One-dimensional Schrödinger Equation. Transmission/Reflection from a step.

Before we proceed with solving time-independent Schrödinger Equation

\[ \hat{H}\psi_n = [ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) ] \psi_n(x) = E_n\psi_n(x) , \]

in various setups, let us examine some of its basic properties in one-dimension. First we notice that the \( \psi(x) \) is a continuous function of \( x \) because otherwise its derivative will diverge to infinity at the point of discontinuity, and the second derivative will diverge even stronger resulting in the infinite total energy of the state. Likewise, in the region where the potential energy \( V(x) \) is infinite the wavefunction has to be zero to ensure that system’s energy containing, in particular, a term \( \int dxV(x)|\psi(x)|^2 \) remains finite.

The first derivative of the wavefunction can be discontinuous; discontinuity in \( d\psi/dx \) will result in the \( \delta \)-functional term in \( d^2\psi/dx^2 \) but under integration it will contribute only a finite amount to energy. We can easily prove that discontinuity in \( d\psi/dx \) can happen only in places where the potential energy goes to infinity. Indeed, consider Eq. (1) and integrate it over small interval of width \( \epsilon \to 0 \) around point \( x \)

\[-\frac{\hbar^2}{2m} \int_{x-\epsilon/2}^{x+\epsilon/2} \psi''(z)dz + \int_{x-\epsilon/2}^{x+\epsilon/2} V(z)\psi(z)dz = E_n \int_{x-\epsilon/2}^{x+\epsilon/2} \psi(z)dz , \]

Since \( \psi(x) \) is continuous to leading order in \( \epsilon \) we can take its value at point \( x \). The first term can be evaluated by parts to yield

\[ \frac{\hbar^2}{2m} \left[ \psi'(x - \epsilon/2) - \psi'(x + \epsilon/2) \right] + \psi(x) \int_{x-\epsilon/2}^{x+\epsilon/2} V(z)dz = E_n\epsilon\psi(x) . \]

In the limit of \( \epsilon \to 0 \) the r.h.s. goes to zero. Also, if \( V(x) \) is finite on the integration interval then the second term on the l.h.s. is also zero in the limit and we arrive at the conclusion that \( \psi'(x) \) is continuous. An interesting case to consider is \( V(x) = u\delta(x - x_0) + U(x) \), where \( U(x) \) is finite and continuous. Since an integral over \( \delta(x - x_0) \) is unity whenever point \( x_0 \) is inside the integration interval we get

\[ \psi'(x_0 + 0) - \psi'(x_0 - 0) = (2mu/\hbar^2)\psi(x_0) , \]

which explains how the wavefunction derivatives relate across the \( \delta \)-functional term in the potential.

The other useful property reflects on the particle conservation law — as the wavefunction \( \psi(x,t) \) evolves in time it remains normalized to unity meaning that the probability density is only redistributed, i.e. its decrease in one place is always exactly compensated by increase in another place. To reveal the continuity Equation for probability density consider Schrödinger Equation and its complex conjugated version

\[ i\hbar\dot{\psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x)\psi(x) , \]

\[ -i\hbar\dot{\psi}^* = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V(x)\psi^* . \]

Now multiply the first Eq. on the left by \( \psi^* \), the second Eq. on the left by \( \psi \) and subtract the second line from the first one. The result is

\[ i\hbar \dot{\rho} = \frac{\hbar^2}{2m} [\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*] = \frac{\hbar^2}{2m} [\nabla(\psi^* \nabla \psi) - \nabla(\psi \nabla \psi^*)] = \nabla\left\{ -\frac{\hbar^2}{2m} [\psi^* \nabla \psi - \psi \nabla \psi^*] \right\} , \]
where $\rho = |\psi|^2$ is the probability density. Introducing current density

$$j = \frac{\hbar}{2im} [\psi^* \nabla \psi - \psi \nabla \psi^*],$$

allows us write the result in the canonical form of the continuity Equation

$$\dot{\rho} + \nabla j = 0.$$  

Particle number conservation can be seen by integrating this relation over the entire space; the integral of the second term vanishes since it can be reduced to the flux through the system’s boundary (zero for the entire space) leaving us with $\dot{N} = 0$.

Let us solve now our first QM problem. We consider a one-dimensional particle incident on the potential step, i.e. we consider $V(x) = \begin{cases} 0 & x \leq 0 \\ V_0 & x > 0 \end{cases}$

We will seek a stationary (time-independent) solution with boundary conditions corresponding to a certain influx of particles incident on the step from the left. For the plane wave $e^{ikx}$ the current flux is given by $j_{\text{inc}} = v = k/m$ and this will be our boundary condition for the incoming wave at $x \to -\infty$. In the regions of negative and positive $x$ we are dealing with the free space Schrödinger Equation, $\psi''(x) = -2mE\psi(x)$ for $x < 0$ and $\psi''(x) = -2m(E-V_0)\psi(x)$ for $x > 0$, and solutions are in the form of plane waves with total energy $E = k^2/2m$:

$$\psi(x < 0) = e^{ikx} + \alpha e^{-ikx}, \quad \psi(x > 0) = \beta e^{ik'x} + \gamma e^{-ik'x}, \quad \text{with } k' = \sqrt{2m(E-V_0)},$$

(we assume here that $E > V_0$; otherwise $k'$ will be purely imaginary and the solution will decay exponentially as $x \to \infty$).

In this problem we will be interested in the transmission and reflection of waves across the step potential. To ensure that the wave is incident only from the left we demand that there is only an outgoing wave $e^{ik'x}$ on the right. This boundary condition requires that the coefficient $\gamma$ above is identically zero, $\gamma = 0$.

To find the remaining coefficients we use matching conditions at $x = 0$ which consist of demanding that the wavefunction is continuous, and that its derivative is continuous too (potential energy is finite everywhere). Thus

$$1 + \alpha = \beta, \quad k(1 - \alpha) = k'\beta.$$  

You can see that this completely fixes the solution. Solving for coefficients $\alpha$ and $\beta$ we get

$$\alpha = \frac{k - k'}{k + k'}, \quad \beta = \frac{2k}{k + k'}.$$
Particle flux associated with the wavefunction component propagating to the left at negative $x$ (backscattered, or reflected, wave) is given by

$$j_{\text{refl}} = |\alpha|^2 (k/m) = |\alpha|^2 j_{\text{inc}},$$

while the flux associated with the wave propagating to the right at positive $x$ (transmitted wave) is given by

$$j_{\text{trans}} = |\beta|^2 (k'/m) = |\beta|^2 (k'/k) j_{\text{inc}}.$$

Transmission/reflection coefficients, $T/R$, are defined as the ratio between the incident and transmitted/reflected fluxes. From our expressions we immediately deduce that

$$T = \frac{4kk'}{(k + k')^2}, \quad R = \frac{(k - k')^2}{(k + k')^2}.$$

The sum $T + R = 1$, as expected, because every particle has to be either transmitted or reflected.

Our solution to the problem was time-independent. A far more elaborate calculation can be done by setting up the initial condition at $t \to -\infty$ in the form of a wave packet moving in the positive $\hat{x}$-direction. The size of the packet is selected to be $\sigma \gg 1/k$, i.e. it is composed of plane waves centered around the mean value of $k = \sqrt{2mE}$ with the spread in momentum space $\Delta k/k \ll 1$. The solution of the time-dependent Schrödinger Equation then leads to this wave packet splitting into two packets, one with relative amplitude $\sqrt{T}$ going to the right for $x > 0$ and the other with the relative amplitude $\sqrt{R}$ going to the left for $x < 0$.

For values of $V_0 > E$ our solution has to be modified. Now the value of $k'$ is purely imaginary $k' = i\sqrt{V_0 - E}$ with the sign selected from the condition that $\psi(x)$ vanishes at $x \to \infty$. Otherwise, the solution is exactly the same. One can easily check that for purely imaginary $k'$ the outgoing flux for $x \to \infty$ is zero. Correspondingly, the reflection coefficient is unity, as expected

$$\alpha = \frac{k - i\text{Im} k'}{k + i\text{Im} k'}, \quad R = |\alpha|^2 = \frac{k^2 + (\text{Im} k')^2}{k^2 + (\text{Im} k')^2} = 1.$$

This result does make sense classically.

We immediately notice that the reflection coefficient is always non-zero as long as there is a step; this behavior in not what is expected in classical mechanics when particles have enough energy to climb the barrier. Moreover, $R$ first decreases as we reduce $V_0$ from positive value, and then increases again for larger negative values of $V_0$ ultimately resulting in a perfect(!) reflection for “jumping into the abyss”, $R \to 1$ for $k' \to \infty$, i.e. there is no danger for falling off the cliff in QM [but it is not recommended to test quantum mechanics on yourself and Grand Canyon]. This has important implications for such processes as absorption of low-energy particles.

Some of this physics is specific to the sharp discontinuity in the $V(x)$ profile. If the step is smeared out into smooth profile—“smooth” is quantified as small variation of $V(x)$ over the particle wavelength $\lambda = 2\pi/\sqrt{2m(E - V(x))}$, i.e. $\lambda dV/dx \ll V(x)$—then with exponential accuracy the classical behavior comes back. For smooth profiles there is nearly perfect transmission for $E > V_0$.  

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Problem 17. Transmission and reflection of the rectangular barrier.
This problem considers particle transmission and reflection from two consecutive steps. Consider
\[ V(x) = \begin{cases} 
0 & |x| > a/2 \\
V_0 > 0 & |x| < a/2 
\end{cases} \]
and a particle with mass \( m \) incident from the left with energy \( E \).

a. Let \( E > V_0 \). By writing down the solution of the time-independent Schrödinger Equation in each of the regions as
\[ \psi(x) = \begin{cases} 
e^{ikx} + \alpha e^{-ikx} & x < -a/2 \\
\beta e^{ik'x} + \gamma e^{-ik'x} & |x| < a/2 \\
\delta e^{ikx} & x > a/2 \end{cases} \]
determine \( k, k', \alpha, \beta, \gamma, \delta \).
b. Calculate transmission and reflection coefficients \( T \) and \( R \) and make sure that you have \( T + R = 1 \).
c. Now consider \( E < V_0 \), and modify your solution accordingly. Calculate \( T \) and \( R \) and make sure that \( T + R = 1 \).
d. Show that in the limit of very large barrier \( V_0 \gg E, 1/ma^2 \) the transmission coefficient remains finite but small
\[ T = 16 \frac{k^2 \kappa^2}{(k^2 + \kappa^2)^2} e^{-2\kappa a}, \quad \kappa = \sqrt{2m(V_0 - E)}. \]

Problem 18. Transmission and reflection from the \( \delta \)-functional barrier.
Consider now an exactly the same setup physics-wise as in the previous problem but with
\[ V(x) = g\delta(x). \]

a. Formulate the solution in different regions and use matching conditions at the origin to fix all unknown coefficients. Calculate \( T \) and \( R \) and verify that \( T + R = 1 \).
b. Compare problems 17 and 18 by taking your answer in problem 17 and considering the limit of \( V_0 \to \infty \) and \( a \to 0 \) in such a way that \( g = V_0 a \) remains constant. Is this limit in agreement with part a)?