Simple one-dimensional potentials

Sourendu Gupta

TIFR, Mumbai, India

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General considerations

In $D = 1$, Schrödinger's differential equation is—

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

Expansion of $|\psi\rangle$ in the eigenstates of $\hat{p}$, means expanding $\psi(x,t)$ in the plane wave basis $\exp[i(px - Et)/\hbar]$. In terms of $\widetilde{V}$, the Fourier transform of $V(x)$, the equation can be written as $2m(E - \widetilde{V}) = p^2$. So, p is real when $E > V$, and imaginary otherwise. When $p > 0$, the wave moves towards increasing x (right-moving), otherwise to the left.

$\hbar/\sqrt{2mV}$ and $\hbar/\sqrt{2mE}$ have dimensions of length. When $1/\lambda = \sqrt{2m(E - V)}/\hbar = p/\hbar$ is real, λ is the wavelength. Otherwise $|\lambda|$ is the range of the wave function.

Degeneracy of eigenvalues

Since Schrödinger's differential equation is of second order, it can be written as two coupled first order equations. For stationary states with energy E, this becomes

$$\frac{d\psi(x;E)}{dx} = \phi(x;E), \quad \text{and} \quad \frac{d\phi(x;E)}{dx} = \frac{\psi(x;E)}{\lambda^2(x)}.$$

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. In matrix form, they are

$$\frac{d}{dx}\begin{pmatrix}\psi\\ \phi\end{pmatrix} = \begin{pmatrix}0 & 1\\ 1/\lambda^2 & 0\end{pmatrix}\begin{pmatrix}\psi\\ \phi\end{pmatrix}.$$

Since the trace vanishes, the two eigenvalues of this matrix, for each E, come with opposite sign. Thus, each energy eigenvalue is doubly degenerate.

Details

The differential equation is first written in the form

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

For an eigenstate of energy E, $\psi_E(x,t) = \psi(x;E)\exp(-iEt/\hbar)$, we can write this as

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

This equation can be decoupled into two coupled first order equations by simply introducing a notation for the derivative

$$\frac{d\psi(x;E)}{dx} = \phi(x;E).$$

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A step potential

Consider a particle moving in a potential step:

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

with $V_0 > 0$. At $x = 0$ there is an impulsive force directed to the left. Classically, if the particle has energy $E < V_0$, it is reflected. If $E > V_0$, then the particle slows down as it crosses the barrier.

Although the potential is discontinuous at $x = 0$, both $\psi(x; E)$ and $\phi(x; E)$ are continuous. So the earlier arguments remain valid. In each of the force-free regions, one can use plane wave solutions. In each of segment, the general solution is a combination of left and right moving waves.

Matching conditions

The wavefunction is

$$\psi(x;E) = \begin{cases} A_1 \mathrm{e}^{ikx} + B_1 \mathrm{e}^{-ikx} & (x < x_0, \quad k = \sqrt{2mE}/\hbar), \\ A_2 \mathrm{e}^{ik'x} + B_2 \mathrm{e}^{-ik'x} & (x > x_0, \quad k' = 1/\lambda), \end{cases}$$

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 $z = \exp(ikx_0)$ and $z' = \exp(ik'x_0)$.

Matching conditions: dimensionless form

Suppose there is an external length scale in the problem: a. Then we can construct the dimensionless distance, $y = x/a$, and the dimensionless wave number $\rho = ka$. The wavefunction is

$$\psi(y;\rho) = \begin{cases} A_1 \mathrm{e}^{i\rho y} + B_1 \mathrm{e}^{-i\rho y} & (y < y_0, \quad \rho = a\sqrt{2mE}/\hbar), \\ A_2 \mathrm{e}^{i\rho' y} + B_2 \mathrm{e}^{-i\rho' y} & (y > y_0, \quad \rho' = 1/\lambda), \end{cases}$$

Derivatives with respect to y are obtained by multiplying the derivative with respect to x by a. So the matching conditions are

$$M(\rho, y_0) \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M(\rho', y_0) \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad \text{where} \quad M(\rho, y_0) = \begin{pmatrix} z & \frac{1}{z} \\ i\rho z & -\frac{i\rho}{z} \end{pmatrix},$$

where $z = \exp(i\rho y_0)$.

A transfer matrix

Using the transfer matrix $T(\rho,\rho',y_0)=M^{-1}(\rho,y_0)M(\rho',y_0)$,

$$\begin{pmatrix}A_1\\B_1\end{pmatrix}=T(\rho,\rho',y_0)\begin{pmatrix}A_2\\B_2\end{pmatrix},\quad\text{and}\quad T(\rho,\rho',y_0)=\begin{pmatrix}\alpha_+z'/z & \alpha_-/zz'\\ zz'\alpha_- & \alpha_+z/z'\end{pmatrix},$$

where $\alpha_\pm=(1\pm\rho'/\rho)/2$. T connects the coefficients on the left to those on the right. T^{-1} is obtained by interchanging ρ and ρ'. If there is an incoming wave on the left of y_0, then there is a reflected wave on the left and a transmitted wave on the right. Since there is then 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

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

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

Quantum vs classical

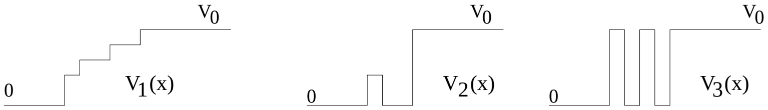
1. In the classical theory, the particle is always transmitted across the barrier when $E > V_0$. In quantum mechanics, there is always reflection, but the amplitude decreases with increasing E.
2. In the classical theory, the particle is always reflected when $E < V_0$. Since $R = 1$, this is also true of quantum mechanics.
3. A classical particle is instantaneously transmitted when $E > V_0$. In quantum mechanics the relative phase between the incident and transmitted wave at the barrier is $\exp[i(\rho - \rho')y_0]$. This phase angle is unobservable. It can always be set to zero by a choice of x_0.
4. In the classical theory, sub-barrier reflection is instantaneous. In quantum mechanics T_{21} has a negative relative phase. Compute the phase. Is there a notion of the delay time?

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, $\hbar/\sqrt{2mE} = \lambda \gg a$. The only other intrinsic length scale of the particle is the range of the wavefunction "under" the barrier: $r = \hbar/\sqrt{2mV_0}$. When $r \gg a$, then the wave cannot possibly resolve the detailed shape of the potential, and one must have $R = 1$. So this feature is universal: true for all potentials.



Check. Any caveats?

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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 $V_0 > 0$. Introduce $y = x/a$, $z = E/V_0$, and choose a trial wavefunction

$$\psi(y;z) = \begin{cases} A_1 \mathrm{e}^{i\rho y} + B_1 \mathrm{e}^{-i\rho y} & (y < -1) \\ A_2 \mathrm{e}^{i\rho' y} + B_2 \mathrm{e}^{-i\rho' y} & (|y| < 1) \\ A_3 \mathrm{e}^{i\rho y} + B_3 \mathrm{e}^{-i\rho y} & (y > 1) \end{cases}$$

where $\rho = a\sqrt{2mE}/\hbar$ and $\rho' = \rho\sqrt{z-1}$. Using the transfer matrix twice, and choosing $B_3 = 0$ as before, one finds the reflection coefficient

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

Resonances: a quantum phenomenon

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 $T = 1$. In terms of dimensional variables, these resonances occur at energies, $E_n^* = n^2\pi^2\hbar^2/(2ma^2)$.

The quantity $r^2 \equiv \rho^2 - {\rho'}^2 = 2mV_0a^2/\hbar^2$ is a "shape" property of the potential, and independent of the energy. Two different potentials (V_0 and a) with the same r have the same physics. Using this shape variable we can write

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

For $2\rho = 2n\pi + \delta$, one finds $R \simeq r^4\delta^2/16n^4\pi^4 \propto \delta^2$. The power of δ is universal in the sense that it is independent of n. However, the constant of proportionality depends on n. Can you trace this universality to an argument about length scales?

Problem 7.1: the square-well potential

Consider the square-well potential ($V_0 > 0$),

$$V(x) = V_0 \left[\Theta(a+x) - \Theta(a-x)\right].$$

1. Rewrite the equations using the dimensionless variables
$$y = x/a, \quad r^2 = \frac{2mV_0a^2}{\hbar^2} \quad \text{and} \quad z = \frac{E}{V_0}.$$
2. Find the bound states, *i.e.*, eigenstates for $z < 0$.
3. Find the scattering states, *i.e.*, eigenstates for $z > 0$.
4. The shape of the potential can be tuned by changing r. What values must r have in order to get a bound state at zero energy ($z = 0$)? What is the range of such a bound state?
5. Find the maximum r for which there is no bound state.
6. Suppose such a value of r is r_*, then if $r = r_* + \delta$, find the properties of bound states which are universal?

Problem 7.2: resonances

For the square barrier and square well problems, consider the scattering states in which there is no left-moving plane wave in the region $x > a$.

1. Is there a phase difference between the right-moving plane waves in the regions $x < -a$ and $x > a$? Can this be understood as a time-delay or time-advance in the region where the potential is non-zero? Does classical mechanics predict any such phenomena? If the answers to the previous two questions are yes, then do the two computations give the same result for the delay or advance? If any of the questions have different answers in classical and quantum mechanics, then explain the physics.
2. How do the phase differences behave near a resonance. Assuming that $A_1 = 1$, plot the track of the complex number A_3 in the complex plane as z changes for fixed r for the barrier and step. Is there universality near resonances?

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Keywords and References

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Matching conditions, transfer matrix, reflected wave, transmitted wave, reflection coefficient, transmission coefficient, relative phase, sub-barrier reflection, resonances, universal behaviour.

References

Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz, chapter 3.
Quantum Mechanics (Vol 1), C. Cohen-Tannoudji, B. Diu and F. Laloë, chapter 1.
Books by Messiah, Merzbacher, and other older texts discuss resonances.
An introduction to universality is given in Section 2 of the paper "How to Renormalize the Schrodinger Equation" by P. Lepage. http://arxiv.org/abs/nucl-th/9706029.