Quantum reflection of cold atoms

Hilmar Oberst and Fujio Shimizu
Institute for Laser Science, University of Electro-Communications, Chofu, Tokyo 182-8585, Japan
E-mail: hilmar@ils.uec.ac.jp, fshimizu@ils.uec.ac.jp

Abstract.

The coherent reflection of ultra-cold neon and helium atoms from silicon surfaces and surface structures is measured and analyzed. When the silicon surface is flat, the reflection is explained by the quantum reflection due to van der Waals attractive potential near the silicon surface. When the silicon surface is modified to form a grating structure, the reflectivity increases dramatically. For certain ranges of surface structure parameters, the reflection may be interpreted as a coherent summation of Fresnel diffraction of the atomic wave at the ridges of the grating structure.

1. Introduction

Waves are deflected and partially reflected at any boundary that causes an abrupt change of the wave vector. In optics, the reflection at a boundary is the most important resource of manipulating an optical wave. The same kind of reflection should in principle also occur for matter waves, but has not been exploited seriously, because the wavelength of a matter wave at room temperature is generally much shorter than the atomic size that characterizes a solid surface. In addition, most particles do not transmit through solid materials coherently. In recent years - owing to the development of cooling techniques for atoms - it has become possible to generate matter waves whose de Broglie wavelength is much longer than the atomic structure of solids. Such matter waves should then be reflected at a solid surface in a similar way as an optical wave, i.e. due to an abrupt change of the wavevector at the boundary. In the case of matter waves this phenomenon has been called 'quantum reflection', and was previously predicted for and observed with helium and hydrogen atoms at superfluid helium surfaces [1]; only recently, the quantum reflection of slow atoms on solid surfaces has also been demonstrated [2, 3], and applied to study atom-surface interactions and to realize new atom-optical devices [4, 5].

In this paper, we summarize our experimental results on the quantum reflection of ultracold, metastable neon and helium atoms on silicon surfaces and surface structures, and present a detailed quantitative analysis of the observed effects. In particular, we demonstrate that the reflectivity increases dramatically when a grating-like surface structure is used instead of a flat surface.

2. Quantum reflection at van der Waals potential tails

The force that a neutral atom feels near a solid surface is caused by attractive van der Waals potential [6]. The atom approaching the surface is constantly accelerated, and its de Broglie wavelength shrinks. The atom therefore is influenced by atomic-size irregularities and is...
ultimately scattered incoherently. For a very slow atom, however, the attractive van der Waals potential is sufficiently steep to partly reflect the atomic wave. The steepness of the potential, \( \phi \), may be scaled as a fractional change of the wavevector over the distance of its de Broglie wavelength,

\[
\phi = \frac{1}{k^2} \frac{dk}{dz},
\]

where \( k = \sqrt{k_0^2 - 2mU(z)/\hbar^2} \) is the local wavevector of the atom of mass \( m \), propagating in the potential \( U(z) \), with the incident wavevector \( k_0 \). For a power law potential \( U(z) = -C_n/z^n \) with \( n > 2 \), \( \phi \) reaches a maximum at a finite distance \( z_{\text{max}} \) and decreases to zero at \( z = 0 \) and \( z = \infty \). Therefore, a slow atom is reflected at some distance away from the surface due to the van der Waals potential, \( U = -C_3/z^3 \). We may expect a large reflectivity if \( \phi_{\text{max}} > 1 \). This gives the maximum velocity of the atom

\[
v \leq \frac{\hbar^3}{m^2 C_3},
\]

and the atom is reflected at around

\[
z_r \approx \frac{mC_3}{\hbar^2}.
\]

For a typical light atom, such as Na in the ground state or Ne in the metastable state, \( C_3 \approx 10^{-49} \text{ Jm}^{-3} \) and \( m \approx 3 \times 10^{-26} \text{ kg} \). Therefore, the reflection will be strong only if the incident velocity \( v < 3 \text{ mm/s} \); due to the gravity acceleration on Earth such low velocities are difficult to achieve for freely propagating atoms. The distance of reflection \( z_r \) is typically a few hundred nanometers, where the surface roughness is averaged out.

The Schrödinger equation with the interaction potential \( U(z) = -C_n/z^n \) can be written in dimensionless form by scaling \( z \) with \( z_s = (mC_n/\hbar^2)^{1/(n-2)} \) and the incident kinetic energy with \( E_s = \hbar^2/(mz_s^2) \equiv mv_s^2 \). We can therefore introduce a more accurate scale of the incident velocity as

\[
v_s \equiv \frac{\hbar}{m} \left( \frac{\hbar^2}{mC_n} \right)^{1/(n-2)}.
\]

The reflectivity then depends only on the scaled incident velocity, i.e. \( R = R(v/v_s) \). Two interesting properties of the quantum reflection can be deduced: The reflectivity increases (1) for atoms with smaller mass and (2) for surfaces with weaker van der Waals interaction. Both effects are clearly seen in our experiments.

The precise form of the van der Waals interaction can be calculated from the imaginary-frequency dipole polarizability \( \alpha(\omega) \) of the atom and the dielectric constant \( \epsilon(\omega) \) of the solid [8, 9, 3]. The potential has two asymptotic forms: \( U(z) = -C_3/z^3 \) for \( z \to 0 \), and \( U(z) = -C_4/z^4 \) for \( z \to \infty \), showing retardation effects [6]. The constants \( C_3 \) and \( C_4 \) can be expressed as

\[
C_3 = \frac{\hbar}{16\pi^2\epsilon_0} \int_0^\infty d\xi \alpha(\alpha) \frac{\epsilon(\alpha)}{\epsilon(\alpha) + 1}, \quad C_4 = \frac{3\hbar\alpha(0)}{32\pi^2\epsilon_0} \frac{\epsilon(0) - 1}{\epsilon(0) + 1} \phi(\epsilon(0)),
\]

where, \( \phi \) is an analytical function [9]. The result for a perfect conductor is obtained by setting \( \epsilon \to \infty \).

For helium - being a relatively simple two-electron atom - the imaginary-frequency dipole polarizability \( \alpha(\omega) \) of the metastable states has been calculated with high precision [7, 10]. Similarly, the dielectric constant of silicon is known over nearly the entire frequency range [11]. Using these values we calculated the van der Waals constants to be \( C_3^{\text{Si}} = 1.23 \times 10^{-48} \text{ Jm}^3 \), \( C_4^{\text{Si}} = 1.77 \times 10^{-55} \text{ Jm}^4 \) for a perfect conductor, and \( C_3^{\text{Si}} = 8.8 \times 10^{-49} \text{ Jm}^3 \), \( C_4^{\text{Si}} = 1.2 \times 10^{-55} \text{ Jm}^4 \) for a silicon surface.
For Ne* we calculate $C_4^\infty = 1.0 \times 10^{-55}$ Jm$^4$ using the value for the static dipole polarizability $\alpha_{Ne}(0) = 3.07 \times 10^{-39}$ Fm$^2$. Similarly, we estimate the constant $C_3^\infty = 1.13 \times 10^{-48}$ Jm$^3$ by using a one-oscillator model for the dipole polarizability, i.e. $\alpha(\xi \omega) \approx \alpha(0)/(1 + (\omega/\omega_a)^2)$, with $\omega_a^{Ne} = 3.1 \times 10^{15}$ s$^{-1}$ [12]. Using the static dielectric function of silicon $\epsilon(0) = 11.7$ we calculate the van der Waals constants to be $C_3^{Si} = 9.5 \times 10^{-49}$ Jm$^3$ and $C_4^{Si} = 6.8 \times 10^{-56}$ Jm$^4$ for a silicon surface.

Using Eq. 4, we obtain for the scaling velocities for He and Ne: $v_s^{He} = 4.89$ cm/s and $v_s^{Ne} = 5.69$ mm/s for the retarded potential, and $v_s^{He} = 2.16$ cm/s and $v_s^{Ne} = 0.94$ mm/s for the unretarded potential. Their ratios are $v_s^{He}/v_s^{Ne} = 8.6$ for the retarded and $v_s^{He}/v_s^{He} = 23$ for the unretarded potential, respectively.

### 3. Experimental setup

![Figure 1. Experimental setup.](image1)

![Figure 2. Atomic image on the detector.](image2)

We measured the reflectivity of metastable neon atoms in the $1s_3(J = 0)$ state and helium atoms in the $1s2s[3S_1]$ state from a flat polished silicon surface. Similar experimental setups were used to prepare the atomic Ne* and He* beams. The setup used for the experiment with helium is shown in Fig. 1.

The atoms were laser-cooled and trapped in magneto-optical traps (MOT). The Ne* atoms are trapped in the $1s_3(J = 2)$ metastable state using the transition at 640 nm. The He* atoms are trapped in the metastable $1s2s[3S_1]$ state using the transition at 1083 nm. The atoms are then released from the trap and hit the silicon surface at grazing angle. The typical angle between the silicon surface and the atomic beam was between 1 to 10 mrad. The technique to release atoms from the trap was slightly different for Ne and He. The Ne atoms were released by optically pumping the atoms into the $1s_3(J = 0)$ state by using the $1s_3 - 2p_3$ transition at 598 nm. Since the atoms in the $1s_3$ state are not influenced by the magnetic field and the laser of the MOT, they drop vertically pulled by gravity. The velocity of the Ne atom at the silicon surface was 3 m/s, corresponding to about 45 cm of free fall. For helium, the same technique
cannot be used, because the optical pumping from a triplet to singlet state is not practical. Consequently, the magnetic field influences the trajectories of He* atoms in the \(2^3S_1\) state. The atoms were therefore released with short pulses of a resonant laser beam at 1083 nm, and the trapping laser beams and coils are switched off simultaneously. This procedure increased the velocity of the He* atoms at the silicon sample, but reduced the influence of magnetic field and stray resonant light. The velocity was varied between 23 to 70 m/s, which was controlled by adjusting the pulse duration and intensity of the releasing laser. The atoms were detected with a micro-channel plate detector (MCP). For the experiment with helium, the high voltage of the MCP detector was gated to select a narrow velocity range. A typical spatial distribution of atom counts on the MCP detector is shown in Fig. 2. The pattern contains the atoms reflected on the silicon plate, as well as those passing behind and in front of the sample. The image is analysed to determine the reflectivity of the atomic beam on the sample.

4. Quantum reflection of Ne* and He* on a flat silicon surface

![Figure 3](image1.png)  
**Figure 3.** Reflectivity of Ne* (1s_3) atoms on a polished, undoped Si plate as a function of the normal incident velocity. The long-dashed line shows the reflectivity expected on a perfect conductor. The solid line shows the case for undoped silicon.

![Figure 4](image2.png)  
**Figure 4.** Reflectivity of He* (2^3S_1) atoms on a polished, undoped Si plate as a function of the normal incident velocity. The long-dashed line shows the reflectivity expected on a perfect conductor. The solid line shows the case for undoped silicon.

Figures 3 and 4 show the experimental results obtained for neon and helium atoms, respectively. The He* data were obtained by varying both the incident velocity and incident angles. They all fit in a single curve, which is expected from the one-dimensional character of the experiment.

We compare the curve to the reflectivity calculated by solving the Schrödinger equation using the calculated van der Waals potentials. For neon the potential was approximated by \(U(z) = -C_4/(z^3(z + l))\), with \(l = C_4/C_3\). We show the reflectivity expected on a perfect conductor, which clearly deviates, and on silicon. For both Ne* and He* the experimental values are close but slightly larger than the reflectivity expected on silicon. The reason for this discrepancy is not yet clear.

We have derived above that the reflectivity increases with decreasing mass \(m\) of the atom. The latter is clearly shown in Figs. 3 and 4, where the velocity to obtain the same reflectivity is ten times larger for He compared to Ne.

In Fig. 5 we plot the reflectivities of Ne* and He* on silicon with the incident velocities scaled by the calculated values for \(v_s\) (Eq. 4). We use only the values for the retarded potential. After
Scaled normal incident velocity $v_{\text{Ne}} = 0.569 \text{ cm/s}$ and $v_{\text{He}} = 4.89 \text{ cm/s}$ for Ne* and He*, respectively. The normal incident velocity to achieve the same reflectivity as on a flat surface was $v_{\text{Ne}} = 0.569 \text{ cm/s}$ and $v_{\text{He}} = 4.89 \text{ cm/s}$.

In the case of the quantum reflection, the reflectivity increases with decreasing van der Waals potential constants $C_3$, $C_4$. The potential constants are approximately proportional to the density of the surface. In order to simulate a low density material, we used grating-like silicon surface consisting of parallel, narrow ridges such as shown in Fig. 6. The structure was formed by chemical etching of silicon with a period of $5 \mu m$ and a size at the top of the ridge of about $100 \text{ nm}$.

The reflectivities measured on this sample with Ne* and He* atomic beams at grazing incidence are shown in Fig. 8 and 9. The improvement of the reflectivity compared to a flat surface is impressive.

The normal incident velocity to achieve the same reflectivity as on a flat surface was 5 to 10 times faster. The reflectivity at relatively fast velocity was more than 100 times larger. We also noticed that the reflectivity of He* and Ne* atoms basically overlap, which nicely confirms the scaling properties of the quantum reflection.

The reflectivity is governed by a wave theory which does not depend on the characteristics of the boundary. The simple example is the Kirchhoff-Helmholtz diffraction theory in optics. Suppose we place knife-edges imperceptibly separated by $\ell$, as shown in Fig. 7, and send a plane wave with normal incidence. The reflected wave is the Poynting-Helmholtz diffraction theory in optics. The reflected wave is the Poynting-Helmholtz diffraction theory in optics. The total intensity is $I_{\text{total}} = I_{\text{incident}} + I_{\text{reflected}} + I_{\text{attenuated}}$, where $I_{\text{incident}}$ is the intensity of the incident wave, $I_{\text{reflected}}$ is the intensity of the reflected wave, and $I_{\text{attenuated}}$ is the intensity of the attenuated wave. The reflected wave is the Poynting-Helmholtz diffraction theory in optics.

The reflectivity of He* and Ne* atoms is shown as a function of the scaled normal incident velocity $v_{\text{Ne}}$ and $v_{\text{He}}$ on silicon as shown in Fig. 5. The reflectivity of He* and Ne* atoms is shown as a function of the scaled normal incident velocity $v_{\text{Ne}}$ and $v_{\text{He}}$ on silicon as shown in Fig. 5.
Figure 6. SEM photograph of the cross-section of the silicon plate. Atoms hit the top of the ridges placed at 5 µm intervals. The top is flat with a width of approximately 100 nm.

Figure 7. Diffraction of an atomic beam from an array of knife edges.

Figure 8. Reflectivity of neon atoms on the sample shown in Fig. 6 as a function of the normal incident velocity. The solid line shows the reflectivity on flat, polished silicon surface.

Figure 9. Reflectivity of helium atoms on the sample shown in Fig. 6 as a function of the normal incident velocity. The solid line shows the reflectivity on a flat, polished silicon surface.

The wavevector $k$ at a small angle $\theta$. The incident wave is diffracted at the tip of the knife edges. The diffracted waves constructively interfere at the direction of $-\theta$ forming the coherent reflected wave. Since $\theta$ is small the propagation of the wave $\Psi(x, y) = \exp(ikx)\psi$ can be described by a parabolic equation

$$2ik \frac{\partial \psi}{\partial x} + \frac{\partial^2 \psi}{\partial y^2} = 0. \quad (7)$$

The parameters that affect the propagation are $k$ and $L$. They are eliminated by normalizing $x$ and $y$ by $x = L\xi$ and $y = \sqrt{L/k}\eta$, obtaining

$$2i \frac{\partial \psi}{\partial \xi} + \frac{\partial^2 \psi}{\partial \eta^2} = 0. \quad (8)$$
6. Conclusion

The reflectivity expected on an array of ideal ridges, i.e. very thin and without van der Waals forces, has been calculated in [13] and is shown as solid line in Fig. 10. This reflectivity represents an upper boundary of ideal ridges, i.e. very thin and without van der Waals forces, which is the same as the scaling law Eq. (9).

\[ \theta T'Y^\wedge = \frac{\theta}{T} = \frac{\gamma}{T} \]

The incident wave is proportional to \( \exp(i\theta Y^\wedge) \), which is written in the original variables

\[ \theta T'Y^\wedge = \frac{\theta}{T} = \frac{\gamma}{T} \]
potentials. The data also clearly demonstrate the scaling properties expected for the quantum reflection on a solid surface. On a surface structure with parallel, narrow ridges the reflectivity depends mainly on the distance between the ridges, the incident wavevector and the incident angle but is insensitive to the material properties. The observed scaling law can be derived by describing the reflection process as the Fresnel diffraction at an array of edges. In order to obtain a quantitative description, the van der Waals interaction near the ridges has to be included in the model.

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