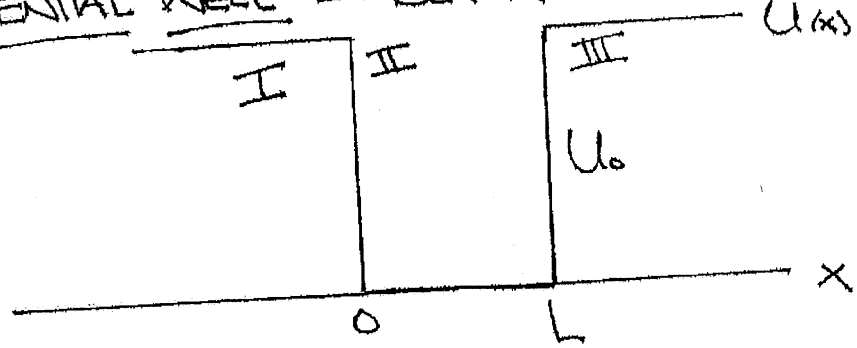
PHYS 262: POTENTIAL WELLS AND BARRIERS, CHAPTER 40

POTENTIAL WELL — BOX WHOSE WALLS ARE NOT INFINITELY STRONG



$$U(x) = \begin{cases} 0 & 0 \le x \le L \\ U_0 & \text{ELSE} \end{cases}$$

WE WANT TO LOOK AT THE BOUND STATE $\Rightarrow E < U_0$

BECAUSE THE WALLS ARE NOT INFINITELY STRONG, THERE IS A NON-ZERO PROBABILITY FOR THE PARTICLE TO BE OUTSIDE THE BOX.

SPLIT INTO 3 REGIONS: I = LEFT OF BOX, II = INSIDE BOX, III = RIGHT OF BOX

IN REGION II: $U = 0 \Rightarrow \Phi_{II} = Ae^{ikx} + Be^{-ikx}$ $\quad E = \frac{(\hbar k)^2}{2M} \Rightarrow k = \sqrt{\frac{2ME}{\hbar^2}}$

IN REGION I OR III: $U = U_0$. NEED TO SOLVE

$$\frac{-\hbar^2}{2M}\frac{d^2\Phi}{dx^2} + U_0\Phi = E\Phi \Rightarrow \frac{-\hbar^2}{2M}\frac{d^2\Phi}{dx^2} = (E - U_0)\Phi$$

$$\Rightarrow \frac{d^2\Phi}{dx^2} = \frac{-2M}{\hbar^2}(E - U_0)\Phi \Rightarrow \frac{d^2\Phi}{dx^2} = \frac{2M}{\hbar^2}(U_0 - E)\Phi$$

NOTICE THAT SINCE $E < U_0$, $U_0 - E > 0$

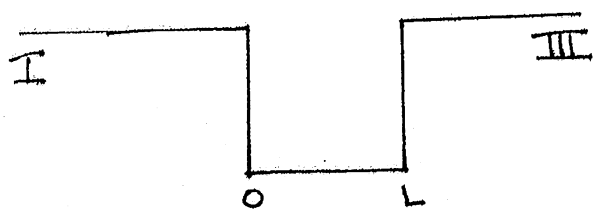
LET $k' = \sqrt{\frac{2M(U_0 - E)}{\hbar^2}} \Rightarrow \frac{d^2\Phi}{dx^2} = k'^2\Phi \Rightarrow \Phi = Ce^{k'x} + De^{-k'x}$

(REGULAR OLD EXPONENTIAL)

NEED DIFFERENT SOLUTIONS FOR REGIONS I AND III $\Rightarrow$

$$\Phi_{I} = Ce^{k'x} + De^{-k'x}$$

$$\Phi_{III} = Fe^{k'x} + Ge^{-k'x}$$



IN REGION I, $x \leq 0$, $\lim\limits_{x \to -\infty} e^{-k'x} = \infty$. THIS CANNOT HAPPEN! THE PROBABILITY TO BE IN REGION I DOES NOT BECOME EXPONENTIALLY LARGE

$\Rightarrow D = 0$

LIKEWISE, IN REGION III, $x \geq L$, $\lim\limits_{x \to \infty} e^{k'x} = \infty$ $\Rightarrow F = 0$

$$\Phi_{I} = Ce^{k'x}$$

$$\Phi_{II} = Ae^{ikx} + Be^{-ikx}$$

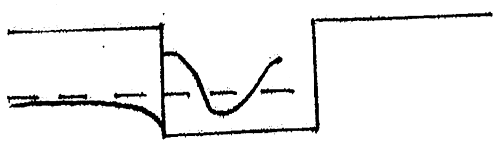
$$\Phi_{III} = Ge^{-k'x}$$

<u>OR</u>

$$\Phi = \begin{cases} Ce^{k'x} & x \leq 0 \\ Ae^{ikx} + Be^{-ikx} & 0 < x < L \\ Ge^{-k'x} & x \geq L \end{cases}$$

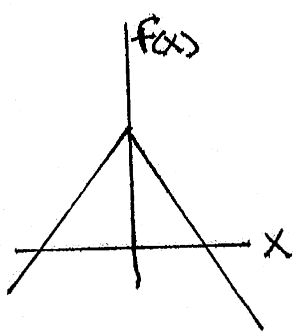
WE REQUIRE THE WAVEFUNCTION AND ITS DERIVATIVE TO BE CONTINUOUS AT THE $x = 0$ AND $x = L$ BOUNDARIES.

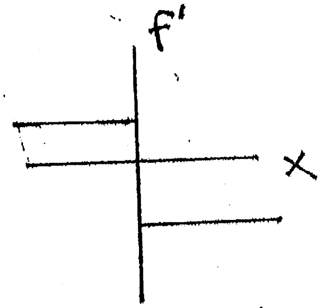
WAVE FUNCTIONS ARE CONTINUOUS SO THAT THERE ARE NO JUMPS IN PROBABILITY.



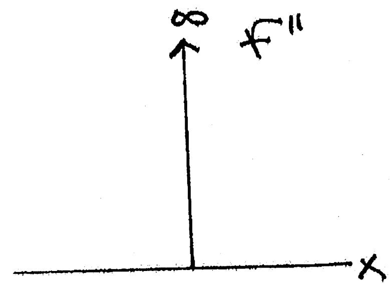
PROB$(X=0)$ IS DIFFERENT WHEN APPROACHING $\emptyset$ FROM LEFT OR RIGHT

THE DERIVATIVE MUST BE CONTINUOUS TO ENSURE THAT THE 2ND DERIVATIVE EXISTS (AS THE SCHRÖDINGER EQN. REQUIRES).





NON-CONTINUOUS DERIVATIVE



$$f'' = \begin{cases} \infty, & X=0 \\ 0, & \text{ELSE} \end{cases}$$

SO WE REQUIRE:

$$\Phi_{I}(0) = \Phi_{II}(0) \qquad \left.\frac{d\Phi_{I}}{dx}\right|_{X=0} = \left.\frac{d\Phi_{II}}{dx}\right|_{X=0}$$

$$\Phi_{II}(L) = \Phi_{III}(L) \qquad \left.\frac{d\Phi_{II}}{dx}\right|_{X=L} = \left.\frac{d\Phi_{III}}{dx}\right|_{X=L}$$

$$\frac{d\Phi_{I}}{dx} = K'Ce^{K'x}, \quad \frac{d\Phi_{II}}{dx} = iK\left(Ae^{iKx} - Be^{-iKx}\right), \quad \frac{d\Phi_{III}}{dx} = -K'Ge^{-K'x}$$

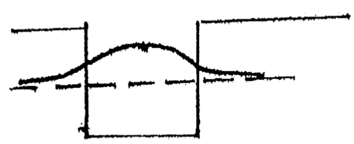
$$C = A + B \qquad K'C = iK(A - B)$$

$$Ae^{iKL} + Be^{-iKL} = Ge^{-K'L} \qquad iK(Ae^{iKL} - Be^{-iKL}) = -K'Ge^{-K'L}$$

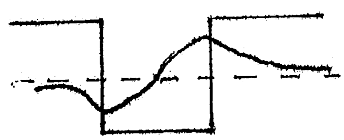
4 EQUATIONS WITH 4 UNKNOWNS. IT CAN BE DONE, BUT IT'S CHALLENGING.

YOU FIND THAT THERE ARE ALTERNATING EVEN AND ODD SOLUTIONS.

EVEN SOLUTION:



ODD SOLUTION:



EVEN SOLUTIONS OBEY THE TRANSCENDENTAL EQUATION: $\tan\left(\frac{KL}{2}\right) = \frac{K'}{K}$

ODD SOLUTIONS OBEY $-\cot\left(\frac{KL}{2}\right) = \frac{K'}{K}$

$K' = \sqrt{\frac{2M(U_0 - E)}{\hbar^2}}$, $K = \sqrt{\frac{2ME}{\hbar^2}}$ $\Rightarrow$ SOLVING THESE EQUATIONS GIVES THE ALLOWED ENERGIES.

$$\frac{K'}{K} = \left(\frac{\frac{2M(U_0 - E)}{\hbar^2}}{\frac{2ME}{\hbar^2}}\right)^{1/2} = \left(\frac{U_0 - E}{E}\right)^{1/2} = \sqrt{\frac{U_0}{E} - 1}$$

As $U_0 \to \infty$, $\frac{K'}{K} \to \infty$

$\Rightarrow$ for EVEN SOLUTIONS $\tan\left(\frac{KL}{2}\right) = \infty \Rightarrow \frac{KL}{2} = \frac{n\pi}{2}$ $(n = 1, 3, 5, \ldots)$

$\Rightarrow KL = n\pi \Rightarrow K = n\pi/L \Rightarrow \sqrt{\frac{2ME}{\hbar^2}} = \frac{n\pi}{L} \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2ML^2}$ = ODD PARTICLE IN A BOX ENERGY

↓

WEIRD!

for ODD SOLUTIONS $-\cot\left(\frac{KL}{2}\right) = -\infty \Rightarrow \frac{KL}{2} = n\pi$ $(n = 1, 3, 5, \ldots)$

$\Rightarrow K = \frac{(2n)\pi}{L} \Rightarrow E = \frac{(2n)^2\pi^2\hbar^2}{2ML^2}$ = EVEN PARTICLE IN A BOX ENERGY

<u>EXAMPLE</u> AN ELECTRON IS IN A BOX WITH SIDES $U_0 = 28.8\,eV$ AND $L = 5\times10^{-10}\,m$. FIND THE ALLOWED ENERGIES FOR THE BOUND STATES.

NEED to SOLVE $\tan\left(\frac{KL}{2}\right) = \frac{K'}{K}$ AND $-\cot\left(\frac{KL}{2}\right) = \frac{K'}{K}$

$$\frac{K'}{K} = \sqrt{\frac{U_0}{E} - 1} = \sqrt{\frac{28.8\,eV}{E} - 1}$$

$\frac{KL}{2} = \sqrt{\frac{2ME}{\hbar^2}}\,\frac{L}{2}$. To get $\frac{KL}{2}$ to BE DIMENSIONLESS (AS REQUIRED to TAKE ITS tan OR cot), K MUST HAVE UNITS 1/meter $\Rightarrow$ E IN Joules.

So LET'S BE TRICKY! $K = \sqrt{\frac{2ME}{\hbar^2}} = \left(\frac{2ME \times 1.6\times10^{-19}\,\frac{J}{eV}}{\hbar^2}\right)^{1/2}$

$$\frac{2M}{\hbar^2} \cdot \frac{1.6\times10^{-19}J}{eV} = \frac{2(9.11\times10^{-31}kg)}{(1.05\times10^{-34}J.s)^2} \cdot \frac{1.6\times10^{-19}J}{eV} = 2.64\times10^{19} \,{}^{1}/_{m^2 \cdot eV}$$

$$\text{UNIT: } \frac{Kg\,J}{J^2 s^2 eV} = \frac{Kg}{J s^2 eV} = \frac{Kg}{Kg\,m^2/s^2 \cdot s^2 eV} = \frac{1}{m^2 \cdot eV}$$

$$\Rightarrow K = \sqrt{\frac{2ME}{\hbar^2}} = \frac{5.138\times10^9}{m}\sqrt{E/eV} \Rightarrow \frac{KL}{2} = 1.285\sqrt{E}$$

$$\Rightarrow \tan(1.285\sqrt{E}) = \sqrt{\frac{28.8}{E} - 1}$$

SINCE E MUST BE LESS THAN 28.8eV ($E < U_0$) THERE ARE 3 SOLUTIONS TO THIS EQUATIONS

$$E_1 = 1.14eV, \quad E_3 = 10.1\,eV, \quad E_5 = 26.25eV$$

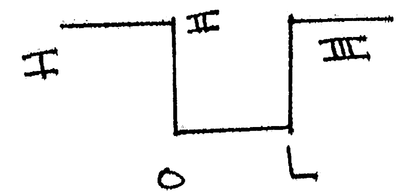
THE OTHER ENERGIES ARE FOUND FROM $-\cot(1.285\sqrt{E}) = \sqrt{\frac{28.8}{E} - 1}$

THERE ARE TWO SOLUTIONS:

$$E_2 = 4.5eV, \quad E_4 = 17.55eV$$

IT'S VERY CONFUSING BUT SINCE THE "EVEN" SOLUTIONS GIVE THE LOWEST ENERGY, THEY ARE LABELLED WITH AN ODD INDEX.

APPENDIX: DERIVATION OF TRANSCENDENTAL EQUATIONS



$$\Phi_{I} = Ce^{K'x}$$

$$\Phi_{II} = Ae^{iKx} + Be^{-iKx}$$

$$\Phi_{III} = Ge^{-K'x}$$

BOUNDARY CONDITIONS:

$$C = A + B \qquad\qquad Ae^{iKL} + Be^{-iKL} = Ge^{-K'L}$$

$$K'C = iK(A-B) \qquad\qquad iK(Ae^{iKL} - Be^{-iKL}) = -K'Ge^{-K'L}$$

$$\downarrow \qquad\qquad \downarrow$$

$$C = A+B \qquad\qquad Ae^{iKL} + Be^{-iKL} = Ge^{-K'L}$$

$$\frac{K'}{iK}C = A-B \qquad\qquad Ae^{iKL} - Be^{-iKL} = \frac{-K'}{iK}Ge^{-K'L}$$

$$\downarrow \qquad\qquad \downarrow$$

$$C\left(1+\frac{K'}{iK}\right) = 2A \qquad\qquad 2Ae^{iKL} = Ge^{-K'L}\left(1-\frac{K'}{iK}\right)$$

$$C\left(1-\frac{K'}{iK}\right) = 2B \qquad\qquad 2Be^{-iKL} = Ge^{-K'L}\left(1+\frac{K'}{iK}\right)$$

$$\downarrow \qquad\qquad \downarrow$$

$$\frac{1+\frac{K'}{iK}}{1-\frac{K'}{iK}} = \frac{A}{B} \qquad\qquad \frac{Ae^{iKL}}{Be^{-iKL}} = \frac{1-\frac{K'}{iK}}{1+\frac{K'}{iK}}$$

$$\downarrow \qquad\qquad \downarrow$$

$$\frac{iK+K'}{iK-K'} = \frac{A}{B} \qquad\qquad \frac{A}{B}e^{2iKL} = \frac{iK-K'}{iK+K'} \rightarrow \frac{A}{B} = \left(\frac{iK-K'}{iK+K'}\right)e^{-2iKL}$$

$$\Rightarrow \frac{iK+K'}{iK-K'} = \left(\frac{iK-K'}{iK+K'}\right)e^{-2iKL} \Rightarrow e^{2iKL}\left(\frac{iK+K'}{iK-K'}\right)^2 = 1$$

$$\Rightarrow \left(e^{iKL}\cdot\frac{iK+K'}{iK-K'}\right)^2 = 1 \Rightarrow e^{iKL}\cdot\frac{iK+K'}{iK-K'} = \pm 1 \rightarrow$$ TWO SOLUTIONS → EVEN AND ODD

$$e^{iKL}\cdot\frac{iK+K'}{iK-K'} = 1 \Rightarrow e^{iKL}(iK+K') = iK-K'$$

$$\Rightarrow iK(e^{iKL}-1) = -K'(e^{iKL}+1) \Rightarrow iK\cancel{e^{iKL/2}}(e^{iKL/2}-e^{-iKL/2}) = -K'\cancel{e^{iKL/2}}(e^{\frac{iKL}{2}}+e^{\frac{-iKL}{2}})$$

$$\Rightarrow iK\left(2i\sin\frac{KL}{2}\right) = -K'2\cos\frac{KL}{2} \Rightarrow -K\sin\frac{KL}{2} = -K'\cos\frac{KL}{2}$$

$$\Rightarrow \frac{\sin\frac{KL}{2}}{\cos\frac{KL}{2}} = \frac{K'}{K} \Rightarrow \tan\frac{KL}{2} = \frac{K'}{K}$$

$$e^{iKL}\cdot\frac{iK+K'}{iK-K'} = -1 \Rightarrow e^{iKL}(iK+K') = -(iK-K') = -iK+K'$$

$$\Rightarrow iK(e^{iKL}+1) = -K'(e^{iKL}-1)$$

$$\Rightarrow iKe^{iKL/2}(e^{iKL/2}+e^{-iKL/2}) = -K'e^{iKL/2}(e^{iKL/2}-e^{-iKL/2})$$

$$\Rightarrow iK\cos\frac{KL}{2} = -K'i\sin\frac{KL}{2} \Rightarrow \frac{\cos KL/2}{\sin KL/2} = \frac{-K'}{K}$$

$$\Rightarrow -\cot\frac{KL}{2} = \frac{K'}{K}$$