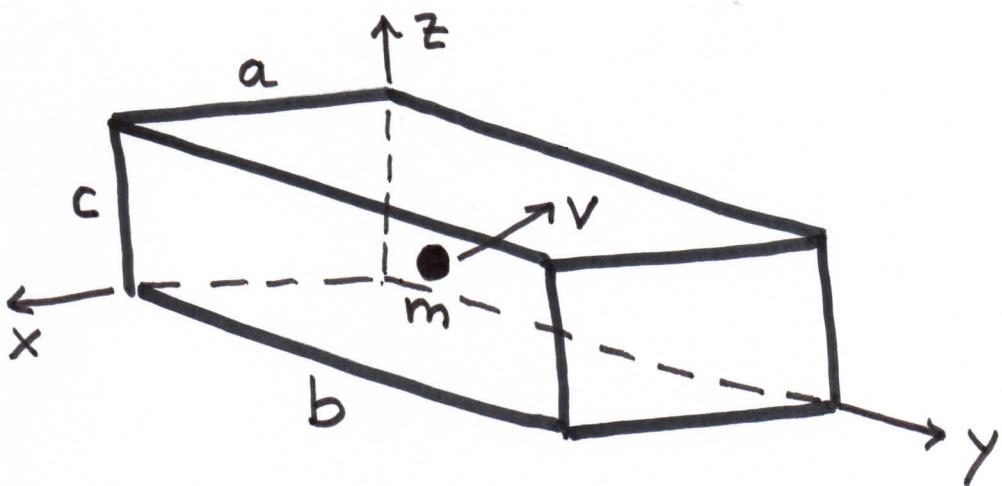


# Particle in 3-D Box

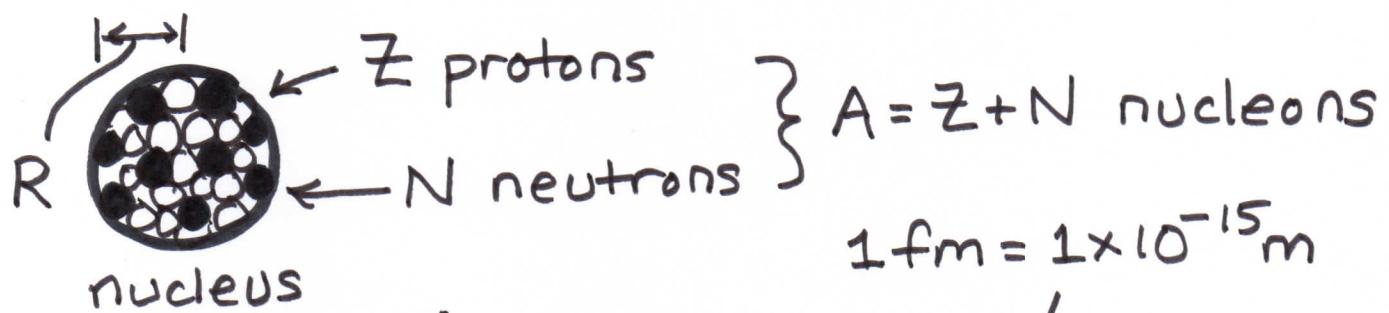


$$\Psi_{n_x n_y n_z}(x, y, z) =$$

$$\sqrt{\frac{8}{abc}} \sin\left(\frac{\pi n_x x}{a}\right) \sin\left(\frac{\pi n_y y}{b}\right) \sin\left(\frac{\pi n_z z}{c}\right)$$

$$E_{n_x n_y n_z} = \frac{\hbar^2}{8m} \left( \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

# Electron Contained in Nucleus?



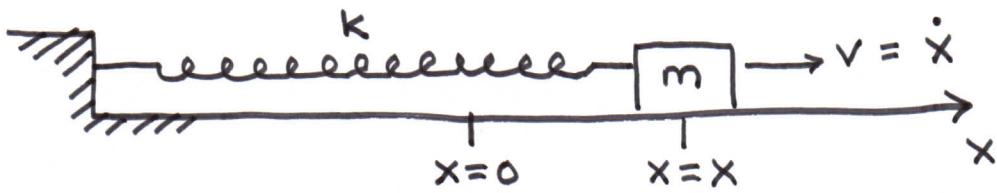
$$R \approx r_0 A^{1/3} \quad r_0 = 1.3 \text{ fm}$$

example: carbon-12 (<sup>12</sup>C)

$$R \approx 1.3 \text{ fm} (12)^{1/3} = 3.0 \times 10^4 \text{ fm} = 3 \times 10^{-6} \text{ nm}$$

$$\begin{aligned} E_{\text{III}} &= \text{lowest energy} && \text{approx.} \\ &= \frac{\hbar^2}{8m} \left( \frac{1^2}{a^2} + \frac{1^2}{b^2} + \frac{1^2}{c^2} \right) && \begin{array}{c} 2R \\ | \\ 2R \\ | \\ 2R \end{array} \\ &= \frac{(hc)^2}{8mc^2} \left( \frac{1}{(6 \times 10^{-6})^2} + \frac{1}{(6 \times 10^{-6})^2} + \frac{1}{(6 \times 10^{-6})^2} \right) \\ &= \frac{1240^2}{8(511,000)} \left[ \frac{3}{(6 \times 10^{-6})^2} \right] \\ &= 3.1 \times 10^{10} \text{ eV} = \boxed{31 \text{ GeV}} \end{aligned}$$

# Classical S.H.O.



$$\vec{F} = -k\vec{x} \rightarrow m\ddot{x} = -kx$$

$$\ddot{x} + \frac{k}{m}x = 0 \leftarrow \text{second-order O.D.E.}$$

Solution is:  $x(t) = c_1 \sin \sqrt{\frac{k}{m}} t + c_2 \cos \sqrt{\frac{k}{m}} t$

where the constants  $c_1$  and  $c_2$  are determined by initial conditions:

$$x(t=0) = c_1 \sin \sqrt{\frac{k}{m}}(0) + c_2 \cos \sqrt{\frac{k}{m}}(0) = c_2 \quad (\text{call } x_0)$$

$$\dot{x}(t=0) = c_1 \sqrt{\frac{k}{m}} \cos \sqrt{\frac{k}{m}}(0) - c_2 \sqrt{\frac{k}{m}} \sin \sqrt{\frac{k}{m}}(0) = c_1 \sqrt{\frac{k}{m}} \quad (\text{call } v_0)$$

---


$$\text{So } x(t) = v_0 \sqrt{\frac{m}{k}} \sin \sqrt{\frac{k}{m}} t + x_0 \cos \sqrt{\frac{k}{m}} t$$

Consider the energy equation:

$$\frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}kA^2$$

↑ amplitude of oscillation

The velocity of the mass at any  $x$ -position is given by:

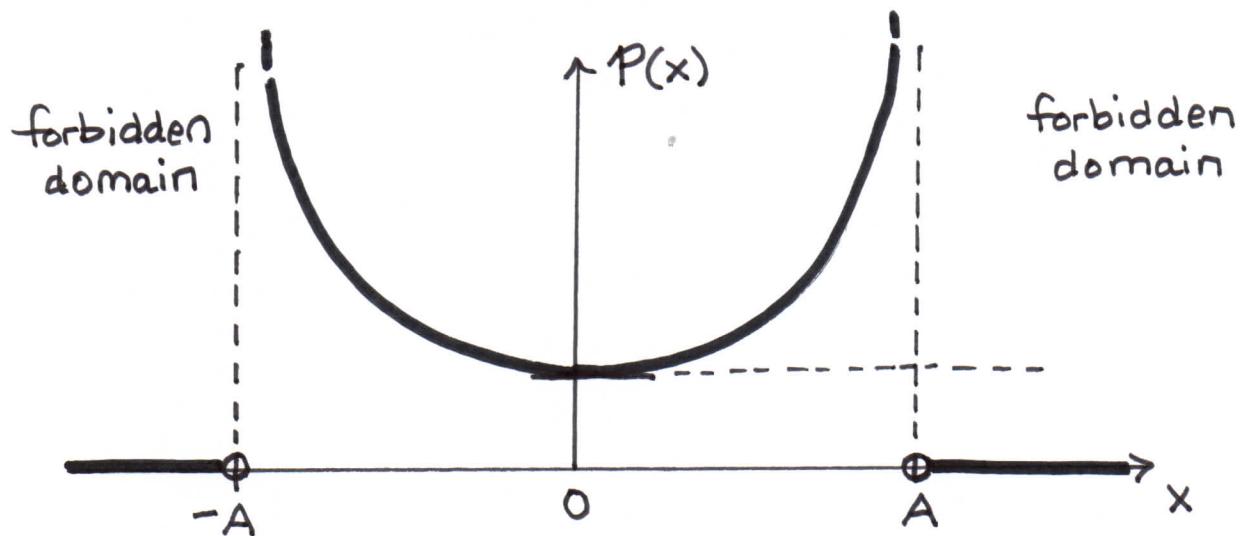
$$v(x) = \sqrt{\frac{k}{m}} \sqrt{A^2 - x^2}$$

$$A = \sqrt{x_0^2 + \frac{m}{k}v_0^2}$$

The probability density  $P(x)$  of finding the oscillating mass at any position (units of  $m^{-1}$ ) is inversely proportional to the mass's speed  $v$ .

$$P(x) = \frac{\alpha}{v} = \frac{\alpha}{\sqrt{\frac{k}{m}} \sqrt{A^2 - x^2}}$$

constant of proportionality



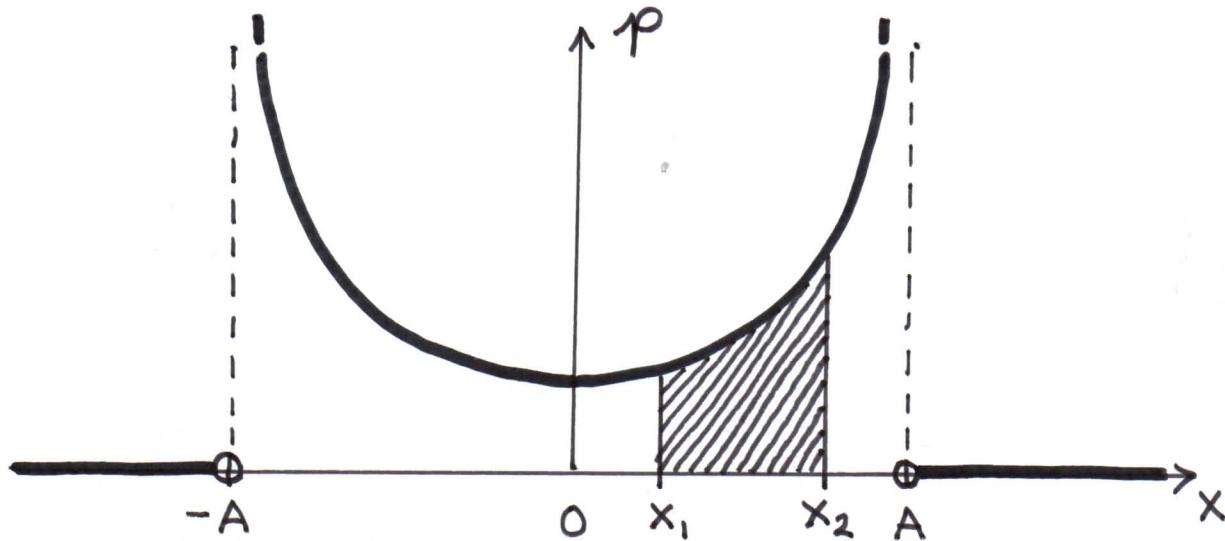
Normalization requires  $\int_{-A}^A P(x) dx = 1$

$$\text{Find } \alpha = \frac{1}{\pi} \sqrt{\frac{k}{m}}$$

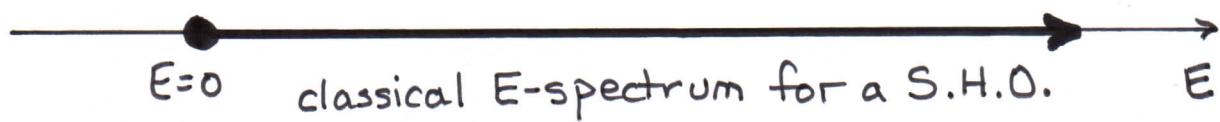
$$\text{So } P(x) = \begin{cases} 0 & \text{for } x < -A \\ \frac{1}{\pi} (A^2 - x^2)^{-1/2} & \text{for } -A < x < A \\ 0 & \text{for } x > A \end{cases}$$

The probability of finding the mass between positions  $x=x_1$ , and  $x=x_2$  at any moment is given by

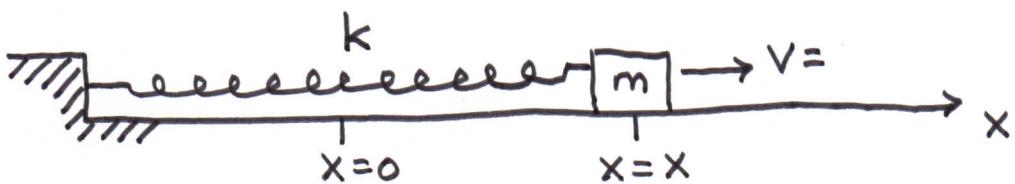
$$P(x_1 < x < x_2) = \int_{x_1}^{x_2} \frac{1}{\pi} (A^2 - x^2)^{-\frac{1}{2}} dx$$



Since the total energy of a classical S.H.O. is  $\frac{1}{2}kA^2 = \frac{1}{2}mv_0^2 + \frac{1}{2}kx_0^2$  and since  $x_0$  and  $v_0$  can be any real numbers of meters or meters/second (forget about limitations on  $v_0$  due to relativity), total energy of a classical S.H.O. can be any non-negative value of joules.



# Quantum Mechanical S.H.O.



- ① Write the Schrödinger Equation for the system using the specific form of the potential energy  $U(x) = \frac{1}{2}kx^2$  for a S.H.O.

$$-\frac{\hbar^2}{2m}\Psi''(x) + \frac{1}{2}kx^2\Psi(x) = E\Psi(x)$$

- ② Recast this equation into "standard form" so as to facilitate a solution.

$$\Psi''(x) + \frac{2m}{\hbar^2} \left[ E - \frac{1}{2}kx^2 \right] \Psi(x) = 0$$

↑ this is a 2<sup>nd</sup> order O.D.E. (homogeneous)

- ③ Solve this equation and find all possible solutions (all possible eigenfunctions  $\Psi_i(x)$  of the operator

$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}kx^2 \right)$  and their corresponding eigenvalues  $E_i$ ).

steady  
energy states

steady  
energy values

Solutions to the Schrödinger Equation for a S.H.O. :

stable energy state  
wave functions  
(eigenfunctions)

$$\Psi_0(x) = C_0 e^{-\frac{m\omega x^2}{2}} \{1\}$$

$$\Psi_1(x) = C_1 e^{-\frac{m\omega x^2}{2}} \left\{ 2\sqrt{\frac{m\omega}{\hbar}} x \right\}$$

$$\Psi_2(x) = C_2 e^{-\frac{m\omega x^2}{2}} \left\{ 4\left(\frac{m\omega}{\hbar}\right)x^2 \right\}$$

$$\Psi_3(x) = C_3 e^{-\frac{m\omega x^2}{2}} \left\{ 8\left(\frac{m\omega}{\hbar}\right)^{3/2} x^3 - 12\sqrt{\frac{m\omega}{\hbar}} x \right\} \quad E_3 = \left(3 + \frac{1}{2}\right)\hbar\omega$$

⋮

$$\Psi_n(x) = C_n e^{-\frac{m\omega x^2}{2}} \left\{ H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \right\}$$

note:  
 $\omega = \sqrt{\frac{k}{m}}$

$$E_0 = \left(0 + \frac{1}{2}\right)\hbar\omega$$

$$E_1 = \left(1 + \frac{1}{2}\right)\hbar\omega$$

$$E_2 = \left(2 + \frac{1}{2}\right)\hbar\omega$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

where the  $C_i$ 's are normalization constants given by:  $C_n = (2^n n! \sqrt{\pi})^{-1/2}$

and the  $H_i$ 's are the Hermite polynomials:

$$H_0(y) = 1$$

$$H_3(y) = 8y^3 - 12y$$

$$H_1(y) = 2y$$

$$H_4(y) = 16y^4 - 48y^2 + 12$$

$$H_2(y) = 4y^2 - 2$$

$$H_5(y) = 32y^5 - 160y^3 + 120y \dots$$

# Hermite Polynomials

The first 11 Hermite polynomials as used in physics:

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x$$

$$H_4(x) = 16x^4 - 48x^2 + 12$$

$$H_5(x) = 32x^5 - 160x^3 + 120x$$

$$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120$$

$$H_7(x) = 128x^7 - 1344x^5 + 3360x^3 - 1680x$$

$$H_8(x) = 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680$$

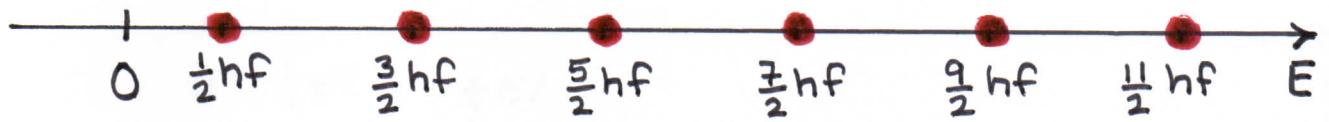
$$H_9(x) = 512x^9 - 9216x^7 + 48384x^5 - 80640x^3 + 30240x$$

$$H_{10}(x) = 1024x^{10} - 23040x^8 + 161280x^6 - 403200x^4 + 302400x^2 - 30240$$

Thus the allowed energies of a quantum mechanical S.H.O. are given by:

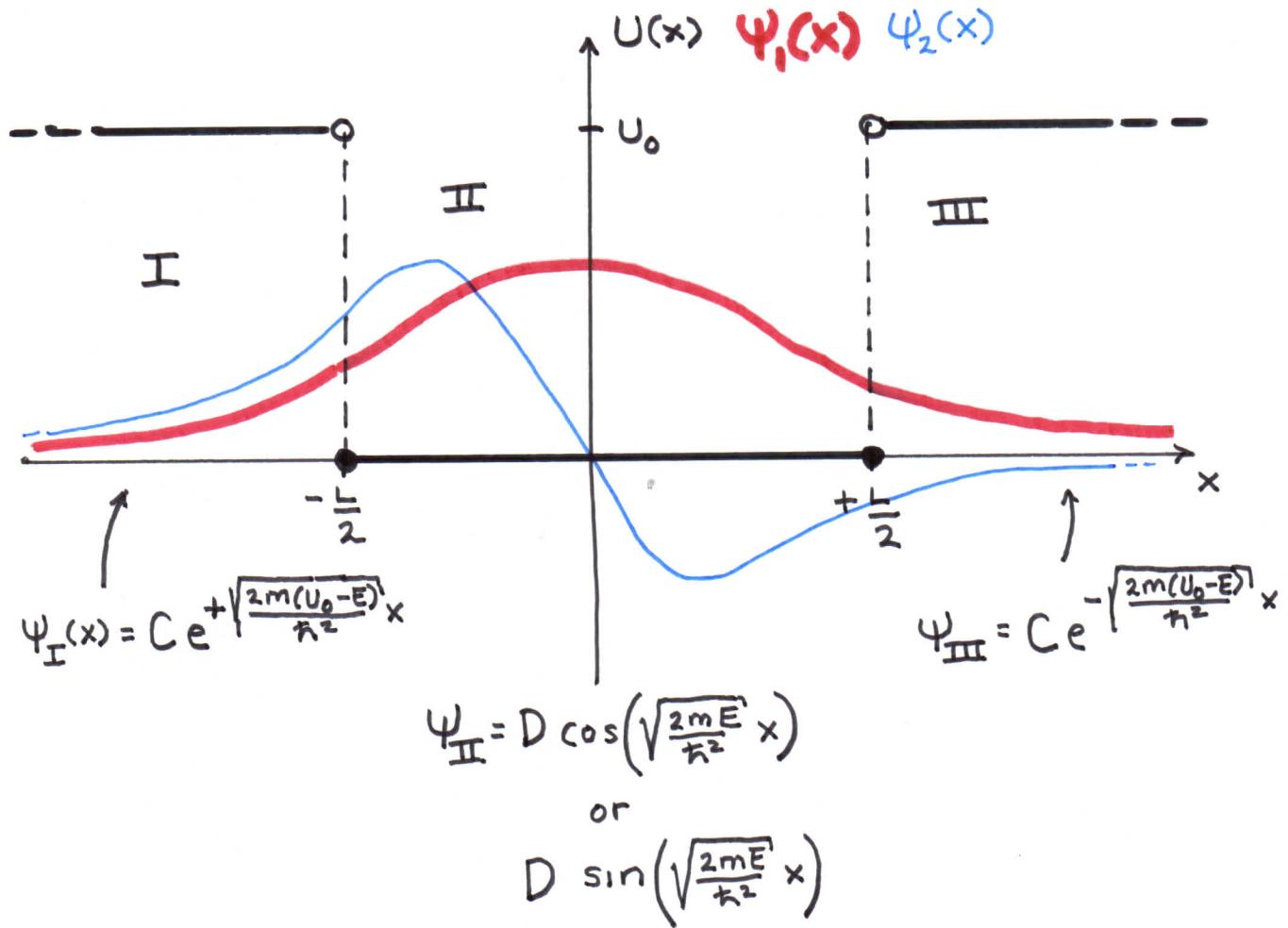
$$E_n = (n + \frac{1}{2})\hbar\omega \text{ or } (n + \frac{1}{2})hf \quad n=0,1,2,\dots$$

$\uparrow$  quantum number

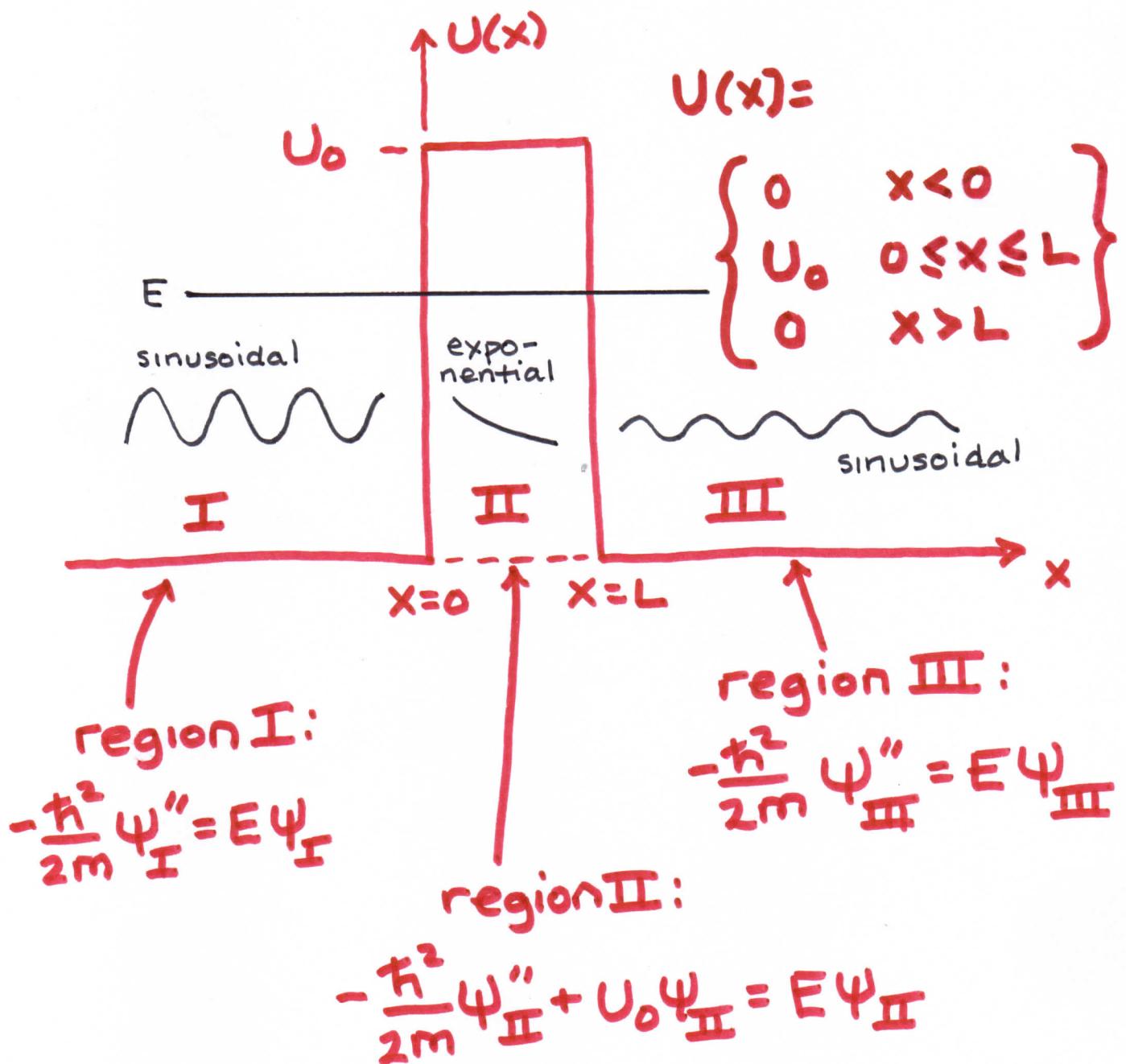


energy spectrum of a quantum mechanical S.H.O.

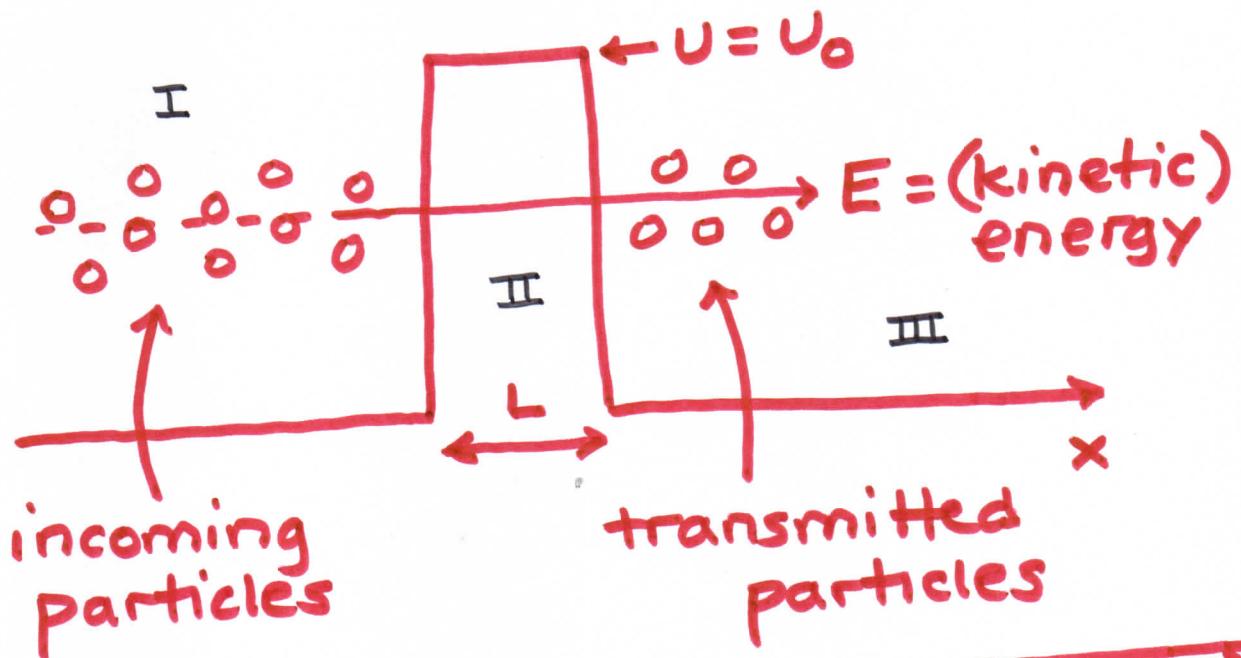
# Finite Square Well



# Finite Barrier



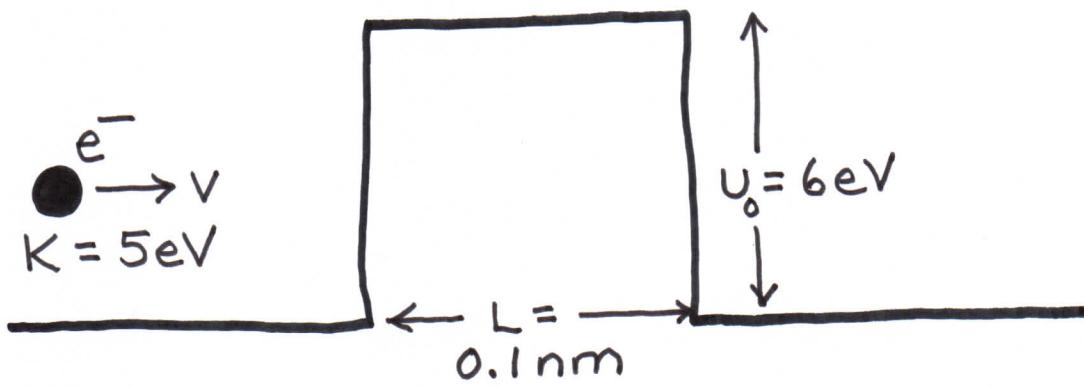
# Barrier Transmission



transmission coefficient  $T \approx e^{-2L\sqrt{\frac{2m(U_0-E)}{\hbar^2}}}$

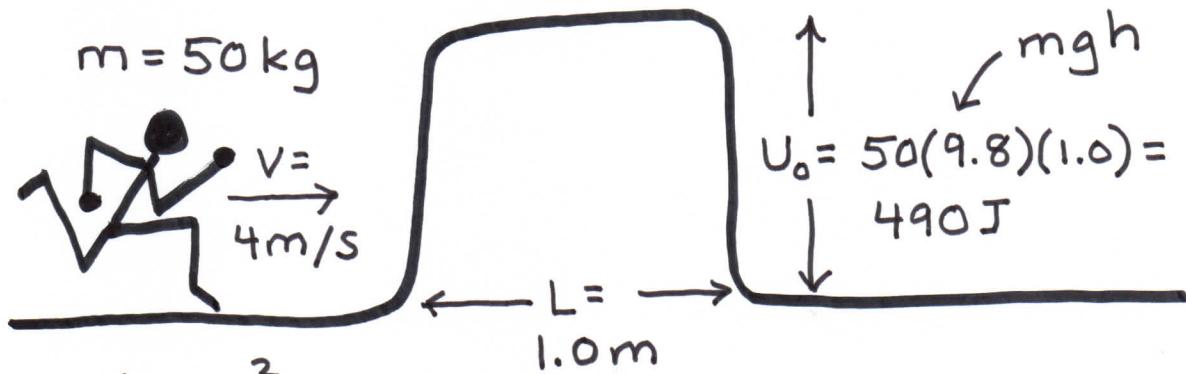
$$T = \frac{(\text{amplitude of sinusoidal } \Psi_{\text{III}})^2}{(\text{amplitude of sinusoidal } \Psi_{\text{I}})^2}$$

# Barrier Penetration Example



$$T = e^{-\frac{-2L\sqrt{2m(U_0-E)}}{\hbar}} = e^{-\frac{-2L\sqrt{2mc^2(U_0-E)}2\pi}{hc}}$$
$$= e^{-\frac{-2(.1)\sqrt{2(511,000)(6-5)}2\pi}{1240}} = \underline{\underline{.359}} \text{ or } \underline{\underline{35.9\%}}$$

# Barrier Penetration Example



$$K = \frac{1}{2}mv^2 =$$

$$\frac{1}{2}(50)(4)^2 = 400 \text{ J}$$

$$T = e^{-\frac{2L\sqrt{2m(U_0 - E)}}{\hbar}} =$$

$$e^{-\frac{2(1.0)\sqrt{2(50)(490 - 400)}}{6.63 \times 10^{-34}}} =$$

$$e^{-1.80 \times 10^{36}} = \frac{1}{10^{7.8 \times 10^{35}}}$$

