68413 Quantum Physics: Wavefunctions in 1D potentials (continued)

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November 28, 2022

1 Potential step

At the last lecture, we talked about solving the time-independent Schrödinger equation in 1D in external potential $V(x)$

$$\hat{H}\Psi(x) = \left[\frac{\hat{p}^2}{2m} + V(x)\right]\Psi(x) = E\Psi(x), \tag{1}$$

i.e. finding $\Psi(x)$ as the eigenfunctions of Hamiltonian H. Noting that in the position representation, the momentum operator $\hat{p} = -i\hbar\mathrm{d}/\mathrm{d}x$, we turned this physics problem into a mathematical one — solving an ODE:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) - E\right]\Psi(x) = 0. \tag{2}$$

1.1 Solving the ODE

In particular, we considered the piecewise-continuous potentials like in Fig. ..., where

$$V(x) = \begin{cases} V_1, & \text{if } x < x_{12} \\ V_2, & \text{if } x \geq x_{12}, \end{cases} \tag{3}$$

and looked for solutions with eigenvalues (energies) $E > V_1, V_2$. In each domain separately, the problem simplifies to

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_1)\right)\Psi_1(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_1^2\right)\Psi_1(x) = 0 \quad \text{for } x < x_{12}, \tag{4}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_2)\right)\Psi_2(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_2^2\right)\Psi_2(x) = 0 \quad \text{for } x \geq x_{12}. \tag{5}$$

Because $E > V_1, V_2$, both $k_1 = \sqrt{2m/\hbar^2(E - V_1)}$ and $k_3 = \sqrt{2m/\hbar^2(E - V_3)}$ can be chosen as real and positive (can you see why? this will be important later!).

Equations for Ψ_1 and Ψ_2 have two solutions each, so the wavefunction are generally written as the linear combinations:

$$\Psi_1(x) = \underbrace{A_1 e^{ik_1x}}_{\rightarrow} + \underbrace{B_1 e^{-ik_1x}}_{\leftarrow}, \quad \Psi_2(x) = \underbrace{A_2 e^{ik_2x}}_{\rightarrow} + \underbrace{B_2 e^{-ik_2x}}_{\leftarrow}, \tag{6}$$

where the arrows indicate the description of a particle propagating to the right (positive x, $\rightarrow$) or to the left (negative x, $\leftarrow$).

1.2 Stitching the solutions

We now *glue* the wavefunction at $x = x_{12}$, demanding that

1. $\Psi(x)$ is continuous everywhere,

$$\Psi_1(x_{12}) = \Psi_2(x_{12}), \tag{7}$$

i.e.

$$A_1 e^{ik_1x_{12}} + B_1 e^{-ik_1x_{12}} = A_2 e^{ik_2x_{12}} + B_2 e^{-ik_2x_{12}}, \tag{8}$$

2. $\Psi'(x)$ is continuous everywhere,

$$\frac{\mathrm{d}}{\mathrm{d}x}\Psi_1(x)|_{x=x_{12}} = \frac{\mathrm{d}}{\mathrm{d}x}\Psi_2(x)|_{x=x_{12}}, \tag{9}$$

i.e.

$$-k_1 A_1 e^{ik_1x_{12}} - ik_1 B_1 e^{-ik_1x_{12}} = ik_2 A_2 e^{ik_2x_{12}} - ik_2 B_2 e^{-ik_2x_{12}}, \tag{10}$$

or

$$k_1\left(A_1 e^{ik_1x_{12}} - B_1 e^{-ik_1x_{12}}\right) = k_2\left(A_2 e^{ik_2x_{12}} - B_2 e^{-ik_2x_{12}}\right), \tag{11}$$

Equations (8) and (15) can be written in the matrix form as:

$$\begin{pmatrix} e^{ik_1x_{12}} & e^{-ik_1x_{12}} & -e^{ik_2x_{12}} & -e^{ik_2x_{12}} \\ k_1 e^{ik_1x_{12}} & -k_1 e^{-ik_1x_{12}} & -k_2 e^{ik_2x_{12}} & k_2 e^{ik_2x_{12}} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{12}$$

1.2.1 Reducing the complexity

Is that enough? 4 variables (A_1, B_1, A_2, B_2) but only 2 equations (Eq. (8),(15)). Perhaps the problem is ill-defined?

Let's define the problem better: we want to understand how a particle incident on the barrier from the left reflects and transmits to the right. In the second medium the particle will *only travel to the right*, so we set $B_2 = 0$. Furthermore, the system of equations in Eq. (8),(15) is linear, so we expect one free parameter, i.e. we can divide (A_1, B_1, A_2, B_2) by any number, for example A_1, and still get a valid solution.

We thus get

$$\Psi_1(x) = e^{ik_1x} + B_1 e^{-ik_1x}, \quad \Psi_2(x) = A_2 e^{ik_2x}, \tag{13}$$

where we explicitly set $A_1 = 1$. Equations (8),(15) become

$$e^{ik_1x_{12}} + B_1 e^{-ik_1x_{12}} = A_2 e^{ik_2x_{12}}, \tag{14}$$

$$k_1 \left(e^{ik_1x_{12}} - B_1 e^{-ik_1x_{12}}\right) = k_2 A_2 e^{ik_2x_{12}}. \tag{15}$$

Diving both sides of the above equations by e^{ik_1x} and moving the constant terms to the RHS, we can express them as:

$$\begin{pmatrix} e^{-2ik_1x_{12}} & -e^{i(k_2-k_1)x_{12}} \\ -k_1 e^{-2ik_1x_{12}} & -k_2 e^{i(k_2-k_1)x_{12}} \end{pmatrix} \begin{pmatrix} B_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} -1 \\ -k_1. \end{pmatrix} \tag{16}$$

1.3 Solutions

$$A_2 = \frac{2k_1}{k_1 + k_2} e^{i(k_1-k_2)x_{12}}, \tag{17}$$

$$B_1 = \frac{k_1 - k_2}{k_1 + k_2} e^{-ik_1x_{12}}, \tag{18}$$

1. do these equations look familiar?
2. what's the maximum value of $|A_2|$ and $|B_1|$?

```python
import numpy as np

M = np.array([
        [np.exp(-2j*k1*x12), -np.exp(-1j*(k2-k1)*x12)],
        [-np.exp(-2j*k1*x12), -k2/k1*np.exp(-1j*(k2-k1)*x12)]
    ])
inh = np.array([-1,-1])
# find v such that M.x = inh
v = np.linalg.solve(M, inh)

# identify (A_2, B_1) = v
```

Listing 1: Solver to the problem of step potential. Note that the second equation has was devided by k_1, so the expressions in M and *inhom* are unitless — this is a standard trick to avoid large or small numbers and possible numerical precision errors.

1.3.1 Current density

The quantify the probabilities of transmission and reflection across the discontinuity, we introduce the current density:

$$J(x) = \frac{\hbar}{m} \Im \left\{ [\Psi(x)]^* \, \Psi'(x) \right\}, \tag{19}$$

and differentiate between the incident

$$J_I(x) = \frac{\hbar}{m} \Im \left\{ \left[A_1 e^{ik_1 x} \right]^* A_1 i k_1 e^{ik_1 x} \right\} = \frac{\hbar k_1}{m} |A_1|^2, \tag{20}$$

transmitted

$$J_T(x) = \frac{\hbar}{m} \Im \left\{ \left[A_2 e^{ik_2 x} \right]^* A_2 i k_2 e^{ik_2 x} \right\} = \frac{\hbar k_2}{m} |A_2|^2, \tag{21}$$

and reflected

$$J_R(x) = \frac{\hbar}{m} \Im \left\{ \left[B_1 e^{-ik_1 x} \right]^* \left(-B_1 i k_1 e^{-ik_1 x} \right) \right\} = \frac{\hbar k_1}{m} |B_1|^2, \tag{22}$$

current densities. We then define *transmission probability* (or transmission) $\mathcal{T}$ and *reflection probability* (or reflection) $\mathcal{R}$:

$$\mathcal{T} = \frac{J_T}{J_I} = \frac{k_2}{k_1} \left| \frac{A_2}{A_1} \right|^2, \quad \mathcal{R} = \frac{J_R}{J_I} = \left| \frac{B_1}{A_1} \right|^2. \tag{23}$$

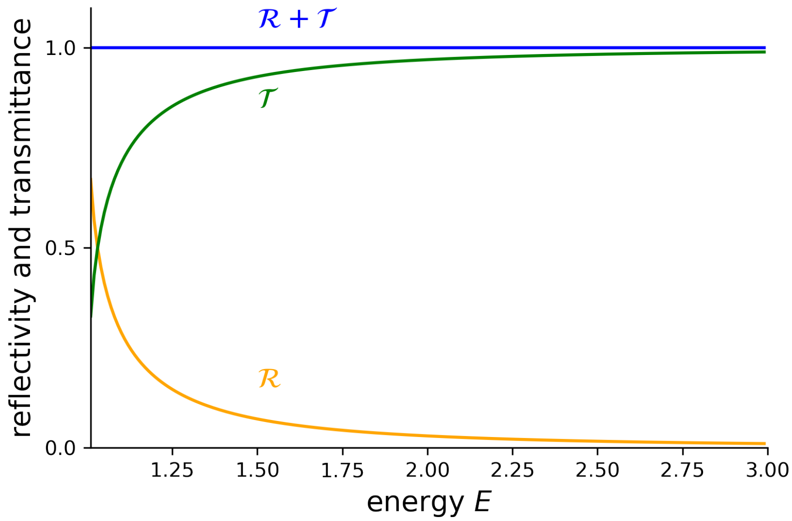

Figure 1: Go to `github` for animated versions

1.3.2 Time evolution of the wavefunction

How does this wavefuction evolve in time? Note that the eigenfunction of the Hamiltonian will evolve according to the time-dependent Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\Psi(x,t) = \hat{H}\Psi(x,t) \rightarrow \Psi(x,t) = e^{-iEt/\hbar}\Psi(x,0). \tag{24}$$

(we'll get back to this problem in the next lecture)

Note

- the wavefunction is continuous, and smooth at the potential discontinuity point x_{12},
- transmitted wavefunction $x > 0$ appears to have a single sin/cos component — but the incident+reflected function are far less regular (better seen in animations as `github`),
- spatial period of oscillations (wavefunction's wavelength) changes with potential regions, but the spatial period of oscillations ($T = \hbar/E$) remains constant (does that remind you of something?),

Play around with the math or the Python code to plot the incident and reflected fields separately.

2 Quantum tunnelling

Now let is consider a case where the piecewise-constant potential exceeds the energy $V(x) = V_2 > E$ over some region $0 < x < L$. Let's also assume that to the potentials to left- and right- are all $< E$:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_1)\right)\Psi_1(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_1^2\right)\Psi_1(x) = 0 \quad \text{for } x < 0, \tag{25}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_2)\right)\Psi_2(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_2^2\right)\Psi_2(x) = 0 \quad \text{for } 0 < x \geq L. \tag{26}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_3)\right)\Psi_3(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_3^2\right)\Psi_3(x) = 0 \quad \text{for } x > L. \tag{27}$$

Because $E < V_2$, we have $k_2^2 = 2m/\hbar^2(E - V_2) < 0$, and so we introduce $k_2 = \pm i\kappa_2$, with $\kappa_2 > 0$ such that the solutions to the wavefunction are

$$\Psi_2(x) = \underbrace{A_2 e^{\kappa_2 x}}_{\nearrow} + \underbrace{B_2 e^{-\kappa_2 x}}_{\searrow}, \tag{28}$$

where the first (second) term grows (decays) exponentially with x, and

$$\Psi_1(x) = \underbrace{A_1 e^{ik_1 x}}_{\rightarrow} + \underbrace{B_1 e^{-ik_1 x}}_{\leftarrow}, \quad \Psi_3(x) = \underbrace{A_3 e^{ik_3 x}}_{\rightarrow} + \underbrace{B_3 e^{-ik_3 x}}_{\leftarrow}, \tag{29}$$

with $k_1 = \sqrt{2m/\hbar^2(E - V_1)}$, $k_3 = \sqrt{2m/\hbar^2(E - V_3)}$.

The boundary conditions (continuity of wavefunction and its derivative), again give us a set of equations for the unknown amplitude coefficients A_i, B_i

$$\boxed{\begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ ik_1 & -ik_1 & \kappa_2 & -\kappa_2 & 0 & 0 \\ 0 & 0 & e^{\kappa_2 L} & e^{-\kappa_2 L} & -e^{ik_3 L} & -e^{ik_3 L} \\ 0 & 0 & \kappa_2 e^{\kappa_2 L} & -\kappa_2 e^{-\kappa_2 L} & -ik_3 e^{ik_3 L} & ik_3 e^{-ik_3 L} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \\ A_3 \\ B_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}} \tag{30}$$

Again, setting the incident wavefunction amplitude as $A_1 = 1$, and noting that the left-propagating component vanished $B_3 = 0$, we can simplify the above to

$$\boxed{\begin{pmatrix} 1 & -1 & -1 & 0 \\ -ik_1 & -\kappa_2 & \kappa_2 & 0 \\ 0 & e^{\kappa_2 L} & e^{-\kappa_2 L} & -e^{ik_3 L} \\ 0 & \kappa_2 e^{\kappa_2 L} & -\kappa_2 e^{-\kappa_2 L} & -ik_3 e^{ik_3 L} \end{pmatrix} \begin{pmatrix} B_1 \\ A_2 \\ B_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} -1 \\ -ik_1 \\ 0 \\ 0 \end{pmatrix}} \tag{31}$$

```python
import numpy as np

M = np.array([
    [1,-1,-1,0],
    [-1j,-k2/k1,k2/k1,0],
    [0,np.exp(k2*L),np.exp(-k2*L),-np.exp(1j*k3*L)],
    [0,np.exp(k2*L),-np.exp(-k2*L),-1j*k3/k2*np.exp(1j*k3*L)]
])
inh = np.array([-1,-1j,0,0])
# find x such that M.x = inh
x = np.linalg.solve(M, inh)
# identify (B_1, A_2, B_2, A_3) = x
```

Listing 2: Solver for the problem of potential barrier.

2.1 Solutions

$$B_1 = \frac{(k_1 - k_3)\kappa_2 \cosh(L\kappa_2) - i(k_1 k_3 + \kappa_2^2)\sinh(L\kappa_2)}{(k_1 + k_3)\kappa_2 \cosh(L\kappa_2) + i(-k_1 k_3 + \kappa_2^2)\sinh(L\kappa_2)}, \tag{32}$$

$$A_3 = \frac{2e^{-ik_3 L} k_1 \kappa_2}{(k_1 + k_3)\kappa_2 \cosh(L\kappa_2) + i(-k_1 k_3 + \kappa_2^2)\sinh(L\kappa_2)}, \tag{33}$$

Since A_3 describes the amplitude of the transmitted wavefunction, we will define *transmission probability* (or transmission) $\mathcal{T} = |A_3|^2$; similarly, we will call $\mathcal{R} = |B_1|^2$ *reflection probability* (or reflection). What are the maximum values of the $\mathcal{T}$ and $\mathcal{R}$?

Our classical intuition suggests that if the potential barrier V_b exceeds the energy if the particle, the transmission $\mathcal{T} = |B_1|^2$ vanishes. However, that would imply vanishing of the numerator of B_1, which cannot happen! Instead, we'll see that $\mathcal{T}$ decays quickly with L.

What is the behavior of transmission $\mathcal{T}$ and reflection $\mathcal{R}$ for $L\kappa_2 \ll 1$ (where $\cosh(L\kappa_2) \approx 1, \sinh(L\kappa_2) \approx L\kappa_2$), assuming $k_1 = k_3$?

$$\mathcal{T} \approx \left[1 + (L\kappa_2)^2 \left(1 + \left(\frac{\kappa_2^2 - k_1^2}{2k_1\kappa_2}\right)^2\right)\right]^{-1} \approx 1 - (L\kappa_2)^2 \left(1 + \left(\frac{\kappa_2^2 - k_1^2}{2k_1\kappa_2}\right)^2\right). \tag{34}$$

(similarly, derive the limit of $\mathcal{R}$)

How about the transmission $\mathcal{T}$ and reflection $\mathcal{R}$ for $L\kappa_2 \gg 1$ (where $\cosh(L\kappa_2) \approx \sinh(L\kappa_2) \approx$

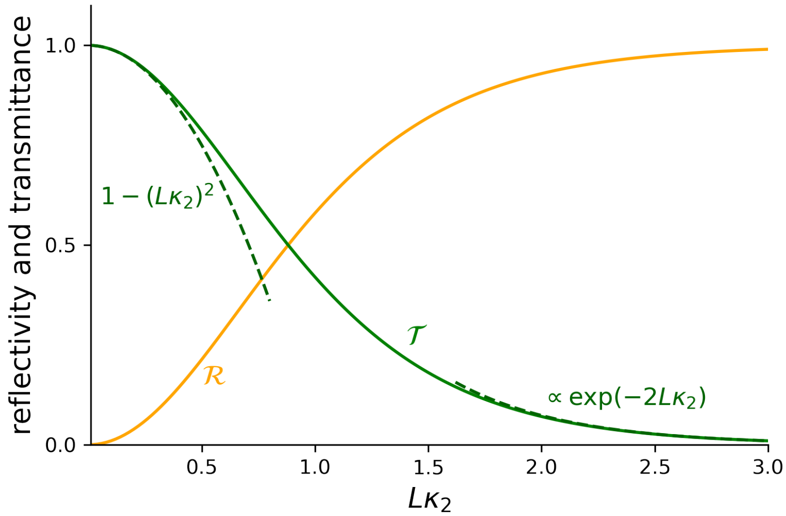

Figure 2: Go to `github` for animated versions

$\exp(L\kappa_2)/2)$, assuming $k_1 = k_3$?

$$\mathcal{T} \approx 4e^{-2\kappa_2 L}\left[1+\left(\frac{\kappa_2^2-k_1^2}{2k_1\kappa_2}\right)^2\right]^{-1}. \tag{35}$$

(similarly, derive the limit of $\mathcal{R}$)

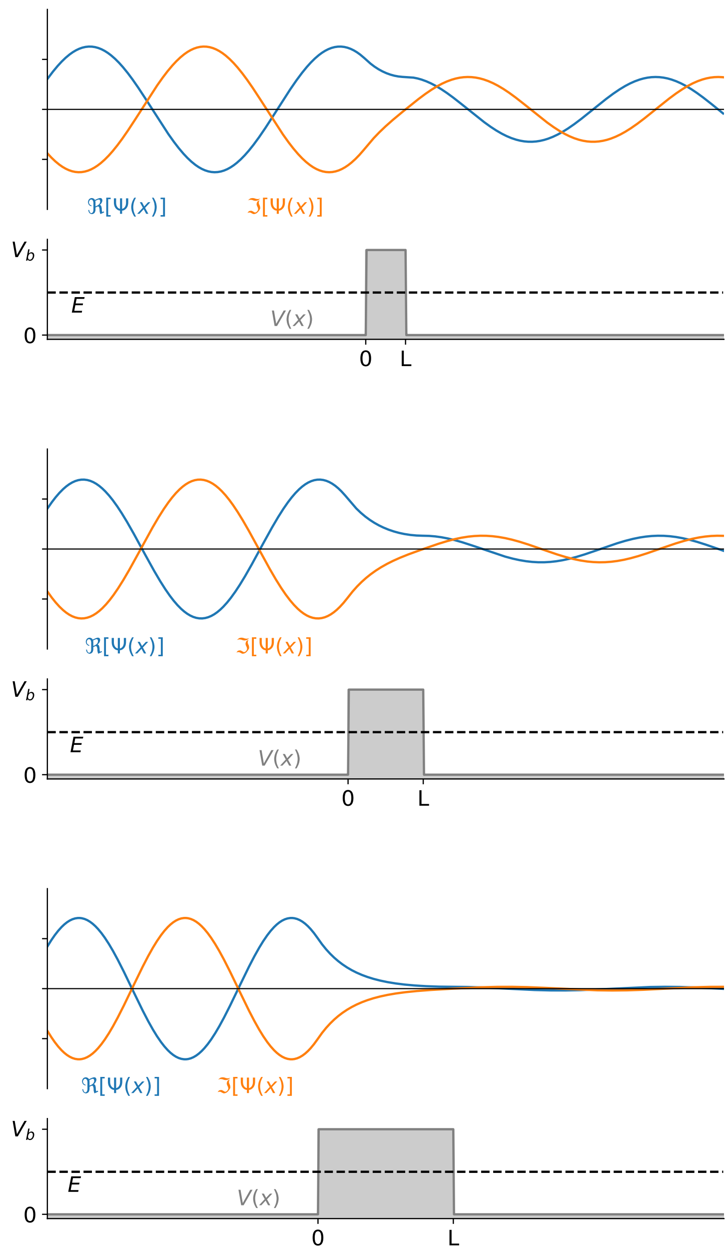

Figure 3: Examples of tunnelling across potential barrier. Go to `github` for animated versions

3 Where from here

3.1 Potential wells and bound states

3.2 Bound state to continuum tunnelling

4 Excercises

1. Derive Eqs. 34 and 35.

2. Limit of transistor technology. Imagine the potential for electron in a transistor as a square potential barrier with $V_b - E = 10^{-1} qV$, where V is a typical voltage in a transistor ($V = 0.3$ V), and q is the electron charge. At what barrier width does the electron transmission $\mathcal{T}$ exceed 10^{-2}? How does this distance compare to the dimensions of the state-of-the-art transistors? Assume electron mass m in calculations.

3. Calculate the transmission ($\mathcal{T}$) of an electron across the barrier of height 13.6 eV (do you know where this comes from?) and width 1 nm, for the electron energy from 1 to 10 eV.

4. Classical limit of the tunnelling: Calculate the transmission of a dog across a tall fence. Model the dog, of mass $m = 10$ kg, as a localised quantum-mechanical wavefunction, and its COM is 1 m below the top of the 1 cm thick fence. For extra points, calculate the de Broglie wavelength of the dog.

5. *(great exam question)* What happens to the transmission in the limit of vanishing barrier width?

6. *(coding challenge)* How to extend Eq. (eq) and code given in ... to tunnelling double barrier?