Quantum Effects in Collisions of Ultracold Atoms with Walls and Nanostructures

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Abstract. We study scattering of ultracold atoms by absorbing surfaces. Loss of flux through inelastic reactions and adsorption is described in an unambiguous and model-independent way by incoming boundary conditions in the semiclassical region near the surface. The near-threshold behaviour of the scattering amplitude is determined by a few parameters of the potential tail beyond the semiclassical region. Investigation of quantum reflection and scattering by flat and spherical surfaces shows that the curvature of the surface strongly influences the range to which the scattering amplitudes are sensitive in the atom-surface interaction.

1. Introduction

The interaction of cold atoms with each other and with surfaces is a topic of intense current interest [1,2]. Technological advances have made it possible to perform experiments with atoms at temperatures in the nanokelvin range [3]. At such low temperatures, quantum effects become important. Ultracold atoms approaching a flat surface are generally lost through inelastic reactions or adsorption if they come to within a few atomic units of the surface. At low enough energy they can be spared this fate through classically forbidden (quantum) reflection in the distant tail of the potential [3–9], see Sec. 2. If the surface is curved, e.g. spherical, the scattering cross section is sensitive to both modulus and phase of the partial wave S-matrix, and the radius of the sphere can be tuned to probe different regions of the atom-surface potential [10]. The theoretical description is given in Sec. 3 and applications are discussed in Sec. 4.

2. Scattering by flat surfaces

For small distances s, a few atomic units or so, the interaction between an atom and a flat surface depends on details of the structure of both atom and surface and is quite complicated. When ultracold atoms enter this "close" region, excitation modes of atom or surface are easily excited, the atom loses energy and is trapped, adsorbed by the surface ("sticking"). Beyond this close region, the atom-surface interaction is well described by a van der Waals potential $-C_3/s^3$. At very large distances, retardation effects become important and an atom in its ground state or in a metastable excited state feels a potential $-C_4/s^4$ [11]. The coefficients $C_{3,4}$ depend on the properties of both atom and surface [12,13]; they can be expressed in terms of the lengths

$$\beta_\alpha = \left(\frac{2M}{\hbar^2}C_\alpha\right)^{1/(\alpha-2)} , \qquad (1)$$

which define typical length scales for quantum mechanical effects associated with the corresponding part of the potential, see Table 1 for examples. The quotient $L = C_4/C_3 =$

$(\beta_4)^2/\beta_3$ has the dimension of a length and is characteristic for the transition zone separating the "small" distance van der Waals regime (which is still beyond the close region of complicated consuming interactions) from the highly retarded regime at very large distances. The true atom-surface potential [14] varies smoothly between these limits,

$$V_{\text{flat}}(s) = -\frac{C_3}{s^3 \, v(s/L)} \, , \tag{2}$$

where $v(x)$ is a shape function with the asymptotic behaviour

$$v(x) \overset{x\to 0}{\sim} 1 \, , \quad v(x) \overset{x\to\infty}{\sim} x \, . \tag{3}$$
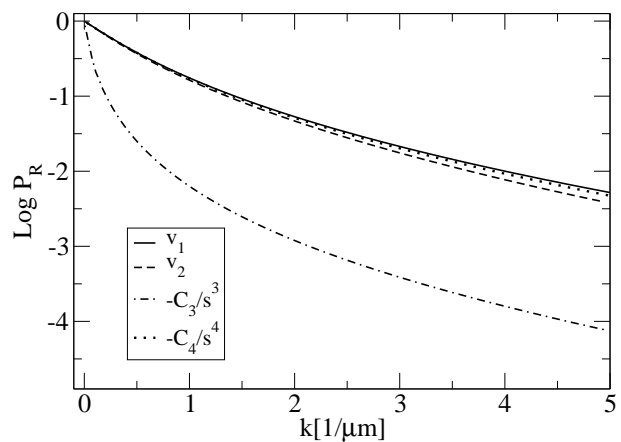
Explicit calculations in this contribution are based on two different shape functions,

$$v_1(x) = 1 + x \, , \quad v_2(x) = \frac{\pi/2}{\arctan\left[\pi/(2x)\right]} \, , \tag{4}$$

which were proposed by Shimizu [9] (v_1) and by Holstein [15] (v_2).

The motion of the atom under the influence of the potential (2) is classical at large distances, where the potential vanishes, and also at "small" distances, as is always the case for potentials more singular than $1/s^2$. In between, there is a nonclassical region where incoming atoms can be reflected without reaching a classical turning point. Ultracold atoms which penetrate this nonclassical region of the attractive potential tail proceed to the close region where they are lost (absorbed); the others are reflected elastically by the nonclassical part of the potential tail ("quantum reflection"). The region where quantum reflection occurs is very far from the surface for near-threshold energies [6, 7]. The amplitude for quantum reflection is obtained by solving the Schrödinger equation for motion normal to the surface with purely incoming boundary conditions at small distances near the surface. These boundary conditions describe the complete loss of all atoms reaching the surface and can be formulated in an unambiguous way using WKB waves, because motion becomes increasingly classical towards smaller distances in the singular attractive potential. Absorptive effects are often formulated with the help of a complex potential, but an energy-independent local complex potential cannot describe total loss of flux at small distances.

Figure 1. Probability for quantum reflection of metastable 2^3S helium atoms from a flat conducting wall. The solid and dashed lines show the results for the potential (2) and shape functions (4); the dot-dashed line shows the result for the nonretarded van der Waals potential $-C_3/s^3$ and the dotted line shows the result for the highly retarded potential $-C_4/s^4$.

Figure 1 shows the probabilities for helium atoms in the metastable 2^3S state being quantum reflected by a flat conducting wall. At energies for which the probabilities are appreciable, quantum reflection is essentially determined by the highly retarded part, $-C_4/s^4$, of the potential. This is a general pattern in the quantum reflection of atoms by flat surfaces [3, 6, 7]. The phase of the amplitude for quantum reflection provides information on time and space shifts involved in the process [16]. These shifts are relatively small, so the effect of the phase is not easily observed in scattering by flat surfaces.

3. Scattering by a sphere

As the simplest non-flat surface, we now turn to scattering by a sphere. Beyond the close region of complicated and consuming atom-surface interactions, the interaction of an atom with a spherical surface is well described by a local potential which depends on the radius R of the sphere and the distance s of the atoms from the surface. For very large R, and s small compared to R but still beyond the close region, the potential behaves as in the case of a flat surface (2). When s is large compared to R, the potential behaves as a nonretarded van der Waals potential $-C_6/s^6$ for "small" distances s (still larger than R) and as a highly retarded potential, $-C_7/s^7$, for large s,

$$V(s) = -\frac{C_6}{s^6 \, v(s/L')} \, , \quad L' = \frac{C_7}{C_6} \, , \tag{5}$$

where $v(x)$ is again a shape function (3) describing the transition from the nonretarded to the highly retarded regime, and L' is a length scale for the transition zone. A potential which satisfies all boundary conditions is, e.g.,

$$V_{\mathrm{sphere}}(s) = -\left[\frac{s^3}{C_3} v\left(\frac{s}{L}\right) + \frac{s^6}{C_6} v\left(\frac{s}{L'}\right) \right]^{-1} \, . \tag{6}$$

For a conducting sphere with radius R, the coefficients $C_{6,7}$ are related to the corresponding coefficients C_3 [14] and C_4 [17] of the flat-surface case by

$$C_6 = 12R^3 C_3 \, , \quad C_7 = \frac{46}{3} R^3 C_4 \quad \Rightarrow \quad L' = \frac{23}{18} L \, . \tag{7}$$

The strengths $C_{6,7}$ can be related to characteristic lengths $\beta_{6,7}$ as in (1); numbers are given in Table 1 for $R = 200$ au and $R = 2000$ au.

Table 1. Lengths (in au) derived from the potential strength parameters $C_3 = 1.9009$ au, $C_4 = 5163$ au for He($2\,^3S$) [18] and $C_3 = 1.889$ au, $C_4 = 1417$ au for Na [19] according to (7), (1)

length	β_3	β_4	L	$\beta_6(200)$	$\beta_7(200)$	$\beta_6(2000)$	$\beta_7(2000)$	L'
He($2\,^3S$)	27 740	8 680	2 716	1 277	1 560	7 184	6 211	3 470
Na	158 300	10 900	750	1 974	1 708	11 100	6 803	959

The scattering of atoms from a sphere is described [20] by the radial Schrödinger equation with the effective potential

$$V_{\mathrm{eff}}(r) = V_{\mathrm{sphere}}(s) + \frac{\hbar^2}{2M} \frac{l(l+1)}{r^2} \, , \quad r = s + R > R \, , \tag{8}$$

for a given angular momentum quantum number l. As in the flat-surface case, the singular attractive potential tail (beyond the close region) allows the absorption of atoms near the surface to be described unambiguously via incoming boundary conditions for $r \to R \Leftrightarrow s \to 0$. Because of loss of flux, the S-Matrix $S_l = e^{2i\delta_l}$ is not unitary and the related scattering phase shift δ_l is complex. For $l = 0$, the radial Schrödinger equation is identical to the equation for normal motion in the flat-surface case, and scattering is essentially quantum reflection by the nonclassical region of the attractive potential tail. The near-threshold behaviour of the s-wave phase shift is

$$\delta_0 \overset{k \to 0}{\sim} -(\bar{a}_R - ib)k + \frac{1}{3}(k\Lambda)^3 \, . \tag{9}$$
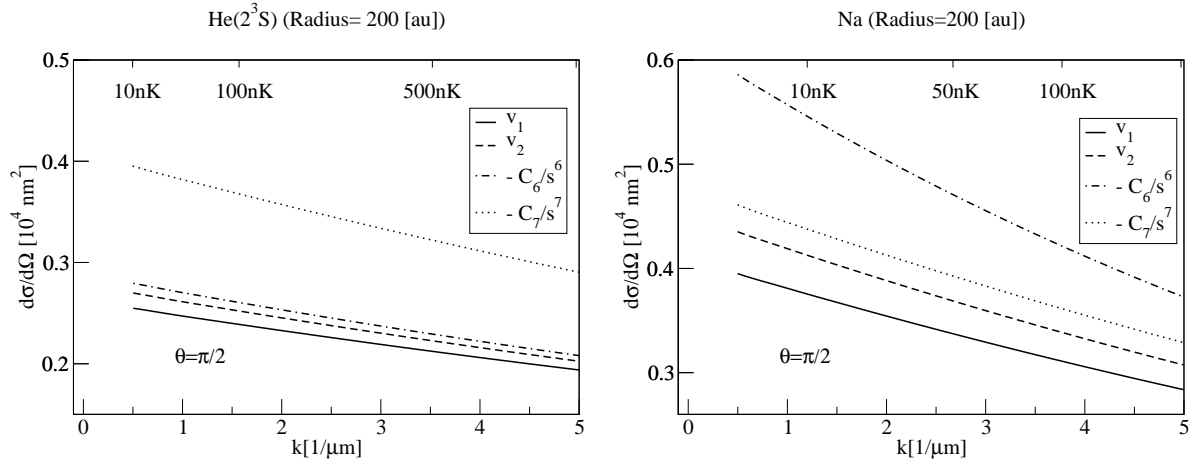
Figure 2. $d\sigma/d\Omega$ at $\theta = \frac{\pi}{2}$ for the elastic scattering of He($2\,^3S$) atoms (left-hand panel) and ground-state sodium atoms (right-hand panel) by an absorbing sphere of radius $R = 200$ au.

Here $\bar{a}_R - ib \equiv \mathcal{A}_0$ is the complex s-wave scattering length; $\bar{a}_R = R + \bar{a}$, and the "mean scattering length" $\bar{a}$, the threshold length b and also Λ are tail parameters determined only by the nonclassical part of the tail of the potential $V_{\text{sphere}}(s)$ [21].

For $l \geq 1$, the effective potential (8) contains a centrifugal barrier instead of just a nonclassical region in the tail. For potentials falling off faster than $1/s^5$, the near-threshold behaviour of the p-wave phase shift δ_1 is determined by a complex p-wave scattering length $\mathcal{A}_1$, $\delta_1 \overset{k\to 0}{\sim} [k\mathcal{A}_1(R)]^3/3$. The contributions of s- and p-waves to the differential cross section give

$$\frac{d\sigma}{d\Omega} \overset{k\to 0}{\sim} |\mathcal{A}_0|^2(1-2bk) + k^2 \left[F(l=0) + \tilde{F}(l=0,1)\cos\theta \right], \tag{10}$$

which is exact up to order $\mathcal{O}(E)$. Here F is a well-defined function of $\mathcal{A}_0$ and Λ, while $\tilde{F}$ also depends on $\mathcal{A}_1$. For homogenous attractive potentials and $R \to 0$, all parameters in (10) can be derived analytically from the corresponding results for repulsive homogenous potentials [21–23].

4. Applications

The isotropic s-wave contribution to (10) can be obtained for $\theta = \frac{\pi}{2}$, $\cos\theta = 0$. Figure 2 shows $d\sigma/d\Omega(\theta = \pi/2)$ for the elastic scattering of He($2\,^3S$) atoms (left-hand panel) and ground-state sodium atoms (right-hand panel) by an absorbing sphere of radius $R = 200$ au for wave numbers k up to $5/\mu$m. This corresponds to temperatures up to $1\ \mu$K for helium and 200 nK for sodium. The dot-dashed lines show the results for a nonretarded van der Waals potential $-C_6/s^6$ and the dotted lines show the results for the highly retarded case $-C_7/s^7$. The solid and dashed lines show the cross sections obtained with the realistic potential (6) for the two versions (4) for the shape factor. Note that the cross section in Fig. 2 is sensitive to both the modulus and the phase of the s-wave S-matrix $e^{2i\delta_0}$; in contrast, the quantum reflection probability in the flat-surface case contains no phase information.

For He($2\,^3S$) the results for $d\sigma/d\Omega$ obtained with (6) are much closer to the van der Waals case than to the retarded case. For sodium, the retarded $-C_7/s^7$ part of the potential is dominant. The results can be understood via the magnitudes of the characteristic lengths β_α associated with the potential strengths C_α according to (1). For helium, $\beta_{6,7}(200)$ are noticeably smaller than $L' = C_7/C_6$ and lie short of the transition zone in the nonretarded van der Waals regime. For sodium, $\beta_{6,7}(200)$ are noticeably larger than L', so the retarded part of the potential dominates
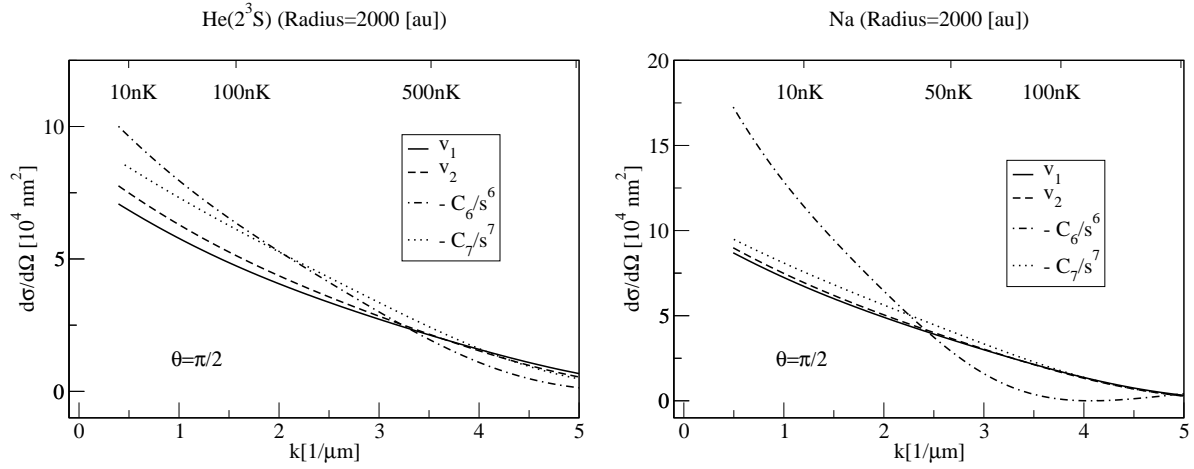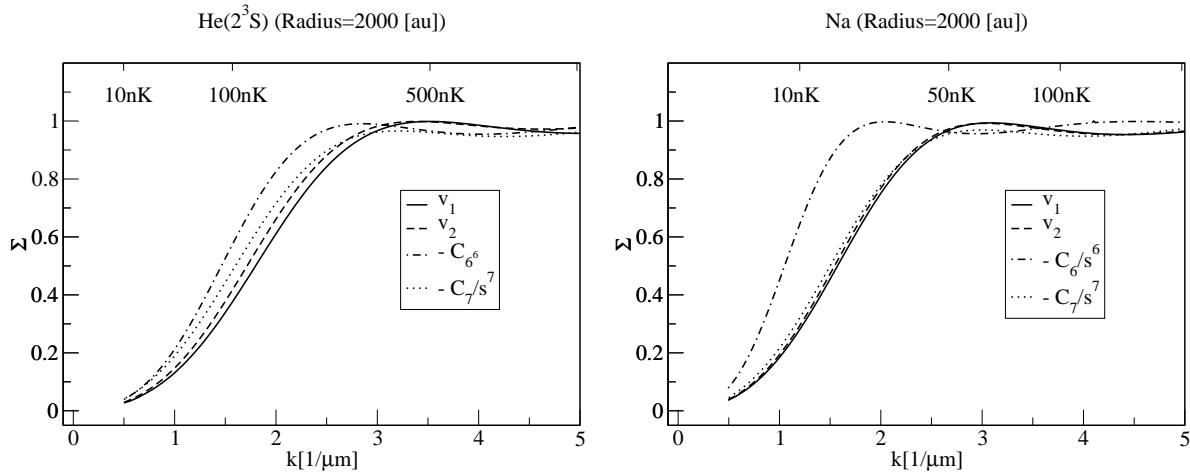
Figure 3. Same as Fig 2, but for $R = 2000$ au.
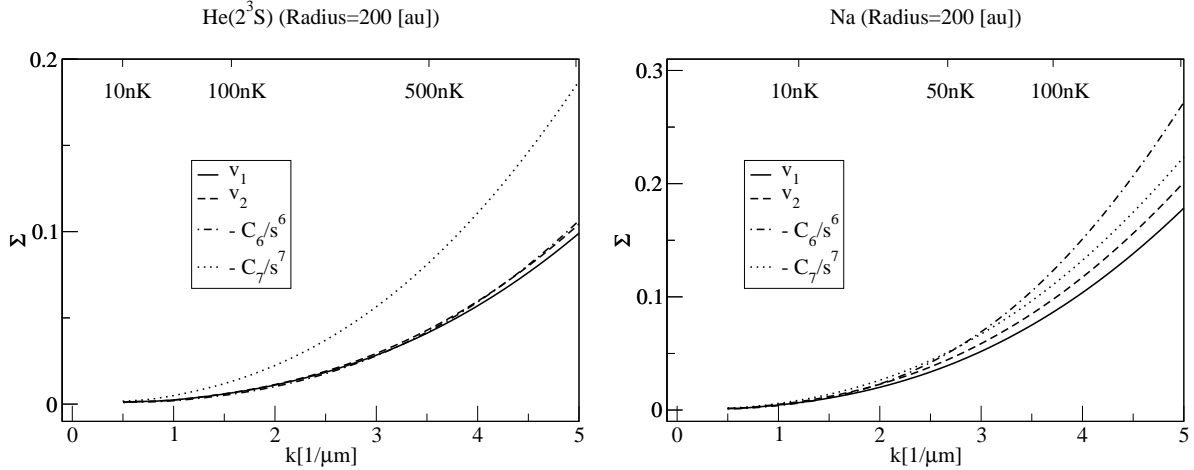
Figure 4. Asymmetry (11) for the elastic scattering of He($2\,{}^3S$) atoms (left-hand panel) and ground-state sodium atoms (right-hand panel) by an absorbing sphere of radius $R = 200$ au.

the result. For sufficiently large radius R of the sphere, $\beta_{6,7}(R)$ are larger than the characteristic length L', even for helium so that the differential cross section is dominated by the retarded part of the potential. This can be seen in Fig. 3 showing the same cross section as Fig. 2, but for $R = 2000$. For $R \to \infty$ we recover the flat-surface case, where the lengths $\beta_{3,4}$ are much larger than the length $L \approx L'$ typical of the transition zone, see Table 1. This explains why quantum reflection by flat surfaces is mainly sensitive to the highly retarded part of the potential.

Further information can be obtained from the dimensionless asymmetry

$$\Sigma(k) \stackrel{\text{def}}{=} \frac{\frac{d\sigma}{d\Omega}(\theta = 0) - \frac{d\sigma}{d\Omega}(\theta = \pi)}{\frac{d\sigma}{d\Omega}(\theta = 0) + \frac{d\sigma}{d\Omega}(\theta = \pi)} = 2k^2 \tilde{F}(l = 0, l = 1) + \text{ higher terms },\qquad (11)$$

which describes the leading deviation from isotropy in (10). Figures 4 and 5 show $\Sigma(k)$ for He($2\,{}^3S$) (left-hand panels) and Na atoms (right-hand panels) for $R = 200$ au and $R = 2000$ au respectively. The asymmetry is clearly more strongly influenced by the nonretarded $-C_6/s^6$ part of the potential for the smaller R value.

He(2^3S) (Radius=2000 [au])   Na (Radius=2000 [au])

Figure 5. Same as Fig. 4, but for $R = 2000$ au.

5. Summary

The absorptive effect of the loss of ultracold atoms at surfaces can be described in an unambiguous and model-independent way via incoming boundary conditions in the semiclassical region of the attractive potential tail. For flat surfaces, quantum reflection in the distant nonclassical part of the potential is mainly sensitive to the highly retarded part of the atom-surface potential. When the surface is spherical, the elastic scattering cross section is sensitive to different regimes of the atom-surface potential, and the nonretarded van der Waals regime becomes increasingly important for smaller radii. Generalizing this result one might conclude that a small radius of curvature makes the amplitudes for quantum reflection and scattering more sensitive to comparatively small distances in the atom-surface potential.

6. References

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