/H} \subseteq \{\sigma \downarrow_{K/H}^K . \, \sigma \in H_K^\perp\}.$$

Now, by Frobenius reciprocity (see [JL04]), we get that

$$d_\sigma = \mathrm{mult}(1, \sigma \downarrow_H^K) = \mathrm{mult}(\sigma, 1 \uparrow_H^K).$$

So, sigma is contained in the induced representation of the trivial representation $1 \uparrow_H^K$ with multiplicity d_σ. By the formula for the induced character (e.g. [JL04], Proposition 21.19), the character $\chi_1 \uparrow_H^K$ of $1 \uparrow_H^K$ is given by

$$\chi_1 \uparrow_H^K (g) = \sum_{g' H \in K/H} \widetilde{1}(g'^{-1} g g'),$$

where $\widetilde{1} = 1 \cdot \mathbf{1}_H$ is the trivial character set to zero except on H. Evaluation at the neutral element e_K yileds

$$\chi_1 \uparrow_H^K (e_K) = \sum_{g' H \in K/H} \widetilde{1}(g'^{-1} e_K g') = \sum_{g' H \in K/H} 1 = |K/H|.$$

Thus, the dimension of the representation $1 \uparrow_H^K$ is $|K/H|$. We already know that the representation contains every representation σ that was lifted from K/H with multiplicity d_σ. Since,

$$\sum_{\widetilde{\sigma} \in \widehat{K/H}} \mathrm{mult}(\sigma, 1 \uparrow_H^K) d_\sigma = \sum_{\widetilde{\sigma} \in \widehat{K/H}} d_\sigma^2 = |K/H|,$$

the lifted representations σ are the only components of $1 \uparrow_H^K$, i.e.

$$1 \uparrow_H^K = \bigoplus_{\widetilde{\sigma} \in \widehat{K/H}} d_\sigma \sigma.$$

Hence, $\mathrm{mult}(1, \sigma \downarrow_H^K) \geq 1$, if and only if $\sigma \downarrow_{K/H}^K \in \widehat{K/H}$. □

Using this identification, we can proof the following.

Lemma 7.7 (Scalar Wave Transform of H-invariant functions – Finite Design Group). *Let $K \leq \mathrm{O}(3)$ be a finite isometry group and H a normal subgroup of G. The scalar wave transform of a function f that is H-invariant is given by*

$$\mathcal{W}_K^{\mathrm{class}} f(\mathbf{k}, \sigma) = \mathcal{W}_{K/H}^{\mathrm{class}} f(\mathbf{k}, \sigma \downarrow_{K/H}^K) \delta_{H_K^\perp}(\sigma) \tag{7.26}$$

for all $\mathbf{k} \in \mathbb{R}^3$, $\sigma \in \widehat{K}$.

Proof. Let $f \in \mathcal{S}(\mathbb{R}^3)$ be H-invariant. Then for $\mathbf{k} \in \mathbb{R}^3$ and $\sigma \in \widehat{K}$

$$\begin{aligned}
\mathcal{W}_K^{\text{class}} f(\mathbf{k}, \sigma) &= \int_{\mathbb{R}^3} \overline{e_{\omega, \mathbf{k}_0, \chi_\sigma}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} \int_K \chi_\sigma(g) e^{-i\mathbf{k} \cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_K(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^3} \int_{K/H} \int_H \chi_\sigma(gh) e^{-i\mathbf{k} \cdot (gh)^{-1}\mathbf{x}} \mathrm{d}\mu_H(h) \mathrm{d}\mu_{K/H}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^3} \int_{K/H} \int_H \sum_{j,k=1}^{d_\sigma} \sigma_{j,k}(g) \sigma_{k,j}(h) e^{-i\mathbf{k} \cdot (gh)^{-1}\mathbf{x}} \mathrm{d}\mu_H(h) \mathrm{d}\mu_{K/H}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{K/H} \int_H \sum_{j,k=1}^{d_\sigma} \sigma_{j,k}(g) \sigma_{k,j}(h) \int_{\mathbb{R}^3} e^{-i\mathbf{k} \cdot g^{-1}\mathbf{x}} \underbrace{f(h\mathbf{x})}_{=f(\mathbf{x})} \mathrm{d}\mathbf{x} \mathrm{d}\mu_H(h) \mathrm{d}\mu_{K/H}(g) \\
&= \sum_{j,k=1}^{d_\sigma} \int_{\mathbb{R}^3} \int_{K/H} \sigma_{j,k}(g) \int_H \sigma_{k,j}(h) \mathrm{d}\mu_H(h) e^{-i\mathbf{k} \cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_{K/H}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x}
\end{aligned}$$

Now, we can apply Lemma 7.6. When $\sigma \downarrow_H^K$ does not contain the trivial representation, then in particular $\int_H \sigma_{k,j}(h) \mathrm{d}\mu_H(h) = 0$ for all $j, k = 1, \ldots, d_\sigma$ by the orthogonality relations. In addition, when $\sigma \in H_K^\perp$ then $\int_H \sigma_{k,j}(h) \mathrm{d}\mu_H(h) = \delta_{k,j}$, so

$$\begin{aligned}
\mathcal{W}_K^{\text{class}} f(\mathbf{k}, \sigma) &= \int_{\mathbb{R}^3} \int_{K/H} \sum_{j=1}^{d_\sigma} \sigma_{j,j}(g) e^{-i\mathbf{k} \cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_{K/H}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \delta_{H_K^\perp}(\sigma) \\
&= \int_{\mathbb{R}^3} \int_{K/H} \chi_\sigma \downarrow_{K/H}^K (g) e^{-i\mathbf{k} \cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_{K/H}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \delta_{H_K^\perp}(\sigma) \\
&= \mathcal{W}_{K/H}^{\text{class}} f(\mathbf{k}, \sigma \downarrow_{K/H}^K) \delta_{H_K^\perp}(\sigma).
\end{aligned}$$

□

We can proof the analog result for the refined scalar wave transform

Lemma 7.8 (Refined Scalar Wave Transform of H-invariant functions – Finite Design Group). *Let $K \leq \mathrm{O}(3)$ be a finite isometry group and H a normal subgroup of G. The refined scalar wave transform of a function f that is H-invariant is given by*

$$\mathcal{W}_K f(\mathbf{k}, \sigma, j) = \mathcal{W}_{K/H} f(\mathbf{k}, \sigma \downarrow_{K/H}^K, j) \delta_{H_K^\perp}(\sigma) \tag{7.27}$$

for all $\mathbf{k} \in \mathbb{R}^3$, $\sigma \in \widehat{K}$.

Proof. The proof is analog to the proof of Lemma 7.7. □

We can again show that the symmetries of f can be reconstructed from the scalar wave transform.

Proposition 7.9 (Reconstruction of Symmetry). *Let $K \leq \mathrm{O}(3)$ be a finite isometry group and $f \in \mathcal{S}(\mathbb{R}^3)$ invariant with respect to a normal subgroup H of K, s.t. f is not invariant with respect to any group H' in between H and K, i.e. $K \leq H' < H$. Then H can be reconstructed from the scalar wave transforms as follows:*

$$H = \bigcap_{\sigma \in \mathrm{supp}(\mathcal{W}_K^{\mathrm{class}} f)} \ker(\sigma) = \bigcap_{\sigma \in \mathrm{supp}(\mathcal{W}_K f)} \ker(\sigma). \tag{7.28}$$

Proof. First, we note that the support of the scalar wave transforms with respect to the second argument is the orthogonal set $H_K^\perp \subseteq \widehat{K}$. It is easily seen that the intersection of the kernels of all elements of $H_K^\perp$ is a normal subgroup:

Let $g, h \in \bigcap_{\sigma \in H_K^\perp} \ker(\sigma)$, i.e. $\sigma(g) = \sigma(h) = \mathrm{id}_{H_\sigma}$ for all $\sigma \in H_K^\perp$. Then also

$$\sigma(h^{-1}g) = \sigma(h^{-1})\sigma(g) = \sigma(h)^*\sigma(g) = \mathrm{id}_{H_\sigma}.$$

When $g \in \bigcap_{\sigma \in H_K^\perp} \ker(\sigma)$ and $h \in K$, then $\sigma(h^{-1}gh) = \sigma(h^{-1})\sigma(g)\sigma(h) = \mathrm{id}_{H_\sigma}$. So, $\widetilde{H} := \bigcap_{\sigma \in H_K^\perp} \ker(\sigma)$ is a normal subgroup of K.

Next, assume that $\widetilde{H}$ is greater that H. Then by definition of $\widetilde{H}$, for all $\sigma \in H_K^\perp$

$$\sigma \downarrow_{\widetilde{H}}^K = 1 \Rightarrow \mathrm{mult}(1, \sigma \downarrow_{\widetilde{H}}^K) = d_\sigma = \mathrm{mult}(\sigma, 1 \uparrow_{\widetilde{H}}^K),$$

using Frobenius reciprocity. Since $1 \uparrow_{\widetilde{H}}^K$ contains all elements of $H_K^\perp$ with multiplicity equal to the dimension, and $H_K^\perp \cong \widehat{K/H}$, we find that $\dim(1 \uparrow_{\widetilde{H}}^K) \geq |K/H| = \frac{|K|}{|H|}$. On the other hand, repeating the argument of Lemma 7.6, we find that $\dim(1 \uparrow_{\widetilde{H}}^K) = |K/\widetilde{H}| = \frac{|K|}{|\widetilde{H}|}$. Thus, $|H| \geq |\widetilde{H}|$, in contradiction to the assumption $H < \widetilde{H}$. Since $H \geq \widetilde{H}$ by the definition of $H_K^\perp$, we find that $\widetilde{H} = H$. □

Unlike in the abelian case, this property does not carry over to the vector-valued wave transform. The action of the compact group on the field vector leads to a modulation of the components of the field when diagonalizing the action. This modulation becomes a translation on the Fourier side, s.t. the reciprocal structure is a superposition of translated versions of the orthogonal group of the symmetry group of the structure.

Now, in the non-abelian compact case, the action of the group on the field vector cannot be diagonalized, but only decomposed into its irreducible components. Moreover, the modulation by a matrix coefficient is not a simple translation on the Fourier side.

Still, we can give an expression for the supports of the wave transforms. In explicit examples, this information could help to reconstruct symmetry information.

Proposition 7.10 (Support of the Wave Transform). *Let $K \leq \mathrm{O}(3)$ be a finite isometry group and $f \in \mathcal{S}(\mathbb{R}^3)$ be invariant with respect to a subgroup H of K. The wave*

transform is supported on the following sets.

$$\operatorname{supp}(\boldsymbol{\mathcal{W}}_K^{\text{class}} f(\mathbf{k},\cdot)) \subseteq \bigcup_{k=1}^{n} \left\{ \sigma \in \widehat{K}.\ \text{mult}\left(\sigma, \sigma_{\mathbb{R}^3}^{(k)^*} \downarrow_H^K \uparrow_H^K\right) \geq 1 \right\}, \quad \mathbf{k} \in \mathbb{R}^3. \tag{7.29}$$

where $\sigma_{\mathbb{R}^3}$ is the standard representation of K on $\mathbb{R}^3$ given by $\sigma_{\mathbb{R}^3}(g)\mathbf{x} = g\mathbf{x}$, that decomposes as

$$\sigma_{\mathbb{R}^3} = \bigoplus_{k=1}^{n} \sigma_{\mathbb{R}^3}^{(k)}.$$

Proof. Let $f \in \mathcal{S}(\mathbb{R}^3)$ be H-invariant. then for all $\mathbf{k} \in \mathbb{R}^3$ and $\sigma \in \widehat{K}$

$$\begin{aligned}
\boldsymbol{\mathcal{W}}_K^{\text{class}} f(\mathbf{k},\sigma) &= \int_{\mathbb{R}^3} \overline{\mathbf{E}_{\omega,\mathbf{k}_0,\chi_\sigma}(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^3} \int_K \chi_\sigma(g) \overline{\sigma_{\mathbb{R}^3}(g)\mathbf{n}(\mathbf{k})} e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_K(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \mathbf{U} \int_{\mathbb{R}^3} \int_K \chi_\sigma(g) \mathrm{diag}(\sigma_{\mathbb{R}^3}^{(k)}(g))_{k=1}^n e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_K(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \mathbf{U}^{-1} \overline{\mathbf{n}(\mathbf{k})}.
\end{aligned}$$

We consider the entries of the matrix-valued integral. At the (ℓ, m)-element of $\sigma_{\mathbb{R}^3}^{(k)}$, we get

$$\begin{aligned}
&\int_{\mathbb{R}^3} \int_K \chi_\sigma(g) \sigma_{\mathbb{R}^3,\ell,m}^{(k)}(g) e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_K(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^3} \int_K \sum_{j=1}^{d_\sigma} \sigma_{j,j}(g) \sigma_{\mathbb{R}^3,\ell,m}^{(k)}(g) e^{-i\mathbf{k}\cdot g^{-1}\mathbf{x}} \mathrm{d}\mu_K(g) f(\mathbf{x}) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^3} \int_{K/H} \int_H \sum_{j=1}^{d_\sigma} \sigma_{j,j}(gh) \sigma_{\mathbb{R}^3,\ell,m}^{(k)}(gh) e^{-i\mathbf{k}\cdot (gh)^{-1}\mathbf{x}} \mathrm{d}\mu_H(h) \mathrm{d}\mu_{K/H}(g) f(\mathbf{x}) \mathrm{d}\mathbf{x}
\end{aligned}$$

Now using the transformation rule for the matrix coefficients, we end up with integrals of the type

$$\int_H \sigma_{i,j}(h) \sigma_{\mathbb{R}^3,l,m}^{(k)}(h) \mathrm{d}\mu_H(h).$$

These integrals vanish when the restriction of σ to H is not contained in the restriction of $\sigma_{\mathbb{R}^3}^*$ to H by the orthogonality relations. In other words, when $\text{mult}(\sigma \downarrow_H^K, \sigma_{\mathbb{R}^3} \downarrow_H^K) = 0$. Thus, the support of the wave transform is contained in the set

$$\{\sigma \in \widehat{K}.\ \text{mult}(\sigma \downarrow_H^K, \sigma_{\mathbb{R}^3} \downarrow_H^K) \geq 1\}.$$

By Frobenius reciprocity and the fact that $\chi_{\sigma\oplus\sigma'} = \chi_\sigma + \chi_{\sigma'}$, we get the result. □

With exactly the same proof, the same result can be shown for the support of the refined wave transform, i.e.

$$\operatorname{supp}(\boldsymbol{\mathcal{W}}_K f(\mathbf{k},\cdot,j)) \subseteq \bigcup_{k=1}^{n} \left\{ \sigma \in \widehat{K}.\ \operatorname{mult}\left(\sigma, \sigma_{\mathbb{R}^3}^{(k)^*} \downarrow_H^K \uparrow_H^K\right) \geq 1 \right\} \tag{7.30}$$

for all $\mathbf{k} \in \mathbb{R}^3$ and all appropriate $j \in \mathbb{N}$.

Outlook

To conclude this work, we shortly discuss some ideas related to the results of this dissertation.

X-Ray Optics and Electron Beams. When considering the generalized von Laue condition (Theorem 6.17) for orientation preserving design groups, i.e. closed subgroups of $\mathrm{SE}(3) := \{(\mathbf{Q}|\mathbf{c}) \in \mathrm{E}(3).\ \det \mathbf{Q} = 1\}$, the result reduces to essentially three different kinds of radiation: plane waves, twisted waves and n-twisted waves. The corresponding minimal design groups are the trivial group for plane waves, the group $R_{\mathbf{e}}$ of rotations about an axis $\mathbb{R}\mathbf{e}$, $\mathbf{e} \in \mathbb{S}^2$, for twisted waves and the corresponding finite rotation group $R_{\mathbf{e}}^{(n)}$ for n-twisted waves.

These are the central cases that lead to a von Laue condition. Our work reduces the problem of structure analysis with these kinds of radiation to a problem of X-ray optics. How can these kind of radiations be produced? In light of the Fourier representations (4.1) and (5.20) for twisted and n-twisted waves, respectively, the task is to phase align the single plane waves in the right way to achieve the needed chirality.

Several approaches to produce analogs of twisted waves for electron beams (e.g. [VTS10], vortex beams) or visible light (e.g. [AD00], high-order Bessel beams) have been proposed. These beams are used as particle traps, for information transmission or in astrophysics.

Using twisted waves for structure analysis turns out to be an even harder task. To vary the radiation parameters, the method for the generation has to be adaptive.

A different approach would be to use electron vortex beams instead of X-rays for the analysis. We believe that the theory developed in this dissertation can be adapted to the use of electron beams instead of electromagnetic waves. A further advantage of this idea is the scalar nature of the electron beam that simplifies the corresponding von Laue condition.

The Diffraction Pattern. We focused on the derivation of a generalized von Laue condition and neglected the possibility of reconstruction from the diffraction pattern. we saw in Chapter 3 that the scatterring of time-harmonic radiation always leads to an analog

of the CDI reconstruction problem that allows in principle to reconstruct a projection of the sample. If this is the goal, it is, of course, preferable to use plane wave radiation.

However, the scattering formula for twisted waves (Theorem 4.5) contains a lot of information on the symmetries of the structure. It might be possible to extract it via a clever transformation of the pattern, even though, we do not see an easy way to do this at the moment.

A simpler approach to use the diffraction patterns for reconstruction is to include the data in a phase retrieval algorithm. It could, for example, be used as an additional constraint set.

Compressed Sensing. A different approach to phase retrieval arose from the field of compressed sensing. In [CSV12], the authors propose a way to reconstruct a general sample from plane wave diffraction patterns that are post-scattered by a random binary matrix. The corresponding algorithm is called PhaseLift and reformulates the phase retrieval problem as a matrix completion problem.

We believe that our framework of the scattering of time-harmonic radiation could provide a different way to use the theory of compressed sensing for phase retrieval. It might be possible to use the difficulty of phase aligning plane waves to our advantage by incorporating the needed randomness in the relative phases of the single plane wave components of the radiation.

A Generalized Bloch-Floquet Theorem. The decomposition of a scalar function into invariant functions via the Zak transform is closely related to the Bloch theorem concerning the electronic Schrödinger equation for a perfect crystal with Bravais lattice $\mathcal{B}$ (see [Blo29], and for a mathematically rigorous account, [RSIV]). It states that the solution space has a basis of eigenstates $\psi_{\mathbf{k}}$ that are of the special form

$$\psi_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}u(\mathbf{x}), \tag{7.31}$$

where $\mathbf{k} \in \mathrm{U}_{\mathcal{B}^\perp}$ is a wave vector in the fundamental domain of the reciprocal lattice $\mathcal{B}^\perp$ of $\mathcal{B}$ and u is $\mathcal{B}$-invariant.

Mathematically it is an application of the Floquet theorem on the solutions of periodic linear differential equations. Even more general, we can decompose arbitrary functions into Bloch waves as follows. Given a Bravais lattice $\mathcal{B}$, every function $f \in \mathcal{S}(\mathbb{R}^3)$ can be written as

$$f(\mathbf{x}) = \frac{1}{\mathrm{V}_{\mathcal{B}^\perp}} \int_{\mathrm{U}_{\mathcal{B}^\perp}} e^{i\mathbf{k}\cdot\mathbf{x}} u(\mathbf{x}, \mathbf{k}) \mathrm{d}\mathbf{k}, \tag{7.32}$$

where u is $\mathcal{B}$-invariant in $\mathbf{x}$. This formulation is sometimes called Bloch-Floquet theorem [SEA03]. It is a direct consequence of the Poisson summation formula and can be proved

as follows. Fourier decomposing f and splitting the integral into the integrals over the fundamental domains of $\mathcal{B}^\perp$, we get

$$\begin{aligned} f(\mathbf{x}) &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{i\mathbf{k}\cdot\mathbf{x}}\widehat{f}(\mathbf{k})\mathrm{d}\mathbf{k} = \sum_{\mathbf{b}'\in\mathcal{B}^\perp}\int_{\mathrm{U}_{\mathcal{B}^\perp}} e^{i(\mathbf{k}+\mathbf{b}')\cdot\mathbf{x}}\widehat{f}(\mathbf{k}+\mathbf{b}')\mathrm{d}\mathbf{k} \\ &= \int_{\mathrm{U}_{\mathcal{B}^\perp}} e^{i\mathbf{k}\cdot\mathbf{x}}\frac{1}{(2\pi)^3}\sum_{\mathbf{b}'\in\mathcal{B}^\perp} e^{i\mathbf{b}'\cdot\mathbf{x}}\widehat{f}(\mathbf{k}+\mathbf{b}')\mathrm{d}\mathbf{k} \\ &= \frac{1}{\mathrm{V}_{\mathcal{B}^\perp}}\int_{\mathrm{U}_{\mathcal{B}^\perp}} e^{i\mathbf{k}\cdot\mathbf{x}} \underbrace{\frac{\mathrm{V}_{\mathcal{B}^\perp}}{(2\pi)^3}\sum_{\mathbf{b}'\in\mathcal{B}^\perp} e^{i\mathbf{b}'\cdot\mathbf{x}}\widehat{f}(\mathbf{k}+\mathbf{b}')}_{=:u(\mathbf{x},\mathbf{k})}\,\mathrm{d}\mathbf{k}. \end{aligned}$$

The $\mathcal{B}$-invariance of u is now seen with the Poisson summation formula:

$$u(\mathbf{x},\mathbf{k}) = \frac{\mathrm{V}_{\mathcal{B}^\perp}}{(2\pi)^3}\sum_{\mathbf{b}'\in\mathcal{B}^\perp} e^{i\mathbf{b}'\cdot\mathbf{x}}\widehat{f}(\mathbf{k}+\mathbf{b}') = \sum_{\mathbf{b}\in\mathcal{B}} e^{-i\mathbf{k}\cdot(\mathbf{x}+\mathbf{b})}f(\mathbf{x}+\mathbf{b}).$$

The relation to the Zak transform becomes clear, when observing that the integrand of (7.32) is actually the Zak transform with respect to the group $H_\mathcal{B}$:

$$e^{i\mathbf{k}\cdot\mathbf{x}}u(\mathbf{x},\mathbf{k}) = \sum_{\mathbf{b}\in\mathcal{B}} e^{-i\mathbf{k}\cdot\mathbf{b}}f(\mathbf{x}+\mathbf{b}) = \mathcal{Z}_{H_\mathcal{B}}f(\mathbf{x},\mathbf{k}).$$

Noting that the unit cell $\mathrm{U}_{\mathcal{B}^\perp}$ of the reciprocal lattice is a parametrization of the quotient group $T/H_{\mathcal{B}^\perp} \cong \widehat{H_\mathcal{B}}$, we find that the Bloch-Floquet decomposition (7.32) is simply the reconstruction formula of the Zak transform: $f(\mathbf{x}) = \mathcal{Z}^{-1}_{H_\mathcal{B}}\mathcal{Z}_{H_\mathcal{B}}f(\mathbf{x},\mathrm{id}_{\mathbb{R}^3})$.

The generalized Zak transform we introduced can thus be used to formulate a generalized Bloch-Floquet theorem. Given an abelian isometry group $H \leq \mathrm{E}(3)$, every function $f \in \mathcal{S}(\mathbb{R}^3)$ can be decomposed as follows:

$$f(\mathbf{x}) = \int_{\widehat{H}} \mathcal{Z}_H f(\mathbf{x},\chi)\mathrm{d}\mu_{\widehat{H}}(\chi). \tag{7.33}$$

The transformation law is analog to the one for classic Bloch waves. The function $\mathcal{Z}_H f(\mathbf{x},\chi)$ is H-invariant in $\mathbf{x}$ up to a phase that is given by the character χ:

$$g\mathcal{Z}_H f(\mathbf{x},\chi) = \mathcal{Z}_H f(g^{-1}\mathbf{x},\chi) = \chi(g)\mathcal{Z}_H f(\mathbf{x},\chi).$$

This generalization of the Bloch theorem could, for example, be useful for studying the electronic structure of objective structures.

Note that this construction can also be generalized to non-abelian compact groups via the Zak transforms introduced in Chapter 7. The corresponding Bloch waves are then not invariant up to a phase, but transform as in equation (7.11) and (7.12). But still, given the wave in a fundamental domain, it is determined in a different fundamental domain up to transformation by an irreducible representation.

APPENDIX A

Fourier analysis

Fourier Analysis on $\mathbb{R}^n$. In this chapter we will cite central results of Fourier analysis without proof, that can be found in almost every textbook about the topic (e.g. [Fri07, SD80, Fol95]). We present the results in a form focusing on the structural content rather than as mere rules of calculus. We begin with the definition on $L^1(\mathbb{R}^n)$.

Definition A.1 (Fourier transform on L^1). *Let $f \in L^1(\mathbb{R}^n)$. Then its Fourier transform $\widehat{f} : \mathbb{R}^n \to \mathbb{C}$ is defined as*

$$\widehat{f}(\mathbf{k}) := \int_{\mathbb{R}^n} f(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}\mathbf{x}, \quad \mathbf{k} \in \mathbb{R}^3. \tag{A.1}$$

We also write $\mathcal{F}(f) := \widehat{f}$.

The following are the main results of the L^1-theory

Lemma A.2 (Riemann-Lebesgue). *The space $\mathcal{F}L^1(\mathbb{R}^n)$ of Fourier transforms of L^1-functions is a subspace of the space of continuous functions that vanish at infinity:*

$$\mathcal{F}L^1(\mathbb{R}^n) \subset C_0(\mathbb{R}^n).$$

Theorem A.3 (Convolution Theorem). *The spaces $L^1(\mathbb{R}^n)$ with convolution and involution $f \mapsto \overline{f_-}$ and $C_0(\mathbb{R}^n)$ with pointwise multiplication and complex conjugation are Banach-*-algebras.*

*The Fourier transform $\mathcal{F} : L^1(\mathbb{R}^n) \to C_0(\mathbb{R}^n)$ is a *-algebra morphism, i.e.*

(i) $\widehat{f * g} = \widehat{f}\widehat{g}$,

(ii) $\widehat{\overline{f_-}} = \overline{\widehat{f}}$.

Theorem A.4 (Inversion Theorem). *Let $f \in L^1(\mathbb{R}^n)$. When $\widehat{f} \in L^1(\mathbb{R}^n)$, then f can be reconstructed pointwise a.e. by*

$$f(\mathbf{x}) = \mathcal{F}^{-1}\widehat{f}(\mathbf{x}) := (2\pi)^{-n} \int_{\mathbb{R}^n} \widehat{f}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}\mathbf{k}, \quad \textit{for a.e. } \mathbf{x} \in \mathbb{R}^3. \tag{A.2}$$

The transformation $\widehat{f} \mapsto \mathcal{F}^{-1}\widehat{f}$ is called inverse Fourier transform.

The Fourier transform on $L^1 \cap L^2$ can uniquely be extended to L^2.

Theorem A.5 (Fourier transform on L^2, Plancherel). *There is a unique continuous map $\mathcal{F} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ that agrees with the Fourier transform on $L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$.*

Moreover, the rescaled version $(2\pi)^{-n/2}\mathcal{F}$ is a unitary transformation (Hilbert space isomorphism), i.e. for all $f, g \in L^2(\mathbb{R}^n)$:

$$\langle (2\pi)^{-n/2}\mathcal{F}f, (2\pi)^{-n/2}\mathcal{F}g\rangle_{L^2(\mathbb{R}^n)} = \langle f, g\rangle_{L^2(\mathbb{R}^n)}.$$

In particular, the Plancherel identity holds:

$$\|f\|_2^2 = (2\pi)^{-n}\|\mathcal{F}f\|_2^2, \quad f \in L^2(\mathbb{R}^n). \tag{A.3}$$

The inverse operator $\mathcal{F}^{-1} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is called inverse Fourier transform on $L^2(\mathbb{R}^n)$ and satisfies

$$\mathcal{F}^{-1}f = (2\pi)^{-n}\mathcal{F}f_- \quad f \in L^2(\mathbb{R}^n).$$

The regular representation $\pi : \mathbb{R}^3 \to \mathrm{U}(L^2(\mathbb{R}^n))$ of the translation group $\mathbb{R}^3$ on the Hilbert space $L^2(\mathbb{R}^3)$ is given by

$$\pi(\mathbf{y})f(\mathbf{x}) := f(\mathbf{x} - \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^3,\ f \in L^2(\mathbb{R}^n).$$

Defining the modulation representation $\widehat{\pi} : \mathbb{R}^3 \to \mathrm{U}(L^2(\mathbb{R}^n))$ of the group $\mathbb{R}^3$ by

$$\widehat{\pi}(\mathbf{y})f(\mathbf{x}) := e^{-i\mathbf{y}\cdot\mathbf{x}}f(\mathbf{x}), \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^3,\ f \in L^2(\mathbb{R}^n),$$

the Fourier transform $\mathcal{F}$ is an intertwining operator for π and $\widehat{\pi}$, i.e.

$$\mathcal{F}\pi = \widehat{\pi}\mathcal{F}. \tag{A.4}$$

The same is true for the unitary version $(2\pi)^{-n/2}\mathcal{F}$, showing that the representations π and $\widehat{\pi}$ are unitary equivalent. This identity is often explicitly stated as translation-modulation duality:

$$\widehat{f(\cdot - \mathbf{y})}(\mathbf{k}) = e^{-i\mathbf{y}\cdot\mathbf{k}}\widehat{f}(\mathbf{k}), \quad \mathbf{x}, \mathbf{k} \in \mathbb{R}^n,\ f \in L^2(\mathbb{R}^n). \tag{A.5}$$

To extend the Fourier transform by duality, we first restrict it to a space of 'nice' functions – the smooth and rapidly decaying Schwartz functions.

Definition A.6 (Schwartz functions). *Define the family of semi-norms*

$$\|\varphi\|_{\boldsymbol{\ell},\mathbf{m}} := \sup_{\mathbf{x}\in\mathbb{R}^n} |\mathbf{x}^{\boldsymbol{\ell}} D^{\mathbf{m}}\varphi(\mathbf{x})|, \quad \boldsymbol{\ell}, \mathbf{m} \in \mathbb{N}_0^n,\ \varphi : \mathbb{R}^n \to \mathbb{C}.$$

The Schwartz space of smooth rapidly decaying functions is defined as

$$\mathcal{S}(\mathbb{R}^n) := \{\varphi \in C^\infty(\mathbb{R}^n).\ \|\varphi\|_{\boldsymbol{\ell},\mathbf{m}} < \infty \text{ for all } \boldsymbol{\ell}, \mathbf{m} \in \mathbb{N}_0^n\}. \tag{A.6}$$

The elements of $\mathcal{S}(\mathbb{R}^n)$ are called Schwartz functions.

Theorem A.7 (Schwartz). *The space $\mathcal{S}(\mathbb{R}^n)$ is a Fréchet space with respect to the locally convex topology induced by the semi-norms $\|\cdot\|_{\boldsymbol{\ell},\mathbf{m}}$, $\boldsymbol{\ell}, \mathbf{m} \in \mathbb{N}_0^n$. It is a locally convex algebra w.r.t. both convolution and pointwise multiplication.*

The Fourier transform $\mathcal{F} : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n)$ and the inverse Fourier transform $\mathcal{F}^{-1} : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n)$ are algebra homomorphisms between the two algebra structures.

Consider a polynomial $p = \sum_{|\mathbf{m}|\leq N} p_{\mathbf{m}} \mathbf{x}^{\mathbf{m}} \in \mathbb{C}[\mathbf{x}, \ldots, \mathbf{x}_n]$, $N \in \mathbb{N}$, and the associated linear transformations

$$D(p) : \ \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n), \ f \mapsto D(p)f := \sum_{|\mathbf{m}|\leq N} p_{\mathbf{m}} D^{\mathbf{m}} f,$$
$$M(p) : \ \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n), \ f \mapsto M(p)f := p(i\cdot) \cdot f.$$

Then the Fourier transform is an intertwining operator for $D(p)$ and $M(p)$, i.e.

$$\mathcal{F}D(p) = M(p)\mathcal{F}.$$

This identity is often explicitly stated as differentiation-multiplication duality:

$$\widehat{\partial_j \varphi}(\mathbf{k}) = i\mathbf{k}_j \widehat{\varphi}(\mathbf{k}), \quad j \in \{1, \ldots, n\}, \ \mathbf{k} \in \mathbb{R}^3, \ \varphi \in \mathcal{S}(\mathbb{R}^n). \tag{A.7}$$

Definition A.8 (Tempered distributions). *The dual space $\mathcal{S}'(\mathbb{R}^n)$ of continuous linear functionals on $\mathcal{S}(\mathbb{R}^n)$ is called the space of tempered distributions. Its elements are called tempered distributions.*

For $1 \leq p \leq \infty$, functions $f \in L^p(\mathbb{R}^n)$ can be seen as tempered distributions by identifying them with the functionals

$$L_f(\varphi) := \int_{\mathbb{R}^n} f\varphi \mathrm{d}\mathcal{L}^n, \quad \varphi \in \mathcal{S}(\mathbb{R}^n).$$

We will not distinguish between the function f and the associated distribution L_f, i.e. we will write $f(\varphi) := L_f(\varphi)$ for $\varphi \in \mathcal{S}(\mathbb{R}^n)$. A nice account of the theory of distributions is found in [Hor83].

The Fourier transform of a tempered distribution is defined as follows:

Theorem A.9 (Fourier transform on $\mathcal{S}'$). *The space $\mathcal{S}'(\mathbb{R}^n)$ of tempered distributions with the weak topology $\sigma(\mathcal{S}'(\mathbb{R}^n), \mathcal{S}(\mathbb{R}^n))$ is a locally convex space.*

The Fourier transform $\mathcal{F} : \mathcal{S}'(\mathbb{R}^n) \to \mathcal{S}'(\mathbb{R}^n)$,defined by

$$\mathcal{F}T(\varphi) := T(\mathcal{F}\varphi), \ \ T \in \mathcal{S}'(\mathbb{R}^n), \ \varphi \in \mathcal{S}(\mathbb{R}^n),$$

is a linear map. The same is true for the inverse Fourier transform $\mathcal{F}^{-1}$ that is defined similarly.

We also write $\widehat{T} := \mathcal{F}T$.

Multiplication and convolution of two tempered distributions are in general not defined. Considering special classes of functions, we can, however, define the multiplication and convolution of tempered distributions with these functions.

Lemma A.10 (Tempered functions). *A function $f : \mathbb{R}^n \to \mathbb{C}$ is called slowly increasing, if there is a $C \geq 0$ and an $N \in \mathbb{N}$, s.t.*

$$|f(\mathbf{x})| \leq C(1 + |\mathbf{x}|^2)^N.$$

Consider the space $\mathcal{T}(\mathbb{R}^n)$ of smooth slowly increasing functions

$$\mathcal{T}(\mathbb{R}^n) := \{f \in C^\infty(\mathbb{R}^n).\ D^{\mathbf{m}} f \text{ slowly increasing for all } \mathbf{m} \in \mathbb{N}_0^n\}.$$

The space $\mathcal{S}(\mathbb{R}^n)$ of Schwartz functions is closed under multiplication with tempered functions, i.e.

$$\mathcal{T}(\mathbb{R}^n) \cdot \mathcal{S}(\mathbb{R}^n) \subseteq \mathcal{S}(\mathbb{R}^n).$$

In particular, the functional L_f, $f \in \mathcal{T}(\mathbb{R}^n)$, is a tempered distribution.

Now, we can define basic operations on the space $\mathcal{S}'(\mathbb{R}^n)$ of tempered distributions.

Corollary A.11 (Basic operations on tempered distributions). *Let $T \in \mathcal{S}'(\mathbb{R}^n)$, $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$, $f \in \mathcal{T}(\mathbb{R}^n)$, $\mathbf{y} \in \mathbb{R}^3$ and $\mathbf{m} \in \mathbb{N}_0^n$. We define*

(i) $T * \varphi \in \mathcal{S}'(\mathbb{R}^n)$ *by* $(T * \varphi)\psi := T(\varphi_- * \psi)$,

(ii) $T \cdot f \in \mathcal{S}'(\mathbb{R}^n)$ *by* $(T \cdot f)\psi := T(f \cdot \psi)$,

(iii) $\pi(\mathbf{y})T \in \mathcal{S}'(\mathbb{R}^n)$ *by* $(\pi(\mathbf{y})T)\psi := T(\pi(-\mathbf{y})\psi)$,

(iv) $D^{\mathbf{m}}T \in \mathcal{S}'(\mathbb{R}^n)$ *by* $(D^{\mathbf{m}}T)\psi := (-1)^{|\mathbf{m}|}T(D^{\mathbf{m}}\psi)$.

The operators $\widehat{\pi}$, $D(p)$, and $M(p)$ for $p \in \mathbb{C}[\mathbf{x}_1, \ldots, \mathbf{x}_n]$ are defined via (ii) and (iv).

These operations satisfy

(1) $\widehat{T * \varphi} = \widehat{T} \cdot \widehat{\varphi}$,

(2) $\widehat{\pi(\mathbf{y})T} = \widehat{\pi}(\mathbf{y})\widehat{T}$,

(3) $\widehat{D(p)T} = M(p)\widehat{T}$.

Note that by (1) the definition of the convolution can be extended to Fourier transforms of tempered functions (e.g. distributions of compact support by Schwartz-Paley-Wiener (e.g. [Die75]).

We collect some results that are used in the main text:

Corollary A.12 (Autocorrelation). *Let $T \in \mathcal{FT}(\mathbb{R}^n)$ be a tempered distribution that is the Fourier transform of a tempered function. Define its autocorrelation function*

$C_T \in \mathcal{S}'(\mathbb{R}^n)$ by

$$C_T := T * \overline{T_-}.$$

Then

$$\widehat{C_T} = |\widehat{T}|^2.$$

Note that $\widehat{T} \in \mathcal{T}(\mathbb{R}^n)$, s.t. $|\widehat{T}|^2$ is well-defined.

Theorem A.13 (Poisson summation formula). *The measure $\delta_{\mathbb{Z}} := \sum_{j\in\mathbb{Z}} \delta_j$ is a tempered distribution. Its Fourier transform is*

$$\widehat{\delta_{\mathbb{Z}}} = 2\pi\delta_{2\pi\mathbb{Z}}.$$

Theorem A.14 (Projection-slice theorem). *Let $\mathbf{k} \in \mathbb{S}^2$ and define the following two operators on $\mathcal{S}(\mathbb{R}^n)$:*

$$\mathrm{p}_{\mathbf{k}} :\ \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbf{k}^\perp),\ \varphi \mapsto \int_{\mathbb{R}} \varphi(\cdot + r\mathbf{k})\mathrm{d}r$$
$$\mathrm{s}_{\mathbf{k}} :\ \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbf{k}^\perp),\ \varphi \mapsto \varphi\big|_{\mathbf{k}^\perp}.$$

The operators are called projection and slice operators, respectively. They satisfy

$$\widehat{\mathrm{p}_{\mathbf{k}}\varphi} = \mathrm{s}_{\mathbf{k}}\widehat{\varphi}.$$

Many measures can also be seen as tempered distribution.

Proposition A.15 (Tempered measures). *A Borel measure μ on $\mathbb{R}^n$ is called tempered measure, if there is an $N \in \mathbb{N}$, s.t.*

$$\int_{\mathbb{R}^n} (1 + |\mathbf{x}|^2)^{-N} \mathrm{d}\mu(\mathbf{x}) < \infty.$$

Every tempered measure is a tempered distribution when identified with the functional $L_\mu \in \mathcal{S}'(\mathbb{R}^n)$ that is defined as

$$L_\mu(\varphi) := \int_{\mathbb{R}^n} \varphi \,\mathrm{d}\mu.$$

Moreover, every positive tempered distribution, i.e. $T\varphi \geq 0$ for all $\varphi \in \mathcal{S}^{\geq 0}(\mathbb{R}^n)$, is a tempered measure.

Fourier Analysis on Locally Compact Abelian Groups. Fourier theory can be extended to a locally compact abelian group G. The role of the complex exponentials $e_{\mathbf{k}}$, $\mathbf{k} \in \mathbb{R}^3$, is played by the characters, i.e. the bounded continuous group homomorphisms from G to $\mathbb{C}^* := \mathbb{C} \setminus \{0\}$. They are collected in the dual grop $\widehat{G}$.

$$\widehat{G} := \{\chi : G \to \mathbb{C}^* \text{ bounded continuous. } \chi(gh) = \chi(g)\chi(h),\ \chi(g^{-1}) = \overline{\chi(g)}\}. \tag{A.8}$$

The Fourier transform on $L^1(G)$ is then defined as follows

Definition A.16 (Fourier Transform on $L^1(G)$). *Let G be a locally compact abelian group and $f \in L^1(G)$. Then the Fourier transform $\mathcal{F}_G f : \widehat{G} \to \mathbb{C}$ of f is defined as*

$$\mathcal{F}_G f(\chi) := \int_G \overline{\chi(g)} f(g) \mathrm{d}\mu_G(g), \tag{A.9}$$

for $\chi \in \widehat{G}$, where μ_G is the Haar measure of G.

The inverse Fourier transform is given by the Fourier inversion theorem.

Theorem A.17 (Fourier Inversion). *Let $f \in L^1(G)$ be continuous with an L^1 Fourier transform $\mathcal{F}_G f \in L^1(\widehat{G})$. Then*

$$f(g) = \int_{\widehat{G}} \chi(g) \mathcal{F}_G f(\chi) \mathrm{d}\mu_{\widehat{G}}(\chi), \tag{A.10}$$

for all $g \in G$, where $\mu_{\widehat{G}}$ is a suitably normalized Haar measure on $\widehat{G}$.

The Fourier transform on $L^1(G)$ can be extended to the space $M^1(G)$ of finite complex measures on G. It is defined as the boounded continuous function on $\widehat{G}$ given by

$$\mathcal{F}_G \mu(\chi) := \int_G \overline{\chi(g)} \mathrm{d}\mu(g), \tag{A.11}$$

for $\mu \in M^1(G)$ and $\chi \in \widehat{G}$.

Most of the results for the Fourier transform can be generalized to the case of locally compact abelian groups. In particular, there is a convolution theorem: For $f_1, f_2 \in L^1(G)$,

$$\mathcal{F}_G(f_1 * f_2) = \mathcal{F}_G f_1 \cdot \mathcal{F}_G f_2, \tag{A.12}$$

where $f_1 * f_2(g) := \int_G f_1(h^{-1}g) f_2(h) \mathrm{d}\mu_G(h)$ for all $g \in G$.

There is also a translation-modulation duality. For $f \in L^1(G)$ and $\chi \in \widehat{G}$,

$$\mathcal{F}_G(f(g^{-1}\cdot))(\chi) = \overline{\chi(g)} \mathcal{F}_G f, \quad g \in G. \tag{A.13}$$

For further results on harmonic analysis on groups, we refer to [Fol95], [Rei68], [Ter85, Ter88], and to the classic account [HR63, HR70].

APPENDIX B

Maxwell's equations

Maxwell's equations are four coupled partial differential equations that govern the behavior of the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$ when an electric charge density ρ_{el} and a current density $\mathbf{J}_{\mathrm{el}}$ is present. They were inferred from suitable experiments in their integral form.

The first of Maxwell's equations is usually called Gauß's law and says that the outward normal electric flux through a closed surface $\partial\Omega$ is proportional to the electric charge contained in Ω. When Ω is suitably regular (e.g. a bounded C^1-domain), then

$$\int_{\partial\Omega} \mathbf{E} \cdot \mathrm{dS} = \frac{1}{\varepsilon_0} \int_{\Omega} \rho_{\mathrm{el}} \, \mathrm{d}\mathcal{L}^3, \qquad \text{(Gauß's law)}$$

where the constant ε_0 is called vacuum permittivity or electric constant. The corresponding outward normal magnetic flux equals zero:

$$\int_{\partial\Omega} \mathbf{B} \cdot \mathrm{dS} = 0.$$

When $\mathbf{E}$ is continuously differentiable, applying the divergence theorem to the left hand sides of these two laws for the choice $\Omega = \mathrm{B}_\varepsilon(\mathbf{x})$ with $\varepsilon > 0$ and $\mathbf{x} \in \mathbb{R}^3$, yields the differential forms of the first two Maxwell equations

$$\begin{aligned} \operatorname{div} \mathbf{E} &= \frac{1}{\varepsilon_0} \rho_{\mathrm{el}}, \\ \operatorname{div} \mathbf{B} &= 0, \end{aligned}$$

in the limit $\varepsilon \to 0$ by continuity. Interpreting the divergence of a vector field as the source strength, one can say that the source of the electric field is the electric charge, while there is non source quantity for the magnetic field.

The third and fourth of Maxwell's equations couple the two fields $\mathbf{E}$ and $\mathbf{B}$ by relating their respective circulations around a closed curve ∂A to the time derivatives of the flux through the surface A enclosed by ∂A, as well as to the current. With A being an orientable two-dimensional submanifold of $\mathbb{R}^3$ that is parametrized by a single chart $\psi : U \to \mathbb{R}^3$, where U is a suitably regular subset of $\mathbb{R}^2$ (e.g. a bounded C^1-domain), they

are

$$\int_{\partial A} \mathbf{E} \cdot \mathrm{ds} = -\partial_t \int_A \mathbf{B} \cdot \mathrm{dS}, \qquad \text{(Faraday's law)}$$

$$\int_{\partial A} \mathbf{B} \cdot \mathrm{ds} = \mu_0 \int_A (\mathbf{J}_{\mathrm{el}} + \varepsilon_0 \partial_t \mathbf{E}) \cdot \mathrm{dS}. \qquad \text{(Ampère's law)}$$

The constant $\mu_0 := 4\pi \cdot 10^{-7} \frac{V \cdot s}{A \cdot m}$ is called vacuum permeability or magnetic constant and defines ε_0 as $\varepsilon_0 := \frac{1}{\mu_0 c^2}$, where $c = 299792458 \frac{m}{s}$ is the speed of light. Using Stoke's theorem on the left hand side, we get the differential forms of these equations, again by a continuity argument.

In summary, Maxwell's equations in differential form (in SI units) are

$$\operatorname{div} \mathbf{E} = \frac{1}{\varepsilon_0} \rho_{\mathrm{el}}, \tag{M1}$$

$$\operatorname{div} \mathbf{B} = 0, \tag{M2}$$

$$\operatorname{curl} \mathbf{E} = -\dot{\mathbf{B}}, \tag{M3}$$

$$\operatorname{curl} \mathbf{B} = \mu_0 (\mathbf{J}_{\mathrm{el}} + \varepsilon_0 \dot{\mathbf{E}}), . \tag{M4}$$

To solve Maxwell's equations for given charge and current densities ρ_{el} and $\mathbf{J}_{\mathrm{el}}$, they are usually reformulated in terms of potentials.

Under appropriate regularity assumptions, the divergence-free magnetic field $\mathbf{B}$ can be written as the curl of a vector field $\mathbf{A}$ – the so-called vector potential:

$$\mathbf{B} = \operatorname{curl} \mathbf{A}. \tag{B.1}$$

Plugging this expression into the differential form of Faraday's law (M3), we find that $\operatorname{curl}(\mathbf{E} + \partial_t \mathbf{A}) = 0$. We can apply the Poincaré lemma and express the argument as a gradient

$$\mathbf{E} + \partial_t \mathbf{A} = -\nabla \varphi, \tag{B.2}$$

where the function φ is called the scalar potential.

The two remaining equations (M1) and (M4) give the dependence of the potentials on the charge and current densities:

$$-\Delta \varphi - \partial_t \operatorname{div} \mathbf{A} = \frac{1}{\varepsilon_0} \rho_{\mathrm{el}}, \tag{B.3}$$

$$-\Delta \mathbf{A} + \nabla \left(\operatorname{div} \mathbf{A} + \frac{1}{c^2} \partial_t \varphi \right) + \frac{1}{c^2} \partial_t^2 \mathbf{A} = \mu_0 \mathbf{J}_{\mathrm{el}}. \tag{B.4}$$

These two equations can be decoupled by making the following observation. Adding a gradient $\nabla \psi$ to the vector potential $\mathbf{A}$ does not change the magnetic field $\mathbf{B}$. To keep the electric field $\mathbf{E}$ unchanged, the scalar potential φ needs to be modified to $\varphi - \partial_t \psi$ following

(B.2). By a suitable choice of ψ, we can achieve that the argument $\operatorname{div}\mathbf{A} + \frac{1}{c^2}\partial_t\varphi$ of the gradient in (B.4) vanishes, since this happens if and only if ψ satisfies the inhomogeneous wave equation

$$-\Delta\psi + \frac{1}{c^2}\partial_t^2\psi = \operatorname{div}\mathbf{A} + \frac{1}{c^2}\partial_t\varphi.$$

This special choice of potentials $\mathbf{A}$ and φ that satisfy

$$\operatorname{div}\mathbf{A} + \frac{1}{c^2}\partial_t\varphi = 0 \tag{B.5}$$

is called Lorenz gauge. Equation (B.5) is called Lorenz gauge condition. As a consequence of this gauge condition, Maxwell's equations (M1)-(M4) reduce to a set of inhomogeneous wave equations for the potentials

$$-\Delta\varphi + \frac{1}{c^2}\partial_t^2\varphi = \frac{1}{\varepsilon_0}\rho_{\text{el}}, \tag{B.6}$$

$$-\Delta\mathbf{A} + \frac{1}{c^2}\partial_t^2\mathbf{A} = \mu_0\mathbf{J}_{\text{el}}. \tag{B.7}$$

An equation of this type

$$\left(-\Delta + \frac{1}{c^2}\partial_t^2\right)u = f \tag{B.8}$$

can be solved by calculating Green's function for the linear differential operator for the wave equation $L := -\Delta + \frac{1}{c^2}\partial_t^2$. This function is defined as the solution $G \in \mathcal{S}'(\mathbb{R}^3 \times \mathbb{R})$ to

$$LG = \delta_0. \tag{B.9}$$

Knowing G, the tempered distribution $u := G * f$ can be defined that solves (B.8). When L^* is the adjoint of L, then for a Schwartz function $\varphi \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R})$

$$\begin{aligned}(Lu)\varphi = u(L^*\varphi) = G * f(L^*\varphi) = G(f_- * L^*\varphi) = G(L^*(f_- * \varphi))\\ = LG(f_- * \varphi) = \delta_0(f_- * \varphi) = (\delta_0 * f)\varphi = L_f(\varphi).\end{aligned}$$

Assuming that $\widehat{G}$ is defined point-wise, by applying a Fourier transform to (B.9), we get

$$\left(|\mathbf{k}|^2 - \frac{\omega^2}{c^2}\right)\widehat{G}(\mathbf{k},\omega) = 1 \quad \text{for all } (\mathbf{k},\omega) \in \mathbb{R}^3 \times \mathbb{R},$$

such that $\widehat{G}(\mathbf{k},\omega) = \frac{c^2}{(c|\mathbf{k}|)^2 - \omega^2}$. What we would like to do now, is to calculate G as the inverse Fourier transform of $\widehat{G}$. But it is not clear how to define the inverse Fourier transform, because $\widehat{G}$ is not a tempered distribution as it is singular at $(c|\mathbf{k}|)^2 = \omega^2$.

We introduce the perturbed version

$$\widehat{G}_\varepsilon(\mathbf{k},\omega) := \frac{c^2}{-\omega^2 + 2i\omega\varepsilon + (c|\mathbf{k}|)^2}, \quad \varepsilon > 0,$$

of $\widehat{G}$ with shifted singularities, s.t. $\widehat{G}_\varepsilon$ is a tempered distribution on $\mathbb{R}^3 \times \mathbb{R}$. We then consider the limit of the inverse Fourier transform of $\widehat{G}_\varepsilon$ for $\varepsilon \to 0$ as a possible Green's function

$$G := \lim_{\varepsilon \to 0} \mathcal{F}_{\mathbf{k}}^{-1} \mathcal{F}_{\omega}^{-1} \widehat{G}_\varepsilon.$$

We start by calculating the one-dimensional inverse Fourier transform $\mathcal{F}_{\omega}^{-1}\widehat{G}_\varepsilon$ by utilizing the residue theorem of complex analysis. Defining the meromorphic function

$$f_\varepsilon(\omega) := \frac{e^{i\omega t}}{c^2} \widehat{G}_\varepsilon(\mathbf{k}, \omega) \quad \text{for } \omega \in \mathbb{C} \setminus \{\omega_1, \omega_2\},$$

where ω_1 and ω_2 are zeros of the denominator, we get

$$\mathcal{F}_{\omega}^{-1}\widehat{G}_\varepsilon(\mathbf{k}, t) = \frac{c^2}{2\pi} \int_{\mathbb{R}} f_\varepsilon(\omega) \mathrm{d}\omega.$$

The function f_ε has singularities at

$$\omega_{1/2} = i\varepsilon \pm \underbrace{\sqrt{(c|\mathbf{k}|)^2 - \varepsilon^2}}_{=:\widetilde{\omega}(\varepsilon)}.$$

For $t \geq 0$, we choose the contour γ_r^+, $r > 0$, from $-r$ to r on the real line and back to r on a semicircle in the upper complex half plane, since in the limit $r \to \infty$, the contributions on the semicircle vanish as $e^{i\omega t} \to 0$ for $\mathrm{Im}(\omega) \to \infty$. For similar reasons, for $t < 0$, we choose the contour γ_r^- going from $-r$ to r on the real line and then back again on a semicircle in the lower complex half plane. In this case, we get

$$\frac{c^2}{2\pi} \int_{\mathbb{R}} f_\varepsilon(\omega) \mathrm{d}\omega = \frac{c^2}{2\pi} \lim_{r \to \infty} \oint_{\gamma_r^-} f_\varepsilon(\omega) \mathrm{d}\omega = 0$$

since the singularities lie in the upper half complex plane. The residues of f_ε at ω_1 and ω_2 are

$$\mathrm{Res}_{\omega_1}(f_\varepsilon) = \frac{-e^{i\omega_1 t}}{2\widetilde{\omega}(\varepsilon)}, \quad \text{and } \mathrm{Res}_{\omega_2}(f_\varepsilon) = \frac{e^{i\omega_2 t}}{2\widetilde{\omega}(\varepsilon)},$$

so we get for $t \geq 0$ that

$$\begin{aligned} \frac{c^2}{2\pi} \int_{\mathbb{R}} f_\varepsilon(\omega) \mathrm{d}\omega &= \frac{c^2}{2\pi} \lim_{r \to \infty} \oint_{\gamma_r^+} f_\varepsilon(\omega) \mathrm{d}\omega = ic^2(\mathrm{Res}_{\omega_1}(f_\varepsilon) + \mathrm{Res}_{\omega_2}(f_\varepsilon)) \\ &= c^2 e^{-i\varepsilon t} \frac{\sin(\widetilde{\omega}(\varepsilon)t)}{\widetilde{\omega}(\varepsilon)}. \end{aligned}$$

At this point we can already take the limit $\varepsilon \to 0$ to get

$$G(\cdot, t) = \mathcal{F}_{\mathbf{k}}^{-1} \lim_{\varepsilon \to 0} \mathcal{F}_{\omega}^{-1} \widehat{G}_\varepsilon(\cdot, t) = c\mathcal{F}_{\mathbf{k}}^{-1} \frac{\sin(ct|\cdot|)}{|\cdot|}.$$

The inverse Fourier transform of the function $\frac{\sin(ct|\cdot|)}{|\cdot|}$ is known to be the distribution $\frac{1}{4\pi ct}\sigma_{ct}$, where σ_{ct} is defined as

$$\sigma_{ct}\varphi := \int_{ctS^2} \varphi \, \mathrm{d}\mathcal{H}^2 \quad \text{for } \varphi \in \mathcal{S}(\mathbb{R}^3).$$

This can easily checked by calculating $\widehat{\sigma}_{ct}$. Thus, Green's function for the inhomogeneous wave equation is

$$G = \begin{cases} \frac{1}{4\pi t}\sigma_{ct}, & t \geq 0, \\ 0, & t < 0. \end{cases} \tag{B.10}$$

For $t \geq 0$, the solution to equation (B.8) is then given by

$$\begin{aligned} u(\mathbf{x},t) = G * f(\mathbf{x},t) &= \frac{1}{4\pi}\frac{\sigma_{ct}}{t} * f(\mathbf{x},t) \\ &= \frac{1}{4\pi}\int_0^\infty \int_{c\tau S^2} \frac{f(\mathbf{x}-\mathbf{y}, t-\tau)}{\tau} \mathrm{d}\mathcal{H}^2(\mathbf{y})\mathrm{d}\tau \\ &= \frac{1}{4\pi}\int_0^\infty \int_{\tau S^2} \frac{f(\mathbf{x}-\mathbf{y}, t-|\mathbf{y}|/c)}{|\mathbf{y}|} \mathrm{d}\mathcal{H}^2(\mathbf{y})\mathrm{d}\tau \\ &= \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{f\left(\mathbf{y}, t-\frac{|\mathbf{x}-\mathbf{y}|}{c}\right)}{|\mathbf{x}-\mathbf{y}|} \mathrm{d}\mathbf{y}. \end{aligned}$$

Applying this to the wave equations (B.6) and (B.7) for the scalar and vector potential, we end up with the so-called retarded potentials solution for Maxwell's equations:

$$\begin{aligned} \varphi(\mathbf{x},t) &= \frac{1}{4\pi\varepsilon_0}\int_{\mathbb{R}^3} \frac{\rho_{\mathrm{el}}\left(\mathbf{y}, t-\frac{|\mathbf{x}-\mathbf{y}|}{c}\right)}{|\mathbf{x}-\mathbf{y}|} \mathrm{d}\mathbf{y}, \\ \mathbf{A}(\mathbf{x},t) &= \frac{\mu_0}{4\pi}\int_{\mathbb{R}^3} \frac{\mathbf{J}_{\mathrm{el}}\left(\mathbf{y}, t-\frac{|\mathbf{x}-\mathbf{y}|}{c}\right)}{|\mathbf{x}-\mathbf{y}|} \mathrm{d}\mathbf{y}. \end{aligned} \tag{B.11}$$

If we had chosen the perturbation of $\widehat{G}$ such that the singularities of f_ε lie in the lower complex half plane, we would have ended up with a different solution that vanishes for $t \geq 0$ and is called the advanced potentials solution.

APPENDIX C

Crystallography

Crystals are macroscopic structures that are highly organized on the atomic scale. They are composed of atoms or molecules in a periodic fashion, i.e. a certain part of the crystal – the so-called unit cell – is repeated in all three space dimensions. Many solids form crystals, because the periodic arrangement is energetically favorable.

Mathematically, the structure of a crystal is described by a crystal lattice, which is the set of the locations of the atoms in space. The periodic structure is extended to infinity what should be seen as an approximation of the macroscopic nature of the crystal. Even though real crystals are three-dimensional, we define crystal structures in arbitrary dimensions.

Definition C.1 (Bravais lattice, Crystal lattice). *An n-dimensional Bravais lattice $\mathcal{B} \subset \mathbb{R}^n$ is a set of the form*

$$\mathcal{B} = \mathbf{A}\mathbb{Z}^n \quad \textit{with } \mathbf{A} \in \mathrm{GL}(n, \mathbb{R}). \tag{C.1}$$

The column vectors $\mathbf{a}_j := (\mathbf{A}_{ij})_i$ are called generators of the Bravais lattice $\mathcal{B}$.

An n-dimensional crystal lattice $\mathcal{L} \subset \mathbb{R}^n$ is a set of the form

$$\mathcal{L} = \mathcal{B} + \mathbf{M} \quad \textit{with } \mathbf{M} \subset \mathbb{R}^n, |\mathbf{M}| < \infty, \tag{C.2}$$

where $\mathcal{B}$ is a Bravais lattice. $\mathcal{B}$ is said to generate the crystal lattice $\mathcal{L}$. The set $\mathbf{M}$ is called a molecule of the crystal lattice.

A unit cell of a Bravais lattice $\mathcal{B}$ or a crystal lattice $\mathcal{L} = \mathcal{B}+\mathbf{M}$ is a set of representatives of the quotient $\mathbb{R}^n/\mathcal{B}$. Given a matrix $\mathbf{A} \in \mathrm{GL}(n, \mathbb{R})$ that generates $\mathcal{B}$, the canonical unit cell $\mathrm{U}_{\mathcal{B}}^{\mathbf{A}}$ is defined as

$$\mathrm{U}_{\mathcal{B}}^{\mathbf{A}} := \mathbf{A}[0, 1)^n.$$

Its volume $\mathrm{V}_{\mathcal{B}}$ is independent of the choice of the generator matrix $\mathbf{A}$ and equals

$$\mathrm{V}_{\mathcal{B}} = |\det \mathbf{A}|.$$

We introduce a canonical form of a crystal lattice $\mathcal{L}$ by defining the canonical generating Bravais lattice $\mathcal{B}_{\mathcal{L}}$ as the generating Bravais lattice with minimal unit cell volume (Note that the generating Bravais lattices of a crystal lattice are partially ordered by their unit

cell volume). Given a generator matrix $\mathbf{A}$ of $\mathcal{B}_\mathcal{L}$, we can also define a canonical molecule $\mathbf{M}_\mathcal{L}^\mathbf{A}$ by choosing the representatives within the canonical unit cell $\mathrm{U}_\mathcal{L}^\mathbf{A}$. In summary, we have the following canonical form of the crystal lattice $\mathcal{L}$:

$$\mathcal{L} = \mathcal{B}_\mathcal{L} + \mathbf{M}_\mathcal{L}^\mathbf{A}, \quad \mathcal{B}_\mathcal{L} = \mathbf{A}\mathbb{Z}^3, \quad \mathbf{M}_\mathcal{L}^\mathbf{A} \subset \mathrm{U}_\mathcal{L}^\mathbf{A} = \mathbf{A}[0,1)^3. \tag{C.3}$$

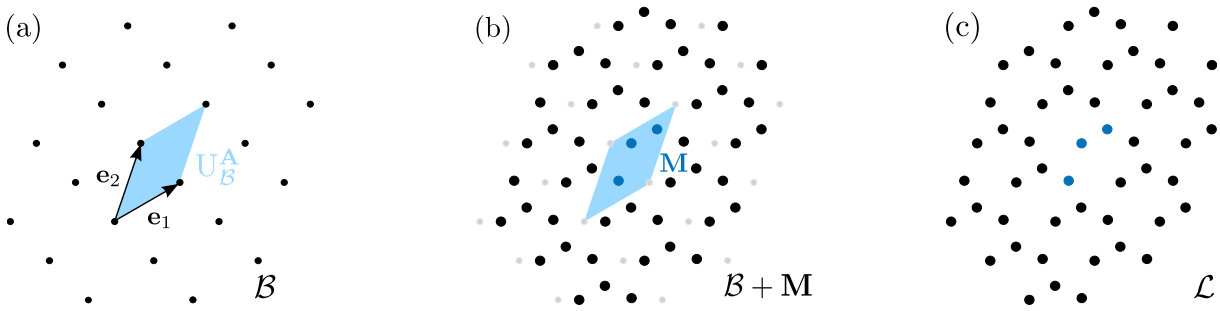


FIGURE C.1. **(a)** A 2-dimensional Bravais lattice $\mathcal{B}$ generated by two vectors $\mathbf{e}_1$ and $\mathbf{e}_2$. The unit cell $\mathrm{U}_\mathcal{B}^\mathbf{A}$ with respect to the generator matrix $\mathbf{A} := (\mathbf{e}_1, \mathbf{e}_2)$ is shaded in light blue. **(b)** A 2-dimensional crystal lattice $\mathcal{B} + \mathbf{M}$ with the Bravais lattice $\mathcal{B}$ shown in (a) (indicated in light gray). The unit cell $\mathrm{U}_\mathcal{B}^\mathbf{A}$ is shaded in light blue and the molecule $\mathbf{M}$ is coloured in dark blue. **(c)** The 2-dimensional crystal lattice $\mathcal{L} = \mathcal{B} + \mathbf{M}$ from (b). The molecule $\mathbf{M}$ is coloured in dark blue. Here $\mathcal{B}_\mathcal{L} = \mathcal{B}$ and $\mathbf{M}_\mathcal{L}^\mathbf{A} = \mathbf{M}$.

An important structure related to a Bravais lattice is its reciprocal lattice. It describes the structure of the lattice in terms of its lattice planes and a plays a prominent role in X-ray Crystallography. Given a Bravais lattice $\mathcal{B} \subset \mathbb{R}^n$, its reciprocal lattice $\mathcal{B}^\perp \subset \mathbb{R}^n$ is defined as

$$\mathcal{B}^\perp := \{\mathbf{k} \in \mathbb{R}^n.\ \mathbf{k} \cdot \mathbf{b} \in 2\pi\mathbb{Z} \text{ for all } \mathbf{b} \in \mathcal{B}\}. \tag{C.4}$$

Given a generator matrix $\mathbf{A} \in \mathrm{GL}(n, \mathbb{R})$, of $\mathcal{B}$, i.e. $\mathcal{B} = \mathbf{A}\mathbb{Z}^3$, it is easily seen that

$$\mathcal{B}^\perp = 2\pi\mathbf{A}^{-T}\mathbb{Z}^n, \tag{C.5}$$

so that $\mathbf{A}^\perp := 2\pi\mathbf{A}^{-T}$ is a generator matrix of $\mathcal{B}^\perp$ which is itself a Bravais lattice. The column vectors $\mathbf{a}_j^\perp := (\mathbf{A}_{ij}^\perp)i$ generate $\mathcal{B}^\perp$ and are related to the generators of $\mathbf{B}$ by

$$\mathbf{a}_i \cdot \mathbf{a}_j^\perp = 2\pi\delta_{ij}.$$

The relation to lattice planes is the following. Given the vector $\mathbf{k}_\iota \in \mathcal{B}^\perp$ with index $\iota \in \mathbb{Z}^n$, i.e. $\mathbf{k}_\iota = \mathbf{A}^\perp\iota$, with ι additionally satisfying $\gcd(\iota_1, \ldots, \iota_n) = 1$, define the sets

$$p_\iota(j) := \{\mathbf{b} \in \mathcal{B}.\ \mathbf{k}_\iota \cdot \mathbf{b} = 2\pi j\} \subset \mathcal{B}, \quad j \in \mathbb{Z}.$$

These sets $p_\iota(j)$ are parallel lattice planes of $\mathcal{B}$. The index ι is called Miller index of the family of lattice planes $(p_\iota(j))_{j\in\mathbb{Z}}$. Obviously,

$$\mathcal{B} = \bigcup_{j\in\mathbb{Z}} p_\iota(j).$$

The importance of the reciprocal lattice for X-ray Crystallography comes from the following fact. The distance λ_ι of two neighboring lattice planes $p_\iota(j)$ and $p_\iota(j+1)$ with Miller index $\iota \in \mathbb{Z}^n$ is

$$\lambda_\iota = \frac{2\pi}{|\mathbf{k}_\iota|}$$

what can be seen from the definition of the lattice planes (Note that every reciprocal lattice vector $\mathbf{k} \in \mathcal{B}^\perp$ can be written as $\mathbf{k} = j\mathbf{k}_\iota = \mathbf{k}_{j\iota}$ with $j \in \mathbb{N}$ and a Miller index ι). As a consequence, plane waves $\widetilde{\mathbf{E}}(\mathbf{x}, t) := \mathbf{n}e^{i\mathbf{k}\cdot\mathbf{x}}$ with wave vector $\mathbf{k} \in \mathcal{B}^\perp$ are constant on $\mathcal{B}$. So, the reciprocal lattice can also be seen as the set of wave vectors, s.t. the corresponding plane waves are invariant with respect to translations by vectors $\mathbf{b} \in \mathcal{B}$. Consider an electric charge density that is invariant with respect to $\mathcal{B}$ – say the electron density of a crystal. The oscillations induced by a plane wave with wave vector $\mathbf{k} \in \mathcal{B}^\perp$ are in phase and lead to constructive interference of the outgoing waves.

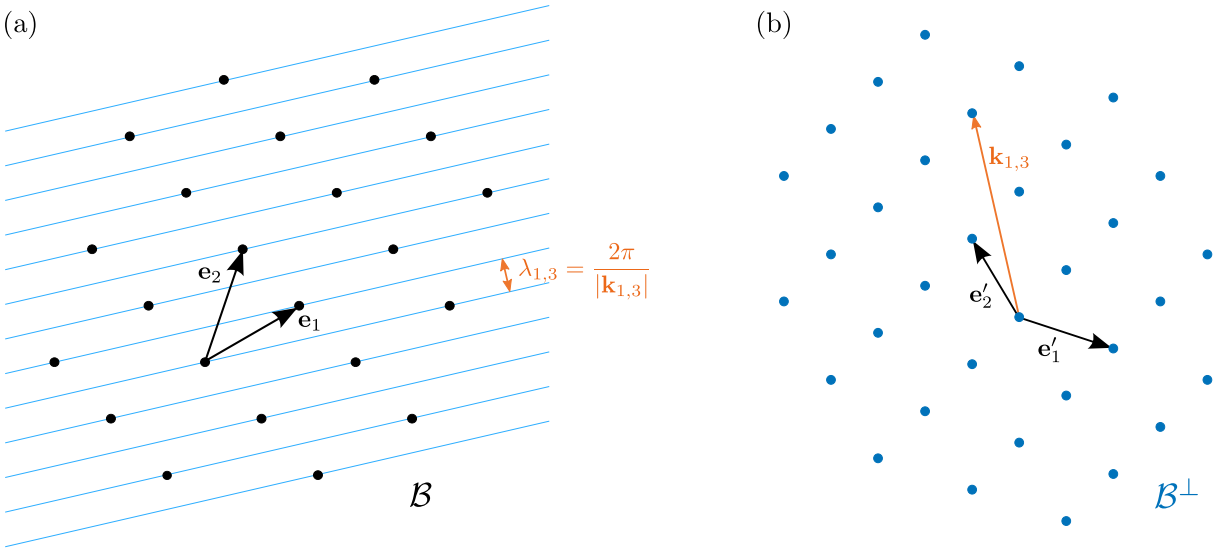


FIGURE C.2. **(a)** The 2-dimensional Bravais lattice $\mathcal{B}$ from Figure (C.1) with two generators $\mathbf{e}_1$ and $\mathbf{e}_2$. The light blue lines show the lattice planes with Miller index $\iota = (1, 3)$ and spacing $\lambda_{1,3} = \frac{2\pi}{|\mathbf{k}_{1,3}|}$. **(b)** The reciprocal lattice $\mathcal{B}^\perp$ of the Bravais lattice $\mathcal{B}$ shown in (a) (up to scaling) with generators $\mathbf{e}_1'$ and $\mathbf{e}_2'$. The reciprocal lattice vector $\mathbf{k}_{1,3}$ shown in orange is normal to the direct lattice planes with Miller index $(1, 3)$ shown in (a).

One might ask the same question for wave vectors $\mathbf{k}$ not on the reciprocal lattice $\mathcal{B}^\perp$. How do the outgoing waves interfere in this case? The answer is quite surprising and a result of a theorem in Fourier analysis. Consider the tempered distribution associated to the Bravais lattice $\mathcal{B} \subset \mathbb{R}^n$:

$$\delta_{\mathcal{B}} := \sum_{\mathbf{b}\in\mathcal{B}} \delta_{\mathbf{b}} \in \mathcal{S}'(\mathbb{R}^n).$$

Then, formally, adding up the phases means evaluating the Fourier transform of $\delta_{\mathcal{B}}$ at $\mathbf{k}$.

Theorem C.2 (Fourier transform of a Bravais lattice). *The Fourier transform of $\delta_{\mathcal{B}}$ is*

$$\widehat{\delta_{\mathcal{B}}} = \frac{(2\pi)^n}{\mathrm{V}_{\mathcal{B}}} \delta_{\mathcal{B}^\perp}. \tag{C.6}$$

Proof. For all $\varphi \in \mathcal{S}(\mathbb{R}^n)$:

$$\widehat{\delta_{\mathcal{B}}}\varphi = \delta_{\mathcal{B}}\widehat{\varphi} = \sum_{\mathbf{k}\in\mathbf{A}\mathbb{Z}^n} \widehat{\varphi}(\mathbf{k}) = \sum_{\mathbf{k}\in\mathbb{Z}^n} \widehat{\varphi}(\mathbf{A}\mathbf{k}).$$

Now,

$$\begin{aligned}
\widehat{\varphi}(\mathbf{A}\mathbf{k}) &= \int_{\mathbb{R}^n} \varphi(\mathbf{x}) e^{-i(\mathbf{A}\mathbf{k})\cdot\mathbf{x}} \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^n} \varphi(\mathbf{x}) e^{-i\mathbf{k}\cdot(\mathbf{A}^T\mathbf{x})} \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^n} \varphi(\mathbf{A}^{-T}\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} \underbrace{|\det(\mathbf{A}^{-T})|}_{=1/|\det(\mathbf{A})|} \mathrm{d}\mathbf{x} = \frac{1}{|\det(\mathbf{A})|} \widetilde{\widehat{\varphi}}(\mathbf{k}),
\end{aligned}$$

with $\widetilde{\varphi}(\mathbf{x}) := \varphi(\mathbf{A}^{-T}\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^n$.
Writing the n-dimensional Fourier transform as the iteration of n one-dimensional Fourier transforms $\widehat{\varphi} = \mathcal{F}_{\mathbf{x}_n} \cdots \mathcal{F}_{\mathbf{x}_1}\varphi$ and iterating the Poisson summation formula, we get

$$\begin{aligned}
\widehat{\delta_{\mathcal{B}}}\varphi &= \frac{1}{|\det(\mathbf{A})|} \sum_{\mathbf{k}\in\mathbb{Z}^n} \widehat{\widetilde{\varphi}}(k) = \frac{(2\pi)^n}{|\det(\mathbf{A})|} \sum_{\mathbf{k}\in\mathbb{Z}^n} \widetilde{\varphi}(2\pi\mathbf{k}) \\
&= \frac{1}{|\det(\mathbf{A})|} \sum_{\mathbf{k}\in\mathbb{Z}^n} \varphi(2\pi\mathbf{A}^{-T}\mathbf{k}) = \left(\frac{(2\pi)^n}{|\det(\mathbf{A})|} \sum_{\mathbf{k}\in 2\pi\mathbf{A}^{-T}\mathbb{Z}^n} \delta_{\mathbf{k}} \right) \varphi \\
&= \frac{(2\pi)^n}{\mathrm{V}_{\mathcal{B}}} \delta_{\mathcal{B}^\perp}\varphi.
\end{aligned}$$

□

This theorem is a generalized version of the Poisson summation formula, which in its distributional formulation says $\widehat{\delta_{\mathbb{Z}}} = 2\pi\delta_{2\pi\mathbb{Z}}$. It says that the outgoing waves add up, when the wave vector belongs to the reciprocal lattice and – more surprisingly – that the waves fully cancel, if it doesn't. This is the mathematical reason for the success of X-ray Crystallography.

Bravais lattices are named after Auguste Bravais who in 1850 gave a classification of Bravais lattices [Bra50]. We state this result here in a modern version (see [EW08]).

Let $\mathcal{B} = \mathbf{A}\mathbb{Z}^n$, $\mathbf{A} \in \mathrm{GL}(n, \mathbb{Z})$, be a Bravais lattice. Define the lattice metric $\mathrm{g}_\mathbf{A}$ on $\mathbb{R}^n$

$$\mathrm{g}_\mathbf{A} := \mathbf{A}^T\mathbf{A}, \quad \text{i.e. } (\mathrm{g}_\mathbf{A})_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j, \ i, j = 1, \dots, n.$$

Then the arithmetic holohedry $\mathrm{H}^a_\mathbf{A}$ of $\mathbf{B}$ w.r.t. $\mathbf{A}$ is defined as

$$\mathrm{H}^a_\mathbf{A} := \{\mathbf{B} \in \mathrm{GL}(n, \mathbb{Z}).\ \mathbf{B}^T\mathrm{g}_\mathbf{A}\mathbf{B} = \mathrm{g}_\mathbf{A}\}, \tag{C.7}$$

where $\mathrm{GL}(n, \mathbb{Z})$ is the group of $n \times n$ integer matrices $\mathbf{B}$ with $\det \mathbf{B} = \pm 1$. Note that $\mathrm{H}^a_\mathbf{A}$ is a subgroup of $\mathrm{GL}(n, \mathbb{Z})$. In words, it is the group of changes of basis that leaves the lattice metric fixed and thus describes fundamental symmetries of the lattice $\mathcal{B}$. Since the arithmetic holohedry depends on the choice of the generator matrix $\mathbf{A}$, we consider conjugacy classes of $\mathrm{H}^a_\mathbf{A}$ in $\mathrm{GL}(n, \mathbb{Z})$.

Definition C.3 (Bravais class). *Let $\mathcal{B} = \mathbf{A}\mathbb{Z}^n$, $\mathbf{A} \in \mathrm{GL}(n, \mathbb{R})$, be a Bravais lattice. The Bravais class $\mathrm{BC}_\mathcal{B}$ of $\mathcal{B}$ is the conjugacy class of the arithmetic holohedry in $\mathrm{GL}(n, \mathbb{Z})$:*

$$\mathrm{BC}_\mathcal{B} := \{\mathbf{B}^{-1}\mathrm{H}^a_\mathbf{A}\mathbf{B}.\ \mathbf{B} \in \mathrm{GL}(n, \mathbb{Z})\}. \tag{C.8}$$

The number of different Bravais classes in n dimensions determines the fundamentally different Bravais lattices. Bravais found this number for three dimensional Bravais lattices:

Theorem C.4 (Bravais classification). *There are exactly 14 Bravais classes in three dimensions.*

In two dimensions there are 5 Bravais classes.

A different classification of Bravais lattices is given by the notion lattice system. It is less fine than the Bravais classification and focuses on orthogonal transformations that fix the lattice. The geometric holohedry of a Bravais lattice $\mathcal{B}$ is defined as the following subgroup of O(3):

$$\mathrm{H}^g_\mathcal{B} := \{\mathbf{Q} \in \mathrm{O}(n).\ \mathbf{Q}\mathcal{B} = \mathcal{B}\}. \tag{C.9}$$

Again, we do not want to distinguish lattices that are related by an orthogonal transformation and thus define:

Definition C.5 (Lattice system). *Let $\mathcal{B} \subset \mathbb{R}^n$ be a Bravais lattice. The lattice system $\mathrm{LS}_\mathcal{B}$ of $\mathcal{B}$ is the conjugacy class of the geometric holohedry in $\mathrm{O}(n)$:*

$$\mathrm{LS}_\mathcal{B} := \{\mathbf{Q}^T\mathrm{H}^g_\mathcal{B}\mathbf{Q}.\ \mathbf{Q} \in \mathrm{O}(n)\}. \tag{C.10}$$

There are 7 lattice systems in three dimensions: triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal and cubic.

The Bravais classification is a subclassification of the classification into lattice systems, i.e. every lattice system is a union of Bravais classes. The different Bravais classes that belong to a lattice system can be defined by different centerings: primitive, body-centered, face-centered and base-centered. In the cubic lattice system, for example, there are three Bravais classes: primitive-centered cubic (pcc or sc for 'simple cubic'), body-centered cubic (bcc) and face-centered cubic (fcc).

Bibliography

[AD00] J. Arlt, and K. Dholakia, *Generation of high-order Bessel beams by use of an axicon*, Optics Communications 177 (2000), pp. 297–301.

[AM11] J. Als-Nielsen and D. McMorrow, *Elements of Modern X-ray Physics*, John Wiley and Sons, New York, (2011).

[BH94] W. R. Bloom, and H. Heyer, *Harmonic Analysis of Probability Measures on Hypergroups*, de Gruyter (1994).

[Blo29] F. Bloch, *Über die Quantenmechanik der Elektronen in Kristallgittern*, Zeitschrift für Physik 52 (1929), pp. 555-600.

[BCL02] H. H. Bauschke, P. L. Combettes, and D. R. Luke, *Phase retrieval, error reduction algorithm, and Fienup variants: a view from convex optimization*, J. Opt. Soc. Am. A, 19 (2002), pp. 1334–1345.

[BCX12] J. M. Ball, Y. Capdeboscq, B. T. Xiao, *On uniqueness for time harmonic anisotropic Maxwell's equations with piecewise regular coefficients*, Math. Models Methods Appl. Sci 22 (2012), 1250036.

[Bra13] W. L. Bragg, *The Structure of Some Crystals as Indicated by Their Diffraction of X-rays*, Proc. R. Soc. Lond. A 89 (1913), pp. 248–277.

[Bra50] A. Bravais, *Mémoire sur les systèmes formés par des point distribués regulièrement sur un plan ou dans l'espace*, Journal de l'Ecole Polytechnique 19 (1850), pp. 1–128.

[BS79] Y. M. Bruck and L. G. Sodin, *On the ambiguity of the image reconstruction problem*, Opt. Commun. 30 (1979), pp. 304–308.

[CEA06] H. N. Chapman, et al., *Femtosecond diffractive imaging with a soft-X-ray free-electron laser*, Nature Physics 2 (2006), pp. 839–843.

[CFT90] T. R. Crimmins, J. R. Fienup, and B. J. Thelen, *Improved bounds on object support from autocorrelation support and application to phase retrieval*, J. Opt. Soc. Am. A, 7 (1990), pp. 3–13.

[CSV12] E. J. Candès, T. Strohmer, and V. Voroninski, *PhaseLift: Exact and Stable Signal Recovery from Magnitude Measurements via Convex Programming*, Communications on Pure and Applied Mathematics, 66 (2013), pp. 1241-1274.

[CW55] W. Cochran, and M. M. Woolfson, *The theory of sign relations between structure factors*, Acta Cryst., 8 (1955), pp. 1–12.

[DEJ] K. Dayal, R. Elliott, and R. D. James, *Objective Formulas*, in preparation.

[Die75] J. Dieudonné, *Éléments d'analyse*, vol. 6, Gauthier-Villars, Paris (1975).

[Els03] V. Elser, *Phase retrieval by iterated projections*, J. Opt. Soc. Am. A, 20 (2003), pp. 40–55.

[EW08] M. El-Batanouny, and F. Wooten, *Symmetry and Condensed Matter Physics – A Computational Approach*, Cambridge University Press (2008).

[Ewa62] P. P. Ewald (editor), *50 Years of X-Ray Diffraction*, reprinted in pdf format for the IUCr XVIII Congress, Glasgow, Scotland (1999), http://www.iucr.org/publ/50yearsofxraydiffraction.

[Fey64] R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics II*, Addison-Weseley (1964).

[Fie82] J. R. Fienup, *Phase retrieval algorithms: a comparison*, Appl. Optics, 21 (1982), pp. 471–476.

[FJJ-1] G. Friesecke, R. D. James, and D. Jüstel, *Design of radiation for nanostructure determination via mathematical modelling of diffraction patterns*, in preparation, ca. 40 pages.

[FJJ-2] G. Friesecke, R. D. James, and D. Jüstel, *Twisting X-rays: design of radiation for nanostructure determination*, in preparation, ca. 4 pages.

[FKL12] W. Friedrich, P. Knipping, and M. von Laue. *Interferenzerscheinungen bei Röntgenstrahlen*, Sitzungsberichte der Mathematisch-Physikalischen Classe der Königlich-Bayerischen Akademie der Wissenschaften zu München, 1912.

[Fol95] G. B. Folland, *A Course in Abstract Harmonic Analysis*, CRC Press (1995).

[Fri07] G. Friesecke, *Lectures on Fourier Analysis*, lecture notes, University of Warwick (2007).

[GEA11] C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, M. Milanesio, G. Ferraris, G. Gilli, P. Gilli, G. Zanotti, and M. Catti, *Fundamentals of Crystallography*, IUCr Texts on Crystallography, 15 (2011).

[GS72] R. W. Gerchberg, and W. O. Saxton, *A practical algorithm for the determination of the phase from image and diffraction plane pictures*, Optik 35 (1972), pp. 237–246.

[Gia76] C. Giacovazzo, *Strengthening of the triplet relationship: a new probabilistic approach in $P\bar{1}$*, Acta Cryst. A, 32 (1976), pp. 967–976.

[Gri99] D. J. Griffiths, *Electromagnetic Theory*, Prentice Hall, (1999).

[Hay82] M. H. Hayes, *The Reconstruction of a Multidimensional Sequence from the Phase or Magnitude of Its Fourier Transform*, IEEE T. Acoust. Speech., 30 (1982), pp. 140–154.

[HK53] H. Hauptman, and J. Karle, *Solution of the Phase Problem. I. The Centrosymmetric Crystal.*, A.C.A. Monograph No. 3 (1953).

[Hor83] L. Hörmander, *The Analysis of Linear Partial Differential Operators I*, Springer (1983).

[HR63] E. Hewitt, and K. A. Ross, *Abstract Harmonic Analysis I*, Springer (1963).

[HR70] E. Hewitt, and K. A. Ross, *Abstract Harmonic Analysis II*, Springer (1970).

[Jac98] J. D. Jackson, *Classical Electrodynamics*, John Wiley and Sons, New York, (1998).

[Jam06] R. D. James, *Objective structures*, J. Mech. Phys. Solids, 54 (2006), pp. 2354–2390.

[Jew75] R. I. Jewett, *Spaces with an Abstract Convolution of Measures*, Advances in Mathematics 18 (1975), pp. 1–101.

[JL04] G. James, and M. Liebeck, *Representations and Characters of Groups*, Second Edition, Cambridge University Press (2004).

[Kut02] G. Kutyniok, *The Zak Transform on Certain Locally Compact Groups*, J. of Math. Sciences 1 (2002), pp. 62-85.

[Las] R. Lasser, Monograph on hypergroups, in preparation.

[MCKS99] J. Miao, P. Charalambous, J. Kirz, and D. Sayre, *Extending the methodology of X-ray crystallography to allow imaging of micrometer-sized non-crystalline specimens*, Nature, 400 (1999), pp. 342344.

[MSS12] J. Miao, R. L. Sandberg, and C. Song, *Coherent X-Ray Diffraction Imaging*, IEEE J. Sel. Top. Quant., 18 (2012), pp. 399–410.

[MSC98] J. Miao, D. Sayre, and H. N. Chapman, *Phase retrieval from the magnitude of the Fourier transforms of nonperiodic objects*, J. Opt. Soc. Am. A, 15 (1998), pp. 16621669.

[Mil96] R. P. Millane, *Multidimensional phase problems*, J. Opt. Soc. Am. A, 13 (1996), pp. 725–734.

[MEA93] R. Miller, G. T. DeTitta, R. Jones, D. A. Langs, C. M. Weeks, and H. A. Hauptman, *On the application of the minimal principle to solve unknown structures*, Science, 259 (1993), pp. 14301433.

[MEA08] S. Marchesini, et al., *Massively parallel X-ray holography*, Nature Photonics 2 (2008), pp. 560-563.

[Osb75] M. S. Osborne, *On the Schwartz-Bruhat Space and the Paley-Wiener Theorem for Locally Compact Abelian Groups*, Journal of Functional Analysis 19 (1975), pp. 40-49.

[Rau05] H. Rauhut, *Time-Frequency and Wavelet Analysis of Functions with Symmetry Properties*, Dissertation, Logos Verlag Berlin (2005).

[Rei68] H. Reiter, *Classical Harmonic Analysis and Locally Compact Groups*, Oxford Mathematical Monographs, Oxford University Press (1968).

[REA01] I. K. Robinson, I. A. Vartanyants, G. J. Williams, M. A. Pfeifer, and J. A. Pitney, *Reconstruction of the Shape of Gold Nanocrystals Using Coherent X-Ray Diffraction*, Phys. Rev. Lett., 87 (2001), 195505.

[RSIV] M. Reed, and B. Simon, *Methods of Modern Mathematical Physics IV: Analysis of Operators*, Academic Press (1978).

[Say52-1] D. Sayre, *The squaring method: a new method for phase determination*, Acta Cryst., 5 (1952), p. 60–65.

[Say52-2] D. Sayre, *Some implications of a theorem due to Shannon*, Acta Cryst., 5 (1952), p. 843.

[SBGC84] D. Shechtman, I. Blech, D. Gratias, J. Cahn, *Metallic Phase with Long-Range Orientational Order and No Translational Symmetry*, Phys. Rev. Lett. 53 (1984), pp. 1951–1954.

[SD80] W. Schempp, and B. Dreseler, *Einführung in die harmonische Analyse*, Teubner (1980).

[SEA03] D. Sjöberg, C. Engström, G. Kristensson, D. Wall, and N. Wellander, *A Floquet-Bloch decomposition of Maxwell's equations, applied to homogenization*, SIAM Multiscale Modeling and Simulation 4 (2003), pp. 149-171.

[Spo04] H. Spohn, *Dynamics of Charged Particles and their Radiation Field*, Cambridge University Press (2004).

[Str94] R. Strichartz, *A Guide to Distribution Theory and Fourier Transforms*, CRC Press, (1994).

[Thi07] P. Thibault, *Algorithmic Methods in Diffraction Microscopy*, PhD Thesis, Cornell University, (2007).

[TEA08] P. Thibault, M. Dierolf, A. Menzel, O. Bunk, C. David, and F. Pfeiffer, *High-Resolution Scanning X-ray Diffraction Microscopy*, Science, 321 (2008), pp. 379–382.

[Ter85] A. Terras, *Harmonic Analysis on Symmetric Spaces and Applications I*, Springer (1985).

[Ter88] A. Terras, *Harmonic Analysis on Symmetric Spaces and Applications II*, Springer (1988).

[US99] I. Usón, and G. M. Sheldrick, *Advances in direct methods for protein crystallography*, Curr. Opin. Struct. Biol., 9 (1999), pp. 643-48.

[Vai03] J. Väisälä, *A Proof of the Mazur-Ulam Theorem*, The American Mathematical Monthly, Vol. 110, No. 7 (2003), pp. 633-635.

[VTS10] J. Verbeeck, H. Tian, and P. Schattschneider, *Production and application of electron vortex beams*, Nature 467 (2010), pp. 301–304.

[WEA06] G. J. Williams, H. M. Quiney, B. B. Dhal, C. Q. Tran, K. A. Nugent, A. G. Peele, D. Paterson, and M. D. de Jonge, *Fresnel Coherent Diffractive Imaging*, Phys. Rev. Lett. 97 (2006), 025506.

[Wig31] E. Wigner, *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren*, Vieweg (1931).

[Wil97] N. J. Wildberger, *Duality and Entropy for Finite Commutative Hypergroups and Fusion Rule Algebras*, J. London Math. Soc. 2 (1997), pp. 275–291.

[Wol09] E. Wolf, *Solution of the Phase Problem in the Theory of Structure Determination of Crystals from X-Ray Diffraction Experiments*, Phys. Rev. Lett. 103 (2009), 075501.

[Wol10] E. Wolf, *Determination of phases of diffracted x-ray beams in investigations of structure of crystals*, Phys. Lett. A, 374 (2010), pp. 491–495.

[Zak67] J. Zak, *Finite Translations in Solid-State Physics*, Phys. Rev. Lett., Vol. 19, Issue 24 (1967), pp. 1385-1387.

Nomenclature

$\mathbf{E}$	electric field, $\mathbf{E}$ $\mathbb{R}^3\times \to \mathbb{R}^3$, page 12
$\mathbf{x}$	space variable, $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)^T \in \mathbb{R}^3$, in cylindrical coordinates $\mathbf{x} = \xi(r, \varphi, z) = (r\cos(\varphi), r\sin(\varphi), z)^T$, page 12
t	time variable, $t \in \mathbb{R}$, page 12
$\mathbf{n}$	complex amplitude, $\mathbf{n} \in \mathbb{C}^3$, page 12
$\mathbf{k}$	wave vector, reciprocal space variable, $\mathbf{k} = (\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)^T \in \mathbb{R}^3$, in cylindrical coordinates $\mathbf{k} = \xi(\widehat{r}, \widehat{\varphi}, \widehat{z}) = (\widehat{r}\cos(\widehat{\varphi}), \widehat{r}\sin(\widehat{\varphi}), \widehat{z})^T$, page 12
ω	angular frequency, $\omega > 0$, page 12
ζ	phase angle, $\zeta \in [0, \pi)$, page 12
c	speed of light, $c = 299792458\frac{m}{s}$, page 12
$\mathbf{B}$	magnetic field, $\mathbf{B}:\ \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$, page 12
ρ_{el}	electric charge density, $\rho_{\text{el}}:\ \mathbb{R}^3 \times \mathbb{R} \to [0, \infty)$, page 12
$\mathbf{J}_{\text{el}}$	electric current density, $\mathbf{J}_{\text{el}}:\ \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$, page 12
$\operatorname{div}\mathbf{F}$	divergence of the vector field $\mathbf{F}$, page 12
$\operatorname{curl}\mathbf{F}$	curl of the vector field $\mathbf{F}$, page 12
∂_t	partial derivative with respect to t, $\partial_t = \frac{\partial}{\partial t}$, page 12
ε_0	vacuum permittivity, electric constant, $\varepsilon_0 = \frac{1}{\mu_0 c^2}$, page 12
μ_0	vacuum permeability, magnetic constant, $\mu_0 = 4\pi{\cdot}10^{-7}\frac{V{\cdot}s}{A{\cdot}m}$, page 12
λ	wavelength, $\lambda > 0$, page 13
f_0	frequency, $f_0 > 0$, page 13
$\Delta\mathbf{F}$	vector Laplacian of the vector field $\mathbf{F}$, $\Delta\mathbf{F} := \nabla(\operatorname{div}\mathbf{F}) - \operatorname{curl}(\operatorname{curl}\mathbf{F})$, page 13
$\widetilde{\mathbf{E}}$	complex electric field, $\operatorname{Re}(\widetilde{\mathbf{E}}) = \mathbf{E}$, page 14

$\widetilde{\mathbf{B}}$ complex magnetic field, $\mathrm{Re}(\widetilde{\mathbf{B}}) = \mathbf{B}$, page 14

$\mathrm{Re}(z)$ real part of a complex number $z \in \mathbb{C}$, $\mathrm{Re}(z) := \frac{z+\overline{z}}{2}$, page 14

$u(\mathbf{x}, t)$ electromagnetic energy density, $u(\mathbf{x}, t) := \frac{1}{2}\left(\varepsilon_0 |\mathbf{E}(\mathbf{x}, t)|^2 + \frac{1}{\mu_0}|\mathbf{B}(\mathbf{x}, t)|^2\right)$ at a point $\mathbf{x} \in \mathbb{R}^3$ and a time $t \in \mathbb{R}$, page 14

$\mathbf{S}(\mathbf{x},\mathrm{t})$ Poynting vector $\mathbf{S}(\mathbf{x}, t) := \frac{1}{\mu_0}\mathbf{E}(\mathbf{x}, t) \times \mathbf{B}(\mathbf{x}, t)$ at a point $\mathbf{x} \in \mathbb{R}^3$ and a time $t \in \mathbb{R}$, page 15

$\mathrm{I}(\mathbf{x})$ electromagnetic intensity $\mathrm{I}(\mathbf{x}) := \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} |\mathbf{S}(\mathbf{x}, t)| \mathrm{d}t$ at a point $\mathbf{x} \in \mathbb{R}^3$, page 16

$\mathbf{E}_{\mathbf{k}} = \mathbf{E}_{\omega,\mathbf{k}_0}$ plane wave with wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0 \in \mathbb{R}^3$, $\mathbf{E}_{\mathbf{k}}(\mathbf{x}) := \mathbf{n}e^{i\mathbf{k}\cdot\mathbf{x}}$ for some $\mathbf{n} \in \mathbf{k}^\perp \setminus \{0\}$ and all $\mathbf{x} \in \mathbb{R}^3$, page 16

$\mathbf{x}^\perp$ orthogonal complement of $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{x}^\perp := \{\mathbf{y} \in \mathbb{C}^3.\ \mathbf{x} \cdot \mathbf{y} = 0\}$, page 16

$e_{\mathbf{k}} = e_{\omega,\mathbf{k}_0}$ scalar plane wave with wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0 \in \mathbb{R}^3$, $e_{\mathbf{k}}(\mathbf{x}) := e^{i\mathbf{k}\cdot\mathbf{x}}$ for $\mathbf{x} \in \mathbb{R}^3$, page 16

$\mathbf{F}_\mathrm{L}$ Lorentz force, $\mathbf{F}_\mathrm{L} := \rho_{\mathrm{el}}\mathbf{E} + \mathbf{J} \times \mathbf{B}$, page 16

$\delta_{\mathbf{x}}$ the δ-distribution at the point $\mathbf{x} \in \mathbb{R}^3$, $\delta_{\mathbf{x}}(\varphi) := \varphi(\mathbf{x})$ for $\varphi \in \mathcal{S}(\mathbb{R}^3)$, page 17

e_{el} elementary charge, page 17

m_{el} mass $m_{\mathrm{el}} \in [0, \infty)$, page 17

Ω compact set $\Omega \subset \mathbb{R}^3$, $\mathrm{supp}(\rho_{\mathrm{el}}) \subseteq \Omega$, page 17

$\mathbf{A}_{\mathrm{el}}$ vector potential $\mathbf{A}_{\mathrm{el}} :\ \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$, $\mathbf{B} = \mathrm{curl}\, \mathbf{A}_{\mathrm{el}}$, page 17

φ_{el} scalar potential $\varphi_{\mathrm{el}} :\ \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$, $\mathbf{E} + \partial_t \mathbf{A}_{\mathrm{el}} = -\nabla\varphi_{\mathrm{el}}$, page 17

∇f gradient of a function f on $\mathbb{R}^3$, page 17

c_{el} scattering constant, $c_{\mathrm{el}} := -\frac{e_{\mathrm{el}}^2}{4\pi\varepsilon_0 m_{\mathrm{el}} c^2}$, page 18

$\mathrm{P}(\mathbf{x}^\perp)$ projection onto the orthogonal complement of a vector $\mathbf{x} \in \mathbb{R}^3$, $\mathrm{P}(\mathbf{x}^\perp) := \left(\mathbf{I} - \frac{\mathbf{x}}{|\mathbf{x}|} \otimes \frac{\mathbf{x}}{|\mathbf{x}|}\right)$, page 18

$\mathbf{I}$ unit matrix, page 18

$\mathbf{v}_1 \otimes \mathbf{v}_2$ the matrix $\mathbf{v}_1\mathbf{v}_2^T$, page 18

$\sphericalangle(\mathbf{x}, \mathbf{y})$ angle between two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, page 18

$C_b(\mathbb{R}^3, \mathbb{C}^3)$ space of bounded continuous complex vector fields on $\mathbb{R}^3$, page 19

$\mathcal{S}(\mathbb{R}^3)$ Schwartz space of rapidly decaying smooth functions on $\mathbb{R}^3$, page 19

$\mathrm{Im}(z)$ imaginary part of a complex number $z \in \mathbb{C}$, $\mathrm{Im}(z) := \frac{z-\overline{z}}{2i}$, page 19

$\mathcal{F}T = \widehat{T}$ the Fourier transform of a tempered distribution $T \in \mathcal{S}'(\mathbb{R}^n)$, $\widehat{T}\varphi := T\widehat{\varphi}$ for all Schwartz functions $\varphi \in \mathcal{S}(\mathbb{R}^n)$, where $\widehat{\varphi}(\mathbf{k}) = \int_{\mathbb{R}^n} \varphi(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} \mathrm{d}\mathbf{x}$, page 20

$\mathrm{dia}(\Omega)$ diameter of the set $\Omega \subseteq \mathbb{R}^3$, $\mathrm{dia}(\Omega) := \sup\{|\mathbf{x} - \mathbf{y}|.\ \mathbf{x}, \mathbf{y} \in \Omega\}$, page 68

$\mathrm{A}(\mathbf{x})$ scattering amplitude $\mathrm{A}(\mathbf{x}) := \mathrm{I}(\mathbf{x})^{1/2}$ at a point $\mathbf{x} \in \mathbb{R}^3$, page 69

$\mathrm{F}(\mathbf{x}; \mathbf{k}, \Omega)$ Fresnel number of a point $\mathbf{x} \in \mathbb{R}^3$ with respect to the wave vector $\mathbf{k} \in \mathbb{R}^3$ and the set $\Omega \subseteq \mathbb{R}^3$, $\mathrm{F}(\mathbf{x}; \mathbf{k}, \Omega) := \frac{\mathrm{dia}(\Omega)^2 |\mathbf{k}|}{2\pi d(\mathbf{x}, \Omega)}$, page 68

$C_c(\mathbb{R}^3)$ space of continuous functions on $\mathbb{R}^3$ with compact support, page 20

$\mathrm{A}(\mathbf{x})$ scattering amplitude $\mathrm{A}(\mathbf{x}) := \mathrm{I}(\mathbf{x})^{1/2}$ at a point $\mathbf{x} \in \mathbb{R}^3$, page 20

$\mathcal{B}$ a Bravais lattice in $\mathbb{R}^3$, $\mathcal{B} = \mathbf{A}\mathbb{Z}^3$ for some $\mathbf{A} \in \mathrm{GL}(3, \mathbb{R})$, page 21

$\mathrm{GL}(n, \mathbb{R})$ general linear group in n dimensions, page 21

$T * \varphi$ convolution of a tempered distribution $T \in \mathcal{S}'(\mathbb{R}^3)$ with a Schwartz function $\varphi \in \mathcal{S}(\mathbb{R}^3)$, $T*\varphi(\psi) := T(\varphi_- * \psi)$ for all $\psi \in \mathcal{S}(\mathbb{R}^3)$, where $\psi_1 * \psi_2(\mathbf{x}) := \int_{\mathbb{R}^3} \psi_1(\mathbf{x} - \mathbf{y}) \psi_2(\mathbf{y}) \mathrm{d}\mathbf{y}$ for $\psi_1, \psi_2 \in \mathcal{S}(\mathbb{R}^3)$, page 21

δ_X the δ-distribution associated to a countable set $X \subset \mathbb{R}^3$, $\delta_X := \sum_{\mathbf{x} \in X} \delta_{\mathbf{x}}$, page 21

$\mathbf{1}_\Omega$ characteristic function of the measurable set $\Omega \subseteq \mathbb{R}^3$, page 21

$\mathcal{S}'(\mathbb{R}^3)$ space of tempered distributions on $\mathbb{R}^3$, page 21

$V_\mathcal{B}$ volume of the unit cell of a Bravais lattice $\mathcal{B}$, $V_\mathcal{B} := |\det(\mathbf{A})|$ with $\mathcal{B} = \mathbf{A}\mathbb{Z}^3$, page 22

$\mathcal{B}^\perp$ reciprocal lattice of a Bravais lattice $\mathcal{B}$, $\mathcal{B}^\perp := \{\mathbf{k} \in \mathbb{R}^3.\ \mathbf{k} \cdot \mathbf{b} \in 2\pi\mathbb{Z} \text{ for all } \mathbf{b} \in \mathcal{B}\}$, page 22

$\mathbf{A}^\perp$ generator matrix of the reciprocal lattice $\mathcal{B}^\perp$ of the Bravais lattice $\mathcal{B} = \mathbf{A}\mathbb{Z}^3$, $\mathbf{A} \in \mathrm{GL}(3, \mathbb{R})$, $\mathbf{A}^\perp := 2\pi\mathbf{A}^{-T}$, page 22

$\mathbf{k}_\iota$ reciprocal lattice vector with Miller index $\iota \in \mathbb{Z}^3$, $\mathbf{k}_\iota := \mathbf{A}^\perp \iota$, page 23

ι Miller index, $\iota \in \mathbb{Z}^3$, $\gcd(\iota_1, \iota_2, \iota_3) = 1$, page 23

λ_ι distance of neighboring lattice planes with Miller index ι, page 23

$\mathrm{U}_{\mathcal{B}}^{\mathbf{A}}$ canonical unit cell of a Bravais lattice $\mathcal{B}$ with respect to the generator matrix $\mathbf{A}$, $\mathrm{U}_{\mathcal{B}}^{\mathbf{A}} := \mathbf{A}[0,1)^3$, page 25

$\varphi_{\mathcal{B}}^{\mathbf{A}}$ canonical unit cell density of a crystal with electron density $\rho_{\mathrm{el}} = \delta_{\mathcal{B}} * \varphi$, $\varphi_{\mathcal{B}}^{\mathbf{A}} := \rho_{\mathrm{el}}\big|_{\mathrm{U}_{\mathcal{B}}^{\mathbf{A}}}$, page 26

$\mathrm{p}_{\mathbf{k}}$ projection operator along $\mathbf{k}$, $\mathrm{p}_{\mathbf{k}}\varphi(\mathbf{x}_0) := \int_{-\infty}^{\infty} \varphi(\mathbf{x}_0 + r\mathbf{k}/|\mathbf{k}|)\mathrm{d}r$ for $\mathbf{x}_0 \in \mathbf{k}^\perp$ and $\varphi \in \mathcal{S}(\mathbb{R}^3)$, page 26

$\mathrm{s}_{\mathbf{k}}$ slice operator, $\mathrm{s}_{\mathbf{k}} : \mathcal{S}(\mathbb{R}^3) \to \mathcal{S}(\mathbf{k}^\perp)$, $\mathrm{s}_{\mathbf{k}}\varphi(\mathbf{x}_0) := \varphi(\mathbf{x}_0)$ for $\mathbf{x}_0 \in \mathbf{k}^\perp$, page 27

$\mathcal{F}^{-1}T$ the inverse Fourier transform of a tempered distribution $T \in \mathcal{S}'(\mathbb{R}^n)$, $(\mathcal{F}^{-1}T)\varphi := T(\mathcal{F}^{-1}\varphi)$ for all Schwartz functions $\varphi \in \mathcal{S}(\mathbb{R}^n)$, where $\mathcal{F}^{-1}\varphi(\mathbf{x}) = \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \varphi(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\mathbf{k}$, page 30

f_- inversion of the function f, $f_-(\mathbf{x}) := f(-\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^3$, page 30

$\mathcal{S}^{\geq 0}(\mathbb{R}^3)$ set of non-negative Schwartz functions, $\mathcal{S}^{\geq 0}(\mathbb{R}^3) := \{\varphi \in \mathcal{S}(\mathbb{R}^3).\ \varphi \geq 0\}$, page 31

$\mathcal{S}_\Omega(\mathbb{R}^3)$ space of Schwartz functions supported on $\Omega \subset \mathbb{R}^3$, $\mathcal{S}_\Omega(\mathbb{R}^3) := \{\varphi \in \mathcal{S}(\mathbb{R}^3).\ \mathrm{supp}(\varphi) \subseteq \Omega\}$, page 31

$\mathrm{supp}(T)$ support of a tempered distribution $T \in \mathcal{S}'(\mathbb{R}^3)$, $\mathrm{supp}(T) := \{\mathbf{x} \in \mathbb{R}^3.\ \forall\ U\mathrm{open},\ \mathbf{x} \in U\ \exists\ \varphi \in \mathcal{S}(U).\ T\varphi \neq 0\}$, page 31

M_ζ phase operator associated to the phase function ζ, $\mathrm{M}_\zeta\varphi := \mathcal{F}^{-1}(e^{i\zeta}\widehat{\varphi})$ for $\varphi \in \mathcal{S}(\mathbb{R}^3)$, page 31

$\mathcal{T}(\mathbb{R}^3)$ space of tempered functions, $\mathcal{T}(\mathbb{R}^3) := \{f \in C^\infty(\mathbb{R}^3).\ D^{\mathbf{m}}f$ slowly increasing for all $\mathbf{m} \in \mathbb{N}_0^3\}$, page 32

$M^1(\Omega)$ space of finite complex Borel measures on a measurable set $\Omega \subseteq \mathbb{R}^3$, page 37

$\mathcal{F}M^1(\Omega)$ space of Fourier transforms of finite complex Borel measures on a measurable set $\Omega \subseteq \mathbb{R}^3$, page 37

$\mathbb{T}$ the torus group, $\mathbb{T} := \mathbb{Z}/2\pi\mathbb{Z}$, page 47

$\mathbb{S}^2$ the 2-sphere in $\mathbb{R}^3$, $\mathbb{S}^2 := \{\mathbf{x} \in \mathbb{R}^3.\ |\mathbf{x}| = 1\}$, page 47

$(\mathbf{Q}|\mathbf{c})$ the isometry on $\mathbb{R}^3$ given by $(\mathbf{Q}|\mathbf{c})(\mathbf{x}) := \mathbf{Q}\mathbf{x} + \mathbf{c}$ for $\mathbf{x} \in \mathbb{R}^3$, with $\mathbf{Q} \in \mathrm{O}(3)$, $\mathbf{c} \in \mathbb{R}^3$, $(\mathbf{Q}|\mathbf{c}) \in \mathrm{E}(3)$, page 47

$\mathrm{O}(n)$ orthogonal group in n dimensions, page 47

$\mathbf{E}_0$ spatial part of the electric field of time-harmonic radiation $\mathbf{E} : \mathbb{R}^3 \to \mathbb{C}^3$, $\mathbf{E}(\mathbf{x}, t) = \mathbf{E}_0(\mathbf{x})e^{-i\omega t}$ for some $\omega > 0$, page 56

$\mathrm{E}(n)$ Euclidean group of isometries of n-dimensional space, page 53

$\mathbf{B}_0$ spatial part of the magnetic fileld of time-harmonic radiation $\mathbf{B} : \mathbb{R}^3 \to \mathbb{C}^3$, $\mathbf{B}(\mathbf{x}, t) = \mathbf{B}_0(\mathbf{x})e^{-i\omega t}$ for some $\omega > 0$, page 56

$C^k(\mathbb{R}^3)$ space of k times continuously differentiable functions, $k \in \mathbb{N}_0$, page 58

R_b^ω space of time-harmonic radiation of frequency $\omega > 0$, page 58

$\mathbf{v}(\tau)$ velocity of a particle at the time τ, $\mathbf{v}(\tau) = \dot{\mathbf{q}}(\tau)$, page 64

$\mathbf{n}(\mathbf{x}, \tau)$ direction from particle to $\mathbf{x}$ at time τ, $\mathbf{n}(\mathbf{x}, \tau) = \frac{\mathbf{x}-\mathbf{q}(\tau)}{|\mathbf{x}-\mathbf{q}(\tau)|}$, page 64

$\boldsymbol{\beta}(\tau)$ relative particle velocity with respect to the speed of light, $\boldsymbol{\beta}(\tau) = \mathbf{v}(\tau)/c$, page 66

$L^1(\mathbb{R}^3)$ (equivalence classes of) integrable functions on $\mathbb{R}^3$, page 70

$\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}$ radiation transform of $\rho_{\mathrm{el}} \in L^1(\mathbb{R}^3)$ with respect to the time-harmonic radiation $\mathbf{E}_0 \in \mathrm{R}_b^\omega$, $\mathcal{R}[\mathbf{E}_0]\rho_{\mathrm{el}}(\mathbf{s}_0) := \int_{\mathbb{R}^3} e^{-i\frac{\omega}{c}\mathbf{s}_0\cdot\mathbf{y}}\mathbf{E}_0(\mathbf{y})\rho_{\mathrm{el}}(\mathbf{y})\mathrm{d}\mathbf{y}$ for $\mathbf{s}_0 \in \mathbb{S}^2$, page 70

$\mathcal{P}$ radiation parameter set, page 72

$\mathcal{O}$ observation parameter set, page 72

χ character of a unitary irreducible representation of a locally compact group, page 77

$((\mathbf{Q}|\mathbf{c})\mathbf{E}_0)$ action of the isometry $(\mathbf{Q}|\mathbf{c}) \in \mathrm{E}(3)$ on the L^∞-vector field $\mathbf{E}_0$, $((\mathbf{Q}|\mathbf{c})\mathbf{E}_0)(\mathbf{x}) = \mathbf{Q}\mathbf{E}_0((\mathbf{Q}|\mathbf{c})^{-1}\mathbf{x})$, page 81

$\mathrm{R}_b^\omega(G)$ space of bounded vector fields that satisfy the design equations for the design group G and frequency $\omega > 0$, page 82

$\mathrm{R}_b^{\omega,\chi}(G)$ space of bounded vector fields that satisfy the design equations for the abelian design group G, the frequency $\omega > 0$ and the character $\chi \in \widehat{G}$, page 83

$\widehat{G}$ dual group of a locally compact abelian group or dual of a compact group, page 83

$H_G^\perp$ orthogonal group of a subgroup $H \leq G$ of a locally compact abelian group G, $H_G^\perp := \{\chi \in \widehat{G}.\ \chi \downarrow_H^G (h) = 1 \text{ for all } h \in H\}$, page 83

$\sigma \downarrow_H^G$ subduced representation of a unitary irreducible representation σ of the locally compact group G to the subgroup $H \leq G$, page 83

J_α Bessel function of the first kind of integer order $\alpha \in \mathbb{Z}$, page 90

$\mathrm{diag}(\mathbf{v})$ diagonal $n \times n$-matrix with components of $\mathbf{v} \in \mathbb{R}^n$ on the diagonal, $(\mathrm{diag}(\mathbf{v}))_{jj} = \mathbf{v}_j$, $j = 1, \ldots, n$, page 90

$\mathcal{H}^m$ the m-dimensional Hausdorff measure, $m \in \mathbb{N}_0$, page 92

$\mathbf{E}_{\mathbf{k}}^{(\alpha)}$ a twisted wave with wave vector $\mathbf{k} \in \mathbb{R}^3$ and phase shift $\alpha \in \mathbb{Z}$, $\mathbf{E}_{\mathbf{k}}^{(\alpha)}(\mathbf{x}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\alpha\widehat{\varphi}}\mathbf{R}_{\widehat{\varphi}}\mathbf{n}e^{i\mathbf{R}_{\widehat{\varphi}}\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}$ for some $\mathbf{n} \in \mathbf{k}^\perp$ and all $\mathbf{x} \in \mathbb{R}^3$, page 93

$e_{\mathbf{k}}^{(\alpha)}$ a scalar twisted wave with wave vector $\mathbf{k} \in \mathbb{R}^3$ and phase shift $\alpha \in \mathbb{Z}$, $e_{\mathbf{k}}^{(\alpha)}(\mathbf{x}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\alpha\widehat{\varphi}}e^{i\mathbf{R}_{\widehat{\varphi}}\mathbf{k}\cdot\mathbf{x}}\mathrm{d}\widehat{\varphi}$ for $\mathbf{x} \in \mathbb{R}^3$, page 93

$\mathrm{SO}(n)$ special orthogonal group in n dimensions, page 115

$\mathcal{F}_G$ Fourier transform on a locally compact abelian or compact group G, page 117

P_K^χ Wigner projection for a compact group K and a character $\chi \in \widehat{K}$, $P_K^\chi f(\mathbf{x}) := \int_K \overline{\chi(g)}(gf)(\mathbf{x})\mathrm{d}\mu_K(g)$ for $f \in C_b(\mathbb{R}^3)$, page 118

$\mathbf{E}_{\omega,\mathbf{k}_0,\chi}$ symmetry-adapted wave with wave vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$ for a character $\chi \in \widehat{G}$ for an isometry group G; when G is compact, then $\mathbf{E}_{\omega,\mathbf{k}_0,\chi} = P_G^\chi \mathbf{E}_{\omega,\mathbf{k}_0}$, page 120

$e_{\omega,\mathbf{k}_0,\chi}$ scalar symmetry-adapted wave with vector $\mathbf{k} = \frac{\omega}{c}\mathbf{k}_0$ for a character $\chi \in \widehat{G}$ for an isometry group G; when G is compact, then $\mathbf{e}_{\omega,\mathbf{k}_0,\chi} = P_G^\chi e_{\omega,\mathbf{k}_0}$, page 120

$\mathcal{Z}_G$ generalized Zak transform for a locally compact abelian or compact group G, page 120

$\mathcal{W}_G$ scalar wave transform for a locally compact abelian or compact closed isometry group G

$\boldsymbol{\mathcal{W}}_G$ wave transform for a locally compact abelian or compact closed isometry group G, page 147

$\sigma_{j,k}$ matrix coefficient of a irreducible unitary representation $\sigma \in \widehat{K}$ of a compact group, page 155

$\sigma \uparrow_H^G$ induced representation of a unitary irreducible representation σ of the subgroup H to the locally compact group $G \geq H$, page 162

$C_0(\mathbb{R}^3)$ space of continuous functions on $\mathbb{R}^3$ vanishing at infinity, page 171

$\int_A \mathbf{v} \cdot \mathrm{dS}$ surface integral of the continuous vector field $\mathbf{v}$ over the oriented surface $(A, \mathbf{n})$ with A a two-dimensional submanifold of $\mathbb{R}^3$ and $\mathbf{n} : A \to \mathbb{R}^3$ a continuous normal vector field on A, $\int_A \mathbf{v} \cdot \mathrm{dS} := \int_A \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}\mathcal{H}^2$, page 177

$\mathrm{B}_\varepsilon(\mathbf{x})$ open ball of radius $\varepsilon > 0$ at a point $\mathbf{x} \in \mathbb{R}^3$, $\mathrm{B}_\varepsilon(\mathbf{x}) := \{\mathbf{y} \in \mathbb{R}^3. \, |\mathbf{y} - \mathbf{x}| < \varepsilon\}$, page 177

$\int_{\mathcal{C}} \mathbf{v} \cdot \mathrm{ds}$ line integral of the continuous vector field $\mathbf{v}$ along the curve $(\mathcal{C}, \tau)$ with $\mathcal{C}$ a one-dimensional submanifold of $\mathbb{R}^3$ and $\tau : \mathcal{C} \to \mathbb{R}^3$ a unit tangent vector field on $\mathcal{C}$, $\int_{\mathcal{C}} \mathbf{v} \cdot \mathrm{ds} := \int_{\mathcal{C}} \mathbf{v} \cdot \tau \, \mathrm{d}\mathcal{H}^1$, page 178

$\mathrm{Res}_x(f)$ Residue of the meromorphic function f at the isolated singularity x, page 180