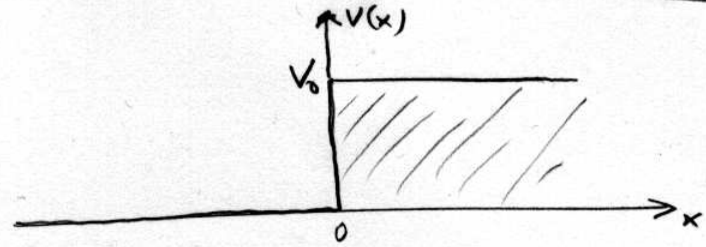
5.4 Scattering off a potential step



$$V(x) = V_0\, \theta(x)$$

- Time-independent Schrödinger equation ($\hat{H}|\psi\rangle = E|\psi\rangle$ in x-representation):

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \text{where} \quad k = \sqrt{2m(E-V)}/\hbar$$

- No physically acceptable solution for $E < 0$

($E \overset{\text{in an eigenstate}}{=} \langle \hat{H} \rangle = \langle \hat{T} + \hat{V} \rangle \geq \langle \hat{V} \rangle \geq V_{min}$ where V_{min} is the minimum of the potential)

Ⓐ $\underset{\sim\sim}{E < V_0}$: (energy of the particle less than the barrier height)

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

(Ae^{ikx} is incoming wave moving from the left to the right)

with $\hbar k = \sqrt{2mE}$, $\hbar\kappa = \sqrt{2m(V_0 - E)}$ real (no term $\sim De^{+\kappa x}$ for $x > 0$ since this would render $\psi(x)$ unnormalizable).

Boundary conditions at $x = 0$:

$$\left.\begin{aligned} &\psi(x) \text{ continuous} \Rightarrow A + B = C \\ &\frac{d\psi}{dx} \text{ continuous} \Rightarrow ik(A - B) = -\kappa C \end{aligned}\right\} \; A + B = \frac{k}{i\kappa}(A - B)$$

$$\boxed{\begin{aligned} \Rightarrow \frac{B}{A} &= \frac{ik+\kappa}{ik-\kappa} = e^{i\alpha} \quad (\alpha\text{-real}) \\ \frac{C}{A} &= \frac{2ik}{ik-\kappa} = 1 + e^{i\alpha} \end{aligned}} \qquad (*)$$

We call $R \equiv \left|\frac{B}{A}\right|^2$ the reflection coefficient. For $E < V_0$ there is no outgoing plane wave at $x > 0$, so transmission to $x \to +\infty$ is zero. This means that the reflection coefficient should be $100\% = 1$. Indeed,

$$R = \left|\frac{ik+\kappa}{ik-\kappa}\right|^2 = 1 \quad \checkmark$$

The matching conditions give us B/A and C/A, but not A itself – A must be obtained from the normalisation of the wavefunction $\psi(x)$. Let's plug in $(*)$ into $\psi(x)$:

$$\psi(x) = \begin{cases} 2A\, e^{i\alpha/2} \cos\left(kx - \frac{\alpha}{2}\right) & x < 0 \\ 2A\, e^{i\alpha/2} \cos\left(\frac{\alpha}{2}\right) e^{-\kappa x} & x > 0 \end{cases}$$

By writing $A = A' e^{-i\alpha/2}$ we can make $\psi(x)$ real if we choose A' real.

- The boundary conditions give us no restriction for E

$\Rightarrow$ <u>the energy eigenvalue spectrum is continuous</u>

- On the right of the step at $x=0$, the wave function is not zero: it penetrates into the classically forbidden region $\left(|\psi(x>0)|^2 \neq 0\right)$, but the probability to find the particle in that region <u>decays exponentially</u> $\sim e^{-2\kappa x}$ with the penetration depth. The probability current density along the x-direction,

$$j = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right) = 0,$$

vanishes, so there is no net particle flow, neither left nor right.

(This is always true as long as $\psi(x)$ is real modulo a constant (x-independent) phase factor.)

The phenomenon of $|\psi(x)|^2 \neq 0$ for $x > 0$ where $E < V$ is known as barrier penetration or tunneling. It is a pure quantum effect.

(B) $E > V_0$: (scattering above the barrier)

Now

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x<0) \quad \hbar k = \sqrt{2mE} \\ Ce^{ik'x} + De^{-ik'x}. & (x<0) \quad \hbar k' = \sqrt{2m(E-V_0)} \text{ real} < \hbar k \end{cases}$$

- Setting $D=0$ implements a boundary condition that we have no wave incident from the right: A wave falls in from the left ($\sim A$), part of it ($\sim B$) gets reflected, another part of it ($\sim C$) gets transmitted.

- Alternatively we can set $A=0$, in which case a wave falls in from the right. ($\sim D$), a part ($\sim C$) gets reflected, another part ($\sim B$) gets transmitted.

- Let's consider the first case ($D=0$) (you can do the case $A=0$ easily yourself — what will be similar, what will be different?). Continuity of ψ and ψ' at $x=0$:

$$\boxed{\left.\begin{aligned} A+B &= C \\ k(A-B) &= k'C \end{aligned}\right\} \Rightarrow \frac{B}{A} = \frac{k-k'}{k+k'}, \quad \frac{C}{A} = \frac{2k}{k+k'}} \quad (*)$$

Now the reflection coefficient is

$$R = \left|\frac{B}{A}\right|^2 = \left(\frac{k-k'}{k+k'}\right)^2 < 1$$

and we have a nonzero transmission coefficient

$$T = 1 - R = \frac{k'}{k}\left|\frac{C}{A}\right|^2 = \frac{4kk'}{(k+k')^2}$$

This definition makes sense when you look at the probability current:

$$j = \begin{cases} \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) = j_{inc} - j_{reflected} & (x<0) \\ \frac{\hbar k'}{m}|C|^2 = j_{transmitted} & (x>0) \end{cases}$$

So $\boxed{R = \left|\frac{j_{refl.}}{j_{inc}}\right| , \quad T = \left|\frac{j_{trans}}{j_{inc}}\right|^2}$

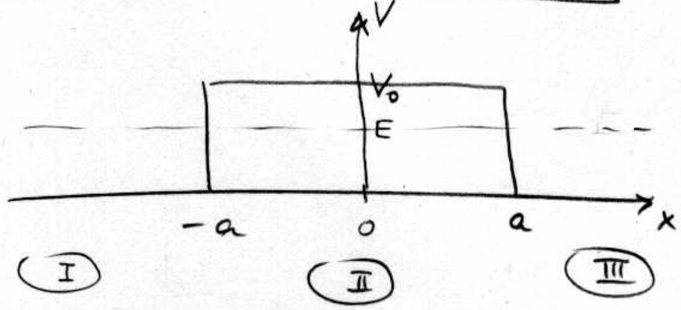
The equality $j_{trans} = j_{inc} - j_{refl}$ (or $R+T=1$) follows from the matching conditions (*).

Both R and T are functions of E through the ratio E/V_0:

$$\boxed{R = \left|\frac{1-\sqrt{1-\frac{V_0}{E}}}{1+\sqrt{1+\frac{V_0}{E}}}\right|^2 , \quad T = \frac{4\,\mathrm{Re}\left(\sqrt{1-V_0/E}\right)}{\left(1+\sqrt{1-V_0/E}\right)^2}}$$

Exercise: plot these as a function of $\varepsilon = \frac{V_0}{E}$!

5.5. The rectangular barrier



$(E < V_0)$

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x<-a) \\ Ce^{-\kappa x} + De^{\kappa x} & (-a<x<a) \\ Fe^{ikx} + Ge^{-ikx} & (x>a) \end{cases} \qquad \begin{aligned} \hbar k &= \sqrt{2mE} \\ \hbar\kappa &= \sqrt{2m(V_0-E)} \end{aligned}$$

- Boundary conditions at $x = -a$:

$$Ae^{-ika} + Be^{ika} = Ce^{\kappa a} + De^{-\kappa a} \qquad (\psi \text{ continuous})$$

$$Ae^{-ika} - Be^{ika} = \frac{i\kappa}{k}\left(Ce^{\kappa a} - De^{-\kappa a}\right) \qquad (\psi' \text{ continuous})$$

$\Rightarrow$ Write as

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \left(1+\frac{i\kappa}{k}\right)e^{\kappa a+ika} & \left(1-\frac{i\kappa}{k}\right)e^{-\kappa a+ika} \\ \left(1-\frac{i\kappa}{k}\right)e^{\kappa a-ika} & \left(1+\frac{i\kappa}{k}\right)e^{-\kappa a-ika} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

- Boundary conditions at $x = +a$ go similarly:

$$\begin{pmatrix} C \\ D \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \left(1-\frac{ik}{\kappa}\right)e^{\kappa a+ika} & \left(1+\frac{ik}{\kappa}\right)e^{\kappa a-ika} \\ \left(1+\frac{ik}{\kappa}\right)e^{-\kappa a+ika} & \left(1-\frac{ik}{\kappa}\right)e^{-\kappa a-ika} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

- Combining these gives after some algebra

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \left(\cosh(2\kappa a) + \frac{i\varepsilon}{2}\sinh(2\kappa a)\right)e^{2ika} & \frac{i\eta}{2}\sinh(2\kappa a) \\ -\frac{i\eta}{2}\sinh(2\kappa a) & \left(\cosh(2\kappa a) - \frac{i\varepsilon}{2}\sinh(2\kappa a)\right)e^{-2ika} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

where $\varepsilon \equiv \frac{\kappa}{k} - \frac{k}{\kappa}$, $\eta \equiv \frac{\kappa}{k} + \frac{k}{\kappa}$, $\eta^2 - \varepsilon^2 = 4$

$$= \frac{\kappa^2 + k^2}{k\kappa}$$

- If we postulate no wave incoming from the right, $G = 0$, then we find

$$\frac{F}{A} = \frac{e^{-2ika}}{\cosh(2\kappa a) + \frac{i\varepsilon}{2}\sinh(2\kappa a)}$$

and

$$\boxed{T = \left|\frac{F}{A}\right|^2 = \frac{1}{\cosh^2(2\kappa a) + \frac{\varepsilon^2}{4}\sinh^2(2\kappa a)} = \frac{1}{1 + \sinh^2(2\kappa a)\left(1 + \frac{\varepsilon^2}{4}\right)} = \frac{1}{1 + \frac{\eta^2}{4}\sinh^2(2\kappa a)}}$$

You can check that $R = \left|\frac{B}{A}\right|^2 = 1 - T$.

So $T \neq 0$, i.e. a fraction of the wave "tunnels" through the barrier even though the energy $E < V_0$ is not large enough to get over the barrier. This tunnel effect is a purely quantum mechanical phenomenon; it describes α-radioactivity and fission of atomic nuclei with large Z, as well as the Josephson effect.

- Limiting cases:

(i) high and wide barrier, $\kappa a \gg 1$:

In this case $\sinh^2(2\kappa a) \approx e^{4\kappa a} \gg 1$ and

$$\boxed{T \approx 16\, e^{-4\kappa a}\left(\frac{k\kappa}{\kappa^2 + k^2}\right)^2}$$ exponentially small tunneling probability

(ii) high and narrow barrier, $V_0 \gg E$, $\kappa \gg k$, $\kappa a \ll 1$,

but $V_0 a$ or $\kappa^2 a$ finite.

In this case $\sinh^2(2\kappa a) \approx (2\kappa a)^2$ and

$$1 + \frac{\eta^2}{4}\sinh^2(2\kappa a) \approx 1 + \left(\frac{\kappa^2 + k^2}{2k\kappa}\right)^2 (2\kappa a)^2$$

$$= 1 + \frac{(2mV_0/\hbar^2)^2\, a^2}{2mE/\hbar^2} = 1 + \frac{2mV_0^2 a^2}{\hbar^2 E}$$

such that

$$T \approx \frac{E}{E + \frac{2m}{\hbar^2} V_0^2 a^2}$$

If we write $g = 2 \lim_{\substack{a \to 0 \\ V_0 \to \infty}} V_0 a$, we can write the

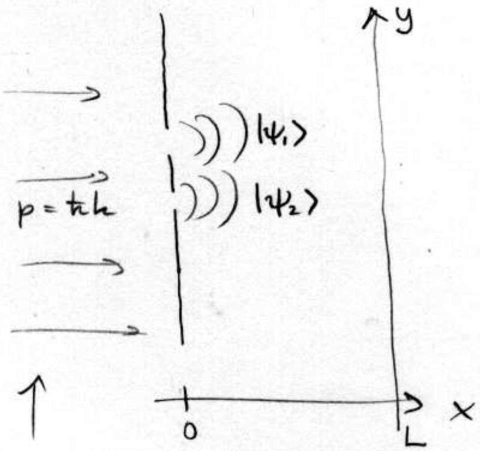
potential as

$$\boxed{\lim_{\substack{a \to 0 \\ V_0 \to \infty \\ g = \text{const}}} V(x) = g\,\delta(x)}$$

and the transmission through this potential barrier as

$$\boxed{T = \frac{E}{E + \frac{mg^2}{2\hbar^2}} \xrightarrow[E \to \infty]{} 1}$$

5.6. The double slit experiment



incoming plane wave $\psi(x) \sim e^{ikx}$

At $x = 0$, the plane wave gets blocked by the screen, except for the holes. Let's call the state corresponding to the wave generated behind the screen from ellectrons passing through the upper slit as $|\psi_1\rangle$, and similarly $|\psi_2\rangle$ for the state corresponding to electrons passing through the lower slit.

- If we don't measure the y-position of the electrons at $x = 0$, then to the right of the screen

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right)$$

and
$$P(x=L,y) = |\langle x=L,y|\psi\rangle|^2 = |\psi(x=L,y)|^2$$
$$= \frac{1}{2}\left|\psi_1(x=L,y) + \psi_2(x=L,y)\right|^2$$
$$= \frac{1}{2}\Big[|\psi_1(x=L,y)|^2 + |\psi_2(x=L,y)|^2 + \underbrace{2\,\mathrm{Re}\left(\psi_1^*(x=L,y)\psi_2(x=L,y)\right)}_{\text{interference term}}\Big]$$

We have only 1 quantum ensemble in state $|\psi\rangle$.

- If we measure the y-position of the electrons @ $x=0$, the wave function collapses to either $|\psi_1\rangle$ or $|\psi_2\rangle$, with 50% probability. It doesn't matter whether we actually check the result of the position measurement, as long as the position detector is turned on, the electrons leave the screen in either state $|\psi_1\rangle$ or state $|\psi_2\rangle$. We have no two equally populated quantum ensembles, one in state $|\psi_1\rangle$, the other with all electrons in state $|\psi_2\rangle$.

For ensemble 1, $P_1(x=L,y) = |\langle x=L,y|\psi_1\rangle|^2 = |\psi_1(x=L,y)|^2$

For ensemble 2, $P_2(x=L,y) = |\psi_2(x=L,y)|^2$

For an electron randomly chosen from these two ensembles,

$$\tilde{P}(x=L,y) = P_{1\,\mathrm{or}\,2}(x=L,y) = |\psi_1(x=L,y)|^2 + |\psi_2(x=L,y)|^2$$

$\longrightarrow$ no interference!

Knowing that the electron went through one of the holes and not the other, without shutting one of the holes, gives $\tilde{P}(x=L,y) = P_{1\,\mathrm{or}\,2}(x=L,y)$, i.e. kills the interference.

Not knowing which hole the electron went through leaves the electrons in state $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right)$, i.e. a linear superposition of probability amplitudes which leads to interference.