Technische Universität München

Max-Planck-Institut für Quantenoptik

A Quantum Information Perspective of Fermionic Quantum Many-Body Systems

Christina V. Kraus

Vollständiger Abdruck der von der Fakultät für Physik
der Technischen Universität München
zur Erlangung des akademischen Grades eines

Doktors der Naturwissenschaften (Dr. rer. nat.)

genehmigten Dissertation.

Vorsitzender : Univ.-Prof. Dr. R. Gross

Prüfer der Dissertation : 1. Hon.-Prof. I. Cirac, Ph. D.
2. Univ.-Prof. Dr. H. Friedrich

Die Dissertation wurde am 14.09.2009 bei der
Technischen Universität München eingereicht und
durch die Fakultät für Physik am 02.11.2009 angenommen.

Abstract

In this Thesis fermionic quantum many-body system are theoretically investigated from a quantum information perspective.

Quantum correlations in fermionic many-body systems, though central to many of the most fascinating effects of condensed matter physics, are poorly understood from a theoretical perspective. Even the notion of "paired" fermions which is widely used in the theory of superconductivity and has a clear physical meaning there, is not a concept of a systematic and mathematical theory so far. Applying concepts and tools from entanglement theory, we close this gap, developing a pairing theory allowing to unambiguously characterize paired states. We develop methods for the detection and quantification of pairing according to our definition which are applicable to current experimental setups. Pairing is shown to be a quantum correlation distinct from any notion of entanglement proposed for fermionic systems, giving further understanding of the structure of highly correlated quantum states. In addition, we show the resource character of paired states for precision metrology, proving that BCS-states allow phase measurements at the Heisenberg limit.

Next, the power of fermionic systems is considered in the context of quantum simulations, where we study the possibility to simulate Hamiltonian time evolutions on a cubic lattice under the constraint of translational invariance. Given a set of translationally invariant local Hamiltonians and short range interactions we determine time evolutions which can and those which can not be simulated. Bosonic and finite-dimensional quantum systems ("'spins") are included in our investigations.

Furthermore, we develop new techniques for the classical simulation of fermionic many-body systems. First, we introduce a new family of states, the fermionic Projected Entangled Pair States (fPEPS) on lattices in arbitrary spatial dimension. These are the natural generalization of the PEPS known for spin systems, and they approximate efficiently ground and thermal states of systems with short-range interaction. We give an explicit mapping between fPEPS and PEPS, allowing to extend previous simulation methods to fermions. In addition, we show that fPEPS naturally arise as exact ground states of certain fermionic Hamiltonians, and give an example that exhibits criticality while fulfilling the area law.

Finally, we derive methods for the determination of ground and thermal states, as well as the time evolution, of interacting fermionic systems using generalized Hartree-Fock theory (gHFT). With the computational complexity scaling polynomially with the number of particles, this method can deal with large systems. As a benchmark we apply our methods to the translationally invariant Hubbard model with attractive interaction and find excellent agreement with known results.

Contents

Chapter 1

Introduction

Quantum mechanical correlations that have no classical analogue are one of the most compelling physical discoveries of the 20th century. The existence of such correlations, called entanglement ("Verschränkung"), was revealed by the famous Einstein-Podolsky-Rosen (EPR) gedanken experiment in the 1930s [1]. Considered by some as a "spooky action at a distance" at that time, the notion of entanglement has transformed into a well-established concept today. A starting point for this development were the inequalities formulated by Bell in 1964 [2]. Violation of a Bell inequality implies the existence of quantum mechanical correlations that cannot be simulated by any classical theory. Nearly twenty years later, Aspect managed to perform the first convincing experiment proving the violation of a Bell inequality [3, 4]. Aspect's striking experiment resulted in the advent of quantum information theory in the early 1990s, where the quantum correlations play the role of a resource for technological applications. Since that time quantum information science has developed into a vibrant research area, ranging from foundational questions of the interpretation on quantum mechanics towards the search for technological application of entanglement [5]. Using knowledge from various fields of physics, mathematics and computer science, the understanding and the control of quantum mechanical systems is at the heart of quantum information theory.

The core of quantum information science is the use of quantum mechanical particles as the carrier of information. Any quantum mechanical two-level system can encode one unit bit of quantum information, and such a system is called qubit in analogy to the bit of classical information theory. The immense success of quantum information theory is due to the interplay of theory and experiment with those qubits: Protocols for quantum cryptography [6], quantum dense coding [7] or quantum teleportation [8] could all be demonstrated in pioneering experiments [9, 10, 11, 12, 13, 14, 15, 16]. Furthermore, it has been predicted that certain computational tasks, such as factoring numbers or simulating quantum mechanical systems, can be carried out exponentially faster using a quantum computer based on qubits than by any known algorithm running on a classical computer. However, the experimental realization of a large-scale quantum computer capable of accomplishing those tasks is, despite major experimental progress, still an unsolved task. Nevertheless, the compelling progress in the field of quantum information sciences

justifies the statement that *"We are currently in the midst of a second quantum revolution. While the first revolution gave us laws for understanding physical reality at very small scales, the second revolution will take these rules and develop new technologies"* [17].

With the beginning of the 21st century intriguing experiments using ultra cold quantum gases (see e.g. [18] for a review) have attracted the attention of the quantum information community. The ground breaking realization of a Bose-Einstein condensate in a system of Rubidium atoms has opened a door towards a new era of condensed matter physics. The present experiments with bosonic and fermionic atoms offer an exciting possibility to verify existing models known from the theory of condensed matter physics and allow to discover and explore new and exotic quantum phases. These systems exhibit strong quantum correlations, and are thus of fundamental interest for the theory of quantum information. Entanglement theory as it is today considers mainly correlations of *few* and *distinguishable* particles. Characterizing entanglement in many-body systems, however, is still an open field of research (see e.g. [19] for a review). The situation gets even more complicated when the particles under consideration are indistinguishable. E.g., by now there is no unique definition of entanglement for fermionic and bosonic systems where the individual particles are indistinguishable (see e.g. [20, 21]). In this respect, the application of tools and techniques from quantum information to condensed matter physics and vice versa is likely to result in interesting insights in questions concerning and even relating both fields. In this regard fermionic systems are especially interesting. Fermions, which are the basic building blocks of matter, are central to many of the most fascinating effects in condensed matter physics, like superconductivity, superfluidity or the quantum Hall effect. The investigation of quantum correlations in fermionic systems is thus the main focus of this Thesis. In the spirit of quantum information science we study these systems from a physical, mathematical and computer theoretical point of view.

We start in Chapter 2 studying quantum correlations in fermionic systems from a conceptual point of view, establishing a pairing theory for fermionic systems. The notion of "pairing" dates back to the 1960s, when Bardeen, Cooper and Schrieffer (BCS) gave an explanation of superconductivity via pairs of fermions with opposite spin and momentum [22]. Since these days it has been believed that there are other systems where the pairing of fermions is the source for interesting physical effects. For example, in 1982 Leggett proposed that the BEC-BCS crossover which is the phase transition of a molecular fermionic Bose-Einstein condensate to a superfluid BCS-phase can be explained via a wave function involving pairs of fermions [23]. In a gas of fermionic atoms in two different spin states a formation of diatomic molecules with bosonic statistics may occur under certain conditions, enabling the formation of a Bose-Einstein condensate. By controlling external parameters via a Feshbach resonance [24, 25, 26] the molecules increase in size and finally the fermionic statistics becomes relevant. In the end, the system become a superfluid due to the formation of Cooper pairs of atoms in two different internal states (see e.g. [27] for a review). Obviously, both phases are characterized by the formation of fermionic pairs. However, recent experiments on the BEC-BCS-crossover have

revealed that the notion of pairing is not so clear in those systems, and a heated debate on the interpretation of observed data has ensued [28, 29, 30, 31]. Thus, the concept of "pairing" in condensed-matter systems requires a new and detailed analysis. Motivated by the significance of experiments with ultra-cold gases for our understanding of condensed matter physics and the lacking clearness of how to understand pairing in those systems, we aim at the formulation of a pairing theory for fermionic particles in analogy to the entanglement theory well established for qubits. We suggest a concise definition of pairing and develop tools for its detection and quantification applicable in present experiments. Our approach is guided by the concepts and tools well known in entanglement theory, like witness operators, convex sets or measures. The theoretical framework we established can be found in Sec. 2.2. A very important question in this context is the relation of pairing to the existing notions of entanglement for indistinguishable fermions. We prove that pairing is not equivalent to any of those concepts, but constitutes a class of correlations on its own. To fill the theory with life, we apply it to relevant physical examples, among others the states introduced by Leggett for the description of the BEC-BCS crossover. Unfortunately, we cannot resolve the pairing debate due to a lack of information on some experimental parameters. Recalling that the resource property of entanglement is central to quantum information processing, we consider in Sec. 2.5 the power of paired states for quantum phase estimation. Here, quantum mechanical probe systems are used to estimate some parameter related to another physical system via the interaction of the probe with the system. The intrinsic uncertainty of quantum mechanics only allows the determination of this parameter to some limited accuracy. Using N classical probe states, this uncertainty can be reduced, but it will scale like $\sim 1/\sqrt{N}$. This so-called Standard Quantum Limit (SQL) can be beaten using quantum mechanical states, and the Heisenberg Limit $\sim 1/N$ can be reached in the best case. We prove that special paired fermionic states allow phase estimation beyond the SQL. Most remarkably, we find an example where the BCS-states available in the laboratory allow quantum metrology at the Heisenberg limit. These results give hope that the pairing of fermionic particles might turn out useful for other applications as well. (The results of this Chapter are published in [32].)

After these conceptual considerations, we aim at getting further insight into the properties of fermionic systems using simulation techniques. The simulation of quantum mechanical systems are burdened by the exponential growth of the underlying Hilbert space, making the simulation of a general quantum many-body system on a classical computer an intractable task. There are two conceptually different approaches to overcome these problems, namely the use of quantum simulators [33] on the one hand and the development of approximation schemes tailored for classical computers on the other hand. We consider both approaches, starting with the idea of quantum simulation in Chapter 3. To be more precise in what we have said above, quantum computers were shown to have the ability of simulating other quantum systems efficiently as long as they evolve according to local interactions [34]. However, due to the limited control in today's experiments, the realization of a universal large-scale quantum computer capable of simulating an arbitrary quantum

system is still an unsolved problem. The need to gain a better understanding in the physics of quantum many-body systems led to the concept of quantum simulators. Here, one assumes only a limited control over the system. Having the ability to engineer only a restricted set of interactions, the fundamental question of quantum simulation is the following: Which systems can be simulated by this limited power? In current experiments of quantum mechanical particles trapped in an optical lattice the experimenter's power is in general limited to applying transformations on individual sites as well as implementing certain short range interactions. We further assume that these operations can only be applied simultaneously on all sites, thus assuming translational symmetry of the problem. Under these restrictions, we study the power of fermions, bosons and distinguishable D-dimensional quantum systems which we also call spin systems. In the case of bosons and fermions we restrict to systems governed by quadratic Hamiltonians. These systems are also called quasi-free, and the corresponding ground and thermal states are known as Gaussian states. The interest in quasi-free systems is due to the fact that while still exactly solvable, certain quadratic Hamiltonians are good approximations for more complicated two-body interactions, like e.g. the BCS-Hamiltonian used in the theory of superconductivity. The relatively simple structure of quadratic Hamiltonians allows us to give a complete characterization of the computational power of these systems. In the case of spin-systems, where we allow for more complicated interactions, we can prove that on-site transformations and nearest-neighbor interaction do not constitute a set capable of simulating an arbitrary interaction. Unfortunately it is not possible to give a complete characterization of the power of spin systems, but we have to restrict to the derivation of no-go theorems for other finite-range interactions as well. All our proof use the mathematical machinery of Lie algebras. (These results can be found in [35].)

As large-scale quantum computers and simulators have not been realized experimentally yet, we have to come back to the simulation of quantum mechanical many-body systems using classical computers. There are basically two different possibilities of tackling the problem of the exponentially growing state space: We can either make an approximation in the simulation of the system, or we can restrict to the exact simulation of systems that can be described by a number of parameters growing only polynomially with the system size. The latter is the content of Chapter 4, where we construct a new family of fermionic states, so called fermionic Projected Entangled Pair States (fPEPS). The construction of fPEPS is motivated by the success of the Projected Entangled Pair States already known for lattice spin systems (see e.g. [36] for a review). These have their roots in the valance-bond picture introduced for the solution of certain spin systems, like the AKLT-model [37], and are the higher dimensional generalization of the $1d$ Matrix Product States (MPS) [38, 39, 40]. In a modern quantum information language, the family of PEPS is best understood by the following construction scheme, most easily explained for the one-dimensional MPS-representation: Starting from a $1d$ spin chain we associated to each site two virtual spins that are in a maximally entangled states with their neighbors. Then we apply to each site a local map from the virtual spins to the physical spin. The family of all states that can be obtained via this procedure is

called MPS, resp. PEPS for higher dimensions. Every PEPS is now described via the local projectors that are applied to each site, i.e. via tensors whose dimensions are related to the dimension of the virtual (bond dimension) and physical spins. PEPS are so useful, since they could be proven to allow an efficient description of ground and thermal states for any short-range interaction in any dimension while using only polynomially many parameters [41].
A naive approach of simulating fermionic systems would use the idea that every fermionic system can be mapped to a spin system via the Jordan-Wigner transformation. However, due to the non-local structure of this transformation, this approach results in an exponential growth of the bond dimension of the projectors for $d > 1$, thus spoiling the reduction of parameters originally achieved. Hence, it seems more appropriate to follow the PEPS construction scheme and build up states by projecting entangled virtual fermionic states onto a physical Hilbert space. We show that as in the case of spins, those states are able to approximate ground and thermal states of local Hamiltonians well. Furthermore, we prove that every fPEPS can be described in the PEPS-language by only doubling the number of parameters. While every state can be approximated well by an fPEPS when only the bond dimension is taken large enough, an interesting question is to ask for classes of fPEPS that are the exact ground state of some short-range interaction Hamiltonian. We consider such a subclass, the so-called Gaussian fPEPS which are quasi-free states obtained via a PEPS-construction. In case of translationally invariant systems we can prove that any Gaussian fPEPS is the ground state of a local Hamiltonian. Furthermore, we can construct an example of a Gaussian fPEPS in two dimensions that exhibits critical behavior, i.e. that has polynomially decaying correlations. This is a remarkable example, since quasi-free fermionic systems have in general a logarithmic correction to the area law mentioned above, while the fPEPS obeys the area law by definition. However, the example we constructed has a vanishing Fermi surface, and the area law does not hold in this case. (The content of this Chapter is an extended version of [42].)

In Chapter 5 we take the other route mentioned above and develop a new approximation scheme for simulating interacting fermionic systems. The existing techniques, like mean-field theory, variational methods or Hartree-Fock theory, generally come along with breaking some symmetry of the system. In the case of generalized Hartree-Fock theory (gHFT) originally introduced by Lieb particle number conservation is broken by using fermionic Gaussian states as the variational states. These incorporate the Slater determinants used in the standard HF ansatz as a limiting case, thus being a generalization of the latter. In [43] this ansatz has been applied to the Hubbard model in $d > 1$, and exact results could be derived for ground and thermal states. However, unless we are dealing with a translationally invariant system, these results come along with complicated optimization problems difficult to handle for large systems. We take the success and the problems of this work as a starting point to develop a formalism to obtain ground and thermal states in the generalized HFT for fermionic systems with arbitrary two-body interaction in any dimension. Since quasi-free fermions are completely characterized by their two-point correlations collected in the covariance matrix (CM), we reformulate the generalized

HFT in terms of equations for the CM. Then the parameter space necessary for the description of the system grows polynomially with the system size, since the CM of a system of M modes is a $2M \times 2M$ matrix. We show that real-time evolution in generalized HFT can be formulated consistently as an evolution equation for the covariance matrix, allowing the simulation of the dynamics for large fermionic systems. Next, we show that the generalized HF ground can be determined via an evolution of the covariance matrix in imaginary time. Furthermore, the CM for thermal states can be found via a fixed-point iteration. We apply the numerical techniques derived in this Chapter to the two-dimensional translationally invariant Hubbard model with attractive interaction, since there exist exact solutions for the energies of ground and thermal states in this case. For a 10×10 lattice we find excellent agreement of our numerical results with the exact solution. We aim at applying our machinery to Hubbard models without translational invariance, as these are under consideration in current experiments. Special instances of the generalized Hubbard model are expected to give rise to the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-phase [44] of Cooper-pairs with non-vanishing center-of-mass momentum, and we hope that our simulations will contribute to the understanding of the quantum phases appearing in cold fermionic gases. (Ref. [45] includes a more concise treatment of these results.)

Chapter 2

Pairing in Fermionic Systems

The notion of pairing in fermionic systems is at least as old as the seminal work of Bardeen, Cooper and Schrieffer explaining superconductivity [22]. The formation of fermionic pairs with opposite spin and momentum is not only the source for the vanishing resistance in solid state systems, but it can also explain many other interesting phenomena, like superfluidity in helium-3 or inside a neutron star.

For instance, with recent progress in the field of ultra cold quantum gases fermionic pairing has gained again a lot of attention [46, 47, 48, 49, 50, 28, 51, 52]. These experiments allow an excellent control over many parameters inherent to the system, offering a unique testing ground for existing theories and an exploration of new and exotic phases. A prominent example is the so-called BEC-BCS crossover. Starting from a mixture of two different spin states of a fermionic gas, two different quantum phases can be obtained using a Feshbach resonance [53, 54]. In one regime, diatomic molecules are formed, and Bose-Einstein condensation can take place. In the other regime, the fermions build loosely bound Cooper pairs, as depicted in Fig. 2.1. In both regimes pairs of fermions emerge, but the notion of pairing is not clear and sometimes even controversial. Recent experiments on the BEC-BCS crossover have caused a heated debate whether or not the obtained data was in agreement with pairing [28, 29, 30, 31]. In addition, pairing without superfluidity [55] has been observed in these experiments, raising fundamental questions on quantum correlations in fermionic many-body systems.

Motivated by these exciting experiments and the central role pairing plays in many physical phenomena, and by the lack of accepted criteria to verify the presence of pairing in a quantum state, we propose a clear and unambiguous definition of pairing intended to capture its two-particle nature and to allow a systematic study of the set of paired states and its properties. We employ methods and tools from quantum information theory to gain a better understanding of the set of fermionic states that display pairing. In particular, we develop tools for the systematic detection and for the quantification of pairing, which are applicable to current experiments. Our approach is inspired by concepts and methods from entanglement theory, thus building a bridge between quantum information science and condensed matter physics.

Since they contain non-trivial quantum correlations, paired states belong to the set of entangled many-body states. However, pairing will turn out to be not equivalent

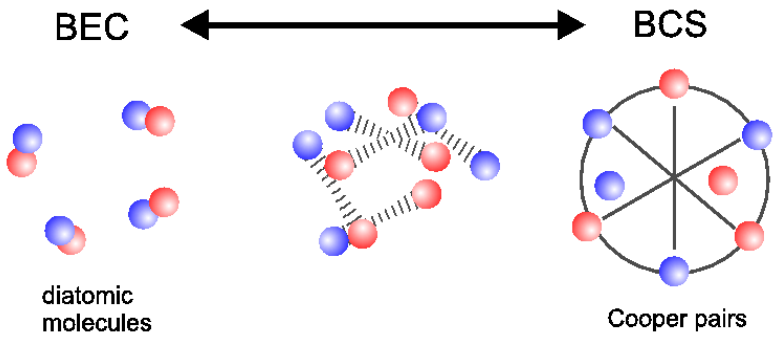

Figure 2.1: BEC-BCS crossover of a fermionic quantum gas. On the BEC-side of the crossover, the fermionic atoms are bound in diatomic molecules with bosonic statistics. These molecules can form a Bose-Einstein condensate. On the BCS-side of the crossover, fermions on the opposite side of the Fermi momentum sphere form Cooper-pairs, and a superfluid phase arises. It has been proposed that these two seemingly distinct regimes of BEC of molecules and BCS superfluidity of Cooper-pairs are continuously connected through the BEC-BCS crossover, where more complicated forms of fermionic pairing are expected to occur.

to any known concept of entanglement in systems of indistinguishable particles [56, 57, 58, 59, 60, 61, 62, 63, 21, 64, 65, 20, 66, 67, 68, 69] but to represent a particular type of quantum correlation of its own. We will show that these correlations can be exploited for quantum phase estimation. Hence pairing constitutes a resource in state estimation using fermions as much as entangled states with spins.

This Chapter is organized as follows: After the introduction of the language necessary for the description of fermionic systems in Sec. 2.1, we will introduce the general framework of pairing theory in Sec. 2.2. This part includes our definition of pairing and methods for its detection and quantification. In order to fill the theory with life we will apply it to two different classes of fermionic states in Secs. 2.3 and 2.4. We start out with pairing in fermionic Gaussian states in Sec. 2.3. The interest in this family of states is two-fold. First, the pairing problem can be solved completely in this case, so that Gaussian states are particularly interesting from a conceptual point of view. Second, there exists a relation between pure fermionic Gaussian states and the BCS-states of superconductivity (see Sec. 2.1.4 for the details) which are examples of paired states par excellence. This enables us to translate methods developed for the detection and quantification of pairing for Gaussian states to the BCS-states. The reader interested in the application of our pairing theory to experimental application is referred to Sec. 2.4. There we study pairing for number conserving states, i.e. states commuting with the number operator. This class includes the states appearing in the BEC-BCS crossover, and we will develop tools for the detection of pairing tailored for these systems. In 2.5 we will show that certain classes of paired states constitute a resource for quantum phase estimation, proving that pairing is a resource similar to entanglement.

2.1 Fermionic states

In this Chapter we review the basic concepts needed for the understanding of fermionic systems. We start out with some notation used for the description of fermionic systems in second quantization in Sec. 2.1.1. As pairing is a special sort of correlation, we continue with a review on quantum correlations and entanglement in systems of indistinguishable particles in Sec. 2.1.2. This general part is followed by the introduction of fermionic Gaussian states and number conserving states in Secs. 2.1.3 and 2.1.4. The latter includes the introduction of BCS-states and their relation to the Gaussian states.

2.1.1 Basic notation

We consider fermions on an M-dimensional single particle Hilbert space $\mathcal{H} = \mathbb{C}^M$. All observables are generated by the creation and annihilation operators $a_j^\dagger$ and $a_j, j = 1, \ldots, M$, which satisfy the canonical anti-commutation relations (CAR) $\{a_k, a_l\} = 0$ and $\{a_k, a_l^\dagger\} = \delta_{kl}$. We say $a_j^\dagger$ creates a particle in mode or single particle state e_j, where $\{e_j\} \subset \mathbb{C}^M$ denotes the canonical orthonormal basis of $\mathcal{H}$. In general, for any normalized $f \in \mathcal{H}$, we define $a_f \equiv \sum_k f_j a_j$, the annihilation operator for mode f. Sometimes a description using the $2M$ hermitian Majorana operators $c_{2j-1} = a_j^\dagger + a_j$, $c_{2j} = (-i)(a_j^\dagger - a_j)$, which satisfy $\{c_k, c_l\} = 2\delta_{kl}$, is more convenient.

The Hilbert space of the many-body system, the antisymmetric Fock space over M modes, $\mathcal{A}_M$, is spanned by the orthonormal Fock basis defined by

$$|n_1, \ldots, n_M\rangle = \left(a_1^\dagger\right)^{n_1} \ldots \left(a_M^\dagger\right)^{n_M} |0\rangle, \tag{2.1}$$

where the vacuum state $|0\rangle$ fulfills $a_j|0\rangle = 0\ \forall j$. The $n_j \in \{0, 1\}$ are the eigenvalues of the the mode occupation number operators $n_j = a_j^\dagger a_j$. The N-particle subspace spanned by vectors of the form (2.1) satisfying $\sum_i n_i = N$ is denoted by $\mathcal{A}_M^{(N)}$. The set of density operators on the Hilbert space $\mathcal{H} = \mathcal{A}_M$, $\mathcal{A}_M^{(N)}$ is denoted by $\mathcal{S}(\mathcal{H})$.

As we have already explained in Chap. 3 linear transformations of the fermionic operators which preserve the CAR are called canonical transformations. They are of the form

$$c_k \mapsto c_k' = \sum_i O_{kl} c_l,$$

where $O \in O(2M)$ is an element of the real orthogonal group. These transformations can be implemented by unitary operations U_O on $\mathcal{A}_M$ which are (for $\det O = 1$) generated by quadratic Hamiltonians in the c_j (see, e.g. [70]). The subclass of canonical operations which commute with the total particle number $N_{\mathrm{op}} = \sum_i n_i$ are called passive transformations. They take a particularly simple form in the complex representation

$$a_k \mapsto a_k' = \sum_l U_{kl} a_l,$$

where U is unitary on the single-particle Hilbert space $\mathcal{H}$, i.e., they describe (quasi)free time evolution of independent particles. Canonical transformations which do not commute with N_{op} are called active. They mix creation and annihilation operators.

2.1.2 Quantum correlations of fermionic states

The notion of "pairing" used in the description of superconducting solids, superfluid liquids, baryons in nuclei, etc. is always associated with a correlated fermionic system. The subject of quantum correlations in fermionic systems is vast [71]. In recent years, there has been renewed interest from the perspective of quantum information theory. There quantum correlations, aka entanglement, of distinguishable systems (qubits) play a crucial role as a resource enabling certain state transformations or information processing tasks. The detailed quantitative analysis of quantum correlations motivated by this has proven to be valuable also in the understanding of condensed matter systems (see [72] for a review).

In contrast to the usual quantum information setting which studies the entanglement of distinguishable particles, the indistinguishable nature of the fermions is of utmost importance in the settings of our interest. The existing concepts for categorizing entanglement in systems of indistinguishable particles fall into two big classes: Entanglement of modes [56, 57, 58, 59, 60, 61, 62, 63, 21] and entanglement of particles. Entanglement of particles has been considered e.g. in [64, 65, 20, 66, 67, 68, 69], leading to the concept of Slater rank [65, 20]. This is the generalization of the Schmidt rank to indistinguishable particles. We show in Sec. 2.2 that our definition of pairing does not coincide with any of the existing ideas. We refrain from giving an exhaustive review on the existing concepts and restrict to the following definition:

Definition 2.1. *A pure fermionic state $\rho_p^{(N)} = |\Psi_p^{(N)}\rangle\langle\Psi_p^{(N)}| \in \mathcal{S}(\mathcal{A}_M^{(N)})$ is called a* product state*, if there exists a passive transformation $a_k \mapsto a'_k$ such that*

$$|\Psi_p^{(N)}\rangle = \prod_{j=1}^{N} a_j'^{\dagger}|0\rangle. \tag{2.2}$$

A state ρ_s is called separable*, if it can be written as the convex combination of product states, i.e.*

$$\rho_s = \sum_{p=1}^{K} \lambda_p \rho_p^{(N_p)}, \tag{2.3}$$

where $\sum_{p=1}^{K} \lambda_p = 1$, $\lambda_p \geq 0$ and all $\rho_p^{(N_p)} \in \mathcal{S}(\mathcal{A}_M^{(N_p)})$ are product states. All other states are said to have "Slater number larger than 1" and are called entangled *in the sense of [65, 20].*

We denote the set of all separable states by $\mathcal{S}_{sep}$ and by $\mathcal{S}_{sep}^{(N)} \equiv \mathcal{S}_{sep} \cap \mathcal{S}(\mathcal{A}_M^{(N)})$ the set of all separable states of particle number N.

Note that the sets $\mathcal{S}_{sep}, \mathcal{S}_{sep}^{(N)}$ of separable states are convex and invariant under passive transformations. Both properties will be useful later on.

Separable states have only correlations resulting from their anti-symmetric nature and classical correlations due to mixing. In the terminology of Refs. [65, 20] they have Slater number one and describe unentangled particles. These states will certainly not contain correlations associated with pairing. Note however that they can be mode-entangled for an appropriate partition of modes.

Besides basis change, there are other operations, which do not create quantum correlations and it is useful to see that the set of separable states is invariant under them. The following lemma shows that this is true for particle number measurements as well as tracing out modes:

Lemma 2.2. *Let $\rho \in \mathcal{S}_{sep}$ be a separable state. Then the state after measuring the particle number $n_h = a_h^\dagger a_h$ in some mode h is separable for both possible outcomes $n_h = 0, 1$.*
Furthermore, $\rho_h \equiv tr_{a_h}[\rho]$, the reduced state obtained by tracing out the mode a_h, is also separable.

Proof. As $\mathcal{S}_{sep}$ is convex, it is sufficient to prove the claim for product states ρ. Let $|\Psi\rangle = \prod_{j=1}^N a_{f_j}^\dagger |0\rangle$ be the vector in Hilbert space corresponding to ρ. Our aim is to show that $|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle$, where $|\Psi_l\rangle$ are product states and $n_h = l$ eigenstates of the occupation number operator n_h. If h is in the span of $\{f_{1\leq k\leq N}\}$ or orthogonal to it, the state already is a n_h eigenstate and we are done. Otherwise, define f_{N+1} orthogonal to the $f_{k\leq N}$ such that $h \in \text{span}\{f_{1\leq k\leq N+1}\}$ and define another orthonormal basis $\{g_j\}$ for the span with $g_1 = h$ and $g_2 \propto f_{N+1} - (h \cdot f_{N+1})h$. Here $(h \cdot f_{N+1})$ denotes the inner product on the single particle Hilbert space. Then we can write

$$|\Psi\rangle = a_{f_{N+1}} a_{f_{N+1}}^\dagger \Pi_{j=1}^N a_{f_j}^\dagger |0\rangle = (x a_{g_1} + y a_{g2}) \Pi_{j=1}^{N+1} a_{g_j}^\dagger |0\rangle,$$

for some $x, y \in \mathbb{C}$. Hence, $|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle$ with $|\Psi_0\rangle = x\Pi_{j=2}^{N+1} a_{g_j}^\dagger |0\rangle$ and $|\Psi_1\rangle = -y a_h^\dagger \Pi_{j=3}^{N+1} a_{g_j}^\dagger |0\rangle$ which both clearly are product states. The reduced state $\text{tr}_h[|\Psi\rangle\langle\Psi|]$ is the statistical mixture of $|\Psi_0\rangle$ and $|\Psi_1\rangle$ and therefore clearly separable. □

We close the Section giving two further properties of separable fermionic states that will turn out useful at different points later on. First, we prove a bound on the two-body operator $a_i^\dagger a_j^\dagger a_k a_l + h.c.$ on separable states:

Lemma 2.3. *Let $\rho \in S_{sep}$ be a separable state. Then*

$$|\text{tr}[(a_i^\dagger a_j^\dagger a_k a_l + h.c.)\rho]| \leq 1/2, \tag{2.4}$$

where i, j, k, l are all different.

Proof. Let $\mathcal{H}_{ijkl}$ be the anti-symmetric Fock space of the single particle spaces spanned by modes $a_i^\dagger, a_j^\dagger, a_k^\dagger, a_l^\dagger$ and define $A_{ijkl} = a_i^\dagger a_j^\dagger a_k a_l + h.c.$. Then $\text{tr}[A_{ijkl}\rho] = \text{tr}[\rho^{(ijkl)} A_{ijkl}]$, where $\rho^{(ijkl)} = \sum_{n=0}^4 \beta_{ijkl}^{(n)} |n\rangle\langle n|$ is a mixed separable state according to Lemma 2.2, and $|n\rangle$ denotes an occupation number basis for the subspace $\mathcal{H}_{ijkl}$.

It is easily checked that A_{ijkl} can have a non-vanishing expectation value only for two-particle states

$$|\mu,\nu\rangle = \left(\sum_{r=i,j,k,l} \mu_r a_r^\dagger\right)\left(\sum_{s=i,j,k,l} \nu_s a_s^\dagger\right)|0\rangle.$$

Using $|2\mathrm{Re}(ab)| \leq |a|^2 + |b|^2$ for any complex numbers a, b and the normalization conditions $\sum_r |\mu_r|^2 = \sum_r |\nu_r|^2 = 1$, one arrives at

$$\begin{aligned} |\mathrm{tr}[A_{ijkl}\rho]| &= 2|\mathrm{Re}[(\mu_i\nu_j - \mu_j\nu_i)(\mu_k\nu_l - \mu_l\nu_k)^*]| \\ &= (|\mu_i|^2 + |\mu_j|^2)(|\mu_k|^2 + |\mu_l|^2) + (|\nu_i|^2 + |\nu_j|^2)(|\nu_k|^2 + |\nu_l|^2) \\ &\leq 0.25 + 0.25 = 0.5. \end{aligned}$$

□

Now we prove that the one-and two-body operators for separable states can be expressed in terms of matrix elements of projectors:

Lemma 2.4. *Let $\rho \in \mathcal{S}_{sep}^{(N)}$ be a pure separable state. Then*

$$\langle n_i\rangle = P_{ii}, \tag{2.5}$$
$$\langle a_i^\dagger a_j^\dagger a_k a_l\rangle = (P\otimes P)_{(ij)(lk)} - (P\otimes P)_{(ij)(kl)}, \tag{2.6}$$

where $P = P^2 = P^\dagger$ is a projector of rank N.

Proof. Consider M modes. We go into the basis where the pure separable state is of the form $|\Phi\rangle = \prod_{i=1}^N a_{\alpha_i}^\dagger|0\rangle$. In this basis

$$\langle a_{\alpha_i}^\dagger a_{\alpha_j}^\dagger a_{\alpha_k} a_{\alpha_l}\rangle_{|\Phi\rangle} = \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl},$$

i.e. (2.6) holds for $P = \mathrm{Id}_N$, where $\mathrm{Id}_N = \mathbb{1}_N \bigoplus 0_{M-N} \in \mathbb{C}^{M\times M}$. Now let $a_i^\dagger = \sum_k U_{ik} a_{\alpha_k}^\dagger$. Then

$$\begin{aligned} \langle a_i^\dagger a_j^\dagger a_k a_l\rangle &= (U\ \mathrm{Id}_N U^\dagger)\otimes(U\mathrm{Id}_N U^\dagger)_{(ij)(lk)} - (U\mathrm{Id}_N U^\dagger)\otimes(U\mathrm{Id}_N U^\dagger)_{(ij)(kl)} \\ &= (P\otimes P)_{(ij)(lk)} - (P\otimes P)_{(ij)(kl)}, \end{aligned}$$

and P is a projector of rank N.

For the one-particle operators, we obtain $\langle n_i\rangle = P_{ii}$, as

$$\begin{aligned} (N-1)\langle n_i\rangle &= \sum_{j\neq i}\langle n_i n_j\rangle = \sum_{j\neq i} P_{ii}P_{jj} - |P_{ij}|^2 = \sum_j P_{ii}P_{jj} - P_{ij}P_{ji} \\ &= \mathrm{tr}[P]P_{ii} - (P^2)_{ii} = (N-1)P_{ii}. \end{aligned}$$

□

2.1.3 Fermionic Gaussian states

Fermionic Gaussian states are represented by density operators that are exponentials of a quadratic form in the Majorana operators. A general multi-mode Gaussian state is of the form

$$\rho = K \exp\left[-\frac{i}{4} c^T G c\right], \tag{2.7}$$

where $c = (c_1, \ldots, c_{2M})$ is a vector of Majorana operators, K is a normalization constant and G is a real anti-symmetric $2M \times 2M$ matrix. Every anti-symmetric matrix can be brought to a block diagonal form

$$OGO^T = \bigoplus_{j=1}^{M} \begin{pmatrix} 0 & -\beta_j \\ \beta_j & 0 \end{pmatrix}, \tag{2.8}$$

by a special orthogonal matrix $O \in SO(2M)$ [73].

From Eq. (2.7) it is clear that Gaussian states have an interpretation as thermal Gibbs states corresponding to a Hamiltonian H that is a quadratic form in the c_k, i.e.,

$$H = \frac{i}{4} c^T G c = \frac{i}{4} \sum_{k>l} G_{kl}[c_k, c_l]. \tag{2.9}$$

The form Eq. (2.8) further shows that every Gaussian state has a normal-mode decomposition in terms of M single-mode "thermal states" of the form $\sim \exp(-\beta a^\dagger a)$. From this one can see that the state is fully determined by the expectation values of quadratic operators $a_i a_j$ and $a_i^\dagger a_j$. These are collected in a convenient form in the real and anti-symmetric covariance matrix Γ which is defined via

$$\Gamma_{kl} = \frac{i}{2} \mathrm{tr}\left(\rho[c_k, c_l]\right). \tag{2.10}$$

It can be brought into block diagonal form by a canonical transformation:

$$O\Gamma O^T = \bigoplus_{i=1}^{M} \begin{pmatrix} 0 & \lambda_j \\ -\lambda_j & 0 \end{pmatrix}. \tag{2.11}$$

For every valid density operator, $\lambda_j \in [-1, 1]$, and the eigenvalues of Γ are given by $\pm i\lambda_j$. Hence, every Γ corresponding to a physical state has to fulfill $i\Gamma \leq \mathbb{1}$ or, equivalently, $\Gamma\Gamma^\dagger \leq \mathbb{1}$. Conversely, to each such Γ corresponds a valid Gaussian density operator where the relation between G and Γ is given by $\lambda_j = \tanh(\beta_j/2)$. The covariance matrix of the ground state of H is obtained in the limit $|\beta_j| \to \infty$ i.e., $\lambda_j \to \mathrm{sign}(\beta_j)$. In fact, this shows that every pure Gaussian state is the ground state to some quadratic Hamiltonian. The purity of the state can be easily determined from the covariance matrix as a Gaussian state is pure if and only if $\Gamma^2 = -\mathbb{1}$ [74].

As mentioned, Gaussian states are fully characterized by their covariance matrix and all higher correlations can be obtained from Γ by Wick's theorem [74] via

$$i^p \mathrm{tr}[\rho c_{j_1} \ldots c_{j_{2p}}] = \mathrm{Pf}(\Gamma_{j_1,\ldots,j_{2p}}), \tag{2.12}$$

where $1 \leq j_1 < \ldots < j_{2p} \leq 2M$ and $\Gamma_{j_1,\ldots,j_{2p}}$ is the corresponding $2p \times 2p$ submatrix of Γ. $\mathrm{Pf}(\Gamma_{j_1,\ldots,j_{2p}})^2 = \det(\Gamma_{j_1,\ldots,j_{2p}})$ is called the Pfaffian.

In some cases it is more appropriate to use a different ordering of the Majorana operators, the so-called q-p-ordering $c = (c_1, c_3, \ldots, c_{2M-1}; c_2, c_4, \ldots, c_{2M})$, opposed to the mode-ordering introduced at the beginning. When using the q-p-ordering, the relation between the real and complex representation is given by

$$c^T = \Omega a^T, \quad \Omega = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ i\mathbb{1} & -i\mathbb{1} \end{pmatrix}, \tag{2.13}$$

where $a = (a_1, \ldots, a_M, a_1^\dagger, \ldots, a_M^\dagger)$. The transformation matrix Ω fulfills $\Omega\Omega^\dagger = 2\mathbb{1}$. In the q-p-ordering the covariance matrix obtains the following block structure:

$$\tilde{\Gamma} = \begin{pmatrix} \Gamma_q & \Gamma_{qp} \\ -\Gamma_{qp}^T & \Gamma_p \end{pmatrix}. \tag{2.14}$$

Finally, for some purposes it is more convenient to define a covariance matrix in terms of creation and annihilation operators. In this so-called complex representation, the CM is of the form

$$\Gamma_c = \frac{1}{4}\Omega^\dagger \tilde{\Gamma} \bar{\Omega} = \begin{pmatrix} Q & R \\ \bar{R} & \bar{Q} \end{pmatrix}, \tag{2.15}$$

where $Q_{kl} = \langle i/2[a_k, a_l] \rangle$, $R_{kl} = \langle i/2[a_k, a_l^\dagger] \rangle$ and $\bar{Q}$ denotes the complex conjugate. Note that $R^\dagger = -R$ and $Q^T = -Q$ and hence $\Gamma_c^T = -\Gamma_c$. The condition $\tilde{\Gamma}\tilde{\Gamma}^\dagger \leq \mathbb{1}$ takes the form $4\Gamma_c\Gamma_c^\dagger \leq \mathbb{1}$.

The description of ρ by its covariance matrix is especially convenient to describe the effect of canonical transformations, i.e. time evolutions generated by quadratic Hamiltonians: if $c_k \mapsto \sum_l O_{kl} c_l$ in the Heisenberg picture then $\Gamma \mapsto O\Gamma O^T$ in the Schrödinger picture. For a passive transformation $a_k \mapsto a'_k = \sum_l U_{kl} a_l$, the q-p-ordered Majorana operators transform as

$$c^T \mapsto c'^T = O_p\, c^T, \quad O_p = \begin{pmatrix} X & Y \\ -Y & X \end{pmatrix}, \tag{2.16}$$

where $X = \mathrm{Re}(U)$ is the real part of the unitary U, and $Y = \mathrm{Im}(U)$ the imaginary part. Note that O_p is both orthogonal and symplectic. The behavior of Γ_c under a passive transformation is particularly simple: Q and R transform according to $Q \mapsto UQU^T$ and $R \mapsto URU^\dagger$.

Passive transformations can be used to transform *pure* fermionic states to a simple standard form, the so-called Bloch-Messiah reduction [75]. We give a simplified derivation of this result in Appendix A. The q-p ordered CM $\tilde{\Gamma}_{\mathrm{BCS}}$ takes the form (2.14) where

$$\Gamma_q = -\Gamma_p = \bigoplus_k \begin{pmatrix} 0 & -2\mathrm{Im}(u_k\bar{v}_k) \\ 2\mathrm{Im}(u_k\bar{v}_k) & 0 \end{pmatrix}, \tag{2.17}$$

$$\Gamma_{qp} = \bigoplus_k \begin{pmatrix} |u_k|^2 - |v_k|^2 & 2\mathrm{Re}(u_k\bar{v}_k) \\ -2\mathrm{Re}(u_k\bar{v}_k) & |u_k|^2 - |v_k|^2 \end{pmatrix}. \tag{2.18}$$

In Hilbert space, the state in standard form is given by

$$|\Psi^{(\bar{N})}_{Gauss}\rangle = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|0\rangle, \tag{2.19}$$

where $u_k, v_k \in \mathbb{C}$, $|u_k|^2 + |v_k|^2 = 1$, $\bar{N} = \sum_k \langle a_k^\dagger a_k\rangle = 2\sum_k |v_k|^2$. Of course we can always even simplify to $u_k, v_k \in \mathbb{R}$ by passive operations. This comprises the kind of "paired" states appearing in the BCS theory of superconductivity [22] with $k \equiv (\vec{k}, \uparrow)$, $-k \equiv (-\vec{k}, \downarrow)$. We will refer to these states as *Gaussian BCS states*. We would like to stress the fact that every pure Gaussian state is a Gaussian BCS state in some basis. The proof is given in Thm. A.2 in Appendix A.

2.1.4 Number conserving fermionic states

For the application to physical systems we are interested in states for which the particle number is a conserved quantity. We call ρ a number conserving state if $[\rho, N_{\mathrm{op}}] = 0$ where N_{op} denotes the total number operator. Thus, the density operator of a number conserving state can be written as a mixture of N_{op}-eigenstates. In particular, all separable states as defined in Def. 2.1 are number conserving.

The Gaussian BCS wave function (2.19) is not number conserving, except for the trivial case that either u_k or v_k vanishes for every mode. However, a relation to these states can be established using the series expansion of the exponential function applied to operators:

$$\begin{aligned} |\Psi^{(\bar{N})}_{Gauss}\rangle &= \prod_k (u_k + v_k P_k^\dagger)|0\rangle \\ &= \left(\prod_k u_k\right) \exp\left[\sum_k \alpha_k P^\dagger\right]|0\rangle = \left(\prod_k u_k\right) \sum_{N=0}^{2M} \frac{1}{N!}\left(\sum_k \alpha_k P^\dagger\right)^N |0\rangle, \end{aligned}$$

where we have introduced the pair creation operator $P_k^\dagger = a_k^\dagger a_{-k}^\dagger$, and the coefficients α_k are related to u_k and v_k via $\alpha_k = v_k/u_k$. We rewrite the above expression in the following way:

$$|\Psi^{(\bar{N})}_{Gauss}\rangle = \sum_{N=0}^{2M} \lambda_N |\Psi^{(N)}_{BCS}\rangle, \tag{2.20}$$

where the number conserving $2N$-particle BCS state is given by

$$|\Psi^{(N)}_{BCS}\rangle = C_N \left(\sum_{k=1}^{M} \alpha_k P_k^\dagger\right)^N |0\rangle. \tag{2.21}$$

Rewriting Eq. (2.21) as

$$|\Psi^{(N)}_{BCS}\rangle = C_N N! \sum_{j_1<j_2<\cdots<j_N} \alpha_{k_1}\ldots\alpha_{k_N} P_{k_1}^\dagger \ldots P_{k_N}^\dagger |0\rangle, \tag{2.22}$$

the normalization constant C_N is seen to be

$$C_N = \left((N!)^2 \sum_{j_1<\ldots<j_N} |\alpha_{j_1}|^2 \ldots |\alpha_{j_N}|^2 \right)^{-1/2}.$$

The coefficients $\lambda_N = \left(\prod_k u_k\right)/(N!C_N)$ can be interpreted as the probability amplitude of being in state $|\Psi^{(N)}_{BCS}\rangle$, since $\sum_N |\lambda_N|^2$=1. We will in general drop the term *number conserving* and refer to states of the form (2.21) as *BCS-states*.

Whenever the distribution of the λ_N is sharply peaked around some average particle number $\bar{N}$, expectation values of relevant observables for the number conserving BCS-states $|\Psi^{(\bar{N})}_{BCS}\rangle$ are approximated well by the expectation values of the Gaussian BCS state in the following way: According to (2.21) the expectation value of any number conserving observable O is given by

$$\langle \Psi^{(\bar{N})}_{Gauss}|O|\Psi^{(\bar{N})}_{Gauss}\rangle = \sum_N |\lambda_N|^2 \langle \Psi^{(N)}_{BCS}|O|\Psi^{(N)}_{BCS}\rangle, \tag{2.23}$$

as O does not couple states with different particle number. If the distribution of the coefficients $|\lambda_N|^2$ is sharply peaked around some average particle number $\bar{N}$, then $\langle \Psi^{(\bar{N})}_{Gauss}|O|\Psi^{(\bar{N})}_{Gauss}\rangle \approx \langle \Psi^{(\bar{N})}_{BCS}|O|\Psi^{(\bar{N})}_{BCS}\rangle$. This relation will turn out very useful later on, as results on Gaussian states can be translated into results on number conserving BCS-states.

2.2 Pairing theory

In this central Section we give the formal framework of our pairing theory. We start with a motivation and the statement of the definition in Subsec. 2.2.1. Next, in Subsec. 2.2.2 we justify the importance of our definition by showing that pairing is not equivalent to any existing definition of entanglement in systems of indistinguishable fermions. Borrowing tools and concepts from entanglement information theory we introduce methods for the detection and quantification of pairing in Subsecs. 2.2.3 and 2.2.4. The formalism developed in this Section is applied to concrete examples in Secs. 2.3 and 2.4.

2.2.1 Motivation and statement of the definition

The simplest system in which we can find pairing consists of two particles and four modes[1]. The prototypical paired state, for example the spin-singlet of two electrons with opposing momenta, is of the form

$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left(a_1^\dagger a_2^\dagger + a_3^\dagger a_4^\dagger \right) |0\rangle. \tag{2.24}$$

The states describing many Cooper pairs in BCS theory are generalizations of $|\Phi\rangle$.

[1] For three modes, all pure two-particle states are of product form.

The state $|\Phi\rangle$ describes correlations between the two particles that cannot be reproduced by any uncorrelated state and it can be completely characterized by one- and two-particle expectations consisting of no more than two creation and annihilation operators each. This is a characteristic of the two-particle property "pairing" that we propose to make the central *defining* property of paired states in the general case of many modes, many particles and mixed states. Since, moreover, we would call the state $|\Phi\rangle$ paired no matter what basis the mode operators a_i refer to and we want it to comprise all BCS-states, we are led to the following list of requirements that a sensible definition of pairing should fulfill:

1. States that have no internal quantum correlation must be unpaired. These are the separable states (2.3).

2. Pairing must reveal itself by properties related to one-and two-particle expectations only.

3. Pairing is be a basis-independent property, i.e. it is invariant under passive transformations.

4. The standard "paired" states appearing in the description of solid state and condensed matter systems, i.e., the BCS-states with wave function (2.21) must be captured by our definition.

Further, it is desirable that there exist examples of paired states that are a resource for some quantum information application.

Let us define:

Definition 2.5. *The set of all operators $\{\mathcal{O}_\alpha\}_\alpha$ on $\mathcal{A}_M$ which are the product of at most two creation and two annihilation operators is called the set of* two-particle operators. *We denote it by A_2.*

These operators capture all one- and two-particle properties of a state ρ and should therefore contain all information about pairing. We will call a state ρ paired, if it can be distinguished from separable states by looking at observables in A_2 alone. This is formalized in the following definition:

Definition 2.6. *A fermionic state ρ is called* paired *if there exists a set of operators $\{\mathcal{O}_\alpha\}_\alpha \subseteq A_2$ such that the expectation values $\{tr[\rho\mathcal{O}_\alpha]\}$ cannot be reproduced by any separable state $\rho_s \in \mathcal{S}_{sep}$.*
States that are not paired are called unpaired.

This definition automatically fulfills our first two requirements. The third, basis independence, clearly holds, since the set of separable states is invariant under passive transformations. We will show in Lemma 2.22 and Subsec. 2.3.2 that the last requirement is met, both for Gaussian and number conserving BCS-states, i.e. all of them are paired. Moreover, in Sec.2.5 we can show that there exist paired states that are a resource for quantum metrology.

For states with a fixed particle number, i.e. $\rho \in \mathcal{S}(\mathcal{A}_M^{(N)})$ it is sufficient to compare with expectation values on N-particle separable states $\rho_s^{(N)} \in \mathcal{S}_{sep}^{(N)}$, as for all other

states the expectation values of $\langle \sum_i n_i \rangle$ and $\langle (\sum_i n_i)^2 \rangle$ differ due to the particle number constraint. For number conserving states, only number conserving observables lead to non-vanishing expectation values and one can thus restrict to linear combinations of $a_i^\dagger a_j$, $a_i^\dagger a_j^\dagger a_k a_l$.

For Gaussian states pairing must reveal itself by properties of the covariance matrix, as all higher correlations can be obtained from it via Eq. (2.12). This important fact enables us to give a complete solution of the pairing problem for fermionic Gaussian states, which we present in Sec. 2.3.

2.2.2 Relation of pairing and entanglement

Paired states are fermionic states exhibiting non-trivial quantum correlations. In particular, by definition paired states are inseparable i.e., entangled in the sense of [65, 20]. This raises immediately the question: Is pairing equivalent to entanglement? First, note that our basis-independent definition clearly has no relation to entanglement of modes, which is basis-dependent. The product states of Def. 2.1 can be mode-entangled for some choice of partition of modes, e.g. $1/\sqrt{2}(a_1^\dagger + a_2^\dagger)|0\rangle$ is entangled in modes $a_1^\dagger$ and $a_2^\dagger$. Further, we provide below examples of entangled, but unpaired states that demonstrate that pairing is not equivalent to entanglement of particles but represents a special type of quantum correlation. First, we show that not every state that is entangled according to the Slater rank criterion is paired:

Lemma 2.7. *There exist states that are entangled according to the Slater rank concept, but not paired.*

Proof. Consider the state $|\Psi_4\rangle = \frac{1}{2}(a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger + a_5^\dagger a_6^\dagger a_7^\dagger a_8^\dagger)|0\rangle$. This state is entangled according to the Slater rank definition, as it has Slater number 2. However, one sees immediately that the one-and two-particle expectations for $|\Psi_4\rangle$ are the same as for

$$\rho_s^{(4)} = \frac{1}{2}|\Phi_1\rangle\langle\Phi_1| + \frac{1}{2}|\Phi_2\rangle\langle\Phi_2|,$$

where $|\Phi_1\rangle = a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger|0\rangle$, $|\Phi_2\rangle = a_5^\dagger a_6^\dagger a_7^\dagger a_8^\dagger|0\rangle$. Since $\rho_s^{(4)}$ is a product state, $|\Psi_4\rangle$ is not paired. One can construct further examples in a similar manner using e.g. other states with higher Slater rank. □

From an intuitive point of view, the state $|\Psi_4\rangle = \frac{1}{2}(a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger + a_5^\dagger a_6^\dagger a_7^\dagger a_8^\dagger)|0\rangle$ is build up of quadruples rather than pairs.

Since pairing is defined via expectation values of one-and two-particle operators only, one might wonder whether pairing is related to entanglement of the two-particle reduced state. To study this relation, we recall the definition of the *two-particle density operator* and the closely related *two-particle density matrix* [76]:

Definition 2.8. *Let ρ be the density operator of a fermionic state. Then $O^{(\rho)}_{(ij)(kl)} = tr[\rho a_i^\dagger a_j^\dagger a_l a_k]$ is called the* two-particle reduced density matrix *(RDM). It is usually not normalized and fulfills $tr[O^{(\rho)}] = \langle N_{op}^2 \rangle - \langle N_{op} \rangle$.*
The operator $\rho_2 = O^{(\rho)}/tr[O^{(\rho)}]$ is called reduced two-particle density operator *(RDO).*

Note the crucial difference between the two-particle RDM and the RDO: While the RDM contains all two-particle correlations of ρ, the RDO corresponds to the two-particle state of any two particles when the rest of the system is discarded. Since pairing is a two-particle property, a natural point of view is to think of it as being related to the entanglement of the two-particle reduced state. However, We would like to emphasize, that pairing is *not* equivalent to entanglement of the RDO, and therefore it is a property of the one- and two-particle expectations:

Lemma 2.9. *Let $|\Psi_{BCS}^{(N)}\rangle$ be a number conserving BCS state as defined in* (2.21) *with $\alpha_k = 1 \ \forall \ k = 1, \ldots, M$. Then $|\Psi_{BCS}^{(N)}\rangle$ is paired for all $M > N$. However, $\rho_{BCS,2}^{(N)}$ is entangled if and only if $M > 3N - 2$.*

Proof. The witness operator (see Sec. 2.2.3) $H_1^{(p)}$ of Thm. 2.20 has a negative expectation value on $|\Psi_{BCS}^{(N)}\rangle$, hence the state is paired in these modes.

To address the entanglement question we calculate first the reduced density operator $\rho_{BCS,2}^{(N)}$ of $|\Psi_{BCS}^{(N)}\rangle$. Let $|i,j\rangle = a_i^\dagger a_j^\dagger |0\rangle$ and consider the subspace spanned by the states $\{|k,-k\rangle, |l,-l\rangle, |k,l\rangle, |k,-l\rangle, |-k,l\rangle, |-k,-l\rangle\}$. In this basis, $\rho_2^{(N)}$ is of the form

$$\rho_2^{(N)} = \frac{1}{4+2a_1} \begin{pmatrix} a_1 & a_2 & 0 \\ a_2 & a_1 & 0 \\ 0 & 0 & \mathbb{1}_4 \end{pmatrix}, \tag{2.25}$$

where $a_1 = (M-1)/(N-1), a_2 = (M-N)/(N-1)$. We use now the following theorem [20] applicable to mixed fermionic states of two particles each living on a single-particle Hilbert space of dimension four:

Theorem 2.10. *Let the mixed state acting on $\mathcal{A}_4$ have a spectral decomposition $\rho = \sum_{i=1}^r |\Psi_i\rangle\langle\Psi_i|$, where r is the rank of ρ, and the eigenvectors $|\Psi_i\rangle$ belonging to nonzero eigenvalues λ_i are normalized as $\langle\Psi_i|\Psi_j\rangle = \lambda_i \delta_{ij}$. Let $|\Psi_i\rangle = \sum_{a,b} w_{ab} a_a^\dagger a_b^\dagger |0\rangle$ in some basis, and define the complex symmetric $r \times r$ matrix C by*

$$C_{ij} = \sum_{abcd} \epsilon^{abcd} w_{ab}^i w_{cd}^j, \tag{2.26}$$

which can be represented using a unitary matrix as $C = U C_d U^T$, with $C_d = diag[c_1, \ldots, c_r]$ diagonal and $|c_1| \geq |c_2| \geq \ldots \geq |c_r|$. The state has Slater number 1 if and only if

$$|c_1| \leq \sum_{i=2}^r |c_i|. \tag{2.27}$$

The spectral decomposition of $\rho_2^{(N)}$ is given by

$$\begin{aligned} \rho_2^{(N)} \ = \ & |\Psi_+\rangle\langle\Psi_+| + |\Psi_-\rangle\langle\Psi_-| + |\Psi_{kl}\rangle\langle\Psi_{kl}| + |\Psi_{k-l}\rangle\langle\Psi_{k-l}| + \\ & |\Psi_{-kl}\rangle\langle\Psi_{-kl}| + |\Psi_{-k-l}\rangle\langle\Psi_{-k-l}|, \end{aligned}$$

where $|\Psi_+\rangle = \sqrt{\frac{a_+}{5+a_+}}|\psi_+\rangle$, $|\Psi_-\rangle = \sqrt{\frac{1}{5+a_+}}|\psi_-\rangle$ and $|\Psi_{\pm k,\pm l}\rangle = \sqrt{\frac{1}{5+a_+}}|\pm k, \pm l\rangle$. Here $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|k,-k\rangle \pm |l,-l\rangle)$ and $a_+ = (2M-N-1)/(N-1)$. Defining $\gamma^2 = 1/(5+a_+)$, one obtains

$$C = \gamma^2 \begin{pmatrix} a_+ & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \tag{2.28}$$

with spectrum $\mathrm{spec}(C) = \gamma^2\{a_+, 1, 1, -1, -1, -1\}$. For $M \leq N$ the state $|\Psi_{BCS}^{(N)}\rangle$ is separable, so we can take $M > N$. Hence, $a_+\gamma^2$ is the eigenvalue with largest absolute value. According to Thm. 2.10, the reduced state is entangled iff $|c_1| > \sum_{i=2}^{r} |c_i|$. For our example, this holds iff $M > 3N - 2$. □

We would like to stress the point that Lemma 2.9 shows the existence of paired states that are not entangled on the two-particle level. Having assured that our definition of pairing does not coincide with entanglement, we now turn to methods of detecting and quantifying pairing.

2.2.3 Methods for detecting pairing

Taking Def. 2.6, we aim at finding tools that can be used for the detection and quantification of pairing. These will be applied to systems of Gaussian states and number conserving states in Secs. 2.3 and 2.4 respectively. In this Section, we exploit the convexity of the set of unpaired states to introduce witness operators and obtain a geometrical picture of the set. The quantification of pairing via pairing measures will be discussed in Sec. 2.2.4.

Pairing witnesses Given a fermionic density operator, we are interested in an operational method to determine whether it is paired or not. As in the case of separability, this simple-sounding question will turn out to be rather difficult to answer in general. Starting from Def. 2.6, it is clear that the set of unpaired states is convex. This suggests the use of the Hahn-Banach separation theorem as a means to certify that a given density operator is not in the set of paired states. In analogy to the entanglement witnesses in quantum information theory [77] we define

Definition 2.11. *A* pairing witness W *is a Hermitian operator that fulfills* $tr[W\rho_u] \geq 0$ *for all unpaired states* ρ_u*, and for which there exists a paired state* ρ *such that* $tr[W\rho] < 0$*. We say that* W detects *the paired state* ρ*.*

The witness defines a hyperplane in the space of density operators such that the convex set of unpaired states lies wholly on that side of the plane characterized by $\mathrm{tr}[\rho W] > 0$. According to the Hahn-Banach theorem [78], for every unpaired state there exists a witness operator which detects it. In principle, a witness operator can be an operator involving an arbitrary number of creation and annihilation operators. However, since definition of pairing refers only to expectation values of operators in A_2, it is enough to restrict to operators from that set. This represents a significant simplification in a two-fold way. First, from a mathematical point of view, witness

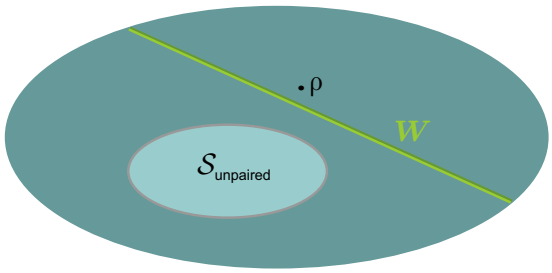

Figure 2.2: Pairing witness W detecting the paired state ρ that lies outside the set of unpaired states $\mathcal{S}_{\text{unpaired}}$.

operators from a finite dimensional set. Second, from an experimental point of view, since operators involving more than two-body correlations are typically very difficult to measure. The construction of entanglement witnesses detecting all entangled states is an unsolved problem in entanglement theory, and we will not be able to give a complete solution to the problem of finding all pairing witnesses either. However, in Section 2.4 we will construct witnesses for a large subclass of BCS-states by using the correspondence between number conserving and Gaussian BCS-states.

Pairing and convex sets Whether a state ρ is paired or not can be determined from a finite set of real numbers, namely the expectation values of a hermitian basis $\{O_\alpha\}$ of A_2. This allows us to reformulate the pairing problem as a geometric question on convex sets in finite-dimensional Euclidean space, describe a complete set of pairing witnesses, and deduce a relation to the ground state energies of quadratic Hamiltonians.

Consider a set $\{O_\alpha, \alpha = 1, \ldots, K\} \subset A_2$ of hermitian operators in A_2 that are not necessarily a basis. Denote by $\vec{O}$ the vector with components O_α. We define the set of all expectation values of $\vec{O}$ for separable states

$$C_{\vec{O}} = \left\{ \vec{v} = \mathrm{tr}[\vec{O}\rho_s] : \rho_s \in S_{sep} \right\} \subset \mathbb{R}^K. \tag{2.29}$$

For a state ρ let $\vec{v}_\rho \equiv \mathrm{tr}[\vec{O}\rho]$. By definition, ρ is paired if $\vec{v}_\rho \notin C_{\vec{O}}$. As the set of separable states is convex, so is $C_{\vec{O}}$. Hence, we can use a result of convex analysis to check if $\vec{v}_\rho \notin C_{\vec{O}}$ [79]:

Lemma 2.12. *Let $C \subset \mathbb{R}^N$ be a closed convex set, and let $\vec{v} \in \mathbb{R}^N$. Then*

$$\vec{v} \in C \Leftrightarrow \ \forall\, \vec{r} \in \mathbb{R}^N : \vec{v} \cdot \vec{r} \geq E(\vec{r}) = \inf_{\vec{w} \in C} \vec{w} \cdot \vec{r}. \tag{2.30}$$

For our purposes, this translates in the following result:

Lemma 2.13. *For a vector of observables $\vec{O} = (O_1 \ldots, O_K)$ let $H(\vec{r}) = \vec{r} \cdot \vec{O}$ and $E(\vec{r}) = \inf_{\rho \in \mathcal{S}_{sep}} \{tr[H(\vec{r})\rho]\}$. Then $W(\vec{r}) \equiv H(\vec{r}) - E(\vec{r})$ is a pairing witness, whenever $E(\vec{r}) \neq \inf_{\text{all}\,\rho} \{tr[\rho H(\vec{r})]\}$.*

If $\{O_\alpha\}$ form a basis of A_2, then $W(\vec{r})$ is a complete set of witnesses in the sense that all paired states are detected by some $W(\vec{r})$, i.e., ρ is unpaired iff $tr[W(\vec{r})\rho] \geq 0 \,\forall\, \vec{r}$.

Proof. The witness property of $W(\vec{r})$ is obvious from the definition of $E(\vec{r})$.

For the second part, "if" is clear and "only if" is seen as follows: By Lemma 2.12, if $\mathrm{tr}[W(\vec{r})\rho] \geq 0 \,\forall\, \vec{r}$ then $\vec{v}_\rho \in C$, i.e. the expectation values can be reproduced by a separable state. But since all expectation values of operators $\in A_2$ can be computed from $\vec{v}_\rho$ this implies all two-particle expectations of ρ can be thus reproduced, i.e. ρ is unpaired. □

For an M-mode system with annihilation operators a_i, a standard choice of O_α is, e.g., given by the real and imaginary parts of $\{(a_i^\dagger a_j^\dagger a_k a_l)_{i>j,k>l}, (a_i^\dagger a_j^\dagger)_{i>j}, (a_i^\dagger a_j)_{i\geq j}\}$, i.e., the dimension of A_2 (as a real vector space) is $K = M^2(M-1)^2/2 + 2M^2$.

Thus Lemma 2.13 gives a necessary and sufficient criterion of pairing and provides a geometrical picture of the pairing problem. While the proof that a state is unpaired will in general be difficult as it requires knowledge of all $E(\vec{r})$ and experimentally the measurement of a complete set of observables, practical sufficient conditions for pairing can be obtained by restricting to a subset $\mathcal{O} \subset A_2$. We will show in Sec. 2.4.1 that for a certain choice of $\{O_\alpha\} \subset A_2$ the set $C_{\vec{O}}$ has a very simple form and allows a good visualization of the geometry of paired states and the detection of all BCS-states up to passive transformations.

To provide a way to determine $E(\vec{r})$ used in Lemma 2.13, we point out an interesting connection to the covariance matrices Γ_c (cf. Eq. (2.15)) of Gaussian states: Even for number conserving states, $E(\vec{r})$ is given by a quadratic minimization problem in terms of Γ_c.

Lemma 2.14. *Let $E(\vec{r})$ and $H(\vec{r})$ be as in Lemma 2.13 and let $\vec{O} = \{a_i^\dagger a_j^\dagger a_k a_l, a_i^\dagger a_j\}$ and group the components of $\vec{r}$ in two subsets $(\vec{r})_{ijkl}$ and $(\vec{r})_{ij}$ corresponding to the one- and two-particle observables, respectively. Then $E(\vec{r})$ is given by a quadratic minimization problem over complex covariance matrices Eq. (2.15), in particular the off-diagonal block R of Γ_c. We have*

$$E(\vec{r}) = \inf_{\substack{R=-R^\dagger \\ 4R^2=-\mathbb{1}}} \left\{ \vec{\gamma}^T M(\vec{r}) \vec{\gamma} + w(\vec{r})^T \vec{\gamma} \right\}, \tag{2.31}$$

where $(\vec{\gamma})_{kl} = \langle a_k^\dagger a_l \rangle = -iR_{lk} + \frac{1}{2}\delta_{kl}$ and the $\vec{r}$-dependent quantities are $[M(\vec{r})]_{(ik)(jl)} = -\vec{r}_{ijkl} + \vec{r}_{ijlk}$ and $[w(\vec{r})]_{kl} = \vec{r}_{kl}$.
The minimization can be extended over all *CMs without changing the result.*

Proof. The minimum $\min_{\rho \in \mathcal{S}_{\mathrm{sep}}} \{\langle H(\vec{r}) \rangle_\rho\}$ is attained for *pure* separable states, i.e., product states. All pure fermionic product states are Gaussian. Then by Wick's theorem the expectation values of the $O_{ijkl} = a_i^\dagger a_j^\dagger a_k a_l$ factorize as $\langle a_i^\dagger a_j^\dagger a_k a_l \rangle_\rho = \langle a_i^\dagger a_j^\dagger \rangle \langle a_k a_l \rangle - \langle a_i^\dagger a_k \rangle \langle a_j^\dagger a_k \rangle + \langle a_i^\dagger a_l \rangle \langle a_j^\dagger a_k \rangle$. Since product states are also number conserving, the first term vanishes. For the other two we use that $\langle a_k^\dagger a_l \rangle = -iR_{lk} + \frac{1}{2}\delta_{kl}$, i.e., they only depend on the off-diagonal block R. The pure state condition $\Gamma^2 = -\mathbb{1}$ translates into $4R^2 = -\mathbb{1}$ for product states $Q = 0$.

We could extend over all CMs γ_c since only the block R appears in the expression to be minimized over and since if $\Gamma_c(Q, R)$ is a valid CM then so is $\Gamma_c(0, R)$. □

This lemma provides a systematic way to construct pairing witnesses.

2.2.4 Pairing measures

A theory of pairing must not only answers the question whether a state is paired or not, but should also give means to quantify the amount of pairing inherent in a state. For this purpose, we introduce the notion of a pairing measure:

Definition 2.15. *Let ρ be an M-mode fermionic state. A pairing measure is a map*

$$\mathcal{M} : \rho \mapsto \mathcal{M}(\rho) \in \mathbb{R}_+,$$

which is invariant under passive transformations and fulfills $\mathcal{M}(\rho) = 0$ for every unpaired state ρ.

In addition, it is often useful to normalize $\mathcal{M}$ such that $\mathcal{M}(\rho_0) = 1$ defines the "unit of pairing". The pair state $|\Phi\rangle$ of Eq. (2.24) would be an obvious choice for this unit, but as we see in Sec. 2.3.4 for Gaussian states a different unit is more natural. Thus we do not include normalization in the above definition.

In the geometric picture of the previous Section, a candidate for a pairing measure that immediately comes to mind is the distance of $\vec{v}_\rho$ from the set C. This measure is positive, and it is invariant under passive transformations, as those correspond to a basis change in the space of expectation vectors. The computation of this distance is, in general, very difficult and there is no evident operational meaning to this quantity. In the following Sections we will introduce a different measure that can be computed for relevant families of states and allow a physical interpretation in terms of quantifying a resource for precision measurements.

2.3 Pairing for Gaussian states

In this Section we study pairing of fermionic Gaussian states. We start with the construction of pairing witnesses in Sec. 2.3.1 which will later be a useful guideline for the construction of pairing witnesses for number conserving states. Then we derive a simple necessary and sufficient criterion for pairing of Gaussian states. In Sec. 2.3.3 we show how pure fermionic Gaussian states can be connected to an $SU(2)$ angular momentum representation. This picture will guide us to the construction of a pairing measure.

2.3.1 Pairing witnesses for Gaussian states

Pairing witnesses for pure Gaussian states emerge naturally from the property that every such state is the ground state of a quadratic Hamiltonian (see Sec. 2.1.3). This leads to the following theorem:

Theorem 2.16. *Let* $0 < \epsilon < 1$ *and let* $0 \leq |v_k|^2 \leq 1 - \epsilon$ *and* $\sum_k |v_k|^2 > 0$. *Then the operator*

$$H = \sum_{k=1}^{M} 2(1 - \epsilon - |v_k|^2)(n_k + n_{-k}) - 2v_k u_k^* P_k^\dagger - 2v_k^* u_k P_k \tag{2.32}$$

is a pairing witness, detecting

$$|\Psi_{Gauss}\rangle = \prod_k (u_k + v_k P_k^\dagger)|0\rangle.$$

Proof. Every Gaussian state is the ground state of a quadratic Hamiltonian. In particular, $|\Psi_{Gauss}\rangle$ is seen to be the ground state of

$$H_0 = \sum_{k=1}^{M} (|u_k|^2 - |v_k|^2)(n_k + n_{-k} - 1) - 2v_k u_k^* P_k^\dagger - 2v_k^* u_k P_k$$

with the help of (2.17)-(2.18), as the Hamiltonian matrix of H_0 and Γ can be brought simultaneously to the standard forms (2.8) resp. (2.11). As $\langle P_k \rangle = 0$ for separable states, the minimal energy for these states is given by

$$E_{\min}^{\text{sep}} = -(1 - 2\epsilon) \sum_k \langle n_k + n_{-k} \rangle - (|u_k|^2 - |v_k|^2).$$

Subtracting this energy, we arrive at the Hamiltonian (2.32). For separable states ρ, the expectation values of $P_k^\dagger$ vanish, so that $\text{tr}[H\rho] \geq 0$. For the Gaussian BCS state, however, $\langle \Psi_{Gauss}|H|\Psi_{Gauss}\rangle = -4\epsilon \sum_k |v_k|^2 < 0$. □

Note that the witness defined in (2.32) is an optimal witness for the state $|\Psi_{Gauss}\rangle$ in the sense that there exists no witness detecting more states than W. Thus, W is tangent to the set of unpaired states.

2.3.2 Complete solution of the pairing problem for fermionic Gaussian states

Every Gaussian state is completely characterized by its covariance matrix, so that the solution of the pairing problem must be related to it. The pairing problem is completely solved by the following theorem:

Theorem 2.17. *Let* ρ *be the density operator of a fermionic Gaussian state with covariance matrix* Γ_c *defined in* (2.15). *Then* ρ *is paired iff* $Q \neq 0$.

Proof. First, note that the condition $Q = 0$ is independent of the choice of basis. If ρ is not paired, then there exists a separable state having the same covariance matrix as ρ. This implies $Q = 0$, as separable states are convex combinations of states with fixed particle number, and thus $\langle i/2[a_k, a_l] \rangle = 0$.

Now, let Γ_c be the covariance matrix of a paired Gaussian state, and assume that $Q = 0$. As R is anti-hermitian, there exists a passive transformation such that $R_{ij} = r_i \delta_{ij}$, and $Q = 0$ is unchanged. But such a covariance matrix can be realized by a separable state fulfilling $\langle n_i \rangle = r_i$ in contradiction to the assumption. □

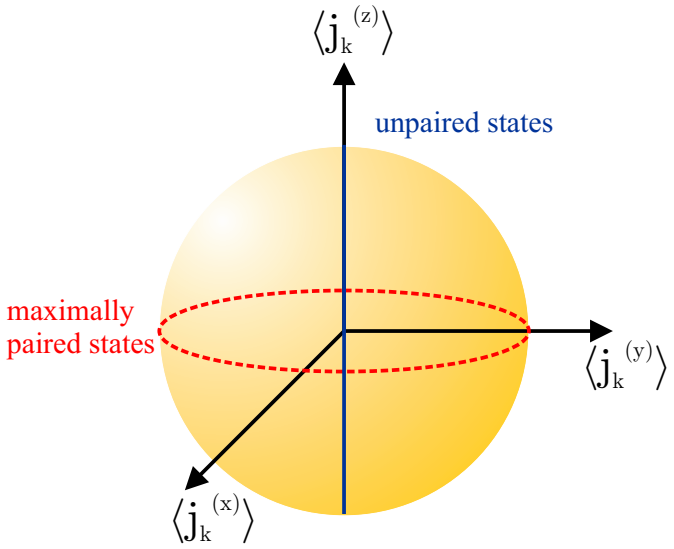

Figure 2.3: Bloch sphere representation of the expectation values of $j_k^{(x)}$, $j_k^{(y)}$ and $j_k^{(z)}$ for a variational BCS state. All pure states lie on the surface of the sphere. Unpaired states lie on the z-axis, while the maximally paired states lie on the equator.

Note that Thm. 2.17 implies that a Gaussian state is unpaired iff it is number conserving.

2.3.3 Angular momentum algebra for Gaussian states

In this Section we will show that pairing of Gaussian states can be understood in terms of an $SU(2)$ angular momentum algebra. The expectation values of the angular momentum operators can be visualized using a Bloch sphere, giving us further understanding of the structure of pairing in Gaussian states. It later leads to the construction of a pairing measure for these states. Define the operators [80, 81]

$$\begin{aligned} j_k^{(x)} &= \frac{1}{2}\left(P_k^\dagger + P_k\right), \\ j_k^{(y)} &= \frac{i}{2}\left(P_k^\dagger - P_k\right), \\ j_k^{(z)} &= \frac{1}{2}\left(1 - n_k - n_{-k}\right). \end{aligned}$$

They fulfill $\left[j_k^{(a)}, j_k^{(b)}\right] = i\varepsilon_{abc} j_k^{(c)}$, $a, b, c \in \{x, y, z\}$, forming an $SU(2)$ angular momentum algebra. For pure Gaussian states in the standard form (2.19) the expectation values of the angular momentum operators are given by $\langle j_k^{(x)}\rangle = \mathrm{Re}(u_k \bar{v_k})$, $\langle j_k^{(y)}\rangle = \mathrm{Im}(u_k \bar{v_k})$, and $\langle j_k^{(z)}\rangle = \frac{1}{2}(1 - 2|v_k|^2)$. As $j^2 = \sum_{i=x,y,z}\langle j_k^{(i)}\rangle^2 = 1/4$ independent of u_k and v_k, the expectation values for every pure Gaussian state lie on the surface of a sphere with radius $1/2$. As we have shown in Thm. 2.17, every unpaired state ρ_u fulfills $\langle j_k^{(x)}\rangle_{\rho_u} = \langle j_k^{(y)}\rangle_{\rho_u} = 0$, so that these states are located on the

z-axis. The states on the equator have $\langle j_k^{(x)}\rangle^2 + \langle j_k^{(y)}\rangle^2 = 1/4$, i.e. they correspond to $|u_k|^2 = |v_k|^2 = 1/2$. The situation is depicted in Fig. 2.3. Referring to the states on the equator as maximally paired is suggested by the fact that they have maximal distance from the set of separable states. This intuitive picture is further borne out by two observations: First, the states on the equator display maximal entanglement between the involved modes [70]. Second, they have the property[2] that they achieve the minimal expectation value of any quadratic witness operator up to basis change. To see this, recall from Sec. 2.1.3 that any quadratic Hamiltonian H of two modes $k, -k$ is up to a common factor and basis change of the form

$$H = \alpha \mathbb{1} + \sin\theta(n_k + n_{-k}) + \cos\theta(P_k^\dagger + P_k).$$

It is a witness (.e., has positive expectation for all product states, if $\alpha \geq |\max\{0, 2\sin\theta\}|$ and does detect some paired state as long as $\sin\theta > -1$. The minimum eigenvalue is $\sin\theta - 1 + \alpha$ and the minimum $\mathrm{tr}(W\rho) = -1$ is attained for $\rho = \frac{1}{2}(1 + P_k^\dagger)|0\rangle\langle 0|(1 + P_k)$.

The pairing measure which is the topic of the next Section will confirm the characterization as maximally paired.

2.3.4 A pairing measure for Gaussian states

The angular momentum representation of paired states depicted in Fig. 2.3 suggests the introduction of a pairing measure via a quantity related to

$$|\langle j_k^{(x)}\rangle|^2 + |\langle j_k^{(y)}\rangle|^2 = |\langle a_k^\dagger a_{-k}^\dagger\rangle|^2.$$

As we are interested in a pairing measure that is invariant under passive transformations we are lead to the following definition:

Definition 2.18. *Let ρ be a fermionic state, and let $Q_{kl} = i/2 tr(\rho[a_k, a_l])$. Then we define*

$$\mathcal{M}_G(\rho) = 2||Q||_2^2 = 2\sum_{kl} |Q_{kl}|^2, \tag{2.33}$$

Lemma 2.19. *$\mathcal{M}_G$ as defined in Eq. (2.18) is a pairing measure fulfilling $\mathcal{M}_G(\rho) \leq M$ for every M-mode Gaussian state.*

Proof. Under a passive transformation $Q \mapsto UQU^T$, and hence $||Q||_2^2$ is invariant. Further, we know by Thm. 2.17 that $Q = 0$ for unpaired states.

It remains to show that for an M-mode Gaussian state ρ we have $\mathcal{M}_G(\rho) \leq M$. Let Γ_c be the $2M \times 2M$ covariance matrix of ρ defined in (2.15). We show first that $\mathcal{M}(\rho)$ is maximized for pure Gaussian states. To do so, recall that an admissible covariance matrix for a Gaussian state in the real representation has to fulfill $i\Gamma \leq 1$ with equality iff Γ is the covariance matrix of a pure Gaussian state. This translates

[2] Maximally entangled states of two qubits share an analogous property about entanglement witnesses [82].

into $\Gamma_c \Gamma_c^\dagger \leq \mathbb{1}$ with equality iff Γ_c belongs to a pure Gaussian state. Using the form of Γ_c given in (2.15), this implies $2\mathrm{tr}[QQ^\dagger + RR^\dagger] \leq \mathrm{tr}[\mathbb{1}] = 2M$. Hence, $||Q||_2^2 \leq M - ||R||_2^2$. It follows that for fixed value of $||R||_2^2$ the value of $||Q||_2^2$ is maximal for a pure Gaussian state. Further, the standard form (2.19)implies that for every value of $||R||$ such a state exists, and that the maximal value is given by $||Q||_2^2 = 2\sum_{k=1}^M |u_k|^2|v_k|^2 \leq M/2$, as $|u_k|^2 + |v_k|^2 = 1$. □

Hence, for every pure Gaussian state with standard form (2.19) the value of the pairing measure is given by $\mathcal{M}_G(\rho) = 4\sum_{k=1}^M |u_k|^2|v_k|^2$. Since $|v_k|^2 = 1 - |u_k|^2$ the measure attains its maximum value for $|u_k|^2 = |v_k|^2 = 1/2$, i.e., for the states already identified as maximally paired.

$\mathcal{M}_G(\rho)$ will appear again when we study the use of paired states for metrology applications, linking the pairing measure to the usefulness of a state for quantum phase estimation and giving support to the "resource" character of paired states.

2.4 Pairing of number conserving states

In the last Section we gave a complete solution to the pairing problem for fermionic Gaussian states. There, Wick's theorem lead to a reduction of the problem to properties of the covariance matrix. For number conserving systems, the situation is more complicated, as now also operators of the form $a_i^\dagger a_j^\dagger a_k a_l$ have to be taken into account. However, we will derive pairing witnesses capable of detecting all number conserving BCS states in Sec. 2.4.1 using the concept of convex sets. For certain classes of BCS states we will construct a family of improved witnesses using the analogy to the Gaussian states. Witnesses have the drawback that they depend on the choice of basis. I.e. even if a witness detects ρ, it does not detect all states related to ρ by a passive transformation. We will show that the eigenvalues of the reduced two-particle density matrix can be used to obtain a sufficient criterion for pairing in Sec. 2.4.2 which is basis independent. We close the Section with the construction of a pairing measure in Sec. 2.4.3.

2.4.1 Pairing of all BCS states and geometry of paired states

In a realistic physical setup it may not be practical to perform all the measurements needed according to Lemma 2.13 to check the necessary and sufficient condition for pairing. Having access only to a restricted set of measurements, necessary criteria for pairing can be derived. In this Section we consider the simplest case of a symmetric measurement involving four modes, i.e. we are looking at the following vector of operators:

$$\vec{O}_3 = \begin{pmatrix} n_k + n_{-k} + n_l + n_{-l} \\ n_k n_{-k} + n_l n_{-l} \\ a_k^\dagger a_{-k}^\dagger a_{-l} a_l + h.c. \end{pmatrix}. \tag{2.34}$$

Remarkably, these expectation values will turn out to be sufficient to detect all BCS states as paired.

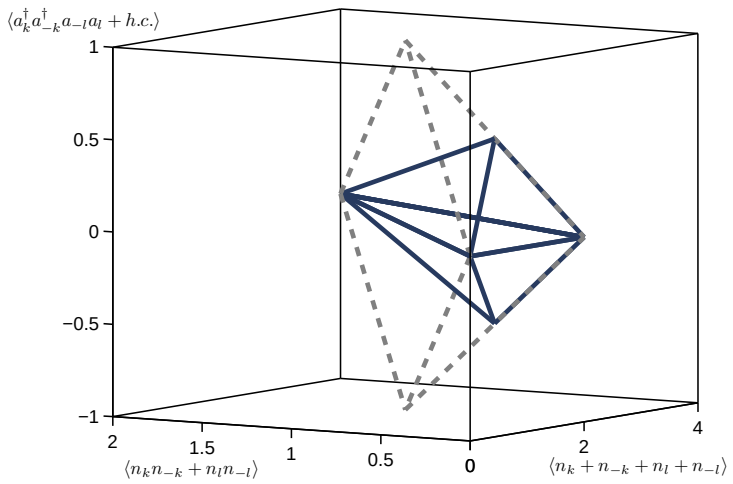

Figure 2.4: Expectation values of the vector Eq. (2.34). For all number conserving states these lie within the convex set $C^{\text{all}}_{\vec{O}_3}$ indicated by the dashed grey lines. The extreme points of the polytope are given by $(0,0,0)$, $(2,0,0)$, $(4,2,0)$ and $(2,1,\pm 1)$. Unpaired states have expectation values in the smaller convex set $C^{\text{unpaired}}_{\vec{O}_3}$ (solid blue) which has extreme points $(0,0,0)$, $(2,0,0)$, $(4,2,0)$ and $(2,1/2,\pm 1/2)$.

We are interested in $C^{\text{unpaired}}_{\vec{O}_3} = \{\text{tr}(\vec{O}_3\rho) : \rho \text{ separable}\}$, the set of all expectation values of $\vec{O}_3$ which correspond to separable states. If for some ρ the vector $\vec{v}_\rho = \text{tr}(\vec{O}_3\rho)$ is found outside of $C^{\text{unpaired}}_{\vec{O}_3}$ then it follows from Lemma 2.13 that ρ is paired. Membership in $C^{\text{unpaired}}_{\vec{O}_3}$ can be easily checked by the following Lemma:

Lemma 2.20. *A number conserving state ρ has expectation values of $\vec{O}_3$ defined in Eq. (2.34) compatible with separability if and only if $tr(H^{(p)}_{k\pm}\rho) \geq 0$ for $k = 1,2,3$, where*

$$\begin{aligned} H^{(p)}_{1\pm} &= \frac{1}{2}(n_k + n_{-k} + n_l + n_{-l}) - (n_k n_{-k} + n_l n_{-l}) \\ &\pm (a_k^\dagger a_{-k}^\dagger a_{-l} a_l + h.c.), \qquad (2.35) \\ H^{(p)}_{2\pm} &= (n_k n_{-k} + n_l n_{-l}) \pm (a_k^\dagger a_{-k}^\dagger a_{-l} a_l + h.c.), \qquad (2.36) \\ H^{(p)}_{3\pm} &= 1 - \frac{1}{2}(n_k + n_{-k} + n_l + n_{-l}) + \frac{1}{2}(n_k n_{-k} + n_l n_{-l}) \\ &\pm \frac{1}{2}(a_k^\dagger a_{-k}^\dagger a_{-l} a_l + h.c.). \qquad (2.37) \end{aligned}$$

Hence, the extremal points of the set $C^{\text{unpaired}}_{\vec{O}_3}$ are given by $tr(H^{(p)}_{k\pm}\rho) = 0$ for three of the witnesses (2.35)-(2.37). The faces of $C^{\text{unpaired}}_{\vec{O}_3}$ consist of points for which at least one of the expectation values $tr(H^{(p)}_{k\pm}\rho)$ vanishes.

$H^{(p)}_{1\pm}$ and $H^{(p)}_{3\pm}$ are also pairing witnesses, while $H^{(p)}_{2\pm}$ is non-negative on all number conserving states.

Proof. As $H^{(p)}_{1\pm}, H^{(p)}_{2\pm}, H^{(p)}_{3\pm}$ are built up of operators that are the product of at most two creation and annihilation operators, we can prove the lemma for separable states. In the first step, we will show that the three operators are positive on all separable states. Then we will show that all states within the set bounded by $H^{(p)}_{1\pm}, H^{(p)}_{2\pm}, H^{(p)}_{3\pm}$ correspond to a separable state. Finally we will show there exist states that are detected as paired by $H^{(p)}_{1\pm}$ and $H^{(p)}_{3\pm}$. Positivity of $H^{(p)}_{2\pm}$ on all number conserving states will be shown in the proof of Lemma 2.20 following below.

To show positivity of $H^{(p)}_{1\pm}, H^{(p)}_{2\pm}, H^{(p)}_{3\pm}$ it is sufficient to show the positivity for pure separable states, as the result for mixed states follows from convexity. From now on, let $\rho \in \mathcal{S}^{(N)}_{sep}$.

$\mathbf{tr}[\mathbf{H}^{(\mathbf{p})}_{\mathbf{1}\pm}\rho] \geq \mathbf{0}$: In Lemma 2.4 we have shown that the expectation values of number conserving one-and two-body operators can be expressed in terms of matrix elements of projectors. Let P be the rank N projector such that

$$\langle a^\dagger_i a^\dagger_j a_k a_l \rangle_\rho = (P \otimes P)_{(ij)(lk)} - (P \otimes P)_{(ij)(kl)},$$

and $\langle n_i \rangle = P_{ii}$. Let $\tilde{P} = P|_{k-k,l,-l}$ the 4×4 principal submatrix of P where the indices run over $k, -k, l, -l$. Then we have the following inequalities:

$$\begin{aligned}
\langle n_k n_{-k} \rangle &= P_{kk}P_{-k-k} - |P_{k-k}|^2 \leq \frac{1}{2}\left(|P_{kk}|^2 + |P_{-k-k}|^2\right) - |P_{k-k}|^2, \\
|\langle a^\dagger_k a^\dagger_{-k} a_{-l} a_l + h.c. \rangle| &= 2|\mathrm{Re}(P_{kl}P_{-k-l} - P_{k-l}P_{-kl})| \\
&\leq 2(|P_{kl}||P_{-k-l}| + |P_{k-l}||P_{-kl}|) \\
&\leq (|P_{kl}|^2 + |P_{-k-l}|^2 + |P_{k-l}|^2 + |P_{-kl}|^2).
\end{aligned}$$

These results imply

$$\mathrm{tr}\left[\rho H^{(p)}_{1\pm}\right] \geq \frac{1}{2}\mathrm{tr}[\tilde{P} - \tilde{P}^2] + |P_{k-k}|^2 + |P_{l-l}|^2.$$

We use the inclusion principle [73], stating that the eigenvalues of a $r \times r$ principal submatrix M_r of a $n \times n$ Hermitian matrix M fulfill $\lambda_k(M) \leq \lambda_k(M_r) \leq \lambda_{k+n-r}(M)$, where the eigenvalues are arranged in increasing order. As P is a projector, we have $0 \leq \lambda_k(P) \leq \lambda_k(\tilde{P}) \leq \lambda_{k+M-r}(P) \leq 1$. Hence,

$$\mathrm{tr}[H^{(p)}_{1\pm}\rho] \geq \frac{1}{2}\mathrm{tr}[\tilde{P} - \tilde{P}^2] \geq \frac{1}{2}\sum_k \lambda_k(\tilde{P})(1 - \lambda_k(\tilde{P})) \geq 0.$$

$\mathbf{tr}[\mathbf{H}^{(\mathbf{p})}_{\mathbf{2}\pm}\rho] \geq \mathbf{0}$: Define $O_1 = n_k n_{-k} + n_l n_{-l} \geq 0$ and $O_2^\pm = 1 \pm a^\dagger_k a^\dagger_{-k} a_{-l} a_l + h.c. \geq 0$. Then $H^{(p)}_{2\pm} = O_1 O_2^\pm$, and as $[O_1, O_2^\pm] = 0$ we conclude that $H^{(p)}_{2\pm} = O_1 O_2^\pm \geq 0$.

$\mathbf{tr}[\mathbf{H}^{(\mathbf{p})}_{\mathbf{3}\pm}\rho] \geq \mathbf{0}$: We will need Lemma 2.2. Note that $\mathrm{tr}[H^{(p)}_{3\pm}\rho] = \mathrm{tr}[H^{(p)}_{3\pm}\rho_{kl}]$, where $\rho_{kl} = \sum_{n=0}^{4}\beta_n|n\rangle\langle n|$, $\beta_n \geq 0$, $\sum_{n=0}^{4}\beta_n = 1$ and $|n\rangle, n = 0,\ldots,4$ are separable n-particle states. Let $\langle H^{(p)}_{3\pm}\rangle_n = \langle n|H^{(p)}_{3\pm}|n\rangle$. Then a straightforward calculation leads to $\langle H^{(p)}_{3\pm}\rangle_0 = 1$, $\langle H^{(p)}_{3\pm}\rangle_1 = \frac{1}{2}$, $\langle H^{(p)}_{3\pm}\rangle_2 = \frac{1}{2}$, $\langle H^{(p)}_{3\pm}\rangle_3 = 0$ and $\langle H^{(p)}_{3\pm}\rangle_4 = 0$. Linearity of the trace implies $\mathrm{tr}[H^{(p)}_{3\pm}\rho] \geq 0$.

Hence, all separable states lie within the set bounded by the planes defined by the witness operators $H^{(p)}_{1\pm}, H^{(p)}_{2\pm}, H^{(p)}_{3\pm}$.

Next, we show that each point within the polytope C^{unpaired} corresponds to a separable state. As S_{sep} is convex, it is sufficient to check that for every extreme point of C^{unpaired} there exists a separable state. This is indeed the case: The extreme points of C^{unpaired} are $(0,0,0)$, $(2,0,0)$, $(4,2,0)$, $(2,1/2,\pm 1/2)$ which correspond for example to the separable states $|0\rangle$, $a^\dagger_k a^\dagger_l|0\rangle$, $a^\dagger_k a^\dagger_{-k} a^\dagger_l a^\dagger_{-l}|0\rangle$ and $(a^\dagger_k + a^\dagger_l)(a^\dagger_{-k} \pm a^\dagger_{-l})/2|0\rangle$ respectively.

It remains to show that $H^{(p)}_{1\pm}$ and $H^{(p)}_{3\pm}$ are pairing witnesses. Define

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(a^\dagger_k a^\dagger_{-k} + a^\dagger_l a^\dagger_{-l})|0\rangle.$$

Then $\mathrm{tr}[H^{(p)}_{1\pm}|\Psi\rangle\langle\Psi|] = \mathrm{tr}[H^{(p)}_{3\pm}|\Psi\rangle\langle\Psi|] = -1$. □

Next, we give a complete characterization of the set $C^{\mathrm{all}}_{\vec{O}_3} = \{\mathrm{tr}(\vec{O}_3\rho) : \rho \in \mathcal{S}(\mathcal{A}^{(N)}_M) : M, N \in \mathbb{N}\}$:

Lemma 2.21. *Every number conserving fermionic state fulfills $tr(H_{k\pm}\rho) \geq 0$, where*

$$H_1 = \frac{1}{2}(n_k + n_{-k} + n_l + n_{-l}) - (n_k n_{-k} + n_l n_{-l}), \tag{2.38}$$

$$H_{2\pm} = (n_k n_{-k} + n_l n_{-l}) \pm (a^\dagger_k a^\dagger_{-k} a_{-l} a_l + h.c.), \tag{2.39}$$

$$H_{3\pm} = 2 - \frac{1}{2}(n_k + n_{-k} + n_l + n_{-l}) \pm (a^\dagger_k a^\dagger_{-k} a_{-l} a_l + h.c.). \tag{2.40}$$

The extremal points of the set $C^{\mathrm{all}}_{\vec{O}_3} = \{tr(\vec{O}_3\rho) : \rho \in \mathcal{S}(\mathcal{A}^{(N)}_M) : M, N \in \mathbb{N}\}$ are given by $tr(H_{k\pm}\rho) = 0$ for three of the witnesses (2.38)-(2.40). The faces of $C^{\mathrm{all}}_{\vec{O}_3}$ consist of points for which at least one of the expectation values $tr(H_{k\pm}\rho)$ vanishes.

Proof. It is sufficient to prove the lemma for $\rho \in \mathcal{S}(\mathcal{A}_N)$, as the result for a general number conserving state follows from convexity.

$\mathbf{tr}[\mathbf{H_1}\rho] \geq \mathbf{0}$: The witness can be rewritten in the form

$$H_1 = \frac{1}{2}(n_k - n_{-k})^2 + \frac{1}{2}(n_l - n_{-l})^2 \geq 0.$$

$\mathbf{tr}[\mathbf{H_{2\pm}}\rho] \geq \mathbf{0}$: This has already been shown in the proof of Thm. 2.21.

$\mathbf{tr}[\mathbf{H_{3\pm}}\rho] \geq \mathbf{0}$: Let $\rho_{kl} = \sum_{n=1}^{4} \beta_n |0\rangle\langle n|$ be the reduced density operator in the modes $\pm k, \pm l$. We can rewrite $H_{3\pm}$ in the form

$$H_{3\pm} = 2 - \frac{1}{2}(n_k + n_{-k} + n_l + n_{-l})(1 \mp (a_k^\dagger a_{-k}^\dagger a_{-l} a_l + h.c.)).$$

Defining $O_{2\mp} = 1 \mp (a_k^\dagger a_{-k}^\dagger a_{-l} a_l + h.c.)$, we obtain $\langle O_{2\mp}\rangle_0 = \langle O_{2\mp}\rangle_1 = \langle O_{2\mp}\rangle_3 = \langle O_{2\mp}\rangle_4 = 1, \langle O_{2\mp}\rangle_2 \leq 2$. This implies

$$\mathrm{tr}[\rho H_{3\pm}] \geq 4 - (\beta_1 + 2\beta_2 + 3\beta_3 + 4\beta_4) \geq 4 - \sum_{n=0}^{4} n\beta_n = 4 - \mathrm{tr}[(n_k + n_{-k} + n_l + n_{-l})\rho_{kl}] \geq 0.$$

As in the proof of Lemma 2.20 it remains to show that the extreme points of C^{all} correspond to some fermionic state. It has been shown in the proof of Lemma 2.20 that $(0,0,0)$, $(2,0,0)$ and $(4,2,0)$ can be reached by some separable state. The remaining two extreme points, $(2,1,\pm 1)$ correspond for example to the state $\frac{1}{\sqrt{2}}(a_k^\dagger a_{-k}^\dagger + a_l^\dagger a_{-l}^\dagger)|0\rangle$. □

We denote by C^{unpaired} and C^{all} the polytopes containing all expectation vectors $\vec{v}_\rho$ corresponding to unpaired states or all number conserving states, respectively. They are bounded by 6 resp. 5 planes defined through the witnesses given in Lemmas 2.20 and 2.21. The situation is depicted in Fig. 2.4.

The witnesses $H_{1\pm}^{(p)}$ given in Eqs. (2.35) allow to detect all number conserving BCS states as paired:

Lemma 2.22. *Except for the trivially unpaired cases $\alpha_k = \delta_{kk_0}$ and $N = M$, the number conserving BCS state $\left|\Psi_{BCS}^{(N)}\right\rangle$ given in Eq. (2.21) is detected by the witness $H_p^{(1)}$ by choosing any two modes (k,l).*

Proof. The first two terms in $H_{1\pm}^{(p)}$ are designed such that their expectation value vanishes for states such as $\left|\Psi_{BCS}^{(N)}\right\rangle$: Since we either have a pair or no particles in the modes $(k,-k)$ we are in an eigenstate with eigenvalue 0 of the operators $n_k + n_{-k} - 2n_k n_{-k}$. The expectation value of the third term is found using the representation Eq. (2.22):

$$\langle a_k^\dagger a_{-k}^\dagger a_{-l} a_l + h.c.\rangle = |C_N|^2 N!^2 \mathrm{Re}(\alpha_k \alpha_l^*) \sum_{\substack{j_1 < \ldots < j_{N-1} \\ j_i \neq k,l}} |\alpha_{j_1}|^2 \ldots |\alpha_{j_{N-1}}|^2,$$

which is nonzero unless $N = M$ or all but one $\alpha_k \neq 0$. The sign can be adjusted by a passive transformation to give $\langle H_{1+}^{(p)}\rangle_{BCS}^{(N)} < 0$. □

This shows that indeed all BCS states are captured as paired by our definition, as desired.

The witnesses $H_{p\pm}^{(1)}$, while detecting every BCS state as paired, are in general far from optimal. However, these states are of great importance in current experiments with ultra cold quantum gases. It has already been shown by Leggett in 1982

[23] that the BCS-states of the form (2.21) can be used to describe the BEC-BCS crossover. Depending on the choice of the coefficients α_k the states describe either a molecular BEC or a superfluid. This motivates the construction of improved witnesses tailored for this class of states. For BCS states realized in nature it is often appropriate to assume some symmetry of the wave function

$$|\Psi_{BCS}^{(N)}(\alpha_k)\rangle = C_N \left(\sum_{k=1}^{2M} \alpha_k P_k^\dagger \right)^N |0\rangle.$$

For example, if $P_k^\dagger = a_{\vec{k}\uparrow}^\dagger a_{-\vec{k}\downarrow}^\dagger$, $P_{k+M}^\dagger = a_{-\vec{k}\uparrow}^\dagger a_{\vec{k}\downarrow}^\dagger$, as it is the case for Cooper pairs, and if we are dealing with an isotropic setting, then $\alpha_k = \alpha_{k+M}$ will hold. It is further often appropriate to assume that the number of modes is much bigger than the number of particles, i.e. $M \gg N$. For this kind of states we will construct pairing witnesses via the correspondence to the Gaussian picture. We sketch the idea of this construction leading to Thm. 2.23, and give the details in the Appendix B.

We have shown in Sec. 2.1.4 the connection of the Gaussian wave function and the number conserving wave function via $|\Psi_{Gauss}\rangle = \sum_{k=1}^N \lambda_N |\Psi_{BCS}^{(N)}(\alpha_k)\rangle$. Consider a number conserving observable O and denote by $\langle O\rangle_{Gauss}$ and $\langle O\rangle_N$ its expectation value for the Gaussian and $2N$-particle BCS wave function respectively. If the distribution of $|\lambda_N|^2$ is sharply peaked around some average particle number $\bar{N}$ with width Δ, then $\langle O\rangle_{Gauss} \approx \langle O\rangle_N$ for any integer $N \in [\bar{N} - \Delta, \bar{N} + \Delta]$. In Thm. 2.16 we have constructed witnesses H for all Gaussian BCS states. As these witnesses are optimal, they suggest to constitute an improved witness detecting the corresponding number conserving BCS state. But H includes terms of the form $P_k^\dagger$ that do not conserve the particle number. Hence, this witness cannot be applied directly to the number conserving case. However, due to Wick's theorem, $\langle P_k^\dagger P_{k+M}\rangle_{Gauss} = \bar{u}_k v_k \langle P_k^\dagger\rangle_{Gauss}$ holds under our symmetry assumption. This suggests that we replace the non-number conserving operator $\bar{u_k} v_k P_k^\dagger$ by the number conserving operator $P_k^\dagger P_{k+M}$. We define operators

$$H_k = 2(1 - \epsilon - |v_k|^2)N_k - 4(P_k^\dagger P_{k+M} + h.c.), \tag{2.41}$$

$$N_k = n_k + n_{-k} + n_{k+M} + n_{-(k+M)}, \tag{2.42}$$

where $0 \leq |v_k|^2 \leq 1 - \epsilon \ \forall k$ for $\epsilon > 0$. Further, we introduce the notation $\alpha_k = v_k/\sqrt{1 - |v_k|^2}$, $\tilde{N} = \sum_{k=1}^M |v_k|^2$ and we denote by N the biggest integer fulfilling $\bar{N} - \tilde{N} \geq 0$. Then the following holds:

Theorem 2.23. *Let $M, \tilde{N} \in \mathbb{N}$ and let $1 \ll N < 2M$. If $1 > \epsilon \geq 18/\sqrt{\pi \bar{N}}$ the Hamiltonian $H(\{v_k\}) = \sum_{k=1}^M H_k$ is a pairing witness detecting*

$$|\Psi_{BCS,sym}^{(N)}\rangle = C_N \left(\sum_{k=1}^{M} \alpha_k (P_k^\dagger + P_{k+M}^\dagger) \right)^N |0\rangle.$$

The proof is given in Appendix B.

2.4.2 Eigenvalues of the two-particle reduced density matrix

In this Section we derive a basis independent condition for detecting pairing. The two-particle reduced density matrix $O^{(\rho)}$ contains all two-particle correlations. A change of basis, $a_i^\dagger \mapsto \sum_k U_{ik} a_k^\dagger$ leaves the spectrum of $O^{(\rho)}$ unchanged since

$$O^{(\rho)}_{(ij),(kl)} \to (U \otimes U)_{(ij),(mn)} O^{(\rho)}_{(mn),(pq)} (U \otimes U)^\dagger_{(pq),(kl)}.$$

Thus, we are lead to the following theorem:

Theorem 2.24. *Let ρ be an unpaired state, and let $O^{(\rho)}$ be its two-particle RDM. Then $\lambda_{max}(O^{(\rho)}) \leq 2$, where λ_{max} denotes the maximal eigenvalue.*

Proof. If ρ is unpaired, then there exists a separable state $\rho_s \in \mathcal{S}_{sep}$ having the same two-particle RDM. Any separable state is of the form $\rho_s = \sum_\alpha \mu_\alpha \rho^{(\alpha)}$, where $\rho^{(\alpha)} = |\psi^{(\alpha)}\rangle\langle\psi^{(\alpha)}|$, $|\psi^{(\alpha)}\rangle = \prod_i a^\dagger_{\alpha_i}|0\rangle$ and $\sum_\alpha \mu_\alpha = 1$. Here, $\{a^\dagger_{\alpha_i}\}_i$ denotes some basis of mode operators. The RDM is of the form $O^{(\rho)} = \sum_\alpha \mu_\alpha O^{(\alpha)}$, where $O^{(\alpha)}$ is the RDM for the state $\rho^{(\alpha)}$. The RDM is calculated in the basis $\{a_i^\dagger\}_i$, and the different bases are related by a unitary transformation $a_i^\dagger = \sum_j U^{(\alpha)}_{ik} a^\dagger_{\alpha_k}$, so that

$$O^{(\alpha)}_{(ij)(kl)} = \mathrm{tr}[\rho^{(\alpha)} a_i^\dagger a_j^\dagger a_l a_k] = (U^{(\alpha)} \otimes U^{(\alpha)})_{(ij)(mn)} O^{(\alpha,0)}_{(mn),(pq)} (U^{(\alpha)} \otimes U^{(\alpha)})^\dagger_{(pq)(kl)},$$

where $O^{(\alpha,0)}_{(mn),(pq)} = \langle a^\dagger_{\alpha_m} a^\dagger_{\alpha_n} a_{\alpha_q} a_{\alpha_p}\rangle_{\rho^{(\alpha)}}$. In the basis of the $\{a^\dagger_{\alpha_i}\}_i$ the expectation value $\langle a^\dagger_{\alpha_m} a^\dagger_{\alpha_n} a_{\alpha_q} a_{\alpha_p}\rangle_{\rho^{(\alpha)}}$ is of the simple form $\langle a^\dagger_{\alpha_i} a^\dagger_{\alpha_j} a_{\alpha_l} a_{\alpha_k}\rangle_{\rho^{(\alpha)}} = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}$. Hence, the spectrum of the $O^{(\alpha)}$ is given by $\underline{\mathrm{spec}(O^{(\alpha)})} = \{0, 2\}\ \forall\, \alpha$. The two-particle RDM is hermitian as $O^\dagger_{(ij)(kl)} = \bar{O}_{(kl)(ij)} = \overline{\langle a_k^\dagger a_l^\dagger a_j a_i\rangle} = \langle a_i^\dagger a_j^\dagger a_l a_k\rangle = O_{(ij)(kl)}$. Then Weyl's theorem [73] implies

$$\lambda_{max}\left(\sum_\alpha \mu_\alpha O^\alpha\right) \leq \sum_\alpha \mu_\alpha \lambda_{max}(O^\alpha) \leq \sum_\alpha 2\mu_\alpha \leq 2.$$

□

Example: An example of a state detected as paired via this criterion is the BCS-state (2.21) with $N = 2, M = 3$ and all α_k equal. The largest eigenvalue of its two-particle RDM is given by $\lambda_{max} = 8/3$.

2.4.3 Pairing measure for number conserving states

In Sec. 2.3.4 we have derived a pairing measure for Gaussian states. The correspondence with number conserving BCS states will be a guideline to derive a measure for number conserving states. The measure of Def. 2.18 involves expectation values of the form $\langle a_k^\dagger a_{-k}^\dagger\rangle$ that vanish for states with fixed particle number. Yet, Wick's theorem suggests that a quantity involving expectation values of the form $\langle P_k^\dagger P_l\rangle$ will lead to a pairing measure. This is indeed the case, which is the content of the following theorem:

Theorem 2.25. *Let ρ be a number conserving pure fermionic state. Then the following quantity defines a pairing measure:*

$$\mathcal{M}(\rho) = \max\left\{\max_{\{a_i^\dagger\}_i}\sum_{kl=1}^{M}|\langle P_k^\dagger P_l\rangle_\rho| - \frac{1}{2}\sum_k\langle n_k\rangle_\rho, 0\right\}, \tag{2.43}$$

where $P_k^\dagger = a_k^\dagger a_{-k}^\dagger$ and the maximum is taken over all possible bases of modes $\{a_i^\dagger\}_i$. For mixed states ρ, a measure can be defined via

$$\mathcal{M}(\rho) = \min\sum_i p_i\mathcal{M}(\rho_i), \tag{2.44}$$

where the minimum is taken over all possible decompositions of $\rho = \sum_i p_i\rho_i$ into pure states ρ_i.

Proof. The positivity of $\mathcal{M}$ and its invariance under passive transformations follow directly from the definition. It remains to show that $\mathcal{M}$ is zero for separable states. We need the following lemma:

Lemma 2.26. *Every pure separable state $\rho \in \mathcal{S}(\mathcal{A}_N)$ fulfills*

$$\sum_{kl=1}^{M}|\langle P_k^\dagger P_l\rangle_\rho| \leq N/2, \tag{2.45}$$

and this bound is tight.

Proof. Using Lemma 2.4, we obtain

$$\sum_{k,l=1}^{M}|\langle P_k^\dagger P_l\rangle| = \sum_{k,l=1}^{M}|P_{kl}P_{-k-l} - P_{k-l}P_{-kl}|, \tag{2.46}$$

where $P = P^2 = P^\dagger$ and $\mathrm{tr}[P] = N$. Using the triangle-inequality we get

$$\begin{aligned}\sum_{k,l=1}^{M}|\langle P_k^\dagger P_l\rangle| &\leq \frac{1}{2}\sum_{k,l}\left(|P_{kl}|^2 + |P_{-k-l}|^2 + |P_{k-l}|^2 + |P_{-kl}|^2\right)\\ &= \frac{1}{2}\mathrm{tr}[P^2] = N/2.\end{aligned}$$

In the last step we have used the property that the sum of the squares of a normal matrix is equal to the sum of squares of its eigenvalues. Taking the square root we obtain the bound of our claim.

The bound is tight, as $P = \mathbb{1}_{2_N}$ implies $\sum_{kl}|\langle P_k^\dagger P_l\rangle| = N/2$ which is obtained for $|\Phi\rangle = \prod_{i=1}^{N} a_i^\dagger|0\rangle$. □

Hence, any separable state of $2N$ particles fulfills $\sum_{kl}|\langle P_k^\dagger P_l\rangle| \leq N$, and this bound can always be achieved, which concludes the proof. □

Example: We close the Section by calculating the value of the pairing measure for two easy examples. Let

$$|\Psi_s\rangle = \bigotimes_{k=1}^{N} \frac{1}{\sqrt{2}} \left(P_k^\dagger + P_{-k}^\dagger \right) |0\rangle, \tag{2.47}$$

$$|\Psi_{BCS}^{(N,M)}\rangle = C_N \left(\sum_{k=1}^{M} P_k^\dagger \right)^N |0\rangle, \tag{2.48}$$

the tensor product of N spin-singlet states and the BCS state with equal weights, respectively. These states have a pairing measure $\mathcal{M}(|\Psi_s\rangle) = N$ resp. $\mathcal{M}(|\Psi_{BCS}^{(N,M)}\rangle = N(M-N)$. Thus, for the spin singlet the pairing measure has in addition the property that it is normalized to 1 and additive, while it is subadditive for $|\Psi_{BCS}^{(N,M)}\rangle$. Further, this example suggests that the pairing of $\mathcal{M}(|\Psi_{BCS}^{(N,M)}\rangle = N(M-N)$ is stronger than for $|\Psi_s\rangle$. We will see indeed in Subsec. 2.5.2 that states of the form $|\Psi_e\rangle$ allow interferometry at the Heisenberg limit.

2.5 Interferometry

The goal of quantum phase estimation is to determine an unknown parameter φ of a Hamiltonian $H_\varphi = \varphi H$ with the highest possible accuracy. The value of φ is inferred by measuring an observable O on a known input state that has evolved under H_φ. In a region where the function $\varphi \mapsto \langle O(\varphi)\rangle$ is bijective, φ can be inferred by inverting $\langle O(\varphi)\rangle$. In a realistic setup, however, $\langle O(\varphi)\rangle$ cannot be determined, as this would require an infinite number of measurements. Instead, one uses the mean value of the measurement results, o, as an estimate of $\langle O(\varphi)\rangle$. This will result in an error $\delta\varphi$ for the parameter to be estimated, as for a given value of φ we have $\langle O(\varphi)\rangle = o \pm \sqrt{\mathrm{Var}(o)}$. Linearizing around the real value of φ, it follows that the uncertainty of φ is given by [83, 84]

$$\langle (\delta\varphi)^2 \rangle = \frac{\mathrm{Var}(O)}{|\partial\langle O\rangle/\partial\varphi|^2}, \tag{2.49}$$

where $\mathrm{Var}(O) = \langle O^2\rangle - \langle O\rangle^2$, and we have used the fact that for many measurement $\mathrm{Var}(O) = \mathrm{Var}(o)$ holds. Further, it can be shown that the minimal uncertainty of φ is bounded by [85, 86]

$$\langle (\delta\varphi)^2 \rangle \mathrm{Var}(H) \geq \frac{1}{4\nu}, \tag{2.50}$$

where ν is the number times the estimation is repeated. Eq. (2.50) derives from the Cramér-Rao bound and is asymptotically achievable in the limit of large ν.

For a given measurement scheme, i.e. for a given input state and a given observable O, the uncertainty in φ can be reduced by using N identical input states and average over the N measurement outcomes. As the preparation of a quantum state is costly, a precision gain which has a strong dependence on N is highly desirable. If these

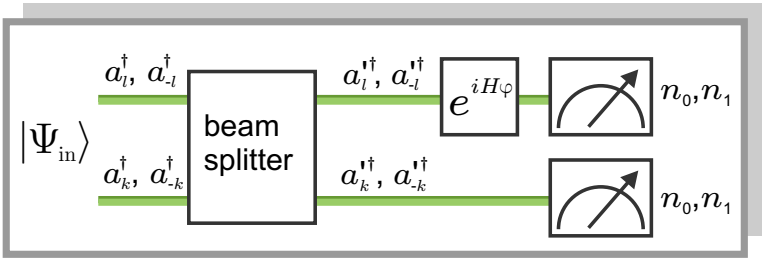

Figure 2.5: Scheme of the Ramsey interferometer setup. The incoming wave function $|\Psi_{\text{in}}\rangle$ enters a beam splitter. Then particles in the modes $a_{\pm l}^\dagger$ evolve under the Hamiltonian $H = H_N$ defined in Eq. 2.53. At the end a particle number measurement is performed on all particles.

probe states are independent of each other, the precision scales like $1/\sqrt{N}$. This is the so-called standard quantum limit (SQL). Using distinguishable or bosonic systems, this limit can be beaten by a factor of $\sqrt{N}$ by using number-squeezed input states [87, 88, 89, 90], N-particle NOON states or maximally entangled GHZ-states $\frac{1}{\sqrt{2}}(|N,0\rangle + |0,N\rangle)$ [84, 91, 92, 93]. Achieving this so-called Heisenberg-limit is the big goal of quantum metrology.

Less is known for fermionic states where number squeezing and coherent N-particle states are prohibited by statistics. Nevertheless, there exist fermionic N-particle state which can achieve the Heisenberg limit for phase measurements in a Mach-Zehnder interferometer setup [94]. Taking the existence of such states as a starting point, we show that paired fermionic states can be used as a resource for phase estimation beyond the SQL. We will consider two different settings. The first setting will be the standard Ramsey-interferometer setup of metrology, where the coupling Hamiltonian is proportional to the number operator. Here, we will see that paired states lead to a precision gain of a factor of 2 compared to separable states. The second setup involves a more complex coupling. Here it will turn out that by using paired states the Heisenberg limit, i.e. a phase sensitivity $(\delta\varphi)^2 \sim 1/N^2$, can be achieved.

2.5.1 Ramsey interferometry with fermions

General setup We consider the standard Ramsey interferometer setup Fig. 2.5 where a state in the modes $\{a_{k_j}^\dagger, a_{l_j}^\dagger\}_{j=-M}^{M}$ undergoes mode mixing at a beam splitter,

$$a_{\pm k_j}^\dagger \rightarrow a_{k_j}'^\dagger = \frac{1}{\sqrt{2}}(a_{\pm k_j}^\dagger + a_{\pm l_j}^\dagger), \tag{2.51}$$

$$a_{\pm l_j}^\dagger \rightarrow a_{\pm l_j}'^\dagger = \frac{1}{\sqrt{2}}(a_{\pm k_j}^\dagger - a_{\pm l_j}^\dagger), \tag{2.52}$$

before evolving under the action of the Hamiltonian

$$H_N = \sum_{j=1}^{M} (n_{l_j} + n_{-l_j}). \tag{2.53}$$

Finally, a particle number measurement is performed on the system, to compute the parity

$$\mathcal{P} = (-1)^{\sum_j n_0^{(j)} + n_1^{(j)}}, \tag{2.54}$$

where $n_0^{(j)} = a_{k_j}'^{\dagger} a'_{k_j}$ and $n_1^{(j)} = a_{-k_j}'^{\dagger} a'_{-k_j}$. According to Eq. (2.49), and using $\mathcal{P}^2 = 1$, the phase sensitivity is given by

$$(\delta\varphi)^2 = \frac{1 - \langle \mathcal{P} \rangle^2}{\left| \frac{\partial}{\partial \varphi} \langle \mathcal{P} \rangle \right|^2}. \tag{2.55}$$

We rewrite the parity operator in a form appropriate for calculations. Noting that the terms for different j commute, we write

$$\mathcal{P} = e^{i\pi \sum_j n_0^{(j)} + n_1^{(j)}} = \prod_j e^{i\pi (n_0^{(j)} + n_1^{(j)})} = \prod_j \sum_{m=0}^{\infty} \frac{(i\pi)^m}{m!} \left(n_0^{(j)} + n_1^{(j)} \right)^m.$$

For the evaluation of the sum we use that $n_{1,2}^2 = n_{1,2}$, so that for $m \geq 2$ we have

$$\begin{aligned} \left(n_0^{(j)} + n_1^{(j)} \right)^m &= \sum_{k=0}^{m} \left(\begin{array}{c} m \\ k \end{array} \right) \left(n_0^{(j)} \right)^k \left(n_1^{(j)} \right)^{m-k} \\ &= n_0^{(j)} + n_1^{(j)} + \sum_{k=0}^{m-1} \left(\begin{array}{c} m \\ k \end{array} \right) n_0^{(j)} n_1^{(j)}. \end{aligned}$$

Then

$$\sum_{m=0}^{\infty} \frac{(i\pi)^m}{m!} \left(n_0^{(j)} + n_1^{(j)} \right)^m =$$

$$1 + \sum_{m=1}^{\infty} \frac{(i\pi)^m}{m!} \left(n_0^{(j)} + n_1^{(j)} \right) + \sum_{m=2}^{\infty} \frac{(i\pi)^m}{m!} \sum_{k=1}^{m-1} \left(\begin{array}{c} m \\ k \end{array} \right) n_0^{(j)} n_1^{(j)} =$$

$$1 - 2 \left(n_0^{(j)} + n_1^{(j)} \right) + 4 n_0^{(j)} n_1^{(j)},$$

by evaluation of the sums. Thus,

$$\mathcal{P} = \prod_{j=1}^{M} \left(1 - 2(n_0^{(j)} + n_1^{(j)}) + 4 n_0^{(j)} n_1^{(j)} \right). \tag{2.56}$$

In the next Section we derive the best possible precision obtainable by using unpaired states, and compare this result to the precision achievable by using paired states. It will turn out that already at two-particle level paired states have more power than the unpaired states for our setup.

Bound on unpaired states for the standard interferometer We derive a lower bound on the phase sensitivity when using an unpaired state of $2N$ particles as input states:

Theorem 2.27. *For the Ramsey interferometer described above the phase sensitivity is bounded by*

$$(\delta\varphi)^2 \geq \frac{1}{2\nu N}, \tag{2.57}$$

when an unpaired state of $2N$ particles is used as input state.

Proof. We will use (2.50), $\langle(\delta\varphi)^2\rangle \mathrm{Var}(H) \geq 1/(4\nu)$, to derive the bound. Hence, we have to estimate an upper bound for the variance of the Hamiltonian H_N defined in (2.53). As H_N as well as H_N^2 contain operators from the set A_2 only, it is sufficient to proof the bound for product states, as for every unpaired state there exists a product state having the same expectations. In Lemma 2.4 we have shown that for pure separable states $\langle n_k n_l\rangle = |P_{kl}|^2 - P_{kk}P_{ll} + P_{kk}\delta_{kl}$, where $P \in \mathbb{C}^{4M\times 4M}$ is a projector of rank $2N$. We arrange the indices as $-l_M, \ldots, l_M, -k_M, \ldots, k_M$ and partition the projector P such that

$$P = \begin{pmatrix} A & B \\ B^\dagger & C \end{pmatrix}, \quad A, B, C \in \mathbb{C}^{2M\times 2M}.$$

As $P^2 = P$, we have $A - A^2 = BB^\dagger$, and the variance of the Hamiltonian H_N is given by

$$\mathrm{Var}(H_N) = \sum_{i=1}^{2M} A_{ii} - \sum_{i,j=1}^{2M} |A_{ij}|^2 = \mathrm{tr}[BB^\dagger], \tag{2.58}$$

as H_N only involves the modes $-l_M \ldots, l_M$. As $\mathrm{rank}(P) = 2N$, there exists some unitary U such that $P = U\mathrm{Id}_{2N}U^\dagger$, where

$$\mathrm{Id}_{2N} = \begin{pmatrix} \mathbb{1}_{2N} & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{C}^{4M\times 4M}.$$

Partitioning the unitary according to

$$U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}, \quad U_{ij} \in \mathbb{C}^{2M\times 2M} \text{ for } i, j = 1, 2,$$

the projector P is of the form

$$P = \begin{pmatrix} U_{11}\mathrm{Id}_{2N}U_{11}^\dagger & U_{11}\mathrm{Id}_{2N}U_{21}^\dagger \\ U_{21}\mathrm{Id}_{2N}U_{11}^\dagger & U_{21}\mathrm{Id}_{2N}U_{21}^\dagger \end{pmatrix}.$$

Using the the above representation of P and the cyclicity of the of the trace, we can write $\mathrm{Var}(H_N) = \mathrm{tr}[\tilde{A}\tilde{B}]$ with hermitian matrices $\tilde{A} = \mathrm{Id}_{2N}U_{11}^\dagger U_{11}\mathrm{Id}_{2N}$, $\tilde{B} = \mathrm{Id}_{2N}U_{21}^\dagger U_{21}\mathrm{Id}_{2N}$. The trace can be interpreted as a scalar product maximized for linearly dependent $\tilde{A}$ and $\tilde{B}$. Exploiting the unitarity of U, one sees immediately that the variance is maximized for $\tilde{A} = c/(1+c)\mathrm{Id}_{2N}$, $\tilde{B} = 1/(1+c)\mathrm{Id}_{2N}$ for some constant c. Hence,

$$\mathrm{Var}(H_N) \leq c/(1+c)^2\mathrm{tr}[\mathbb{1}_{2N}] \leq N/2.$$

Inserting this into Eq. (2.50), we find that $(\delta\varphi)^2 \geq \frac{1}{2\nu N}$. ∎

Interferometry with two particles In a first step we show that already a two-particle paired state can beat the bound for the phase sensitivity derived for unpaired states (2.57). Hence pairing manifests itself as useful quantum correlation already at the two-particle level. We show the following:

Theorem 2.28. *Using the paired state*

$$|\Psi_{\rm in}^{(2)}\rangle = \left(\sum_{j=1}^{M} \alpha_j a_{k_j}^\dagger a_{-k_j}^\dagger + \beta_j a_{l_j}^\dagger a_{-l_j}^\dagger\right)|0\rangle, \tag{2.59}$$

with normalization $\sum_j |\alpha_j|^2 + |\beta_j|^2 = 1$ *as input state for the Ramsey interferometer described above, we can achieve an optimal phase sensitivity given by*

$$(\delta\varphi)^2_{\rm min} = \frac{1}{2\left(1 + 2\sum_{j=1}^{M} {\rm Re}(\alpha_j \bar{\beta}_j)\right)} \geq \frac{1}{4}. \tag{2.60}$$

Proof. Take $|\Psi_{\rm in}^{(2)}\rangle$ as the input state. After an application of the beam splitter transformation (2.51) and an evolution under the Hamiltonian (2.53), the output state is of the form

$$\begin{aligned} |\Psi_{\rm out}^{(2)}\rangle &= \sum_{j=1}^{M} |\psi_j\rangle, \\ |\psi_j\rangle &= \left[q_j^{(+)}\left(a_{k_j}^\dagger a_{-k_j}^\dagger + e^{2i\varphi} a_{l_j}^\dagger a_{-l_j}^\dagger\right) + q_j^{(-)} e^{i\varphi}\left(a_{l_j}^\dagger a_{-k_j}^\dagger + a_{k_j}^\dagger a_{-l_j}^\dagger\right)\right]|0\rangle, \end{aligned}$$

where $q_j^{(\pm)} = (\alpha_j \pm \beta_j)/2$. For the calculation of the expectation value of the parity operator given in (2.56), we use that terms of the form $n_x^{(j)} n_{x'}^{(j')}$ where $x, x' = 0, 1$ give vanishing expectation value for the state $|\Psi_{\rm out}^{(2)}\rangle$ if $j \neq j'$. Hence, the expectation value of the parity operator simplifies to the calculation of

$$\langle \mathcal{P}\rangle = 1 + \sum_j \langle 4 n_0^{(j)} n_1^{(j)} - 2(n_0^{(j)} + n_1^{(j)})\rangle. \tag{2.61}$$

From Eq. (2.51) we see that we have to evaluate terms of the form

$$\begin{aligned} \langle n_0^{(j)} + n_1^{(j)}\rangle &= \frac{1}{2}\langle n_{k_j} + n_{l_j} + n_{-k_j} + n_{-l_j} + a_{k_j}^\dagger a_{l_j} + a_{l_j}^\dagger a_{k_j} + a_{-k_j}^\dagger a_{-l_j} + a_{-k_j}^\dagger a_{-l_j}\rangle \\ \langle n_0^{(j)} n_1^{(j)}\rangle &= \frac{1}{4}\langle (n_{k_j} + n_{l_j})(n_{-k_j} + n_{-l_j})\rangle + \frac{1}{4}\langle a_{k_j}^\dagger a_{-l_j}^\dagger a_{-k_j} a_{l_j} + h.c.\rangle \\ &+ \frac{1}{4}\langle a_{k_j}^\dagger a_{-k_j}^\dagger a_{-l_j} a_{l_j} + h.c.\rangle + \frac{1}{4}\langle (n_{k_j} + n_{l_j})(a_{-k_j}^\dagger a_{-l_j} + a_{-l_j}^\dagger a_{-k_j})\rangle \\ &+ \frac{1}{4}\langle (n_{-k_j} + n_{-l_j})(a_{k_j}^\dagger a_{l_j} + a_{l_j}^\dagger a_{k_j})\rangle. \end{aligned} \tag{2.62}$$

Since $(n_{k_j} + n_{l_j})|\psi_j\rangle = |\psi_j\rangle \ \ \forall j$, we obtain

$$\begin{aligned} \langle 4 n_0^{(j)} n_1^{(j)} - 2(n_0^{(j)} + n_1^{(j)})\rangle &= \langle a_{k_j}^\dagger a_{-k_j}^\dagger a_{-l_j} a_{l_j} + a_{k_j}^\dagger a_{-l_j}^\dagger a_{-k_j} a_{l_j} + h.c.\rangle \\ &+ \langle (n_{k_j} + n_{l_j})(n_{-k_j} + n_{-l_j})\rangle - \langle n_{k_j} + n_{-k_j} + n_{l_j} + n_{-l_j}\rangle \\ &= -4|q^{(+)}|^2 \sin^2\varphi \end{aligned} \tag{2.63}$$

by direct calculation. Thus, the expectation value of the parity operator is given by

$$\langle \mathcal{P} \rangle = 1 - \sin^2 \varphi \left(1 + 2 \sum_{j=1}^{M} \mathrm{Re}(\alpha_j \bar{\beta}_j) \right). \tag{2.64}$$

Using the formula for $(\delta\varphi)^2$, Eq. (2.55), we obtain (2.60).

The minimal bound of 1/4 can be obtained for a state where $\alpha_k = \beta_k \; \forall \; k$, since in this case the normalization constraint implies $2 \sum_j |\alpha_j|^2 = 1$. □

Thm. 2.28 shows that there exist two-particle paired states exceeding the bound on unpaired states given in (2.57). However, since for pure two-particle states pairing is equivalent to entanglement we will study next an example where the nature of pairing is clearly the reason for an improved phase sensitivity.

Interferometry with $2N$-particle BCS-states Generalizing this result, it follows immediately that states of the form $|\Psi_{\mathrm{in}}^{(2)}\rangle^{\otimes N}$, will lead to a phase sensitivity $(\delta\varphi)^2_{\mathrm{min}} = 1/\left[2N(1 + 2\sum_{j=1}^{M} \mathrm{Re}(\alpha_j \bar{\beta}_j))\right]$. In this Section we will show that the same result can be achieved using BCS-states.

Theorem 2.29. *Take the paired state*

$$|\Psi_{\mathrm{in}}^{(2N)}\rangle = c' \left(\sum_{j=1}^{M} \alpha_j a_{k_j}^\dagger a_{-k_j}^\dagger + \beta_j a_{l_j}^\dagger a_{-l_j}^\dagger \right)^N |0\rangle, \tag{2.65}$$

where we use the normalization condition $\sum_j |\alpha_j|^2 + |\beta_j|^2 = 1$ as the input state for the Ramsey type interferometer defined above. Then the optimal phase sensitivity is given by

$$(\delta\varphi)^2 = \frac{1}{2\bar{N}(1 + 2\sum_j \mathrm{Re}(\alpha_j \bar{\beta}_j))}. \tag{2.66}$$

Proof. As in previous Sections we will use the correspondence to the Gaussian state

$$\begin{aligned} |\Psi_{in,Gauss}^{(2\bar{N})}\rangle &= c \exp\left[\sum_{j=1}^{M} \alpha_j a_{k_j}^\dagger a_{-k_j}^\dagger + \beta_j a_{l_j}^\dagger a_{-l_j}^\dagger \right] |0\rangle \\ &= c \prod_j (1 + \alpha_j a_{k_j}^\dagger a_{-k_j}^\dagger)(1 + \beta_j a_{l_j}^\dagger a_{-l_j}^\dagger)|0\rangle \end{aligned}$$

where $|N - \bar{N}| \ll \bar{N}$ for the calculation. After the state has passed through the interferometer, it has transformed into the output state

$$\begin{aligned} &|\Psi_{out,Gauss}^{(2\bar{N})}\rangle = \\ &\prod_j \left[1 + q_j^{(+)}(a_{k_j}^\dagger a_{-k_j}^\dagger + a_{l_j}^\dagger a_{-l_j}^\dagger) + q_j^{(-)}(a_{l_j}^\dagger a_{-k_j}^\dagger + a_{k_j}^\dagger a_{-l_j}^\dagger) + \alpha_j \beta_j a_{k_j}^\dagger a_{-k_j}^\dagger a_{l_j}^\dagger a_{-l_j}^\dagger \right] |0\rangle. \end{aligned}$$

Since $|\Psi^{(2\bar{N})}_{out,Gauss}\rangle$ is a product of terms with support in disjoint subspaces of modes $\pm k_j, \pm l_j$, we can evaluate each factor $1 - 2(n_0^{(j)} + n_1^{(j)}) + 4n_0^{(j)}n_1^{(j)}$ of the parity operators $\mathcal{P}$ (2.56) independently. Making use of (2.62) and the fact that

$$\langle (n_{k_j} + n_{l_j})(a^\dagger_{-k_j}a_{-l_j} + a^\dagger_{-l_j}a_{-k_j})\rangle = \langle a^\dagger_{-k_j}a_{-l_j} + a^\dagger_{-l_j}a_{-k_j}\rangle$$

the expectation value of the parity operator is readily computed to be

$$\langle \mathcal{P}\rangle_{Gauss} = \prod_j (1 - |c|^2|\alpha_j + \beta_j|^2 \sin^2\varphi).$$

We expand the last expression for small values in φ and obtain

$$\langle \mathcal{P}\rangle = 1 - \varphi^2|c|^2 \sum_j |\alpha_j + \beta_j|^2.$$

As only number operators are involved, $\langle \mathcal{P}\rangle_{Gauss} \approx \langle \mathcal{P}\rangle_N$, where $\langle \ldots\rangle_N$ denotes the expectation value of $\mathcal{P}$ for the state $|\Psi^{(2N)}_{\text{in}}\rangle$. With the help of (2.49) we obtain

$$(\delta\varphi)^2 = \frac{1}{2|c|^2 \sum_j |\alpha_j + \beta_j|^2.}$$

Using $\bar{N} = |c|^2 \sum_k |\alpha_k|^2 + |\beta_k|^2 = |c|^2$, one arrives at (2.66). The minimal value $(\delta\varphi)^2 = 1/(4N)$ is obtained when $\alpha_j = \beta_j \; \forall\, j$. □

The above result shows that the use of paired states results in a precision gain of up to a factor of 2 compared to the best precision obtainable for unpaired states (2.57).

Relation to the pairing measure The pairing measure derived in Sec. 2.3.4 and 2.4.3 quantifies the precision gain obtainable by the use of paired states. To see this, denote by $|\Psi^{(2\bar{N})\prime}_{in,Gauss}\rangle$ the state after the beam splitter transformation. Then the value of the pairing measure defined in Def. 2.18, $\mathcal{M}_G(\rho) = \sum_{kl} |\langle a_k a_l\rangle|^2$, for this state is given by

$$\mathcal{M}_G\left(|\Psi^{(2\bar{N})\prime}_{in,Gauss}\rangle\right) = \frac{N^2}{2}\left(1 + 2\sum_j \mathrm{Re}(\alpha_j\bar{\beta}_j)\right).$$

Comparison with Eq. (2.66) leads to the observation

$$(\delta\varphi)^2 = \frac{\bar{N}}{4\mathcal{M}_G\left(|\Psi^{(2\bar{N})\prime}_{in,Gauss}\rangle\right)}. \tag{2.67}$$

The above relation demonstrates that $\mathcal{M}_G$ is indeed quantifying a useful resource present in paired states. Whether this interpretation can be extended to mixed states will not be explored here.

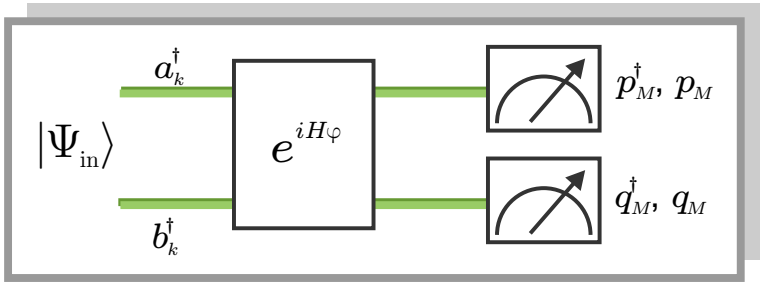

Figure 2.6: Setup which allows interferometry with paired states at the Heisenberg limit. Particles in modes $a_k^\dagger$ and $b_k^\dagger$ evolve under the complex coupling Hamiltonian H (for the detailed form of H refer to the text). In the end particle numbers are measured.

2.5.2 Interferometry involving a pair-interaction Hamiltonian

So far we have seen that paired states lead to a gain of a factor of 2 in precision compared to unpaired states in a Ramsey-type interferometer. This Section will show that paired states are even more powerful and can lead to a precision gain of a factor of N when measuring the phase of a pair-interaction Hamiltonian.

We consider a setup where two fermionic states enter the ports A and B of an interferometer. The particles entering port A can occupy the modes $\{a_k^\dagger\}_{k=-M}^{M}$, while the particles entering through port B can occupy the modes $\{b_k^\dagger\}_{k=-M}^{M}$. Then the two states evolve under the Hamiltonian $H_c = H_\infty, H_F$ defined in (2.78) resp. (2.81) and a particle number measurement is performed at the end. The situation is depicted in Fig 2.6. We will compare the power of paired states over unpaired ones for two different settings. We start by introducing some basic notation:

Prerequisites We define pair operators $P_k^\dagger = a_k^\dagger a_{-k}^\dagger$ and $Q_k^\dagger = b_k^\dagger b_{-k}^\dagger$ and their equally weighted superpositions

$$p_M^\dagger = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} P_k^\dagger, \quad q_M^\dagger = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} Q_k^\dagger. \tag{2.68}$$

The operators $p_M^\dagger$ and $q_M^\dagger$ fulfill the commutation relations

$$[p_M^\dagger, p_M] = -1 + \frac{1}{M}\hat{N}_a \tag{2.69}$$

$$[q_M^\dagger, q_M] = -1 + \frac{1}{M}\hat{N}_b, \tag{2.70}$$

where $n_k = a_k^\dagger a_k$ so that $N_a = \sum_k (n_k + n_{-k})$, and $N_b = \sum_k (m_k + m_{-k})$ with $n_k = a_k^\dagger a_k$ and $m_k = b_k^\dagger b_k$ being the number operators for particles in modes $a_k^\dagger$ and $b_k^\dagger$ respectively.

We compare the power of two paired states and two unpaired states entering through port A and B. The bound for unpaired states will be derived again via (2.50). Due to the structure of the input states, $\langle H_c\rangle$ and $\langle H_c^2\rangle$ are expectation values of operators from A_2, it is sufficient to compare the power of paired states to those of separable states. As paired states we take products of BCS-states in modes a and b,

$$|\Psi_N^{(M)}\rangle \;=\; |N\rangle_a^{(M)}|N\rangle_b^{(M)}, \tag{2.71}$$

where $|N\rangle_a^{(M)} = c_N^{(M)}(p_M^\dagger)^N|0\rangle$ and $|N\rangle_b^{(M)} = c_N^{(M)}(q_M^\dagger)^N|0\rangle$ with normalization constant $c_N^{(M)} = (NM!/M^N)^{-\frac{1}{2}}$. The separable input state states are of the form

$$|\Phi_N\rangle = |\phi^{(2N)}\rangle_a|\phi^{(2N)}\rangle_b, \tag{2.72}$$

where $|\phi^{(2N)}\rangle_{a,b}$ are separable states in the modes $a_k^\dagger$ and $b_k^\dagger$ respectively.

After the input state has evolved under the Hamiltonian $H_c\varphi$ into the state $|\Psi_N^{(M)}(\varphi)\rangle = e^{iH_c\varphi}|\Psi_N^{(M)}\rangle$ an observable O is used as an estimator to determine the parameter φ to a precision given by (2.49). Instead of working in the Schrödinger picture of state evolution it turns out to be more convenient to tackle the problem in the Heisenberg picture. There O evolves according to

$$O \to O' = e^{-iH_c\varphi}Oe^{iH_c\varphi} \equiv O(\varphi).$$

We are interested in the phase sensitivity for small φ, so that we can expand (2.49) in powers of φ. First, an expansion of the observable O leads to

$$O(\varphi) = O - i\varphi[H_c, O] - \frac{1}{2}\varphi^2(H_c^2O + OH_c^2 - 2H_cOH_c) + \mathcal{O}(\varphi^3). \tag{2.73}$$

Next, if the input state $|\Psi_N^{(M)}\rangle$ is an eigenvector of O with eigenvalue 0, we obtain the following simple expressions for $\langle O\rangle$ and $\mathrm{Var}(O)$:

$$\left|\frac{\partial}{\partial\varphi}\langle O\rangle\right|^2 \;=\; 4\varphi^2|\langle H_cOH_c\rangle|^2 + \mathcal{O}(\varphi^3), \tag{2.74}$$

$$\mathrm{Var}(O) \;=\; \varphi^2\langle H_cO^2H_c\rangle + \mathcal{O}(\varphi^3). \tag{2.75}$$

In this case the phase fluctuation $(\delta\varphi)^2$ simplifies to

$$(\delta\varphi)^2 = \frac{\langle H_cO^2H_c\rangle}{4|\langle H_cOH_c\rangle|^2} + \mathcal{O}(\varphi). \tag{2.76}$$

An observable fulfilling this property is

$$O = \left(\frac{1}{2}(p_M^\dagger p_M - q_M^\dagger q_M)\right)^2 \equiv \left(J_z^{(M)}\right)^2. \tag{2.77}$$

The commutation relations for $p_M^\dagger$ and $q_M^\dagger$ (2.69) imply that in the limit of infinitely many modes, $M \to \infty$, the operators $p_M^\dagger$ and $q_M^\dagger$ become bosonic. We start out with a scenario where the input states are in the bosonic limit and then turn our attention to a setting where the fermionic nature is apparent.

2.5.2.1 Bosonic limit

In this Section we consider the scenario $M \to \infty$, i.e. we are in the limit where the fermionic particles exhibit bosonic commutation relations. The limit is understood for the expectation values of the operators. We consider a coupling of the form $H_c = \varphi H_\infty$ where

$$H_\infty = \frac{1}{2}(p_\infty^\dagger q_\infty + q_\infty^\dagger p_\infty), \tag{2.78}$$

and measure $(J_\infty^{(z)})^2$.

Bound on unpaired states We start deriving the best precision for unpaired states using (2.50). For the calculation we use a finite M for input state, coupling Hamiltonian and measurement and then take the limit $M \to \infty$, i.e. we take $H_M = \frac{1}{2}(p_M^\dagger q_M + q_M^\dagger p_M)$ and $(J_z^{(M)})^2$ defined in (2.77). Then

$$\lim_{M\to\infty} \langle \phi_{a,b} | H_M | \phi_{a,b} \rangle = 0$$

due to the conservation of particle number. Hence,

$$\lim_{M\to\infty} \mathrm{Var}(H_M) = \lim_{M\to\infty} \langle H_M^2 \rangle = \lim_{M\to\infty} (\langle p_M^\dagger p_M \rangle + \langle q_M^\dagger q_M \rangle)^2 = 0,$$

as $\langle p_M^\dagger p_M \rangle = \frac{1}{M} \sum_{kl} |\langle P_k^\dagger P_l \rangle|^2 \leq N/M$. The last inequality results from the bound of the pairing measure on unpaired states Thm. 2.25. The same holds for $\langle q_M^\dagger q_M \rangle$. Thus, in the limit $M \to \infty$ the variance of H_∞ vanishes. This implies that unpaired states are of no use at all for a phase estimation in this setting, since $(\delta\varphi)^2 \to \infty$.

Phase estimation using paired states Now we use the paired input state defined in (2.71) as the input state for the interferometer. We can prove the following:

Theorem 2.30. *For suitable paired input states, the interferometer depicted in Fig 2.6, where $H = H_\infty$ is defined in Eq.* (2.78)*, allows to estimate the coupling parameter φ to a precision*

$$(\delta\varphi)^2_{\mathrm{inf}} = \frac{1}{2N^2}. \tag{2.79}$$

Proof. Consider the interferometric setup depicted in Fig. 2.6, where the $2N$-particle input state and the coupling Hamiltonian are defined in Eqs. (2.71) and (2.78) respectively. We will again use a finite M for input state, coupling Hamiltonian and measurement and then take the limit $M \to \infty$, i.e. we use $|\Psi_{\mathrm{in}}\rangle = |N\rangle_a^{(M)} |N\rangle_b^{(M)}$, $H_M = \frac{1}{2}(p_M^\dagger q_M + p_M^\dagger q_M)$ and $(J_z^{(M)})^2$. In Appendix C.1 we show that

$$\begin{aligned} \langle H_M (J_z^{(M)})^2 H_M \rangle &= \frac{1}{8} \alpha_N^2 \alpha_{N+1}^2 (\alpha_{N+1}^2 - \alpha_{N-1}^2)^2, \\ \langle H_M (J_z^{(M)})^4 H_M \rangle &= \frac{1}{32} \alpha_N^2 \alpha_{N+1}^2 (\alpha_{N+1}^2 - \alpha_{N-1}^2)^4, \end{aligned} \tag{2.80}$$

where $\alpha_N = \sqrt{N\left(1-\frac{N-1}{M}\right)}$. Thus using (2.76), we obtain

$$(\delta\varphi)^2_M = \frac{1}{2\alpha^2_{N+1}\alpha^2_N} + \mathcal{O}(\varphi).$$

Taking the limit $M \to \infty$ leads to the result of the theorem. □

2.5.2.2 Interferometry far from the bosonic limit

In the preceding Section we have studied the power of paired states in the bosonic limit. The power of bosonic particles for interferometry has been known for quite a while. Hence, the use of paired states where the fermionic nature of the particles survives might be a more interesting question. In this Section we show that even far from the bosonic limit paired states can achieve a precision gain of order N for quantum metrology. To this end we consider a coupling Hamiltonian of the form $H_c = \varphi H_F$ where

$$H_F = \sum_{k=1}^{\infty} P_k^\dagger Q_k + P_k Q_k^\dagger. \tag{2.81}$$

Bound on product states First, we give a bound for the phase sensitivity achievable by using product states at the input:

Theorem 2.31. *Using product states of $2N$ particles as input states for the interferometric setting depicted in Fig. 2.6, the phase φ of the coupling Hamiltonian $H_c = \varphi H_F$, where H_F is defined in Eq.* (2.81)*, can not be measured to a precision better than $(\delta\varphi)^2 \geq 1/(16N)$.*

Proof. For every product state of the form (2.72) we have $\langle H_F\rangle = 0$ due to particle number conservation. Hence, $\mathrm{Var}(H_F) = \langle H_F^2\rangle$. We will bound this expectation value:

$$\begin{aligned}\langle H_F^2\rangle &= \sum_{k\neq l}\langle P_k^\dagger P_l\rangle\langle Q_l^\dagger Q_k\rangle + c.c. + \sum_k \langle P_k^\dagger P_k\rangle\langle Q_k Q_k^\dagger\rangle \\ &\leq 2\left(\sum_{k\neq l}|\langle P_k^\dagger P_l\rangle|^2\right)^{1/2}\left(\sum_{k\neq l}|\langle Q_k^\dagger Q_l\rangle|^2\right)^{1/2} + \sum_k \langle P_k^\dagger P_k\rangle\langle Q_k Q_k^\dagger\rangle + c.c.\,.\end{aligned}$$

From Lemma 2.26 we know that $\left(\sum_{k\neq l}|\langle P_k^\dagger P_l\rangle|^2\right)^{1/2} \leq \sqrt{N}$. Further,

$$\begin{aligned}\langle P_k P_k^\dagger\rangle &= \langle 1-(n_k-n_{-k})^2 - n_k n_{-k}\rangle \leq 1, \\ \sum_k \langle P_k^\dagger P_k\rangle &\leq N.\end{aligned}$$

Thus, $\mathrm{Var}(H_F) \leq 2\sqrt{N}\sqrt{N} + 2N = 4N$ which leads immediately to our result via (2.50). □

The power of paired states We show next that the bound derived on product states can be beaten by a factor of $\sqrt{N}$ using paired states.

Theorem 2.32. *Using paired states of the form* (2.71) *as input states for the interferometric setting depicted in fig. 2.6, the phase φ of the coupling Hamiltonian $H_c = \varphi H_F$, with H_F as in* (2.81) *can be measured to a precision*

$$(\delta\varphi)^2 = \frac{M(M-1)}{8N(M-N)(M-1+MN-N^2)}. \tag{2.82}$$

For the proof see Appendix C.2. This theorem implies $(\delta\varphi)^2 \sim 1/N^2$ for all $M \geq 2N$.

Concluding remarks In conclusion we have shown that paired states are a resource for quantum metrology. Theorem 2.32 is the main result of this Section. We have remarked already at the beginning of this Chapter that it has been proven before that the Heisenberg limit can be achieved using fermionic particles [94]. However, these states were constructed in an abstract way, while we prove that the BCS-states that can be created easily in an experimental setup are a very powerful resource for quantum metrology.

2.6 Application to experiments and conclusion

In summary, we have developed a pairing theory for fermionic states. We have given a precise definition of pairing based on a minimal list of natural requirements. We have seen that pairing is neither equivalent to entanglement of the whole state nor of its two-particle reduced density operator but represents a different kind of quantum correlation. Within the framework of fermionic Gaussian states we could give a complete solution of the pairing problem. For number conserving states we have given sufficient conditions for the detection of pairing that can be verified by current experimental techniques, e.g. via spatial noise correlations [95, 96, 97], and prescribed a systematic way to construct complete families of pairing witnesses.

Another important point of our work is the utility of fermionic states for quantum metrology. While it has been shown that fermionic states can in principle achieve the Heisenberg limit for precision measurements in a Ramsey-type interferometer [94], we could prove the usefulness of states that are available in the laboratory. Furthermore, the resource leading to the improved phase sensitivity is the pairing according to our definition and not the entanglement according to any of the existing concepts. This observation gives hope that pairing of fermions will turn out as a useful resource for different sorts of quantum information applications in the future. In addition, the optimal precision for the Ramsey-type setup is proportional to the pairing measure introduced from an intuitive picture in Secs. 2.3.4 and 2.4. This endows the measure with an operational meaning.

Unfortunately, one of our initial motivations of giving a characterization of pairing, the pairing debate [28, 29, 30, 31], could not be resolved so far. To do so we need

access to the proportionality factor linking the quantity plotted in Fig. 4 of [28] to the local pair correlation correlation function $G_2(r,r) = \langle \Psi_\downarrow^\dagger(r)\Psi_\uparrow^\dagger(r)\Psi_\uparrow(r)\Psi_\downarrow(r)\rangle$.

The results we have presented are just a first step in understanding pairing and its relation to other types of quantum correlations. We hope that the pairing theory we have developed will help to get a better understanding of correlated many-body systems and provide a new perspective on quantum correlations, and may in addition serve as a starting point for further inquiries. For instance, the pairing theory developed so far has some formal analogies to the theory of generalized entanglement [98, 99]. Furthermore, another possibility is to look for a finer characterization of pairing. For example, $\sum_{k=1}^{2} P_k^\dagger|0\rangle$ and $\sum_{k=1}^{M} P_k^\dagger|0\rangle$ represent paired states of rather different nature. Thus, the development of witnesses or measures which allow to determine over how many modes the pairs in a given states extend is an interesting question. Further, one could think of relating these differences to applications in metrology or elsewhere. Next, the role of higher order correlations could be explored. The set of unpaired states contains both separable and highly correlated states. This is, for example, reflected in the fact that there are unpaired states which can be transformed to paired ones by single-mode particle number measurements. For example, the unpaired state $(a_1^\dagger a_2^\dagger a_3^\dagger + a_4^\dagger a_5^\dagger a_6^\dagger)|0\rangle$ can be transformed into a paired state by measuring particle number in mode $b = a_3 + a_6$. A theory of higher-order correlated states could be developed along the lines discussed here: Define e.g. the nth-order correlated those states whose expectation values on nth-order observables cannot be reproduced by $m < n$-correlated states.

Up to now we have concentrated on fermionic states. But the question of pairing in bosonic systems might be equally interesting and relevant for recent experiments [100]. While our theoretical framework can be directly applied to the bosonic case, the criteria for its detecting have to be adapted since bosons obey canonical *commutation* relations. Moreover, so far we have considered finitely many modes only, and it is an obvious question whether generalizing to an infinite dimensional single-particle space gives rise to new phenomena.

Tools and methods from entanglement theory have been very useful in analyzing pairing. One very important such tool, however, is missing: Positive maps. These are transformations which do not correspond to a physical operations but nevertheless, when applied to a subsystem in a separable state with the rest, map density operators to (unnormalized) density operators and thus provide strong necessary conditions for separability. The most prominent case in the qubit case is the partial transpose of a subsystem, that leads even to a necessary and sufficient condition in the case of two qubits [101, 102]. Finding an analogy might prove very useful for the analysis of many-body correlations. Another important object in the theory of entanglement is the set of LOCC operations (local operations and classical communication), i.e., the operations that cannot create entanglement. In the case of pairing, the analogous set would contain passive operations and discarding modes, as seen above, while measurements do not belong to this set. Are there other physical transformations that cannot create pairing? Do paired states, then, possibly allow to implement such transformations similar to entanglement enabling non-LOCC operations?

Chapter 3

Quantum Simulations in Translationally Invariant Systems

In the last Chapter we have applied concepts and methods from quantum information theory to gain further insight into the quantum correlations of fermionic systems. From now on we focus on the possibility to obtain information on quantum mechanical systems, especially fermions, using simulation techniques and approximation methods. Our goal is to approximate the ground and thermal states, as well as the dynamical properties of the system.

The simulation of the time evolution of quantum mechanical many-body systems is a daunting task, as the underlying Hilbert space grows exponentially with the number of particles. This observation lead Feynman already in 1982 to the following question [33]: Can physics be simulated by a universal computer?. The universal computer he had in mind should be composed out of elements that are locally interconnected, as it is the case, e.g. for a cellular automaton. He noticed that quantum mechanical systems are much more appropriate than classical ones to achieve this task:

"Trying to find a computer simulation of physics, seems to me to be an excellent program to follow out...And I'm not happy with all the analyses that go with just the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem because it doesn't look so easy."[33]

Following these lines, Llyod could prove in his pioneering work of 1996 [34] that Feynman's hypothesis was correct: Quantum computers can indeed be used to simulate any local quantum system, and we can efficiently simulate quantum mechanical time evolutions—provided that we have sufficient coherent control on the system [103]. In this direction enormous progress has been made during the last years, in particular in systems of optical lattices [104] and ion traps [105, 106, 107, 108]. Moreover, it was realized that quantum simulators [109] are much less demanding than quantum computers and, in fact, pioneering experiments simulating quantum phase transitions in systems of cold atomic gases [104] have already turned some of the vision [110] into reality.

One of the fundamental questions in the field of quantum simulations is the fol-

lowing: Given a set of interactions we can engineer with a particular system, which are the Hamiltonians that can be simulated? Concerning *gates*, i.e., discrete time unitary evolutions, it has been shown in the early days of quantum information theory that almost any two-qubit gate is *universal* [111, 112]. Similarly, any fixed entangling two-body interaction was shown to be capable of simulating any other two-body Hamiltonian when supplemented by the set of all local unitaries [113, 114]. The many-body analogue of this problem was solved in [115, 116] and the efficiency of quantum simulations was studied in various contexts (cf. [117, 118, 119, 120]).

All these schemes are based on the addressing of sites, i.e., local control. Imagine now that we have a chain in which we cannot address each particle individually but only apply global single-particle and nearest-neighbor interactions. Can we simulate the evolution of a next-to-nearest neighbor interaction Hamiltonian, or obtain some long-range (e.g., dipole) coupling, or even a three-particle interaction Hamiltonian?

In our work we will concentrate on the case in which the interactions at hand are short range and *translationally invariant* as it is approximately the case in different experimental set-ups, like in the case of atoms in optical lattices or in many other systems that naturally appear in the context of condensed matter and statistical physics. In order to make the problem mathematically tractable and to exploit its symmetries we will consider periodic boundary conditions, even though typically physical systems have open ones. In this sense, our results may not be directly applicable to certain physical situations. In any case, we expect that our work will be a step forward to the establishment of what can and cannot be simulated with certain quantum systems, namely spins, fermions and bosons.

This Chapter is organized as follows: In Sec. 3.1 we give a concise statement of the problem as well as an introduction in the techniques of quantum simulation. Next, we give some preliminaries on quadratic Hamiltonians in Sec. 3.2. Sec. 3.3 will then treat fermionic and Sec. 3.4 bosonic systems. Both start with the one-dimensional case which is then generalized to arbitrary dimensional cubic lattices. Finally spin systems are addressed in Sec. 3.5.

3.1 Statement of the problem

Consider a cubic lattice of N sites with periodic boundary conditions in arbitrary spatial dimension. Assume that we can implement every Hamiltonian from a given set $\mathcal{S} = \{\mathcal{H}_1, \mathcal{H}_2, \ldots\}$ of translationally invariant Hamiltonians and in this way achieve every unitary time evolution of the form $e^{i\mathcal{H}_j t}$ for arbitrary $t \in \mathbb{R}$. Note that this assumes that both $\pm\mathcal{H}_j$ are available. The question we are going to address is the following: Which evolutions can be simulated by concatenating evolutions generated by the elements of $\mathcal{S}$?. Our main interest lies in sets which contain all on-site Hamiltonians and specific nearest-neighbor interactions. The situation is depicted in Fig. 3.1.

The natural language for tackling this problem is the one of Lie algebras [121, 122] since the set of reachable interactions is given by the Lie algebra $\mathcal{L}$ generated by the

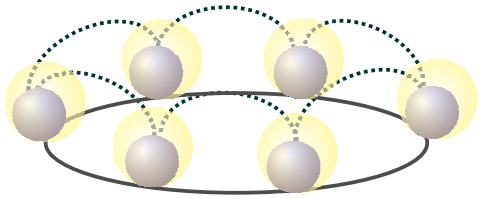

Figure 3.1: One-dimensional translationally invariant lattice with periodic boundary conditions. On-site interaction (yellow dots) and nearest-neighbor interactions (dashed lines) are implemented in a translationally invariant way.

set $i\mathcal{S}$. This follows from the *Lie -Trotter formulae* [123, 124]

$$\begin{aligned} e^{\alpha L_k+\beta L_l} &= \lim_{n\to\infty}\left(e^{\alpha L_k/n}e^{\beta L_l/n}\right)^n, \quad \alpha,\beta\in\mathbb{R}, \\ e^{[L_k,L_l]} &= \lim_{n\to\infty}\left(e^{L_k/\sqrt{n}}e^{L_l/\sqrt{n}}e^{-L_k/\sqrt{n}}e^{-L_l/\sqrt{n}}\right)^n, \end{aligned}$$

where L_k is a representation of the generator $i\mathcal{H}_k$. When applying the Lie-Trotter formulae to the elements of $i\mathcal{S}$ we can obtain all commutators and real linear combinations of its elements, i.e., we end up with the Lie algebra generated by $\mathcal{S}$. Conversely, it follows from the Baker-Campbell-Haussdorff formula [125, 126, 127] that all simulatable interactions can be written in this way. We will study the cases of D-dimensional 'spin' systems ($\mathcal{L}\subset su_{D^N}$) as well as quadratic Hamiltonians in fermionic ($\mathcal{L}\subset so_{2N}$) and bosonic ($\mathcal{L}\subset sp_{2N}$) operators. Whereas in the case of quadratic bosonic and fermionic Hamiltonians a rather exhaustive characterization of simulatable time evolutions is possible, a full characterization of simulatable spins systems still remains an open problem.

3.2 Quadratic Hamiltonians

This Section will introduce the basic notions and the notation used in Secs. 3.3, 3.4. The presentation is a collection of tools widely used in the literature on translationally invariant quasi-free fermionic [128, 129, 70, 130] and bosonic [131, 132] systems. We consider a system of N fermionic or bosonic modes characterized by a quadratic Hamiltonian

$$\mathcal{H}=\sum_{k,l=1}^{N} A_{kl}a_k a_l + B_{kl}a_k a_l^\dagger + C_{kl}a_k^\dagger a_l + D_{kl}a_k^\dagger a_l^\dagger. \tag{3.1}$$

Here, $a_k^\dagger$ and a_k are creation and annihilation operators satisfying the canonical (anti)-commutation relations

$$\text{CAR: } \{a_k,a_l\} = 0, \quad \{a_k,a_l^\dagger\}=\delta_{kl} \text{ (fermions)}, \tag{3.2}$$

$$\text{CCR: } [a_k,a_l] = 0, \quad [a_k,a_l^\dagger]=\delta_{kl} \text{ (bosons)}. \tag{3.3}$$

By defining a vector $\alpha = (a_1, \ldots, a_N, a_1^\dagger, \ldots a_N^\dagger)$ and a *Hamiltonian matrix*

$$\tilde{H} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{3.4}$$

Eq.(3.1) can be written in the compact form $\mathcal{H} = \alpha \tilde{H} \alpha^T$. The Hermiticity of $\mathcal{H}$ implies the relations

$$B = B^\dagger,\ C = C^\dagger\ , A = D^\dagger. \tag{3.5}$$

We will identify Hamiltonians which differ by multiples of the identity as they give rise to undistinguishable time evolutions. The commutation relations can then be exploited to symmetrize the Hamiltonian matrix $\tilde{H}$ such that

$$A = \tau A^T, D = \tau D^T, B = \tau C^T, \tag{3.6}$$

where $\tau = 1$ for bosons and $\tau = -1$ in the case of fermions. Instead of working with $2N$ creation and annihilation operators it is often convenient to introduce $2N$ hermitian operators c_k via

$$c_k = (a_k^\dagger + a_k)/\sqrt{2},\ \ c_{k+N} = i(a_k^\dagger - a_k)/\sqrt{2}. \tag{3.7}$$

In the case of fermions these are the Majorana operators obeying the anti-commutation relation

$$\{c_k, c_l\} = \delta_{kl}. \tag{3.8}$$

For bosons the c_k are the position and c_{k+N} momentum operators, and the commutation relations can be expressed in terms of the symplectic matrix σ via

$$[c_k, c_l] = i\sigma_{kl},\ \ \sigma = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix},\ \ \mathbb{1} \in \mathbb{R}^{N\times N}. \tag{3.9}$$

Eq. (3.1) can now be written in the form

$$\mathcal{H} = \frac{\sqrt{\tau}}{2} \sum_{k,l} H_{kl} c_k c_l, \quad H = \begin{pmatrix} X & W \\ \tau W^T & Y \end{pmatrix}. \tag{3.10}$$

Exploiting again the commutation relations we can choose the Hamiltonian matrix H real and (anti-) symmetric with $H = \tau H^T$. The Hamiltonian matrices of the two representations are related via

$$\tilde{H} = \frac{\sqrt{\tau}}{4} \begin{pmatrix} X - Y - i(W + \tau W^T) & X + Y + i(W - \tau W^T) \\ X + Y - i(W - \tau W^T) & X - Y + i(W + \tau W^T) \end{pmatrix}.$$

Time evolution

We are interested in time evolutions generated by quadratic Hamiltonians of the form in Eq. (3.1). These are canonical transformations which preserve the (anti-) commutation relations and act (in the Heisenberg picture) linearly on the c_k's:

$$e^{i\mathcal{H}t} c_k e^{-i\mathcal{H}t} = \sum_{l=1}^{N} T_{lk} c_l\ . \tag{3.11}$$

In the fermionic case the CAR are preserved iff $T \in O(2N)$ is an element of the orthogonal group in $2N$ dimensions. This group has two components corresponding to elements with determinant ± 1. As time evolution has to be in the part connected to the identity (for $t = 0$) we have that $T \in SO(2N)$ is an element of the special orthogonal group. For bosons the preservation of the commutation relations implies that T is a symplectic matrix, i.e. $T\sigma T^T = \sigma$. Both groups $SO(2N)$ and $Sp(2N)$ are Lie groups and we can express T in terms of the exponential map acting on the respective Lie algebra, i.e., $T = e^{tL}$. We use the infinitesimal version of Eq. (3.11) to derive a simple relation between the generator L and the Hamiltonian matrix H. We make use of the Baker-Campbell-Hausdorff formula

$$e^{iA}Be^{-iA} = \sum_{m=0}^{\infty} \frac{1}{m!}[A, B]_m, \tag{3.12}$$

where $[A, B]_m = [A, [A, B]_{m-1}]$ and $[A, B]_0 \equiv B$, and expand to first order in Δt. For fermions, this leads to

$$e^{i\mathcal{H}\Delta t}c_k e^{-i\mathcal{H}\Delta t} = c_k - \Delta t \sum_{k,l} H_{lk}c_l + \mathcal{O}\left((\Delta t)^2\right) \tag{3.13}$$

while for bosons we obtain

$$e^{i\mathcal{H}\Delta t}c_k e^{-i\mathcal{H}\Delta t} = c_k + \Delta t \sum_{k,l} (H\sigma^T)_{lk}c_l. \tag{3.14}$$

As $T = e^{\Delta t L}\sum_{kl}(\delta_{kl} + \Delta t L_{lk})c_l$, we can immediately read off

$$L = -H, \quad \text{for fermions} \tag{3.15}$$

$$L = H\sigma^T \quad \text{for bosons.} \tag{3.16}$$

Translationally invariant systems

We will throughout consider translationally invariant systems on cubic lattices in d spatial dimensions with periodic boundary conditions. Hence, the indices of the Hamiltonian matrix H_{kl} which correspond to two points on the lattice are d-component vectors $k, l \in \mathbb{Z}_m^d$ where m is the edge length of the cube, i.e., $N = m^d$. The translational invariance is expressed by the fact that the matrix elements G_{kl}, of the blocks $G \in \{X, Y, W\}$ of H depend only on the relative distance $k - l$. Taking into account the periodic boundary conditions, $k - l$ is understood modulo m in each component. Such matrices are called *circulant*, and we will denote by $\mathcal{C}_A$ and $\mathcal{C}_S$ the set of circulant symmetric and antisymmetric matrices, respectively. All circulant matrices can be diagonalized simultaneously by Fourier transformation [73]

$$\hat{G} \equiv \mathcal{F}^{\otimes d} G \mathcal{F}^{\dagger \otimes d} = \operatorname{diag}\left[\sum_{k \in \mathbb{Z}_m^d} G_k e^{-\frac{2\pi i}{m}kl}\right]_l, \tag{3.17}$$

$$\mathcal{F}_{pq} = \frac{1}{\sqrt{m}} e^{\frac{2\pi i}{m}pq}, \quad p, q \in \mathbb{Z}_m, \tag{3.18}$$

where $G_k \equiv G_{k,0}$ is the entry of the k-th off-diagonal of the matrix G. It follows from (3.17) that all circulant matrices mutually commute.

3.3 Simulations in fermionic systems

In this Section we study the set of interactions that can be simulated in a translationally invariant fermionic system starting with quadratic local transformations and nearest neighbor-interactions. Making use of the fact that the blocks X, Y and W in Eq. (3.10) mutually commute we calculate the commutator $L'' = [L, L']$ of two generators L and L' given by

$$L^{(\prime)} = \begin{pmatrix} X^{(\prime)} & W^{(\prime)} \\ -W^{(\prime)T} & Y^{(\prime)} \end{pmatrix}, \tag{3.19}$$

and obtain

$$\begin{aligned} L'' &= \begin{pmatrix} X'' & W'' \\ -W''^T & -X'' \end{pmatrix}, \\ X'' &= W'W^T - WW'^T, \\ W'' &= W(Y' - X') - W'(Y - X). \end{aligned} \tag{3.20}$$

Note that by Eq. (3.20) every commutator has the symmetry $Y'' = -X''$. Hence, if we start with a set $\mathcal{S}$ of Hamiltonians with corresponding generators $\mathcal{S}_\mathcal{L} = \{L_1, L_2, \ldots\}$, then every element of the generated Lie algebra $\mathcal{L}$ has this form up to linear combinations of elements in $\mathcal{S}_\mathcal{L}$. On the level of Hamiltonians this symmetry corresponds to real tunneling/hopping coefficients $B_{kl} = -C_{lk} \in \mathbb{R}$ in Eq. (3.1). We will denote by $\mathcal{R}$ the vector space of all matrices of the form (3.19) for which $Y = -X$.

Let us now introduce the elements of the set $\mathcal{S}_\mathcal{L}$ corresponding to all local Hamiltonians and specific nearest-neighbor interactions. Every generator L of a local Hamiltonian is proportional to

$$E = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}. \tag{3.21}$$

For giving an explicit form to the nearest-neighbor interaction, we define a matrix $M^{(v)}$ via

$$M^{(v)}_{kl} = \delta_{l,k+v}, \tag{3.22}$$

where $v, k, l \in \mathbb{Z}_m^d$ and the addition is modulo m in each of the components. This leads to the properties

$$M^{(v_1)} M^{(v_2)} = M^{(v_1+v_2)}, \quad M^{(0)} = \mathbb{1}. \tag{3.23}$$

Moreover, we define the matrices

$$M_+^{(v)} = M^{(v)} + M^{(-v)}, \quad M_-^{(v)} = M^{(v)} - M^{(-v)}, \tag{3.24}$$

$$H_X^{(v)} = \begin{pmatrix} M_-^{(v)} & 0 \\ 0 & -M_-^{(v)} \end{pmatrix}, \tag{3.25}$$

$$H_{W(\pm)}^{(v)} = \begin{pmatrix} 0 & M_{(\pm)}^{(v)} \\ M_{(\pm)}^{(v)T} & 0 \end{pmatrix}, \tag{3.26}$$

where the indices X and W refer to a non-vanishing X- and W-block respectively. Denoting by $e_i \in \mathbb{Z}_m^d$ the basis vectors $(e_i)_j = \delta_{ij}$, every Hamiltonian matrix corresponding to a nearest-neighbor interaction along e_i is of the form

$$H_0 \equiv \begin{pmatrix} X_0 & W_0 \\ -W_0^T & Y_0 \end{pmatrix} = \begin{pmatrix} xM_-^{(e_i)} & wM^{(e_i)} + \tilde{w}M^{(-e_i)} \\ -(\tilde{w}M^{(e_i)} + wM^{(-e_i)}) & yM_-^{(e_i)} \end{pmatrix}, \tag{3.27}$$

where $x, y, w, \tilde{w} \in \mathbb{R}$. We will now start studying one-dimensional systems and then generalize to the d-dimensional case.

3.3.1 Simulations in one-dimensional fermionic systems

In this Section we consider quadratic fermionic Hamiltonians with translational symmetry on a ring of m sites. We will give an exhaustive characterization of nearest-neighbor Hamiltonians which are universal for the simulation of all interactions obeying the symmetry $Y = -X$, when supplemented by all on-site Hamiltonians. The results depend on whether m is even or odd.

Theorem 3.1. *Consider a translationally invariant fermionic systems of m sites on a ring with periodic boundary conditions. Starting with all one-particle transformations which are proportional to the matrix E defined in* (3.21) *and one nearest-neighbor interaction H_0 of the form* (3.27) *we can simulate the following set of interactions depending on the symmetry properties of X_0, Y_0 and W_0:*

1. *$m = 2n + 1$ odd:*
   - (a) *$X_0 = Y_0, W_0 \in \mathcal{C}_S$: No further interaction can be simulated.*
   - (b) *$X_0 \neq Y_0$ or $W_0 \notin \mathcal{C}_S$: The space $\mathcal{R}$ (i.e. $X = -Y$) can be simulated.*
2. *$m = 2n$ even:*
   - (a) *$X_0 = Y_0, W_0 \in \mathcal{C}_S$: No further interaction can be simulated.*
   - (b) *$W_0 \in \mathcal{C}_A$ or $W_0 = 0$: The space spanned by*

$$\mathcal{I} \equiv \{H_X^{((2k-1)e_1)}, H_{W+}^{(2ke_1)}, H_{W-}^{((2k-1)e_1)}\}_{k\in\mathbb{N}}$$

   can be simulated. (For the definition of H_X and H_W see Eqs. (3.25), (3.26) *).*

(c) $W_0 \notin \mathcal{C}_A, H_0 \in \mathcal{R}$*: The space* $\mathcal{R}$ *can be simulated.*

(d) $W_0 \notin \mathcal{C}_A, H_0 \notin \mathcal{R}$*: The space spanned by*

$$\mathcal{J} \equiv \{H_X^{(ke_1)}, H_W^{(2ke_1)}, H_W^{((2k-1)e_1)} - H_W^{((2(k-1)-1)e_1)}\}_{k\in\mathbb{N}}$$

can be simulated.

Proof. For the proof we will need the relations

$$\begin{aligned}
[H_X^{(ke_1)}, E] &= 2H_{W-}^{(ke_1)}, && (3.28)\\
[E, H_W^{(ke_1)}] &= H_X^{(ke_1)}, && (3.29)\\
[H_X^{(ke_1)}, H_X^{(le_1)}] &= 0, && (3.30)\\
[H_X^{(ke_1)}, H_W^{(le_1)}] &= 2(H_W^{((l+k)e_1)} - H_W^{((l-k)e_1)}), && (3.31)\\
[H_W^{(ke_1)}, H_W^{(le_1)}] &= H_X^{((l-k)e_1)}. && (3.32)
\end{aligned}$$

For $X_0 = Y_0, W_0 \in \mathcal{C}_S$, $[H_0, E] = 0$ according to (3.20) so that we cannot simulate any further interaction (up to multiples of E). This proves (1a) and (2a).

If $W_0 \notin \mathcal{C}_S$ or $X_0 \neq Y_0$, we will show in the first step by induction over k that the set $\mathcal{I}$ defined in (2b) can be simulated. For $k = 1$, we can get $H_X^{(e_1)}$ and $H_{W-}^{(e_1)}$ by taking the commutator of H_0 with the one-particle transformation E: If $W_0 \in \mathcal{C}_S$, then $[H_0, E] \sim H_{W-}^{(e_1)}$ and $H_X^{(e_1)}$ can be obtained using (3.29). If $X_0 = Y_0$, then $[H_0, E] \sim H_X^{(e_1)}$ and we get $H_{W-}^{(e_1)}$ by (3.28). If $W_0 \notin \mathcal{C}_S$ and $X_0 \neq Y_0$, then

$$[H_0, E]/(\tilde{w}_0 - w) + [[H_0, E], E]/2(x_0 - y_0) \sim H_{W-}^{(e_1)},$$

and according to (3.29) we also get $H_X^{(e_1)}$. From (3.31) we see that we get

$$H_{W+}^{(2e_1)} = [H_X^{(e_1)}, H_{W-}^{(e_1)}]/2 + 2E.$$

Now let $k \geq 1$. Using (3.31) and (3.29) we get

$$[H_X^{(e_1)}, H_{W+}^{(2ke_1)}] + H_{W-}^{((2k-1)e_1)} = H_{W-}^{((2(k+1)-1)e_1)},$$

which implies that we also get $H_X^{((2(k+1)-1)e_1)}$. As

$$[H_X^{(e_1)}, H_{W-}^{((2(k+1)-1)e_1)}] + H_{W+}^{(2e_1)} = H_{W+}^{(2(k+1)e_1)},$$

we have shown that we can simulate $\mathcal{I}$. Using the relations (3.28) - (3.32), we see that $\mathcal{I}$ is closed under the commutator bracket.

If $m = 2n + 1$, $\mathcal{I}$ is a basis of all possible interactions of the space $\mathcal{R}$ because of the periodic boundary conditions. To see this, define for an arbitrary k the number $k' = k+n+1$. As $2k' \bmod m = 2k+1$, we see that $H_X^{((2k'-1)e_1)} = H_X^{(2ke_1)}, H_{W-}^{((2k'-1)e_1)} = H_{W-}^{(2ke_1)}$ and $H_{W+}^{(2k'e_1)} = H_{W+}^{(2(k+1)e_1)}$, which proves (1b).

Now let $m = 2n$. If $W_0 \in \mathcal{C}_A$ or $W_0 = 0$, then

$$H_0 = \tilde{H} + w_0 H_W^{(e_1)}, \quad \tilde{H} = \begin{pmatrix} x_0 M_-^{(e_1)} & 0 \\ 0 & y_0 M_-^{(e_1)} \end{pmatrix} \notin \mathcal{I}.$$

The elements of $\mathcal{I}$ are the only ones that can be simulated as

$$[\tilde{H}, H_{W\pm}^{(le_1)}] = (x_0 - y_0)[H_X^{(e_1)}, H_{W\pm}^{(le_1)}] \in \mathcal{I},$$

where $l = 2k, 2k-1$ respectively and $\tilde{H}$ commutes with $H_X^{((2k-1)e_1)}$. This proves (2b).

If $W_0 \notin \mathcal{C}_A$ and $H_0 \in \mathcal{R}$, then

$$H_0 = x_0 H_X^{(e_1)} - \tilde{w}_0 H_{W-}^{(e_1)} + (w_0 + \tilde{w}_0) H_W^{(e_1)},$$

so that we can extract $H_W^{(e_1)}$. According to (3.31)

$$[H_X^{((2k-1)e_1)}, H_W^{(e_1)}] = 2(H_W^{(2ke_1)} - H_W^{(-2(k-1)e_1)}),$$

so that we can get $H_W^{(2ke_1)}$ as $H_W^{(0)} = E$, and we can simulate $H_X^{(2ke_1)}$ using (3.29). It remains to show that we can simulate $H_W^{((2k-1)e_1)}$. Note that the possibility of simulating $H_W^{(ke_1)}$ implies that we can get $H_W^{(-ke_1)}$, as

$$H_W^{(ke_1)} + [[H_W^{(ke_1)}, E], E]/2 = H_W^{(-ke_1)}.$$

According to (3.32)

$$[H_W^{(e_1)}, H_{W+}^{(2ke_1)}] = H_W^{((2k+1)e_1)} + H_W^{(-(2k-1)e_1),}$$

so that we can get $H_W^{((2k-1)e_1)}$ as $H_W^{(-e_1)}$ is available. This proves (2c).

Finally we consider the case where $W_0 \notin \mathcal{C}_A$ and $H_0 \notin \mathcal{R}$. Then

$$\begin{aligned} H_0 &= \tilde{H} + \tilde{w}_0 H_{W-}^{(e_1)}, \\ \tilde{H} &= \begin{pmatrix} X_0 & (w_0 + \tilde{w}_0) M^{(e_1)} \\ -(w_0 + \tilde{w}_0) M^{(-e_1)} & Y_0 \end{pmatrix} \notin \mathcal{I}. \end{aligned}$$

We will now calculate the commutator of $\tilde{H}$ with all elements of $\mathcal{I}$ in order to see if we get additional interactions. From

$$[\tilde{H}, H_X^{((2k-1)e_1)}] = -2(w_0 + \tilde{w}_0) H_{W-}^{(2ke_1)}$$

we see that we can get $H_W^{(2ke_1)}$, as $H_{W+}^{(2ke_1)} \in \mathcal{I}$ and using (3.29) we get $H_X^{(2ke_1)}$. As

$$[H_X^{(ke_1)}, H_W^{(2le_1)}] = 2(H_W^{((2l+k)e_1)} - H_W^{((2l-k)e_1)}),$$

we have shown that the set $\mathcal{J}$ can be simulated. Using (3.28)-(3.32), we see that $\{\mathcal{J}, \tilde{H}\}$ is closed under the commutator bracket, which proves (2d). □

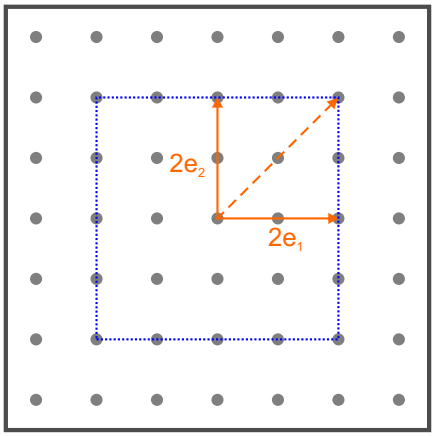

Figure 3.2: Two-dimensional fermionic lattice with box B_2 (see proof of Thm. 3.2). The interactions along e_1 and e_2 (solid arrows) are used to simulate the interactions in the direction $2(e_1 + e_2)$ (dashed arrow).

3.3.2 Simulations in d-dimensional fermionic systems

This Section will generalize the previous results to systems in d spatial dimensions. The following theorem shows that certain nearest-neighbor interactions are universal for simulating the space $\mathcal{R}$ (i.e. $Y = -X$) on a d-dimensional cube.

Theorem 3.2. *Consider a fermionic systems on a d-dimensional translationally invariant cubic lattice with m^d sites and periodic boundary conditions. Then the following sets of nearest-neighbor interactions together with all on-site transformations are complete for simulating the space $\mathcal{R}$:*

1. *$m = 2n + 1$ odd:*

$$H_0^{(e_i)} = \begin{pmatrix} x_i M_-^{(e_i)} & w_i M^{(e_i)} + \tilde{w}_i M^{(-e_i)} \\ \tilde{w}_i M^{(e_i)} + w_i M^{(-e_i)} & y_i M_-^{(e_i)} \end{pmatrix},$$

   where $i = 1, \ldots, d$, $x_i \neq y_i$ or $w_i \neq \tilde{w}_i$ for all i.

2. *$m = 2n$ even: d interactions $H_0^{(e_i)}$ of the above form where $x_i = -y_i, w_i \neq -\tilde{w}_i$ for all i and 2^d interactions of the form $H_W^{(\sum_{i=1}^d c_i e_i)}$, $c_i \in \{0, \pm 1\}$.*

Proof. We start with an odd number of fermions, $m = 2n + 1$. For the proof we will consider interactions with a maximal interaction range in each direction e_i of the lattice. To do so, we define for every integer $z \in \mathbb{N}$ the d-dimensional cube of edge length $2z$, $B_z = \{v \in \mathbb{Z}_m^d \,|\, \|v\|_\infty \leq z\}$. Then a Hamiltonian $H^{(v^{(z)})}$ where $v^{(z)} = (v_1^{(z)}, \ldots, v_d^{(z)}) \in B_z$ couples a given lattice site s only with sites which lie in a cube of edge size $2z$ with s in its center. We will show by induction over z that $H_X^{(v)}$ and $H_W^{(v)}$ can be simulated. We start with a minimal edge length of 2, i.e. $z = 1$ and define $\mathcal{N}_v = \{i \,|\, |v_i| = 1\}$ with cardinality $|\mathcal{N}_v|$. We will show that

$H_X^{(v^{(1)})}, H_W^{(v^{(1)})}$ can be simulated for $|\mathcal{N}_{v^{(1)}}| = 1, \ldots, d$, i.e., for an arbitrary number of non-vanishing components of the vector $v^{(1)}$. For $|\mathcal{N}_{v^{(1)}}| = 1$, the vector $v^{(1)}$ has only one non-vanishing component $v^{(1)} = \pm e_i$, and the situation is as the one of theorem 3.1. Hence $H_X^{(\pm e_i)}$ and $H_W^{(\pm e_i)}$ can be simulated for arbitrary i. Now let $|\mathcal{N}_{v^{(1)}}| = r > 1$, $j \in \mathcal{N}_{v^{(1)}}$, i.e. we want to simulate an interaction in the direction of the diagonals as depicted in Fig. 3.2. As $|\mathcal{N}_{v^{(1)} - v_j^{(1)} e_j}| = r - 1$ we know by induction over the cardinality of $\mathcal{N}_{v^{(1)}}$ that $H_W^{(v^{(1)} - v_j^{(1)} e_j)}$ can be simulated. Then we get $H_X^{(v^{(1)})}$ as

$$[H_W^{(-v_j^{(1)} e_j)}, H_W^{(v^{(1)} - v_j^{(1)} e_j)}] = H_X^{(v^{(1)})},$$

and $H_W^{(v^{(1)})}$ can be obtained according to Theorem 3.1. Now we consider boxes with edge length bigger than 2 assuming that $H_X^{(v^{(z)})}$ and $H_W^{(v^{(z)})}$ can be constructed for all $v^{(z)} \in B_z$, and let $v^{(z+1)} = (v_1^{(z+1)}, \ldots, v_1^{(z+1)}) \in B_{z+1}$. First we show that there exist $p^{(z)}, q^{(z)} \in B_z$ such that $p^{(z)} + q^{(z)} = v^{(z+1)}, p^{(z)} - q^{(z)} \in B_z$ (see Fig. 3.3). Therefore we define the set $\mathcal{Z}_v = \{i | |v_i^{(z+1)}| = z + 1\}$. If we take $q^{(z)} = \sum_{i \in \mathcal{Z}_v} \frac{v_i}{|v_i|} e_i$ and $p^{(z)} = v^{(z+1)} - q^{(z)}$ then by definition $p^{(z)}, q^{(z)} \in B_z$ and $p^{(z)} + q^{(z)} = v^{(z+1)}$. As for all $i \in \mathcal{Z}_v$ we have $|(p^{(z)} - q^{(z)})_i| = (|v_i| - 2) \leqq z - 1$ and for all $i \notin \mathcal{Z}_v$ we have $|(p^{(z)} - q^{(z)})_i| = (|v_i|) \leqq z$, it follows that $p^{(z)} - q^{(z)} \in B_z$. Using now the commutator relation

$$[H_X^{(q^{(z)})}, H_W^{(p^{(z)})}] = 2(H_W^{(v^{(z+1)})} - H_W^{(p^{(z)} - q^{(z)})}),$$

(see Eq.(3.31)) we obtain that $H_W^{(v^{(z+1)})}$ can be simulated, and from (3.29) we know that we also get $H_X^{(v^{(z+1)})}$.

Now consider the case where $m = 2n$. If $x_i = -y_i, w_0 \neq -\tilde{w}_i \; \forall i$, we can simulate $H_X^{(ke_i)}$ and $H_X^{(ke_i)}$ for all i and k according to Theorem 3.1 (2c). Like in the case $m = 2n + 1$ we can simulate $H_X^{(kv^{(1)})}$ for all $v^{(1)} \in B_1$, but according to Theorem 3.1 (2b) simulating $H_W^{(kv^{(1)})}$ seems not to be possible. So we include these nearest-neighbor interactions in our initial set. The rest of the proof is then like in the case $m = 2n + 1$, and we see that the space $\mathcal{R}$ can be simulated. □

3.4 Simulations in bosonic systems

In the following Section we will study simulations in translationally invariant bosonic systems using quadratic on-site Hamiltonians and nearest-neighbor interactions. According to Eq. (3.16) the generators are of the form

$$L = \sigma^T \begin{pmatrix} -W & Y \\ -X & W \end{pmatrix},$$

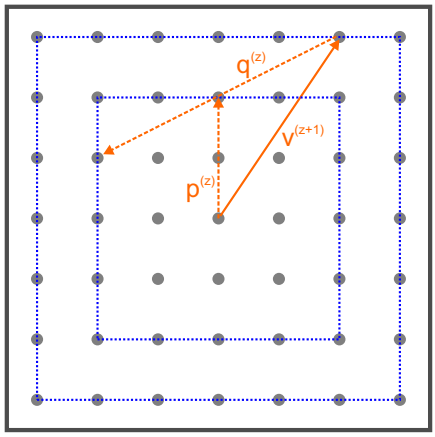

Figure 3.3: Boxes B_z and B_{z+1}. Any vector $v^{(z+1)} \in B_{z+1}$ can be decomposed into a sum of vectors from B_z, i.e., $v^{(z+1)} = p^{(z)} + q^{(z)}$ where $p^{(z)}, q^{(z)} \in B_z$, such that $q^{(z)} - p^{(z)} \in B_z$ (see proofs of Thms. 3.2 and 3.4).

and their commutator $L'' = [L, L']$ is given by

$$L'' = \begin{pmatrix} -W'' & Y'' \\ -X'' & W''^T \end{pmatrix}, \tag{3.33}$$

$$X'' = -X'(W + W^T) + X(W' + W'^T), \tag{3.34}$$

$$Y'' = Y(W' + W'^T) - Y'(W + W^T), \tag{3.35}$$

$$W'' = W''^T = X'Y - XY'. \tag{3.36}$$

As in the fermionic case all commutators obey a symmetry which is in this case $W'' = W''^T$ corresponding to reflection symmetry (point symmetry) of the Hamiltonian and we will denote the vector space of all point symmetric Hamiltonians by $\mathcal{P}$. This means that all simulated interactions are point symmetric up to linear combinations of the initial Hamiltonians.

Every generator L of an arbitrary on-site Hamiltonian is of the form

$$E_{(x_E, y_E, w_E)} = \begin{pmatrix} -w_E \mathbb{1} & y_E \mathbb{1} \\ -x_E \mathbb{1} & w_E \mathbb{1} \end{pmatrix}, \; x_E, y_E, w_E \in \mathbb{R}. \tag{3.37}$$

Generators corresponding to a nearest-neighbor interaction along an axis e_i are of the form

$$L^{(e_i)} = \begin{pmatrix} -W & Y \\ -X & W^T \end{pmatrix} = \begin{pmatrix} -wM^{(e_i)} + \tilde{w}M^{(-e_i)} & yM_+^{(e_i)} \\ xM_+^{(e_i)} & \tilde{w}M^{(e_i)} + wM^{(-e_i)} \end{pmatrix}, \tag{3.38}$$

where $x, y, w, \tilde{w} \in \mathbb{R}$ and $M^{(v)}$ has been defined in (3.22).

We define $L_W^{(v)} = \left(-M_+^{(v)} \right) \oplus M_+^{(v)}$ and

$$L_X^{(v)} = \begin{pmatrix} 0 & 0 \\ -M_+^{(v)} & 0 \end{pmatrix}, \; L_Y^{(v)} = \begin{pmatrix} 0 & M_+^{(v)} \\ 0 & 0 \end{pmatrix}, \tag{3.39}$$

where the indices X, Y and W correspond to a non-zero X-, Y- and W-block respectively.

3.4.1 Simulations in one-dimensional bosonic systems

In this Section we show that for one-dimensional bosonic systems an arbitrary nearest-neighbor interaction is complete for simulating the vector space $\mathcal{P}$ (i.e. $W = W^T$) when supplemented by all on-site Hamiltonians.

Theorem 3.3. *Consider bosonic systems with quadratic Hamiltonians on a one-dimensional translationally invariant lattice with periodic boundary conditions. The set of all possible one-mode transformations $E_{(x_E,y_E,w_E)}$ in* (3.37) *together with one arbitrary nearest-neighbor interaction given by L in Eq.*(3.38) *is universal for simulating the space $\mathcal{P}$ of all point symmetric interactions.*

Proof. First we will show that an arbitrary interaction with $X = Y = 0, W = W^T$ can be brought from the W-block in the X and Y-block:

$$\left[\begin{pmatrix} -W & 0 \\ 0 & W \end{pmatrix}, \begin{pmatrix} 0 & -\frac{1}{2} \\ 0 & 0 \end{pmatrix}\right] = \begin{pmatrix} 0 & W \\ 0 & 0 \end{pmatrix}, \tag{3.40}$$

$$\left[\begin{pmatrix} -W & 0 \\ 0 & W \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ -\frac{1}{2} & 0 \end{pmatrix}\right] = \begin{pmatrix} 0 & 0 \\ -W & 0 \end{pmatrix}. \tag{3.41}$$

Thus it is sufficient to show that an arbitrary W-block can be obtained. Let us start with a nearest-neighbor interaction of the form $L_Y^{(e_1)}$. As

$$[L_Y^{(e_1)}, E_{(1,0,0)}] = L_W^{(e_1)}$$

we also get $L_X^{(e_1)}$ according to (3.40). Now $[L_Y^{(e_1)}, L_X^{(e_1)}] - 2E_{(0,0,1)} = L_W^{(2e_1)}$, so that we also get $L_X^{(2e_1)}$ and $L_Y^{(2e_1)}$. As $[L_Y^{(ke_1)}, L_X^{(e_1)}] = L_W^{((k+1)e_1)} + L_W^{((k-1)e_1)}$ we can simulate $\mathcal{P}$.

Finally it remains to show that we can get $L_Y^{(e_1)}$ from an arbitrary nearest-neighbor interaction. If $y \neq 0$ in (3.38), then $[[L^{(e_1)}, E_{(0,0,1/2)}], E_{(-1,0,0)}] = yL_W^{(e_1)}$ so that we get $L_Y^{(e_1)}$ according to (3.40). If $y = 0, x \neq 0$, then $[[L^{(e_1)}, E_{(0,0,1/2)}], E_{0,1,0}] = xL_W^{(e_1)}$ and we get $L_Y^{(e_1)}$ as before. If $x = y = 0, w \neq 0$, then $[L^{(e_1)}, E_{(0,-1,0)}] = (w + \tilde{w})L_Y^{(e_1)}$. □

3.4.2 Simulations in d-dimensional bosonic systems

The following generalizes the previous result to cubic lattices in arbitrary spatial dimensions in cases where nearest neighbor interactions along all axes and diagonals are available.

Theorem 3.4. *Consider a system of bosonic modes on a d-dimensional translationally invariant lattice with periodic boundary conditions. The set of all on-site transformations together with all nearest-neighbor interactions corresponding to $L^{(\sum_i c_i e_i)}, c_i \in \{0, \pm 1\}, i = 1 \ldots, d$ with L as in Eq.* (3.38) *is complete for simulating the space $\mathcal{P}$ of all possible point symmetric interactions.*

Proof. Like in the d-dimensional fermionic case let $B_z = \{v | \|v\|_\infty \leq z\}, z \in \mathbb{N}, v^{(z)} \in B_z$. From Thm. 3.3 we know that it is sufficient to show that $L_W^{(v)}$ can be simulated

for arbitrary v. By induction over z we will show that $L_W^{(v^{(z)})}$ can be simulated for all $v^{(z)} \in B_z$. For $z = 1$ we know from Thm. 3.3 that all interactions described by $v^{(1)} \in B_1$ can be simulated as we have chosen our initial Hamiltonians appropriately. Now assume that $L_W^{(v^{(z)})}$ can be simulated for all $v^{(z)} \in B_z$, and let $v^{(z+1)} \in B_{z+1}$. Then there exist $p^{(z)}, q^{(z)} \in B_z$ such that $p^{(z)} + q^{(z)} = v^{(z+1)}, p^{(z)} - q^{(z)} \in B_z$ (see Fig. 3.3). As

$$[L_X^{(p^{(z)})}, L_Y^{(q^{(z)})}] = L_W^{(v^{(z+1)})} - L_W^{(p^{(z)}-q^{(z)})},$$

we can simulate $L_W^{(v^{(z+1)})}$. □

3.5 Simulations in spin systems

In this Section we will consider translationally invariant quantum lattice systems where a D-dimensional Hilbert space is assigned to each of the sites. We refer to these systems as *spins* although, of course, the described degrees of freedom do not have to be spin-like. The main result of this Section is that within the translationally invariant setting universal sets of interactions cannot exist. These results are based on the following Lemma involving Casimir operators, i.e., operators which commute with every element of the Lie algebra [121, 122]:

Lemma 3.5. *Consider a Lie-Algebra $\mathcal{L}$ and subalgebra $\mathcal{L}' = [\mathcal{L}, \mathcal{L}]$. Let $\mathcal{S}_\mathcal{L}$ be a set of generators for $\mathcal{L}$ and C a Casimir operator of $\mathcal{L}$ fulfilling*

$$tr[CG] = 0 \; \forall G \in \mathcal{S}_\mathcal{L} \setminus \mathcal{L}'. \tag{3.42}$$

Then for every $K \in \mathcal{L}$ we have that $tr[CK] = 0$.

Proof. Every $K \in \mathcal{L}$ can be written as

$$K = \sum_{L \in \mathcal{L}'} \alpha_L L + \sum_{G \in \mathcal{S}_\mathcal{L} \setminus \mathcal{L}'} \beta_G G \; , \quad \alpha_L, \beta_G \in \mathbb{C}. \tag{3.43}$$

Since we can write any $L \in \mathcal{L}'$ as $L = [L_1, L_2]$, $L_i \in \mathcal{L}$ we have that

$$\mathrm{tr}[CL] = \mathrm{tr}[C[L_1, L_2]] = \mathrm{tr}[[CL_1, L_2]] = 0$$

where we have used that C is a Casimir operator, i.e., $\forall L \in \mathcal{L} : [C, L] = 0$. Hence if we take the trace of Eq. (3.43) with C we get

$$\mathrm{tr}[CK] = \sum_{G \in \mathcal{S}_\mathcal{L} \setminus \mathcal{L}'} \beta_G \mathrm{tr}[CG]$$

which vanishes according to the assumption in Eq. (3.42). □

Let us now exploit Lemma 3.5 in the translationally invariant setting in order to rule out the universality of interactions corresponding to certain sets of generators $\mathcal{S}_\mathcal{L}$. The following results are stated for one-dimensional systems but they can be applied to d-dimensional lattices by grouping sites in $d - 1$ spatial dimensions.

We use Casimir operators of the form

$$C = \sum_{k=1}^{m} \gamma_k T^k \ , \quad \gamma_k \in \mathbb{C} \ , \tag{3.44}$$

where $T|i_1, i_2, \ldots, i_m\rangle = |i_2, i_3, \ldots, i_m, i_1\rangle$ is the translation operator which shifts the lattice by one site. To simplify notation we define an operator

$$\tau(X) = \sum_{j=1}^{m} T^j X T^{\dagger j} \ , \tag{3.45}$$

which symmetrizes any operator X with respect to the translation group. If X does not act on the entire lattice we will slightly abuse notation and write X instead of $X \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$.

Theorem 3.6. *Consider a translationally invariant spin system on a ring of length m. If f is a non-trivial factor of m then there is no universal set of Hamiltonians with interaction range smaller than f which generates all translationally invariant interactions. In particular if m is even, nearest-neighbor interactions cannot generate all next-to-nearest neighbor Hamiltonians.*

Proof. Let us introduce a basis of the Lie algebra su_{D^m} of the form $i\sigma_{j_1} \otimes \cdots \otimes \sigma_{j_m}$, $j_k \in \mathbb{Z}_{D^2}$ where σ_k is traceless except for $\sigma_0 = \mathbb{1}$ and $\mathrm{tr}[\sigma_k^2] = 2$ for all $k > 0$. For $D = 2$ these are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.46}$$

and for $D > 2$ we can simply choose all possible embeddings thereof. Let $m = f \cdot f'$ and consider a Casimir operator of the form in Eq. (3.44) with $\gamma_k = \delta_{k,f}$, i.e., $C = T^f$. We first show that for every Hamiltonian $H \in su_{D^m}$ with interaction range smaller than f we have $\mathrm{tr}[CH] = 0$. To see this note that the shift operator T^f contracts the trace of a tensor product as

$$\mathrm{tr}\big[T^f \sigma_{j_1} \otimes \cdots \otimes \sigma_{j_m}\big] = \prod_{\beta=1}^{f} \mathrm{tr}\left[\prod_{\alpha=0}^{f'-1} \sigma_{j_{(\beta+\alpha f)}}\right]. \tag{3.47}$$

In order to arrive at formula (3.47) expand the translation operator T^f in the computational basis

$$T^f = \sum_{i_1,\ldots,i_m} |i_1 \ldots i_m\rangle\langle i_{m-(f-1)} i_{m-(f-2)} \ldots i_1 \ldots i_{m-f}|,$$

and find that

$$\mathrm{tr}\big[T^f \sigma_{j_1} \otimes \cdots \otimes \sigma_{j_m}\big] = \sum_{i_1,\ldots,i_m} \langle i_{m-(f-1)}|\sigma_{j_1}|i_1\rangle\langle i_{m-(f-2)}|\sigma_{j_2}|i_2\rangle \ldots \langle i_{m-f}|\sigma_{j_m}|i_m\rangle.$$

Rearranging the order of the factors and using $(f'-1)f = m - f$ leads to

$$\prod_{\beta=1}^{f} \sum_{i_\beta, i_{f+\beta}, \ldots} \langle i_{m-(f-\beta)} | \sigma_{j_\beta} | i_\beta \rangle \langle i_\beta | \sigma_{j_{(f+\beta)}} | i_{f+\beta} \rangle \cdot \ldots$$

$$\ldots \cdot \langle i_{(f'-2)f+\beta} | \sigma_{j_{((f'-1)f+\beta)}} | i_{(f'-1)f+\beta} \rangle = \prod_{\beta=1}^{f} \mathrm{tr} \left[\prod_{\alpha=0}^{f'-1} \sigma_{j_{(\beta+\alpha f)}} \right].$$

If the interaction range of H is smaller than f then it can be decomposed into elements of the form $\tau(\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_f})$. Since σ_k is traceless for all $k > 0$, all these terms amount to a vanishing trace in Eq. (3.47) so that we have indeed $\mathrm{tr}[CH] = 0$. This means we can apply Lemma 3.5 to the set $\mathcal{S}_\mathcal{L}$ corresponding to all interactions with range smaller than f.

Now consider a two-body interaction between site one and site $f+1$ of the form $\tilde{H} = \tau\big(\sigma_j^{(1)} \sigma_j^{(1+f)}\big)$. From Eq. (3.47) we get

$$\mathrm{tr}[C\tilde{H}] = m \mathrm{tr}[\sigma_j^{(1)} \sigma_j^{(1+f)}] \prod_{\beta=2}^{f} \mathrm{tr}[\mathbb{1}] = 2mD^f,$$

such that by Lemma 3.5 we conclude that $\tilde{H}$ cannot be simulated. □

The following shows that a universal set of nearest-neighbor interactions cannot exist irrespective of the factors of m:

Theorem 3.7. *Consider a ring of length m. Then the set $\mathcal{S}_\mathcal{L}$ corresponding to all on-site Hamiltonians and nearest-neighbor interactions is not universal for simulating all translationally invariant Hamiltonians. In particular for $D = 2$ a product Hamiltonian*

$$H = \tau\Big(\sigma_{j_1} \otimes \cdots \otimes \sigma_{j_m}\Big) \tag{3.48}$$

cannot be simulated if σ_1, σ_2 and σ_3 all occur an odd number of times.

Proof. We use the Casimir operator $C = T - T^\dagger$ and the set of generators $\mathcal{S}_\mathcal{L} = i\{\tau(\sigma_k \otimes \sigma_l)\} \subset su_{2^m}$. As $\mathrm{tr}[CG] = 0$ for all $G \in \mathcal{S}_\mathcal{L}$ we can again apply Lemma 3.5. Consider now the above product Hamiltonian H or if $D > 2$ its embedding respectively. Using Eq. (3.47) with $f = 1, f' = m$ we obtain

$$\mathrm{tr}[CH] = m \mathrm{tr} \left[\prod_{k=1}^{m} \sigma_{i_k} - \prod_{l=1}^{m} \sigma_{i_l}^T \right]. \tag{3.49}$$

Since $\sigma_i^T = (-1)^{\delta_{i,2}} \sigma_i$ and by assumption σ_2 appears an odd number of times we get $\mathrm{tr}[CH] = 2m \mathrm{tr}\big[\prod_{k=1}^{m} \sigma_{i_k}\big]$ which is non-zero iff σ_1 and σ_3 appear and odd number of times as well. □

Clearly, one can derive other no-go theorems in a similar manner from Lemma 3.5. However, we end this Section by providing some examples of interactions which *can* be simulated. For this we define $g_{kl} = \tau(\sigma_k \otimes \sigma_l)$.

Theorem 3.8. *Consider a translationally invariant system of m qubits ($D = 2$) on a ring. By using on-site Hamiltonians and nearest-neighbor interactions the following interactions can be simulated:*

$$\tau(\sigma_i \otimes \sigma_i \otimes \sigma_i), \tag{3.50}$$

$$J_{ij}^{(r_j)} = \tau(\sigma_i \otimes \sigma_j \otimes \ldots \sigma_j \otimes \sigma_i), \tag{3.51}$$

where $i, j \in \{1, 2, 3\}$ and r_j denotes the number of σ_j matrices. Moreover, for $m = 5$ one can simulate next-to-nearest neighbor interactions of the form $N_i = \tau(\sigma_i \otimes \mathbb{1} \otimes \sigma_i \otimes \mathbb{1} \otimes \mathbb{1})$.

Proof. We will restrict our proof to the pairs $i = 1, j = 2$ as the other interactions can be obtained in an analogous way. We start proving (3.50). The Hamiltonian (3.50) can be simulated due to $[g_{21}, g_{13}]/(2i) = \tau(\sigma_1 \otimes \sigma_1 \otimes \sigma_1)$. For proving (3.51), we start with $[g_{13}, g_{11}]/(2i) = J_{12}^{(1)}$. As $[J_{12}^{(r_2)}, g_{31}]/(2i) = J_{12}^{(r_2-1)} - J_{12}^{(r_2+1)}$, $J_{12}^{(0)} = g_{11}$, we have shown (3.51).

Now we will prove that the next-to-nearest neighbor interaction can be achieved for $m = 5$, $i = 1$ ($i = 2, 3$ follow similarly). Using (3.51), we see that $\tau(\sigma_1 \otimes \sigma_1 \otimes \sigma_1 \otimes \sigma_1 \otimes \mathbb{1})$ can be simulated, as $[g_{23}, J_{21}^{(3)}]/(2i) + J_{(21)}^{(2)} = \tau(\sigma_1 \otimes \sigma_1 \otimes \sigma_1 \otimes \sigma_1 \otimes \mathbb{1})$, and similarly we get $\tau(\sigma_3 \otimes \sigma_3 \otimes \sigma_3 \otimes \sigma_3 \otimes \mathbb{1})$. As $[[g_{11}, g_{23}], g_{32}]/4 = 2N_1 - \tau(\sigma_1 \otimes \sigma_1 \otimes \sigma_1 \otimes \sigma_1 \otimes \mathbb{1}) - \tau(\sigma_3 \otimes \sigma_3 \otimes \sigma_3 \otimes \sigma_3 \otimes \mathbb{1})$ we can extract N_1. □

3.6 Summary of the results and conclusion

Before coming to the conclusion we give a a simplified summary of the main results. Hamiltonians and interactions are meant to be translationally invariant throughout and it is assumed that interactions along different directions can be implemented independently.

- *Fermions:* All simulated evolutions have *real* tunneling/hopping amplitudes. Within this set generic nearest-neighbor interactions are universal for the simulation of any translationally invariant interaction when supplemented with all on-site Hamiltonians. Whereas for cubes with odd edge length the proof of universality requires interactions along all axes and diagonals, the diagonals are not required for even edge length.

- *Bosons:* All simulated evolutions are point symmetric. Within this set every nearest-neighbor interaction (available along axes and diagonals) is universal for the simulation of any translationally invariant interaction when supplemented with all on-site Hamiltonians.

- *Spins:* There is no universal set of nearest-neighbor interactions. Moreover, if f is a factor of the edge length m of the cubic lattice then there is no universal set of interactions with interaction range smaller than f. In particular, if m is even, not all next-to-nearest neighbor interactions can be simulated from nearest neighbor ones. Sets of Hamiltonians that can be simulated have been constructed.

In conclusion, we have presented a characterization of universal sets of translationally invariant Hamiltonians for the simulation of interactions in quadratic fermionic and bosonic systems given the ability of engineering local and nearest neighbor interactions. Thereby the Lie algebraic techniques of quantum simulation restrict the space of reachable interactions to Hamiltonians with real hopping amplitudes in the case of fermions and to point symmetric interactions in the case of bosons.

For spins the situation appears to be more difficult and a complete characterization of interactions that can be simulated remains to be found. As a first step, we have identified Hamiltonians that cannot be simulated using short range interactions only. Furthermore, we have introduced a technique based on the Casimir operator of the corresponding Lie algebra which allows one to find Hamiltonians that cannot be simulated with a given set of interactions.

In this work we have considered the question of what can be simulated leaving aside the question of the efficiency. In this context it is important to remark the fact that the number of applications of the original Hamiltonians in order to obtain a result bounded by some given error scales polynomially in the Trotter expansion. The scaling with the total number of particles depends on the number of commutators that are required to obtain the Hamiltonian.

Finally, whereas we have shown that it is not possible to perform certain simulations for spin systems it is still possible to perform those simulations by encoding the qubits in a different way.

Chapter 4

Fermionic Projected Entangled Pair States (fPEPS)

After the considerations on the power of fermionc, bosonic and spin systems for quantum simulations in Chapter 3, we concentrate from now on on the possibilities of simulating fermionic systems on a classical computer. To this end, we aim at constructing a family of states that allow a good approximation of ground and thermal state properties of the system while depending on few parameters only. For spin systems on a lattice with local, i.e., short–range interactions, such families could be found in recent years. In one spatial dimension, Matrix Product States (MPS) [39, 40] which underly [133, 134] the successful Density Matrix Renormalization Group algorithm [135, 136] provide a good approximation to the ground state of any gapped local Hamiltonian [137, 138]. Projected Entangled Pair States (PEPS) [139, 140] (cf. also [37, 141, 142]), which naturally extend MPS to higher spatial dimensions, approximate spin states at any finite temperature [41, 143], and have been successfully used to simulate spin systems which cannot be dealt with otherwise [144, 145, 146, 147, 148]. In one spatial dimension, it is possible to adapt the methods based on MPS to fermionic systems using the Jordan-Wigner transform [149], which maps fermions into spins while keeping the interactions local. In higher dimensions, however, this is no longer possible: Fermionic operators at different locations anticommute, which effectively induces nonlocal effects when mapping fermions to spins. Thus, the use of PEPS to describe fermionic systems is no longer justified (see however [150, 151] for different approaches).

In the following we introduce a new family of states, the fermionic Projected Entangled Pair States (fPEPS), which naturally extend the PEPS to fermionic systems. According to their definition, fPEPS are well suited to describe fermionic systems with local interactions. They can be, in turn, efficiently described in terms of standard PEPS at the price of having to double the number of parameters. This automatically implies that the algorithms introduced to simulate ground and thermal states, as well as the time evolution of spin systems using PEPS [139, 140], can be readily adapted to fPEPS. We also show that certain fPEPS are exact ground states of local fermionic Hamiltonians, in as much the same way as PEPS are for spins [152, 153]. In particular, we give the explicit construction of a Gaussian

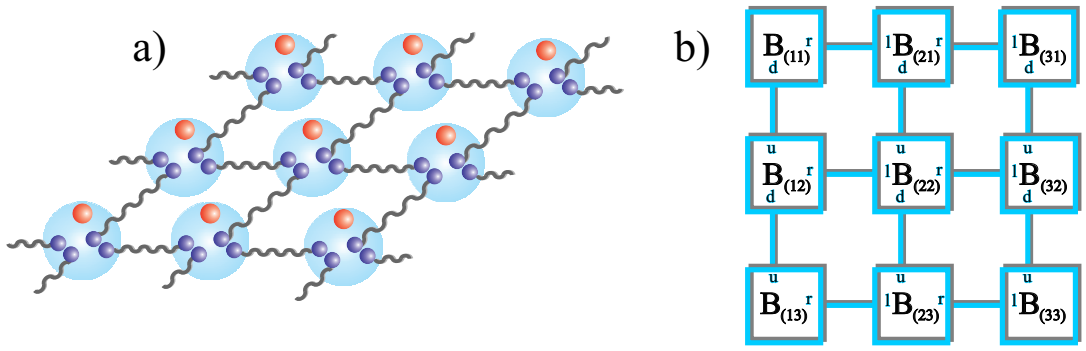

Figure 4.1: a) Construction of a PEPS in two dimensions. The balls joined by lines represent pairs of maximally entangled D-dimensional auxiliary spins, which are then mapped to the physical spins (red), as illustrated by the light blue spheres. b) Contraction of the tensor network performed by the map $\mathcal{C}$ given in Eq. (4.2) for a 3×3 lattice. The horizontal and vertical lines linking adjacent tensors B indicate the contraction of the corresponding indices l and r resp. u and d.

Hamiltonian which has an fPEPS as its exact ground state. Remarkably, the state is critical, i.e. gapless with polynomially decaying correlations, yet obeying an entropic area law [154], in contrast to what happens with other free fermion systems [155, 156].

In Sec. 4.1 we review the PEPS-construction and explain why PEPS are well suited to describe spin systems with local interactions in thermal equilibrium. Based on this idea we construct the family of fPEPS in Sec. 4.2, and show their relation to the PEPS-description for spin systems in Sec. 4.3. Then we consider a subfamily of fPEPS for which we can build local parent Hamiltonians, i.e. those for which they are exact ground states, in Sec 4.4. Finally, in Sec. 4.5 we give a particular example which exhibits criticality. For the sake of simplicity, we will concentrate on two spatial dimensions.

4.1 MPS and PEPS for spin systems

This Section gives a short review of the basic concepts of Projected Entangled Pair States for spin systems. These states can be understood best using the valence bond state construction: For simplicity, let us consider a $2D$ lattice of $N \equiv N_h \cdot N_v$ spin-1/2 particles, with states $|0\rangle$ and $|1\rangle$. The nodes have coordinates (h, v), where $h = 1, \ldots, N_h$ is the horizontal and $v = 1, \ldots, N_v$ the vertical position on the lattice. To each node with coordinates (h, v) we associate four auxiliary spins of dimension D. Each of them is in a maximally entangled state $|I\rangle = 1/\sqrt{D} \sum_{n=1}^{D} |n, n\rangle$ with one of its neighbors, as indicated by the curly lines in Fig. 4.1a. $|I\rangle$ is called the entangled bond, and D the bond dimension. The state of all maximally entangled virtual particles, $|\Psi_R\rangle$, is called resource state. Next we apply a linear operator, also called "projector" (blue spheres in Fig. 4.1a), to each node mapping the auxiliary

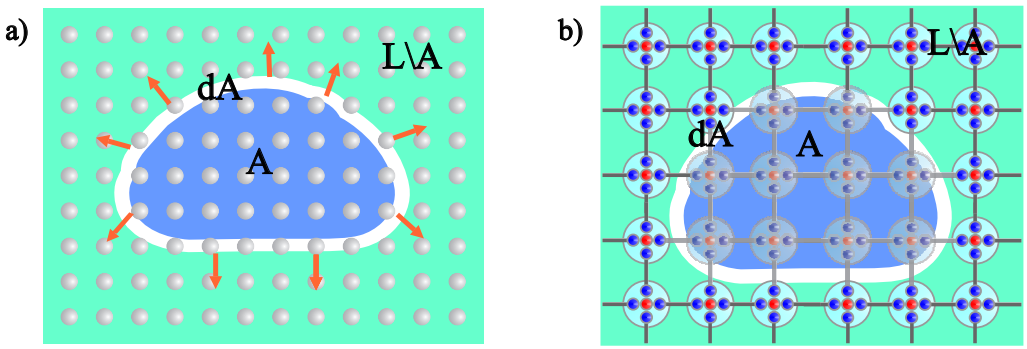

Figure 4.2: a) Area law for a lattice spin system with short-rang interaction. Only spins (grey spheres) on the boundary dA give rise to the correlations (orange arrows) between the region A and the rest of the system, $L\backslash A$. b) PEPS fulfill the area law by construction. The entropy of the reduced density operator $\rho_A = \mathrm{tr}_{L\backslash A}[\rho]$ is upper bounded by the rank of ρ_A. For every PEPS $\mathrm{rank}(\rho_A)$ scales with the size of the boundary dA .

spins onto the physical ones. Every map is of the form

$$P_{(h,v)} = \sum_{l,r,u,d=0}^{D-1} \sum_{k=0}^{1} \left(B_{(h,v)}\right)^{[k]}_{l,r,u,d} |k\rangle\langle l,r,u,d|, \tag{4.1}$$

where $(B_{(h,v)})$ is a five-index tensor. Due to the special structure of the resource state $|\Psi_R\rangle$, the state after the projection is given by

$$|\Psi\rangle = \sum_{k_1,\ldots,k_N=0}^{1} \mathcal{C}\left(\left(B_{(1,1)}\right)^{[k_{(1,1)}]}, \ldots, \left(B_{(N_h,N_v)}\right)^{[k_{(N_h,N_v)}]}\right) |k_{(1,1)} \ldots k_{(N_h,N_v)}\rangle. \tag{4.2}$$

The function $\mathcal{C}$ performs a contraction of the tensor network as depicted in Fig. 4.1b.

In the following we review some important properties of the PEPS. First, if the bond dimension D is high enough every state can be described as a PEPS, since the entangled bonds can be used as a resource for teleportation. Second, and more important, PEPS allow for an efficient description of ground and thermal state of physical systems described by a Hamiltonian with short-range interaction, $H = \sum_\lambda h_\lambda$, where h_λ acts on a finite region of the lattice only. We briefly review the ideas that have led to this result and sketch the proof given in [41]. We start with some general considerations regarding zero and finite temperature properties of a system with Hamiltonian H. Since H is local, ground and thermal states are expected to depend on few parameters only, so that these states occupy only a small part of the exponentially large Hilbert space. PEPS can be described by a number of parameters that scales polynomially with the system size, rising the question if these states lie exactly in the region of the Hilbert space we are interested in. A hint that this might hold true is given by the fact that all PEPS fulfill the so-called *area law* (see [154] for a review). The area law states that the entropy of a subsystem A of a lattice spin system L with short-range interaction grows linearly with the size of

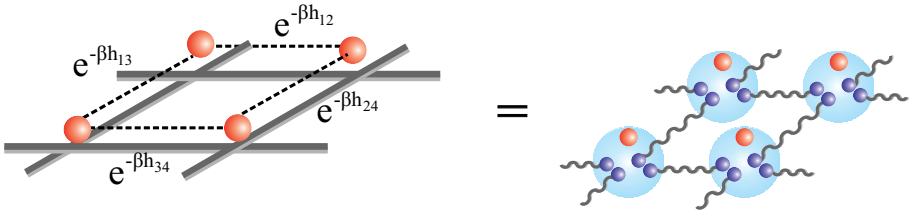

Figure 4.3: Why PEPS approximate thermal states well: $\exp[-\beta h_{ij}]$ can be implemented using local maps only if an entangled pair is available.

the boundary of A. In an intuitive picture only spins in the boundary of the region of A, dA will give rise to correlations of A with $L\backslash A$, as depicted in Fig. 4.2a. The PEPS defined above fulfill the area law by definition, which can be understood with the help of Fig. 4.2b. The entropy S_A of the subsystem A is upper bounded by the rank of the reduced density operator $\rho_A = \mathrm{tr}_{L\backslash A}[\rho]$, where ρ is the density operator of the whole system [5]. Due to the PEPS-construction, we see immediately that $\mathrm{rank}(\rho_A) \leq N_{dA}$, where N_{dA} denotes the number of bonds linking the region A with the rest of the system.

These general considerations on spin systems have suggested for some time that the family of PEPS can efficiently describe ground and thermal states of short-range interacting systems, and this hypothesis could finally be proven to hold true in [41]. The idea of the proof is the following: Consider the Hamiltonian $H = \sum_\lambda h_\lambda$ and assume for simplicity that each h_λ acts on two neighboring spins only. We first rewrite the unnormalized density operator as $e^{-\beta H} = \mathrm{tr}_B[|\Psi\rangle\langle\Psi|]$, where $|\Psi\rangle = e^{-\beta H/2} \otimes \mathbb{1} |\chi\rangle_{AB}$ is a purification of the thermal state $e^{-\beta H}$ [157] and $|\chi\rangle_{AB}$ a pairwise maximally entangled state of each spin with another one, the latter playing the role of an environment. We argue now that $|\Psi\rangle$ can be expressed as a PEPS, considering first the simplest case where $[h_\lambda, h_{\lambda'}] = 0$, so that $|\Psi\rangle = \prod_\lambda e^{-\beta h_\lambda/2} \otimes \mathbb{1} |\chi\rangle_{AB}$. The action of each of the terms $e^{-\beta h_\lambda/2} \otimes \mathbb{1}$ on two spins in neighboring nodes can be viewed as follows: Include in each node one auxiliary spin such that they are in a maximally entangled state and apply local maps to the real and auxiliary spin in each node. Finally project the auxiliary spins on the state $|0\rangle$. By proceeding in the same way for each term $e^{-\beta h_\lambda/2}$, we end up with the PEPS description (see Fig. 4.3). This is valid for all values of β, in particular for $\beta \to \infty$, i.e., for the ground state. In case that the local Hamiltonians do not commute, a more sophisticated proof is required [41]. One can, however, understand qualitatively why the construction remains to be valid by using a Trotter decomposition to approximate $e^{-\beta H} \approx \prod_{m=1}^{M} \prod_\lambda e^{-\beta h_\lambda/2M}$ with $M \gg 1$. Again, this allows for a direct implementation of each $\exp[-\beta h_\lambda/2M]$ using one entangled bond, yielding M bonds for each vertex of the lattice. Since, however, the entanglement induced by each $\exp[-\beta h_\lambda/2M]$ is very small, each of these bonds will only need to be weakly entangled, and the M bonds can thus be well approximated by a maximally entangled state of low dimension. Note that the spins belonging to the purification do not play any special role in this construction, and thus we will omit them in the

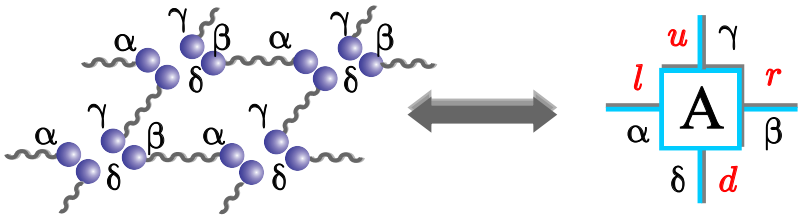

Figure 4.4: Ordering of the virtual modes on the lattice and tensor A. We associate to each lattice site four virtual modes, such that the local basis is of the form $(\alpha^\dagger_{(h,v)})^l(\beta^\dagger_{(h,v)})^r(\gamma^\dagger_{(h,v)})^u(\delta^\dagger_{(h,v)})^d|0\rangle$, where $u,d,l,r \in \{0,1\}$. Then $\alpha_{(h,v)}$ is in an entangled state with the mode $\beta_{(h-1,v)}$ to its left, and $\gamma_{(h,v)}$ is entangled with the mode $\delta_{(h,v-1)}$ above. The tensor A corresponding to the local projector is a five-index tensor (the physical mode is not shown in the figure).

following.

4.2 Construction of fPEPS

We will now extend the PEPS construction explained above to fermionic systems, in such a way that the same arguments apply. We consider fermions on a lattice, and work in second quantization. For a Hamiltonian $H = \sum h_\lambda$, each term h_λ must contain an even number of fermionic operators, in order for the Trotter decomposition to be still possible. Thus, we just have to find out how to express the action of $e^{-\beta h_\lambda}$ in terms of auxiliary systems. This is very simple: one just has to consider that the auxiliary particles are fermions themselves, forming maximally entangled states, and write a general operator which performs the mapping as before. To this end we associate to each node (h,v) four auxiliary fermionic modes, with creation operators $\alpha^\dagger_{(h,v)}, \beta^\dagger_{(h,v)}, \gamma^\dagger_{(h,v)}, \delta^\dagger_{(h,v)}$, respectively. Now we have to decide on the form of the maximally entangled states of two neighboring virtual modes ν and $\bar\nu$. Fermionic states have a definite parity, and for the even resp. odd parity sector the most general pure two-mode state is of the form

$$|\phi_e\rangle = \left(u + v\nu^\dagger\bar\nu^\dagger\right)|0\rangle, \tag{4.3}$$

$$|\phi_o\rangle = \left(u\nu^\dagger + v\bar\nu^\dagger\right)|0\rangle, \tag{4.4}$$

where e and o refers to even and odd parity respectively. The states $|\phi_{e,o}\rangle$ have some non-trivial quantum correlation iff $u,v \in \mathbb{C}\backslash\{0\}$. But then both these states can be mapped to the state

$$|\varphi_{\max}\rangle = \frac{1}{\sqrt{2}}\left(1 + f^\dagger\bar f^\dagger\right)|0\rangle, \tag{4.5}$$

via a local operation: In case of $|\phi_e\rangle$ apply $P_e = \langle 0|_{\nu\bar\nu}\bar f^\dagger\bar\nu(v + uf^\dagger\nu)$, in case of $|\phi_e\rangle$ apply $P_e = \langle 0|_{\nu\bar\nu}\bar f^\dagger\bar\nu(uf^\dagger + v\nu)$. Thus, wlog. we can use entangled states of the form $|\varphi_{\max}\rangle$ for the entangled bonds, as the action of the local transformation can

be absorbed via a redefinition of the local projectors. We define

$$H_{(h,v)} = \frac{1}{\sqrt{2}}\left(1+\beta^\dagger_{(h,v)}\alpha^\dagger_{(h+1,v)}\right), \tag{4.6}$$

$$V_{(h,v)} = \frac{1}{\sqrt{2}}\left(1+\delta^\dagger_{(h,v)}\gamma^\dagger_{(h,v+1)}\right), \tag{4.7}$$

which create maximally entangled states between adjacent sites, as shown in Fig. 4.4. Next we have to consider the form of the local projectors. The most general operator involving four virtual modes and one physical mode $a_{(h,v)}$ is of the form

$$Q_{(h,v)} = \sum (A_{(h,v)})^{[k]}_{lrud} a^{\dagger k}_{(h,v)} \alpha^l_{(h,v)} \beta^r_{(h,v)} \gamma^u_{(h,v)} \delta^d_{(h,v)}, \tag{4.8}$$

where the sum runs from 0 to 1 for all indices. However, as the physical state must be of definite parity as well, the operator $Q_{(h,v)}$ must also commute with the parity operator. This requirement imposes an additional condition on the tensors $(A_{(h,v)})$, namely $(u+d+l+r+k) \bmod 2 = c$, were c is fixed for each node[1]. If $c=0$ the map is parity-preserving, while the choice $c=1$ defines a parity-changing map.

The fermionic projected entangled states (fPEPS) is now obtained via

$$|\Psi\rangle = \langle \prod_{(h,v)} Q_{(h,v)} \prod_{(h,v)} H_{(h,v)} V_{(h,v)} \rangle_{\text{aux}} \, |\text{vac}\rangle, \tag{4.9}$$

where the expectation value is taken in the vacuum of the auxiliary modes, and $|\text{vac}\rangle$ denotes the vacuum of the physical fermions. Note that the definition of fPEPS straightforwardly extends to systems with both more than one physical mode per site and more than one mode per bond, as well as to open boundaries or higher spatial dimensions.

4.3 Relation between fPEPS and PEPS

The goal of this Section is to find an efficient description of any fPEPS in terms of standard PEPS. This will enable us to use the methods introduced for PEPS [139, 140] in order to determine physical observables, as well as to perform simulations of ground or thermal states, and time evolution. We have to identify the Fock space of the fermionic modes with the Hilbert space of spins. For that, we sort the lattice sites according to $(v-1)N_h + h$, where $v = 1, \ldots, N_v$, $h = 1, \ldots, N_h$ and associate $a_1^{\dagger k_1} \ldots a_N^{\dagger k_N} |\text{vac}\rangle$ to the spin state $|k_1, \ldots, k_N\rangle$. Then we write $|\Psi\rangle$ in that basis, and express it as a PEPS in terms of tensors B (4.1). The goal is to find the relation between the tensors B corresponding to the spin description and A corresponding to the fermionic description. In principle, the fPEPS to PEPS transformation can be done straightforwardly by adding extra bonds to the PEPS which take care of

[1] In fact one can freely choose c for all but one $Q_{(h,v)}$: Since, e.g., the bond (4.6) is invariant under $(i\beta_{(h,v)} + \beta^\dagger_{(h,v)})(i\alpha_{(h+1,v)} + \alpha^\dagger_{(h+1,v)})$, the corresponding maps (4.8) can be right multiplied with it, switching their parity.

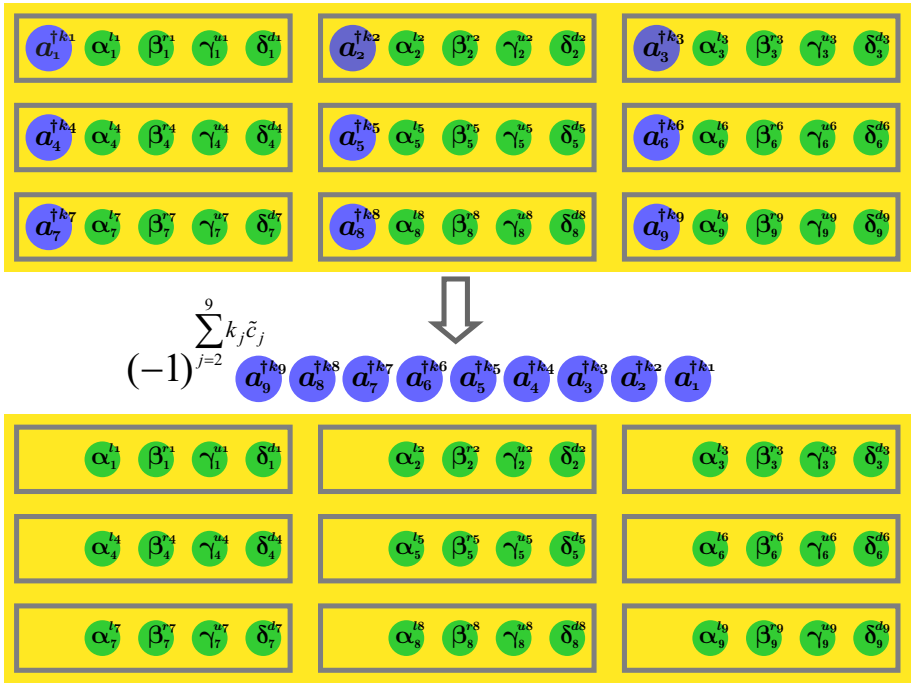

Figure 4.5: Derivation of the relation of fPEPS and PEPS for a 3×3 lattice, step 1. In order to apply the projector $\mathcal{P}$ to the virtual system, we first commute all physical modes $a^\dagger$ to the left of all virtual modes α, β, γ, δ. This action gives rise to local and global phases only.

the signs which arise from reordering the fermionic operators. However, this would lead to a number of bonds per link that scales linearly with the system size and thus to a dimension which is exponential in N. Remarkably, it is possible to express every fPEPS as a PEPS by introducing only *one* additional bond per horizontal link as follows: Replace each fermionic bond by a bond of maximally entangled spins, adding one additional horizontal qubit bond everywhere except at the boundaries (see Fig. 4.8). This means that the tensor B will have now two more indices, say l' and r', which are associated to those new bonds. Then, we find the relation

$$(B_{h,v})^{[k]}_{lrr'ud} = (-1)^{f_{(h,v)}(k,u,d,l,r)} (A_{h,v})^{[k]}_{lrud} (-1)^{(d+l)r'}, \tag{4.10}$$

for $h = 1$, while for $h > 1$ we have

$$(B_{h,v})^{[k]}_{ll'rr'ud} = \quad (-1)^{f_{(h,v)}(k,u,d,l,r)} (A_{h,v})^{[k]}_{lrud} (-1)^{dr'} \delta_{l',(r'+u+d) \bmod 2}, \tag{4.11}$$

where $f_{(h,v)}(k,u,d,l,r)$ is a function which only depends on the local indices, and $r' = 0$ for $h = N_h$.

Let us now explain how to obtain this result. Consider an fPEPS of the form (4.9) which we want to bring into the normal ordered form by commuting the fermionic operators. To this end, we perform the following three steps on the total projector $\mathcal{P} = \prod Q_{(h,v)}$ (see Fig. 4.5, 4.6, 4.7), observing that local sign contributions can be absorbed in the tensors $(A_{(h,v)})^{[k]}_{lrud}$:

First, commute all physical modes to the left, as depicted in Fig. 4.5 for a 3×3 lattice. Commuting $a^\dagger_{N_h,N_v}$ to the very left results in a contribution $(-1)^{k_{N_h,N_v}\sum_{(h,v)\neq(N_h,N_v)} c_{(h,v)}}$, since for all (h,v) the operators $Q_{(h,v)}$ have the fixed parity $c_{(h,v)}$. We continue with the next operator $a^\dagger_{N_{h-1},N_v}$ and so on, and finally arrive at

$$P = (-1)^{S_{\text{phys},1}} \prod_{v=N_v}^{1} \prod_{h=N_h}^{1} a^{\dagger k_{(h,v)}}_{(h,v)} \prod_{v=1}^{N_v} \prod_{h=1}^{N_h} \alpha^{l_{(h,v)}}_{(h,v)} \beta^{r_{(h,v)}}_{(h,v)} \gamma^{u_{(h,v)}}_{(h,v)} \delta^{d_{(h,v)}}_{(h,v)}, \tag{4.12}$$

where $S_{\text{phys},1} = \sum_{(h,v)} k_{(h,v)} \tilde{c}_{(h,v)}$. Here we have introduced site-dependent constants $\tilde{c}_{(h,v)} = \sum_{(h',v')<(h,v)} c_{(h',v')}$. Thus, $S_{\text{phys},1}$ gives only a local contribution. We still have to bring the physical modes in normal order, $\prod_{v=1}^{N_v}\prod_{h=1}^{N_h} a^{\dagger k_{(h,v)}}_{(h,v)}$, giving rise to a sign $(-1)^{S_{\text{phys},2}}$, where $S_{\text{phys},2} = \frac{1}{2}\sum_{(h,v)\neq(h',v')} k_{(h,v)}k_{(h',v')} = \frac{1}{2}p(p-1)$, and $p = \sum_{(h,v)} k_{(h,v)}$ is the parity of the fPEPS; since the latter is fixed, this yields a global phase. In total, commuting all physical modes to the left gives rise to a sign contribution $(-1)^{S_{\text{phys}}}$, where $S_{\text{phys}} = S_{\text{phys},1} + S_{\text{phys},2}$, the first term giving rise to local sign contributions while the latter gives a global phase.

Next, we contract the horizontal bonds. This can be done by reordering the modes of the tensors acting on each horizontal line independently. Thus, consider the operators on the first horizontal line, $L_1 \equiv Q_{(1,1)}Q_{(2,1)}\dots Q_{(N_h,1)}$ and abbreviate the indices $(h,1) \equiv h$, as well as $N_h = N$. Then L_1 is of the form

$$L_1 = \left[\alpha_1^{l_1}\beta_1^{r_1}\gamma_1^{u_1}\delta_1^{d_1}\right]\left[\alpha_2^{l_2}\beta_2^{r_2}\gamma_2^{u_2}\delta_2^{d_2}\right]\left[\alpha_3^{l_3}\beta_3^{r_3}\gamma_3^{u_3}\delta_3^{d_3}\right]\dots\left[\alpha_N^{l_N}\beta_N^{r_N}\gamma_N^{u_N}\delta_N^{d_N}\right], \tag{4.13}$$

where we have put square brackets around the modes on each site for better visualization. Since the horizontal bonds are of the form $H_h = \frac{1}{\sqrt{2}}(\mathbb{1} + \beta_h^\dagger \alpha_{h+1}^\dagger)|0\rangle$, we reorder the modes in L_1 as $[\alpha_{h+1}^{l_{h+1}}\beta_h^{r_h}]$:

$$\begin{aligned} L_1 &= (-1)^{\sum_{h=1}^{N-1} l_{h+1}(u_h+d_h+r_h)}\times \\ &\alpha_1^{l_1}\left[\left(\alpha_2^{l_2}\beta_1^{r_1}\right)\gamma_1^{u_1}\delta_1^{d_1}\right]\left[\left(\alpha_3^{l_3}\beta_2^{r_2}\right)\gamma_2^{u_2}\delta_2^{d_2}\right]\dots\left[\left(\alpha_N^{l_N}\beta_{N-1}^{r_{N-1}}\right)\gamma_{N-1}^{u_{N-1}}\delta_{N-1}^{d_{N-1}}\right]\beta_N^{r_N}\left[\gamma_N^{u_N}\delta_N^{d_N}\right]. \end{aligned}$$

Each term $l_{h+1}(u_h + d_h + r_h)$ results from moving the mode α_{h+1} to the left of the modes $\beta_h\gamma_h\delta_h$, as shown in Fig 4.6. Now we contract all the horizontal bonds except the one at the boundary, resulting in a delta-function $\delta_{r_h,l_{h+1}}$ $(h = 1,\dots,N-1)$ for each contracted bond, so that

$$L_1 = (-1)^{S^{(v=1)}_{(H,\text{OBC})}}\alpha_1^{l_1}\left[\gamma_1^{u_1}\delta_1^{d_1}\right]\left[\gamma_2^{u_2}\delta_2^{d_2}\right]\dots\left[\gamma_{N-1}^{u_{N-1}}\delta_{N-1}^{d_{N-1}}\right]\beta_N^{r_N}\left[\gamma_N^{u_N}\delta_N^{d_N}\right],$$

with only local sign contributions $S^{(v=1)}_{(H,\text{OBC})} = \sum_{h=1}^{N_h-1} r_h(u_h + d_h + r_h)$. In case of OBC we are done with the horizontal contraction, while in case of PBC the modes α_1 and β_N remain to be contracted. To this end we move α_1 to the right of the modes γ_j, δ_j, $j = 1\dots,N-1$. After the contraction of the bond, we are left with

$$L_1 = (-1)^{S^{(v=1)}_{(H,\text{PBC})}}\left[\gamma_1^{u_1}\delta_1^{d_1}\right]\left[\gamma_2^{u_2}\delta_2^{d_2}\right]\dots\left[\gamma_{N-1}^{u_{N-1}}\delta_{N-1}^{d_{N-1}}\right]\left[\gamma_N^{u_N}\delta_N^{d_N}\right],$$

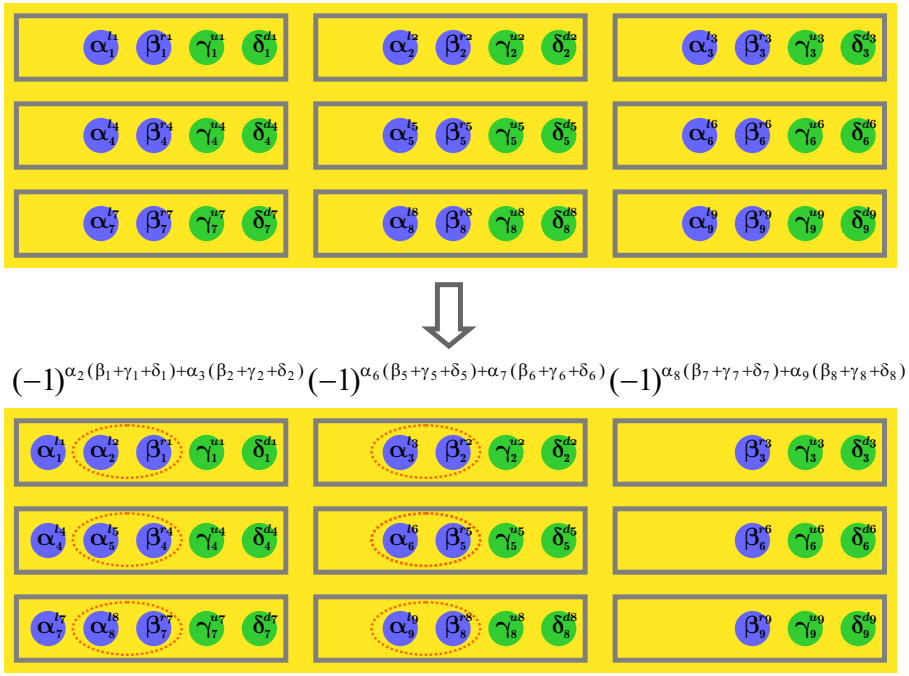

Figure 4.6: Derivation of the relation of fPEPS and PEPS for a 3×3 lattice, step 2. As the physical modes have been separated from the virtual modes in the last step, we can consider the virtual modes only. The horizontal bonds can be contracted on each line independently. For PBC this gives rise to local sign contributions only, while a non-local contribution occurs in case of PBC when we contract the boundary bond.

where $S^{(h=1)}_{(H,\mathrm{PBC})} = S^{(h=1)}_{(H,\mathrm{OBC})} + l_1 \sum_{v=1}^{N-1}(u_h + d_h)$. In summary, the contraction of the horizontal bonds for open boundary conditions gives rise to only local sign-contributions of the form $(-1)^{S^{(v)}_{(H,\mathrm{OBC})}}$ for each line horizontal $v = 1, \ldots, N_v$, where

$$S^{(v)}_{(H,\mathrm{OBC})} = \sum_{h=1}^{N_h-1} r_{(h,v)}(u_{(h,v)} + d_{(h,v)} + r_{(h,v)}), \tag{4.14}$$

while in case of periodic boundary conditions we obtain for each horizontal line $v = 1, \ldots, N_v$ a non-local sign-contribution of the form $(-1)^{S^{(v)}_{(H,\mathrm{PBC})}}$, where

$$S^{(v)}_{(H,\mathrm{PBC})} = S^{(v)}_{(H,\mathrm{OBC})} + l_{(1,v)}\Pi(N_h, v), \tag{4.15}$$

and $\Pi(h, v) = \sum_{j>h}(u_{(j,v)} + d_{(j,v)})$.

In the last step we contract the vertical bonds, proceeding columnwise from $h = 1$, as shown in Fig. 4.7. We denote by $\tilde{P}$ the product of all remaining operators,

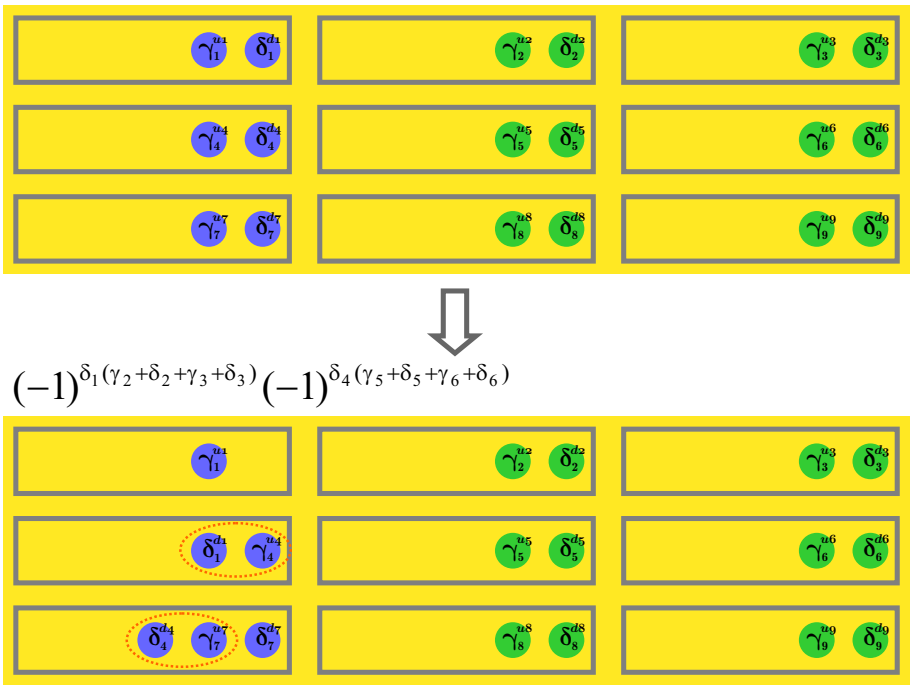

Figure 4.7: Derivation of the relation of fPEPS and PEPS for a 3×3 lattice, step 3. After the contraction of all horizontal bonds in step 2 we finally contract the vertical bonds proceeding columnwise, starting with the first vertical line. The contraction gives rise to non-local sign contributions for both, open and periodic boundary conditions.

$$\tilde{P} = \begin{matrix} \left[\gamma_{(1,1)}^{u_{(1,1)}}\delta_{(1,1)}^{d_{(1,1)}}\right] & \left[\gamma_{(2,1)}^{u_{(2,1)}}\delta_{(2,1)}^{d_{(2,1)}}\right] & \cdots & \left[\gamma_{(N_h,1)}^{u_{(N_h,1)}}\delta_{(N_h,1)}^{d_{(N_h,1)}}\right] \times \\ \left[\gamma_{(1,2)}^{u_{(1,2)}}\delta_{(1,2)}^{d_{(1,2)}}\right] & \left[\gamma_{(2,2)}^{u_{(2,2)}}\delta_{(2,2)}^{d_{(2,2)}}\right] & \cdots & \left[\gamma_{(N_h,2)}^{u_{(N_h,2)}}\delta_{(N_h,2)}^{d_{(N_h,2)}}\right] \times \\ \vdots & \vdots & \cdots & \vdots \\ \left[\gamma_{(1,N_v)}^{u_{(1,N_v)}}\delta_{(1,N_v)}^{d_{(1,N_v)}}\right] & \left[\gamma_{(2,N_v)}^{u_{(2,N_v)}}\delta_{(2,N_v)}^{d_{(2,N_v)}}\right] & \cdots & \left[\gamma_{(N_h,N_v)}^{u_{(N_h,N_v)}}\delta_{(N_h,N_v)}^{d_{(N_h,N_v)}}\right]. \end{matrix}$$

We move all operators of the form $\delta_{(1,v)}^{d_{(1,v)}}$, $v = 1, \ldots, N_v - 1$ down one line, which results in a non-local contribution $(-1)^{d_{(1,v)}\Pi_{(1,v)}}$ for each $v = 1, \ldots, N_h - 1$:

$$\tilde{P} = \begin{matrix} & \left[\gamma_{(1,1)}^{u_{(1,1)}}\right] & \left[\gamma_{(2,1)}^{u_{(2,1)}}\delta_{(2,1)}^{d_{(2,1)}}\right] & \cdots & \left[\gamma_{(N_h,1)}^{u_{(N_h,1)}}\delta_{(N_h,1)}^{d_{(N_h,1)}}\right] \times \\ (-1)^{d_{(1,1)}\Pi(1,1)}. & \left[\delta_{(1,1)}^{d_{(1,1)}}\gamma_{(1,2)}^{u_{(1,2)}}\right] & \left[\gamma_{(2,2)}^{u_{(2,2)}}\delta_{(2,2)}^{d_{(2,2)}}\right] & \cdots & \left[\gamma_{(N_h,2)}^{u_{(N_h,2)}}\delta_{(N_h,2)}^{d_{(N_h,2)}}\right] \times \\ (-1)^{d_{(1,2)}\Pi(1,2)}. & \left[\delta_{(1,2)}^{d_{(1,2)}}\gamma_{(1,3)}^{u_{(1,3)}}\right] & \left[\gamma_{(2,3)}^{u_{(2,3)}}\delta_{(2,3)}^{d_{(2,3)}}\right] & \cdots & \left[\gamma_{(N_h,3)}^{u_{(N_h,3)}}\delta_{(N_h,3)}^{d_{(N_h,3)}}\right] \times \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ (-1)^{d_{(1,N_v-1)}\Pi(1,N_v-1)}. & \left[\delta_{(1,N_v-1)}^{d_{(1,N_v-1)}}\gamma_{(1,N_v)}^{u_{(1,N_v)}}\right]\delta_{(1,N_v)}^{d_{(1,N_v)}} & \left[\gamma_{(2,N_v)}^{u_{(2,N_v)}}\delta_{(2,N_v)}^{d_{(2,N_v)}}\right] & \cdots & \left[\gamma_{(N_h,N_v)}^{u_{(N_h,N_v)}}\delta_{(N_h,N_v)}^{d_{(N_h,N_v)}}\right]. \end{matrix}$$

The contraction of all but the boundary bond on the first vertical line gives rise to a local contribution $(-1)^{d_{(1,v)}}$ for $v = 1, \ldots, N_v - 1$, and we are left with

$$\tilde{P} = \prod_{v=1}^{N-1} (-1)^{d_{(1,v)}\Pi(1,v)} \times$$

$$\begin{array}{rcccc} & \begin{bmatrix} \gamma_{(1,1)}^{u_{(1,1)}} \end{bmatrix} & \begin{bmatrix} \gamma_{(2,1)}^{u_{(2,1)}} \delta_{(2,1)}^{d_{(2,1)}} \end{bmatrix} & \cdots & \begin{bmatrix} \gamma_{(N_h,1)}^{u_{(N_h,1)}} \delta_{(N_h,1)}^{d_{(N_h,1)}} \end{bmatrix} \times \\ (-1)^{d_{(1,1)}} \cdot & & \begin{bmatrix} \gamma_{(2,2)}^{u_{(2,2)}} \delta_{(2,2)}^{d_{(2,2)}} \end{bmatrix} & \cdots & \begin{bmatrix} \gamma_{(N_h,2)}^{u_{(N_h,2)}} \delta_{(N_h,2)}^{d_{(N_h,2)}} \end{bmatrix} \times \\ (-1)^{d_{(1,2)}} \cdot & & \begin{bmatrix} \gamma_{(2,3)}^{u_{(2,3)}} \delta_{(2,3)}^{d_{(2,3)}} \end{bmatrix} & \cdots & \begin{bmatrix} \gamma_{(N_h,3)}^{u_{(N_h,3)}} \delta_{(N_h,3)}^{d_{(N_h,3)}} \end{bmatrix} \times \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ (-1)^{d_{(1,N_v-1)}} \cdot & \begin{bmatrix} \delta_{(1,N_v)}^{d_{(1,N_v)}} \end{bmatrix} & \begin{bmatrix} \gamma_{(2,N_v)}^{u_{(2,N_v)}} \delta_{(2,N_v)}^{d_{(2,N_v)}} \end{bmatrix} & \cdots & \begin{bmatrix} \gamma_{(N_h,N_v)}^{u_{(N_h,N_v)}} \delta_{(N_h,N_v)}^{d_{(N_h,N_v)}} \end{bmatrix}. \end{array}$$

For OBC, all bonds on the first vertical line are contracted now, while for PBC we still have to contract the boundary bond. To this end, we commute the mode $\delta_{(1,N_v)}$ next to the mode $\gamma_{(1,1)}$. Due to the fixed parity of the bonds this gives also a sign contribution $(-1)^{d_{(1,N_v)}\Pi(1,N_v)}$, while the contraction of the bond results in a local contribution $(-1)^{d_{(1,N_v)}}$. In summary, the contraction of vertical bonds results in a non-local sign-contribution for all but the most right vertical line, $(-1)^{S^{(h)}_{(H,\mathrm{OBC})}}$, $(h = 1, \ldots, N_h - 1)$, where

$$S^{(h)}_{(H,\mathrm{OBC})} = d_{(h,v)}\Pi_{(h,v)}. \tag{4.16}$$

In addition we get a local sign-contributions $(-1)^{d_(h,v)}$ for $h = 1, \ldots, N_h$ and $v = 1, \ldots, N_v - 1$.

Summary: From the contraction scheme we have explained above we conclude that every fPEPS obtained via a projection described by tensors A can be represented as a PEPS obtained via the application of projectors described by tensors B in the following way: First, all local sign contributions can be absorbed via the following redefinition of the tensors:

$$\begin{aligned} &h, v = 1, \ldots, N_{h,v} - 1: && (\tilde{A}_{(h,v)})^{[k]}_{lrud} = (-1)^{r(u+d)}(-1)^{r+d}(A_{(h,v)})^{[k]}_{lrud}, \\ &h = N_h, v = 1, \ldots, N_v - 1: && (\tilde{A}_{(h,v)})^{[k]}_{lrud} = (-1)^{d}(A_{(h,v)})^{[k]}_{lrud}, \\ &v = N_v, h = 1, \ldots, N_h - 1: && (\tilde{A}_{(h,v)})^{[k]}_{lrud} = (-1)^{r(u+d)}(-1)^{r}(A_{(h,v)})^{[k]}_{lrud}. \end{aligned} \tag{4.17}$$

All non-local signs, however, can be computed if the respective parity $\Pi(h, v)$ is available at each site. This can be achieved by adding an additional bond passing this information to the left, as depicted in Fig. 4.8:

$$\begin{aligned} &h = 2, \ldots, N_h - 1: && (B_{(h,v)})^{[k]}_{ll'rr'ud} = (\tilde{A}_{(h,v)})^{[k]}_{lrud}(-1)^{dr'}\delta_{l',(u+d+r')\bmod 2}, \\ &h = N_h: && (B_{(N_h,v)})^{[k]}_{ll'rud} = (\tilde{A}_{(N_h,v)})^{[k]}_{lrud}\delta_{l',(u+d+r')\bmod 2}, \\ &h = 1: && (B_{(1,v)})^{[k]}_{lrr'ud} = (\tilde{A}_{(1,v)})^{[k]}_{lrud}(-1)^{(d+l)r'}. \end{aligned} \tag{4.18}$$

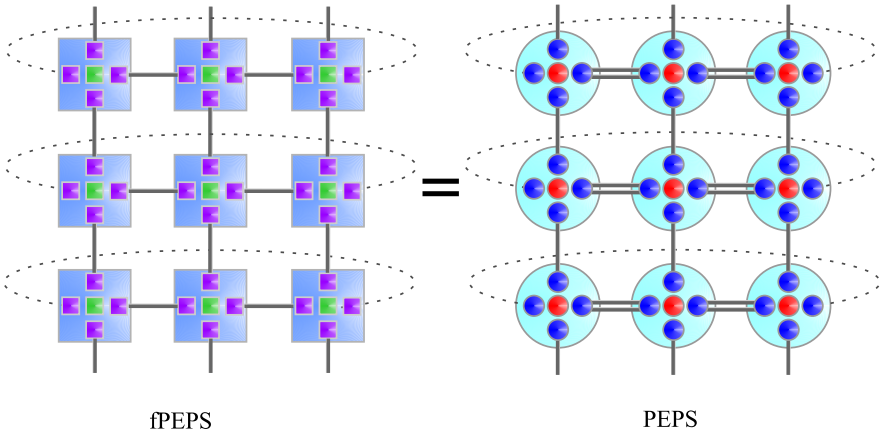

Figure 4.8: Every fPEPS can be represented as a PEPS at an extra cost of at most one additional bond per link (shown for a 3×3 PBC lattice).

Note that the same proof applies to open boundaries, as well as systems with more physical or virtual modes per site, without the need for further extra bonds to compute $\Pi(h, v)$. Similarly, one can derive a corresponding result for higher dimensions.

4.4 Fermionic Gaussian states and parent Hamiltonians

It would be desirable if there existed classes of Hamiltonians that have an fPEPS of low bond dimension as their exact ground state. In this Section we encounter such a family of states, the class of Gaussian fPEPS. These enable us to show that fPEPS naturally appear as ground states of free local Hamiltonians. As we have given a detailed introduction to the class of Gaussian states in Sec. 2.1.3 we only repeat the facts necessary for the understanding of the following Section. Fermionic Gaussian states constitute an important subclass of states, as they appear as ground and thermal states of quadratic Hamiltonians, corresponding to free fermion or BCS-states. They are completely characterized by their covariance matrix (CM) $\Gamma_{kl}^{(x,y)} = \mathrm{tr}[\frac{i}{2}[c_k^{(x)}, c_l^{(y)}]\rho]$, where $c_k^{(1)} = a_k^\dagger + a_k$ and $c_k^{(2)} = (-i)(a_k^\dagger - a_k)$ are Majorana operators fulfilling the CAR $\{c_k, c_l\} = 2\delta_{kl}$. Maps that transform Gaussian input states to Gaussian output states, so called Gaussian maps, have been introduced in Ref. [70]. These maps can equivalently be defined via their action on the covariance matrix of the input state. Applying the Jamiolkowski duality [158, 159] between maps and states to a fermionic system, the most general Gaussian map $\mathcal{E} : \Gamma_{\mathrm{in}} \to \Gamma_{\mathrm{out}}$ could be shown to have the form [70]

$$\mathcal{E}(\Gamma_{\mathrm{in}}) = B(D + \Gamma_{\mathrm{in}}^{-1})^{-1} B^T + A, \tag{4.19}$$

where

$$\mathcal{G} = \begin{pmatrix} A & B \\ -B^T & D \end{pmatrix} = -\mathcal{G}^T \,, \;\; \mathcal{G}\mathcal{G}^T \leq \mathbb{1} \,, \tag{4.20}$$

with block matrices A, B and D, and $\mathcal{G}$ can be understood as the covariance matrix of the state dual to the map $\mathcal{E}$. A map transforming pure states into pure states has to fulfill $\mathcal{G}\mathcal{G}^T = \mathbb{1}$. Since we are interested in ground states of physical systems we focus from now on on the set of pure fermionic Gaussian states.

In the following we construct the family of all translationally invariant pure Gaussian fPEPS with one bond of the form H resp. V (see Eqs. (4.6), (4.7)) between adjacent sites. The state of the virtual system is already translationally invariant and Gaussian, and we denote its CM by $\Gamma_{\text{in}} = \oplus\omega_{h,v}$ where $\omega_{h,v}$ is the CM of the maximally entangled horizontal resp. vertical bonds. Then the desired family of states can be obtained by applying the same Gaussian map to each node $\vec{n} = (h, v)$ of the lattice: $\mathcal{G} = \oplus_{\vec{n}}\tilde{\mathcal{G}}$, where $\tilde{\mathcal{G}}\tilde{\mathcal{G}}^T = \mathbb{1}$.

We show now that all Gaussian fPEPS constructed in this way are ground states of local Hamiltonians. To this end we follow an approach similar to that presented in [160] where an analogous result could be derived for bosonic systems. We derive first the form of the covariance matrix obtained after applying the channel $\mathcal{G}$ to Γ_{in}. Then we show that this CM corresponds to the ground state of a local Hamiltonian. The translational invariance of the problem suggests an approach in Fourier space. We introduce the Fourier transform of the the mode operators

$$\hat{f}_{\vec{\phi}} = \left(\frac{1}{\sqrt{N}}\right)^2 \sum_{\vec{n}} e^{-\frac{2\pi}{N} i\vec{\phi}\cdot\vec{n}} f_{\vec{n}}, \tag{4.21}$$

where f is either a physical or virtual mode, and we have introduced the reciprocal lattice vector $\vec{\phi} = (\frac{2\pi k_h}{N_h}, \frac{2\pi k_v}{N_v})$. We consider now the CM of the output state in the qp-ordered form, i.e. we write

$$\Gamma_{\text{out}} = \begin{pmatrix} \Gamma_{\text{out}}^{(1,1)} & \Gamma_{\text{out}}^{(1,2)} \\ \Gamma_{\text{out}}^{(2,1)} & \Gamma_{\text{out}}^{(2,2)} \end{pmatrix}, \tag{4.22}$$

where $\Gamma_{\text{out}}^{(r,s)} = \langle \frac{i}{2}[c^{(r)}, c^{(s)}]\rangle$, $r, s = 0, 1$. The translationally invariant construction is reflected in the fact that the blocks $\Gamma_{\text{out}}^{(r,s)}$ are circulant matrices. Hence, they all can be diagonalized simultaneously by a Fourier transformation $\mathcal{F}$. The Fourier transform of Γ_{out}, $\hat{G}_{\text{out}} = \mathcal{F}\Gamma_{\text{out}}\mathcal{F}^\dagger$, has diagonal blocks

$$\hat{G}_{\text{out}}^{(r,s)} = \mathcal{F}\langle\frac{i}{2}[c^{(r)}, c^{(s)}]\rangle\mathcal{F}^\dagger = \langle\frac{i}{2}[\hat{d}^{(r)}, \hat{d}^{(s)\dagger}]\rangle = \text{diag}\left(g^{(r,s)}(\vec{\phi})\right), \tag{4.23}$$

where $g^{(r,s)}(\vec{\phi}) \in \mathbb{C}$ are the eigenvalues of the blocks $\Gamma_{\text{out}}^{(r,s)}$. The operators $\hat{d}_{\vec{\phi}}^{(r)}$ are the Fourier transformed Majorana operators,

$$\hat{d}_{\vec{\phi}}^{(r)} = \left(\frac{1}{\sqrt{N}}\right)^2 \sum_{\vec{n}} e^{-\frac{2\pi}{N} i\vec{\phi}\cdot\vec{n}} c_{\vec{n}}^{(r)},$$

while the Majorana operators in the reciprocal lattice space are given by $\hat{c}^{(1)}_{\vec{\phi}} = \hat{a}^\dagger_{\vec{\phi}} + \hat{a}_{\vec{\phi}}$, $\hat{c}^{(2)}_{\vec{\phi}} = (-i)(\hat{a}^\dagger_{\vec{\phi}} - \hat{a}_{\vec{\phi}})$, where $\hat{a}_{\vec{\phi}}$ is defined in (4.21). The CM in the reciprocal lattice space, $(\hat{\Gamma}^{(x,y)}_{\text{out}})_{\vec{\phi}_1,\vec{\phi}_2} = \langle \frac{i}{2}[\hat{c}^{(x)}_{\vec{\phi}_1}, \hat{c}^{(y)}_{\vec{\phi}_2}]\rangle$ can be obtained from $\hat{G}_{\text{out}}$ with the help of the relation

$$\begin{pmatrix} \hat{c}^{(1)}_{\vec{\phi}} \\ \hat{c}^{(2)}_{\vec{\phi}} \\ \hat{c}^{(1)}_{-\vec{\phi}} \\ \hat{c}^{(2)}_{-\vec{\phi}} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & i & 1 & -i \\ -i & 1 & i & 1 \\ 1 & -i & 1 & i \\ i & 1 & -i & 1 \end{pmatrix}\begin{pmatrix} \hat{d}^{(1)}_{\vec{\phi}} \\ \hat{d}^{(2)}_{\vec{\phi}} \\ \hat{d}^{(1)\dagger}_{\vec{\phi}} \\ \hat{d}^{(2)\dagger}_{\vec{\phi}} \end{pmatrix}, \tag{4.24}$$

and we use in the following $\hat{G}_{\text{out}}$ to derive properties of $\hat{\Gamma}_{\text{out}}$. To this end, we regroup the modes such that $\hat{G}_{\text{out}} = \bigoplus_{\vec{\phi}} \hat{G}_{\text{out}}(\vec{\phi})$ is a direct sum of blocks corresponding to the same lattice vector, i.e.

$$\hat{G}_{\text{out}}(\vec{\phi}) = \begin{pmatrix} g^{(1,1)}(\vec{\phi}) & g^{(1,2)}(\vec{\phi}) \\ g^{(2,1)}(\vec{\phi}) & g^{(2,2)}(\vec{\phi}) \end{pmatrix}, \tag{4.25}$$

and derive properties of the eigenvalues $g^{(r,s)}(\vec{\phi})$. Since $\hat{G}^\dagger_{\text{out}} = (\mathcal{F}\Gamma_{\text{out}}\mathcal{F}^\dagger)^\dagger = -\hat{G}_{\text{out}}$ it follows immediately that $g^{(1,1)}(\vec{\phi}) \equiv ip(\vec{\phi})/d(\vec{\phi})$, $g^{(2,2)}(\vec{\phi}) \equiv i\tilde{p}(\vec{\phi})/d(\vec{\phi})$, where $p(\vec{\phi}), \tilde{p}(\vec{\phi}), d(\vec{\phi}) \in \mathbb{R}$ and $g^{(1,2)}(\vec{\phi}) = -\bar{g}^{(1,1)}(\vec{\phi}) \equiv q(\vec{\phi})/d(\vec{\phi})$ with $q(\vec{\phi}) \in \mathbb{C}$. It will become clear soon why we have introduced $d(\vec{\phi})$. Further, as the Fourier transform is unitary, we have $\hat{G}^2_{\text{out}}(\vec{\phi}) = -\mathbb{1}$, implying

$$\begin{aligned} p(\vec{\phi})^2 + |q(\vec{\phi})|^2 &= 1, \\ \tilde{p}(\vec{\phi})^2 + |q(\vec{\phi})|^2 &= 1, \\ (p(\vec{\phi}) + \tilde{p}(\vec{\phi}))q(\vec{\phi}) &= 0. \end{aligned}$$

From the last equation we get $\tilde{p}(\vec{\phi}) = -p(\vec{\phi})$ or $q(\vec{\phi}) = 0$. In the latter case this requires $p(\vec{\phi})^2 = \tilde{p}(\vec{\phi})^2 = 1$. But then $ip(\vec{\phi})$ and $i\tilde{p}(\vec{\phi})$ are the eigenvalues of $\hat{G}_{\text{out}}(\vec{\phi})$, and due to the antisymmetry of Γ we have $p(\vec{\phi}) = -\tilde{p}(\vec{\phi})$ as well. Thus,

$$\hat{G}_{\text{out}}(\vec{\phi}) = \frac{1}{d(\vec{\phi})}\begin{pmatrix} ip(\vec{\phi}) & q(\vec{\phi}) \\ -q(\vec{\phi}) & -ip(\vec{\phi}) \end{pmatrix}. \tag{4.26}$$

To obtain information on $p(\vec{\phi})$, $q(\vec{\phi})$ and $d(\vec{\phi})$ we use that the channel $\mathcal{E}$ describes a translationally invariant map. This implies that the blocks A, B and D are block diagonal, and thus commute with the Fourier transform. Since for pure states $\Gamma^{-1} = -\Gamma$ holds, we have

$$\hat{G}_{\text{out}} = \mathcal{F}\Gamma_{\text{out}}\mathcal{F}^\dagger = \mathcal{F}B(D + \Gamma^{-1}_{\text{in}}(\vec{\phi}))^{-1}B^T\mathcal{F}^\dagger + A = B(D - \hat{G}_{\text{in}}(\vec{\phi}))^{-1}B^T + A, \tag{4.27}$$

where $\hat{G}_{\text{in}} = \mathcal{F}G_{\text{in}}\mathcal{F}^\dagger$. We use that $(D - \hat{G}_{\text{in}}(\vec{\phi}))^{-1} = \text{adj}(D - \hat{G}_{\text{in}}(\vec{\phi}))/\det(D - \hat{G}_{\text{in}}(\vec{\phi}))$ where adj denotes the adjugate matrix [73], and we define $d(\vec{\phi}) = \det(D -$

$\hat{G}_{\text{in}}(\vec{\phi})$). As Γ_{in} is the covariance matrix of a system of maximally entangled states between nearest neighbors, its Fourier transform $\hat{G}_{\text{in}}(\vec{\phi})$ is built out of terms of the form $e^{i\phi_{1,2}}$ only. Thus, $d(\vec{\phi}) = \det(D - \hat{G}_{\text{in}}(\vec{\phi}))$ and $\text{adj}(D - \hat{G}_{\text{in}}(\vec{\phi}))$ are polynomials of low order in $\phi_{1,2}$. As B and A are local operators, we see that p and q are polynomials of low degree as well.

Now we are in a position to show that every translationally invariant fPEPS is the ground state of a local Hamiltonian. To this end we define the Hamiltonian $H = i \sum_{kl} h_{kl} c_k c_l$, where h is defined through its representation in reciprocal lattice space via $\hat{h}(\vec{\phi}) = d(\vec{\phi})\hat{\Gamma}_{\text{out}}(\vec{\phi})$, where $\hat{\Gamma}_{\text{out}}(\vec{\phi})$ is obtained from $\hat{G}_{\text{out}}(\vec{\phi})$ with the help of Eq. (4.24):

$$\hat{\Gamma}(\vec{\phi}) = \frac{1}{d(\vec{\phi})} \begin{pmatrix} 0 & \text{Re}(q(\vec{\phi})) & -\text{Im}(q(\vec{\phi})) & p(\vec{\phi}) \\ -\text{Re}(q(\vec{\phi})) & 0 & p(\vec{\phi}) & \text{Im}(q(\vec{\phi})) \\ \text{Im}(q(\vec{\phi})) & -p(\vec{\phi}) & 0 & \text{Re}(q(\vec{\phi})) \\ -p(\vec{\phi}) & -\text{Im}(q(\vec{\phi})) & -\text{Re}(q(\vec{\phi})) & 0 \end{pmatrix}. \tag{4.28}$$

Then, since $\hat{\Gamma}_{\text{out}}(\vec{\phi})$ and $\hat{h}(\vec{\phi})$ are diagonal in the same basis, H has the state with covariance matrix Γ_{out} as its ground state (c.f. Sec. 2.1.3), and unless H is gapless — corresponding to zeros of $d(\vec{\phi})$ — the ground state is unique. Moreover, since the degree of $p(\vec{\phi})$ and $q(\vec{\phi})$ is bounded by twice the number of virtual modes per site, it follows that H is local.

4.5 Example of a critical fPEPS

Let us now give an example of a local Hamiltonian which has a critical fPEPS as its exact ground state. We start giving the channel description of the fPEPS, and prove then its criticality by showing that the state has polynomially decaying correlation functions. Further, we give the explicit form of a parent Hamiltonian of this fPEPS. Finally, we express the channel in terms of local projectors, relating the channel description to the construction of fPEPS introduced in Sec. 4.2.

Construction of the example

We consider the class of Gaussian fPEPS defined above and use the trick of calculating the output state with the help of the Fourier transformed CM of the output state, $\hat{G}_{\text{out}}$ (4.27). Before giving the form of the channel, we calculate the covariance matrix of the entangled bonds, $\Gamma_{\text{in}} = \bigoplus \omega_{h,v}$, where $\omega_{h,v}$ is the covariance matrix of an entangled horizontal or vertical bond:

$$\omega_{h,v} = \text{circ}(0,1,0,\ldots) \otimes X - \text{circ}(0,\ldots,0,1) \otimes X^T, \quad X = \begin{pmatrix} 0 & \sigma_x \\ 0 & 0 \end{pmatrix}, \tag{4.29}$$

where σ_x denotes the Pauli x-matrix. Here we have ordered the modes according to $(c_\alpha^{(1)}, c_\alpha^{(2)}, c_\beta^{(1)}, c_\beta^{(2)})$ resp. $(c_\gamma^{(1)}, c_\gamma^{(2)}, c_\delta^{(1)}, c_\delta^{(2)})$ for the horizontal resp. vertical bonds.

$\mathrm{circ}(x_1,\ldots,x_n)$ denotes the circulant matrix, where $x_1,\ldots,x_n$ are the entries of the first row. The Fourier transform of $\omega_{h,v}$ is given by

$$\hat{\omega}_{h,v} = \mathcal{F}\omega_{h,v}\mathcal{F}^\dagger = \bigoplus_{\phi_{1,2}} X e^{i\phi_{1,2}} - X^T e^{-i\phi_{1,2}}. \tag{4.30}$$

Then, when grouping the modes for each lattice site according to $(c_\alpha^{(1)}, c_\alpha^{(2)}, c_\beta^{(1)}, c_\beta^{(2)}, c_\gamma^{(1)}, c_\gamma^{(2)}, c_\delta^{(1)}, c_\delta^{(2)})$, the Fourier transformed covariance matrix of the bonds, $\hat{G}_{\mathrm{in}} = \mathcal{F}\Gamma_{\mathrm{in}}\mathcal{F}^\dagger$ becomes block diagonal, i.e. $\hat{G}_{\mathrm{in}} = \bigoplus_{\vec{\phi}} \hat{G}_{\mathrm{in}}(\vec{\phi})$, where

$$\hat{G}_{\mathrm{in}}(\vec{\phi}) = \begin{pmatrix} 0 & -e^{i\phi_1}\sigma_x & 0 & 0 \\ e^{i\phi_1}\sigma_x & 0 & 0 & 0 \\ 0 & 0 & 0 & -e^{i\phi_2}\sigma_x \\ 0 & 0 & e^{i\phi_2}\sigma_x & 0 \end{pmatrix}. \tag{4.31}$$

Now we give the explicit form of the channel describing the local map, $\mathcal{G} = \bigoplus_{\vec{n}} \tilde{\mathcal{G}}_{\vec{n}}$, where the direct sum is taken over all lattice sites with coordinates $\vec{n}$, and take the modes ordered as $(c_a^{(1)}, c_a^{(2)}, c_\alpha^{(1)}, c_\alpha^{(2)}, c_\beta^{(1)}, c_\beta^{(2)}, c_\gamma^{(1)}, c_\gamma^{(2)}, c_\delta^{(1)}, c_\delta^{(2)})$. We take a translationally invariant channel, i.e. $\tilde{\mathcal{G}}_{\vec{n}} \equiv \tilde{\mathcal{G}}\ \forall \vec{n}$. Referring to Eq. (4.20), $\tilde{\mathcal{G}}$ has blocks of the following form:

$$\begin{aligned} A &= \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \qquad B = \frac{1}{2}\begin{pmatrix} 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & -1 & -1 \end{pmatrix} \\ D &= \frac{1}{4}\begin{pmatrix} 0 & 0 & 2 & 2 & 1 & -1 & 1 & -1 \\ 0 & 0 & 2 & 2 & -1 & 1 & -1 & 1 \\ -2 & -2 & 0 & 0 & 1 & -1 & 1 & -1 \\ -2 & -2 & 0 & 0 & -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 & 0 & 0 & 2 & 2 \\ 1 & -1 & 1 & -1 & 0 & 0 & 2 & 2 \\ -1 & 1 & -1 & 1 & -2 & -2 & 0 & 0 \\ 1 & -1 & 1 & -1 & -2 & -2 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{4.32}$$

With the help of (4.24) we arrive at

$$\hat{\Gamma}_{\mathrm{out}} = \bigoplus_{\vec{\phi}} \frac{1}{d(\vec{\phi})} \begin{pmatrix} 0 & q(\vec{\phi}) & 0 & p(\vec{\phi}) \\ -q(\vec{\phi}) & 0 & p(\vec{\phi}) & 0 \\ 0 & -p(\vec{\phi}) & 0 & q(\vec{\phi}) \\ -p(\vec{\phi}) & 0 & -q(\vec{\phi}) & 0 \end{pmatrix}, \tag{4.33}$$

where the functions p, q and d are given by

$$p(\vec{\phi}) = \sin(\phi_1) - \sin(\phi_2), \tag{4.34}$$

$$q(\vec{\phi}) = \cos(\phi_1)\cos(\phi_2), \tag{4.35}$$

$$d(\vec{\phi}) = 1 - \sin(\phi_1)\sin(\phi_2). \tag{4.36}$$

In the next step we show that this fPEPS describes a critical system.

Decay of the correlation functions

We prove criticality by considering the asymptotic behavior of the correlation functions in position space. For large systems we can replace the discrete Fourier transform by a continuous one. Let $\xi = p, q$ and define

$$\xi_{n_1,n_2} \equiv \langle i c^{(1)}_{(1,1)} c^{(y_\xi)}_{(n_1,n_2)} \rangle = \frac{1}{(2\pi)^2} \int_0^{2\pi} \frac{\xi(\phi_1,\phi_2)}{d(\phi_1,\phi_2)} e^{in_1\phi_1} e^{in_2\phi_2} d\phi_1 d\phi_2, \tag{4.37}$$

where $y_p = 1$ and $y_q = 2$ for p- and q-correlations respectively. We make the substitution $z = e^{i\phi_1}$ so that $dz = iz d\phi_1$, and arrive at

$$\frac{p(z,\phi_2)}{d(z,\phi_2)} = i\frac{z^2 - 1 - 2iz\sin\phi_2}{2iz - (z^2-1)\sin\phi_2}, \tag{4.38}$$

$$\frac{q(z,\phi_2)}{d(z,\phi_2)} = i\frac{(z^2+1)\cos\phi_2}{2iz - (z^2-1)\sin\phi_2}. \tag{4.39}$$

Then ξ_{n_1,n_2} can be written as

$$\xi_{n_1,n_2} = \frac{1}{2\pi} \int_0^{2\pi} d\phi_2 e^{in_2\phi_2} I^{(\xi)}_{n_1,n_2}(\phi_2), \tag{4.40}$$

$$I^{(\xi)}_{n_1,n_2}(\phi_2) = \frac{1}{2\pi i} \oint_C dz \frac{\xi(z,\phi_2)}{d(z,\phi_2)} z^{n_1-1}, \tag{4.41}$$

where C is the closed loop on the unit circle in the complex plane. Since $d(z,\phi_2)^{-1}$ has poles at $z_\pm = i\left(1 \pm |\cos\phi_2|\right)/\sin\phi_2$ and p as well as q are holomorphic at $z_\pm$, the integral $I^{(\xi)}_{n_1,n_2}(\phi_2)$ is proportional to the residue within C according to the residue theorem. As only z_- lies within the unit circle we obtain

$$I^{(\xi)}_{n_1,n_2}(\phi_2) = \frac{\xi(z_0,\phi_2)}{\partial_z d(z,\phi_2)|_{z=z_0}}. \tag{4.42}$$

In the following we give a detailed calculation of these integrals.

Calculation of p-correlations With the help of (4.38) we obtain

$$\begin{aligned} I^{(p)}_{n_1,n_2}(\phi_2) &= \frac{1}{2\pi i} \oint_C dz\, i\frac{z^2 - 1 - 2iz\sin\phi_2}{2iz - (z^2-1)\sin\phi_2} z^{n_1-1} \\ &= i^{n_1+1}(1 - |\cos\phi_2|)^{n_1} \frac{|\cos\phi_2|}{(\sin\phi_2)^{n_1+1}}. \end{aligned}$$

The p-correlations are obtained via (4.40):

$$\begin{aligned} p_{n_1,n_2} &= \frac{1}{2\pi} \int_0^{2\pi} d\phi_2\, e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2) \\ &= \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} d\phi_2\, e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2) + \frac{1}{2\pi} \int_{\pi/2}^{3/2\pi} d\phi_2\, e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2) \\ &= \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} d\phi_2\, e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2) + e^{in_2(\phi_2+\pi)} I^{(p)}_{n_1,n_2}(\phi_2+\pi). \end{aligned} \tag{4.43}$$

The symmetry $I^{(p)}_{n_1,n_2}(\phi_2+\pi) = (-1)^{n_1+1} I^{(p)}_{n_1,n_2}(\phi_2)$ leads to

$$p_{n_1,n_2} = \frac{1}{2\pi}(1-(-1)^{n_1+n_2}) \int_{-\pi/2}^{\pi/2} d\phi_2 \; e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2). \tag{4.44}$$

For $\phi_2 \in [-\pi/2, \pi/2]$ we have $|\cos\phi_2| = \cos\phi_2$. Then $I^{(p)}_{n_1,n_2}(\phi_2)$ simplifies to the following expression:

$$I^{(p)}_{n_1,n_2}(\phi_2) = i^{n_1+1} \frac{\cos\phi_2}{1-\cos\phi_2} \left(\tan\frac{\phi_2}{2}\right)^{n_1+1}. \tag{4.45}$$

Note that $I^{(p)}_{n_1,n_2}(-\phi_2) = (-1)^{n_1+1} I^{(p)}_{n_1,n_2}(\phi_2)$. For n_1 even (odd) $I^{(p)}_{n_1,n_2}(\phi_2)$ is an odd (even) function, and only the sine (cosine)-part of the exponential $e^{in_2\phi_2}$ gives a non-vanishing contribution. This corresponds to the real part of the integral, and hence

$$p_{n_1,n_2} = \frac{1}{2\pi}(1-(-1)^{n_1+n_2}) 2\mathrm{Re}\left[\int_0^{\pi/2} d\phi_2 \; e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2)\right]. \tag{4.46}$$

Calculation of q-correlations Application of the residue theorem results in

$$\begin{aligned} I^{(q)}_{n_1,n_2}(\phi_2) &= \frac{1}{2\pi i}\oint_C dz \; i\frac{(z^2+1)\cos\phi_2}{2iz-(z^2-1)\sin\phi_2} z^{n_1-1} \\ &= i^{n_1-1}\frac{(1-|\cos\phi_2|)^{n_1}}{(\sin\phi_2)^{n_1+1}}\cos\phi_2. \end{aligned}$$

Using $I^{(q)}_{n_1,n_2}(\phi_2+\pi) = (-1)^{n_1} I^{(q)}_{n_1,n_2}(\phi_2)$ we obtain

$$q_{n_1,n_2} = \frac{1}{2\pi}(1+(-1)^{n_1+n_2}) \int_{-\pi/2}^{\pi/2} d\phi_2 \; e^{in_2\phi_2} I^{(q)}_{n_1,n_2}(\phi_2). \tag{4.47}$$

For $\phi \in [-\pi/2, \pi/2]$ we have $I^{(p)}_{n_1,n_2}(\phi_2) = -I^{(q)}_{n_1,n_2}(\phi_2)$, resulting in

$$q_{n_1,n_2} = -\frac{1}{2\pi}(1+(-1)^{n_1+n_2}) 2\mathrm{Re}\left[\int_0^{\pi/2} d\phi_2 \; e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2)\right]. \tag{4.48}$$

Asymptotic behavior of the integral To prove criticality we are interested in the asymptotic behavior of the integral

$$J_{n_1,n_2} = \int_0^{\pi/2} d\phi_2 \; e^{in_2\phi_2} I^{(p)}_{n_1,n_2}(\phi_2). \tag{4.49}$$

The correlations are symmetric under the exchange of n_1 and n_2. This follows from translational invariance and can also be seen directly from the form of $p(\phi_1,\phi_2)$ and $q(\phi_1,\phi_2)$. Hence, to determine the asymptotic behavior, we can assume wlog.

b) n_1+n_2 odd ($q=0$)			
n_2	1	n_1	$2n_1$
$p(n_1)$	n_1^{-2}	n_1^{-3}	n_1^{-2}

a) n_1+n_2 even ($p=0$)			
n_2	1	n_1	$2n_1$
$q(n_1)$	n_1^{-3}	n_1^{-2}	n_1^{-2}

Table 4.1: Asymptotic decay of the correlation functions p and q along the axes ($n_2=1$), the diagonal ($n_2=n_1$) and in the direction $n_2=2n_1$.

$n_1 \gg 1$. In this limit, the absolute value of $I^{(p)}_{n_1,n_2}(\phi_2)$ attains its maximum for $\phi_2 = \pm\arccos(1/n-1) \to \pi/2$. We rewrite

$$I^{(p)}_{n_1,n_2}(\phi_2) = i^{n_1+1} c(\phi_2) e^{(n_1+1)t(\phi_2)},$$

where $c(\phi_2) = \frac{\cos\phi_2}{1-\cos\phi_2}$ and $t(\phi_2) = \log\left(\tan\frac{\phi_2}{2}\right)$ and expand $c(\phi_2)$ and $t(\phi_2)$ around $\pi/2$:

$$\frac{\cos\phi_2}{1-\cos\phi_2} = -\left(\phi_2-\frac{\pi}{2}\right) + \left(\phi_2-\frac{\pi}{2}\right)^2 + \mathcal{O}\left((\phi_2-\frac{\pi}{2})^3\right), \tag{4.50}$$

$$\log\left(\tan\frac{\phi}{2}\right) = \left(\phi_2-\frac{\pi}{2}\right) + \frac{1}{6}\left(\phi_2-\frac{\pi}{2}\right)^3 + \mathcal{O}\left((\phi_2-\frac{\pi}{2})^5\right). \tag{4.51}$$

Substituting $\phi_2 \to \phi_2 - \frac{\pi}{2}$ the integral attains the form

$$J_{n_1,n_2} = i^{n_1+n_2+1}\int_{-\pi/2}^{0} d\phi_2 J(n_1,n_2,\phi_2), \tag{4.52}$$

$$J(n_1,n_2,\phi_2) = e^{in_2\phi_2}\left(-\phi_2+\phi_2^2\right) e^{(n_1+1)\phi_2+\phi_2^3/6(n_1+1)}(1+\mathcal{O}(\phi_2^3)). \tag{4.53}$$

We use $J_{n_1,n_2} = \int_{-\infty}^{0} d\phi_2 J(n_1,n_2,\phi_2) - \int_{-\infty}^{-\pi/2} d\phi_2 J(n_1,n_2,\phi_2)$, and obtain

$$\int_{-\infty}^{0} d\phi_2 J(n_1,n_2,\phi_2) = \frac{3+n_1+in_2}{(1+n_1+in_2)^3} + \mathcal{O}\left(\frac{1}{n_1^4},\frac{1}{n_2^4}\right),$$

while the second integral can be bounded by

$$\left|\int_{-\infty}^{-\pi/2} d\phi_2 J(n_1,n_2,\phi_2)\right| \leq e^{-(n_1+1)\pi/2}\left|\int_{-\infty}^{-\pi/2} d\phi_2 e^{1/6(n_1+1)\phi_2^3}\left(-\phi_2+\phi_2^2\right)\left(1+\mathcal{O}\left(\phi_2^3\right)\right)\right|.$$

This gives rise to only an exponentially small correction that can be neglected in the asymptotic limit. Summarizing, we see that the p-correlations are non-vanishing

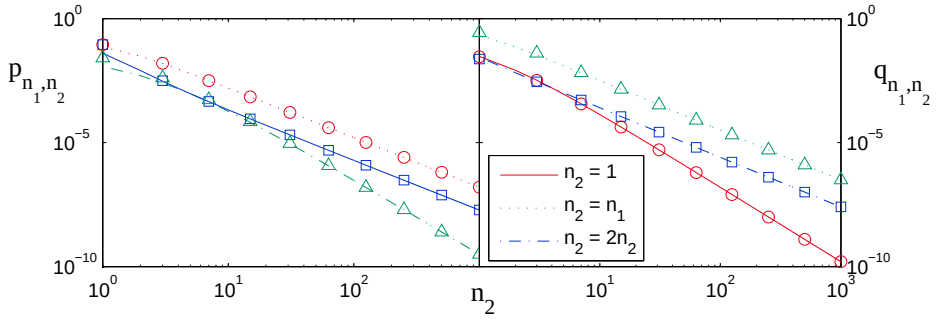

Figure 4.9: Exact value and asymptotic scaling of the correlations $p_{n_1,n_2} = \langle ic^{(1)}_{(1,1)} c^{(1)}_{(n_1,n_2)} \rangle$ (left) and $q_{n_1,n_2} = \langle ic^{(1)}_{(1,1)} c^{(2)}_{(n_1,n_2)} \rangle$ (right) in direction of the axis ($n_2 = 1$, red), along the diagonal ($n_2 = n_1$, green) and along the direction $(n_1, 2n_1)$ (blue). We conclude criticality of the system from the polynomial decay of the correlations.

only for $n_1 + n_2$ odd, while q-correlations are non-vanishing only for $n_1 + n_2$ even:

$$p_{n_1,n_2} \sim (1 - (-1)^{n_1+n_2}) \operatorname{Re}\left(\frac{3 + n_1 + in_2}{(1 + n_1 + in_2)^3}\right), \tag{4.54}$$

$$q_{n_1,n_2} \sim (1 + (-1)^{n_1+n_2}) \operatorname{Im}\left(\frac{3 + n_1 + in_2}{(1 + n_1 + in_2)^3}\right). \tag{4.55}$$

Table 4.1 summarizes the asymptotic behavior of p and q for $n_2 = 1, n_2, 2n_1$. In Fig. 4.9 we have plotted the asymptotic scaling and the exact value for the correlations obtained via numerical integration for three different directions along the lattice. The algebraic decay of the correlation functions implies criticality of the system. Hence, we have found the ground state of a critical system obeying an area law. To understand why this is no contradict the violation of the area law expected for particle number conserving free fermionic systems [155, 156] we determine next the explicit form of the parent Hamiltonian.

Calculation of the parent Hamiltonian

As we have explained in Sec. 4.4, the parent Hamiltonian H of an fPEPS with covariance matrix $\hat{\Gamma}_{\text{out}}(\vec{\phi})$ is given by $H = \sum_{kl} h_{kl} c_k c_l$, where h is defined through its representation in reciprocal lattice space via $\hat{h}(\vec{\phi}) = d(\vec{\phi})\hat{\Gamma}_{\text{out}}(\vec{\phi})$. Using the form of $\hat{\Gamma}_{\text{out}}$ given in (4.33) and the relations

$$\begin{aligned} i\hat{c}^{(1)}_{\vec{\phi}} \hat{c}^{(2)}_{\vec{\phi}} &= 1 - 2\hat{a}^\dagger_{\vec{\phi}} \hat{a}_{\vec{\phi}}, \\ i\left(\hat{c}^{(1)}_{\vec{\phi}} \hat{c}^{(2)}_{-\vec{\phi}} + \hat{c}^{(2)}_{\vec{\phi}} \hat{c}^{(1)}_{-\vec{\phi}}\right) &= 2\left(\hat{a}^\dagger_{\vec{\phi}} \hat{a}^\dagger_{-\vec{\phi}} - \hat{a}_{\vec{\phi}} \hat{a}_{-\vec{\phi}}\right), \end{aligned}$$

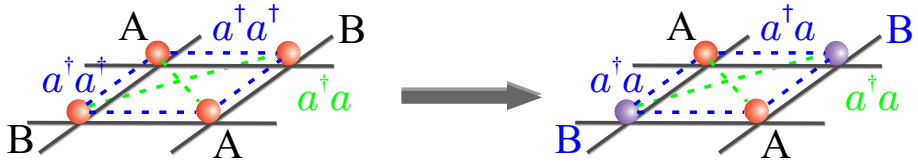

Figure 4.10:
Critical Hamiltonian $H_{\rm crit}$. Hopping of the form $a_x^\dagger a_y$ occurs along the diagonals, while non number conserving operators $a_x^\dagger a_y^\dagger$ act along the edges (left). Applying a particle-hole transformation on the B sublattice, $H_{\rm crit}$ can be converted into a number conserving Hamiltonian with hopping terms along the edges and the diagonals (right).

we obtain the Hamiltonian in position space:

$$H = 4\sum_{\vec{\phi}\geq 0} p(\vec{\phi})\left(\hat{a}^\dagger_{\vec{\phi}}\hat{a}^\dagger_{-\vec{\phi}} - \hat{a}_{\vec{\phi}}\hat{a}_{-\vec{\phi}}\right) + 4q(\vec{\phi})\left(1 - \hat{a}^\dagger_{\vec{\phi}}\hat{a}_{\vec{\phi}} - \hat{a}^\dagger_{-\vec{\phi}}\hat{a}_{-\vec{\phi}}\right). \tag{4.56}$$

We split the calculation:

$$\begin{aligned}
\sum_{\vec{\phi}} q(\vec{\phi})\hat{a}^\dagger_{\pm\vec{\phi}}\hat{a}_{\pm\vec{\phi}} &= \sum_{\vec{\phi},\vec{n}} \cos\left(\frac{2\pi}{N}k_1\right)\cos\left(\frac{2\pi}{N}k_2\right) e^{\pm\frac{2\pi}{N}i\vec{\phi}\vec{n}} e^{\mp\frac{2\pi}{N}i\vec{\phi}'\vec{n}'} a^\dagger_{\vec{n}} a_{\vec{n}'} \\
&= \frac{1}{4}\left(\delta_{n_1',n_1-1} + \delta_{n_1',n_1+1}\right)\left(\delta_{n_2',n_2-1} + \delta_{n_2',n_2+1}\right) a^\dagger_{\vec{n}} a_{\vec{n}'}, \\
\sum_{\vec{\phi}} p(\vec{\phi})\hat{a}^\dagger_{\vec{\phi}}\hat{a}^\dagger_{-\vec{\phi}} &= \sum_{\vec{\phi}} \left[\sin\left(\frac{2\pi}{N}k_1\right) - \sin\left(\frac{2\pi}{N}k_2\right)\right] e^{\frac{2\pi}{N}i\vec{\phi}\vec{n}} e^{\frac{2\pi}{N}i\vec{\phi}'\vec{n}'} a^\dagger_{\vec{n}} a^\dagger_{\vec{n}'} \\
&= \frac{1}{2i}\left[\delta_{n_1,n_1'}(\delta_{n_2',n_2-1} - \delta_{n_2',n_2+1}) + \delta_{n_2,n_2'}(\delta_{n_1',n_1-1} - \delta_{n_1',n_1+1})\right] a^\dagger_{\vec{n}} a^\dagger_{\vec{n}'},
\end{aligned}$$

and obtain a parent Hamiltonian of the form (see Fig. 4.10)

$$\begin{aligned}
H_{\rm crit} &= 2i\sum_{(h,v)} a^\dagger_{(h,v)}a^\dagger_{(h,v+1)} - a^\dagger_{(h,v)}a^\dagger_{(h+1,v)} + \text{h.c.} \\
&\quad - \sum_{(h,v)} a^\dagger_{(h,v)}(a_{(h+1,v+1)} + a_{(h+1,v-1)}) + \text{h.c.}.
\end{aligned}$$

As we have explained above, the ground state of H is unique unless $d(\vec{\phi}) = 0$. We see from (4.36) that we can ensure that by considering only N_h, N_v odd. Note that, although $H_{\rm crit}$ is not particle conserving, it can be converted into a particle conserving Hamiltonian via a simple particle–hole transformation in the B sublattice. This new Hamiltonian possesses a spectrum with a Dirac point separating the modes with positive and negative energies. Thus, the Fermi surface has zero dimension, which explains why our results do not contradict the violation of the area law expected for free fermionic systems [155, 156].

Calculation of the projectors

Finally we derive the form of the projectors

$$Q_{(h,v)} = \sum (A_{(h,v)})^{[k]}_{lrud} a^{\dagger k}_{(h,v)} \alpha^{l}_{(h,v)} \beta^{r}_{(h,v)} \gamma^{u}_{(h,v)} \delta^{d}_{(h,v)}, \tag{4.57}$$

corresponding to the channel (4.32). To this end we show that we can decompose the channel in an orthogonal transformation acting on the virtual modes followed by projecting the modes β, γ and δ on the vacuum. Finally, the remaining modes α are identified with the physical modes a. Summarizing, we want to show that

$$\mathcal{E}(\Gamma_{\text{in}}) = \mathcal{E}_{\text{vac},\beta,\gamma,\delta}(O\Gamma_{\text{in}}O^T),$$

where O is an orthogonal transformation and $\mathcal{E}_{\text{vac},\beta,\gamma,\delta}$ is the channel that maps the modes β, γ and δ on each site on the vacuum. Following [70], $\mathcal{E}_{\text{vac},\beta,\gamma,\delta}$ is represented by a covariance matrix $\mathcal{G}_0 = \bigoplus \tilde{\mathcal{G}}_0$, where the direct sum is taken over all lattice sites, and $\tilde{\mathcal{G}}_0$ is of the form (4.20) with

$$\begin{aligned} A_0 &= \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad B_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \\ D_0 &= \begin{pmatrix} \tilde{D}_0 & 0 \\ 0 & 0_2 \end{pmatrix}, \quad \tilde{D}_0 = \bigoplus_{j=1}^{3} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \end{aligned} \tag{4.58}$$

Then it follows by direct calculation that $B = B_0 O$, $D = O^T D_0 O$, where the orthogonal matrix O is of the form

$$O = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2\sqrt{6}} & -\frac{1}{2\sqrt{6}} & -\frac{1}{\sqrt{3}} & -\frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ -\frac{1}{2} & 0 & \frac{1}{2\sqrt{6}} & -\frac{1}{2\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ -\frac{1}{2} & 0 & -\frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{2\sqrt{3}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & \frac{1}{2} & -\sqrt{\frac{3}{8}} & \frac{1}{2\sqrt{6}} & -\frac{1}{2\sqrt{3}} & 0 & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \\ 0 & -\frac{1}{2} & -\sqrt{\frac{3}{8}} & -\frac{1}{2\sqrt{6}} & \frac{1}{2\sqrt{3}} & 0 & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} \\ 0 & -\frac{1}{2} & 0 & \sqrt{\frac{2}{3}} & -\frac{1}{2\sqrt{3}} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{\sqrt{6}} & \frac{1}{2\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}, \tag{4.59}$$

and $\mathcal{E}(\Gamma_{\text{in}}) = B_0(D_0 - O\Gamma_{\text{in}}O^T)^{-1}B_0^T + A_0$. Decomposing the channel in this way allows a calculation of the projector as follows: The orthogonal transformation O is a canonical transformation on the Majorana operators that has a unitary representation in Fock space, $c_k \mapsto c'_k = U c_k U^\dagger$, where

$$U = \exp\left[-\frac{1}{4}\sum_{k,l} u_{k,l} c_k c_l\right], \tag{4.60}$$

is unitary and $u = u^T$ is real. The matrix u can be obtained via the relation $Uc_kU^\dagger = (e^u c)_k$, implying $O = e^u$. The matrix elements of the projector can be obtained via the relation

$$\langle k|_a \langle 0|_{\beta,\gamma,\delta} U^\dagger |0\rangle_a \stackrel{!}{=} \sum A^k_{lrud} \langle 0|_a \langle 0|_{\alpha,\beta,\gamma,\delta} (a^\dagger)^k \alpha^l \beta^r \gamma^u \delta^d |0\rangle_a, \tag{4.61}$$

where $|k\rangle_a = \left(a^\dagger\right)^k |0\rangle_a$, and we have made, as explained above, the identification $\alpha \equiv a$ on the left side of the equation. In this way we obtain the following result:

$$\begin{array}{llll} A^0_{0000} = x_+, & A^0_{1111} = x_+, & & \\ A^0_{1010} = x_-, & A^0_{0110} = -x_+, & A^0_{0101} = -x_-, & A^0_{1001} = -x_+, \\ A^0_{1100} = x_+, & A^0_{0011} = x_+, & & \\ & & & \\ A^1_{1000} = x_-, & A^1_{0100} = -x_+, & A^1_{0010} = -x_+, & A^1_{0001} = -x_-, \\ A^1_{1110} = -x_+, & A^1_{1101} = -x_-, & A^1_{1011} = x_-, & A^1_{0111} = -x_+, \end{array} \tag{4.62}$$

where $x_\pm = (1 \pm i)/4$. As the channel is mapping a Gaussian input state to a Gaussian output state it is a Gaussian map and can thus be written as the exponential of a quadratic form in the modes:

$$Q = \exp\left[(i\alpha + \beta)(-\gamma + i\delta) + \alpha\beta + \gamma\delta + a^\dagger(-i\alpha - \beta - \gamma + i\delta)\right]. \tag{4.63}$$

4.6 Conclusion

Motivated by the success of PEPS for the description of spins we have introduced the class of fermionic Projected Entangled Pair States (fPEPS) in this Chapter. Theses states are obtained by applying fermionic linear maps to maximally entangled fermionic states placed between nearest neighbors. This construction resembles the construction of PEPS and is well suited to describe ground and thermal states of local fermionic Hamiltonians, both free and interacting, in the same way as PEPS are suited to describe ground states of local spin systems. We have then shown how fPEPS can be used for simulating fermionic systems, since they can be transformed into PEPS at the cost of only one additional horizontal bond between neighboring sites, and we have provided an explicit mapping for the corresponding tensors. Further, we have investigated the role of fPEPS as ground states of local Hamiltonians. To this end, we have introduced Gaussian fPEPS and shown that they naturally arise as ground states of quasi-free local Hamiltonians. Finally, we have used these tools to demonstrate the existence of local free fermionic Hamiltonians which are critical without violating the area law. One might ask if it is also possible to find fPEPS with low bond dimension that are the exact ground state of more complicated Hamiltonians, e.g. the Hubbard type Hamiltonians that we will encounter in the next Chapter. This is a line of research we pursue at the moment.

Chapter 5

Interacting Fermionic Systems in Generalized Hartree-Fock Theory

In the last Chapter we have constructed a new family of fermionic states, the fPEPS, well suited for the description of physical systems with local interaction. We have explained that all ground and thermal states of these systems can be approximated arbitrarily well by an fPEPS as long as the bond-dimension D is taken large enough. For numerical applications the bond dimension becomes the main bottleneck, since the number of multiplications required for the contraction of the tensor network on an $L\times L$ lattice scales as $\sim L^2D^{12}$ [145]. Hence, the development of an approximation technique tailored to the system under investigation might be another promising approach. In this Chapter we take this route to study strongly correlated fermionic many-body systems with two-body interaction, all described by a Hamiltonian

$$H = -\sum_{kl} t_{kl} a_k^\dagger a_l + \sum_{klmn} u_{klmn} a_k^\dagger a_l^\dagger a_m a_n. \tag{5.1}$$

These models are used among others for the description of superconductivity in BCS-theory, the Kondo effect or, most prominently, the Hubbard model [161]

$$H_{\text{Hubbard}} = -\sum_{x,y,\sigma} t_{xy} a_{x\sigma}^\dagger a_{y\sigma} + \sum_x u_x n_{x\uparrow} n_{x\downarrow} + \sum_{x,\sigma} \mu_{x\sigma} n_{x\sigma}. \tag{5.2}$$

The Hubbard model describes fermions with two different spin states ($\sigma =\uparrow,\downarrow$) on a lattice that can tunnel between sites x and y, and have attractive ($u_x < 0$) or repulsive ($u_x > 0$) interaction. The tunneling Hamiltonian $H_{\text{hopp}} = -\sum_{x,y\sigma} t_{xy} a_{x\sigma}^\dagger a_{y\sigma}$ as well as the interaction Hamiltonian $H_{\text{int}} = \sum_x u_x n_{x\uparrow} n_{x\downarrow}$ alone are easy to analyze. However, the sum of the two terms and their interplay with the filling $\sum_{x,\sigma} \mu_{x\sigma} n_{x\sigma}$ is believed to describe many fascinating effects of condensed-matter physics, and we just give a brief overview on various possible phases of this model. More details can be found e.g. in [162]. In the attractive regime, and for equal spin population the Hubbard model describes e.g. superfluids or Luther-Emery liquids that exhibit exponential decay of spin correlations For imbalanced spin population the appearance of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-phase is predicted [163, 164, 165].

This is a superfluid phase of Cooper pairs with non-vanishing center-of-mass momentum. In the repulsive regime ($u_x > 0$) the Hubbard model can exhibit e.g. Mott insulator, ferromagnetic and antiferromagnetic phases [166]. Current experiments with ultra cold fermionic quantum gases allow the realization of the Hubbard model in optical lattices, giving hope to gain further insight into interesting properties of the model [18], like the BEC-BCS crossover. Due to its immense importance for the understanding of fermionic many-body systems the Hubbard model has undergone an intense theoretical investigation in recent years (see e.g. [167] for a review). This includes the exact solution for certain instances of the model in $1D$ by Lieb and Wu [168, 169] or exactly solvable Gaudin-Yang-models using the Bethe ansatz and generalizations thereof (see e.g.[170, 171, 172, 173, 174]). In all other cases, we have to confine ourselves to numerical approximation schemes, like Density-Matrix-Renormalization Group (DMRG) [175, 176] or Quantum Monte Carlo (QMC) [177] techniques. While DMRG works only in one dimension, QMC for fermions leads to negative probabilities, known as the fermioic sign problem. Another approach uses special trial wave functions like Gutzwiller [178] or projected wave functions (see e.g. [179, 180, 181]).

One prominent approach for approximating ground and thermal states of the Hubbard model is the Hartree-Fock theory, where the energy for an N-particle system is minimized with respect to a Slater determinant formed from N orthonormal one-particle functions. The Slater determinant will break certain symmetries of the system, like translational or rotational invariance. One might think of using other trial wave functions that break other symmetries of the systems. One possible idea is to give up particle number conservation using a grand canonical ensemble, as it is done, for example, in the BCS-theory of superconductivity. The states that are now allowed as variational ansatz states are the fermionic Gaussian states we have already encountered at different points throughout this Thesis. Since the Slater determinants used in Hartree-Fock theory are a special case of this approach, the variational approach within the set of fermionic Gaussian states is a known as generalized Hartree-Fock theory (gHFT). This approach has been applied by Lieb [43] to the Hubbard model, deriving analytic solutions for gHF ground and thermal states. Though being exact, these results involve complicated optimization conditions that are hard to solve numerically for big systems without translational invariance and periodic boundary conditions.

In this Chapter we show how to overcome these problems by developing numerical techniques allowing the determination of ground and thermal states in generalized Hartree-Fock theory applicable to large systems governed by any Hamiltonian of the form (5.1). In order to make this Chapter self-contained we start with a short summary of the properties of fermionic Gaussian states that are necessary for the understanding of the Chapter in Sec. 5.1. This brief review also allows us to argue why we believe that the gHFT is very well suited to capture the physical properties of the Hubbard model. Then we derive in Sec. 5.2 consistent equations for real time evolution in gHFT. These can be seen as an analogue of the Gross-Piteavskii equations [182] long known for bosons. This result is of special interest as dynamical experiments on many-body systems have become possible in recent years,

among others Hanbury-Brown-Twiss experiments [183] or BEC-BCS crossover experiments [46]. These evolution equations further motivate the determination of the gHF ground state via an approach closely related to the known technique of imaginary time evolution, which we explain in Sec. 5.3. A slightly different approach is taken in Sec. 5.4, where we show how the finite temperature gHF states can be found using a fixed-point iteration. We close the Chapter with an application of our techniques to the two-dimensional translationally invariant Hubbard model in Sec. 5.5, and compare our results for ground and thermal state to the exact solutions derived in [43].

5.1 Toolbox of generalized Hartree-Fock Theory

In this Section we summarize the tools necessary for the understanding of this Chapter. Our goal is to find the ground and thermal states as well as the dynamics of a system governed by the Hamiltonian H given in (5.1). We approach the problem in the Majorana picture and define $c_k = a_k^\dagger + a_k$, $c_{k+M} = (-i)(a_k^\dagger - a_k)$, where M is the number of modes and $k = 1, \ldots, M$. These operators satisfy the canonical anti-commutation relations (CAR) $\{c_k, c_l\} = 2\delta_{kl}$. The Hamiltonian H in this picture is given by

$$H(T,U) = i\sum T_{kl} c_k c_l + \sum_{klmn} U_{klmn} c_k c_l c_m c_n = H_{\text{hopp}} + H_{\text{int}}, \tag{5.3}$$

where $T_{kl}, U_{klmn} \in \mathbb{R}$. The CAR allow to antisymmetrize T and U such that $T^T = -T$ while U is antisymmetric under the exchange of any adjacent indices. Gaussian states are fully characterized by their second moments collected in the real and anti-symmetric covariance matrix (CM) $\Gamma_{kl} = \langle \frac{i}{2}[c_k, c_l] \rangle$ from which all higher correlations can be obtained via Wick's theorem:

$$i^p \text{tr}[\rho c_{j_1} \ldots c_{j_{2p}}] = \text{Pf}(\Gamma|_{j_1 \ldots j_{2p}}), \tag{5.4}$$

where $1 \leq j_1 < \ldots < j_{2p} \leq 2M$ and $\Gamma_{j_1,\ldots,j_{2p}}$ is the corresponding $2p \times 2p$ submatrix of Γ. $\text{Pf}(\Gamma_{j_1,\ldots,j_{2p}})^2 = \det(\Gamma_{j_1,\ldots,j_{2p}})$ is called the Pfaffian. Γ is the CM of a physical state iff $i\Gamma \leq \mathbb{1}$, while pure states have to fulfill $\Gamma^2 = -\mathbb{1}$. Every Gaussian state is the ground state of a quadratic Hamiltonian $H_Q = i\sum_{kl} h_{kl} c_k c_l$, with real and antisymmetric Hamiltonian matrix h. All Gaussian states remain Gaussian under the time evolution governed by a quadratic Hamiltonian, and the CM transforms according to $\Gamma(t) = O(t)\Gamma(0)O(t)^T$, where $O(t) = e^{th/4}$ is an orthogonal transformation.

We argue now why we believe that the gHFT is well suited for an approximation of physical properties of the Hubbard model. It has been proven in Ref. [43] Thm. 2.9 that the generalized HF ground states of all interacting two-body Hamiltonians are pure states. Further, as we know from the results of [75] and Appendix A every pure Gaussian state can be brought into a standard form $|\Psi\rangle = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|0\rangle$, where $|u_k|^2 + |v_k|^2 = 1 \ \forall k$. But these are exactly the states used to derive the properties of superfluids in BCS theory. Further, if for all k either $u_k = 0$ or $v_k = 0$, then we can arrive at a product state of particles with either zero, one,

or two particles with opposite spin at each lattice site. Thus, the pure Gaussian states capture two extreme cases of the Hubbard model, the Mott phase as well as the superfluid phase, and are hence good candidates as variational states for that model.

5.2 Real time evolution

In the following we derive equations capturing the dynamics of a system governed by an interaction Hamiltonian of the form (5.3) in gHFT. The key idea is to use the covariance matrix for the description of the dynamical evolution. In the Heisenberg picture, where the time evolution of the Majorana operators is given by $c_k(t) = e^{iH(T,U)t}c_k e^{-iH(T,U)t}$, the covariance matrix evolves according to

$$\frac{d}{dt}\Gamma_{\alpha\beta}(t) = \langle [c_\alpha(t)c_\beta(t), H(T,U)]\rangle. \tag{5.5}$$

As $H(T,U)$ involves terms quartic in the Majorana operators this evolution clearly takes us out of the Gaussian setting. We truncate this transformation imposing that Wick's theorem holds, i.e. we write

$$\langle c_i c_j c_k c_l\rangle = -(\Gamma_{ij}\Gamma_{kl} - \Gamma_{ik}\Gamma_{jl} + \Gamma_{il}\Gamma_{jk}). \tag{5.6}$$

With the help of the commutation relation

$$[c_\alpha c_\beta, c_i c_j] \;=\; 2(c_i c_\alpha \delta_{j\beta} - c_i c_\beta \delta_{j\alpha} - c_\beta c_j \delta_{i\alpha} + c_\alpha c_j \delta_{i\beta})$$

we can calculate the contributions for the hopping and the interaction term to be

$$\begin{aligned}\langle [c_\alpha c_\beta, H_{\text{hopp}}]\rangle &= 4[T,\Gamma]_{\alpha\beta},\\ \langle [c_\alpha c_\beta, H_{\text{int}}]\rangle &= 24[\text{tr}_B[U\Gamma],\Gamma]_{\alpha\beta},\end{aligned}$$

where we have defined $\text{tr}_B[U\Gamma]_{ij} = \sum_{kl} U_{ijkl}\Gamma_{lk}$. This implies the following time evolution for the covariance matrix:

$$\dot\Gamma_{\alpha\beta}(t) = 4[\bar h(\Gamma(t)),\Gamma(t)]_{\alpha\beta}, \tag{5.7}$$

$$\bar h(\Gamma(t)) = T + 6\text{tr}_B[U\Gamma(t)]. \tag{5.8}$$

This equation can be formally integrated:

$$\begin{aligned}\Gamma(t) &= O(t)\Gamma(0)O(t)^T,\\ O(t) &= \mathcal{T}\exp\left(4\int_0^t \bar h(\Gamma(t'))dt'\right),\end{aligned} \tag{5.9}$$

where $\mathcal{T}$ denotes the time ordering operator. Note that due to the anti-symmetry of $\bar h(\Gamma(t'))$ Eq. (5.9) guarantees that the matrix $O(t)$ is an orthogonal transformation. Hence, when starting with a valid covariance matrix $\Gamma(0)$, our approximation scheme ensures that we remain within the set of Gaussian states. Further, from what we

have said in Sec. 5.1 it follows that the dynamical evolution under the interaction Hamiltonian $H(T,U)$ can be understood as time evolution under a *quadratic but state-dependent* Hamiltonian

$$H_Q(\Gamma) \;=\; i\sum_{kl}\bar{h}(\Gamma(t))_{kl}c_kc_l. \tag{5.10}$$

Our approximation scheme does not only ensure that we always remain within the set of Gaussian states, but it also conserves energy and particle number, as we show in the following:

Conservation of the particle number Let H be a number conserving Hamiltonian, i.e. $[H,\hat{N}]=0$, and write the particle number operator as $\hat{N}=\sum_{i=k}^{M}a_i^\dagger a_i = \frac{M}{2}+\frac{i}{4}\sum_{kl}\tilde{N}_{kl}c_kc_l$, where $\tilde{N}_{kl}=\delta_{l,k+M}$ for $k=1,\ldots,M$ and $\tilde{N}_{kl}=\delta_{l,k-M}$ for $k=M+1,\ldots,2M$. Then

$$0=\mathrm{tr}[\rho[H,\hat{N}]]=\frac{i}{4}\sum_{kl}\tilde{N}_{kl}\langle[H,c_kc_l]\rangle=\frac{i}{4}\mathrm{tr}[\tilde{N}\dot{\Gamma}(t)]=-i\frac{d}{dt}\langle\hat{N}(t)\rangle.$$

Conservation of the energy For a closed system the energy should be a conserved quantity, too. Using Wick's theorem we can calculate the energy to be $E(t)=\mathrm{tr}[H\rho]=-\mathrm{tr}[(T+3\mathrm{tr}_B[U\Gamma])\Gamma]$. Then

$$\dot{E}(t) \;=\; \sum_{kl}\frac{\partial E}{\partial\Gamma_{kl}}\dot{\Gamma}_{kl}=4\mathrm{tr}[\bar{h}(\Gamma)[\bar{h}(\Gamma),\Gamma]]=0.$$

In conclusion, we have shown that the application of Wick's theorem to the evolution equation of a system governed by a two-body interaction Hamiltonian leads to a consistent dynamical equation that can be considered as the analogue of the Gross-Pitaevskii equation known for bosons [182]. The truncation of the evolution is equivalent to an evolution under an effective state-dependent quadratic Hamiltonian. The particle number as well as the energy remain conserved quantities within this approximation. In the following Section we will see that this approximation scheme leads to a dynamical equation for the determination of the ground state of the system.

5.3 Ground states

In principle, the ground state in generalized HF-theory can be found via a direct minimization

$$\min_{\rho\,\text{Gaussian}}\mathrm{tr}[H\rho]=\min_{i\Gamma\leq\mathbb{1}}\sum_{ij}\left\{T_{ij}\Gamma_{ij}-3\sum_{i,j,k,l}U_{ijkl}\Gamma_{ij}\Gamma_{kl}\right\}. \tag{5.11}$$

For the translationally invariant Hubbard model this problem could be reduced to an optimization over two parameters only [43]. Generically, this constrained quadratic

minimization problem is a daunting task. We attack this problem from a different perspective. A well-known approach for the determination of the ground state $|\phi_0\rangle$ of a Hamiltonian H is imaginary time evolution. Starting with an arbitrary initial state $|\Psi\rangle$, the application of the operator e^{-Ht} will result in the ground state for $t \to \infty$ as long as $|\Psi\rangle$ has non-vanishing overlap with $|\phi_0\rangle$. This can be seen directly by writing $|\Psi\rangle = \sum_i c_i |\phi_i\rangle$, where $|\phi_i\rangle$ and E_i are eigenvectors and the corresponding eigenvalues of H. Then

$$\frac{e^{-Ht}|\Psi\rangle}{\|e^{-Ht}|\Psi\rangle\|^{1/2}} = \frac{\sum_i e^{-E_i t} c_i |\phi_i\rangle}{\|e^{-Ht}|\Psi\rangle\|^{1/2}} \to |\phi_0\rangle \text{ for } t \to \infty. \tag{5.12}$$

Due to the exponential growth of the state space with the number of modes this approach can be applied to small systems only. The idea is to apply the Gaussian approximation, i.e. Wick's theorem, to derive an evolution equation for the covariance matrix which only scales quadratically with the number of modes. Starting with an arbitrary pure Gaussian state $\rho(0)$, the evolution under H in imaginary time,

$$\rho(t) = \frac{e^{-Ht}\rho(0)e^{-Ht}}{\mathrm{tr}[e^{-2Ht}\rho(0)]}, \tag{5.13}$$

clearly takes us out of the setting of Gaussian states. But we could discretize the evolution and find for small time steps Δt the best Gaussian approximation at each step. However, due to the truncation it is not clear that this procedure will converge. And even if we find a steady state is is not clear that this will be the ground state of the system. Another possible approach is to use the quadratic but state-dependent effective Hamiltonian $H_Q(\Gamma)$ that is derived from $H(T, U)$ for the imaginary time evolution. As $H_Q(\Gamma)$ is a quadratic operator we will stay in the space of Gaussian states. But as the Hamiltonian is state-dependent it is the outcome of this procedure is not clear. But we are lucky, and we show in the next Subsections that both approaches are equivalent and lead indeed to the desired solution. To be precise, we show that the following is equivalent:

1. Direct minimization of the energy Eq. (5.11) in generalized Hartree-Fock theory.

2. Imaginary time evolution of the state ρ with the quartic Hamiltonian for small time steps Δt followed by an approximation of $\rho(t + \Delta t)$ by a Gaussian state.

3. Imaginary time evolution of ρ with the quadratic but state-dependent Hamiltonian $H_Q(\Gamma)$.

5.3.1 Minimization of the energy

In order to obtain the generalized Hartree-Fock ground state we have to solve the minimization problem

$$\min_{\rho \text{ Gaussian}} E(\rho) = \min_{\rho \text{ Gaussian}} \mathrm{tr}[H\rho] = \min_{i\Gamma \leq \mathbb{1}} \left\{ \sum_{ij} T_{ij}\Gamma_{ij} - 3 \sum_{i,j,k,l} U_{ijkl}\Gamma_{ij}\Gamma_{kl} \right\}. \tag{5.14}$$

The condition $i\Gamma \leq \mathbb{1}$ is fulfilled iff $\mathbb{1} - i\Gamma = (A + iB)(A + iB)^\dagger$, where A and B are real matrices, from which we derive

$$\Gamma = AB^T - BA^T, \tag{5.15}$$
$$\mathbb{1} = AA^T + BB^T. \tag{5.16}$$

The problem can be reformulated as an optimization problem using Lagrange multipliers. The Lagrangian is given by

$$\begin{aligned}\mathcal{L} &= \sum_{ij} T_{ij}(AB^T - BA^T)_{ij} - 3\sum_{ijkl} U_{ijkl}(AB^T - BA^T)_{ij}(AB^T - BA^T)_{kl} \\ &\quad + \sum_{i,k,l} \lambda_{kl}(A_{ki}A_{li} + B_{ki}B_{li} - \delta_{kl}),\end{aligned} \tag{5.17}$$

where $\lambda^T = \lambda$ are the Lagrange multipliers. The necessary condition for a local minimum are given by

$$\frac{\partial \mathcal{L}}{\partial A_{\alpha\beta}} = 2(\bar{h}B + \lambda A)_{\alpha\beta} = 0, \tag{5.18}$$
$$\frac{\partial \mathcal{L}}{\partial B_{\alpha\beta}} = 2(-\bar{h}A + \lambda B)_{\alpha\beta} = 0. \tag{5.19}$$

It has been proven in Ref. [43] that the HF ground state is always pure, i.e. $\Gamma^2 = -\mathbb{1}$. Using this information and (5.15) and (5.16) we arrive at the following necessary conditions for a minimum:

$$[\bar{h}(\Gamma), \Gamma] = 0, \tag{5.20}$$
$$\Gamma^2 = -\mathbb{1}. \tag{5.21}$$

These two equations are non-linear matrix equations and thus hard to solve, both analytically and numerically, for large systems. But we will see in the next Subsection that these equations appear as the steady-state conditions of imaginary time evolution.

5.3.2 Imaginary time evolution

From Eq. (5.13) we see that the evolution of the density operator ρ under the Hamiltonian H in imaginary time is given by

$$\dot{\rho}(t) = -\{H, \rho(t)\} + 2\rho(t)\mathrm{tr}[H\rho(t)], \tag{5.22}$$

so that the covariance matrix evolves according to

$$\dot{\Gamma}_{kl}(t) = -i\mathrm{tr}[\{H, c_k c_l\}\rho(t)] + 2i\Gamma_{kl}\mathrm{tr}[H\rho(t)]. \tag{5.23}$$

As we show in Appendix D both approaches for imaginary time evolution, number 2 and 3 described right before the beginning of Subsec. 5.3.1, lead to the same evolution equation of the covariance matrix:

$$-\frac{1}{4}\dot{\Gamma} = \Gamma\bar{h}(\Gamma)\Gamma + \bar{h}(\Gamma). \tag{5.24}$$

Starting from a pure Gaussian state both approaches ensure that we always remain in the set of pure Gaussian states. Thus $\Gamma(t+\Delta t) = O(t+\Delta t)\Gamma(t)O(t+\Delta t)^T$, where $O(t+\Delta t) = e^{A(t)\Delta t}$ is an orthogonal transformation, i.e. $A(t)^T = -A(t)$. Then

$$\Gamma(t+\Delta t) - \Gamma(t) = [A, \Gamma(t)]\Delta t + \mathcal{O}\left((\Delta t)^2\right) \stackrel{!}{=} -4(\Gamma\bar{h}\Gamma + \bar{h})\Delta t + \mathcal{O}\left((\Delta t)^2\right).$$

The solution of this equation is given by

$$O(t) = \mathcal{T}\exp\left[\int_0^t A(t')dt'\right], \tag{5.25}$$

$$A(t) = -2[\bar{h}(\Gamma), \Gamma]. \tag{5.26}$$

The steady-state is obtained for $O(t) = \mathbb{1}$ or equivalently $[\bar{h}(\Gamma), \Gamma] = 0$. But this is exactly the necessary condition for the generalized Hartree-Fock ground state derived in Eq. (5.20), while (5.21) holds true as we always stay in the set of pure states. Thus, instead of solving the highly non-linear matrix equations Eq. (5.20) and (5.21) we can solve Eq. (5.25) numerically and arrive at the ground state.

5.4 Thermal states

As we have seen in the last Section, the generalized Hartree-Fock ground state can be obtained via an imaginary time evolution. To learn about the finite temperature properties in gHFT we have to consider the approximation to the Gibbs state $\rho \sim e^{-\beta H}$, where $\beta = \frac{1}{k_B T}$ is the inverse temperature. We recall that the Gibbs state minimizes the free energy, $F(\rho) = E(\rho) - \beta^{-1}S$. Thus, we have to solve

$$\min_{\rho \text{ Gaussian}} F(\rho) = \min_{\rho \text{ Gaussian}} \left\{E(\rho) - \beta^{-1}S(\rho)\right\}.$$

An expression for the energy has already been given in Eq. (5.14). For the calculation of the entropy we consider a one-mode Gaussian state in its standard form

$$\rho = \frac{e^{-\beta a^\dagger a}}{1+e^{-\beta}} = \frac{1+\lambda}{2}|0\rangle\langle 0| + \frac{1-\lambda}{2}|1\rangle\langle 1|, \tag{5.27}$$

where $\pm i\lambda$ are the eigenvalues of the covariance matrix Γ. The entropy $S = -\mathrm{tr}[\rho \ln \rho]$ is given by

$$S(\rho) = \ln 2 - \frac{1}{2}\left[(1-\lambda)\ln(1-\lambda) + (1+\lambda)\ln(1+\lambda)\right], \tag{5.28}$$

so that for M modes we have

$$S = M\ln 2 - \frac{1}{2}\mathrm{tr}\left[(\mathbb{1} + i\Gamma)\ln(\mathbb{1} + i\Gamma)\right]. \tag{5.29}$$

Thus, using (5.14) the generalized HF Gibbs state is obtained via the following minimization problem:

$$\min_{\rho \text{ Gaussian}} F(\rho) =$$
$$\min_{i\Gamma \leq \mathbb{1}} \left\{ -\mathrm{tr}[(T + 3\mathrm{tr}_B[U\Gamma])\Gamma] - \beta^{-1} \left(M \ln 2 - \frac{1}{2}\mathrm{tr}[(\mathbb{1} + i\Gamma)\ln(\mathbb{1} + i\Gamma)] \right) \right\}.$$

In analogy to the minimization of the energy in Sec. 5.3.1 we use Eqs. (5.15) and (5.16) to transform this minimization problem into an optimization with Lagrange multipliers $\lambda = \lambda^T$ and Lagrangian

$$\mathcal{L} = E(A,B) - \beta^{-1} S(A,B) - \sum_{i,j} \lambda_{ij}(AA^T + BB^T - \delta_{ij}). \tag{5.30}$$

Here, $E(A,B)$ is as in Eq. (5.11). Since we have already done the optimization of the energy term in Sec. 5.3.1, we consider now to the entropy term. With the help of $\ln(\mathbb{1} - X) = -\sum_{k=1}^{\infty} \frac{1}{k} X^k$ (see e.g. [184]) we obtain

$$\mathrm{tr}[(\mathbb{1} + i\Gamma)\ln(\mathbb{1} + i\Gamma)] = -\sum_{k,l} \frac{1}{k}(-i)^k (\Gamma^k + i\Gamma^{k+1})_{ll}.$$

Taking the derivative of the entropy wrt. to Γ_{mn} we arrive at

$$\frac{\partial S}{\partial \Gamma_{mn}} = \left[-\frac{i}{2}(\mathbb{1} - i\Gamma) \sum_{k=0}^{\infty} (i\Gamma)^k + \frac{i}{2} \sum_{k=1}^{\infty} \frac{1}{k} (i\Gamma)^k \right]_{mn} = -\frac{i}{2} \left[\mathbb{1} + \ln(\mathbb{1} - i\Gamma) \right]_{mn},$$

where we have made use of the formula $(\mathbb{1} - X)^{-1} = \sum_{k=0}^{\infty} X^k$ [184]. Then we obtain the following necessary conditions for a minimal entropy:

$$[h_F(\Gamma), \Gamma] = 0, \tag{5.31}$$
$$h_F(\Gamma)(\mathbb{1} + \Gamma^2) = 0, \tag{5.32}$$
$$h_F(\Gamma) = \bar{h} - \frac{i}{4\beta} \ln \frac{\mathbb{1} + i\Gamma}{\mathbb{1} - i\Gamma}. \tag{5.33}$$

It has been proven in Thm. 2.8 of Ref. [43] that the quasi-free state minimizing the free energy is always a Gibbs-state of the form $\rho \sim \exp[-\beta^{-1} h_A]$, where h_A is a quadratic operator on a finite Hilbert space. Since we consider the finite temperature case, i.e. $\beta < \infty$ this implies that Eq. (5.32) can be fulfilled only for $h_F = 0$ leading to the following implicit equation for the covariance matrix:

$$\Gamma = i \tanh\left[2i\beta \bar{h}(\Gamma) \right]. \tag{5.34}$$

This equation can be solved numerically via a fixed-point iteration.

5.5 Application: The $2d$-Hubbard-Model

As a benchmark, we apply the numerical methods derived in the last Sections to the two-dimensional translationally invariant Hubbard model with attractive interaction. The Hamiltonian of the system is given by

$$H_- = \sum_{x,y\in\Lambda,\sigma} t_{x,y}^{\text{hopp}} a_{x,\sigma}^\dagger a_{y,\sigma} - u\sum_{x\in\Lambda}\left(n_{x\uparrow}-\frac{1}{2}\right)\left(n_{x\downarrow}-\frac{1}{2}\right) - \mu\sum_{x,\sigma} n_{x,\sigma}, \tag{5.35}$$

where x and y are points on the two-dimensional lattice Λ, and $\sigma = \uparrow, \downarrow$ denotes the spin degree of freedom. The hermitian $|\Lambda|\times|\Lambda|$ matrix t^{hopp} is called *hopping matrix*. In the following we take t^{hopp} to be real and consider nearest-neighbor hopping, i.e. $t_{xy}^{\text{hopp}} = \tau$ when x and y are nearest-neighbors, and $t_{xy}^{\text{hopp}} = 0$ otherwise. For $u > 0$ the second term in H_- is an attractive on-site interaction between particles of opposite spin. Further, we have included a chemical potential μ. In Ref. [43] it is shown that in this case the ground state energy as well as the free energy of the Gibbs state can be obtained via a two-parameter optimization of the *pressure functional*

$$\begin{aligned}&\mathcal{P}(\beta,\mu) = (2\beta^{-1}\ln 2 + \mu)|\Lambda| \\ &- \min_{d^2\le\eta}\left\{-2\beta^{-1}\text{tr}\left[\ln\cosh\frac{\beta}{2}\sqrt{(t^{\text{hopp}}-\mu\mathbb{1})^2 - 2ud(t^{\text{hopp}}-\mu\mathbb{1}) + u^2\eta}\right] + u\eta|\Lambda|\right\}.\end{aligned} \tag{5.36}$$

The free energy is related to this functional via $F(\beta,\mu) = -\mathcal{P}(\beta,\mu)$, while the ground state energy $E(\mu)$ can be obtained when taking the limit $\beta\to\infty$:

$$E(\mu) = \min_{d^2\le\eta}\left\{-\text{tr}\left[\sqrt{(t^{\text{hopp}}-\mu\mathbb{1})^2 - 2ud(t^{\text{hopp}}-\mu\mathbb{1}) + u^2\eta}\right] + u\eta|\Lambda|\right\} - \mu|\Lambda|. \tag{5.37}$$

We consider a 10×10 lattice and compare our numerical values for the ground state energy as well as the free energy to the results obtained via the optimization of (5.36) and (5.37). We set the strength of hopping as the energy scale of the system, i.e. $\tau = 1$, and we take $\mu = 0$.

Ground state energy To obtain the ground state energy we use imaginary time evolution according to Eq. (5.25), i.e. $\Gamma(t) = O(t)\Gamma_0 O(t)^T$, where

$$\begin{aligned} O(t) &= \mathcal{T}\exp\left[\int_0^t A(t')dt'\right], \\ A(t) &= -2[\bar{h}(\Gamma),\Gamma], \end{aligned}$$

and $\bar{h}(\Gamma) = T + 6\text{tr}_B[U\Gamma(t)]$. We discretize the time-ordered integral, such that $O(t+\Delta t) = e^{A(t)\Delta t}O(t)$, and expand the exponential to first order,

$$e^{A\Delta t} = \frac{\mathbb{1}+\frac{1}{2}A\Delta t}{\mathbb{1}-\frac{1}{2}A\Delta t} + \mathcal{O}\left((\Delta t)^2\right),$$

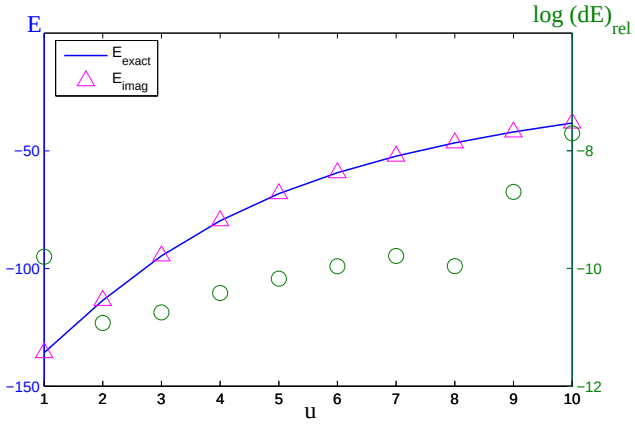

Figure 5.1: Generalized Hartree-Fock ground state energy E_0 for the two-dimensional translationally invariant Hubbard model (c.f. Eq. (5.35)) with attractive interaction on a 10×10 lattice for $\tau = 1$, $\mu = 0$ and $u \in [1, 10]$. The red line shows the exact gHF ground state energy, E_{exact}, obtained from Eq. (5.37), while the triangles correspond to the energy obtained via imaginary time evolution, E_{imag} (c.f. text for the details of the numerical realization). The relative error, $(dE)_{\text{rel}}$, is plotted in logarithmic units.

which ensures that $O(t + \Delta t)$ is orthogonal. Starting from a covariance matrix Γ_0 of an arbitrary pure state, we evolve for a time $10^5 \Delta t$, where $\Delta t = 10^{-3}$. In Fig. 5.1 we compare this approach (triangles) to the exact solution given by Eq. (5.37) (red line) for an interaction strength $u = 1, 2, \ldots, 10$. We find excellent agreement of the ground state energy obtained via imaginary time evolution, $E_{\text{imag}}(u)$, and the exact solution, $E_{\text{exact}}(u)$, with a relative error (green circles) upper bounded by $(dE)_{\text{rel}} = |E_{\text{imag}} - E_{\text{exact}}|/|E_{\text{exact}}| < 2 \cdot 10^{-8}$.

Free energy The gHF Gibbs state is given by the implicit equation (5.34), derived in Sec. 5.4:

$$\Gamma = i \tanh \left[2i\beta \bar{h}(\Gamma) \right] .$$

We start either at a) $\beta = \infty$, i.e. we take the ground state of the system (which can be obtained for example via the minimization of the energy explained above), or b) at $\beta = 0$, i.e. we take the maximally mixed state $\rho \sim \mathbb{1}$, as the initial state for the iteration. Then we change the temperature in steps $\Delta\beta$ and obtain the new Gibbs state via a fixed-point iteration. In Fig. 5.2 we give the results for both approaches, taking as an example an interaction strength of $u = -6$, a temperature $\beta \in [0, 1]$, and change β in steps $\Delta\beta = 0.01$. Again, we have set the hopping energy as the energy scale of the system, i.e. we take $\tau = 1$, and take zero chemical potential. For a better visualization of the result we have added a model independent term to the free energy, plotting $F^* = F + 2\beta^{-1} \ln 2|\Lambda|$. The blue line depicts the exact solution, F^*_{exact}, obtained from the minimization of the pressure functional Eq. (5.36), while the triangles show the numerical solution, F^*_{num}. We also show the relative error

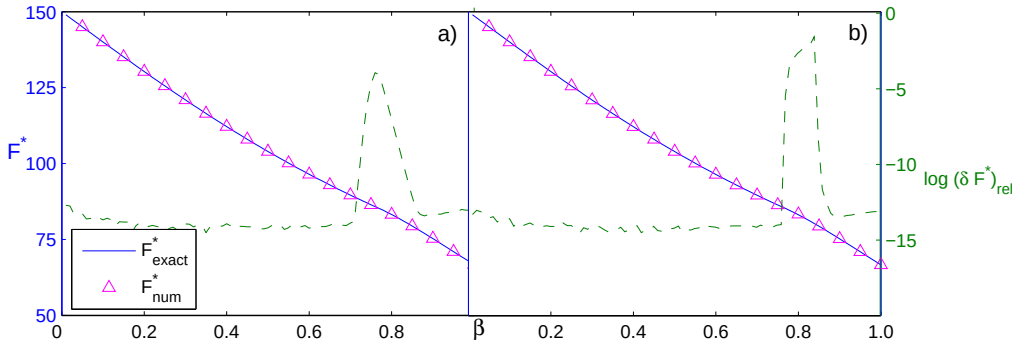

Figure 5.2: Comparison of the exact solution for the free energy in generalized Hartree-Fock theory (blue line) with the numerical solution of Eq. (5.34) (triangles) via a fixed point iteration starting from a) the ground state and $\beta = 1$, b) the completely mixed state and $\beta = 0$. For a better visualization of the result we have plotted $F^* = F + 2\ln 2\beta^{-1}|\Lambda|$. We take $\tau = 1$, $u = -6$ and $\mu = 0$. The green dotted line shows the relative error of the numerical solution compared to the exact result in logarithmic units (c.f. text for an explanation of the error peak).

$dF^*_{\mathrm{rel}} = |F^*_{\mathrm{exact}} - F^*_{\mathrm{num}}|/|F^*_{\mathrm{exact}}|$ in logarithmic units. There is excellent agreement of our approach with the exact solution. However, we find a slightly bigger error in a region of $\beta \approx 0.8$. We argue now why this discrepancy might occur. As it has been shown in Ref. [43], whenever $(t^{\mathrm{hopp}} - \mu\mathbb{1})$ is unitarily equivalent to $-(t^{\mathrm{hopp}} - \mu\mathbb{1})$ and $1 < \frac{u}{|\Lambda|}\mathrm{tr}[|t^{\mathrm{hopp}} - \mu\mathbb{1}|^{-1}] \leq \infty$ holds true, the pressure defined in (5.36) is non-analytic at a finite critical temperature β_c uniquely determined via

$$1 = \frac{u}{2|\Lambda|}\mathrm{tr}\left[\left|t^{\mathrm{hopp}} - \mu\mathbb{1}\right|^{-1}\tanh\left(\frac{\beta_c}{2}\left|t^{\mathrm{hopp}} - \mu\mathbb{1}\right|\right)\right]. \tag{5.38}$$

Since in our case $\mu = 0$ and t^{hopp} is antisymmetric, we find a critical temperature $\beta_c \approx 0.77$, and it is exactly in the region around β_c that we see the increased deviation of F^*_{num} from the exact solution. The numerical accuracy might be improved by decreasing $\Delta\beta$ or taking a higher accuracy for the fixed-point iteration. Currently, we stop the iteration process for a fixed temperature as soon as $||\Gamma_n(\beta) - \Gamma_{n+1}(\beta)|| < 10^{-6}$. Another idea is to take for each value of β the minimal value of approach a) and b).

Since the translationally invariant two-dimensional Hubbard model is only a benchmark for our numerical routines, we do not investigate these ideas in more detail here. Summarizing, we can state that the numerical methods developed in the last Sections allow in general the determination of the ground state energy as well as the Gibbs free energy for our toy model to very high accuracy. These results give hope that we can successfully apply our procedures to physically relevant scenarios as well. Further, we learn that more care has to be taken in parameter regimes where quantum phase transitions occur, and we have suggested possible approaches to achieve solution of high accuracy in these regions as well.

5.6 Conclusion

Summarizing, we have developed numerical methods to approximate the time evolution and the ground and thermal states of finite fermionic systems with arbitrary two-body interaction, $H(T,U) = i\sum T_{kl}c_k c_l + \sum_{klmn} U_{klmn}c_k c_l c_m c_n$, in any dimension. Our approach makes use of the generalized Hartree-Fock theory, where pure and mixed quasi-free states are used as variational input states such that the whole problem can be considered on the level of the covariance matrices.

The dynamical evolution of the system within this approximation leads to an evolution equation of the covariance matrix that can be seen as an analogue of the Gross-Pitaevskii equation known for bosons. The solution of this equation is given by a time-dependent orthogonal transformation of the CM that can be easily implemented numerically. Furthermore, this evolution is equivalent to the dynamics of a system governed by a *quadratic but state-dependent* Hamiltonian $H_Q(\Gamma)$. This result is a starting point to attack the problem of finding the variational ground state via an imaginary time evolution with $H_Q(\Gamma)$. The dynamical evolution we can derive for the CM in that way can be reformulated as a time-dependent orthogonal transformation as well, and leads to a steady-state that is indeed the gHF ground state. In case of thermal states the minimization of the free energy leads to an implicit equation for the covariance matrix that allows a solution using a fixed-point iteration.

So far we have performed first numerical applications of our methods to the translationally invariant $2D$ Hubbard model with attractive interaction at half filling, since this problem has been reduced to a simple optimization problem in [43]. For a 10×10 lattice we have obtained results for the ground state energies in a regime of $u/\tau \in [0, 10]$, and we have seen that our results are in excellent agreement with the exact solution. In the case of thermal states, we have considered an interaction strength $u = -6$ in a temperature region $\beta \in [0, 1]$, and have found excellent agreement with the results of [43]. However, we have seen slightly bigger errors in a parameter regime where the model exhibits a quantum phase transition

The application of the framework presented in this Chapter to physically relevant scenarios, where, e.g., translational invariance is broken, and its numerical optimization is work in progress [45]. One important goal is to investigate regimes of the Hubbard model away from half-filling where exotic quantum phases, like the FFLO-phase, are expected to arise.

Chapter 6

Conclusions and Outlook

Fermionic particles are the basic building blocks of matter, and their quantum correlations are central to many fascinating physical effects. In this Thesis we have investigated a broad range of topics related to these systems from the perspective of quantum information theory.

The first part of this Thesis, Chapter 2, is devoted to conceptual considerations regarding quantum correlations in fermionic many-body systems. So far there have been various attempts to adapt the framework of entanglement theory developed for distinguishable spin-systems to a system of indistinguishable particles, none of which has lead to a conclusive result. Thus, in our approach to characterize correlations in these systems we use a different approach, taking the well-established notion of "paired" fermions in solid state and condensed matter systems as a starting point to develop a pairing theory for fermionic systems. Starting from a minimal list of requirements a paired state should fulfill we propose a definition of pairing, and develop methods for its detection and quantification applicable to current experiments. Our approach is guided by concepts and tools known in entanglement theory, like convex sets or witness operators. Further, we show that pairing is distinct from any of the existing notions of quantum correlations introduced for systems of indistinguishable particles. In addition, we show that pairing is a resource for high-precision phase estimation. Most remarkably, certain instances of the BCS-states of superconductivity, that are all captured as paired by our definition, can be proven to allow quantum metrology at the Heisenberg limit.

The idea to come up with a pairing theory for fermions was initially motivated by current experiments on ultra cold quantum gases. We set as a goal the definition, detection and quantification of pairing, as well as to study its resource character and to find its relation with known concepts of quantum correlations in fermionic systems. We not only achieved all these goals, but in the course of our work we have encountered numerous questions for further investigations, and we just mention some of the most interesting ones. First, one might think of generalizing the notion of pairing to higher order correlations, what might lead to an understanding of the complete fermionic Fock space. Next, one could also take the other road and try to find finer characterizations of pairing, which could lead to equivalence classes of paired states that cannot be transformed into each other by certain phys-

ical transformations, in analogy to the GHZ- and W-states well known in quantum information theory. Furthermore, other methods for the detection of pairing might be developed. Especially, the concept of positive maps that has turned out so powerful in the spin-setting could not be applied successfully to fermions yet. Another possible way to follow is to try to come up with quantum information applications other than metrology where the pairing of fermions plays the role of the resource.

After these conceptual considerations, the second part of this Thesis, Chapters 3-5, is devoted to simulations of fermionic systems. The simulation of quantum mechanical systems falls into two big classes, namely simulation on a classical computer and quantum simulation. We start in Chap. 3 with the latter one, including bosonic and finite dimensional quantum systems in our investigations. Considering a translationally invariant lattice of arbitrary dimensions, we ask what time evolutions can and which cannot be be simulated given certain sets of translationally invariant Hamiltonians. Using the machinery of Lie algebras we can give a full characterization in the case of quasi-free bosonic and fermionic systems, while we can only derive no-go theorem in the case of spin systems. However, the technique of finding Hamiltonians that cannot be simulated with the help of Casimir operators might turn out useful for other questions in the field of quantum simulation.

Finally, we consider the simulation of fermionic systems with the help of algorithms tailored for a classical computer. In this case the exponential growth of the quantum mechanical state space generally demands for an approximation in the determination of ground and thermal states, as well as the time evolution of the system. One possible approach is the construction of a class of states that describe relevant physical systems with few parameters sufficiently well. To this end we introduce the family of fermionic Projected Entangled Pair States (fPEPS) in Chapter 4, that are the generalization of the Projected Entangled Pairs States (PEPS) known for spin systems. The fPEPS do not only approximate ground and thermal states of fermionic systems with local interaction well, they can also be mapped to the PEPS-representation by only doubling the number of parameters. Thus, the well-developed numerical tools of PEPS can also be used for the simulation of fermionic systems. The application of the fPEPS to numerical simulations is one major line of research to follow in the future. Another line of thought is the determination of fPEPS of low bond dimension that are the exact ground state of some fermionic system. In the case of quasi-free fermions we introduce the class of Gaussian fPEPS all of which turn out to be ground states of some short-range Hamiltonian. We provide an example of a critical fPEPS in two dimensions, which is remarkable, since only states with vanishing Fermi surface can fulfill an area law in $2D$. This example could be a starting point for finding further examples of this kind, and perhaps even to categorize critical free-fermionic systems. Currently, we are interested in finding fEPS that are ground states of local Hamiltonians with hopping and two-body interaction, and we could see first indications that such examples might exist.

Due to the rich structure of quantum phases described by the Hubbard model, its investigation has occupied physicists for decades. Since this model is realized in systems of ultra cold quantum gases in optical lattices, it is currently in the center of investigation both from a theoretical and experimental perspective. In the

final Chapter of this Thesis, Chap. 5, we develop a framework for the simulation of fermionic systems described by any Hamiltonian with two-body interaction. Starting from the idea of generalized Hartree-Fock theory (gHFT), where pure and mixed quasi-free states are taken as variational states, we could derive a dynamical evolution equation for the covariance matrix of the system that can be understood as an analogue of the Gross-Pitaevskii equation known for bosons. The gHF ground states can be found as steady-states of an imaginary time evolution of the covariance matrix (CM), while the CM of thermal states is given by an implicit equation solvable by a fixed-point iteration. Since the covariance matrix depends only polynomially on the number of modes, our approach can be applied to large physical systems as they appear in current experimental setups. We hope that the numerical application to the Hubbard model will give information on interesting quantum phases captured by this system, e.g. the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO)-states [44] in the regime of attractive interaction.

In conclusion, this Thesis presents important results for the understanding of fermionic systems and their correlations. The understanding gained by the introduction of the pairing theory and the possibilities for numerical simulation of fermionic many-body systems with the help of fPEPS and the formalism based on gHFT are the main results of our work. The interplay of quantum information science and condensed matter physics has turned out as a very fruitful approach for our investigations, and we hope that the interaction of these two different fields of physics will lead to many interesting insights in the future.

Appendix A

A standard form for pure fermionic Gaussian states

In the following we give a derive a standard form for all pure fermionic Gaussian states. After completing the proof we found out that this result had already been obtained in [75] and is known as Bloch-Messiah reduction. However, as we think that our derivation of the result is more transparent, we would like to present it here. Recall that in Sec. 2.1.3 we have introduced the complex representation of the covariance matrix given by

$$\Gamma_c = \frac{1}{4}\Omega^\dagger \tilde{\Gamma} \bar{\Omega} = \begin{pmatrix} Q & R \\ \bar{R} & \bar{Q} \end{pmatrix}, \tag{A.1}$$

where $Q_{kl} = \langle \frac{i}{2}[a_k, a_l] \rangle$, $R_{kl} = \langle \frac{i}{2}[a_k, a_l^\dagger] \rangle$ and $\bar{Q}$ denotes the complex conjugate. Note that $R^\dagger = -R$ and $Q^T = -Q$ and hence $\Gamma_c^T = -\Gamma_c$. Every anti-hermitian matrix can be diagonalized and every anti-symmetric complex matrix can be block-diagonalized by a unitary transformation. The following lemma gives a necessary and sufficient condition that Q and R can be (block-) diagonalized simultaneously:

Lemma A.1. *Let Q, R be complex $n \times n$ matrices and assume that $Q = -Q^T$ and $R = -R^\dagger$. Then $RQ = -Q\bar{R}$ if and only if there exists a unitary U such that*

$$UQU^T = \bigoplus_k q_k \sigma_y \equiv Q_0 \tag{A.2}$$

$$URU^\dagger = \bigoplus_k i r_k \mathbb{1}_2 \equiv R_0, \tag{A.3}$$

where σ_y is the Pauli y-matrix, and $q_k, r_k \in \mathbb{R}$.

Proof. If Q and R are in the standard form (A.2) and (A.3), then it follows immediately that $RQ = -Q\bar{R}$.

Now let $RQ = -Q\bar{R}$. As R is anti-hermitian, R can be diagonalized by a unitary U and has only complex eigenvalues, i.e.

$$RU = U \begin{pmatrix} ir_1 I_1 & & \\ & \ddots & \\ & & ir_m I_m \end{pmatrix},$$

where I_k is the identity on the eigenspace E_k of R corresponding to the eigenvalues ir_k. Let e_k be an eigenvector of R corresponding to the eigenvalues ir_k, i.e. $Rv_K = ir_k e_k$. Then $RQ\bar{e}_k = Q\bar{R}\bar{e}_k = ir_k Q\bar{e}_k$, and Qe_k is an eigenvector of R corresponding to the eigenvalue ir_k. Hence,

$$Q\bar{U} = U \begin{pmatrix} Q_1 & & \\ & \ddots & \\ & & Q_n \end{pmatrix},$$

where Q_k are block matrices and $\dim(Q_k) = \dim(E_k)$. Next, we show that the dimension of the eigenspaces of R is always even. To do so, note that $[Q\bar{Q}, R] = 0$, and hence $Q\bar{Q}$ and R are simultaneously diagonalizable: $XQ\bar{Q}X^\dagger = \mathrm{diag}(q_i)$ and $XRX^\dagger = \mathrm{diag}(ir_i)$, where X is unitary, and the eigenspaces of R and $Q\bar{Q}$ have the same dimension. Further, as Q is antisymmetric, there exists a unitary Y such that $YQY^T = \bigoplus_k q_k \sigma_y$. As a consequence, $Q\bar{Q} = Y \bigoplus_k (-q_k)\mathbb{1}_2 Y^\dagger$, i.e. the spectrum of $Q\bar{Q}$ as well as of R is doubly degenerate: $\dim(E_k) = 2d_k$. Now we are nearly done. As Q is antisymmetric, so are the blocks Q_i, and hence there exists a family V_i of unitary matrices of dimension $2d_i$ such that $V_i Q_i V_i^T = \bigoplus_k q_k^{(i)} \sigma_y$. Defining $W = \bigoplus_k V_k$ we find that $W^\dagger Q W^T = Q_0$ and $W^\dagger R W = R_0$. □

With this Lemma we are now in the position to state the following theorem about pure fermionic Gaussian states:

Theorem A.2. *For every pure fermionic Gaussian state $|\Psi\rangle$ there exists a basis of modes $\{a_k\}$ such that $|\Psi\rangle = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|0\rangle$, where $|u_k|^2 + |v_k|^2 = 1\ \forall k$.*

Proof. If $|\Psi\rangle = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|0\rangle$, then its covariance matrix $\Gamma_{c,kl} = \mathrm{tr}[i/2\rho[A_k, A_l]]$, where $A = (a_1, a_{-1}, \ldots, a_M, a_{-M}, a_1^\dagger a_{-1}^\dagger, \ldots)$ is of the form

$$\begin{aligned} \Gamma_c &= \begin{pmatrix} Q & R \\ \bar{R} & Q \end{pmatrix} \\ Q &= \bigoplus_k v_k \bar{u}_k \, \sigma_y, \quad R = \frac{i}{2} \bigoplus_k (1 - |v_k|^2). \end{aligned}$$

Now let Γ_c be the covariance matrix of a pure state, i.e.

$$\Gamma_c \Gamma_c^\dagger = \begin{pmatrix} QQ^\dagger + RR^\dagger & QR^T + RQ^T \\ \bar{R}Q^\dagger + \bar{Q}R^\dagger & \bar{R}R^T + \bar{Q}Q^T \end{pmatrix} = \frac{\mathbb{1}}{4}. \tag{A.4}$$

The equation is satisfied iff $QQ^\dagger + RR^\dagger = \frac{1}{4}\mathbb{1}$ and $Q\bar{R} = -RQ$. The last condition implies that Q and R can be (block-)diagonalized simultaneously and attain the standard form (A.2) and (A.3) according to lemma A.1. Hence, there exists a unitary U such that $UQU^T = \bigoplus_k q_k \sigma_y$ and $URU^\dagger = i \bigoplus_k r_k \mathbb{1}_2$. As $QQ^\dagger + RR^\dagger = \mathbb{1}/4$ must be fulfilled, we have the condition $4(|q_k|^2 + |r_k|^2) = 1 \forall k$. Define u_k and r_k via $r_k = (1 - 2|v_k|^2)/2$ and $q_k = \bar{u}_k v_k$. Then we see that $|\Psi\rangle = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|0\rangle$ for some particular choice of basis. □

Appendix B

Proof of Thm. 2.23

In the following we provide all the details leading to Thm. 2.23, starting with the bound on separable states:

Lemma B.1. *Let $\rho \in S_{sep}$ with $tr[N_{op}\rho] = N$ and let $H(\{v_k\})$ be as in Thm. 2.23. Then* $\mathrm{tr}[H(\{v_k\})\rho_s] \geq 0$.

Proof. The operator H_k acts non-trivially only on the modes $a_k^\dagger, a_{-k}^\dagger, a_{k+M}^\dagger, a_{-(k+M)}^\dagger$. Denote by ρ_k the reduced density operator obtained when tracing out all but these four modes. According to Lemma 2.2, $\rho_k = \sum_{n=0}^4 \beta_k^{(n)} |n\rangle\langle n|$ is a convex combination of separable n-particle states $|n\rangle\langle n|$. We proved in Lemma 2.3 that $|\mathrm{tr}[(P_k^\dagger P_{k+M} + h.c.)\rho_s]| \leq 1/2$. Hence

$$\langle H(\{v_k\})\rangle \geq 2N(1-\epsilon) - 2\sum_{k=1}^{M}(|v_k|^2\langle N_k\rangle + \beta_k^{(2)}).$$

Now $2\beta_k \leq \langle N_k\rangle \leq 4$ and $|v_k|^2 \leq 1-\epsilon$ so that $|v_k|^2\langle N_k\rangle + \beta_k^{(2)}) \leq 4$. Due to the particle number constraint $\sum_{k=1}^M \langle N_k\rangle = N$ this value can be taken for $k = 1, \ldots, N/4$. Hence,

$$-2\sum_{k=1}^{M}(|v_k|^2\langle N_k\rangle + \beta_k^{(2)}) \geq -2\cdot 4(1-\epsilon)N/4$$

so that $\langle H(\{v_k\})\rangle \geq 0$. □

To show the witness character of $H(\{v_k\})$ we also have to prove that there exists a BCS state that is detected by the Hamiltonian. We will need the following theorem about the distribution described by the $|\lambda_N|^2$ in (2.20):

Theorem B.2. *Let $|\Psi_{Gauss}\rangle = \sum_{N=0}^M \lambda_N^{(M)} |\Psi_{BCS}^{(N)}\rangle$ like in (2.19), (2.21). If $\sum_{k=1}^M |u_k|^2|v_k|^2 = \mathcal{O}(N^\gamma)$ for some $\gamma > 0$, then in the limit $N \to \infty$ the $|\lambda_N|^2$ converge to a normal distribution,*

$$|\lambda_N|^2 = \frac{1}{\sqrt{2\pi}\sigma_{\bar{N}}} \exp\left[-\frac{(N-\bar{N})^2}{2\sigma_{\bar{N}}^2}\right],$$

where $2\bar{N} = 2\sum_{k=1}^{M} |v_k|^2$ *is the mean particle number for the variational state, and the variance is given by* $\sigma_{\bar{N}}^2 = 4\sum_{k=1}^{M} |v_k|^2|u_k|^2$.

Proof. For the proof we will need a theorem from probability theory known as Lyapunov's central limit theorem [185]:

Theorem B.3. *(Lyapunov's central limit theorem)*
Let $X_1, X_2, \ldots$ *be independent random variables with distribution functions* $F_1, F_2, \ldots$, *respectively, such that the expectation value* $E(X_n) = \mu_n$ *and the variance* $\mathrm{Var}(X_n) = \sigma_n^2$ *fulfill* $\mu_n, \sigma_n < \infty$ *and at least one* $\sigma_n > 0$. *Let* $S_n = X_1 + \cdots + X_n$ *and* $s_n = \sqrt{\mathrm{Var}(S_n)} = \sqrt{\sigma_1^2 + \cdots + \sigma_n^2}$. *If the Lyapunov condition*

$$\frac{1}{s_n^{2+\delta}} \sum_{k=1}^{n} E|X_k - \mu_k|^{2+\delta} \xrightarrow[n\to\infty]{} 0$$

is satisfied for some $\delta > 0$ *then the normalized partial sums* $\frac{S_n - ES_n}{s_n}$ *converge in distribution to a random variable with normal distribution with mean* $\mu = 0$ *and variance* $\sigma = 1$.

Consider the observables $X_k = n_k + n_{-k}$, $k = 1, \ldots, M$, where $n_{\pm k} = 0, 1$ is the number of particles with quantum numbers $\pm k$ respectively. The X_k can be considered as classical random variables since they commute mutually. In the variational BCS-state the random variable $S_M = \sum_{k=1}^{M} X_k$ is distributed according to the probability distribution

$$\begin{aligned} P(S_M = 2N) &= \sum_{k_1 < \ldots < k_M = 1}^{M} |v_{k_1}|^2 \ldots |v_{k_N}|^2 |u_{k_{N+1}}|^2 \ldots |u_{k_M}|^2 \\ &= \left(\prod_k |u_k|^2 \right) \sum_{k_1 < \ldots < k_M = 1}^{M} \frac{|v_{k_1}|^2 \ldots |v_{k_N}|^2}{|u_{k_1}|^2 \ldots |u_{k_N}|^2} \qquad \text{(B.1)} \\ &= \frac{|C|^2}{(N!)^2 |C_N|^2} = |\lambda_N^{(M)}|^2. \qquad \text{(B.2)} \end{aligned}$$

With the help of Thm. B.3 applied to the random variable S_M we can now complete the proof of Thm. B.2, i.e. show that $\lambda_N^{(M)}$ converges to a normal distribution for large M. We start calculating the expectation value μ_k of X_k. For a BCS-state, X_k takes the values $X_k = 0, 2$, as particles with quantum numbers $\pm k$ always appear in pairs. As

$$P(X_k = 0) = |u_k|^2, \quad P(X_k = 2) = |v_k|^2,$$

we get $\mu_k = 2|v_k|^2$ and

$$E(S_M) = 2\sum_k |v_k|^2 \equiv 2\bar{N}.$$

For calculating the variance, note that $X_k^2 = n_k^2 + n_{-k}^2 + 2n_k n_{-k} = 0, 4$, and

$$P(X_k^2 = 0) = |u_k|^2, \;\; P(X_k^2 = 4) = |v_k|^2.$$

Hence

$$\mathrm{Var}(X_k) = 4|u_k|^2|v_k|^2, \qquad s_M^2 = 4\sum_k |u_k|^2|v_k|^2.$$

To apply the central limit theorem, we consider $E(|X_k - \mu_k|^4)$. Using

$$P(|X_k - \mu_k|^4 = \mu_k^4) = |u_k|^2, \;\; P(|X_k - \mu_k|^4 = (2-\mu_k)^4) = |v_k|^2, \;\; \mu_k = 2|v_k|^2$$

we arrive at

$$\begin{aligned} E(|X_k - \mu_k|^4) &= 16|u_k|^2|v_k|^2(|u_k|^6 + |v_k|^6) \leq 16|u_k|^2|v_k|^2(|u_k|^2 + |v_k|^2) \\ &= 16|u_k|^2|v_k|^2. \end{aligned}$$

Setting $\delta = 2$ in the Lyapunov condition, we obtain

$$\frac{1}{s_M^4}\sum_{k=1}^{M} E(|X_k - \mu_k|^4) \leq \frac{4}{s_M^2} = \mathcal{O}(N^{-\gamma}) \to 0,$$

where we have applied the assumption of the theorem $\sum_{k=1}^{M} |v_k|^2|u_k|^2 = \mathcal{O}(N^\gamma)$ in the last step. The central limit theorem implies that S_M converges to a normal distribution with expectation values $2\bar{N} = 2\sum_k |v_k|^2$ and variance $\sigma_{\bar{N}}^2 = 4\sum_k |v_k|^2|u_k|^2$. □

With this result at hand we can prove the following:

Lemma B.4. *Let $H(\{v_k\})$ and $|\Psi_{BCS}^{(N)}\rangle$ be defined as in Thm. 2.23. If $\epsilon > 18/\sqrt{\pi\bar{N}}$, then*

$$\langle \Psi_{BCS,sym}^{(N)} | H(\{v_k\}) | \Psi_{BCS,sym}^{(N)} \rangle \;\; < 0.$$

Proof. We will use the correspondence of variational and number conserving BCS-states, deriving first a bound for $|\langle H(\{v_k\})\rangle_{\mathrm{Gauss}} - \langle H(\{v_k\})\rangle_N|$, where $|\Psi_{\mathrm{Gauss}}\rangle = \sum_{k=1}^{2M} \lambda_n |\Psi_{BCS,sym}^{(n)}\rangle$ with $|\Psi_{BCS,sym}^{(n)}\rangle$ like in Thm. 2.23. To do so, we will need that the $|\lambda_n|^2$ are normally distributed. From $|u_k|^2 = 1 - |v_k|^2 \geq \epsilon$ where $\epsilon > 18/(\sqrt{2\pi\bar{N}})$ and $\sum_{k=1}^{2M} |v_k|^2 = \bar{N}$, it follows that $\sigma_{\bar{N}} = \sum_{k=1}^{2M} |v_k|^2|u_k|^2 \geq \epsilon\bar{N} = \mathcal{O}(\sqrt{N})$. Hence, we know from Thm. B.2 that the $|\lambda_n|^2$ describe a normal distribution around $\bar{N} \approx N$ with standard deviation $\sigma_{\bar{N}}$.

Now, write $H(\{v_k\}) = H_0 - 2W + 2(1-\epsilon)\sum_{k=1}^{M} N_k$, where

$$\begin{aligned} H_0 &= -2\sum_{k=1}^{M} |v_k|^2 N_k, \\ W &= 2\sum_k P_k^\dagger P_{k+M} + P_{k+M}^\dagger P_k. \end{aligned}$$

We start with a bound for $|\langle H_0\rangle_{var} - \langle H_0\rangle_N| \leq T_1 + T_2$, where

$$\begin{aligned} T_1 &= \left| \sum_{\Delta\in[-\sigma_{\bar{N}}^2,\sigma_{\bar{N}}^2]} |\lambda_{N+\Delta}|^2 (\langle H_0\rangle_{N+\Delta} - \langle H_0\rangle_N) \right|, \\ T_2 &= \left| \sum_{\Delta\notin[-\sigma_{\bar{N}}^2,\sigma_{\bar{N}}^2]} (|\lambda_{N+\Delta}|^2 (\langle H_0\rangle_{N+\Delta} - \langle H_0\rangle_N) \right|. \end{aligned} \tag{B.3}$$

A bound for T_2 can be easily derived noting that

$$|\langle H_0\rangle_n - \langle H_0\rangle_{n'}| = 8 \left| \sum_k |v_k|^2 \left(\langle n_k\rangle_n - \langle n_k\rangle_{n'}\right) \right|, \tag{B.4}$$

and for $n = N + \Delta \geq N$ we have $\sum_k |v_k|^2(\langle n_k\rangle_n - \langle n_k\rangle_N) \leq \sum_k |v_k|^2\langle n_k\rangle_n \leq n$, as $|v_k|^2 \leq 1$. Hence,

$$\begin{aligned} T_2 &\leq 16 \left| \sum_{\Delta\notin[0,\sigma_{\bar{N}}^2]} |\lambda_{N+\Delta}|^2 |N+\Delta| \right| \\ &\leq 8\frac{\sigma_{\bar{N}}}{\sqrt{2\pi}} e^{-\sigma_{\bar{N}}^2/2} + 4N\left(1 - \mathrm{Erf}(\sigma_{\bar{N}}/\sqrt{2})\right) \\ &\leq 8\frac{\sigma_{\bar{N}}}{\sqrt{2\pi}} + 4N\left(1 - \mathrm{Erf}(\sigma_{\bar{N}}/\sqrt{2})\right), \end{aligned}$$

where we have approximated the sum by an integral in the second step. For bounding T_1, we will show first that for $n = N + \Delta$ where $\Delta \in [-\sigma_{\bar{N}}^2, \sigma_{\bar{N}}^2]$ we have $\langle n_k\rangle_n - \langle n_k\rangle_{n-1} \geq 0$. Expanding the BCS wave function

$$|\Psi_{BCS,sym}^{(n)}\rangle = C_n n! \sum_{j_1<\ldots<j_n=1}^{2M} \alpha_{j_1}\ldots\alpha_{j_n} P_{j_1}^\dagger \ldots P_{j_n}^\dagger |0\rangle,$$

the expectation value of the number operator is easily calculated to be $\langle n_k\rangle_n = |C_n|^2(n!)^2|\alpha_k|^2 S_k^{(n-1)}$, where

$$S_k^{(n)} = \sum_{\substack{j_1<\ldots<j_n=1 \\ j_i\neq k}}^{2M} |\alpha_{j_1}|^2 \ldots |\alpha_{j_n}|^2.$$

If $0 < |v_k|^2 \leq 1-\epsilon$, there exists a lower bound on the coefficients $|\alpha_k|^2 = |v_k|^2/\sqrt{1-|v_k|^2} \geq b \;\forall\; k$. Then $S_k^{(n-1)}$ and $S_k^{(n-2)}$ are related via

$$S_k^{(n-1)} \geq b\frac{2M-(n-1)}{n-1} S_k^{(n-2)}.$$

In the proof of Thm. B.2 we show that

$$\frac{|\lambda_n|^2}{|\lambda_{n-1}|^2} = \frac{|C_{n-1}|^2((n-1)!)^2}{|C_n|^2(n!)^2},$$

resulting in

$$\langle n_k\rangle_n - \langle n_k\rangle_{n-1} \geq \left(b\frac{2M-(n-1)}{n-1} - \frac{|\lambda_n|^2}{|\lambda_{n-1}|^2}\right)|C_n|^2(n!)^2|\alpha_k|^2 S_k^{(n-2)}.$$

For $n = N+\Delta$ and $\Delta \in [-\sigma_N^2, \sigma_N^2]$ the normal distribution of the $|\lambda_n|^2$ implies $|\lambda_n|^2/|\lambda_{n-1}|^2 = \exp[(2\Delta-1)/(2\sigma_N^2)] \leq e$. Hence,

$$b\frac{2M-(n-1)}{n-1} - \frac{|\lambda_n|^2}{|\lambda_{n-1}|^2} \geq 0 \Leftrightarrow b \geq e\frac{n}{2M-(n-1)} > 3\frac{n-1}{2M-(n-1)}.$$

For $M = q(n-1)$, this is equivalent to $|\alpha_k|^2 \geq 3/(2q-1)$, which can be achieved for $q \gg 1$. The last condition is satisfied, as we are considering dilute systems, where $M \gg \bar{N}$. Thus, $\langle n_k\rangle_n - \langle n_k\rangle_{n-1} \geq 0$, implying $\sum_k |v_k|^2(\langle n_k\rangle_n - \langle n_k\rangle_{n-1}) \leq 1$, as $|v_k|^2 \leq 1$. Using (B.4) and a telescope sum, we conclude that

$$T_1 \;\leq\; 8\left|\sum_{\Delta\in[-\sigma_{\bar{N}},\sigma_{\bar{N}}]}(|\lambda_{N+\Delta}|^2|\Delta|\right| \leq 8\left|\sum_{\Delta}|\lambda_{N+\Delta}|^2|\Delta|\right| = 16\frac{\sigma_{\bar{N}}}{\sqrt{2\pi}}.$$

Next, we derive the bound for the operator W. Its expectation value is given by

$$\langle W\rangle_n = |C_n|^2(n!)^2 2\sum_k |\alpha_k|^2 \sum_{\substack{j_1<\ldots<j_{n-1}\\ j_i\neq k,k+M}}^{2M} |\alpha_{j_1}|^2\ldots|\alpha_{j_{n-1}}|^2.$$

For $n \in [N-\Delta, N+\Delta]$, we use the same argumentation we have used for bounding $\langle n_k\rangle_n - \langle n_k\rangle_{n-1}$, to obtain

$$\langle W\rangle_n - \langle W\rangle_{n-1} \leq 2.$$

Further, $\langle n_k\rangle_n = \langle P_k^\dagger P_{k-M}^\dagger + h.c.\rangle_n/2 + \langle n_k n_{k+M}\rangle_n$ due to the symmetry $\alpha_k = \alpha_{k+M}$. Hence, $\langle W\rangle_n \leq 2n$. Thus, up to a factor of 2 we obtain the same bound as for H_0. Putting all the pieces together we find that

$$|\langle H(\{v_k\})\rangle_{var} - \langle H(\{v_k\})\rangle_N| \leq 2(1-\epsilon) + \frac{72}{\sqrt{2\pi}}\sigma_N + 12N\left(1-\mathrm{Erf}(\sigma_N/\sqrt{2})\right).$$

In the limit of large x, the error function $\mathrm{Erf}(x/\sqrt{2\pi})$ can be approximated by the following formula:

$$1-\mathrm{Erf}(x/\sqrt{2}) = 2\frac{\exp[-x^2/2]}{\sqrt{2\pi}}(x^{-1}-x^{-3}+\ldots).$$

As $\sigma_N = \mathcal{O}(\sqrt{N})$, we conclude

$$12N(1 - \mathrm{Erf}(\sigma_{\bar{N}}/\sqrt{2})) \leq \frac{24}{\epsilon\sqrt{2\pi}}\sigma_{\bar{N}} \exp[-\sigma_{\bar{N}}^2/2] \to 0$$

for $N \gg 1$. A straightforward calculation results in

$$\langle H(\{v_k\})\rangle_{var} = -4N\epsilon,$$

leading immediately to the statement of the theorem. □

Appendix C

Interferometry with paired states

In this Section we give the details for the derivation of the formulae used in Sect. 2.5.2. We start with some basic formula that will turn out useful later on.

Some useful formula

Notation We briefly summarize the notation necessary to follow the calculation. We use to different kinds of modes, a_k and b_k that are used to build the pair operators $P_k = a_k^\dagger a_{-k}^\dagger$ and $Q_k^\dagger = b_k^\dagger b_{-k}^\dagger$ and their equally weighted superpositions

$$p_M^\dagger = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} P_k^\dagger, \quad q_M^\dagger = \frac{1}{\sqrt{M}} \sum_{k=1}^{M} Q_k^\dagger.$$

The operators $p_M^\dagger$ and $q_M^\dagger$ fulfill the commutation relations

$$\begin{aligned} [p_M^\dagger, p_M] &= -1 + \frac{1}{M}\hat{N}_a \\ [q_M^\dagger, q_M] &= -1 + \frac{1}{M}\hat{N}_b, \end{aligned}$$

where $N_a = \sum_k (n_k + n_{-k})$, $N_b = \sum_k (m_k + m_{-k})$ and $n_k = a_k^\dagger a_k$, $m_k = b_k^\dagger b_k$. Further, we define states

$$\begin{aligned} |N\rangle_p^{(M)} &= c_N^{(M)} (p_M^\dagger)^N |0\rangle, \\ |N\rangle_q^{(M)} &= c_N^{(M)} (q_M^\dagger)^N |0\rangle, \end{aligned}$$

with normalization constant $c_N^{(M)}$ to be determined later.

Relation to angular momentum algebra Calculations for interferometric setups are often done with the help of angular momentum operators. We follow these lines by introducing the following set of operators:

$$J_x^{(M)} = \frac{1}{2}\left(p_M^\dagger q_M + p_M q_M^\dagger\right), \tag{C.1}$$

$$J_y^{(M)} = \frac{i}{2}\left(q_M^\dagger p_M - p_M^\dagger q_M\right), \tag{C.2}$$

$$J_z^{(M)} = \frac{1}{2}\left(p_M^\dagger p_M - q_M^\dagger q_M\right). \tag{C.3}$$

These operators fulfill the commutation relations

$$\begin{aligned}
[J_x^{(M)}, J_y^{(M)}] &= iJ_z^{(M)} - \frac{i}{2M}\left(p_M^\dagger p_M \hat{N}_b - q_M^\dagger q_M \hat{N}_a\right), \\
[J_y^{(M)}, J_z^{(M)}] &= iJ_x^{(M)}\left(1 + \frac{1}{M} - \frac{1}{2M}(\hat{N}_a + \hat{N}_b)\right), \\
[J_z^{(M)}, J_x^{(M)}] &= iJ_y^{(M)}\left(1 + \frac{1}{M} - \frac{1}{2M}(\hat{N}_a + \hat{N}_b)\right),
\end{aligned}$$

which are to lowest order the $SU(2)$ commutation relations explaining the used nomenclature. In this language, we can write $O = (n_M^{(-)})^2 = (J_z^{(M)})^2$. These operators will turn out to be useful for the derivation of the phase sensitivity far from the bosonic limit.

Calculation of the normalization constant $c_N^{(M)}$ Next we derive an explicit expression for the normalization constant $c_N^{(M)}$ of the states $|N\rangle_p^{(M)}$. As

$$\langle N|N\rangle_a^{(M)} = |c_N^{(M)}|^2 \langle 0|(p_M)^N (p_M^\dagger)^N|0\rangle \stackrel{!}{=} 1,$$

we must first find an expression for $p_M(p_M^\dagger)^N|0\rangle$. Using the commutation relation $[p_M^\dagger, p_M] = 1 - \frac{1}{M}\hat{N}_a$ and the fact that $\hat{N}_a(p_M^\dagger)^N|0\rangle = 2N(p_M^\dagger)^N|0\rangle$ as $(p_M^\dagger)^N|0\rangle$ is a state with $2N$ particles one can derive the following expression:

$$\begin{aligned}
p_M(p_M^\dagger)^N|0\rangle &= p_M p_M^\dagger (p_M^\dagger)^{N-1}|0\rangle \\
&= \left(1 - \frac{\hat{N}_a}{M} + p_M^\dagger p_M\right)(p_M^\dagger)^{N-1}|0\rangle \\
&= \left(1 - 2\frac{N-1}{M}\right)(p_M^\dagger)^{N-1}|0\rangle + p_M^\dagger p_M p_M^\dagger (p_M^\dagger)^{N-2}|0\rangle \\
&= \left(1 - 2\frac{N-1}{M}\right)(p_M^\dagger)^{N-1}|0\rangle + p_M^\dagger \left(1 - \frac{\hat{N}_a}{M} + p_M^\dagger p_M\right)(p_M^\dagger)^{N-2}|0\rangle \\
&= \left(1 - 2\frac{N-1}{M} + 1 - 2\frac{N-2}{M}\right)(p_M^\dagger)^{N-1}|0\rangle + (p_M^\dagger)^2 p_M (p_M^\dagger)^{N-2}|0\rangle \\
&= \left(N - 2N\cdot\frac{N}{M} + \frac{2}{M}\sum_{k=1}^{N} k\right)(p_M^\dagger)^{N-1}|0\rangle = \alpha_N^2 (p_M^\dagger)^{N-1}|0\rangle
\end{aligned} \tag{C.4}$$

where we have introduced

$$\alpha_N = \sqrt{N\left(1 - \frac{N-1}{M}\right)}. \tag{C.5}$$

The bracket $\langle 0|(p_M)^N(p_M^\dagger)^N|0\rangle$ can thus be evaluated to

$$\langle 0|(p_M)^N(p_M^\dagger)^N|0\rangle = \prod_{k=1}^{N}(N+1-k)\left(1-\frac{N-k}{M}\right) = N\frac{M!}{M^N}, \tag{C.6}$$

so that we get the following result for the normalization constant:

$$c_N^{(M)} = \left(N\frac{M!}{M^N}\right)^{-\frac{1}{2}}.$$

Relation between $c_N^{(M)}$ and $c_{N-1}^{(M)}$ Starting from Eq. (C.6) we obtain

$$\begin{aligned} c_{N-1}^{(M)} &= \left[\prod_{k=1}^{N-1}((N-1)+1-k)\left(1-\frac{N-1-k}{M}\right)\right]^{-\frac{1}{2}} \\ &= \left[\prod_{r=2}^{N}(N+1-r)\left(1-\frac{N-r}{M}\right)\right]^{-\frac{1}{2}} = \alpha_N c_N^{(M)}. \end{aligned} \tag{C.7}$$

Useful commutation relations The following lemma is a collection of commutation relations needed later on:

Lemma C.1. *The following commutation relations hold:*

$$[n_{\pm k}, p_M^\dagger] = \frac{1}{\sqrt{M}}P_k^\dagger \tag{C.8}$$

$$[P_k, p_M^\dagger] = \frac{1}{\sqrt{M}}(1-n_k-n_{-k}) \tag{C.9}$$

$$\begin{aligned} [J_z^{(M)}, \sum_{k=1}^{M}P_k^\dagger Q_k^\dagger] &= \frac{1}{2\sqrt{M}}\sum_{k=1}^{M}(m_k+m_{-k})P_k^\dagger q_M^\dagger \\ &\quad -\frac{1}{2\sqrt{M}}\sum_{k=1}^{M}(n_k+n_{-k})Q_k^\dagger p_M^\dagger \end{aligned} \tag{C.10}$$

Proof. We start with the calculation of (C.8):

$$[n_k, p_M^\dagger] = \frac{1}{\sqrt{M}}[a_k^\dagger a_k, P_k^\dagger] = \frac{1}{\sqrt{M}}a_k^\dagger[a_k, a_k^\dagger]a_{-k}^\dagger = \frac{1}{\sqrt{M}}P_k^\dagger$$

$$[n_{-k}, p_M^\dagger] = \frac{1}{\sqrt{M}}[a_{-k}^\dagger a_{-k}, P_k^\dagger] = \frac{1}{\sqrt{M}}a_{-k}^\dagger a_k^\dagger[a_{-k}, a_k^\dagger] = \frac{1}{\sqrt{M}}P_k^\dagger$$

Next, we derive (C.9).

$$\begin{aligned}
[P_k, p_M^\dagger] &= \frac{1}{\sqrt{M}}[P_k, P_k^\dagger] = \frac{1}{\sqrt{M}}[a_{-k}a_k, a_k^\dagger a_{-k}^\dagger] \\
&= \frac{1}{\sqrt{M}}a_{-k}[a_k, a_k^\dagger]a_{-k}^\dagger + \frac{1}{\sqrt{M}}a_k^\dagger[a_{-k}, a_{-k}^\dagger]a_k \\
&= \frac{1}{\sqrt{M}}(1-n_{-k})(1-2n_k) + \frac{1}{\sqrt{M}}n_k(1-2n_{-k}) \\
&= \frac{1}{\sqrt{M}}(1-n_k-n_{-k})
\end{aligned}$$

The derivation of (C.10) is a little more involved. First, we calculate the commutator of $p_M^\dagger p_M$ with $\sum_{k=1}^M P_k^\dagger Q_k^\dagger$ using (C.9) and the hermitian conjugate of (C.9), $[p_M, P_k^\dagger] = \frac{1}{\sqrt{M}}(1-n_k-n_{-k})$:

$$\begin{aligned}
[p_M^\dagger p_M, \sum_{k=1}^M P_k^\dagger Q_k^\dagger] &= \sum_{k=1}^M [p_M, P_k^\dagger]Q_k^\dagger = p_M^\dagger q_M^\dagger - p_M^\dagger \sum_{k=1}^M (n_k + n_{-k})Q_k^\dagger \\
&= p_M^\dagger q_M^\dagger + \frac{2}{\sqrt{M}}\sum_{k=1}^M P_k^\dagger Q_k^\dagger - \frac{1}{\sqrt{M}}\sum_{k=1}^M (n_k+n_{-k})Q_k^\dagger p_M^\dagger
\end{aligned}$$

In the same way we get

$$[q_M^\dagger q_M, \sum_{k=1}^M P_k^\dagger Q_k^\dagger] = p_M^\dagger q_M^\dagger + \frac{2}{\sqrt{M}}\sum_{k=1}^M P_k^\dagger Q_k^\dagger - \frac{1}{\sqrt{M}}\sum_{k=1}^M (m_k+m_{-k})P_k^\dagger q_M^\dagger.$$

Subtraction of the two equations leads to (C.10). □

Action of the operators p_M, $p_M^\dagger$, $P_k^\dagger$ and P_k on $|N\rangle_a$. In order to obtain the action of the Hamiltonians used in our interferometric setups the following results will turn out useful:

Lemma C.2. *The operators $p_M^\dagger$, p_M, $P_k^\dagger$ and P_k act in the following way on the state $|N\rangle$*

$$p_M|N\rangle_p^{(M)} = \alpha_N|N-1\rangle_p^{(M)}, \tag{C.11}$$

$$p_M^\dagger|N\rangle_p^{(M)} = \alpha_{N+1}|N+1\rangle_p^{(M)} \tag{C.12}$$

$$P_k^\dagger|N\rangle_p^{(M)} = \alpha_{N+1}\frac{\sqrt{M}}{N+1}n_k|N+1\rangle_p^{(M)} \tag{C.13}$$

$$P_k|N\rangle_p^{(M)} = \frac{1}{\alpha_N}\frac{N}{\sqrt{M}}(1-n_k)|N-1\rangle_p^{(M)}, \tag{C.14}$$

where α_N was defined in Eq. (C.5).

Proof. The first expression, (C.11) is Eq. (C.4). For the (C.12) we use (C.7):

$$p_M^\dagger |N\rangle_p^{(M)} = c_N^{(M)} p_M^\dagger (p_M^\dagger)^N |0\rangle = \frac{c_N^{(M)}}{c_{N+1}^{(M)}} |N+1\rangle_p^{(M)} = \alpha_{N+1} |N+1\rangle_p^{(M)}.$$

□

To obtain (C.13) we use the commutation relation (C.8) N times:

$$n_k (p_M^\dagger)^N |0\rangle = \left(p_M^\dagger n_k + \frac{1}{\sqrt{M}} P_k^\dagger \right) (p_M^\dagger)^{N-1} |0\rangle = \ldots \frac{N}{\sqrt{M}} P_k^\dagger (p_M^\dagger)^{N-1} |0\rangle.$$

The relation for the normalization constants $c_N^{(M)}/c_{N+1}^{(M)} = \alpha_N^{(M)}$ derived in (C.7) leads to the desired result.

To arrive at (C.14) we use induction over N. For $N = 1$ we have $c_1^{(M)} = 1, p_1 = 1$. Thus, the commutation relation (C.9) leads to

$$P_k |1\rangle = P_k p_M^\dagger |0\rangle = \frac{1}{\sqrt{M}} (1 - n_k - n_{-k}) |0\rangle = \frac{1}{\alpha_1} \frac{1}{\sqrt{M}} |0\rangle.$$

For the induction step we use (C.8) and (C.13) to obtain

$$\begin{aligned}
P_k (p_M^\dagger)^{N+1} |0\rangle &= \left(p_M^\dagger P_k + \frac{1}{\sqrt{M}} (1 - n_k - n_{-k}) \right) (p_M^\dagger)^N |0\rangle \\
&= p_M^\dagger \frac{N}{\sqrt{M}} (1 - n_k) (p_M^\dagger)^{N-1} |0\rangle + \frac{1}{\sqrt{M}} (1 - n_k - n_{-k}) (p_M^\dagger)^N |0\rangle \\
&= \frac{N+1}{\sqrt{M}} (p_M^\dagger)^N |0\rangle - \frac{2}{\sqrt{M}} (p_M^\dagger)^N |0\rangle \\
&\quad - \frac{N}{\sqrt{M}} \left(n_k p_M^\dagger - \frac{1}{\sqrt{M}} P_k^\dagger \right) (p_M^\dagger)^{N-1} |0\rangle \\
&= \left(\frac{N+1}{\sqrt{M}} - \frac{N+2}{\sqrt{M}} n_k + \frac{1}{\sqrt{M}} n_k \right) (p_M^\dagger)^N |0\rangle \\
&= \frac{N+1}{\sqrt{M}} (1 - n_k) (p_M^\dagger)^N |0\rangle
\end{aligned}$$

Again, $c_N^{(M)}/c_{N+1}^{(M)} = \alpha_N^{(M)}$ leads to the desired result.

C.1 Quasi-bosonic limit

This Section shows in detail the derivation of the formulae used in Sec. 2.5.2.1. The Hamiltonian H_M can be rewritten as

$$H_M = \frac{1}{2} \left(p_M^\dagger q_M + p_M q_M^\dagger \right) = J_M^{(x)}.$$

For the calculation of the phase sensitivity given in (2.76) we have to determine

$$\langle H_M O H_M\rangle = \langle \Psi_N^{(M)}|J_x^{(M)}(J_z^{(M)})^2 J_x^{(M)}|\Psi_N^{(M)}\rangle,$$
$$\langle H_M O^2 H_M\rangle = \langle \Psi_N^{(M)}|J_x^{(M)}(J_z^{(M)})^4 J_x^{(M)}|\Psi_N^{(M)}\rangle.$$

In the following we calculate $J_z^{(M)}J_x^{(M)}|N,N\rangle$ and $(J_z^{(M)})^2J_x^{(M)}|N,N\rangle$, as the norm of these vectors is the desired expectation value. We start with $J_x^{(M)}|N,N\rangle$, using (C.12) and (C.11):

$$\begin{aligned} J_x^{(M)}|N,N\rangle &= \frac{1}{2}\left(p_M q_M^\dagger + p_M^\dagger q_M\right)|N,N\rangle \\ &= \frac{1}{2}\alpha_N\alpha_{N+1}\left(|N+1,N-1\rangle + |N-1,N+1\rangle\right). \end{aligned}$$

In this way it is easy to see that

$$\begin{aligned} J_z^{(M)}J_x^{(M)}|N,N\rangle &= \frac{1}{2}\left(p_M p_M - q_M^\dagger q_M\right)J_x^{(M)}|N,N\rangle \\ &= \frac{1}{2}\alpha_N\alpha_{N+1}\left(\alpha_{N+1}^2-\alpha_{N-1}^2\right)\left(|N+1,N-1\rangle - |N-1,N+1\rangle\right) \end{aligned}$$

$$\begin{aligned} \left(J_z^{(M)}\right)^2 J_x^{(M)}|N,N\rangle &= \frac{1}{2}\left(p_M p_M - q_M^\dagger q_M\right)J_z^{(M)}J_x^{(M)}|N,N\rangle \\ &= \frac{1}{2}\alpha_N\alpha_{N+1}\left(\alpha_{N+1}^2-\alpha_{N-1}^2\right)\left(|N+1,N-1\rangle - |N-1,N+1\rangle\right) \end{aligned}$$

Combining these results we arrive at

$$\begin{aligned} \langle J_x^{(M)}(J_z^{(M)})^2 J_x^{(M)}\rangle &= \frac{1}{8}\alpha_N^2\alpha_{N+1}^2(\alpha_{N+1}^2-\alpha_{N-1}^2)^2 \\ \langle J_x^{(M)}(J_z^{(M)})^4 J_x^{(M)}\rangle &= \frac{1}{32}\alpha_N^2\alpha_{N+1}^2(\alpha_{N+1}^2-\alpha_{N-1}^2)^4. \end{aligned} \tag{C.15}$$

C.2 Interferometry far from the bosonic limit

In this Section we give the details of the calculations in Sec. 2.5.2.2. We have to calculate $\langle H_F(J_z^{(M)})^2 H_F\rangle$ and $\langle H_F(J_z^{(M)})^4 H_F\rangle$.

Action of H on the input state In the first step, we derive an expression for the action of H on the input state:

Lemma C.3. *Let $|\Psi_N^{(M)}\rangle = |N\rangle_a^{(M)}|N\rangle_b^{(M)} \equiv |N,N\rangle$ be the input state of the interferometer and let $H_F = \sum_{k=1}^\infty P_k^\dagger Q_k + Q_k^\dagger P_k$ be the interaction Hamiltonian. Then*

$$\begin{aligned} H_F|\Psi_N^{(M)}\rangle &= \frac{\alpha_{N+1}}{\alpha_N}N\left(|N+1,N-1\rangle + |N-1,N+1\rangle\right) \\ &- \frac{N(N-1)}{M}\frac{1}{\alpha_N\alpha_{N-1}}\sum_{k=1}^M P_k^\dagger Q_k^\dagger\left(|N,N-2\rangle + |N-2,N\rangle\right). \end{aligned}$$

Proof. Using (C.13) and (C.14) we see that for all $k \leq M$

$$(P_k^\dagger Q_k + Q_k^\dagger P_k)|N,N\rangle = \frac{\alpha_{N+1}}{\alpha_N}\frac{N}{N+1}[n_k(1-m_k)|N+1,N-1\rangle + (1-n_k)m_k|N-1,N+1\rangle],$$

and $(P_k^\dagger Q_k + Q_k^\dagger P_k)|N,N\rangle = 0$ for $k > M$. Summation over k leads to

$$H_F|N,N\rangle = \sum_{k=1}^{M}\frac{\alpha_{N+1}}{\alpha_N}N(|N+1,N-1\rangle + |N-1,N+1\rangle) - \frac{\alpha_{N+1}}{\alpha_N}\frac{N}{N+1}\sum_{k=1}^{M} n_k m_k(|N+1,N-1\rangle + |N-1,N+1\rangle). \quad \text{(C.16)}$$

From (C.13) we see that $n_k|N\rangle = \frac{N}{M}\frac{1}{\alpha_N}P_k^\dagger|N-1\rangle$ implying

$$n_k m_k(|N+1,N-1\rangle + |N-1,N+1\rangle) = \frac{(N-1)(N+1)}{M}\frac{1}{\alpha_{N+1}\alpha_{N-1}}(|N,N-2\rangle + |N-2,N\rangle).$$

Plugging this in (C.16) leads to the desired result. □

Calculation of $J_z^{(M)}H|N,N\rangle$ and $(J_z^{(M)})^2H|N,N\rangle$ Next, we derive an expression for $J_z^{(M)}H|N,N\rangle$ and $(J_z^{(M)})^2H|N,N\rangle$, as the length of these vectors gives rise to the desired overlap:

Lemma C.4. *Let $V = N/(\alpha_{N+1}\alpha_N)$, $a = (\alpha_{N+1}^2 - \alpha_N^2)$ and $y = (\alpha_N^2 - \alpha_{N-2}^2 - 4/M)$. Then*

$$J_z^{(M)}H|N,N\rangle = V\left(x - \frac{1}{N+1}y\sum_{k=1}^{M} n_k m_k\right)(|N+1,N-1\rangle - |N-1,N+1\rangle)$$

$$\left(J_z^{(M)}\right)^2 H|N,N\rangle = V\left(x^2 - \frac{1}{N+1}y^2\sum_{k=1}^{M} n_k m_k\right)(|N+1,N-1\rangle + |N-1,N+1\rangle).$$

Proof. For the proof we will need the commutation relation $[J_z^{(M)}, \sum_{k=1}^{M} P_k^\dagger Q_k^\dagger]$ given in (C.10) and the action of H on $|N,N\rangle$ derived in lemma C.3. Using

$$J_z^{(M)}(|N,N-2\rangle \pm |N-2,N\rangle) = (\alpha_N^2 - \alpha_{N-2}^2)(|N,N-2\rangle \mp |N-2,N\rangle),$$

and (C.10), we can further obtain

$$\begin{aligned}
& J_z^{(M)} \sum_{k=1}^{M} P_k^\dagger Q_k^\dagger (|N, N-2\rangle \pm |N-2, N\rangle) \\
= & \sum_{k=1}^{M} P_k^\dagger Q_k^\dagger (\alpha_N^2 - \alpha_{N-2}^2)(|N, N-2\rangle \mp |N-2, N\rangle) \\
& + \frac{1}{\sqrt{M}} \sum_{k=1}^{M} (m_k + m_{-k}) P_k^\dagger (\alpha_{N-1} |N, N-1\rangle \pm \alpha_{N+1} |N-2, N+1\rangle \\
& - \frac{1}{\sqrt{M}} \sum_{k=1}^{M} (n_k + n_{-k}) Q_k^\dagger (\alpha_{N+1} |N+1, N-2\rangle \pm \alpha_{N+1} |N-1, N\rangle \\
= & \left(\alpha_N^2 - \alpha_{N-1}^2 - \frac{4}{M} \right) \sum_{k=1}^{M} P_k^\dagger Q_k^\dagger (|N, N-2\rangle \mp |N-2, N\rangle).
\end{aligned}$$

using (C.13) leads to the desired result. □

Calculation of the expectation values The result for the expectation values is summarized in the following lemma:

Lemma C.5. *For the input state $|N, N\rangle$ the following equations hold:*

$$\langle N, N | H_F (J_x^{(M)})^2 H_F | N, N \rangle = \frac{2N(M-N)(M+MN-N^2-1)(M+1-2N)^2}{M^3(M-1)},$$

$$\langle N, N | H_F (J_x^{(M)})^4 H_F | N, N \rangle = \frac{2N(M-N)(M+MN-N^2-1)(M+1-2N)^4}{M^5(M-1)},$$

Proof. For the proof we use lemma C.4 to obtain

$$\begin{aligned}
\langle N, N | H_F (J_x^{(M)})^2 H_F | N, N \rangle &= V^2 \left(2x^2 + \frac{2y^2}{(N+1)^2} T_{nnmm} - \frac{4xy}{N+1} T_{nm} \right), \\
\langle N, N | H_F (J_x^{(M)})^4 H_F | N, N \rangle &= V^2 \left(2x^4 + \frac{2y^4}{(N+1)^2} T_{nnmm} - \frac{4x^2y^2}{N+1} T_{nm} \right),
\end{aligned}$$

where the matrix elements T_{nnmm} and T_{nm} are given by

$$\begin{aligned}
T_{nm} &= \sum_{k=1}^{M} \langle N+1, N-1 | n_k m_k | N+1, N-1 \rangle, \\
T_{nnmm} &= \sum_{k,l=1}^{M} \langle N+1, N-1 | n_k n_l m_k m_l | N+1, N-1 \rangle.
\end{aligned}$$

To evaluate these matrix elements, we write the state $|N\rangle$ in the form

$$|N\rangle_p = c_N^{(M)} \left(\frac{1}{\sqrt{M}} \sum_{j=1}^{M} P_j^\dagger \right)^N |0\rangle = g_N^{(M)} N! \sum_{j_1<j_2<\ldots<j_N=1}^{M} P_{j_1}^\dagger \ldots P_{j_N}^\dagger |0\rangle,$$

and the normalization constant $g_N^{(M)}$ fulfills

$$|g_N^{(M)}|^2 (N!)^2 = \frac{N!(M-N)!}{M!}.$$

With this result and from

$$n_k|N\rangle = g_N^{(M)} N! P_k^\dagger \sum_{\substack{j_1<j_2<\ldots<j_N=1 \\ j_i \neq k}}^{M} P_{j_1}^\dagger \ldots P_{j_N}^\dagger |0\rangle$$

we can deduce that

$$\begin{aligned} \langle N|n_k|N\rangle &= |g_N^{(M)}|^2 (N!)^2 \left(\begin{array}{c} M-1 \\ N-1 \end{array} \right) = \frac{N}{M}, \\ \langle N|n_k n_l|N\rangle &= |g_N^{(M)}|^2 (N!)^2 \left(\begin{array}{c} M-2 \\ N-2 \end{array} \right) = \frac{N(N-1)}{M(M-1)}. \end{aligned}$$

Putting all the pieces together one arrives at the formulas stated above. □

Appendix D

Derivation of the evolution equation

In the following we give the details of the calculations of Subsec. 5.3.2.

Imaginary time evolution with H

We have to evaluate $\mathrm{tr}[H\rho(t)]$ and $\mathrm{tr}[\{H_2, c_k c_l\}\rho(t)]$ using Wick's theorem.

Calculation of $\mathbf{tr}[H\rho(t)]$:

$$\begin{aligned} \mathrm{tr}[H\rho(t)] &= \sum_{ij} T_{ij}\Gamma_{ij} - \sum_{ijkl} U_{ijkl}(\Gamma_{ij}\Gamma_{kl} - \Gamma_{ik}\Gamma_{jl} + \Gamma_{il}\Gamma_{jk}) = -\mathrm{tr}[\Gamma h_3(\Gamma)], \\ h_3(\Gamma) &= T + 3\mathrm{tr}_B[U\Gamma]. \end{aligned} \tag{D.1}$$

Calculation of $\mathbf{tr}[\{H, c_k c_l\}\rho(t)]$: We split the calculation into the evaluation of the terms $\mathrm{tr}[\{H_2, c_k c_l\}\rho(t)]$ and $\mathrm{tr}[\{H_4, c_k c_l\}\rho(t)]$:

$$\begin{aligned} \mathrm{tr}[\{H_2, c_k c_l\}\rho(t)] =& -\sum_{i,j\neq k,l} T_{ij}\langle c_i c_j c_k c_l + c_k c_l c_i c_j\rangle + 4T_{kl} \\ & - \sum T_{ik}\langle c_i c_k c_k c_l + c_k c_l c_i c_k\rangle + T_{kj}\langle c_k c_j c_k c_l + c_k c_l c_k c_j\rangle + (k \leftrightarrow l) \\ =& \, 2\sum_{i,j\neq k,l} T_{ij}(\Gamma_{ij}\Gamma_{kl} - \Gamma_{ik}\Gamma_{jl} + \Gamma_{il}\Gamma_{jk}) + 4T_{kl} \\ =& \, 2\sum_{i,j\neq k,l} (T_{ij}\Gamma_{ij})\Gamma_{kl} - 4\sum_{i,j\neq k,l} T_{ij}\Gamma_{ik}\Gamma_{jl} + 4T_{kl} \\ =& \sum_{ij} (T_{ij}\Gamma_{ij} - 2T_{kj}\Gamma_{kj} - 2T_{lj}\Gamma_{lj})\Gamma_{kl} + 4T_{kl} - 4\sum_{ij} T_{ij}\Gamma_{ik}\Gamma_{jl} \\ & + 4\sum (T_{ik}\Gamma_{ik}\Gamma_{kl} + T_{lj}\Gamma_{lk}\Gamma_{jl}) \\ =& \, -2\mathrm{tr}[T\Gamma]\Gamma_{kl} + 4(\Gamma T\Gamma + T)_{kl} \end{aligned}$$

$$
\begin{aligned}
&-i\mathrm{tr}[\{H_4, c_k c_l\}\rho(t)] = -i\sum U_{ijmn}\langle c_i c_j c_m c_n c_k c_l + c_k c_l c_i c_j c_m c_n\rangle = \\
&-i\sum_{i,j,m,n\neq k,l} U_{ijmn}\langle c_i c_j c_m c_n c_k c_l + c_k c_l c_i c_j c_m c_n\rangle - 24i\sum_{i,j} U_{ijlk}\langle c_i c_j\rangle \\
&-4i\sum_{i,j,m,n\neq k,l} U_{ijmk}(\langle c_i c_j c_m c_l\rangle + \langle c_l c_i c_j c_m\rangle) + U_{ijml}(\langle c_i c_j c_m c_k\rangle + \langle c_k c_i c_j c_m\rangle) \\
&= -i\sum_{i,j,m,n\neq k,l} U_{ijmn}\langle c_i c_j c_m c_n c_k c_l + c_k c_l c_i c_j c_m c_n\rangle - 24\sum_{i,j} U_{ijlk}\Gamma_{ij}
\end{aligned}
$$

Now, we perform the following simplification using Wick's theorem:

$$
\begin{aligned}
& -i\sum_{i,j,m,n\neq k,l} U_{ijmn}\langle c_i c_j c_m c_n c_k c_l + c_k c_l c_i c_j c_m c_n\rangle \\
= \quad & -2i\sum_{i,j,m,n\neq k,l} U_{ijmn}\langle c_i c_j c_m c_n c_k c_l\rangle \\
= \quad & 2\sum_{i,j,m,n\neq k,l} U_{ijmn}(-\Gamma_{ij}\langle c_m c_n c_k c_l\rangle + \Gamma_{im}\langle c_j c_n c_k c_l\rangle - \Gamma_{in}\langle c_j c_m c_k c_l\rangle \\
& \qquad +\Gamma_{ik}\langle c_j c_m c_n c_l\rangle - \Gamma_{il}\langle c_j c_m c_n c_k\rangle) \\
= \quad & 2\sum_{i,j,m,n\neq k,l} U_{ijmn}\left(-3\Gamma_{ij}\langle c_m c_n c_k c_l\rangle + \Gamma_{ik}\langle c_j c_m c_n c_l\rangle - \Gamma_{il}\langle c_j c_m c_n c_k\rangle\right) \\
= \quad & 6\sum_{i,j,m,n\neq k,l} U_{ijmn}\Gamma_{ij}\Gamma_{mn}\Gamma_{kl} - 24\sum_{i,j,m,n\neq k,l} U_{ijmn}\Gamma_{ik}\Gamma_{jm}\Gamma_{nl}
\end{aligned}
$$

We treat the two terms independently:

$$
\begin{aligned}
& 6\sum_{i,j,m,n\neq k,l} U_{ijmn}\Gamma_{ij}\Gamma_{mn}\Gamma_{kl} \\
= \quad & 6\ \mathrm{tr}[\Gamma\mathrm{tr}[U\Gamma]]\Gamma_{kl} \\
& -24\sum_{j,m,n}(U_{kjmn}\Gamma_{kj}\Gamma_{mn} + U_{ljmn}\Gamma_{lj}\Gamma_{mn})\Gamma_{kl} \\
& +24\sum_{m,n}(U_{klmn}\Gamma_{kl}\Gamma_{mn} + 2U_{kmln}\Gamma_{km}\Gamma_{ln})\Gamma_{kl} \\
& +24\sum_{m,n}(U_{lkmn}\Gamma_{ll}\Gamma_{mn} + 2U_{lmkn}\Gamma_{lm}\Gamma_{kn})\Gamma_{kl} \\
& -24\sum_{j,m,n}(U_{kjmn}\Gamma_{kj}\Gamma_{mn} + U_{ljmn}\Gamma_{lj}\Gamma_{mn})\Gamma_{kl} - 24\sum_{m,n} U_{klmn}\Gamma_{kl}\Gamma_{mn}\Gamma_{kl} \\
= \quad & 6\ \mathrm{tr}[\Gamma\mathrm{tr}[U\Gamma]]\Gamma_{kl} + 24\sum_{m,n} U_{klmn}(\Gamma_{mn}\Gamma_{kl}^2 - 2\Gamma_{km}\Gamma_{ln}) \\
& -24\sum_{j,m,n}(U_{kjmn}\Gamma_{mn}\Gamma_{kj} + U_{ljmn}\Gamma_{lj}\Gamma_{mn})\Gamma_{kl}
\end{aligned}
$$

$$
\begin{aligned}
& - \sum_{i,j,m,n\neq k,l} U_{ijmn}\Gamma_{ik}\Gamma_{jm}\Gamma_{nl} \\
= \quad & - \sum_{i,j,m,n} U_{ijmn}\Gamma_{ik}\Gamma_{jm}\Gamma_{nl} \\
& + \sum_{m,n}(U_{mkln}\Gamma_{mk}\Gamma_{kl}\Gamma_{nl} + U_{lmnk}\Gamma_{lk}\Gamma_{mn}\Gamma_{kl}) \\
& + \sum_{j,m,n} U_{ljmn}\Gamma_{lk}\Gamma_{jm}\Gamma_{nl} - \sum_{m,n}(2\, U_{lkmn}\Gamma_{lk}\Gamma_{km}\Gamma_{nl} - U_{lmnk}\Gamma_{lk}\Gamma_{mn}\Gamma_{kl}) \\
& + \sum_{j,m,n} \Gamma_{jk}\Gamma_{kn}\Gamma_{nl} - \sum_{m,n}(U_{lkmn}\Gamma_{lk}\Gamma_{km}\Gamma_{nl} + U_{mkln}\Gamma_{mk}\Gamma_{kl}\Gamma_{nl} \\
& + \sum_{j,m,n} U_{jlmn}\Gamma_{jk}\Gamma_{ln}\Gamma_{nl} - \sum_{m,n}(U_{mlkn}\Gamma_{mk}\Gamma_{lk}\Gamma_{nl} + U_{nlmk}\Gamma_{nk}\Gamma_{lm}\Gamma_{kl}) \\
& + \sum_{j,m,n} U_{jmkn}\Gamma_{mk}\Gamma_{mk}\Gamma_{nl} - \sum_{m,n}(U_{lmkn}\Gamma_{lk}\Gamma_{mk}\Gamma_{nl} + U_{mlkn}\Gamma_{mk}\Gamma_{lk}\Gamma_{nl}) \\
& + \sum_{j,m,n} U_{jmln}\Gamma_{jk}\Gamma_{ml}\Gamma_{nl} - \sum_{m,n}(U_{mkln}\Gamma_{mk}\Gamma_{kl}\Gamma_{nl} + U_{mnlk}\Gamma_{mk}\Gamma_{nl}\Gamma_{kl}) \\
& + \sum_{j,m,n} U_{jmnk}\Gamma_{mk}\Gamma_{mn}\Gamma_{kl} - \sum_{m,n}(U_{lnmn}\Gamma_{lk}\Gamma_{nm}\Gamma_{kl} + 2U_{nlmk}\Gamma_{nk}\Gamma_{lm}\Gamma_{kl}) \\
= \quad & -(\Gamma \mathrm{tr}[U\Gamma]\Gamma)_{kl} + 2\sum_{j,m,n}(U_{ljmn}\Gamma_{jk}\Gamma_{ml}\Gamma_{nl} - U_{kjmn}\Gamma_{jk}\Gamma_{km}\Gamma_{nl}) \\
& + 2\sum_{m,n} U_{klmn}(\Gamma_{kl}\Gamma_{mk}\Gamma_{nl} - \Gamma_{mn}\Gamma_{kl}^2) + \sum_{j,m,n}(U_{kjmn}\Gamma_{mn}\Gamma_{kj} + U_{ljmn}\Gamma_{mn}\Gamma_{lj})\Gamma_{kl}
\end{aligned}
$$

The second term in the last expression vanishes, as it is symmetric under exchange of k and l in the Γ's, but antisymmetric in the U. Taking all pieces together, we obtain

$$
-i\mathrm{tr}[\rho\{H_4, c_k c_l\}] = 24\mathrm{tr}[U\Gamma]_{kl} - 24(\Gamma\mathrm{tr}[U\Gamma]\Gamma)_{kl} + 6\mathrm{tr}[\Gamma\mathrm{tr}[U\Gamma]]\Gamma_{kl}
$$

Imaginary time evolution with $\bar{H}$

First, $\mathrm{tr}[\bar{H}\rho(t)] = -\mathrm{tr}[\bar{h}\Gamma]$. With the helpof Wick's theorem, we obtain

$$
\begin{aligned}
& -i\mathrm{tr}[\rho(t)\{\bar{H}, c_k c_l\}] \\
= \quad & -i\sum_{i,j} i\bar{h}_{ij}\langle c_i c_j c_k c_l + c_k c_l c_i c_j\rangle \\
= \quad & \sum_{i,j\neq k,l} \bar{h}_{ij}\langle c_i c_j c_k c_l + c_k c_l c_i c_j\rangle - 4\bar{h}_{kl} \\
& + 2\sum_{i} \bar{h}_{ik}(\langle c_i c_l\rangle + \langle c_l c_i\rangle) - 4\bar{h}_{lk} + 2\sum_{j} \bar{h}_{lj}(\langle c_j c_k\rangle + \langle c_k c_j\rangle) - 4\bar{h}_{lk} \\
= \quad & 2\sum_{i,j\neq k,l} \bar{h}_{ij}(-\Gamma_{ij}\Gamma_{kl} + \Gamma_{ik}\Gamma_{jl} - \Gamma_{il}\Gamma_{jk}) - 4\bar{h}_{kl}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & -2 \sum_{i,j\neq k,l} \bar{h}_{ij}\Gamma_{ij}\Gamma_{kl} + 4 \sum_{i,j\neq k,l} \bar{h}_{ij}\Gamma_{ik}\Gamma_{jl} - 4\bar{h}_{kl} \\
= \quad & -2\sum_{i,j} \bar{h}_{ij}\Gamma_{ij}\Gamma_{kl} - 4\bar{h}_{kl} \\
& +4\sum_{j}(\bar{h}_{kj}\Gamma_{kj} + \bar{h}_{lj}\Gamma_{lj})\Gamma_{kl} - 4\bar{h}_{kl}\Gamma_{kl} - 4\bar{h}_{lk}\Gamma_{lk}\Gamma_{kl} \\
& +4\sum_{i,j} \bar{h}_{ij}\Gamma_{ij}\Gamma_{ik}\Gamma_{jl} - 4\sum_{j}(\bar{h}_{lj}\Gamma_{lk}\Gamma_{jl} + \bar{h}_{jk}\Gamma_{jk}\Gamma_{kl}) + 4\bar{h}_{lk}\Gamma_{lk}\Gamma_{kl} + 4\bar{h}_{lk}\Gamma_{lk}\Gamma_{kl} \\
= \quad & 2\mathrm{tr}[\bar{H}\Gamma]\Gamma_{kl} - 4(\Gamma\bar{h}\Gamma + \bar{h})_{kl}
\end{aligned}
$$

Bibliography

[1] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. **47**, 777 (1935).

[2] J. S. Bell, Physics **1**, 195 (1964).

[3] A. Aspect, J. Dalibard, and G. Roger, Phys. Rev. Lett. **49**, 1804 (1982).

[4] A. Aspect, P. Grangier, and G. Roger, Phys. Rev. Lett. **47**, 460 (1981).

[5] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, 2000).

[6] A. K. Ekert, Phys. Rev. Lett. **67**, 661 (1991).

[7] C. H. Bennett and S. J. Wiesner, Phys. Rev. Lett. **69**, 2881 (1992).

[8] C. H. Bennett *et al.*, Phys. Rev. Lett. **70**, 1895 (1993).

[9] D. Boschi, S. Branca, F. De Martini, L. Hardy, and S. Popescu, Phys. Rev. Lett. **80**, 1121 (1998).

[10] D. Bouwmeester, P. J.W., M. Mattle, Manfred Eibl, H. Weinfurter, and A. Zeilinger, Nature **390**, 575 (1997).

[11] A. Furusawa *et al.*, Science **23**, 706 (1998).

[12] T. Jennewein, G. Weihs, J. W. Pan, and A. Zeilinger, Phys. Rev. Lett. **88**, 017903 (2001).

[13] K. Mattle, H. Weinfurter, P. G. Kwiat, and A. Zeilinger, Phys. Rev. Lett. **76**, 4656 (1996).

[14] D. S. Naik, C. G. Peterson, A. G. White, A. J. Berglund, and P. G. Kwiat, Phys. Rev. Lett. **84**, 4733 (2000).

[15] J. W. Pan, D. Bouwmeester, H. Weinfurter, and A. Zeilinger, Phys. Rev. Lett. **80**, 3891 (1998).

[16] W. Tittel, J. Brendel, H. Zbinden, and N. Gisin, Phys. Rev. Lett. **84**, 4737 (2000).

[17] J. P. Dowling and G. J. Milburn, Philosophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences **361**, 1655 (2003).

[18] I. Bloch, J. Dalibard, and W. Zwerger, Reviews of Modern Physics **80**, 885 (2008).

[19] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Reviews of Modern Physics **80**, 517 (2008).

[20] K. Eckert, J. Schliemann, D. Bruss, and M. Lewenstein, Annals of Physics **299**, 88 (2002).

[21] M.-C. Banuls, J. I. Cirac, and M. M. Wolf, Physical Review A **76**, 022311 (2007).

[22] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[23] A. Leggett, Modern Trends in the Theory of Condensed Matter, edited by A. Pekalsky, R. Przystawa, (Springer-Verlag, Berlin, 1980) .

[24] E. Tiesinga, B. J. Verhaar, and H. T. C. Stoof, Phys. Rev. A **47**, 4114 (1993).

[25] S. Inouye, R. Andrews, J. Stenger, H. Miesner, and W. Stamper-Kurn, D.M. anf Ketterle, Nature **392**, 153 (1998).

[26] E. R. I. Abraham *et al.*, Phys. Rev. A **55**, R3299 (1997).

[27] R. Grimm, Ultracold fermi gases in the bec-bcs crossover: a review from the innsbruck perspective, in *Ultracold Fermi Gases, Proceedings of the International School of Physics "Enrico Fermi", Course CLXIV, Varenna, 20 - 30 June 2006*, edited by M. Inguscio, W. Ketterle, and C. Salomon.

[28] G. B. Partridge, K. E. Strecker, R. I. Kamar, M. W. Jack, and R. G. Hulet, Physical Review Letters **95**, 020404 (2005).

[29] G. B. Partridge, W. Li, R. I. Kamar, Y. Liao, and R. G. Hulet, Science **27**, 311 (2006).

[30] M. W. Zwierlein and W. Ketterle, Science **314**, 54a (2006).

[31] G. B. Partridge, W. Li, R. I. Kamar, Y. Liao, and R. G. Hulet, Science **314**, 54b (2006).

[32] C. V. Kraus, M. M. Wolf, J. I. Cirac, and G. Giedke, Physical Review A **79**, 012306 (2009).

[33] R. Feynman, Int. J. Theor. Phys. **21**, 467 (1982).

[34] S. Lloyd, Science **273**, 1073 (1996).

[35] C. V. Kraus, M. M. Wolf, and J. I. Cirac, Physical Review A **75**, 022303 (2007).

[36] F. Verstraete, J. I. Cirac, and V. Murg, Advances in Physics **57**, 143 (2008).

[37] A. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Commun. Math. Phys. **115**, 477 (1988).

[38] M. Fannes, B. Nachtergaele, and R. Werner, Comm. Math. Phys. **144**, 443 (1990).

[39] A. Klümper, A. Schadschneider, and J. Zittartz, J. Phys. A **24**, L955 (1991).

[40] A. Klümper, A. Schadschneider, and J. Zittartz, Z. Phys. B **87**, 281 (1992).

[41] M. B. Hastings, Phys. Rev. B **73**, 085115 (2006).

[42] C. V. Kraus, N. Schuch, F. Verstraete, and J. I. Cirac, arXiv.org:0904.4667, (2009).

[43] V. Bach, E. H. Lieb, and J. P. Solovej, J. Stat. Phys. **76**, 3 (1994).

[44] A. I. larkin and Y. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **47**, 1136 (1964).

[45] C. V. Kraus and J. I. Cirac, in preparation.

[46] M. Greiner, C. Regal, and D. Jin, Nature **426**, 537 (2003).

[47] S. Jochim *et al.*, Science **302**, 2101 (2003).

[48] M. W. Zwierlein *et al.*, Phys. Rev. Lett. **91**, 250401 (2003).

[49] M. Zwierlein, J. Abo-Shaeer, A. Schirotzek, C. Schunck, and W. Ketterle, Nature **435**, 1047 (2005).

[50] M. Zwierlein, C. Schunck, A. Schirotzek, and W. Ketterle, Nature **442**, 154 (2005).

[51] M. W. Zwierlein *et al.*, Physical Review Letters **92**, 120403 (2004).

[52] C. A. Regal, M. Greiner, and D. S. Jin, Physical Review Letters **92**, 040403 (2004).

[53] J. Cubizolles, T. Bourdel, S. J. Kokkelmans, G. V. Shlyapnikov, and C. Salomon, Phys. Rev. Lett. **91**, 240401 (2003).

[54] C. A. Regal, C. Ticknor, J. Bohn, and D. Jin, Nature **424**, 47 (2003).

[55] C. Schunck, Y. Shin, A. Schirotzek, M. Zwierlein, and W. Ketterle, Science **316**, 867 (2007).

[56] P. Zanardi, Phys. Rev. A **65**, 042101 (2002).

[57] P. Zanardi and X. Wang, J. Phys. A:Math. Gen. **35**, 7947 (2002).

[58] D. Larsson and H. Johannesson, Physical Review A **73**, 042320 (2006).

[59] M. M. Wolf, Physical Review Letters **96**, 010404 (2006).

[60] D. Gioev and I. Klich, Physical Review Letters **96**, 100503 (2006).

[61] M. Cramer, J. Eisert, and M. B. Plenio, Physical Review Letters **98**, 220603 (2007).

[62] Y. Shi, Phys. Rev. A **67**, 024301 (2003).

[63] R. Paškauskas and L. You, Phys. Rev. A **64**, 042310 (2001).

[64] H. M. Wiseman and J. A. Vaccaro, Phys. Rev. Lett. **91**, 097902 (2003).

[65] J. Schliemann, J. I. Cirac, M. Kuś, M. Lewenstein, and D. Loss, Phys. Rev. A **64**, 022303 (2001).

[66] M. R. Dowling, A. C. Doherty, and H. M. Wiseman, Physical Review A **73**, 052323 (2006).

[67] J. Schliemann, D. Loss, and A. H. MacDonald, Phys. Rev. B **63**, 085311 (2001).

[68] N. Schuch, F. Verstraete, and J. I. Cirac, Phys. Rev. A **70**, 042310 (2004).

[69] N. Schuch, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **92**, 087904 (2004).

[70] S. Bravyi, Quant. Inf. Comput. **5**, 216 (2005).

[71] G. D. Mahan, *Many-Particle Physics*, 3rd ed. (Kluwer Academic, 2000).

[72] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).

[73] R. Horn and C. Johnson, *Matrix Analysis* (Cambridge University Press, 1985).

[74] V. Bach, E. Lieb, and J. Solovej, Journal of Statistical Physics **76**, 3 (1994).

[75] C. Bloch and A. Messiah, Nuclear Physics **39**, 95 (1962).

[76] A. Coleman and V. Yukalov, *Reduced Density Matrices* (Springer-Verlag, 2000).

[77] M. Horodecki, P. Horodecki, and R. Horodecki, Physics Letters A **223**, 1 (1996).

[78] W. Rudin, *Functional Analysis*, 2nd ed. (McGraw-Hill, 1991).

[79] R. Rockafellar, *Convex Analysis* (Princeton University Press, 1970).

[80] P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

[81] R. A. Barankov and L. S. Levitov, Phys. Rev. Lett. **93**, 130403 (2004).

[82] R. A. Bertlmann, K. Durstberger, B. C. Hiesmayr, and P. Krammer, Physical Review A **72**, 052331 (2005).

[83] D. J. Wineland, J. J. Bollinger, W. M. Itano, and D. J. Heinzen, Phys. Rev. A **50**, 67 (1994).

[84] J. J. Bollinger, W. M. Itano, D. J. Wineland, and D. J. Heinzen, Phys. Rev. A **54**, R4649 (1996).

[85] S. L. Braunstein and C. M. Caves, Phys. Rev. Lett. **72**, 3439 (1994).

[86] S. L. Braunstein, C. M. Caves, and G. Milburn, Annals of Physics **247**, 135 (1996).

[87] K. Eckert *et al.*, Physical Review A **73**, 013814 (2006).

[88] B. Yurke, S. L. McCall, and J. R. Klauder, Phys. Rev. A **33**, 4033 (1986).

[89] M. J. Holland and K. Burnett, Phys. Rev. Lett. **71**, 1355 (1993).

[90] P. Bouyer and M. A. Kasevich, Phys. Rev. A **56**, R1083 (1997).

[91] C. C. Gerry, Phys. Rev. A **61**, 043811 (2000).

[92] W. J. Munro, K. Nemoto, G. J. Milburn, and S. L. Braunstein, Phys. Rev. A **66**, 023819 (2002).

[93] S. F. Huelga *et al.*, Phys. Rev. Lett. **79**, 3865 (1997).

[94] B. Yurke, Phys. Rev. Lett. **56**, 1515 (1986).

[95] E. Altman, E. Demler, and M. D. Lukin, Phys. Rev. A **70**, 013603 (2004).

[96] T. Rom *et al.*, Nature **444**, 733 (2006).

[97] M. Greiner, C. A. Regal, J. T. Stewart, and D. S. Jin, Phys. Rev. Lett. **94**, 110401 (2005).

[98] L. Viola and H. Barnum, Entanglement and subsystems, entanglement beyond subsystems, and all that, in *Proceedings of the Boston Colloquium for Philosophy of Science on "Foundations of Quantum Information and Entanglement", Boston, March 23–24, 2006.*

[99] A. A. Klyachko and A. S. Shumovsky, Journal of OPtics B **5**, S322 (2003).

[100] S. Riedl *et al.*, Physical Review A **78**, 053609 (2008).

[101] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).

[102] M. Horodecki, P. Horodecki, and R. Horodecki, Physics Letters A **223**, 1 (1996).

[103] C. Zalka, Proc. Roy. Soc. Lond. A **454**, 313 (1998).

[104] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature **415**, 39 (2002).

[105] D. Leibfried, R. Blatt, C. Monroe, and D. Wineland, Rev.Mod. Phys. **75**, 281 (2003).

[106] D. Porras and J. I. Cirac, Phys. Rev. Lett. **92**, 207901 (2004).

[107] D. Porras and J. I. Cirac, Phys. Rev. Lett. **93**, 263602 (2004).

[108] D. Porras and J. I. Cirac, Phys. Rev. Lett. **96**, 250501 (2006).

[109] E. Jane, G. Vidal, W. Dür, P. Zoller, and J. I. Cirac, Quant. Inf. Comput. **3**, 15 (2003).

[110] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).

[111] D. Deutsch, A. Barenco, and A. Ekert, Proc. R. Soc. Lond. A **449**, 669 (1995).

[112] S. Lloyd, Phys. Rev. Lett. **75**, 346 (1995).

[113] J. L. Dodd, M. A. Nielsen, M. J. Bremner, and R. T. Thew, Phys. Rev. A **65**, 040301(R).

[114] M. A. Nielsen, M. J. Bremner, J. L. Dodd, A. M. Childs, and C. M. Dawson, Phys. Rev. A **66**, 022317 (2002).

[115] M. J. Bremner, J. L. Dodd, M. A. Nielsen, and D. Bacon, Phys. Rev. A **69**, 012313 (2004).

[116] M. J. Bremner, D. Bacon, and M. A. Nielsen, Phys. Rev. A **71**, 052312 (2005).

[117] C. H. Bennett *et al.*, Phys. Rev. A **66**, 012305 (2002).

[118] P. Wocjan, M. Rötteler, D. Janzing, and T. Beth, Phys. Rev. A **65**, 042309 (2002).

[119] P. Wocjan, M. Rötteler, D. Janzing, and T. Beth, Quant. Inf. Comput. **2**, 133 (2002).

[120] G. Vidal and J. I. Cirac, Phys. Rev A **66**, 022315 (2002).

[121] W. Fulton and J. Harris, *Representation Theory* (Springer, 1991).

[122] J. F. Cornwell, *Group Theory in Physics Vol. 1 and 2* (Academic Press).

[123] H. F. Trotter, Proc. Am. Math. soc. **10**, 545 (1959).

[124] P. R. Chernoff, J. Functional Analysis **2**, 238 (1968).

[125] F. Haussdorff, Ber. Ver. Saechs. Akad. Wiss. Leipzig,Math.-Phys.Kl. **58**, 19 (1906).

[126] E. B. Dynkin, Math. Rev. **11**, 80 (1949).

[127] E. B. Dynkin, Am. Math. Soc. Transl. **9**, 470 (1950).

[128] E. Lieb, T. Schulz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).

[129] H. Araki, Bogoliubov tranformation and fock representation of canonical anti-commutator relations, in *Operator Algebras and Mathematical Physics* Vol. 62, Contemporary Mathematics, Iowa City (1987).

[130] M. M. Wolf, Phys. Rev. Lett. **96**, 010404 (2006).

[131] K. Audenaert, J. Eisert, M. B. Plenio, and R. F. Werner, Phys. Rev. A **66**, 042327 (2002).

[132] N. Schuch, J. I. Cirac, and M. M. Wolf, Comm. Math. Phys. **267**, 65 (2006).

[133] S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995).

[134] F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004).

[135] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).

[136] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).

[137] M. Hastings, J. Stat. Mech. , P08024 (2007).

[138] F. Verstraete and J. I. Cirac, Phys. Rev. B **73**, 094423 (2006).

[139] F. Verstraete and J. I. Cirac, (2004), cond-mat/0407066.

[140] F. Verstraete, V. Murg, and J. I. Cirac, Advances in Physics **57**, 143 (2008).

[141] N. Maeshima, Y. Hieida, Y. Akutsu, T. Nishino, and K. Okunishi, Phys. Rev. E , 016705 (2001).

[142] Y. Nishio, N. Maeshima, A. Gendiar, and T. Nishino, (2004), cond-mat/0401115.

[143] M. B. Hastings, Phys. Rev. B **76**, 035114 (2007).

[144] A. Isacsson and O. F. Syljuasen, Phys. Rev. E **74**, 026701 (2006).

[145] V. Murg, F. Verstraete, and J. I. Cirac, Phys. Rev. A **75**, 033605 (2007).

[146] V. Murg, F. Verstraete, and J. I. Cirac, Phys. Rev. B **79**, 195119 (2009).

[147] J. Jordan, R. Orus, and G. Vidal, Phys. Rev. B **79**, 174515 (2009).

[148] M. Troyer, private communication .

[149] P. Jordan and Wigner, Z. Phys. **47**, 631 (1928).

[150] F. Verstraete and J. I. Cirac, J.Stat.Mech. **0509**, 012 (2005).

[151] G. Evenbly and G. Vidal, arXiv:0710.0692.

[152] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quant. Inf. Comput. **7**, 401 (2007).

[153] D. Perez-Garcia, F. Verstraete, J. I. Cirac, and M. M. Wolf, Quant. Inf. Comput. **8**, 0650 (2008).

[154] J. Eisert, M. Cramer, and M. Plenio, arXiv:0808.3773.

[155] M. M. Wolf, Phys. Rev. Lett. **96**, 010404 (2006).

[156] D. Gioev and I. Klich, Phys. Rev. Lett. **96**, 100503 (2006).

[157] F. Verstraete, J. J. Garcia-Ripoll, and J. I. Cirac, Phys. Rev. Lett. **93**, 207204 (2004).

[158] A. Jamiolkowski, Rep. Math. Phys. **3**, 275 (1972).

[159] F. Verstraete and H. Verschelde, quant-ph/0202124.

[160] N. Schuch, M. M. Wolf, and J. I. Cirac, Commun. Math. Phys **267**, 65 (2006).

[161] J. Hubbard, Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences **276**, 238 (1963).

[162] M. Rasetti, Series on Advances in Statistical Mechanics **7** (1991).

[163] P. Fulde and R. A. Ferrell, Phys. Rev. **135**, A550 (1964).

[164] A. Larkin and O. Ovchinnikov, Zh. Eskp. Teor. Fiz. **47**, 1136 (1994).

[165] R. Casalbuoni and G. Nardulli, Rev. Mod. Phys. **76**, 263 (2004).

[166] H. Tasaki, Journal of Physics: Condensed Matter **10**, 4353 (1998).

[167] E. H. Lieb, The Hubbard Model: Some Rigorous Results and Open Problems, in *Advances in Dynamical Systems and Quantum Physics*, Internat. Press, 1993.

[168] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[169] H. Shiba, Phys. Rev. B **6**, 930 (1972).

[170] G. Orso, Physical Review Letters **98**, 070402 (2007).

[171] H. Hu, X.-J. Liu, and P. D. Drummond, Physical Review Letters **98**, 070403 (2007).

[172] T. B. Bahder and F. Woynarovich, Phys. Rev. B **33**, 2114 (1986).

[173] G. Ortiz, R. Somma, J. Dukelsky, and S. Rombouts, Nuclear Physics B **707**, 421 (2005).

[174] F. Pan, J. P. Draayer, and W. E. Ormand, Physics Letters B **422**, 1 (1998).

[175] A. E. Feiguin and F. Heidrich-Meisner, Physical Review B **76**, 220508 (2007).

[176] M. Tezuka and M. Ueda, Physical Review Letters **100**, 110403 (2008).

[177] G. G. Batrouni, M. H. Huntley, V. G. Rousseau, and R. T. Scalettar, Phys. Rev. Lett. **100**, 116405 (2008).

[178] M. C. Gutzwiller, Phys. Rev. **137**, A1726 (1965).

[179] A. Paramekanti, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **87**, 217002 (2001).

[180] S. Pathak, V. B. Shenoy, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **102**, 027002 (2009).

[181] M. E. Pezzoli and F. Becca, Ground-state properties of the disordered hubbard model in two dimensions, arXiv.org:0906.4870.

[182] L. Pitaevskii and S. Stringari, *BoseEinstein Condensation* (Clarendon Press, Oxford, 2003).

[183] M. Henny *et al.*, Science **284**, 296 (1999).

[184] R. Horn and C. Johnson, *Topics in Matrix Analysis* (Cambridge University Press, 1985).

[185] P. Billingsley, *Probability and Measure*, 3rd ed. (Wiley-Interscience, 1995).

Acknowledgements

I am very deeply grateful for the support and guidance I have obtained from my Thesis advisor Ignacio Cirac throughout the course of my Ph.D. Having the opportunity of getting the guidance of a person who has on the one hand such a deep understanding of physics and on the other hand huge pedagogical abilities is a privilege every Ph.D. student can dream of. I acknowledge his immense patience, his constant encouragement and his great kindness. Learning and discussing physics from and with him has been a unique opportunity for me and has inspired me in many ways. I will always stay in his debt.

Throughout the course of my Thesis I had the opportunity of collaborating with various people, and I would like to acknowledge their contributions in chronological order. In the beginning of my Ph.D. I got the possibility to learn from Michael Wolf, who unfortunately moved to Copenhagen. I am very grateful for his help and guidance.

The pairing theory was developed in close collaboration with Géza Giedke. I could not have been more lucky to get advice from a person who has such a broad knowledge of various fields of physics. I highly acknowledge the huge amount of time he devoted to my education, his readiness for discussions and his patience.

I am very grateful to Frank Verstraete who was willing to host me in Vienna for a period of two months to work on the development of the fPEPS. During this time I could learn a lot about MPS and PEPS from him and his co-workers, especially from Enrique Rico. Apart from this, I acknowledge the kind hospitality of Frank and his group which contributed a big deal that I felt well in Vienna.

During the final part of my work on the fPEPS I collaborated with Norbert Schuch. His big enthusiasm, his readiness for discussions and explanations and his willingness to share ideas have been of great help for me.

Though I never worked on a project with her, I would also like to acknowledge the help I received from Mari Carmen Bañuls, who was always willing to discuss with me. Further, she taught me a lot about programming.

This work profited from discussions with Karl-Gerd Vollbrecht, Juan Jose Garcia-Ripoll, David Peres-Garcia, Miguel Aguado, Matteo Rizzi and others.

I acknowledge the effort of Thomas Schulte-Herbrüggen in his position as coordinator of the Ph.D. program QCCC. Further, I appreciate the initiatives of my fellow Ph.D students from the QCCC-program in our seminars and in the organization of the workshop.

During my time at MPQ I had the opportunity to share the office with (in chronological order) Maria Eckholt, Christine Muschik, Gorka Azcune, Henning

Christ, Oliver Buerschaper and Fabio Mezzacapo. I am very happy that I could get to know them all, and I am thankful for the good time we had together discussing physics and more, and for their support concerning work and beyond.

This work has been supported by the Ph.D. program Quantum Computation, Communication and Control (QCCC) of the Elitenetzwerk Bayern (ENB).