68413 Quantum Physics: Wavefunctions in 1D potentials

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1 Potential step

Previously, we began to discuss 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 $\hat{H}$. 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 Eq. (2)

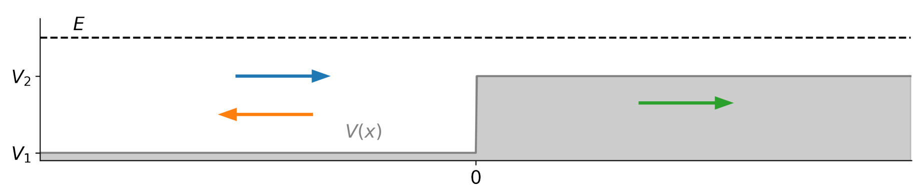

Figure 1: Step potential as described in Eq. (3).

In particular, we considered the piecewise-continuous potentials like in Fig. 1, where

$$V(x) = \begin{cases} V_1, & \text{if } x < 0 \\ V_2, & \text{if } x \geq 0, \end{cases} \tag{3}$$

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

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

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

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:

$$\Psi_1(x) = \underbrace{A_1 e^{ik_1 x}}_{\rightarrow} + \underbrace{B_1 e^{-ik_1 x}}_{\leftarrow}, \quad \Psi_2(x) = \underbrace{A_2 e^{ik_2 x}}_{\rightarrow} + \underbrace{B_2 e^{-ik_2 x}}_{\leftarrow}, \tag{6}$$

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 the point of potential discontinuity $x = 0$, demanding that

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

$$\Psi_1(0) = \Psi_2(0), \tag{7}$$

i.e.

$$A_1 + B_1 = A_2 + B_2, \tag{8}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}x}\Psi_1(x)|_{x=0} = \frac{\mathrm{d}}{\mathrm{d}x}\Psi_2(x)|_{x=0}, \tag{9}$$

i.e.

$$k_1 (A_1 - B_1) = k_2 (A_2 - B), \tag{10}$$

Equations (8) and (14) can be written in the matrix form as:

$$\begin{pmatrix} e^{ik_1x_{12}} & e^{-ik_1x_{12}} & -e^{ik_2x_{12}} & -e^{ik_2x_{12}} \\ k_1e^{ik_1x_{12}} & -k_1e^{-ik_1x_{12}} & -k_2e^{ik_2x_{12}} & k_2e^{ik_2x_{12}} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{11}$$

1.2.1 Reducing the complexity

Are the above boundary conditions enough? We have 4 uknown variables (A_1, B_1, A_2, B_2) but only 2 equations (Eq. (8),(14)). Perhaps the problem is ill-defined?

Let's define it better: we want to understand how a particle incident on the barrier *from the left* reflects back, and transmits *to the right* (see the blue, orange, and green arrows in Fig. 1). In the second medium the particle will only travel to the right, so we set $B_2 = 0$ in Eq. (6). Furthermore, equations (8) and (14) form a linear set of equations, so we expect that any solution of (A_1, B_1, A_2, B_2), divided by any non-zero number will still yield a valid solution. In particular, setting $A_1 = 1$ we can simpligy Eq. (6) to

$$\Psi_1(x) = e^{ik_1x} + B_1e^{-ik_1x}, \quad \Psi_2(x) = A_2e^{ik_2x}. \tag{12}$$

Equations (8) and (14) become

$$1 + B_1 = A_2, \tag{13}$$

$$k_1\left(1 - B_1\right) = k_2A_2. \tag{14}$$

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

$$\begin{pmatrix} 1 & -1 \\ -k_1 & -k_2 \end{pmatrix} \begin{pmatrix} B_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} -1 \\ -k_1. \end{pmatrix} \tag{15}$$

1.3 Solutions

From the above we can quickly identify a solution:

$$A_2 = \frac{2k_1}{k_1 + k_2}, \quad B_1 = \frac{k_1 - k_2}{k_1 + k_2}. \tag{16}$$

Consider:

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

Symbolic solution in Mathematica While solving the set of 2 equations is straightforward, more complicated systems with N domains, will yield systems of $2(N-1)$ equations. Let's use this as an opportunity to learn some basic Wolfram Mathematica — a powerful software for symbolic calculations. Here's a listing of the Mathematica script solving Eq. (15):

```
M = {{1,-1},
        {-1,-k2/k1}};
b = {-1, -1};
ln = LinearSolve[M,b];
B1 = ln[[1]]//FullSimplify
A2 = ln[[2]]//FullSimplify
```

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 inh are unitless. This is a standard trick to avoid large or small numbers and possible numerical precision errors — it's not strickly necessary for symbolic calculation, but a great habit to get into! Code available for download at GitHub.

Numerical solution in Python Note that once we know the values of all the parameters, the above equations can be also solved numerically. Here's a listing of the Python code solving Eq. (15):

```
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 2: Solver to the problem of step potential. Note that the second equation has was devided by k_1, so the expressions in M and inh are unitless. This is a standard trick to avoid large or small numbers and possible numerical precision errors. Code available for download at GitHub.

1.3.1 Examples

In Fig. 2 we show a few example solutions of the problem of step potential.

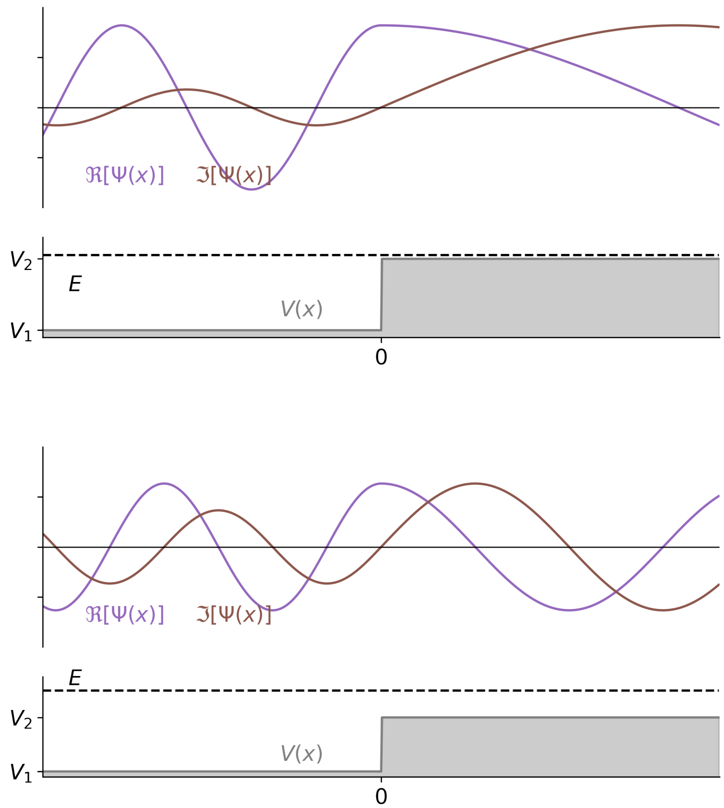

Figure 2: Step potential as described in Eq. (3) with (top) $(V_1, V_2, E) = (0, 3, 3.1)$ and (bottom) $(V_1, V_2, E) = (0, 2, 3)$. Throughout these notes, we set $m = \hbar = 1$ for simplicity. You can find animations in the lecture slides, or try to generate them yourself using the available code.

Consider:

- the wavefunction is continuous, and smooth at the potential discontinuity point $x = 0$,
- 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),
- 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 you've seen in the electromagnetic course?

1.4 Transmission and reflection

To quantify the probabilities of transmission and reflection across the step discontinuity, we introduce the current density (we will derive this quantity at the next lecture):

$$J(x) = \frac{\hbar}{m} \Im \left\{ [\Psi(x)]^* \, \Psi'(x) \right\}, \tag{17}$$

and differentiate between the incident current density (see Eq. (6))

$$J_I(x) = \frac{\hbar}{m} \Im \left\{ \left[A_1 e^{ik_1 x}\right]^* A_1 i k_1 e^{ik_1 x} \right\} = \frac{\hbar k_1}{m} |A_1|^2, \tag{18}$$

transmitted current density

$$J_T(x) = \frac{\hbar}{m} \Im \left\{ \left[A_2 e^{ik_2 x}\right]^* A_2 i k_2 e^{ik_2 x} \right\} = \frac{\hbar k_2}{m} |A_2|^2, \tag{19}$$

and reflected current density

$$J_R(x) = \frac{\hbar}{m} \Im \left\{ \left[B_1 e^{-ik_1 x}\right]^* \left(-B_1 i k_1 e^{-ik_1 x}\right) \right\} = \frac{\hbar k_1}{m} |B_1|^2. \tag{20}$$

We then define *transmission probability* (or transmission) $\mathcal{T}$ and *reflection probability* (or reflection) $\mathcal{R}$ as the ratios of the above currents:

$$\mathcal{T} = \frac{J_T}{J_I} = \frac{k_2}{k_1} \left| \frac{A_2}{A_1} \right|^2, \quad \mathcal{R} = \frac{J_R}{J_I} = \left| \frac{B_1}{A_1} \right|^2. \tag{21}$$

In Fig. 3 we plot the transmission $\mathcal{T}$, reflection $\mathcal{R}$, and $\mathcal{T} + \mathcal{R}$, as a function of energy E, for the problem of step potential with $(V_1, V_2) = (0, 1)$.

Consider:

- what's the limit of transmission for $E \to V_2$?
- what's the significance of $\mathcal{T} + \mathcal{R} = 1$?

Time evolution of the wavefunction In the lecture we showed some animations of the wavefunctions oscillating with time. While we haven't yet discussed the time-dependent Schrödinger equation, let us skip ahead a bit, and note that eigenfunction of the Hamiltonian, with eigenvalues (energy) E, will evolve in time according to

$$\Psi(x, t) = e^{-iEt/\hbar} \Psi(x, 0). \tag{22}$$

We'll get back to this problem in the next lecture.

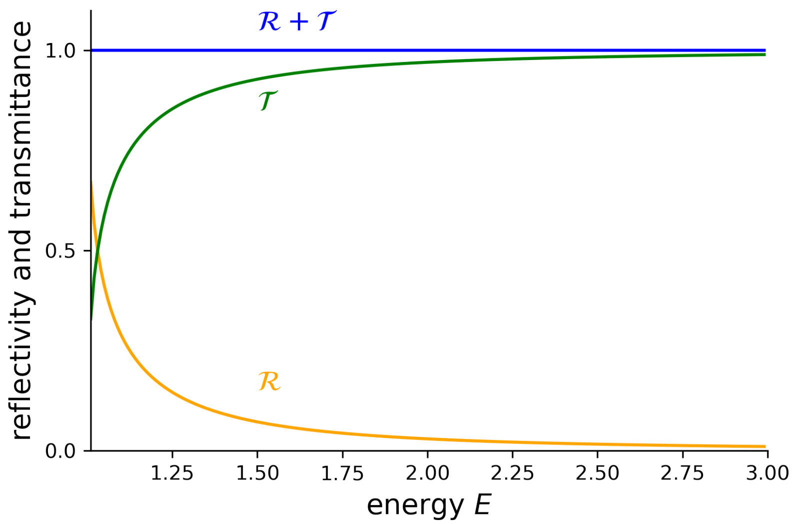

Figure 3: Transmission $\mathcal{T}$, reflection $\mathcal{R}$, and $\mathcal{T}+\mathcal{R}$, as a function of energy E, for the problem of step potential with $(V_1, V_2) = (0, 1)$.

2 Quantum tunnelling

Now that we have developed the necessary mathematical apparatus, let's challenge out classical notions of what's allowed and what's forbidden in quantum mechanics.

We start by considering a 1D system where the piecewise-constant potential exceeds the energy $V(x) = V_2 > E$ over some region $0 < x < L$, while outside of that region the potentials are all 0:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\right)\Psi_1(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_1^2\right)\Psi_1(x) = 0 \quad \text{for } x < 0, \tag{23}$$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V_2)\right]\Psi_2(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_2^2\right)\Psi_2(x) = 0 \quad \text{for } 0 < x \leq L, \tag{24}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}E\right)\Psi_3(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k_3^2\right)\Psi_3(x) = 0 \quad \text{for } L < x. \tag{25}$$

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

$$\Psi_2(x) = \underbrace{A_2 e^{\kappa_2 x}}_{\nearrow} + \underbrace{B_2 e^{-\kappa_2 x}}_{\searrow}, \tag{26}$$

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

$$\Psi_1(x) = \underbrace{A_1 e^{ik_1 x}}_{\rightarrow} + \underbrace{B_1 e^{-ik_1 x}}_{\leftarrow}, \quad \Psi_3(x) = \underbrace{A_3 e^{ik_3 x}}_{\rightarrow} + \underbrace{B_3 e^{-ik_3 x}}_{\leftarrow}, \tag{27}$$

with $k_1 = k_3 = \sqrt{2m/\hbar^2 E}$.

The boundary conditions

$$\Psi_1(0) = \Psi_2(0), \quad \Psi_1'(0) = \Psi_2'(0) \tag{28}$$

$$\Psi_2(L) = \Psi_3(L), \quad \Psi_2'(L) = \Psi_3'(L) \tag{29}$$

, again give us a set of equations for the unknown amplitude coefficients A_i, B_i

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

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

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

Symbolic solution in Mathematica

```
M = {
        {1,-1,-1,0},
        {-\\[ImaginaryI],-\\[Kappa]2/k1,\\[Kappa]2/k1,0},
        {0,Exp[\[Kappa]2 L],Exp[-\[Kappa]2 L],-Exp[\[ImaginaryI] k3 L]},
        {0,Exp[\[Kappa]2 L],- Exp[-\[Kappa]2 L],
         -\[ImaginaryI] k3/\[Kappa]2 Exp[\[ImaginaryI] k3 L]}
};
b = {-1, -\[ImaginaryI],0,0};
ln = LinearSolve[M,b];
B1 = ln[[1]]//FullSimplify
A2 = ln[[2]]//FullSimplify
B2 = ln[[3]]//FullSimplify
A3 = ln[[4]]//FullSimplify
```

Listing 3: Solver for the problem of potential barrier, developed as an extension of the code given in Listing 1. Code available for download at GitHub.

Numerical solution in Python

```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 4: Solver for the problem of potential barrier, developed as an extension of the code given in Listing 2. Code available for download at GitHub.

2.1 Solutions

Using the symbolic solver, or pen and paper, we can find the following solutions to Eq. (31):

$$B_1 = \frac{(k_1-k_3)\kappa_2\cosh(L\kappa_2) - i(k_1k_3+\kappa_2^2)\sinh(L\kappa_2)}{(k_1+k_3)\kappa_2\cosh(L\kappa_2) + i(-k_1k_3+\kappa_2^2)\sinh(L\kappa_2)}, \tag{32}$$

$$A_2 = -\frac{2k_1(k_3-i\kappa_2)}{(\kappa_2+ik_1)(\kappa_2+ik_3)+(k_1+i\kappa 2)(k_3+i\kappa_2)e^{2\kappa_2 L}}, \tag{33}$$

$$B_2 = \frac{2e^{2\kappa_2 L}k_1(-ik_3+\kappa_2)}{(\kappa_2+ik_1)(k_3-i\kappa_2)+(\kappa_2-ik_1)(k_3+i\kappa_2)e^{2\kappa_2 L}}, \tag{34}$$

$$A_3 = \frac{2e^{-ik_3L}k_1\kappa_2}{(k_1+k_3)\kappa_2\cosh(L\kappa_2) + i(-k_1k_3+\kappa_2^2)\sinh(L\kappa_2)}, \tag{35}$$

Using these formulas, in Fig. 5 we plot several solution of to the quantum tunnelling problem.

2.2 Transmission and reflection

Here again we can quantify the reflection and transmission probabilities using the current densities J_I, J_R and J_T the calculate $\mathcal{R}$ and $\mathcal{T}$ introduced in Eq. (21). Since we'll consider the transmission over the barrier, the transmitted current will be defined by A_3 (see Eq. (27)) simply as $\mathcal{T} = |B_1|^2$.

Our classical intuition suggests that if the potential barrier V_b exceeds the energy of the particle, the transmission $\mathcal{T}_{\text{classical}}$ should be identically 0. However, that would imply vanishing of the numerator of B_1 (see Eq. (32)), which cannot happen! Instead, we can plot $\mathcal{T}$ as a function of parameter $\kappa_2 L$, which auspiciously pops up in Eq. (32), and see that $\mathcal{T}$ decays quickly with L. How quickly?

Let's study the behavior of transmission $\mathcal{T}$ in two regimes:

- for $L\kappa_2 \ll 1$ (where $\cosh(L\kappa_2) \approx 1 + (L\kappa_2)^2/2, \sinh(L\kappa_2) \approx L\kappa_2$), assuming $k_1 = k_3$?

$$\mathcal{T} \approx \left[1 + (L\kappa_2)^2\left(1 + \left(\frac{\kappa_2^2 - k_1^2}{2k_1\kappa_2}\right)^2\right)\right]^{-1} \approx 1 - (L\kappa_2)^2\left(1 + \left(\frac{\kappa_2^2 - k_1^2}{2k_1\kappa_2}\right)^2\right). \tag{36}$$

  (derive the above, and the corresponding $\mathcal{R}$)

- for $L\kappa_2 \gg 1$ (where $\cosh(L\kappa_2) \approx \sinh(L\kappa_2) \approx \exp(L\kappa_2)/2$), assuming $k_1 = k_3$?

$$\mathcal{T} \approx 4e^{-2\kappa_2 L}\left[1 + \left(\frac{\kappa_2^2 - k_1^2}{2k_1\kappa_2}\right)^2\right]^{-1}. \tag{37}$$

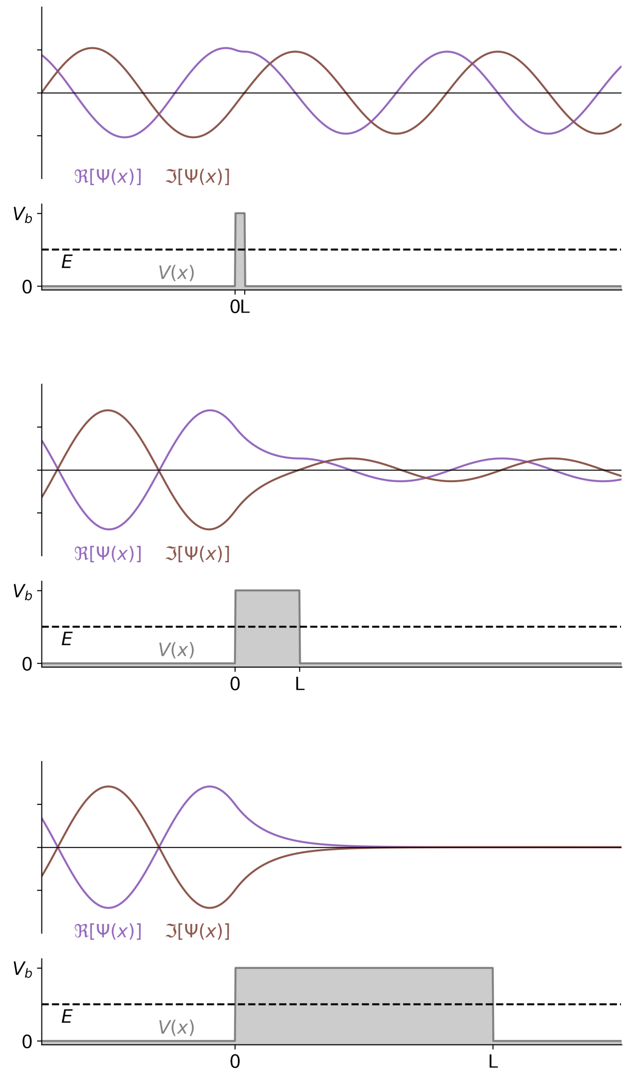

Figure 4: Examples of tunnelling across potential barrier, with $(V_b, E) = (4, 2)$, and increasing barrier length such that $L\kappa_2 = (0.3, 2, 8)$. Go to the lecture slides for animated versions

(derive the above, and the corresponding $\mathcal{R}$)

3 Problems

1. Derive Eqs. 36 and 37, and the corresponding expressions for the reflection $\mathcal{R}$.

2. Explore the limits 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

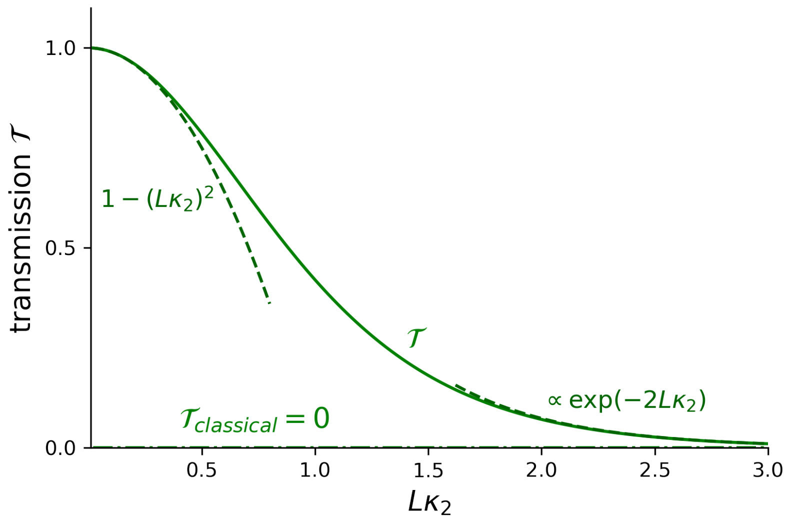

Figure 5: Go to github for animated versions

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?

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. *(great exam question)* What happens to the transmission in the limit of vanishing barrier width? How about simultaneously growing V_b and shrinking L?

5. *(coding challenge)* How to extend Eq. (31) and code given in Listings 3 and 4 to tunnelling through a double barrier?