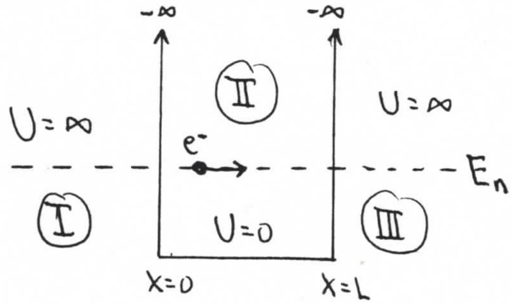
Physics 360 - Lecture Notes #1

I) Particle in a Box



Recall that in Region II

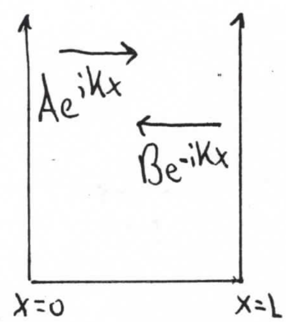
$$\frac{d^2\psi_{II}}{dx^2} = -K_{II}^2\psi_{II} \quad , \quad K_{II} = \sqrt{\frac{2mE}{\hbar^2}}$$

the solutions are: $\psi_{II}(x) = A\sin K_{II}x + B\cos K_{II}x$

This solution can be expressed somewhat differently by recalling Euler's identities:

$$e^{i\theta} = \cos\theta + i\sin\theta$$
$$e^{-i\theta} = \cos\theta - i\sin\theta$$

Then, $\psi_{II}(x) = A'e^{iK_{II}x} + B'e^{-iK_{II}x}$



where $A'e^{iKx}$ = wave traveling in positive x-direction

$B'e^{-iKx}$ = wave traveling in negative x-direction

Applying the continuity conditions at $x=0$ gives:

$$\psi_{I}(x=0) = \psi_{II}(x=0)$$
$$0 = A'e^0 + B'e^0 = A'+B' \Rightarrow A' = -B'$$

Continuity at $x=L$ gives: $\psi_{II}(x=L) = \psi_{III}(x=L)$

$$A'e^{iK_{II}L} + B'e^{-iK_{II}L} = 0$$
$$A'\left(e^{iK_{II}L} - e^{-iK_{II}L}\right) = 0 \quad (\text{since } A' = -B')$$

$2iA'\sin(K_{II}L) = 0$

This is valid only if $K_{II}L = n\pi \Rightarrow K_{IIn} = \frac{n\pi}{L}$

Thus the solutions are: $\psi_{II}(x) = 2iA'\sin(K_{IIn}L)$

and the allowed energies are $E_n = \frac{\hbar^2 K_{IIn}^2}{2m} = E_0 n^2$ as before

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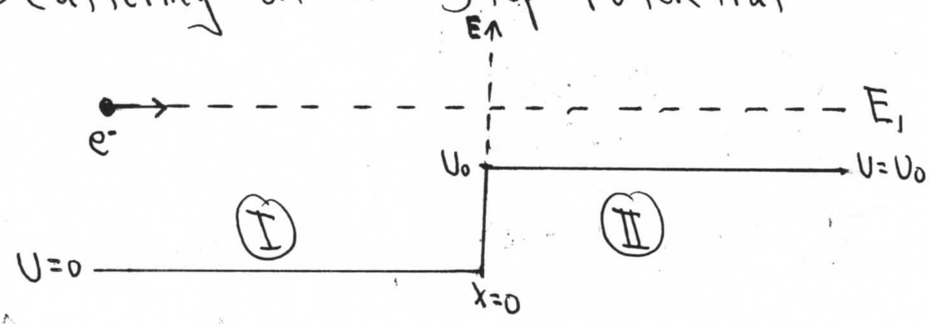
Let's use this complex arithmetic to solve other interesting problems. We will find that using complex exponentials makes solutions easier to find and understand.

(II) Scattering at a Step Potential



In this problem, the energy of the incident e^- is greater than the step height: $E_1 > U_0$

A classical particle should just slow down upon passing over the step. But in quantum mechanics, a reflection occurs. The e^- experiences a force $F = -dU/dx$ at the step because the potential abruptly changes at $x=0$. Since the e^- is modeled as a wave, this wave will experience a disturbance there and be partially reflected. Some of the waves will make it pass the step and thus be transmitted.

Let's write down and solve the Schrodinger equation in regions (I) and (II).

In Region I:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} + \underbrace{U(x)}_{0}\psi_I = E\psi_I \Rightarrow \frac{d^2\psi_I}{dx^2} = \frac{-2mE}{\hbar^2}\psi_I = -K_I^2\psi_I$$

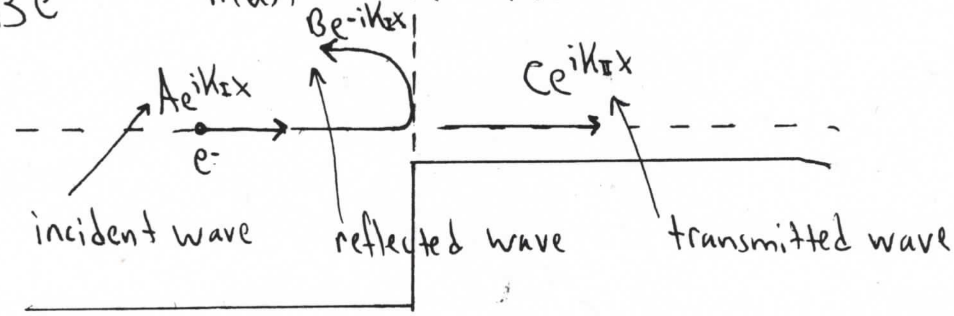
The solutions are the same as those for an infinite square well:

$$\psi_I(x) = Ae^{iK_Ix} + Be^{-iK_Ix} \quad , \quad K_I = \sqrt{\frac{2mE}{\hbar^2}}$$

Now it makes sense what ψ_I is composed of:

Ae^{iK_Ix} must be an incident wave

Be^{-iK_Ix} must be a reflected wave



In Region II:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + U(x)\psi_{II} = E\psi_{II} \quad , \text{ where } U(x) = U_0$$

$$\frac{d^2\psi_{II}}{dx^2} = -\frac{2m}{\hbar^2}(E-U_0)\psi_{II} = K_{II}^2\psi_{II} \quad , \quad K_{II} = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$$

Solutions are the same as those for an infinite square well:

$$\psi_{II}(x) = \underbrace{Ce^{iK_{II}x}}_{\text{wave traveling to the right}} + \underbrace{De^{-iK_{II}x}}_{\text{wave traveling to the left}} \quad , \quad K_{II} = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$$

The term $Ce^{iK_{II}x}$ must be the transmitted wave

The term $De^{-iK_{II}x}$ must be a reflected wave, but since there is nothing to reflect from in the region $x > 0$, the coefficient $D = 0$ (since there is no reflected wave).

The solution in Region II is then

$$\psi_{II}(x) = Ce^{iK_{II}x}$$

The arbitrary constants A, B, and C must be chosen such that $\psi(x)$ and $\frac{d\psi}{dx}$ are continuous at $x = 0$.

Continuity at $x=0$: $\psi_I(x=0) = \psi_{II}(x=0)$.

$$A + B = C$$

$$\left.\frac{d\psi_I}{dx}\right]_{x=0} = \left.\frac{d\psi_{II}}{dx}\right]_{x=0}$$

$$iK_I A - iK_I B = iK_{II} C$$

$$K_I(A-B) = K_{II} C$$

but $C = A+B$, thus

$$K_I(A-B) = K_{II}(A+B)$$

$$(K_I - K_{II})A = (K_I + K_{II})B$$

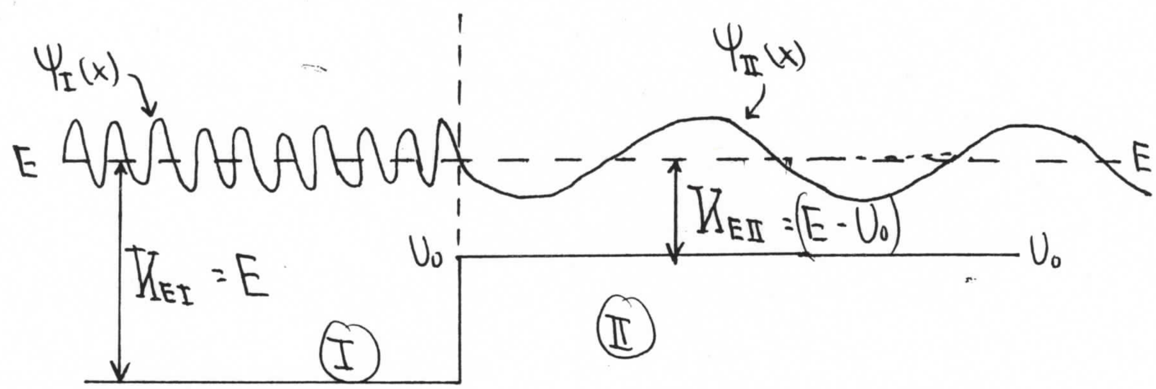
The reflected amplitude $B = \left(\frac{K_I - K_{II}}{K_I + K_{II}}\right)A$

The transmitted amplitude $C = A+B = \left(\frac{2K_I}{K_I + K_{II}}\right)A$

The solution to Schrödinger's equation is then

$$\left\{\begin{array}{ll} \psi_I(x) = Ae^{ik_I x} + A\left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)e^{-ik_I x} & , x \le 0, \quad k_I = \sqrt{\frac{2mE}{\hbar^2}} \\ \psi_{II}(x) = A\left(\frac{2k_I}{k_I + k_{II}}\right)e^{ik_{II} x} & , x \ge 0, \quad k_{II} = \sqrt{\frac{2m(E-U_0)}{\hbar^2}} \end{array}\right\}$$

A sketch of the wavefunctions is below:



We can see that the wavelength in Region II is longer than that in Region I because the kinetic energy of the e^- in Region I is greater than that in Region II

$$K_{EI} > K_{EII} \Rightarrow \frac{P_I^2}{2m} > \frac{P_{II}^2}{2m} \Rightarrow P_I > P_{II} \Rightarrow \frac{h}{\lambda_I} > \frac{h}{\lambda_{II}} \Rightarrow \boxed{\lambda_{II} > \lambda_I}$$

This is basically a scattering problem, and recall from your electromagnetism course that scattered waves ~~are~~ are characterized by a reflection R and transmission T coefficient:

$$R = \frac{\text{reflected flux}}{\text{incident flux}} = \frac{v_I |B|^2}{v_I |A|^2} = \frac{|B|^2}{|A|^2} = \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)^2$$

v_I and v_{II} are the velocities of the e^- in Region I and II

$$\text{flux} \equiv \frac{\text{Probability}}{(\text{Area})(\text{Time})} = \text{Probability per unit area per unit time.}$$

$$T = \frac{\text{transmitted flux}}{\text{incident flux}} = \frac{v_{II}|C|^2}{v_I|A|^2}$$

but $v_I = \frac{p_I}{m} = \frac{\hbar k_I}{m}$, similarly, $v_{II} = \frac{\hbar k_{II}}{m}$

Then, $$T = \frac{k_{II}}{k_I}\frac{|C|^2}{|A|^2} = \frac{k_{II}}{k_I}\left(\frac{4k_I^2}{[k_I+k_{II}]^2}\right) = \frac{4k_Ik_{II}}{(k_I+k_{II})^2}$$