# PHYS229: Wavefunctions in 1D potentials

Dr Mikołaj K. Schmidt
mikolaj.schmidt@mq.edu.au

## 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 $\hat{p} = -i\hbar d/dx$, we turned this physics problem into a mathematical one — solving an ODE:

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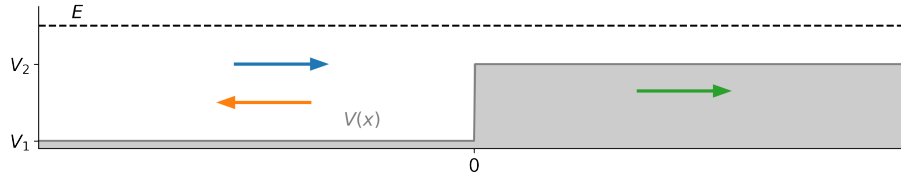
### 1.1 Solving Eq. (2)



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

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

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

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

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

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

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 $\Psi_1$ and $\Psi_2$ 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 *stitch* 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,

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

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

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

Dividing both sides of the above equations by $e^{ik_1x}$ and moving the constant terms to the RHS, we can express them as:
$$\begin{pmatrix} 1 & -1 \\ -k_1 & -k_2 \end{pmatrix} \begin{pmatrix} B_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} -1 \\ -k_1. \end{pmatrix} \tag{15}$$

2

## 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):

```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 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.
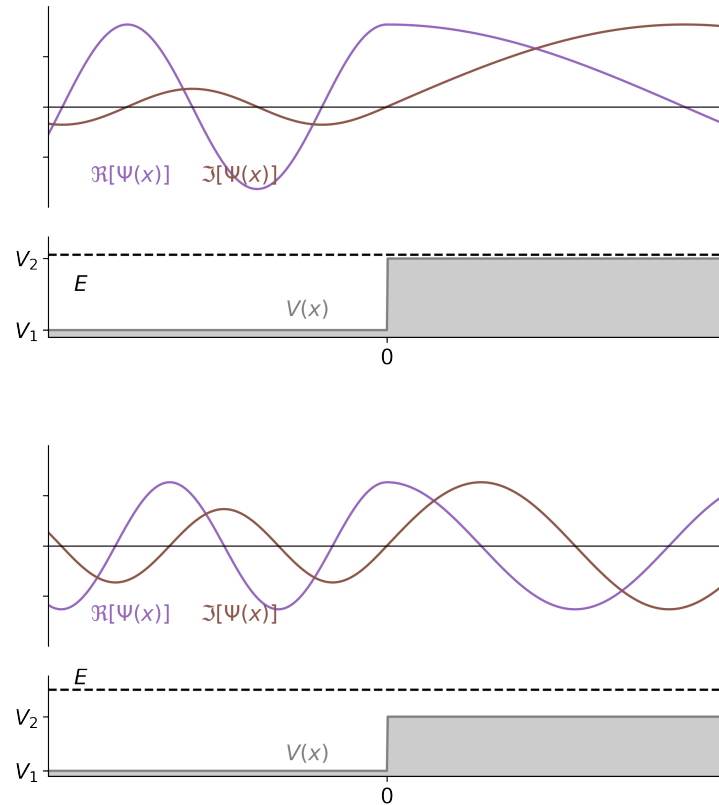


Figure 2: Step potential as described in Eq. (3) with (top) $(V_1, V_2, E) = (0, 3, 3.1)$ and (bottom) $(V_1, V_2, E) = (0, 2, 3)$. Throughout these notes, we set $m = \hbar = 1$ for simplicity. You can find animations in the lecture slides, or try to generate them yourself using the available code.

> 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):

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

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

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

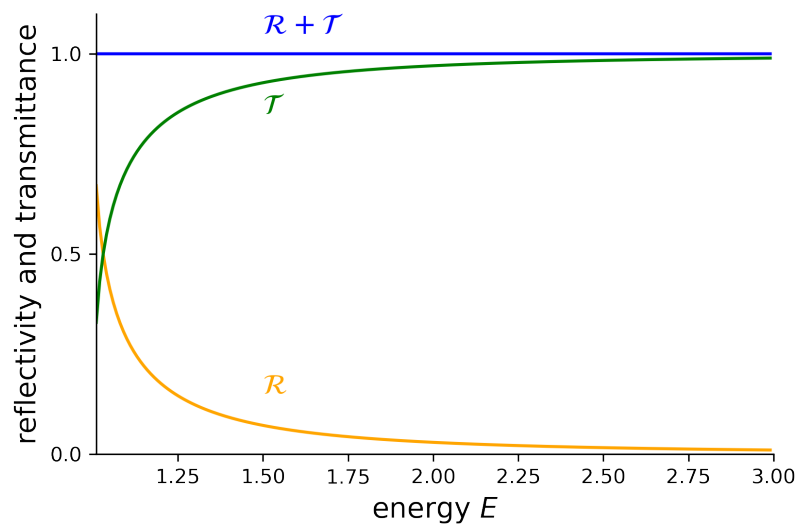We'll get back to this problem in the next lecture.

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:

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

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

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

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},
        {-I, -k2/k1, k2/k1, 0},
        {0, Exp[k2 L], Exp[-k2 L], -Exp[I k3 L]},
        {0, Exp[k2 L], -Exp[-k2 L], -I k3/k2 Exp[I k3 L]}
};
b = {-1, -I, 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):

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

$$A_2 = -\frac{2k_1(k_3 - i\kappa_2)}{(\kappa_2 + ik_1)(\kappa_2 + ik_3) + (k_1 + i\kappa2)(k_3 + i\kappa_2)e^{2\kappa_2 L}}, \tag{33}$$

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

$$A_3 = \frac{2e^{-ik_3 L}k_1 \kappa_2}{(k_1 + k_3)\kappa_2 \cosh(L\kappa_2) + i(-k_1 k_3 + \kappa_2^2) \sinh(L\kappa_2)}, \tag{35}$$

8

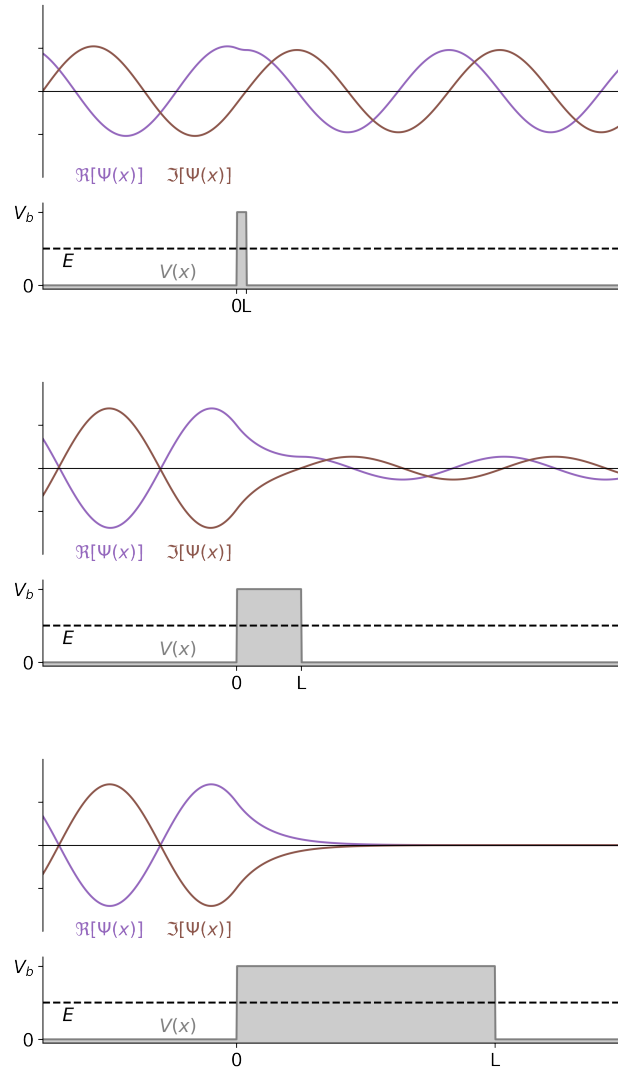Using these formulas, in Fig. 5 we plot several solution of to the quantum tunnelling problem.



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

## 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 $\mathcal{T}_{classical}$ 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?
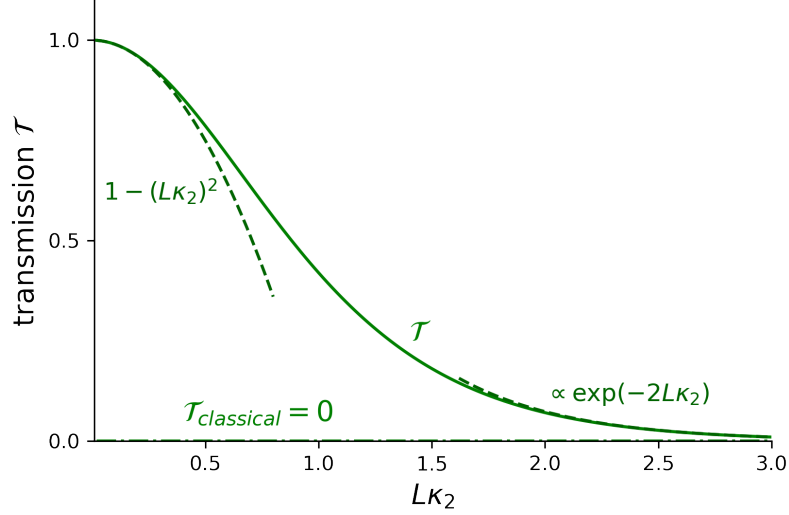


Figure 5: Go to `github` for animated versions

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 $k_1 = k_3$?

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

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

10

## 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 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?