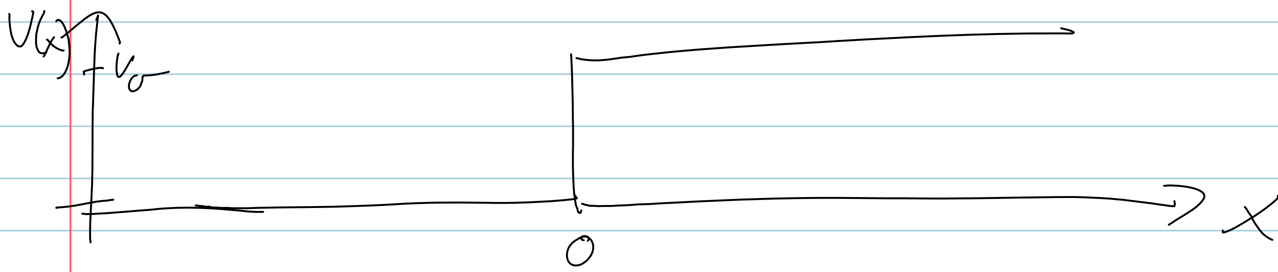
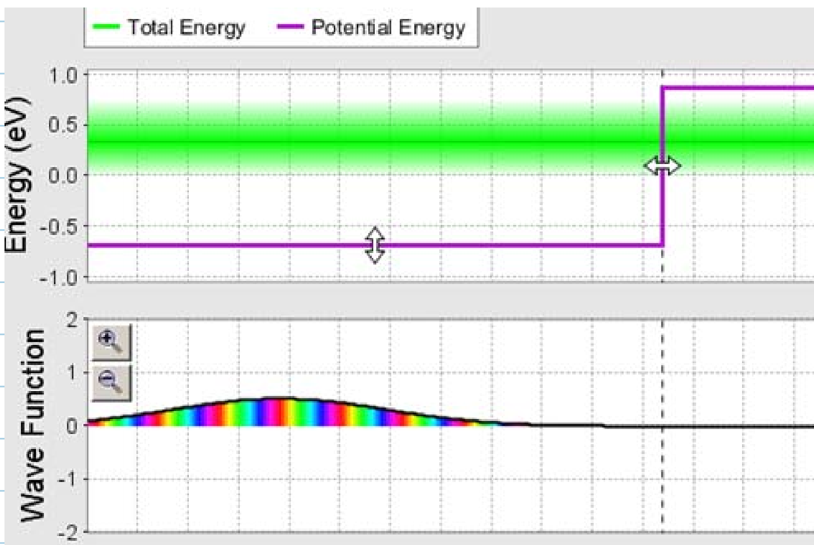
L29 Potential Step E<0

7.4 Potential Step



Simulation (see PhET website) shows:
wave packets (incoming from left)
- with low energy bounce
- with higher energy are partly reflected ...

7.4.1 E < V_0



a) Ansatz of solution of time independent Schrödinger Equation

$$\psi(x) = \begin{cases} A_+ e^{ikx} + A_- e^{-ikx} & x<0 \\ B_+ e^{\kappa x} + B_- e^{-\kappa x} & x>0 \end{cases}$$

$$k = \frac{\sqrt{2mE}}{\hbar} \qquad \kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

b) Physical constraints

$B_+ = 0$ (otherwise exponentially increasing wave function)

But note: total wave function cannot be normalized
(as for free particles momentum eigenstates)
==> interpretation as probability flux (probability current density)

c) Matching conditions

$$\psi(x), \quad \frac{\partial}{\partial x}\psi(x) \quad \text{continuous at } x = 0$$

$$\boxed{\begin{aligned} \psi(x): &\quad A_+ + A_- = B_- \qquad && (\mathrm{I}) \\ \frac{\partial}{\partial x}\psi(x): &\quad ikA_+ - ikA_- = -\kappa B_- \qquad && (\mathrm{II}) \end{aligned}}$$

NOTE:

as we see here, there are three amplitudes to be determined, and there are two linear constraints. This means, we get a family of non-trivial solutions for any value of energy E (remember that the variables k and κ are function of the energy!).

As a result, we can express two of the amplitudes as a function of the third one:

$$\underline{(ik)\mathrm{I} + \mathrm{II}:} \quad 2ikA_+ = (ik - \kappa)B_-$$

$$\Rightarrow \quad B_- = \frac{2ik}{ik - \kappa} A_+$$

$$\boxed{B_- = \frac{2k}{k + i\kappa} A_+}$$

$$\underline{ik\mathrm{I} - \mathrm{II}:} \quad 2ikA_- = (ik + \kappa)B_-$$

$$A_- = \frac{ik + \kappa}{2ik} B_-$$

$$= \frac{ik + \kappa}{ik - \kappa} A_+$$

$$\boxed{A_- = \frac{k - i\kappa}{k + i\kappa} A_+}$$

Note: $\frac{k - i\kappa}{k + i\kappa} = e^{i\varphi}$ for some angle φ

Proof: $\left|\frac{k-i\kappa}{k+i\kappa}\right| = \sqrt{\frac{k-i\kappa}{k+i\kappa}\,\frac{k+i\kappa}{k-i\kappa}} = 1$

This means that the incoming and returning amplitude have differ only by the phase, but have the same magnitude.

d) solution:

$$\psi_E(x) = \begin{cases} A_+\left(e^{ikx} + \frac{k-i\kappa}{k+i\kappa}\, e^{-ikx}\right) \\ A_+\, \frac{2k}{k+i\kappa}\, e^{-\kappa x} \end{cases}$$

Potential Step: 0<E< V_0

Eigenstates for energy eigenvalue range $0<E<V_0$

$$\Psi_E(x) = \begin{cases} A_+e^{ikx} + A_-e^{-ikx} & x \leq 0 \\ B_+e^{\kappa x} + B_-e^{-\kappa x} & x > 0 \end{cases}$$

$$\kappa = \frac{1}{\hbar}\sqrt{2m(V_0-E)}$$

$$k = \frac{1}{\hbar}\sqrt{2mE}$$

<u>Well behaved wave function:</u>
No exponential growth as $|x| \to \infty$: $B_+ = 0$

<u>Continuity of Ψ(x) and d/dx Ψ(x):</u>

$$\begin{aligned} \Psi: \quad & A_+ + A_- &= B_- \\ \frac{d}{dx}\Psi: \quad & ikA_+ - ikA_- &= -\kappa B_- \end{aligned}$$

This is a phase factor $e^{i\phi}$

Three complex Amplitudes, two complex linear constraints
➔ matching conditions can always be fulfilled by setting

$$B_- = \frac{2k}{k+i\kappa}A_+ \qquad A_- = \frac{k-i\kappa}{k+i\kappa}A_+$$

<u>Clicker Question:</u>
Are the eigenspaces here
A) degenerate
B) non-degenerate?

<u>Solution:</u>

$$\Psi_E(x) = A_+\begin{cases} e^{ikx} + \frac{k-i\kappa}{k+i\kappa}e^{-ikx} & x \leq 0 \\ \frac{2k}{k+i\kappa}e^{-\kappa x} & x > 0 \end{cases}$$

A_+: normalization:
$\int \Psi_{E'}^*(x)\, \Psi_E(x) = \delta(E-E')$

The normalization is important in order to get the time evolution of initial states right! We omit here the explicit calculation ...

Note that the normalization condition shown above is what we need for the expansion of the initial state into the eigenstate. This normalization condition can be satisfied for all remaining terms of the ansatz (including spatial oscillations as we go to minus infinity), but it would be incompatible with the exponential growth connected with the amplitude B+!

e) **interpretation**

1) Incoming wave gets reflected, but particles can penetrate the barrier ...

2)wave packet in simulation is a superposition of these solutions with a range of values of eigen-energies E!

3) for each value of E there is exactly one eigenfunction, so the eigenspaces are non-degenerate. (Compare this to the case of the free particle, where we had two linear independent eigenfunction for each value of E: momentum eigenstates with positive or negative momentum.)

Solving Strategies: potential step

$$\boxed{\frac{d}{d\,t}|\Psi(t)\rangle = -\frac{i}{\hbar}H|\Psi(t)\rangle}$$

Initial state: $|\Psi(0)\rangle$ mass: m

$$\kappa = \frac{1}{\hbar}\sqrt{2m(V_0 - E)} \qquad k = \frac{1}{\hbar}\sqrt{2mE}$$

1) Find Eigensystem of H:

$$\hat{H} = \frac{\hat{P}_x^2}{2m} + V(\hat{X})$$

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi_E(x) = E\,\Psi_E(x)}$$

Solution for $0<E<V_0$:

$$\Psi_E(x) = A_+\begin{cases} e^{ikx} + \frac{k-i\kappa}{k+i\kappa}e^{-ikx} & x \le 0 \\ \frac{2k}{k+i\kappa}e^{-\kappa x} & x > 0 \end{cases}$$

$0<E<V_0$ non-degenerate continuous set of eigenvalues

2) Decompose initial state into eigenstates of H

(Will eventually need also eigenstates E>V_0)

$$|\Psi(0)\rangle = \int dE\,\langle\Psi_E|\Psi(0)\rangle\,|\Psi_E\rangle$$

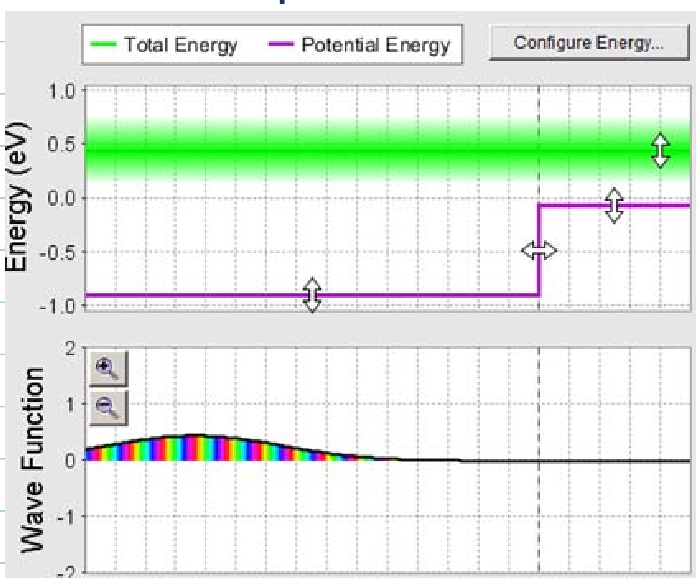
$$\boxed{\langle\Psi_E|\Psi(0)\rangle = \int dx\,\Psi_E^*(x)\,\Psi(x,0)}$$

3) Write down final solution

$$|\Psi(t)\rangle = \int dE\,\langle\Psi_E|\Psi(0)\rangle\,e^{-i\frac{Et}{\hbar}}|\Psi_E\rangle$$

$$\boxed{\Psi(x,t) = \int dE\,\langle\Psi_E|\Psi(0)\rangle\,e^{-i\frac{Et}{\hbar}}\,\Psi_E(x)}$$

7.4.2 Potential step for E> V



Once the energy in the particles (wave packets) is above the barrier, we observe that part are transmitted over the barrier, while some part is reflected. (A classical particle in the analogue situation would always pass the barrier!)

To understand this behaviour, we once more calculate the eigenstates of the system, now in the new range E> V!

Step 1: Mathematical Ansatz

Eigenstates for energy eigenvalue range E>V_0

$$\Psi_E(x) = \begin{cases} A_+ e^{ik_1 x} + A_- e^{-ik_1 x} & x \leq 0 \\ B_+ e^{ik_2 x} + B_- e^{-ik_2 x} & x > 0 \end{cases}$$

$$k_1 = \frac{1}{\hbar}\sqrt{2mE}$$

$$k_2 = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$$

Step 2: Physical constraints

There are no additional physical constraints to be imposed on the formal mathematical solutions of step 1.

Step 3: boundary conditions

The constraint of the wave function being continuous at the interface gives two constraints that are linear and homogeneous in the amplitudes A+, A-, B+, B-.

So we have:

4 amplitudes

2 constraints

==> 2 free parameters (amplitudes)

As a result, we can expect once again a continuous eigenspectrum. The most general solution will then be parameterized by two parameters.

We can choose A+ and B-, which happen to be the amplitudes of waves coming from the left (minus infinity), and from the right (plus infinity).

The most general solution can be written as a linear combination of two solutions:

Solution set 1: set B- = 0, so there are no incoming waves from the right.

Solution set 2: set A+ = 0, so no incoming wave from the right.

Each set contains solutions now parameterized by only one parameter, which will then be fixed the normalization condition. The solutions will differ (they are linearly independent), so the eigenspace to the continous eigenspectrum of E will be degenerate: for each value of E we have again two solutions (like for a free particle). The most general eigenstate is a linear combination of the two solutions from set 1 and set 2.

We can search for solution set 1 and set 2 independently

Step 4: Searching for restricted solution set (here set 1)

Continuity of Ψ(x) and d/dx Ψ(x):

$$\begin{aligned} \Psi: \quad & A_+ + A_- &=& \; B_+ \\ \frac{d}{dx}\Psi: \quad & ik_1 A_+ - ik_1 A_- &=& \; k_2 B_+ \end{aligned}$$

Choice: flux only from $-\infty$

➔ set B_ = 0

From here we find

Three complex amplitudes (A_-, A_+, B_+), two complex linear constraints

➔ matching conditions can always be fulfilled by setting

$$A_- = \frac{k_1 - k_2}{k_1 + k_2} A_+ \qquad B_+ = \frac{2k_1}{k_1 + k_2} A_+$$

arriving at the solution set 1:

Solution:

$$\Psi_E(x) = A_+ \begin{cases} e^{ik_1x} + \frac{k_1-k_2}{k_1+k_2} e^{-ik_1x} & x \leq 0 \\ \frac{2k_1}{k_1+k_2} e^{-ik_2x} & x > 0 \end{cases}$$

where the amplitude A+ will be determined again by the normalization condition

NOTE: there is a corresponding set of solutions (solution set 2) which are obtained by setting A+ = 0 after step 3!!