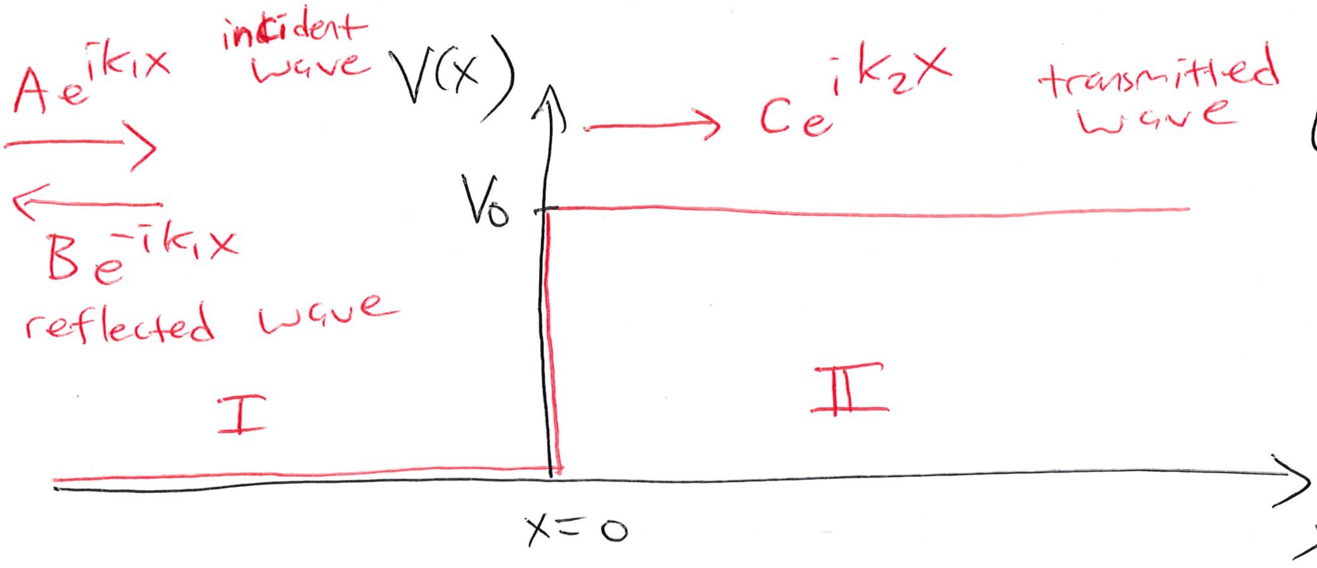
1D Scattering

Scattering involves shooting a wavepacket at a target, and observing the outgoing particle(s).

As we have seen, a wave packet can be built from a linear superposition of plane waves, and the dynamics of a plane wave is much simpler. By choosing the appropriate boundary conditions, we can study scattering with plane waves.

As the simplest example, consider scattering from a potential step:



Region I: $E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$

Region II: $(E-V_0)\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$

$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$,

$\psi_{II}(x) = Ce^{ik_2x}$ solve Sch. eq. in regions I and II separately, provided

$$E = \frac{\hbar^2 k_1^2}{2m},$$

$$E = \frac{\hbar^2 k_2^2}{2m} + V_0.$$

(assuming $E > V_0$)

The coefficient A is determined by the incident probability current:

$$j_{in} = \frac{1}{2m}\left(\psi_{in}^* \frac{\hbar}{i}\frac{d\psi_{in}}{dx} - \psi_{in}\frac{\hbar}{i}\frac{d\psi_{in}^*}{dx}\right)$$

$$\psi_{in}(x) = A e^{ik_1 x}$$

$$j_{in} = \frac{\hbar k_1}{m}|A|^2.$$

How do we determine the coefficients B + C ?

i) The wavefunction must be continuous at $x=0$, otherwise the momentum would blow up:

$$\psi_I(0) = \psi_{II}(0)$$

ii) The first derivative of ψ must be continuous at $x=0$, otherwise the kinetic energy would blow up:

$$\psi_{I}'(0) = \psi_{II}'(0).$$

i) $A + B = C$

ii) $ik_1(A-B) = ik_2 C$

$$\Rightarrow \quad A - B = \frac{k_2}{k_1} C$$

$$2A = \left(1 + \frac{k_2}{k_1}\right) C$$

$$\Rightarrow \quad C = \frac{2k_1}{k_1+k_2} A$$

$$B = C - A = \frac{k_1 - k_2}{k_1 + k_2} A$$

Current conservation:

$$j_{in} = \frac{\hbar k_1}{m} |A|^2 \qquad \text{incident current}$$

$$j_{tr} = \frac{\hbar k_2}{m} |C|^2 \qquad \text{transmitted } \text{"}$$

$$j_{re} = -\frac{\hbar k_1}{m} |B|^2 \qquad \text{reflected } \text{"}$$

Let $R = \dfrac{|j_{re}|}{|j_{in}|}$ = reflection probability

and $T = \left| \dfrac{j_{tr}}{j_{in}} \right|$ = transmission probability

$$R = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

$$T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2} = \frac{4k_1 k_2}{(k_1+k_2)^2}$$

$$R + T = 1$$

Note that R is independent of the sign of the potential step; a step down is equally effective at reflecting the wavepacket as a step up. Note that a classical particle with $E > V_0$ would <u>not</u> be reflected by the step.

<u>Q: what if $E < V_0$?</u>

$$\psi_I(x) = A e^{ik_1 x} + B e^{-ik_1 x}$$

$$\psi_{II}(x) = C e^{-K_2 x},$$

$$K_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

(exponentially growing solution is not normalizable).

i) $A + B = C$

ii) $ik_1(A - B) = -K_2 C$

$$A - B = i\frac{K_2}{k_1} C$$

$$C = \frac{2k_1}{k_1 + iK_2} A$$

$$B = \frac{k_1 - iK_2}{k_1 + iK_2} A$$

Since ψ_{II} is real,

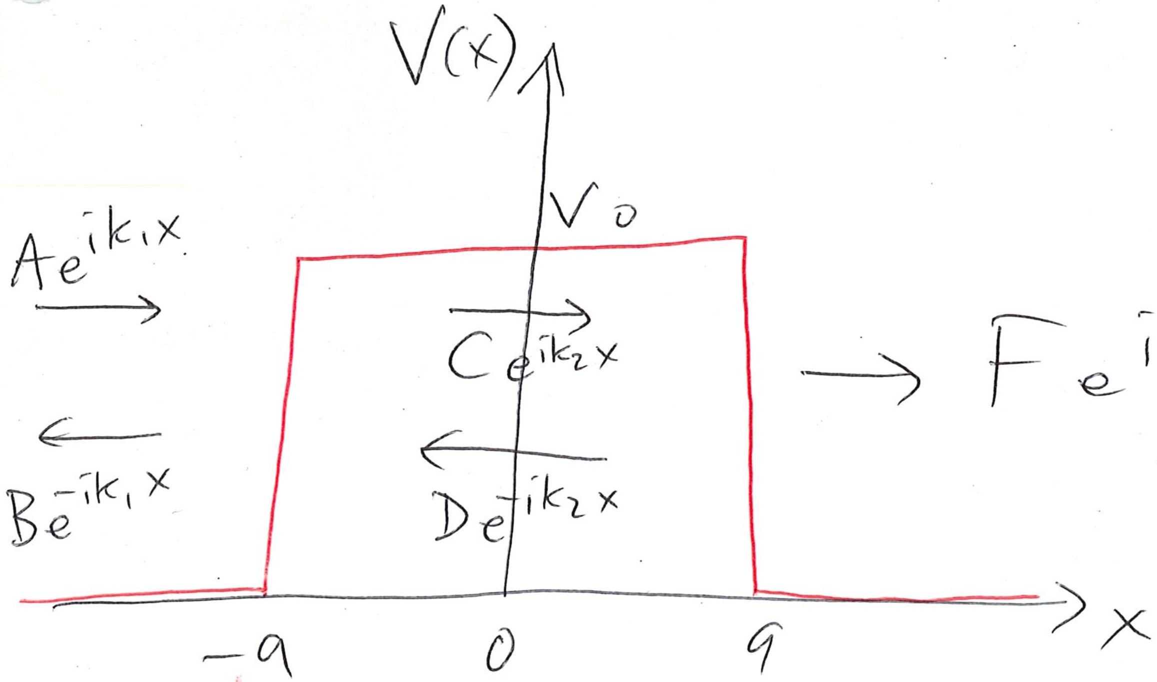
$$j_{tr} = 0$$

$$T = 0, \quad R = \left|\frac{B}{A}\right|^2 = \underline{1}$$

All particles are reflected, as in the classical case.

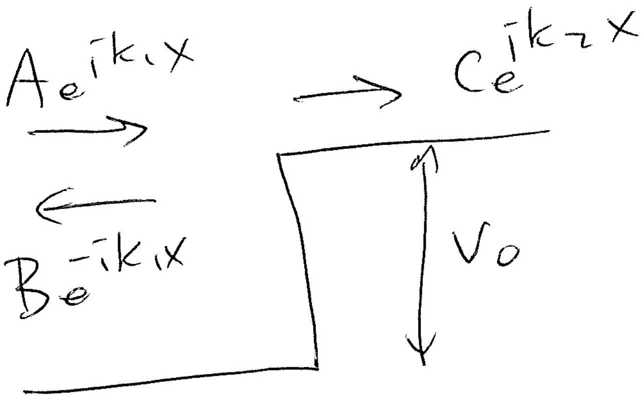
More on piecewise-constant potentials in 1D

i) Scattering from a rectangular barrier revisited ($E > V_0$)



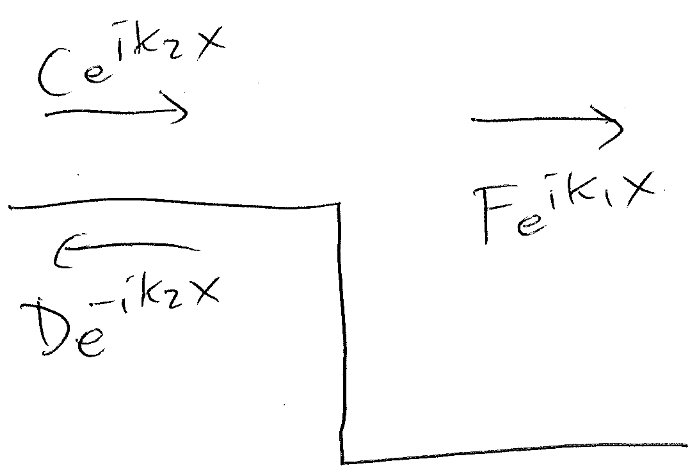
Solve using Huygen's principle in 1D

For a single step up, we would have



$$C = \frac{2k_1}{k_1+k_2} A$$

For a single step down, we would have



$$D = \frac{k_2-k_1}{k_1+k_2} C$$

$$F = \frac{2k_2}{k_1+k_2} C$$

Let $t_1 = \dfrac{2k_1}{k_1+k_2}$ $\quad r_1 = \dfrac{k_2-k_1}{k_1+k_2}$

$t_2 = \dfrac{2k_2}{k_1+k_2}$ $\quad r_2 = \dfrac{k_2-k_1}{k_1+k_2}$

$$\frac{F}{A} = t_1 e^{i2k_2a} t_2$$

$$+ t_1 e^{i2k_2a} r_2 e^{i2k_2a} r_1 e^{i2k_2a} t_2$$

$$+ t_1 e^{i2k_2a} r_2 e^{i2k_2a} r_1 e^{i2k_2a} r_2 e^{i2k_2a}$$

$$\times r_1 e^{i2k_2a} t_2 + \cdots$$

$$= t_1 t_2 e^{i2k_2a} \left(1 + r_1 r_2 e^{i4k_2a} + (r_1 r_2)^2 e^{i8k_2a} + \cdots \right)$$

$$= \frac{t_1 t_2 e^{i2k_2a}}{1 - r_1 r_2 e^{i4k_2a}}$$

Now $t_1 t_2 = \dfrac{4k_1k_2}{(k_1+k_2)^2} = T_1$

(trans. prob. for a single step).

and $\quad r_1 r_2 = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 = R_1$

(refl. prob. for a single step).

Note that $\quad T_1 + R_1 = 1$.

$$t_{12} = \frac{F}{A} = \frac{T_1 e^{i2k_2a}}{1 - R_1 e^{i4k_2a}}$$

$$T_{12} = |t_{12}|^2 = \frac{T_1^2}{(1 - R_1 e^{i4k_2a})(1 - R_1 e^{-i4k_2a})}$$

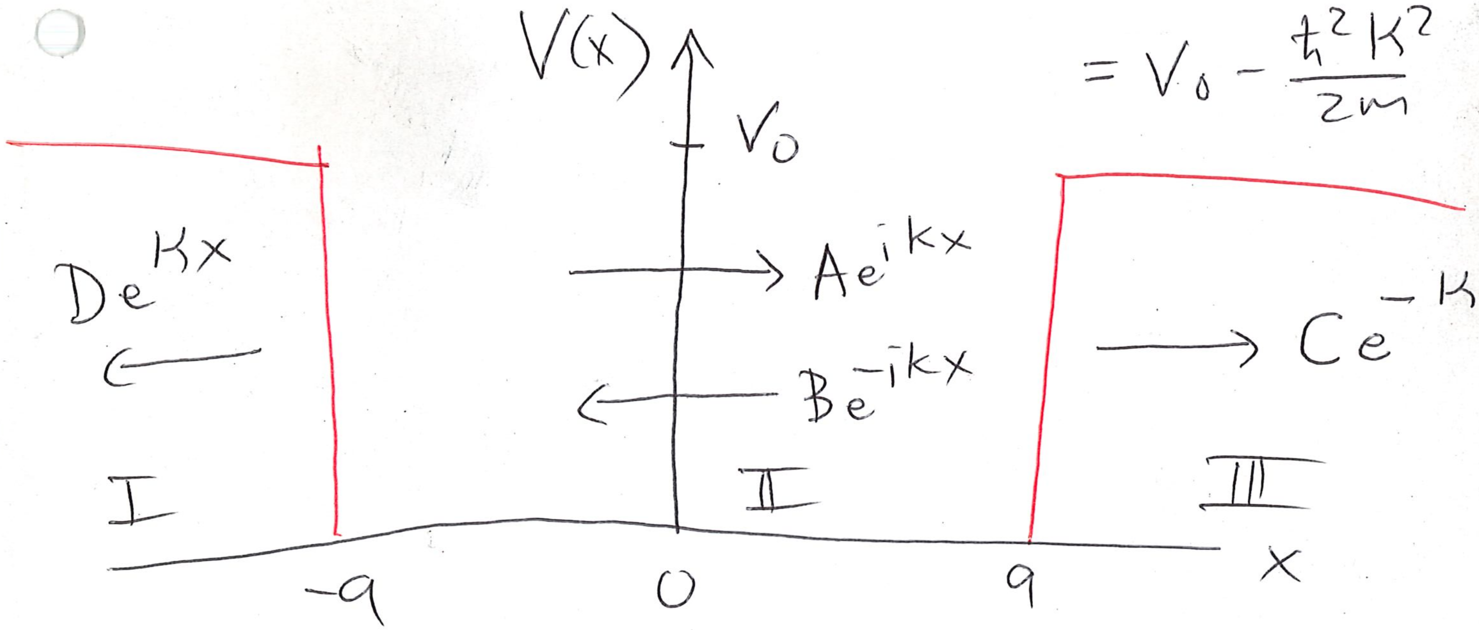
$$= \frac{T_1^2}{1 + R_1^2 - 2R_1 \cos 4k_2a}$$

$$= \frac{1}{1 + \frac{4R_1}{(1-R_1)^2} \sin^2(2k_2a)}$$

This is the same answer we got before by another method.

ii) Bound states in a rectangular potential well ($E < V_0$)

$$E = \frac{\hbar^2 k^2}{2m} = V_0 - \frac{\hbar^2 K^2}{2m}$$



Standard method:

$\psi_I(-a) = \psi_{II}(-a)$

$\psi_I'(-a) = \psi_{II}'(-a)$

$\psi_{II}(a) = \psi_{III}(a)$

$\psi_{II}'(a) = \psi_{III}'(a)$

One of the coefficients A, B, C, D can be fixed by normalization. The remaining four variables (including E) can be determined by solving this system of four equations. (See Goswami, 4.2)

<u>Another (easier) way:</u>

$$r = \frac{B}{A} = \frac{k - iK}{k + iK} \equiv e^{i\theta}$$

A bound state, or standing wave, is a stationary solution:

$$e^{ik2a}\, r\, e^{ik2a}\, r = 1$$

$$r^2 e^{i4ka} = 1$$

$$r e^{i2ka} = \pm 1 \qquad \text{let } L = 2a$$

$$e^{i(kL+\theta)} = \pm 1$$

$$e^{i(kL+\theta)} = e^{i\pi n} = \begin{cases} +1, & n \text{ even} \\ -1, & n \text{ odd} \end{cases}$$

$$\boxed{\begin{gathered} kL + \theta(k) = n\pi, \\ \theta = -2\tan^{-1}\left(\frac{K}{k}\right) \end{gathered}}$$

$\Rightarrow$ determines allowed values of k_n and hence E_n.

<u>Special case</u>: $V_0 \gg E \Rightarrow K \gg k$

$\tan^{-1}(\infty) = \frac{\pi}{2}$ $\qquad k_n L - \pi = n\pi$

$$k_n = \frac{(n+1)\pi}{L}, \quad n = 0, 1, 2, \ldots$$

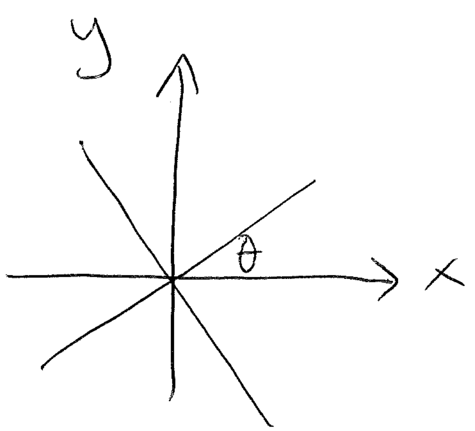
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}(n+1)^2$$

$\Rightarrow$ particle in a box.

One can also write

$$\tan^{-1}\left(\frac{K}{k}\right) = k_n a - \frac{n\pi}{2}$$

$$\frac{K}{k} = \tan\left(k_n a - \frac{n\pi}{2}\right)$$



$$\frac{K}{k} = \tan ka, \quad n \text{ even}$$

or

$$\frac{K}{k} = -\cot ka, \quad n \text{ odd}$$

$$Lk - 2\tan^{-1}\left(\frac{K}{k}\right) = n\pi$$

If $L \to 0$ or $V_0 \to 0$, then only one solution exists: $n=0$.

$\boxed{\text{An attractive potential always forms at least one bound state in 1D.}}$

$\theta \to 0$ as $E \to V_0$, so the total # of bound states is, in general, determined by

$$V_0 > E_n = \frac{\hbar^2 k_n^2}{2m} \simeq \frac{\hbar^2 \pi^2 n^2}{2m L^2}$$

$$n_{max} \simeq \mathrm{Int}\sqrt{\frac{2mL^2 V_0}{\pi^2 \hbar^2}}$$