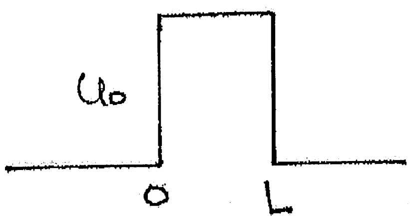
PHYS 262 - TUNNELING AND HARMONIC OSCILLATOR, CHAPTER 40

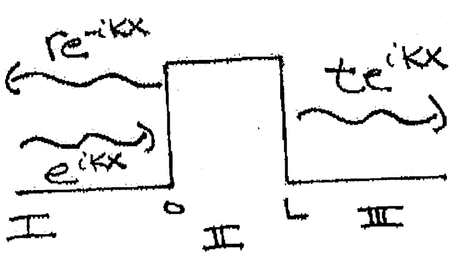
FOR A POTENTIAL BARRIER, WE HAVE THE POSSIBILITY OF A PARTICLE TO "TUNNEL" THROUGH IT.



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

WE ASSUME $E < U_0$. CLASSICALLY A PARTICLE STARTING ON THE LEFT SIDE OF THE BARRIER COULD NEVER REACH THE RIGHT HAND SIDE. BUT IN QUANTUM MECHANICS, INSIDE THE BARRIER, $\Phi = Ae^{K'x} + Be^{-K'x} \rightarrow$ NOT ZERO. TO MATCH BOUNDARY CONDITIONS, WE MUST HAVE A NON-ZERO Φ FOR $X \ge L$, SO THERE IS A PROBABILITY FOR THE PARTICLE TO GO THROUGH.

WE USE SLIGHTLY DIFFERENT NOTATION HERE:



e^{iKx} = INCIDENT WAVE

re^{-iKx} = REFLECTED WAVE

te^{iKx} = TRANSMITTED WAVE

$$\Phi_{I} = e^{iKx} + re^{-iKx} \qquad K = \sqrt{\frac{2ME}{\hbar^2}}$$

$$\Phi_{II} = Ae^{K'x} + Be^{-K'x} \qquad K' = \sqrt{\frac{2M(U_0 - E)}{\hbar^2}}$$

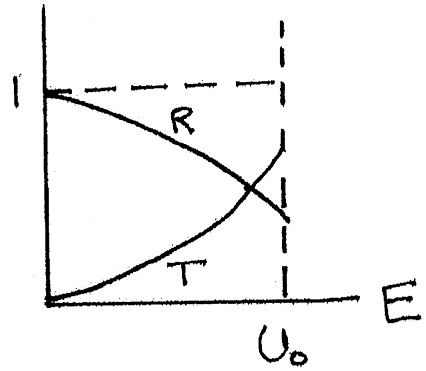
$$\Phi_{III} = te^{iKx}$$

THE PROBABILITY OF TRANSMISSION IS $T = |t|^2$

THE PROBABILITY OF REFLECTION IS $R = |r|^2$

BY MATCHING WAVEFUNCTIONS AND DERIVATIVES AT BOUNDARIES, WE FIND

$$\boxed{R = \frac{\sinh^2(k'L)}{\sinh^2(k'L) + \frac{4E(U_0-E)}{U_0^2}}} \qquad \boxed{T = \frac{\frac{4E(U_0-E)}{U_0^2}}{\sinh^2(k'L) + \frac{4E(U_0-E)}{U_0^2}}} \qquad \sinh(k'L) = \frac{e^{k'L} - e^{-k'L}}{2}$$



WHEN T IS SMALL, IT MUST BECAUSE $\sinh^2 k'L \gg 1 \Rightarrow k'L \gg 1$

$\Rightarrow \sinh(k'L) \approx \frac{1}{2} e^{k'L} \Rightarrow \sinh^2(k'L) \cong \frac{1}{4} e^{2k'L}$

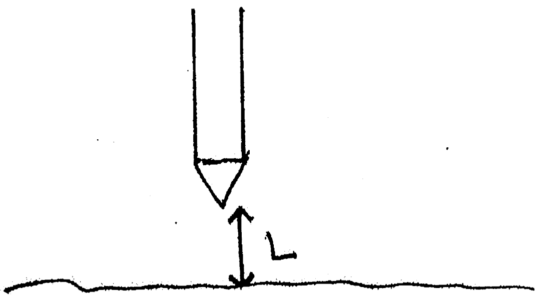
$$\Rightarrow T \cong \frac{\frac{4E(U_0-E)}{U_0^2}}{\frac{1}{4}e^{2k'L}} \Rightarrow \boxed{T = \frac{16E(U_0-E)}{U_0^2} e^{-2k'L}}$$

<u>EXAMPLE</u> WHAT IS PROBABILITY FOR AN ELECTRON TO TUNNEL THROUGH A $U_0 = 5\,\text{eV}$ BARRIER IF $E = 3\,\text{eV}$ AND $L = 1\times10^{-9}\,\text{m}$?

$U_0 - E = 2\,\text{eV} = 3.2\times10^{-19}\,\text{J}$ $\quad k' = \sqrt{\frac{2m(U_0-E)}{\hbar^2}} = \left(\frac{2\cdot 9.11\times10^{-31}\,\text{kg}\cdot 3.2\times10^{-19}\,\text{J}}{1.05\times10^{-34}\,\text{J·s}}\right)^{1/2} = 7.3\times10^{9}/\text{m}$

$$\Rightarrow T = \frac{16(3\,\text{eV})(2\,\text{eV})}{(5\,\text{eV})^2} e^{-2(7.3\times10^9)(1\times10^{-9})} = 1.8\times10^{-6}$$

AN EXAMPLE OF TUNNELING OCCURS IN THE SCANNING TUNNELING MICROSCOPE (STM). IT USES A PROBE TO APPLY A VERY LARGE U_0 ABOVE THE SURFACE OF A SAMPLE. ELECTRONS FROM THE SURFACE TUNNEL TO THE PROBE TO CREATE A CURRENT.

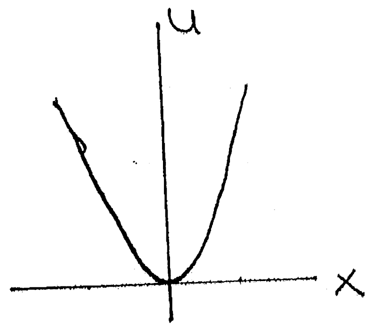


THE NUMBER OF TUNNELING ELECTRONS IS PROPORTIONAL TO T. SINCE T IS SO SENSITIVE TO THE VALUE OF L, YOU CAN USE THE CURRENT TO FIGURE OUT HOW CLOSE THE PROBE IS TO THE SURFACE. LETTING THE PROBE SCAN OVER THE SURFACE CREATES A 3D TOPOGRAPHIC MAP WITH ATOMIC RESOLUTION (p. 1532)

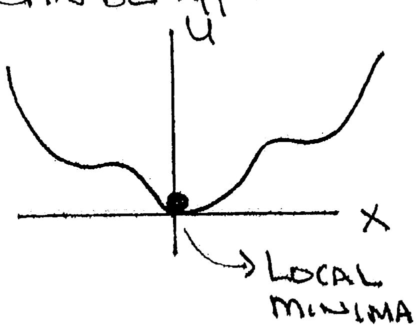
__HARMONIC OSCILLATOR__ – ONE OF THE MOST IMPORTANT QM PROBLEMS IS THE HARMONIC OSCILLATOR.

$F = -K_0 X$ (HOOKE'S LAW) K_0 = SPRING CONSTANT

$U = \frac{1}{2} K_0 X^2$



WE USE HARMONIC OSCILLATOR A __LOT__ BECAUSE ANY POTENTIAL ENERGY CAN BE APPROXIMATED AS ONE.



$$U(x) = U(0) + \frac{dU}{dx}\Big|_0 x + \frac{1}{2}\frac{d^2U}{dx^2}\Big|_0 x^2 + \ldots$$

AT MINIMA $\frac{dU}{dx} = 0 \Rightarrow U = \frac{1}{2}\frac{d^2U}{dx^2} X^2 = \frac{1}{2} K_0 X^2$

THE STATIONARY STATES ARE A LITTLE BIT HARDER to WRITE DOWN:

$$\Phi_n = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \exp\left(-\frac{M\omega x^2}{2\hbar}\right) H_n\left(\sqrt{\frac{M\omega}{\hbar}}x\right)$$

$H_n(y)$ = HERMITE POLYNOMIALS

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n}\left(e^{-y^2}\right)$$

THOUGH IT'S EASIER to USE THE RECURSIVE RELATIONSHIP to FIND THEM.

$$\boxed{\frac{dH_n}{dy} = 2y H_n - H_{n+1}}$$

$$H_0 = 1,\quad H_1 = 2y,\quad H_2 = 4y^2 - 2,\quad H_3 = 8y^3 - 12y, \ldots$$

$$\Rightarrow \Phi_0 \propto \exp\left(-\frac{M\omega x^2}{2\hbar}\right), \quad E_0 = \tfrac{1}{2}\hbar\omega$$

$$\Phi_1 \propto \exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(2\sqrt{\frac{M\omega}{\hbar}}x\right), \quad E_1 = \tfrac{3}{2}\hbar\omega$$

$$\Phi_2 \propto \exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(4\frac{M\omega}{\hbar}x^2 - 2\right), \quad E_2 = \tfrac{5}{2}\hbar\omega$$

$\vdots$ $\qquad\qquad\qquad\qquad$ $\vdots$

THE SCHRÖDINGER EQUATION FOR THE HARMONIC OSCILLATOR IS <u>NOT EASY</u> TO SOLVE! (IT REQUIRES A SERIES SOLUTION.)

$$-\frac{\hbar^2}{2M}\frac{d^2\Phi}{dx^2} + \frac{1}{2}K_0 x^2 \Phi = E\Phi$$

IT TURNS OUT THAT THE ALLOWED ENERGY VALUES ARE VERY SIMPLE: $\boxed{E_n = (n+\frac{1}{2})\hbar\omega}$ $n = 0, 1, 2, 3, \ldots$

$$\boxed{\omega = \sqrt{\frac{K_0}{M}}}$$

$E_0 = \frac{1}{2}\hbar\omega$ IS CALLED THE ZERO POINT ENERGY. A QM HARMONIC OSCILLATOR CAN NEVER BE AT REST BECAUSE THAT WOULD VIOLATE THE UNCERTAINTY PRINCIPLE.

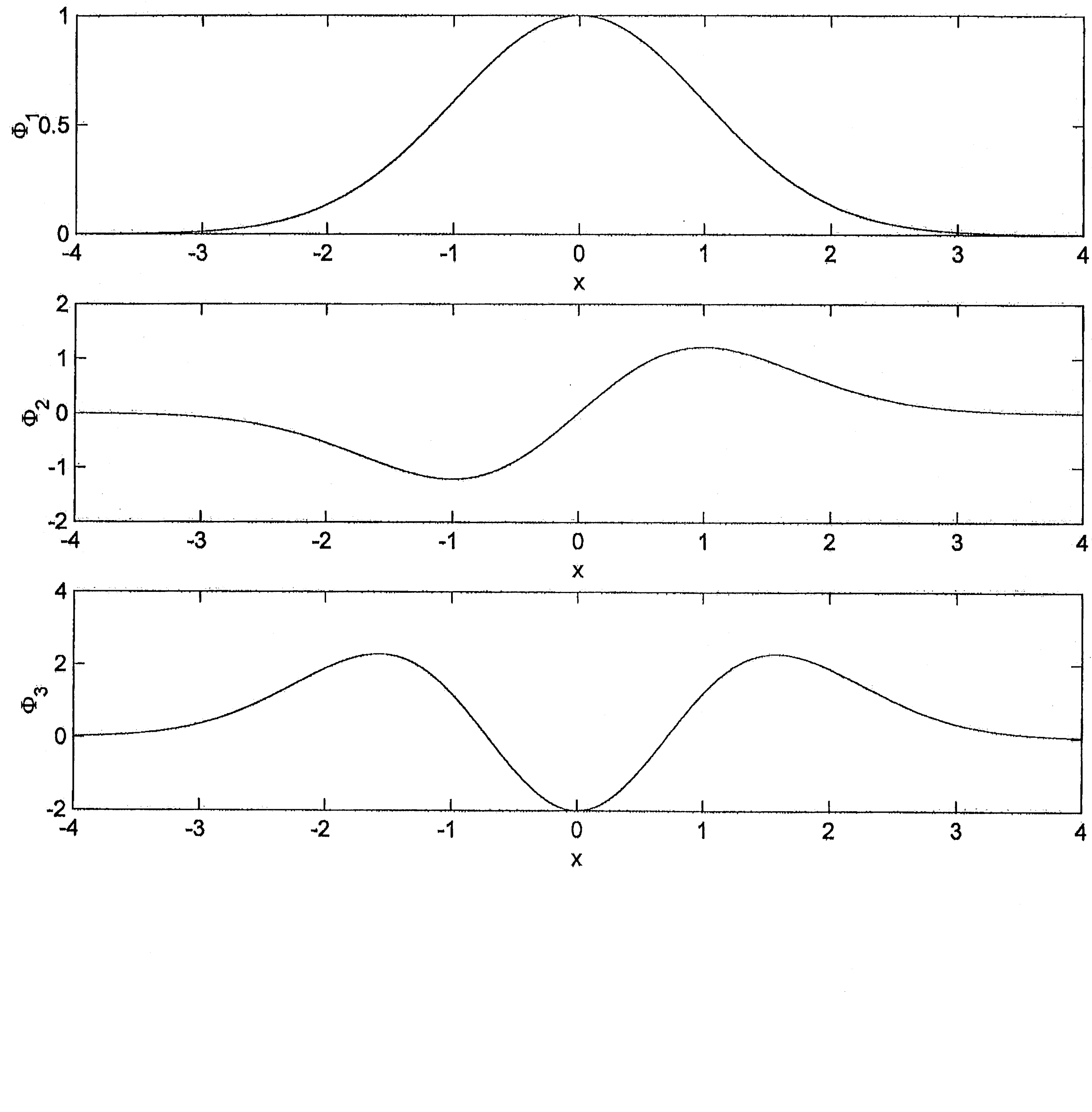
<u>EXAMPLE</u> - WHAT ARE THE ALLOWED ENERGIES OF AN ELECTRON CONNECTED TO A $K_0 = 1600\,N/m$ SPRING?

$$\frac{K_0}{M} = \frac{1600\,N/m}{9.11\times10^{-31}\,kg} = 1.76\times10^{33}/s^2 \Rightarrow \omega = 4.19\times10^{16}/s$$

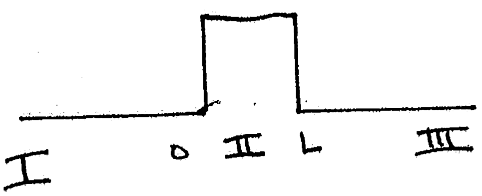
$$\left(\text{UNIT}: \frac{N}{kg\,m} = \frac{kg\,m/s^2}{kg\,m} = 1/s^2\right)$$

$$E_n = (n+\tfrac{1}{2})(6.583\times10^{-16}\,eV\cdot s)(4.19\times10^{16}/s) = (n+\tfrac{1}{2})\,27.6\,eV$$

$$E_0 = 13.8\,eV,\ E_1 = 41.4\,eV,\ E_2 = 69\,eV, \ldots$$


1
0.5
0
Φ_1
-4
-3
-2
-1
0
1
2
3
4
x
2
1
0
-1
-2
Φ_2
-4
-3
-2
-1
0
1
2
3
4
x
4
2
0
-2
Φ_3
-4
-3
-2
-1
0
1
2
3
4
x

Appendix - Derivation of R and T:



$$\Phi_I = e^{ikx} + r e^{-ikx} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Phi_{II} = A e^{k'x} + B e^{-k'x} \qquad k' = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

$$\Phi_{III} = t e^{ikx}$$

B.C.'s at $X=0$: $1 + r = A + B$

$$ik(1-r) = k'(A-B)$$

$X = L$: $A e^{k'L} + B e^{-k'L} = t e^{ikL}$ $\Rightarrow$ $A e^{k'L} + B e^{-k'L} = t e^{ikL}$

$k'(A e^{k'L} - B e^{-k'L}) = ik t e^{ikL}$ $\quad \frac{k'}{ik}(A e^{k'L} - B e^{-k'L}) = t e^{ikL}$

$$\Rightarrow A e^{k'L} + B e^{-k'L} = \frac{k'}{ik}\left(A e^{k'L} - B e^{-k'L}\right) \Rightarrow$$

$$A e^{k'L}\left(1 - \frac{k'}{ik}\right) = -B e^{-k'L}\left(1 + \frac{k'}{ik}\right) \Rightarrow A e^{k'L}\frac{(ik-k')}{ik} = -B e^{-k'L}\frac{(ik+k')}{ik}$$

$$\Rightarrow A = -B e^{-2kL}\frac{(ik+k')}{(ik-k')}$$

$$1 + r = A + B \Rightarrow 1 + r = -B e^{-2k'L}\frac{(ik+k')}{ik-k'} + B = B\left(1 - \frac{e^{-2k'L}(ik+k')}{ik-k'}\right)$$

$$= \frac{B}{ik-k'}\left(ik - k' - e^{-2k'L}(ik+k')\right) = \frac{B}{ik-k'}\left(ik(1 - e^{-2k'L}) - k'(1 + e^{-2k'L})\right)$$

$$= \frac{B}{ik-k'}\left(ik e^{-k'L}(e^{k'L} - e^{-k'L}) - k' e^{-k'L}(e^{k'L} + e^{-k'L})\right)$$

$$= \frac{B e^{-k'L}}{ik-k'}\left(ik\, 2\sinh k'L - k'\, 2\cosh k'L\right) = \frac{2B e^{-k'L}}{ik-k'}\left(ik \sinh k'L - k' \cosh k'L\right)$$

$$\sinh x = \frac{1}{2}(e^{x} - e^{-x}) \qquad \cosh x = \frac{1}{2}(e^{x} + e^{-x})$$

$$\Rightarrow 1+r = \frac{2Be^{-k'L}}{ik-k'}\left(ik\sinh(k'L) - k'\cosh(k'L)\right)$$

$$ik(1-r) = k'(A-B) \Rightarrow 1-r = \frac{k'}{ik}\left(-Be^{-2k'L}\frac{(ik+k')}{ik-k'} - B\right)$$

$$= \frac{-k'B}{ik}\left(e^{-2k'L}\frac{(ik+k')}{ik-k'} + 1\right) = \frac{-k'}{ik}\frac{B}{ik-k'}\left(e^{-2k'L}(ik+k') + (ik-k')\right)$$

$$= \frac{-k'}{ik}\frac{B}{ik-k'}\left(ik(1+e^{-2k'L}) - k'(1-e^{-2k'L})\right) = \frac{-k'}{ik}\frac{2Be^{-k'L}}{ik-k'}\left(ik\cosh(k'L) - k'\sinh(k'L)\right)$$

$$\Rightarrow 1-r = \frac{2Be^{-k'L}}{ik-k'}\left(-k'\cosh(k'L) + \frac{k'^2}{ik}\sinh(k'L)\right)$$

$$1+r = \frac{2Be^{-k'L}}{ik-k'}\left(ik\sinh(k'L) - k'\cosh(k'L)\right)$$

$$1-r = \frac{2Be^{-k'L}}{ik-k'}\left(-k'\cosh(k'L) + \frac{k'^2}{ik}\sinh(k'L)\right)$$

$$\Rightarrow \frac{1+r}{1-r} = \frac{ik\sinh(k'L) - k'\cosh(k'L)}{-k'\cosh(k'L) + \frac{k'^2}{ik}\sinh(k'L)}$$

Notice: If $\frac{1+r}{1-r} = \frac{a}{b} \Rightarrow (1+r)b = (1-r)a \Rightarrow r(a+b) = a-b$

$$\Rightarrow r = \frac{a-b}{a+b}$$

$$\Rightarrow r = \frac{ik\sinh(k'L) - \cancel{k'\cosh(k'L)} + \cancel{k'\cosh(k'L)} - \frac{k'^2}{ik}\sinh(k'L)}{ik\sinh(k'L) - k'\cosh(k'L) - k'\cosh(k'L) + \frac{k'^2}{ik}\sinh(k'L)}$$

$$\Rightarrow r = \frac{\left(ik - \frac{k'^2}{ik}\right)\sinh(k'L)}{\left(ik + \frac{k'^2}{ik}\right)\sinh(k'L) - 2k'\cosh(k'L)} = \frac{\frac{(ik)^2 - k'^2}{ik}\sinh(k'L)}{\frac{(ik)^2 + k'^2}{ik}\sinh(k'L) - 2k'\cosh(k'L)\cdot\frac{ik}{ik}}$$

$$\Rightarrow r = \frac{(-K^2-K'^2)\sinh(K'L)}{(-K^2+K'^2)\sinh(K'L) - 2iKK'\cosh(K'L)} = \frac{-(K^2+K'^2)\sinh(K'L)}{(-K^2+K'^2)\sinh(K'L) - 2iKK'\cosh(K'L)}$$

$$R = |r|^2 = rr^* = \frac{-(K^2+K'^2)\sinh(K'L)}{(-K^2+K'^2)\sinh(K'L) - 2iKK'\cosh(K'L)} \cdot \frac{-(K^2+K'^2)\sinh(K'L)}{(-K^2+K'^2)\sinh(K'L) + 2iKK'\cosh(K'L)}$$

$$= \frac{(K^2+K'^2)^2\sinh^2(K'L)}{(-K^2+K'^2)^2\sinh^2(K'L) + 4K^2K'^2\cosh^2(K'L)}$$

$$\cosh^2 x = \left(\frac{e^x+e^{-x}}{2}\right)^2 = \frac{e^{2x}+e^{-2x}+2}{4} \qquad \sinh^2 x = \left(\frac{e^x-e^{-x}}{2}\right)^2 = \frac{e^{2x}+e^{-2x}-2}{4}$$

$$\Rightarrow \cosh^2 x - \sinh^2 x = \frac{2}{4} + \frac{2}{4} = 1$$

$$\Rightarrow R = \frac{(K^2+K'^2)^2\sinh^2(K'L)}{(-K^2+K'^2)^2\sinh^2 + 4K^2K'^2(1+\sinh^2 K'L)} = \frac{(K^2+K'^2)^2\sinh^2(K'L)}{\left[(-K^2+K'^2)^2+4K^2K'^2\right]\sinh^2(K'L) + 4K^2K'^2}$$

$$(-K^2+K'^2)^2 + 4K^2K'^2 = K^4 - 2K^2K'^2 + K'^4 + 4K^2K'^2 = K^4 + 2K^2K'^2 + K'^4 = (K^2+K'^2)^2$$

$$\Rightarrow R = \frac{(K^2+K'^2)^2\sinh^2(K'L)}{(K^2+K'^2)^2\sinh^2(K'L) + 4K^2K'^2} = \frac{\sinh^2(K'L)}{\sinh^2(K'L) + \frac{4K^2K'^2}{(K^2+K'^2)^2}}$$

$$K^2 = \frac{2mE}{\hbar^2} \quad K'^2 = \frac{2m(U_0-E)}{\hbar^2} \Rightarrow K^2+K'^2 = \frac{2mU_0}{\hbar^2}$$

$$\Rightarrow R = \frac{\sinh^2(k'L)}{\sinh^2(k'L) + \frac{4\left(\frac{2m}{\hbar^2}\right)^2 E(U_0 - E)}{\left(\frac{2m}{\hbar^2}\right)^2 U_0^2}} \Rightarrow \boxed{R = \frac{\sinh^2(k'L)}{\sinh^2(k'L) + \frac{4E(U_0-E)}{U_0^2}}}$$

THE PARTICLE EITHER REFLECTS OR IS TRANSMITTED

R = PROBABILITY FOR REFLECTION

T = PROBABILITY OF TRANSMISSION

$$\Rightarrow R + T = 1 \Rightarrow T = 1 - R$$

$$\Rightarrow T = 1 - \frac{\sinh^2(k'L)}{\sinh^2(k'L) + \frac{4E(U_0-E)}{U_0^2}} = \frac{\sinh^2(k'L) + \frac{4E(U_0-E)}{U_0^2} - \sinh^2(k'L)}{\sinh^2(k'L) + \frac{4E(U_0-E)}{U_0^2}}$$

$$\Rightarrow \boxed{T = \frac{\frac{4E(U_0-E)}{U_0^2}}{\sinh^2(k'L) + \frac{4E(U_0-E)}{U_0^2}}}$$

PROBLEM : 40.51 p.1545

Show that $\Phi = Cx\exp\left(-\frac{M\omega x^2}{2\hbar}\right)$ is Φ_1 for HARMONIC OSCILLATOR

SCHRÖ. EQN. $-\frac{\hbar^2}{2M}\frac{d^2\Phi}{dx^2} + \frac{1}{2}K_0 x^2 \Phi = E\Phi$

Notice $\omega = \sqrt{\frac{K_0}{M}} \Rightarrow K_0 = M\omega^2 \Rightarrow \frac{1}{2}K_0 x^2 = \frac{1}{2}M\omega^2 x^2$

$$\frac{d\Phi}{dx} = C\exp\left(-\frac{M\omega x^2}{2\hbar}\right) + Cx\exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(-\frac{M\omega}{2\hbar}\cdot 2x\right)$$

$$= C\exp\left(-\frac{M\omega x^2}{2\hbar}\right) - Cx^2\left(\frac{M\omega}{\hbar}\right)\exp\left(-\frac{M\omega x^2}{2\hbar}\right) = C\exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(1-x^2\frac{M\omega}{\hbar}\right.$$

$$\frac{d^2\Phi}{dx^2} = C\exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(-\frac{M\omega x}{\hbar}\right)\left(1-x^2\frac{M\omega}{\hbar}\right) + C\exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(0 - 2x\frac{M\omega}{\hbar}\right)$$

$$= C\exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(-\frac{M\omega x}{\hbar}\right)\left(1 - x^2\frac{M\omega}{\hbar} + 2\right) = Cx\exp\left(-\frac{M\omega x^2}{2\hbar}\right)\left(-\frac{M\omega}{\hbar}\right)\left(3-x^2\frac{M\omega}{\hbar}\right.$$

$$\Rightarrow \frac{d^2\Phi}{dx^2} = \Phi\left(3 - x^2\frac{M\omega}{\hbar}\right)\left(-\frac{M\omega}{\hbar}\right)$$

$$-\frac{\hbar^2}{2M}\frac{d^2\Phi}{dx^2} = -\frac{\hbar^2}{2M}\left(-\frac{M\omega}{\hbar}\right)\Phi\left(3-x^2\frac{M\omega}{\hbar}\right) = \frac{\hbar\omega}{2}\left(3-x^2\frac{M\omega}{\hbar}\right)\Phi$$

$$= \frac{3}{2}\hbar\omega\Phi - \frac{1}{2}M\omega^2 x^2\Phi$$

$$\Rightarrow -\frac{\hbar^2}{2M}\frac{d^2\Phi}{dx^2} + \frac{1}{2}M\omega^2 x^2\Phi = \frac{3}{2}\hbar\omega\Phi \Rightarrow E = \frac{3}{2}\hbar\omega$$