# One-dimensional potentials: potential step



Figure I: Potential step of height  $V_0$ . The particle is incident from the left with energy E.

We analyze a time independent situation where a current of particles with a welldefined energy is incident on the barrier. The time-independent SE is

$$
\hat{H}u(x) = Eu(x) \tag{15-1}
$$

$$
-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2}(x) + V(x)u(x) = Eu(x)
$$
\n(15-2)

$$
\frac{d^2u}{dx^2} = -\frac{2m}{\hbar^2} [E - V(x)]u(x)
$$
\n(15-3)

Qualitative features of solutions for regions of constant  $V_1$ :

If  $E - V_1 > 0$ , the solutions are of the form  $e^{\pm i k_1 x}$  with  $\frac{\hbar^2 k^2}{2m} = E - V_1$ ,  $k_1$  real.

**Interpretation.**  $\frac{\hbar^2 k^2}{2m}$  is the KE of the particle with total energy E in a region of potential  $V_1$ , the  $e^{\pm ikx}$  wavefunctions correspond to particles traveling left / right.



Figure II: In a region where the particle energy is greater than the (constant) potential, the solutions of the SE are plane waves  $e^{\pm ikx}$ , where  $E - V_1 = \hbar^2 k^2 / 2m$  is the kinetic energy of the particle in that region.

If  $E - V_1 < 0$ , the solutions are of the form  $e^{\pm \kappa_1 x}$  with  $\frac{\hbar^2}{2}$ κ m  $\frac{1^2}{2} = V_1 - E, \; \kappa_1$ real. These are damped exponentials with a decay length constant  $\kappa_1$  (decay length  $\kappa_1^{-1}$ ), where  $\frac{\hbar^2 \kappa_1^2}{2m} = V_1 - E$  represents the "missing" kinetic energy of the particle As  $E \to V$ , the decay length  $\kappa_1^{-1}$  becomes longer and longer.



Figure III: In a region where the particle energy is less than the (constant) potential, the solutions of the SE are exponentially growing or decaying functions,  $e^{\pm \kappa x}$ , where  $V_1 - E = \hbar^2 \kappa^2 / 2m$  is the "missing kinetic energy" of the particle in that region.



interface, an evanescent (non-traveling, exponentially decaying wave) builds up inside the vacuum. The closer we are to the critical angle for total internal reflection, the longer the decay length of the evanescent wave. This phenomenon is analogous to a particle entering a classically forbidden region with  $V_1 > E$ . The less forbidden the region, the longer the decay length.

*Note.* There is a non-zero probability to find the particle with energy  $E$  in a "classically forbidden region" with  $E < V_1$ . The less the region is forbidden (the smaller  $V_1 - E$ ), the further the particle penetrates into the forbidden region (the longer the decay length  $\kappa_1$ <sup>-1</sup>). The phenomenon is similar to total internal reflection inside glass at a glass-vacuum interface.

The light field has non-zero amplitude in the "forbidden region". How do we know? Approach with a second prism. The evanescent (decaying) field existing in the vacuum is converted back into a traveling wave in the second prism.

Similarly, a particle can tunnel through a potential barrier even if its energy is insufficient to surpass it.

Back to potential step Assume  $E > V_0$ : define



Figure V: The light field "tunneling" through the forbidden region can be detected as it emerges on the other side in a second prism.



Figure VI: As a particle tunnels through a barrier and emerges from the other side, the energy E and the Broglie wavelength  $2\pi/k$  remain the same. The amplitude of the emerging wave is smaller than that of the incident wave.



Figure VII: Potential step

$$
\frac{\hbar^2 k^2}{2m} = E
$$
\n
$$
\frac{\hbar^2 q^2}{2m} = E - V_0
$$
\n(KE in region  $x < 0$ )\n
$$
\frac{\hbar^2 q^2}{2m} = E - V_0
$$
\n(KE in region  $x > 0$ )\n
$$
\tag{15-5}
$$

The most general solution is

$$
Ae^{ikx} + Be^{-ikx} \qquad \text{in the region } x < 0 \tag{15-6}
$$

$$
Ce^{iqx} + De^{-iqx}
$$
 in the region  $x > 0$  (15-7)

� If we choose as the initial condition a particle incident from the left  $(A \neq 0)$ , then the particle can be transmitted to the RHS ( $C \neq 0$ ), or, as we shall see, partially reflected by the barrier in spite of  $E > V_0$  ( $B \neq 0$ ). However, if no particle is incident from the right then  $D = 0$ .

### Calculate the particle current (or flux)

In region  $x < 0$ :

$$
j_{\leq} = \frac{\hbar}{2im} \left( u^* \frac{du}{dx} - \left( \frac{du^*}{dx} \right) u \right) \tag{15-8}
$$

$$
= \frac{\hbar}{2im} \left[ \left( A^* e^{-ikx} + B^* e^{ikx} \right) \left( ikA e^{ikx} - ikB e^{-ikx} \right) - \text{ c.c.} \right] \tag{15-9}
$$

$$
= \frac{\hbar k}{2m} \left[ |A|^2 + AB^* e^{2ikx} - A^* B e^{-2ikx} - |B|^2 - \text{c.c.} \right] \tag{15-10}
$$

$$
= \frac{\hbar k}{m} \left[ |A|^2 - |B|^2 \right] \quad \to \quad \text{net current for } x < 0 \tag{15-11}
$$

We define the reflection amplitude  $r = \frac{B}{A}$ , and the reflection coefficient as  $R = |r|^2 =$  $\left|\frac{B}{A}\right|$  $\frac{B}{A}$ |<sup>2</sup>.

For  $x > 0$ :

$$
j_{>} = \frac{\hbar q}{m} |C|^2
$$
 (15-12)

Continuity of wavefunction at  $x = 0$ :

$$
\psi(x \to 0) = A + B = \psi(x \gets 0) = C \tag{15-13}
$$

In spite of the potential step, the derivative of the wavefunction must also be continuous:

$$
\left(\frac{du}{dx}\right)_{x=\epsilon} - \left(\frac{du}{dx}\right)_{x=-\epsilon} = \int_{-\epsilon}^{\epsilon} dx \frac{d}{dx} \left(\frac{du}{dx}\right)
$$
\n(15-14)

$$
= -\frac{2m}{\hbar^2} \int_{-\epsilon}^{\epsilon} dx [E - V(x)] u(x) = 0 \qquad (15-15)
$$

For future applications, we note that if the potential contains a delta function term  $\lambda \delta(x - a)$ , with some magnitude of the delta function  $\lambda$ , then the same calculation gives

$$
\left(\frac{du}{dx}\right)_{x=a+\epsilon} - \left(\frac{du}{dx}\right)_{x=-a-\epsilon} = \frac{2m}{\hbar^2} \int_{a-\epsilon}^{a+\epsilon} dx \lambda \delta(x-a) u(\lambda) \tag{15-16}
$$

$$
=\frac{2m}{\hbar^2}\lambda u(a)\tag{15-17}
$$

To summarize, we have the following rules:

**Rule 1.** The wavefunction  $u(x)$  is always continuous

**Rule 2.** The first spatial derivative of the wavefunction  $\frac{du}{dx}$  is continuous if the potential does not contain  $\delta$ -function like terms. (It may contain potential steps).

**Rule 2.1.** if the potential contains a term  $\lambda \delta(x - a)$ , the the first derivative  $\frac{du}{dx}$  is discontinuous at  $x = a$  amnd satisfies the relation

$$
\left(\frac{du}{dx}\right)_{x=a+\epsilon} - \left(\frac{du}{dx}\right)_{x=a-\epsilon} = \frac{2m}{\hbar^2} \lambda u(a) \tag{15-18}
$$



Figure VIII: A discontinuity in the slope of the wavefunction occurs at a delta function potential. The difference in wavefunction slopes is proportional to the strength of the  $\delta$  potential, and to the value of the wavefunction at the cusp.



Solve for  $B, C$  in terms of  $A$ 

$$
C = A + B = \frac{k}{q}(A - B)
$$
 (15-21)

$$
A\left(1 - \frac{k}{q}\right) = -B\left(1 + \frac{k}{q}\right) \tag{15-22}
$$

$$
A\frac{q-k}{q} = -B\frac{q+k}{q} \tag{15-23}
$$

$$
B = \frac{k - q}{k + q}A\tag{15-24}
$$

$$
C = A + B = A + \frac{k - q}{k + q}A = \frac{2}{k + q}A
$$
 (15-25)

$$
r = \frac{B}{A} = \frac{k - q}{k + q} \tag{15-26}
$$

Transmission amplitude

\n
$$
t = \frac{C}{A} = \frac{2k}{k+q} \qquad (15-27)
$$

$$
|r|^2 = \left|\frac{B}{A}\right|^2 = \left(\frac{k-q}{k+q}\right)^2 \qquad (15-28)
$$

$$
|t|^2 = \left|\frac{C}{A}\right|^2 = \frac{4k^2}{(k+q)^2} \qquad (15-29)
$$

$$
\text{Reflection current} \qquad \qquad j_{\leftarrow} = \frac{\hbar k}{m} |B|^2 = \frac{\hbar k}{m} \left(\frac{k-q}{k+q}\right)^2 |A|^2 \qquad (15-30)
$$

Transmission current 
$$
j_{\to,x>0} = \frac{\hbar q}{m} |C|^2 = \frac{\hbar k}{m} \frac{4kq}{(k+q)^2} |A|^2
$$
 (15-31)

$$
\text{Net current for } x < 0 \qquad j < = \frac{\hbar k}{m} (|A|^2 - |B|^2) = \frac{\hbar k}{m} |A|^2 \frac{4kq}{(k+q)^2} \qquad (15-32)
$$

$$
\text{Net current for } x > 0 \qquad \qquad j > = \frac{\hbar q}{m} |C|^2 = \frac{\hbar k}{m} \frac{4kq}{(k+q)^2} |A|^2 \qquad (15-33)
$$

The current obeys the continuity equation (see problem set)

$$
\frac{\partial j}{\partial x} + \frac{\partial}{\partial t} |\psi|^2 = 0 \tag{15-34}
$$

Here we are considering stationary states,  $\frac{\partial}{\partial t} |\psi|^2 = 0$  (no change of probability density in time),  $\implies j = \text{const}$ , current is continuous across the potential step,

$$
j_{\leq} = j_{>},\tag{15-35}
$$

or

$$
j_{\text{inc}} = j_{\to,\text{x}<0} = \frac{\hbar k}{m} |A|^2 = j_{\text{refl}} + j_{\text{trans}}
$$
 (15-36)

$$
= j_{\leftarrow, x < 0} + j_{\rightarrow, x > 0} \tag{15-37}
$$

$$
= \frac{\hbar k}{m} |B|^2 + \frac{\hbar q}{m} |C|^2.
$$
 (15-38)

*Note.*  $|r|^2 + |t|^2 \neq 1$  because the particle velocity is different for  $x > 0$  from that for  $x < 0$ .

## Discussion of results

In contrast to classical mechanics, there is some reflection at the potential step even though the energy of the particle is sufficient to surpass it. This is familiar from optics, where a step-like change in the index of refraction (e.g., air-glass interface) leads to partial reflection. The particle reflection is a consequence of the matching of the wavefunction and its derivative at the boundary. Again, this is similar to optics where the matching of th electromagnetic fields at the boundary results in a reflected field.

Note. For a very smooth change of potential (or refractive index in optics) there is not reflection. What is smooth? A change over many wavelengths. Changes of the potential over a distance l short compared to a wavelength  $\lambda = \frac{2\pi}{k}$  result in reflection. Slow changes of potential over many  $\lambda$  do not result in reflection if particle energy exceeds barrier height.



Figure IX: A potential that varies smoothly over many de Broglie wavelengths does not produce partial reflection if the particle energy is sufficient to surpass it.

Intermediate region  $l \sim \lambda$ : we expect resonance phenomena (non-monotonic changes of reflection probability with particle energy). For the potential step, the reflection probability

$$
|r|^2 \to 0 \qquad \text{for } k \to q \qquad (E \gg V_1), \text{and} \qquad (15-39)
$$

$$
|r|^2 \to 1 \qquad \text{for } q \to 0 \qquad (E \gg V_1), \text{as expected.} \tag{15-40}
$$

(15-41)

Interestingly, the reflection probability can be written as

$$
|r|^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_1}}{\sqrt{E} + \sqrt{E - V_1}}\right)^2
$$
 (15-42)

i.e. it does not depend explicitly on  $\hbar$ . However, the reflection is still inherenetly nonclassical in that the potential needs to change abruptly compared to the particle's de Broglie wavelength, that depends on  $\hbar$ .

**Solution for**  $E < V_0$ : We define

$$
\frac{\hbar^2 k^2}{2m} = E \tag{15-43}
$$

$$
\frac{\hbar^2 \kappa^2}{2m} = V_0 - E \qquad \qquad \text{("missing KE to surpass barrier")} \tag{15-44}
$$

Most general solution

$$
Ae^{ikx} + Be^{-ikx} \qquad \text{for } x < 0 \tag{15-45}
$$

$$
Ce^{-\kappa x} + De^{\kappa x} \qquad \text{for } x > 0 \tag{15-46}
$$

The  $e^{+\kappa x}$  term is not normalizable,  $D=0$ 

We can go through the same procedure as before using the continuity of  $\psi_1\psi'$ at  $x = 0$ , or use the previous calculation if we set  $q \to i\kappa$  (Ce<sup>iqx</sup>  $\to C e^{-\kappa x}$  then). Consequently,

$$
|r|^2 = \left|\frac{B}{A}\right|^2 = \left|\frac{k - i\kappa}{k + iq}\right|^2 = \frac{k^2 + \kappa^2}{k^2 + \kappa^2} = 1\tag{15-47}
$$

$$
|t|^2 = \left|\frac{C}{A}\right|^2 = \left|\frac{2k}{k + i\kappa}\right|^2 = \frac{4k^2 + \kappa^2}{k^2 + \kappa^2} \neq 0\tag{15-48}
$$

(15-49)

A part of the wave penetrates the barrier, which is why the 'transmission' amplitude does not vanish. Note, however, that there is no associated particle current: Since  $Ce^{-kx}$  does not have a spatially varying phase, the particle current

$$
j = \frac{\hbar}{2im} \left( \psi^* \frac{\partial \psi}{\partial x} - \text{ c.c.} \right) \tag{15-50}
$$

vanishes for  $x > 0$ ,

$$
j_{<} = \frac{\hbar k}{m}(|A|^2 - |B|^2) = 0\tag{15-51}
$$

$$
j_{>}=0\tag{15-52}
$$

The net current is zer0 in steady-state because all particles are reflected.

Note. The reflected wave has an energy-dependent phase shift

$$
r = \frac{B}{A} = \frac{k - i\kappa}{k + i\kappa} \tag{15-53}
$$

$$
=\frac{(k-i\kappa)^2}{k^2+\kappa^2} \tag{15-54}
$$

$$
=\frac{k^2 - \kappa^2 - 2ik\kappa}{k^2 + \kappa^2} \tag{15-55}
$$

$$
=e^{i\phi} \tag{15-56}
$$

with tan  $\phi = -\frac{2k\kappa}{k^2 - \kappa^2}$ 

The phase shift of the wave is important in 3D scattering problems.

### Can we localize the particle in the forbidden region?



Figure X: The wavefunction for  $E < V_0$  protrudes into the forbidden region  $x > 0$ . Can the particle be observed there?

To be sure that we have measured the particle inside the barrier, and not outside, we must measure its position at least with accuracy  $\Delta x \approx \kappa^{-1}$ . Then according to Heisenberg uncertainty, a momentum kick exceeding  $\Delta p \geq \frac{\hbar}{\Delta x} \sim \hbar \kappa$  will be transferred onto the particle.

### How much energy do we transfer?

$$
\Delta E = E(p + \Delta p) - E(p) \tag{15-57}
$$

$$
=\frac{(p+\Delta p)^2}{2m} - \frac{p^2}{2m}
$$
\n(15-58)

$$
=\frac{p\Delta p}{m} + \frac{(\Delta p)^2}{2m} \tag{15-59}
$$

$$
p = \hbar k \tag{15-60}
$$

 $p\Delta p$  can be positive or negative,  $(\Delta p)^2$  is always positive. the transferred energy is on average

$$
\langle \Delta E \rangle = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2m(\Delta x)^2} = \frac{\hbar^2 \kappa^2}{2m} = V_0 - E \tag{15-61}
$$

According to Heisenberg uncertainty, the measurement that localizes the particle inside the barrier transfers enough energy to allow the particle to be legitimately there.

Rule. A positive KE  $E - V_1 > 0$  corresponds to a spatially oscillating wavefunction  $e^{\pm ikx}$  with rate constant k (oscillation period  $\lambda = \frac{2\pi}{k}$ ). A negative ("missing") KE  $E - V_1 < 0$  corresponds to a spatially decaying or growing wavefunction  $e^{\pm} \kappa x$  with decay rate constant  $\kappa$  (decay length  $\kappa^{-1}$ ).

The "missing" KE is associated with the size of the region  $(\kappa^{-1})$  that the particle occupies in the classically forbidden space.