

## 4. TIME-INDEPENDENT SCHRÖDINGER EQUATION

The solution of the TDSE is a rather formidable problem even in 1D. The underlying problem is not just that it is a partial differential equation of second order in  $x$  and first order in  $t$ , but that we must consider both of these variables at once. As a consequence, the space and time dependence of the wavefunction may be very complicated. We have seen one example of this complexity before: The Gaussian free-particle state function is a combination of spatial and time-dependent factors.

One way to solve the TDSE is to seek solutions that have a particularly simple form, i.e.

$$\Psi(x, t) = \psi(x)\xi(t)$$

These product functions are called **separable solutions** of the partial differential equation (PDE). In Quantum Mechanics, they are called **stationary-state wavefunctions**. One can find these stationary-state wavefunctions using a method called **separation of variables**. For example, substituting the above expression for  $\Psi(x, t)$  into the TDSE, one gets:

$$\xi(t) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x, t)\psi(x) \right] = \psi(x) i\hbar \frac{\partial \xi(t)}{\partial t}$$

or:

$$\frac{1}{\psi(x)} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x, t)\psi(x) \right] = i\hbar \frac{1}{\xi(t)} \frac{\partial \xi(t)}{\partial t}$$

The last equation is almost separable, since, in general, the potential energy can depend on both  $x$  and  $t$ . If we assume that  $V(x, t) = V(x)$ , i.e. the potential energy is time-independent, then the LHS is only a function of  $x$  and the RHS is only a function of  $t$ . Therefore, the two sides can be equal if they are constant. This gives us two equations:

$$\begin{cases} \frac{1}{\psi(x)} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) \right] = \alpha \rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = \alpha\psi(x) \\ i\hbar \frac{1}{\xi(t)} \frac{\partial \xi(t)}{\partial t} = \alpha \rightarrow i\hbar \frac{\partial \xi(t)}{\partial t} = \alpha\xi(t) \end{cases}$$

### Notes:

- The fact that we can obtain these two equations at all, provided that  $V$  does not depend on time, proves that **stationary state wavefunctions** exist for systems with a time-independent potential energy.
- A system whose potential energy is time-independent is said to be **conservative**. Hence, stationary states exist for conservative systems.
- The solution of the second equation [for  $\xi(t)$ ] is very simple, and is given by:

$$\xi(t) = \xi(0)e^{-i\alpha t / \hbar}$$

The Born interpretation of  $\psi(x,t)$  provides a clue to the physical meaning of the separation constant  $\alpha$ . The wavefunction of a stationary state oscillates at a frequency  $\omega = \alpha / \hbar$ . From the de Broglie-Einstein relation, one has that  $E = \hbar\omega = \alpha$ . Hence, we can represent  $\alpha$  as the total energy of the particle in the state represented with this wavefunction, i.e.

$$\xi(t) = \xi(0)e^{-iEt/\hbar}$$

- The first equation then becomes:

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi_E(x) = E\psi_E(x)$$

This is the time-independent SE (TISE), which is an equation of a very special form. There is a differential operator representing the total energy of the system, which operates on the unknown function  $\psi_E(x)$  to produce the same function  $\psi_E(x)$  multiplied by a parameter  $E$ . Mathematicians call an equation of this form an **eigenvalue equation**:

- $\psi_E(x)$  is the eigenfunction
- $E$  is the corresponding eigenvalue

### Summary:

The results presented in this section can be summarized as follows:

- If a microscopic system is conservative, then there exist special quantum states of the system, called stationary states, in which the energy is sharp.
- Even if the number of these eigenstates is infinite, the energies of the bound states form a discrete list.
- If there is a one-to-one correspondence between the quantized energies of a quantum system and its bound state, or stationary-state wavefunctions, then the bound state energy is **non-degenerate**. If there are stationary states for which there correspond more than one distinct spatial functions, such bound states are called **degenerate**.

## A. STATIONARY STATES FOR A FREE PARTICLE

Let's try to solve the TISE for a free particle, for which  $V(x) = 0$ , i.e.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E\psi(x) \rightarrow \frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + E\psi(x) = 0$$

This is a homogeneous, second-order partial differential equation with constant coefficients, and the solution of this equation is of the form:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

This function is not normalizable, since it does not decay for  $|x| \rightarrow \infty$ . Two properties follow from the impossibility of normalizing this function:

- The energies are not quantized, i.e. all values  $E > 0$  are allowed.
- The energies are degenerate ( $+k$  and  $-k$ ).

One can avoid this problem by introducing a finite domain, which will be discussed in the next lectures.

## B. POTENTIAL STEP

Our next task is to solve the TISE for one-dimensional single-particle system whose potential energy is piecewise constant. A piecewise constant potential is one that is constant for all values of  $x$  except at a finite number of discontinuities-points, where it changes from one constant value to another. One of the simplest piecewise-constant potentials is the [potential step](#)

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases} \rightarrow V(x) = V_0 \Theta(x)$$

shown graphically in the figure below.

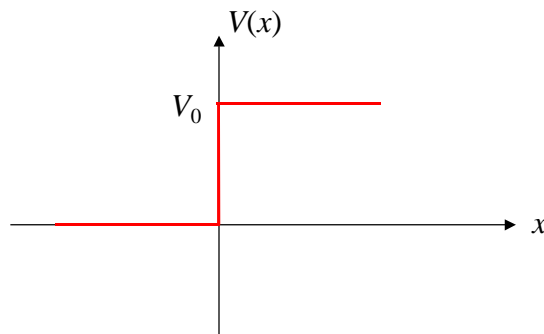


Figure 1. Potential step (an example of a piecewise constant potential).

Our task is to solve the following problem: We assume that we have a beam of particles incident from the left that encounters an impulsive force at  $x=0$ . We will consider two cases: (a) when the energy  $E$  of the particle is less than  $V_0$ , and (b) when the energy of the particle is greater than  $V_0$ .

### Case (a): $E < V_0$ :

For this particular case, we need to distinguish between two separate regions:

- On the left from the potential step,  $E > V(x) \rightarrow$  classically-allowed region
- On the right from the potential step,  $E < V(x) \rightarrow$  classically-forbidden region
- $x=0$  is called a turning point  $\rightarrow$  point that separates the classically-allowed from the classically forbidden regions (see the figure below).

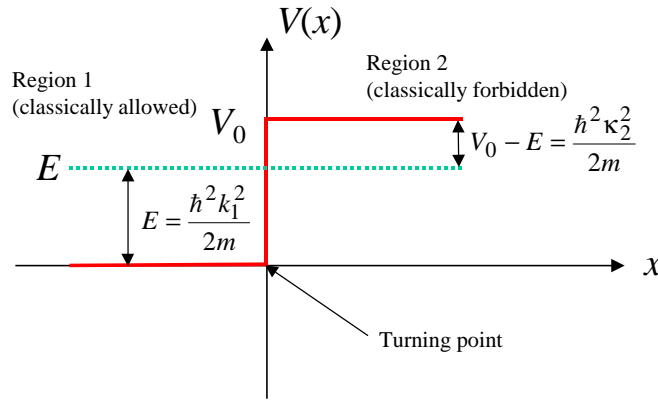


Figure 2. Description of the various regions for case (a).

The solution procedure for this type of problems is the following one:

- Write down the TISE for each region in which the potential energy is constant. Solve the TISE up to arbitrary constants.
- If necessary, apply the asymptotic condition to get physically admissible state functions.
- Match the wavefunctions and the derivatives of the wavefunctions at each of the turning points.

Following the above-outlined procedure, we get the following general expressions for the wavefunctions in region 1 and region 2:

$$\psi(x) = \begin{cases} A^{(1)} e^{ik_1 x} + B^{(1)} e^{-ik_1 x} = \psi_1(x), & k_1 = \sqrt{\frac{2mE}{\hbar^2}} \\ A^{(2)} e^{-\kappa_2 x} = \psi_2(x), & \kappa_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \end{cases}$$

The unknown coefficients that appear in the above expression are calculated from the requirement that  $\psi(x)$  be continuous and smooth, which implies that it must also have continuous first derivative. Therefore, using the boundary conditions:

$$\begin{cases} \psi_1(0) = \psi_2(0) \\ \left. \frac{d\psi_1(x)}{dx} \right|_{x=0} = \left. \frac{d\psi_2(x)}{dx} \right|_{x=0} \end{cases}$$

we get:

$$\begin{cases} B^{(1)} = \frac{k_1 - i\kappa_2}{k_1 + i\kappa_2} A^{(1)} \\ A^{(2)} = \frac{2k_1}{k_1 + i\kappa_2} A^{(1)} \end{cases}$$

**Important notes:**

- $|B^{(1)}| = |A^{(1)}|$ , which means that in region 1, two waves of equal amplitude travel in the opposite direction and with the same phase velocity. Because of this, the wavefunction in region 1 represents a standing wave.
- The above observation suggest that the probability of reflection  $R(E)=1$  and that of transmission  $T(E)=0$ . This result is just what we would expect were we applying classical physics to the problem.
- In region 2, the wavefunction represents an evanescent wave, whose amplitude equals to

$$|\psi_2(x)| = \frac{2k_1}{\sqrt{k_1^2 + \kappa_2^2}} |A^{(1)}| e^{-\kappa_2 x}$$

This is consistent with the previous observation that all incident particles with  $E < V_0$  are reflected back. Therefore, we might say that **no probability flow is associated with evanescent waves**.

**Case (b):  $E > V_0$ :**

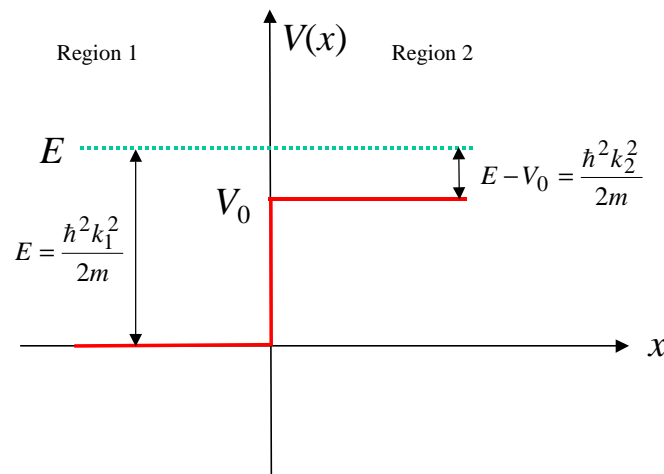


Figure 3. Graphical description of the variables used for this case.

Following the procedure described in part (a), we get the following general expressions for the wavefunctions in region 1 and region 2:

$$\Psi(x) = \begin{cases} A^{(1)} e^{ik_1x} + B^{(1)} e^{-ik_1x} = \Psi_1(x), & k_1 = \sqrt{\frac{2mE}{\hbar^2}} \\ A^{(2)} e^{ik_2x} = \Psi_2(x), & k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \end{cases}$$

The unknown coefficients that appear in the above expression are again calculated from the requirement that  $\Psi(x)$  be continuous and smooth, which implies that it must also have continuous first derivative. Therefore, using the boundary conditions:

$$\begin{cases} \Psi_1(0) = \Psi_2(0) \\ \left. \frac{d\Psi_1(x)}{dx} \right|_{x=0} = \left. \frac{d\Psi_2(x)}{dx} \right|_{x=0} \end{cases}$$

in this particular case we obtain:

$$\begin{cases} B^{(1)} = \frac{k_1 - k_2}{k_1 + k_2} A^{(1)} \\ A^{(2)} = \frac{2k_1}{k_1 + k_2} A^{(1)} \end{cases}$$

### Important notes:

- Since all coefficients are real and their magnitude is in general not equal to one, we might conclude that the wavefunction for continuum stationary states is of the following general form:

$$\Psi(x) = \begin{cases} \text{incident wave} + \text{reflected wave} & \rightarrow \text{source} \\ \text{transmitted wave} & \rightarrow \text{detector} \end{cases}$$

We want to define the following two quantities:

- $\rho(E) = B^{(1)} / A^{(1)} \rightarrow$  reflection probability amplitude
- $\tau(E) = A^{(2)} / A^{(1)} \rightarrow$  transmission probability amplitude

Then, we can write:

$$\Psi(x) = \begin{cases} A^{(1)} e^{ik_1x} + \rho(E) A^{(1)} e^{-ik_1x} = \Psi_1(x), & x < 0 \\ \tau(E) A^{(1)} e^{ik_2x} = \Psi_2(x), & x \geq 0 \end{cases}$$

- From the probability amplitudes, one can calculate the reflection and transmission coefficients. To do so, we return to the probability current densities - the fluxes - for the

incident, reflected and transmitted waves. If we use the expression for the probability current, of the form

$$J(x) = -\frac{i\hbar}{2m} \left( \frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right)$$

we arrive at the following results:

$$J_1 = -\frac{e\hbar k_1}{2m} \left[ 1 - |\rho(E)|^2 \right] |A^{(1)}|^2 = J_{inc} + J_{ref}, \quad x < 0$$

$$J_2 = -\frac{e\hbar k_2}{2m} |\tau(E)|^2 |A^{(1)}|^2 = J_{trans}, \quad x \geq 0$$

If we look at the result at region 1, the probability current density  $J_1$  equals the sum of the incident current and a reflected current. In region 2, we have a transmitted current  $J_2$ . We can, therefore, define a reflection probability  $R(E)$  and transmission probability  $T(E)$  in the following manner:

$$R(E) = \left| \frac{J_{ref}}{J_{inc}} \right| = \left| \frac{-\frac{q\hbar k_1}{m} |\rho(E)|^2 |A^{(1)}|^2}{-\frac{q\hbar k_1}{m} |A^{(1)}|^2} \right| = |\rho(E)|^2, \text{ and}$$

$$T(E) = \left| \frac{J_{trans}}{J_{inc}} \right| = \left| \frac{-\frac{q\hbar k_2}{m} |\tau(E)|^2 |A^{(1)}|^2}{-\frac{q\hbar k_1}{m} |A^{(1)}|^2} \right| = \frac{k_2}{k_1} |\tau(E)|^2 .$$

Since a particle is either reflected or transmitted, we must have that

$$T(E) + R(E) = 1 .$$

For our particular problem, this gives us:

$$R(E) = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2 \text{ and } T(E) = \frac{4k_1 k_2}{(k_1 + k_2)^2} .$$

Therefore, in contrast to the case  $E < V_0$ , our result for  $E > V_0$  does not conform to the predictions of classical physics.

### Example:

Consider a step potential of height  $V_0 = 0.3$  eV. The effective mass of the electrons is assumed to be  $0.067 m_0$ , where  $m_0$  is the free electron mass.

Using the expressions we derived in this section, we can immediately calculate  $R(E)$  and  $T(E)$  for this step potential. The energy dependence of these two coefficient is shown in the figure below.

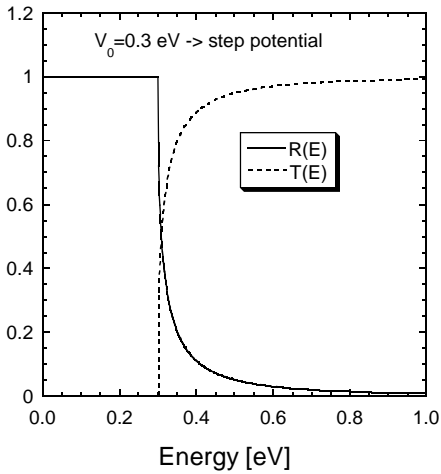


Figure 4. Transmission and reflection coefficient for a step potential as a function of the incident carrier energy.

An interesting thing to plot is the magnitude squared of the wavefunctions in regions (1) and (2) as a function of position. The behavior of  $|\psi_i(x)|^2$  ( $i=1$  for region 1 and  $i=2$  for region 2) is shown on the next figure. We use  $E=0.25$  eV and  $A^{(1)}=1$ . Note that the energy of the particles  $E$  is smaller than the barrier height. Therefore, we expect to see standing wave pattern in region 1 [since  $R(E)=1$  for this case] and evanescent (exponentially-decaying solution) in region 2.

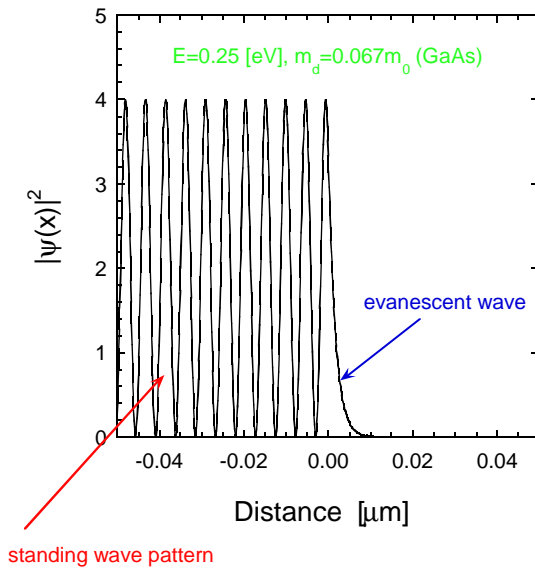


Figure 5. The magnitude squared of the wavefunction for carrier energy less than the barrier height.