Quantum reflection as the reflection of subwaves*

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This paper studies quantum reflection with recent research on reflection coefficient. Based on the analytical transfer matrix method, a novel explanation for this phenomenon is proposed that quantum reflection is the reflection of subwaves, which originate inherently from the inhomogeneity of the fields and is always neglected in the semiclassical regime. Comparison with exact formula and the numerical calculations for different potentials has confirmed the reliability and the validity of the proposed theory.

Keywords: quantum reflection, cold atom, analytical transfer matrix method
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1. Introduction

Quantum reflection which is referred to the classically forbidden reflection has become a subject of profound importance due to its close relationship with ultracold atoms and Bose–Einstein Condensates. With the recent explosive growth of experiments on cold atoms near surfaces,[1−9] new atom-optical devices based on quantum reflection are not far beyond our reach. Past experiments have already demonstrated an atomic mirror,[5] a reflective diffraction grating,[6] a hologram for atoms[7] and a normal-incidence atomic mirror.[8] In earlier theoretical works, Böheim and Brenig and Carraro and Cole[2] established an extremely low critical normal kinetic energy required for observing quantum reflection from a surface. Based on a coarse criterion for the breakdown of the Wentzel–Kramers–Brillonic (WKB) approximation, the resulted value represents merely a rough and rather conservative estimate of the critical energy.[2] A recent theory on quantum reflection, formulated by Côté, Friedrich, and co-workers,[10,11] is based on straightforward matching of a WKB wave function to an exact or good approximate solution of the Schrödinger equation. This new theory is much more accurate in producing the threshold and the high-energy behaviour of the reflectivity and has been successfully extended to a large group of potentials such as attractive homogeneous potential tails.[12]

Recently a general and exact expression of the reflection coefficient for a quantum particle through an arbitrary potential barrier based on the analytical transfer matrix (ATM) method was formulated.[13] In this paper, this expression is extended to study the quantum reflection issue and a novel explanation for this phenomenon is proposed that quantum reflection is the reflection of subwaves. This work may provide a deeper insight into the foundation of quantum mechanics, which is just the law of wave motion in different potentials.

2. Theory

2.1. Quantum reflection is reflection of the subwaves

We start from the general analysis of the expression of the reflection coefficient briefly. Let us consider an arbitrary continuous attractive potential which has its support on the interval $[0, s]$ as shown in Fig. 1 and particles of mass m incident from the left with energy $E = \hbar^2 k^2/(2m)$. Since we focus ourselves on quantum reflection, we set $V(x) = V(0)$ for $x < 0$ to avoid the reflection of an abrupt step at $x = 0$. Without loss of generality, for $x > s$, we set $V(x) = 0$ and the reflection coefficient is defined with respect to a reference, which is chosen to be $x = 0$ in Fig. 1. Then the region $[0, s]$ is divided into l segments with homogeneous potential energy $V_j = V\left(x_{j-1} + d_j/2\right)$ and

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the thickness d_j $(j = 1, 2, \cdots, l)$. At each step there will be reflection and transmission of waves which may have previously undergone reflection and transmission themselves.

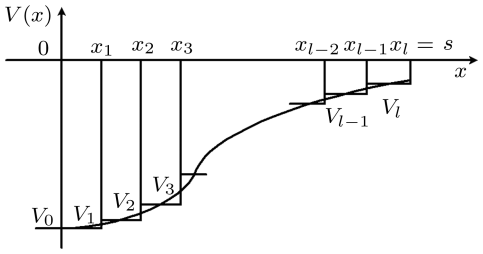


Fig. 1. Arbitrary attractive potential has support $[0, s]$.

Solutions of the Schrödinger equation at $x \leq 0$ and $x \geq s$ can be written as

$$\psi(x) = \begin{cases} A_0 \exp(\mathrm{i}\kappa_0 x) + B_0 \exp(-\mathrm{i}\kappa_0 x), & x \leq 0, \\ A_s \exp(\mathrm{i}\kappa_s x), & x \geq s \end{cases} \quad (1)$$

with $\kappa_0 = \sqrt{2m(E - V_0)}/\hbar, \kappa_s = \sqrt{2mE}/\hbar$. According to the ATM method, we have

$$\begin{bmatrix} \psi(0) \\ \psi'(0) \end{bmatrix} = \prod_{j=1}^{l} M_j(d_j) \begin{bmatrix} \psi(s) \\ \psi'(s) \end{bmatrix}, \quad (2)$$

here we denote differentiations with respect to x by primes, the matrix corresponding to the jth segment is given by

$$\boldsymbol{M}(d_j) = \begin{bmatrix} \cos(\kappa_j d_j) & -\kappa_j^{-1} \sin(\kappa_j d_j) \\ \kappa_j \sin(\kappa_j d_j) & \cos(\kappa_j d_j) \end{bmatrix}, \quad (3)$$
$$(j = 1, 2, \ldots, l).$$

Substituting Eq. (1) and $r = B_0/A_0$ in Eq. (2) gives

$$\left[-\mathrm{i}\kappa_0 \frac{1-r}{1+r} \ 1 \right] \prod_{j=1}^{l} M_j(d_j) \begin{bmatrix} 1 \\ \mathrm{i}\kappa_s \end{bmatrix} = 0. \quad (4)$$

As $l \to \infty$, solving Eq. (4), one will obtain the expression of the reflection coefficient

$$r = \frac{r_{01} + r_{ls} \exp\left[\mathrm{i}2 \int_0^s K(x)\mathrm{d}x\right]}{1 + r_{01} r_{ls} \exp\left[\mathrm{i}2 \int_0^s K(x)\mathrm{d}x\right]}, \quad (5)$$

where r_{01} and r_{ls} denote the reflection coefficients related to the wavenumbers κ_0, κ_1 and κ_l, κ_s, respectively.[13,14] The wavenumber $K(x)$ that consists of the main waves and subwaves can be cast into the form

$$K(x) = \kappa(x) + \frac{q(x)\kappa'(x)}{q^2(x) + \kappa^2(x)}. \quad (6)$$

The main waves refer to the incident wave and the transmitted waves in all segments without experience of any reflection, while the subwaves refer to the waves undergone once or multi-reflections. The relation between the main wavenumber $\kappa(x)$ and the classical momentum $p(x)$ is $\kappa(x) = \sqrt{2m(E - V(x))}/\hbar = p(x)/\hbar$. And it has already been pointed out in our previous works[13−15] that the wavenumber of the subwaves can be written as $q\kappa'/(q^2 + \kappa^2)$, where $q(x) = -\psi'(x)/\psi(x)$ is already completely specified by Eqs. (1) and (2). The physical insight of the scattered subwaves will be discussed later.

It should be noted that the r_{ij} in Eq. (5) which take the form

$$r_{ij}(x = a) = \frac{\kappa_i - \kappa_j}{\kappa_i + \kappa_j} \quad (7)$$

describe the behaviour of the subwaves if the point $x = a$ is not a classical turning point. Since the potential is always continuous at the reference (for example in Fig. 1 the reference is $x = 0$). As the thickness of the segments $d_1 \to 0$ through finer divisions of the potential profile, there is $\kappa_0 - \kappa_1 \to 0$, thus r_{01} will always approach zero. Then we can rewrite Eq. (5) as

$$\begin{aligned} r &= r_{ls} \exp\left[\mathrm{i}2 \int_0^s K(x)\mathrm{d}x\right] \\ &= r_{ls} \exp\left[\mathrm{i}2 \int_0^s \left(\kappa(x) + \frac{q\kappa'}{(q^2 + \kappa^2)}\right) \mathrm{d}x\right]. \end{aligned} \quad (8)$$

Since $E > V(x)$, $\kappa(x)$ is always a positive real quantity, so does the integral of $\kappa(x)$, this gives

$$\left| \exp(\mathrm{i}2 \int_0^s \kappa(x)\mathrm{d}x) \right| \equiv 1, \quad (9)$$

which means that the main waves have no effect on the reflection probability $R = rr*$, they can only affect the phase of r. As a result, modulus of the reflection coefficient $|r|$ can be written as

$$|r| = \left| r_{ls} \exp\left[\mathrm{i}2 \int_0^s \frac{q\kappa'}{(q^2 + \kappa^2)} \mathrm{d}x\right] \right|. \quad (10)$$

Note that, Eq. (10) describes purely the behaviour of the subwaves. This final expression indicates that quantum reflection is resulted from the reflection of the subwaves.

2.2. The subwaves

The concept of the subwaves was first introduced by the exact ATM quantization condition which takes the form[15−19]

$$\int_{x_1}^{x_2} \kappa(x)\mathrm{d}x + \varphi(s) = (n+1)\pi, \ n = 0, 1, 2, \ldots, \quad (11)$$

where x_1, x_2 are the classical turning points defined by $E = V(x_{1,2})$, $\varphi(s)$ denotes the phase contribution of the scattered subwaves and is given by

$$\varphi(s) = \int_{x_1}^{x_2} \frac{q\kappa'}{q^2+\kappa^2}\,\mathrm{d}x. \tag{12}$$

In order to illustrate the physics insight of the subwaves, let us consider a stepped potential well as shown in Fig. 2. Requiring the eigenfunction $\psi(x)$ of the bound states corresponding to the eigenvalues $V_3 > E > V_1$ and its first derivative $\psi'(x)$ to be continuous, one obtains

$$\begin{aligned}&\exp[\mathrm{i}2(\kappa_1 d_1 + \kappa_2 d_2 - \phi_{10} - \phi_{23})]\\ &+ r_{12}\exp[\mathrm{i}2(\kappa_1 d_1 - \phi_{10})]\\ &+ r_{21}\exp[\mathrm{i}2(\kappa_2 d_2 - \phi_{23})] = 1,\end{aligned} \tag{13}$$

where $\phi_{10} = \arctan(\alpha_0/\kappa_1)$, $\phi_{32} = \arctan(\alpha_3/\kappa_2)$ denote the half-phase shift at the boundaries of the well and $\kappa_i = \sqrt{2m(E-V_i)}/\hbar$, $\alpha_j = \sqrt{2m(V_j-E)}/\hbar$ $(i = 1, 2,\ j = 0, 3)$. By purely algebraic methods, Eq. (13) can be recast into the form of ATM quantization condition

$$(\kappa_1 d_1 + \kappa_2 d_2) + \varphi(s) = n\pi + \phi_{10} + \phi_{32}. \tag{14}$$

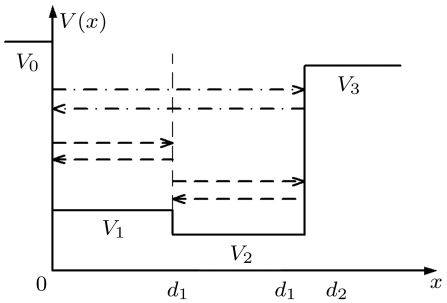


Fig. 2. The stepped potential well.

If we set $V_1 = V_2$, then we obtain $\varphi(s) = 0$ in Eq. (14), it follows that $\varphi(s)$ denotes the phase contribution picked up by the scattered subwaves which result from the interface at $x = d_1$. Extending this simple potential to an arbitrary one, we find that the wavenumber $q\kappa'/(q^2+\kappa^2)$ represents the scattered subwaves which originate inherently from the inhomogeneity of the fields and can always be neglected in the semiclassical regime.

3. Examples

To clarify the validity of our theory on quantum reflection, test calculations have been performed with several concrete examples covering different possible situations.

A fundamentally important example in quantum reflection is the Woods–Saxon step potential

$$V(x) = -\frac{V_0}{1+\exp(x/L)}, \tag{15}$$

for which the exact reflection probability is shown by Landau and Lifshitz[20]

$$R = \left\{\frac{\sinh[\pi(p_1-p_2)L/\hbar]}{\sinh[\pi(p_1+p_2)L/\hbar]}\right\}^2. \tag{16}$$

This potential is the mean field potential for the nucleons inside the atomic nucleus. Numerical comparisons between the proposed method and the exact one are plotted in Figs. 3 and 4. It is shown that the results calculated from Eqs. (10) and (16) agree very well.

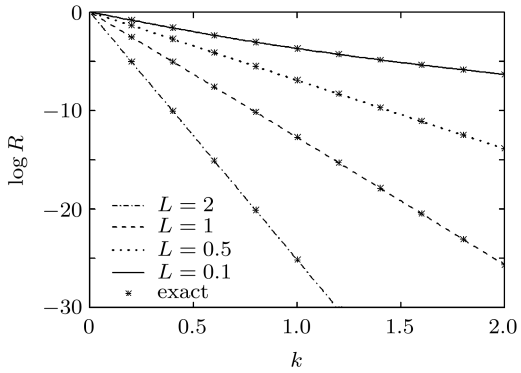


Fig. 3. Probability for reflection by the potential steps Eq. (15) as a function of k for various values of parameter L ($V_0 = 0.5$).

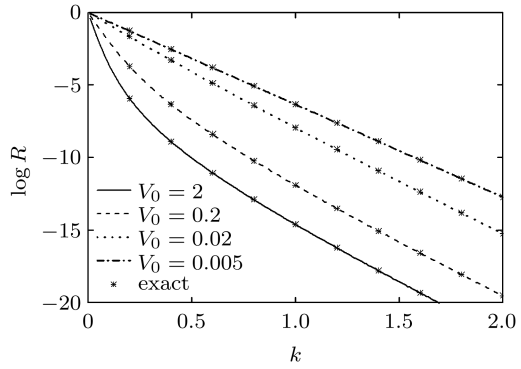


Fig. 4. Probability for reflection by the potential steps Eq, (15) as a function of k for various values of parameter V_0 ($L = 0.5$).

For the second example, consider a potential given by[10]

$$V(x) = -\frac{V_0}{1+\{\ln[1+\exp(x/L)]\}^{\alpha}}, \tag{17}$$

which shows the form of a long-range attractive tail of atom–atom or atom–ion interaction, namely

$$V_\alpha(x) = -\frac{\hbar^2}{2m}\frac{\beta^{\alpha-2}}{x^\alpha} \tag{18}$$

with $\beta^{\alpha-2} = 2mV_0L^\alpha/\hbar^2$.

Reflection probabilities for $\alpha = 8$ and $\alpha = 3$ are shown in Figs. 5 and 6, respectively. Again, we obtain the same results as those of numerical calculation in Ref. [10]. To the best of our knowledge, this is the first expression that can describe the quantum reflection of the attractive potential tails at any particle energy.

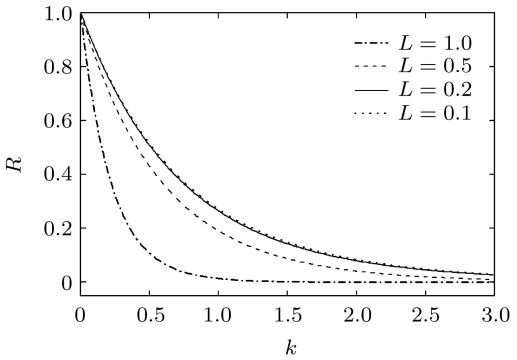


Fig. 5. Probability for reflection by the potential steps Eq. (17) as a function of k for $\alpha = 8$ and various values of the parameter L.

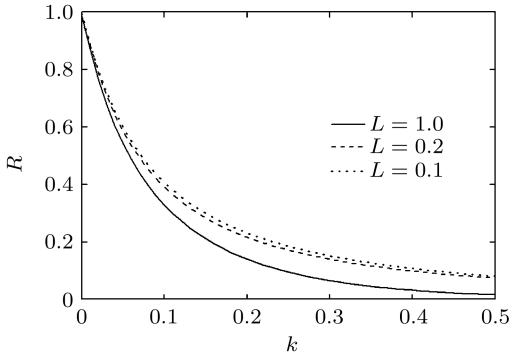


Fig. 6. Probability for reflection by the potential steps Eq. (17) as a function of k for $\alpha = 3$ and various values of the parameter L.

We illustrate two examples that are not related to the attractive long-range tails. The third example, which is equal to the BSEC (bound states embedded into the continuum) potential on the positive semiaxis, is discussed in detail in Ref. [21]. The potential of the bound state at the energy $E = E_{\rm BSEC}$ is

$$V(x) = -2\frac{\mathrm{d}}{\mathrm{d}x}\left\{\frac{c^2\sin^2(k_{\rm b}x)}{k_{\rm b}^2 + c^2\left(\dfrac{x}{2} - \dfrac{\sin(2k_{\rm b}x)}{4k_{\rm b}}\right)}\right\}, \quad x \geq 0, \tag{19}$$

where $k_{\rm b} = \sqrt{E_{\rm BSEC}}$. It is remarkable that although the potential is energy independent, the $|r(E)|$ has a resonance character at selected energy points even for the above-barrier motion.[21]

The reflection coefficient modulus $|r(E)|$ for various values of the parameter c is calculated and shown in Fig. 7. Our results are the same with those in Ref. [21].

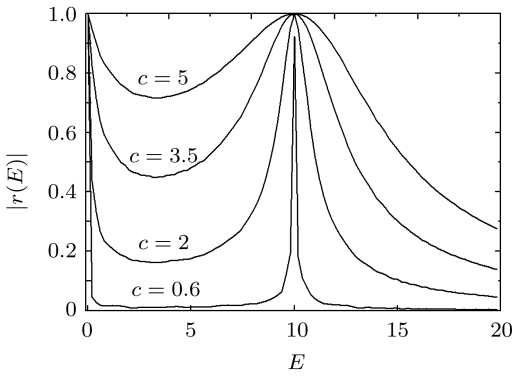


Fig. 7. The modulus of the reflection coefficient $|r(E)|$ for potentials having BSEC on the semiaxis $0 \leq x < \infty$ at energy $E_{\rm BSEC} = 10$.

The last example of above-barrier quantum reflection is a potential that has been calculated by transmission-line method in Ref. [22], namely

$$U(x) = \begin{cases} \dfrac{U_0}{2}[1 + \cos(2k_\Lambda x)], & 0 < x < N\Lambda, \\ 0, & x < 0, x > N\Lambda, \end{cases} \tag{20}$$

where Λ is the period of the potential, $k_\Lambda = \pi/\Lambda$ and U_0 is the potential amplitude. This example presents quantum reflection of cold atoms from a periodic light-induced dipole potential. As is well known in optics, reflection can be enhanced by periodic structures, this example shows that periodic potential can also enhance the reflection of atoms with certain energy.[22] Using the dimensionless variables $\varepsilon = 2mE/\hbar^2k_\Lambda^2$, $V = 2mU/\hbar^2k_\Lambda^2$, and $\xi = k_\Lambda x$, we find that the one dimensional Schrödinger equation becomes

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} + V(\xi)\psi(\xi) = \varepsilon\psi(\xi). \tag{21}$$

The reflection probability shown in Fig. 8 was calculated for potential height $V_0 = 40$, and N of 10, 100, and 1000 potential cells by using Eq. (10). The results fit well with those calculated with the transmission-line method in Ref. [22].

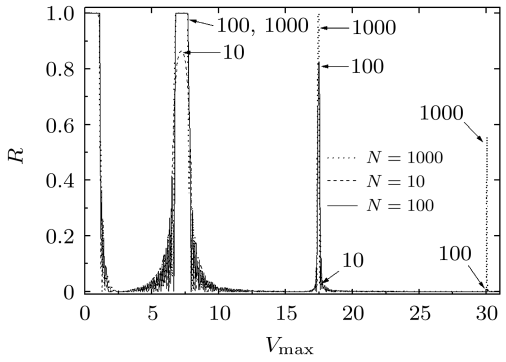


Fig. 8. Probability for reflection by the periodic cosine potential Eq. (21), for different numbers of potential cells $N = 10$, $N = 100$ and $N = 1000$ in dashed, solid, and dotted curves, respectively.

The last two examples demonstrate that the probability for reflection occurs above a barrier can also be described by Eq. (10) exactly.

4. Conclusion

In conclusion, the ATM method is used to treat quantum reflection and a novel explanation is proposed that quantum reflection is the reflection of subwaves. The proposed theory has also been applied to four different concrete examples, including Woods-Saxon step, a potential with long-range attractive tail, a BSEC potential on the positive semiaxis and a periodic cosine potential with a rectangle envelope. As a result, Eq. (10) is found to be applicable to all the quantum reflection problems for any particle energy.

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