Quantum scattering in one dimension

Abstract

Quantum scattering in one dimension with some tricks for a fast solution.

Index Terms

quantum,scattering,tunneling,wave function

Contents

I. Introduction

Let us consider the Schrodinger equation with a simple one dimensional potential. For completeness will start with the time dependent equation which we will convert to time independent one.

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} \quad = \quad H\psi(x,t), \tag{1}$$

where the Hamiltonian H is defined as

$$H \quad = \quad -\hbar^2\frac{\partial^2}{\partial x^2}+V(x). \tag{2}$$

$V(x)$ in Eq. (2) represents the potential. We will be solving for energy eigen-states which satisfy the following equation:

$$H\psi(x,t) = E\,\psi(x,t). \tag{3}$$

Plugging the expression in Eq. (3) into Eq. (1), we get:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} \quad = \quad E\,\psi(x,t), \tag{4}$$

We can convert this partial differential equation into ordinary differential equation by seperation of variables: $\psi(x,t)\equiv\psi(x)\phi(t)$.

Inserting this into Eq. (4), we get:

$$i\hbar\frac{d\phi(t)}{dt} \quad = \quad E\,\phi(x,t), \tag{5}$$

where the time independent part drops from the equation. The solution to Eq. (5) is given by

$$\phi(t) \quad = \quad \phi(0)e^{-iEt}, \tag{6}$$

where $\phi(0)$ represents the initial value. Therefore $\psi(x,t)$ is of the following form:

$$\psi(x,t) = \psi(x)\phi(0)e^{-iEt}. \tag{7}$$

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Plugging the expression in Eq. (7) into Eq. (1) with the Hamiltonian given in Eq. (2), we get:

$$\left[-\hbar^2 \frac{d^2}{dx^2} + V(x)\right]\psi(x) \quad = \quad E\,\psi(x), \tag{8}$$

where the time dependent part, $\phi(t)$, drops from the equation. Eq. (8) is the differential equation we will have to solve for various potentials $V(x)$.

II. Free-particle solutions

Consider a particle of mass m and momentum p propagating freely along $x-$ axis. Since there is no potential involved, we have $V(x) = 0$. Therefore, the Schrodinger equation simplifies to

$$\left[-\hbar^2 \frac{d^2}{dx^2}\right]\psi(x) \quad = \quad E\,\psi(x), \tag{9}$$

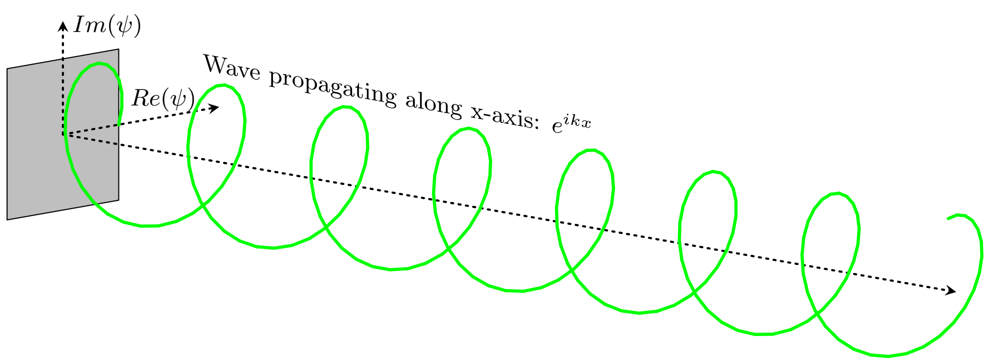

Figure 1: A wave freely propagating along $x-$axis. The transverse axes show real and imaginary parts of the wave.

III. Scattering from a rectangular potential

Here we will present a super-fast way of solving the scattering problem by building in the boundary conditions to the wave function. This will help significantly in solving for the unknown coefficients. Consider the rectangular potential in Fig. (2):

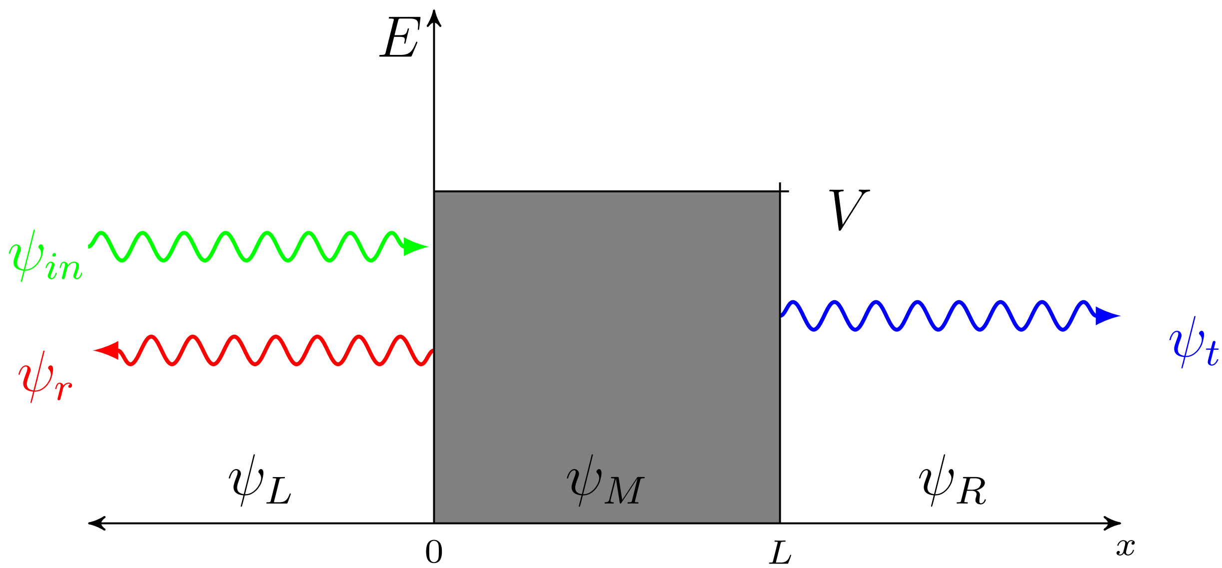

Figure 2: A potential of height V extending from 0 to L.

ψ_{in}, ψ_r and ψ_t represent the incoming, reflected and transmitted wave-functions, respectively. They are plane-waves, i.e., their functional form is $e^{\pm ikx}$. The functional form of the wave for $0 < x < L$ depends on the energy of the incoming wave (E) relative to the height of the potential(V). If $E < V$, the wave function will be of the form $e^{\pm k'x}$, or equivalently $\cosh k'x$ and $\sinh k'x$ where $k' = \sqrt{2m(V-E)}/\hbar$. Although the functional forms look different, they can be translated into each other by the transformation $k' \to ik'$. We will first assume $E < V$, and use $\cosh k'x$ and $\sinh k'x$ in the middle region.

A. *How not to solve the problem*

The textbook method of solution has the following strategy: You start with generic coefficients for the functions in three regions:

$$\psi = \begin{cases} \psi_L = \psi_{in} + \psi_r = Ae^{ikx} + Be^{-ikx}, & x < 0 \\ \psi_M = C\cosh k'x + D\sinh k'x, & 0 < x < L \\ \psi_R = \psi_t = Ee^{ikx}, & x > L. \end{cases} \tag{10}$$

You then require the continuity of ψ and ψ' at $x = 0$ and $x = L$. That results in a matrix equation that can be solved for B, C, D and E. It will be a tedious calculation which we can totally avoid with some out of box thinking.

B. *A faster solution*

There is no reason for solving the problem from left to right. We can think backwards, and assign coefficients starting from the transmitted wave. We can also be a bit smarter and try to satisfy the boundary conditions while we are assigning the coefficient. Let's define ψ_R first:

$$\psi_R = Ce^{ik(x-L)}, \tag{11}$$

where we introduced an extra phase e^{-ikL} for ψ_R for two good reasons:

1. We will be imposing the boundary condition at $x = L$ with will cancel out the phase. This will simplify the subsequent calculations.
2. The phase naturally arises as the wave travels a distance of L even when $V = 0$. This means the phase in C will be purely due to the potential barrier.

Let's think about ψ_M which will involve $cosh k'x$ and $\sinh k'x$. We will be imposing the continuity at $x = L$. Wouldn't it be wonderful if one of the functions dropped at the boundary? We can make that happen if we shift the arguments and use $\cosh k'(x-L)$ and $\sinh k'(x-L)$. So let's do the following:

$$\psi_M = C\cosh k'(x-L) + C\frac{ik}{k'}\sinh k'(x-L), \tag{12}$$

which satisfies the continuity of the wave-function and its derivative at $x = L$ by construction! Now we need to construct ψ_L:

$$\psi_L = Ae^{ikx} + Be^{-ikx} \tag{13}$$

We will require $\psi_L(0) = \psi_M(0)$ and $\frac{d}{dx}\psi_L(0) = \frac{d}{dx}\psi_M(0)$, which results in

$$\begin{aligned} A+B &= C(\cosh k'L - \frac{ik}{k'}\sinh k'L) \\ A-B &= C(-\frac{k'}{ik}\sinh k'L + \cosh k'L) \end{aligned} \tag{14}$$

Solving for C and B is very easy:

$$C = \frac{1}{\cosh k'L - i\frac{k^2-k'^2}{2kk'}\sinh k'L}A \tag{15}$$

$$B = -i\frac{k'^2+k^2}{2kk'}\sinh k'L\, C \tag{16}$$

$$= \frac{-i\frac{k'^2+k^2}{2kk'}\sinh k'L}{\cosh k'L - i\frac{k^2-k'^2}{2kk'}\sinh k'L}A, \tag{17}$$

where $k' = \sqrt{2m(V-E)}/\hbar$ and $k = \sqrt{2mE}/\hbar$. The transmission and reflection strength can be defined as C/A and B/A

$$t \equiv \frac{C}{A} = \frac{1}{\cosh k'L - i\frac{k^2-k'^2}{2kk'}\sinh k'L} \tag{18}$$

$$= \frac{1}{\sqrt{1+\frac{V^2}{4E(V-E)}\sinh^2 k'L}}e^{i\theta_t} \tag{19}$$

$$r \equiv \frac{B}{A} = \frac{-i\frac{V}{2\sqrt{E(V-E)}}\sinh k'L}{\cosh k'L - i\frac{k^2-k'^2}{2kk'}\sinh k'L} \tag{20}$$

$$= \frac{\frac{V}{2\sqrt{E(V-E)}}\sinh k'L}{\sqrt{1+\frac{V^2}{4E(V-E)}\sinh^2 k'L}}e^{i\theta_r}, \tag{21}$$

where we simplified the denumerator as follows:

$$
\begin{aligned}
\text{Denum} &= \left|\cosh k'L - i\frac{k^2-k'^2}{2kk'}\sinh k'L\right| && (22)\\
&= \sqrt{\cosh^2 k'L + \left[\frac{k^2-k'^2}{2kk'}\right]^2 \sinh^2 k'L} && (23)\\
&= \sqrt{1+\sinh^2 k'L + \left[\frac{k^2-k'^2}{2kk'}\right]^2 \sinh^2 k'L} && (24)\\
&= \sqrt{1+\left(1+\left[\frac{k^2-k'^2}{2kk'}\right]^2\right)\sinh^2 k'L} && (25)\\
&= \sqrt{1+\left[\frac{k^2+k'^2}{2kk'}\right]^2 \sinh^2 k'L} && (26)\\
&= \sqrt{1+\frac{V^2}{4E(V-E)}\sinh^2 k'L} && (27)
\end{aligned}
$$

Note that the coefficients in Eq. (21) are complex numbers, and the phases are given by

$$
\begin{aligned}
\theta_t &= \arctan\left(\frac{k^2-k'^2}{2kk'}\tanh k'L\right) && (28)\\
&= \arctan\left(\frac{2E-V}{\sqrt{E(V-E)}}\tanh\left[\frac{\sqrt{2m(V-E)}}{\hbar}L\right]\right) && (29)\\
\theta_r &= -\frac{\pi}{2}+\theta_t. && (30)
\end{aligned}
$$

Let's look at a low energy limit as a sanity check of our reflection angle. Assume a very high potential i.e., $V \gg E$. In this case, the argument of arctan goes to $-\infty$, which yields an angle of $-\pi/2$ of for the transmitted wave. Therefore, we conclude that the reflected wave will gain an wave shift of $-\pi$, which is equaivalent to π since we can add multiples of 2π. This is what one would expect for classical reflection of a wave.

C. E>V case

When $E > V$, we will have a negative number in the square root and k' will be a purely imaginary number. Furthermore we can use the equality $\sinh(ix) = i\sin(x)$ for $x \in \mathbb{R}$. So we can actually combine $E > V$ and $E < V$ cases into a single expression:

$$
|t|^2 = \frac{1}{1+\frac{V^2}{4E|E-V|}\left|\sin\left[\frac{\sqrt{2m(E-V)}}{\hbar}L\right]\right|^2}. \quad (31)
$$

In order to plot the coefficients, it is a good idea to define unitless quantities. One thing we can do is to normalize energy E with respect to the height of the potential V and define a unitless measure of the potential depth: So, let's define $\mathcal{E} = E/V$ and $\mathcal{L} = \frac{\sqrt{2mV}}{\hbar}L$. In these units, the transmission coefficient can be rewritten as:

$$
|t|^2 = \frac{1}{1+\frac{1}{4\mathcal{E}|\mathcal{E}-1|}\left|\sin\left[\sqrt{1-\mathcal{E}}\mathcal{L}\right]\right|^2}, \quad (32)
$$

which is a good representation to see how things change as energy of the incoming wave and the potential depth is varied. One important observation is that the transmission coefficient in Eq. (31) will be equal to 1 when $\sqrt{1-\mathcal{E}}\mathcal{L} = n\pi$, where n is an integer. These are the resonance wavelengths where integer number of half-wavelengths can fit in the potential barrier.

D. Exploring the reflections and transmissions

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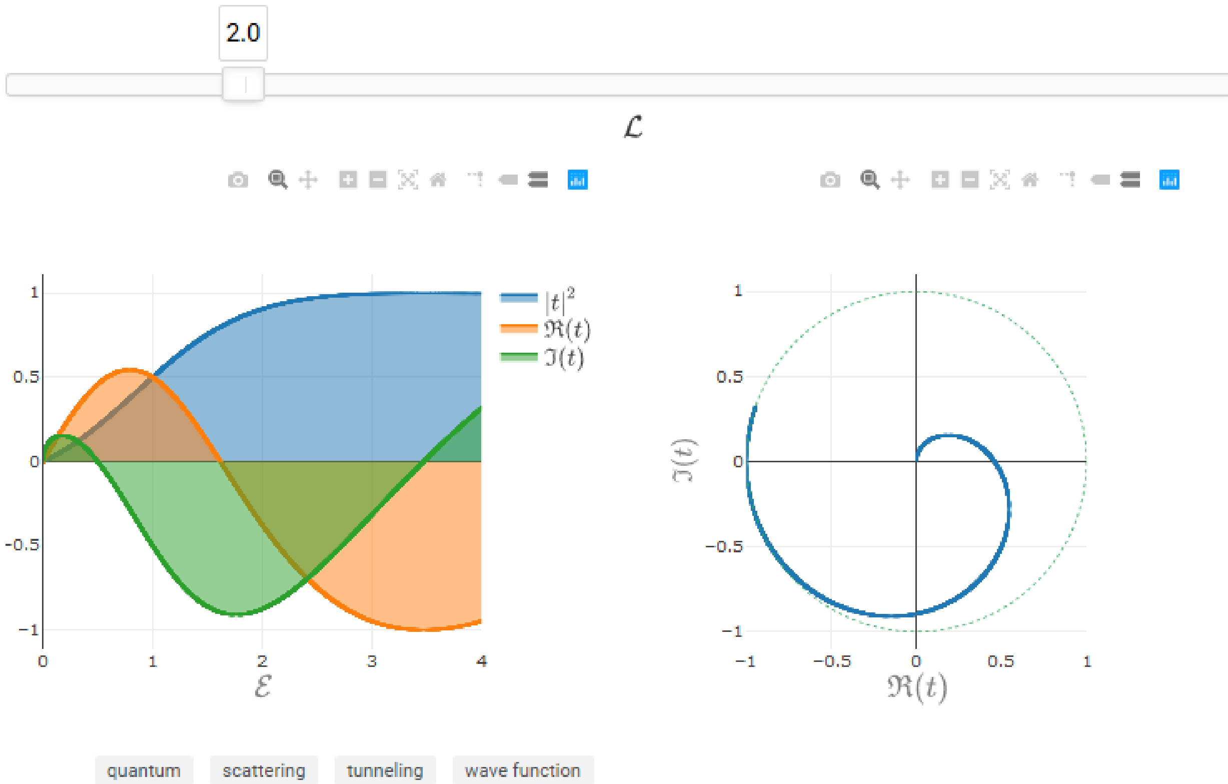

Figure 3: Scattering amplitudes and phases here.