Simple one-dimensional potentials

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Outline

General considerations

We consider Schrödinger's equation in one space dimension with a time-independent potential—

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = V(x)\psi(x,t) - \frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}.$$

Note that $\hbar/\sqrt{2mE}$ (and $\hbar/\sqrt{2mV}$) have the dimensions of a length. The solutions can be expanded in a complete basis of plane waves: $\phi(x,t) = \exp[i(px - Et)/\hbar]$. The eigenvalue equation can be formally written as $2m(E - V) = p^2$.

When $E < V$, one finds that p is imaginary, and the eigenfunction is exponential. Real values of p (and hence pure plane waves) are obtained when $E > V$. When $p > 0$, the wave moves towards increasing x and is called a right-moving wave. When $p < 0$ the wave moves to the left. The length scale $\sqrt{2m(E - V)}/\hbar$ is the wavelength when it is real. Otherwise the length scale $\sqrt{2m|E - V|\hbar}$ is the range of the wave function.

Degeneracy of eigenvalues

Since Schrödinger's equation is a second order differential equation, the eigenvalue equation for stationary states can be written as the set

$$\frac{d\psi(x;E)}{dx} = \phi(x;E), \quad \text{and} \quad \frac{d\phi(x;E)}{dx} = \frac{2m[E-V(x)]}{\hbar^2}\psi(x;E).$$

Thus, specification of $\phi(x;E)$ and $\psi(x;E)$ at any point allows us to find the values of these functions anywhere, through the above equations. Writing the above equations in the matrix form

$$\frac{d}{dx}\begin{pmatrix}\psi\\ \phi\end{pmatrix} = \begin{pmatrix}0 & 1\\ 2m(E-V)/\hbar^2 & 0\end{pmatrix}\begin{pmatrix}\psi\\ \phi\end{pmatrix},$$

formally, the eigenvalues of the matrix equation give $p/i\hbar$. Since the trace of the matrix vanishes, the two "eigenvalues" come with opposite sign. Thus, each energy eigenvalue is doubly degenerate.

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A step potential

Consider a particle moving in a potential step:

$$V(x) = V_0\Theta(x) = \begin{cases} 0 & (x < 0), \\ V_0 & (x > 0). \end{cases}$$

We will take V_0 to be positive. Hence, at $x = 0$ there is an impulsive force directed to the left. Classically, if the particle has kinetic energy less than V_0, it is reflected. If the initial kinetic energy is larger than V_0, then the particle slows down as it crosses the barrier.

The discontinuity in the potential does not invalidate the conditions discussed previously. The energy eigenstates $\psi(x; E)$ are continuous across $x = 0$, as are the derivatives $\psi'(x; E)$. In each of the force-free regions, $x < 0$ and $x > 0$, one can try the plane wave solutions. In each of these segments, the general solution is a combination of left and right moving waves.

Matching conditions

The wavefunction is

$$\psi(x;E) = \begin{cases} A_1 \mathrm{e}^{ikx} + B_1 \mathrm{e}^{-ikx} & (x < x_0, \quad k = \sqrt{2mE}/\hbar), \\ A_2 \mathrm{e}^{ik'x} + B_2 \mathrm{e}^{-ik'x} & (x > x_0, \quad k' = \sqrt{2m(E-V_0)}/\hbar), \end{cases}$$

where $x_0 = 0$. When $E > V_0$ we see that k' is real, in agreement with classical reasoning.

At x_0 the two halves of the wavefunction and its derivatives must be matched up. The matching conditions are

$$M(k,x_0)\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M(k',x_0)\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad \text{where} \quad M(k,x_0) = \begin{pmatrix} z & \frac{1}{z} \\ ikz & -\frac{ik}{z} \end{pmatrix},$$

where we have used the shorthand notation $z = \exp(ikx_0)$.

A transfer matrix

We can now write down a transfer matrix across the discontinuity—

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T(k,k',x_0) \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad \text{and} \quad T(k,k',x_0) = \begin{pmatrix} \alpha_+ z'/z & \alpha_-/zz' \\ zz'\alpha_- & \alpha_+ z/z' \end{pmatrix},$$

where $z = \exp(ikx_0)$, $z' = \exp(ik'x_0)$ and $\alpha_\pm = (1 \pm k'/k)/2$. This transfer matrix connects the coefficients on the left to those on the right. The inverse transfer matrix can be obtained by interchanging k and k'. When there is an incoming wave on the left of x_0. There is then a reflected wave on the left and a transmitted wave on the right. Since there is no incoming wave on the right, $B_2 = 0$. The reflection coefficient is $R = |B_1/A_1|^2$. From the transfer matrix above, we find

$$R = \left| \frac{k - k'}{k + k'} \right|^2 .$$

When $E \gg V_0$, we find that $R \to 0$, and for $E \leq V_0$ one has $R = 0$. The transmission coefficient is $T = 1 - R$.

Quantum vs classical

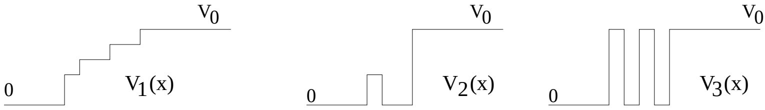
1. In the classical theory, the particle is always transmitted across the barrier when $E > V_0$. In the quantum theory, there is always a reflected wave. The amplitude of this wave decreases with increasing E.
2. In the classical theory the particle is instantaneously transmitted when $E > V_0$. In the quantum theory the relative phase angle between the incident and transmitted wave **at the barrier** is $\exp[i(k - k')x_0]$. This phase angle is immaterial, as can be seen by the fact that it can always be shifted to zero by a choice of x_0. Hence the transmission is instantaneous.
3. In the classical theory, the particle is always reflected when $E < V_0$. Since $R = 1$, this is also true of the quantum theory.
4. In the classical theory, sub-barrier reflection is instantaneous. In the quantum theory T_{21} has a relative phase angle which is negative. (**Compute this**) This means that the reflection is delayed.

Universality: a quantum phenomenon

Deform the step barrier to any general barrier—

$$V(x) = \begin{cases} 0 & (x < -a) \\ V_0 & (x > a), \end{cases}$$

and any shape in the range $|x| < a$. In this potential, consider incoming waves with $E \to 0$ on the left. The wavelength of such waves is $\sqrt{2mE}/\hbar$, and is much larger than a. The range of the wavefunction "under" the barrier is then $r = \sqrt{2mV_0}/\hbar$. When $r \gg a$, then the wave cannot possibly resolve the detailed shape of the potential, and one must have $R = 1$. This result seems to be universal in the limit $k \to 0$ and $r \gg a$.



Check. Any caveats?

Outline

The potential

Consider the potential

$$V(x) = V_0 \left[\Theta(a-x) - \Theta(x+a)\right] = \begin{cases} 0 & (|x| > a), \\ V_0 & (|x| < a), \end{cases}$$

where $V_0 > 0$. This is a finite potential barrier. Choose the trial wavefunction

$$\psi(x; E, \lambda) = \begin{cases} A_1 \mathrm{e}^{ikx} + B_1 \mathrm{e}^{-ikx} & (x < -a) \\ A_2 \mathrm{e}^{ik'x} + B_2 \mathrm{e}^{-ik'x} & (|x| < a) \\ A_3 \mathrm{e}^{ikx} + B_3 \mathrm{e}^{-ikx} & (x > a) \end{cases}$$

where $k = \sqrt{2mE}/\hbar$ and $k' = \sqrt{2m(E - V_0)}/\hbar$. Using the transfer matrix twice, and choosing $B_3 = 0$ as before, one finds the reflection coefficient

$$R = \frac{(k^2 - k'^2)^2 \sin^2(2ka)}{4k^2 k'^2 + (k^2 - k'^2)^2 \sin^2(2ka)}.$$

Resonances: a quantum phenomenon

In terms of the dimensionless quantities $\rho = ka$ and $\rho' = k'a$, the reflection coefficient for the square barrier is

$$R = \frac{(\rho^2 - {\rho'}^2)^2 \sin^2(2\rho)}{4\rho^2{\rho'}^2 + (\rho^2 - {\rho'}^2)^2 \sin^2(2\rho)}.$$

The wavelength of the incident wave $(2\pi/k)$ is an exact multiple of the barrier width whenever $2\rho = 2n\pi$. For such energies, one finds that $R = 0$ and $T = 1$. These energies, $E^*_n = n^2\pi^2\hbar^2/(2ma^2)$, are called **resonances**. Since $\rho^2 - {\rho'}^2 = 2mV_0a^2/\hbar^2 = \gamma^2$ is independent of the energy, in the vicinity of a resonance, *i.e.*, for $2\rho = 2n\pi + \delta$, one finds that $R \simeq \gamma^4\delta^2/16n^4\pi^4 \propto \delta^2$. The power of δ is **universal** in the sense that it does not depend on the particular resonance, *i.e.*, it is independent of n. However, the constant of proportionality depends on n. **Can you trace this universality to an argument about length scales?**

Outline

References

1. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. Part of the material in this lecture can be found in chapter 3 of this book.
2. Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 1 of this book contains some discussion of the step and square barriers.
3. More discussion of resonances can be found in many of the older textbooks of quantum mechanics (see, for example, the books by Messiah, Merzbacher, and so on).
4. An introduction to renormalization for the Schrödinger's equation is given in Section 2 of the paper "How to Renormalize the Schrodinger Equation" by P. Lepage. The paper is available at the URL `http://arxiv.org/abs/nucl-th/9706029`.