PH 107 :Quantum Physics and Applications

Tunnelling application and Simple Harmonic Oscillator

Lecture 18: 15-02-2022

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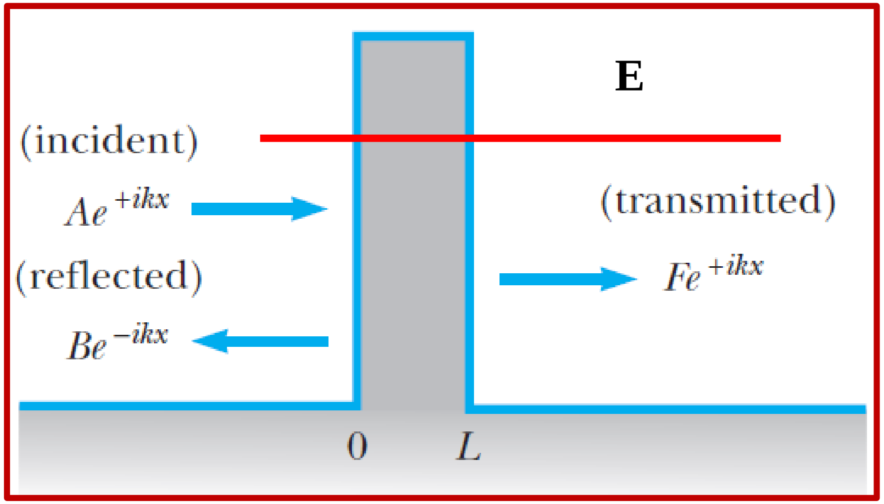
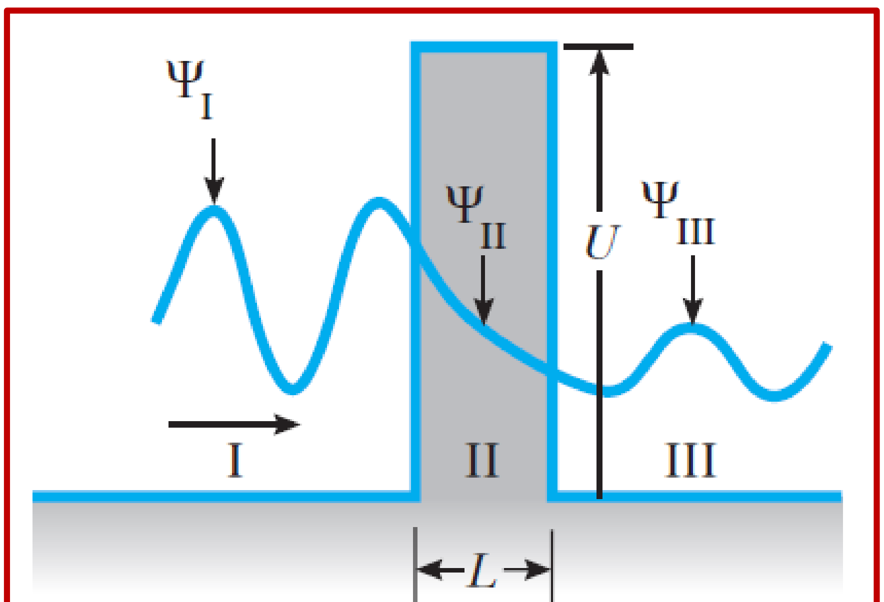
Recap (Potential Barrier, E<V_o)

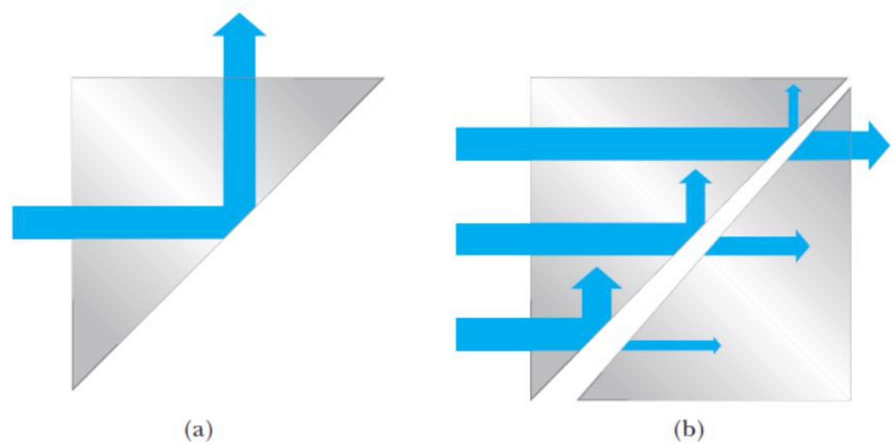


$$T(E) = \left[1 + \frac{1}{4}\left(\frac{V_0^2}{E(V_0 - E)}\right)\sinh^2 \alpha L\right]^{-1}$$

$$\sinh \alpha L = (e^{\alpha L} - e^{-\alpha L})/2 \; ; \; \alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$$



Tunneling Application



For αL>> 1

$$\sinh^2(\alpha L) = \left(\frac{e^{\alpha L} - e^{-\alpha L}}{2}\right)^2 = \frac{1}{4}\left(e^{2\alpha L} + e^{-2\alpha L} - 2\right) \approx \frac{1}{4}e^{2\alpha L}$$

Also neglecting 1 in comparison to other term in expression of T

$$\boxed{\text{For } \alpha L >> 1, \qquad T \approx \frac{16E(V_0 - E)}{V_0^2}e^{-2\alpha L}}$$

E<< Vo

For αL<< 1

$$\sinh^2(\alpha L) = \left(\frac{e^{\alpha L} - e^{-\alpha L}}{2}\right)^2 \approx \alpha^2 L^2$$

(keeping only leading terms in αL)

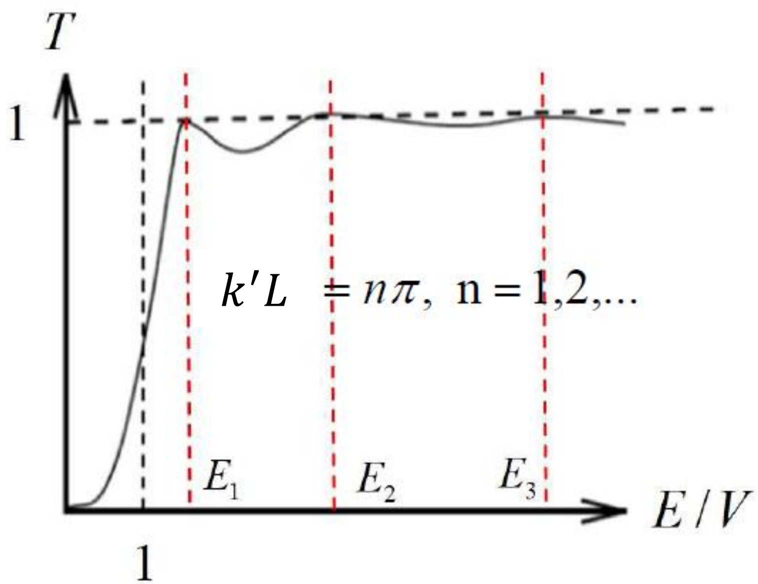
$$\frac{V_0^2}{4E(V_0 - E)} = \frac{1}{4(E/V_0)(1 - E/V_0)} \approx \frac{1}{4(E/V_0)}$$

$$T = \left[1 + \frac{1}{4}\left(\frac{V_0^2}{E(V_0 - E)}\right)\sinh^2(\alpha L)\right]^{-1} \Rightarrow \therefore T = \left[1 + \frac{1}{4}\left(\frac{V_0^2}{E(V_0 - E)}\right)\alpha^2 L^2\right]^{-1}$$

$$\Rightarrow \therefore T = \left[1 + \frac{m^2 V_0^2 L^2}{\hbar^4 k^2}\right]^{-1}$$

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

Transmission resonances: The E>V_0 case



$$T(E) = \left[1 + \frac{1}{4}\left(\frac{V_0^2}{E(E-V_0)}\right)\sin^2 k'L\right]^{-1}$$

$$(k')^2 = \frac{2m}{\hbar^2}(E - V_0)$$

- At high energies and weak potentials, particle would not feel the effect of the barrier.
- For total transmission/ transmission resonance.

$\sin^2 k'L = \mathbf{0}$ or $k'L = n\pi$ where n = 1, 2,3

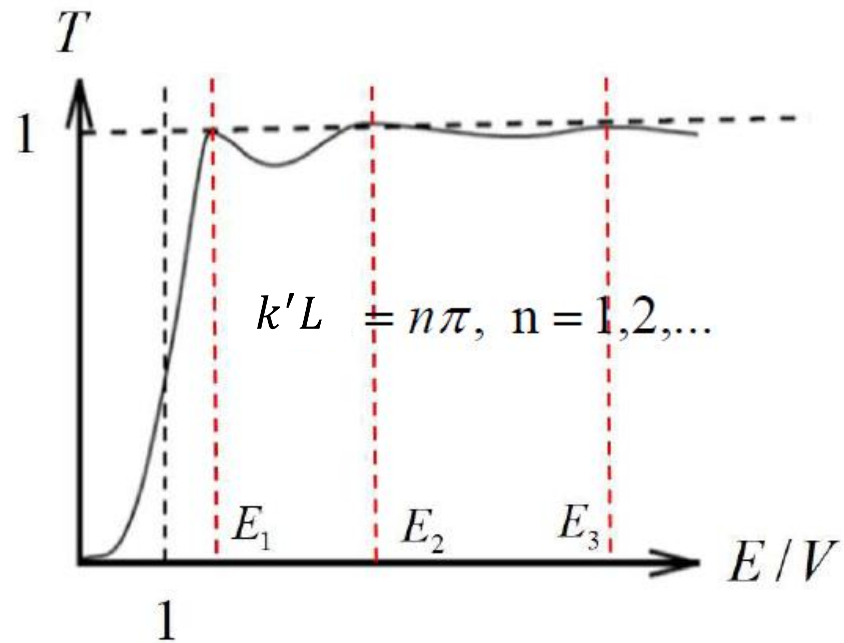
$$\boxed{E_n = V_o + \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

Phenomena of 100% transmission through a barrier at specific energies is called "Transmission Resonance".

Transmission resonances: The $E>V_0$ case

Incident energy of the particle;

$$E_n = V_o + \frac{n^2\pi^2\hbar^2}{2ma^2} \quad ; n = 1, 2, 3$$

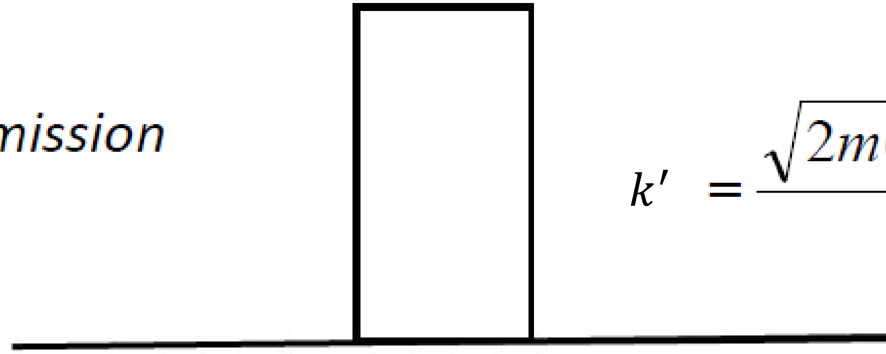


- The maxima of T coincides with energy eigen values of infinite square well potential. These are known as resonances.

- **Ramsauer-Townsend effect:** **S**cattering of low energy electron from noble atoms. Noble gases become nearly transparent to electrons of specific energy.

- **Size Resonance** : MeV energy neutrons pass transparently through nuclei at resonant energies.

Condition for transmission resonance



$$k' = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

$$k'L = n\pi, \ \mathrm{n} = 1,2,\ldots$$

$$L = n\frac{\pi}{k'} = n\left(\frac{\pi}{2\pi / \lambda'}\right) = n\left(\frac{\lambda'}{2}\right)$$

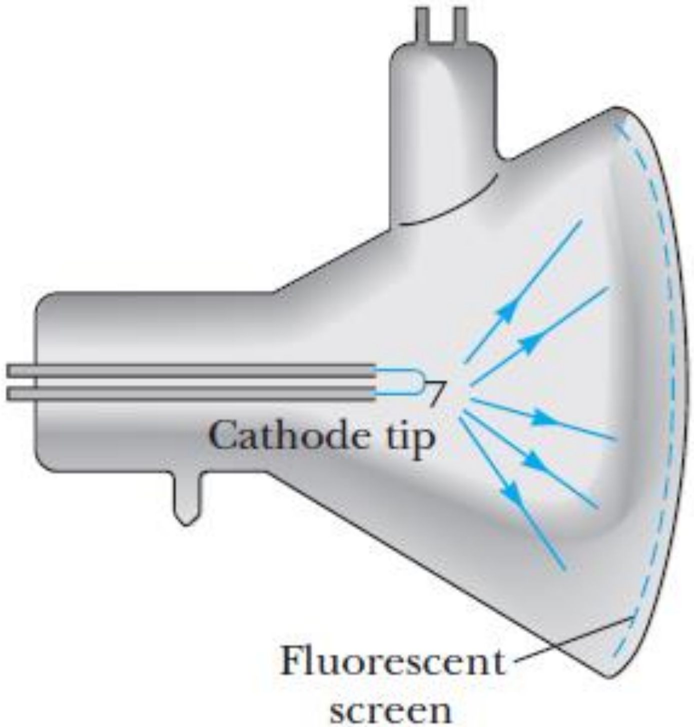
λ' *is the wavelength of the particle in the barrier region.*

Tranmission resonances occur when the length of the barrier is half intergral of the wavelength of the particle in the barrier region.

Tunneling Application 2: Field-emission

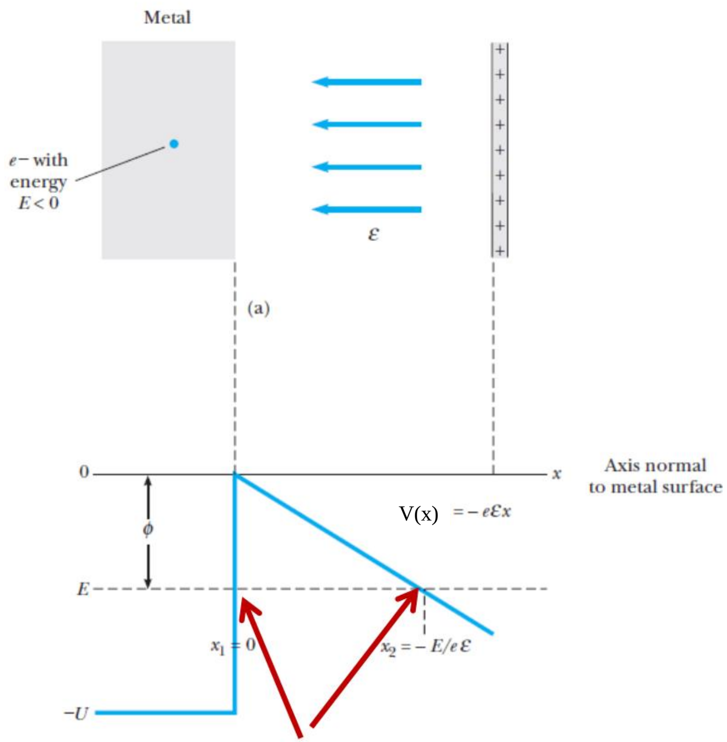
- Electrons are emitted from a metal under the action of a strong electric field (*Cold emission*).

- Escaping electrons used in image to determine with structural details of the surface



Tunneling Application 2: Field-emission

- Mobile electrons attracted to the surface by the positively charged plate.
- Free metal electrons are bound by a potential well of depth U. The total energy of electron is negative.
- Beyond surface x > 0, electron is attracted by force (eε). Its potential energy V(x) = - eε*x*.
- By virtue of wave character electron tunnel through this barrier.



Classical turning points

$$T(E) \simeq \exp\left(-\frac{2}{\hbar}\sqrt{2m}\int\sqrt{V(x)-E}\,dx\right)$$

$$T(E)_{\mathrm{FE}} \simeq \exp\left(\left\{-\frac{4}{3e\hbar}\sqrt{2m}|E|^{3/2}\right\}\frac{1}{\epsilon}\right)$$

$$\simeq \exp\left(-\frac{\epsilon_c}{\epsilon}\right)$$

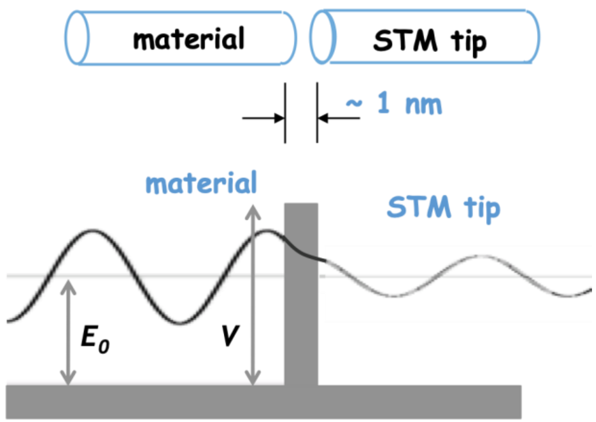
Characteristic field strength for emission

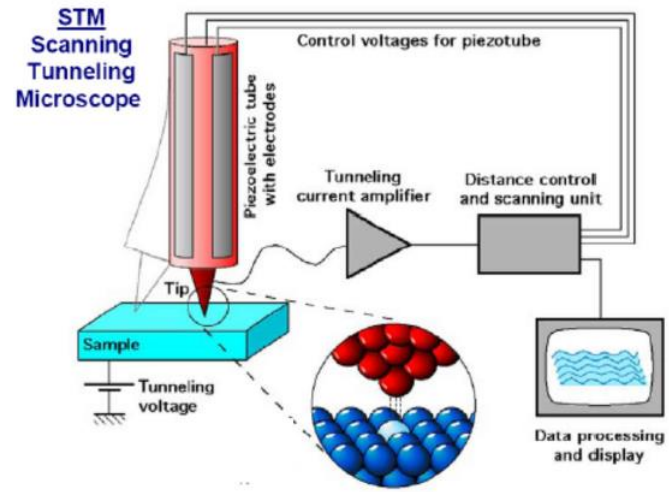
$$\varepsilon_c = \frac{4\sqrt{2m}|E|^{3/2}}{3e\hbar}$$

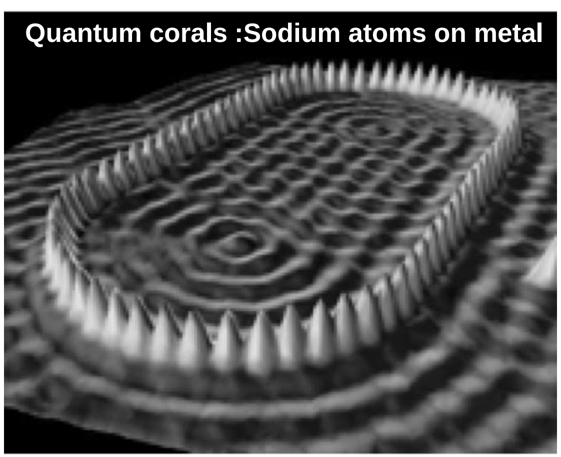
Tunneling Application 3:Scanning Tunneling Microscope

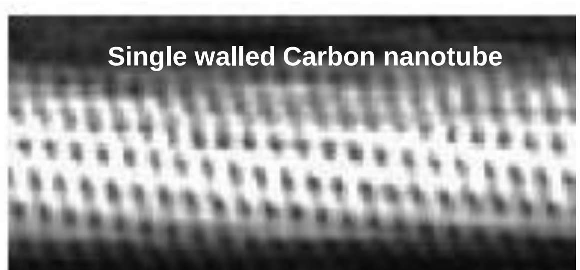
- Due to quantum effect of barrier penetration, the electron density of material (wave function) extends beyond the surface.

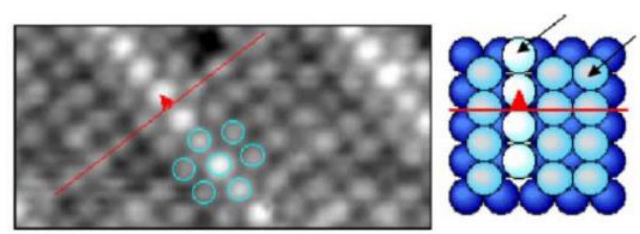
- One can exploit the tunneling effect to measure the electron density on the surface.



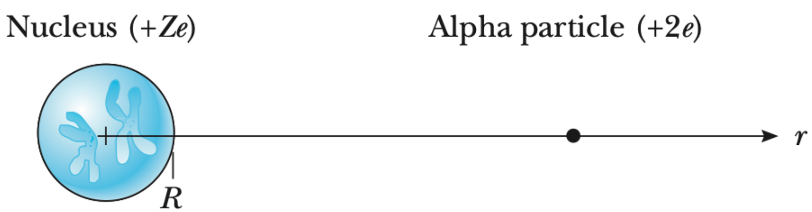








Tunneling Application 4 : Alpha-Decay



$$^{232}_{92}U \rightarrow \,^{4}_{2}H_{e} + \,^{228}_{90}Th$$

Table 7.1 Characteristics of Some Common α Emitters

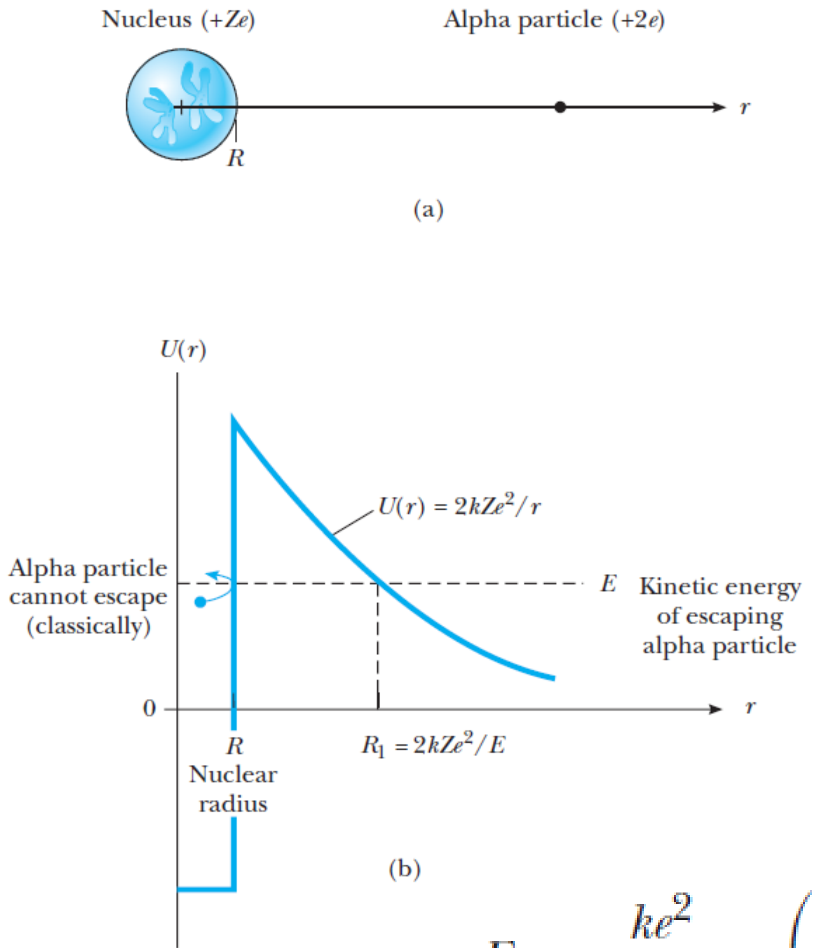
Element	α Energy	Half-Life*
$^{212}_{84}\mathrm{Po}$	8.95 MeV	2.98×10^{-7} s
$^{240}_{96}\mathrm{Cm}$	6.40 MeV	27 days
$^{226}_{88}\mathrm{Ra}$	4.90 MeV	1.60×10^{3} yr
$^{232}_{90}\mathrm{Th}$	4.05 MeV	1.41×10^{10} yr

*Note that half-lives range over 24 orders of magnitude when α energy changes by a factor of 2.

Decay of radioactive elements with emission of **α**-particles (helium nuclei) was puzzling until 1928 (Gamow and Gurney).

- α-particles have energy in the range of 4-9 ev
- **Half-life time of emitter varies enormously. This can be explained by tunnelling.**

α-decay (example 13.0, Chapter 13, Serway)



$$Coulomb\ barrier, U(r) \sim 30\ MeV$$

$$R \sim 10\ fm$$

$$T(E)_\alpha \approx exp\left(-4\pi Z\sqrt{\frac{E_0}{E}} + 8\sqrt{\frac{ZR}{r_0}}\right)$$

$r_0 = 7.25\ fm$ **is like the "Bohr radius" of the α particle.**

$$E_0 = \frac{ke^2}{2r_0} = \left(\frac{ke^2}{2a_0}\right)\left(\frac{a_0}{r_0}\right) = (13.6\ \mathrm{eV})(7295) = 0.0993\ \mathrm{MeV}$$

Decay Rate = Collison frequency (f = v/2R) X T(E)

α-decay

Decay rate: $\lambda = fT(E)_\alpha$

$$\lambda \approx 10^{21} exp\left(-4\pi Z\sqrt{\frac{E_0}{E}} + 8\sqrt{\frac{ZR}{r_0}}\right)$$

Half-life time of the emitter

$$t_{1/2} = \frac{\ln 2}{\lambda}$$

Sensitivity of tunnelling rate to small changes in particle energy accounts for the wide range of half-lives observed for α emitters

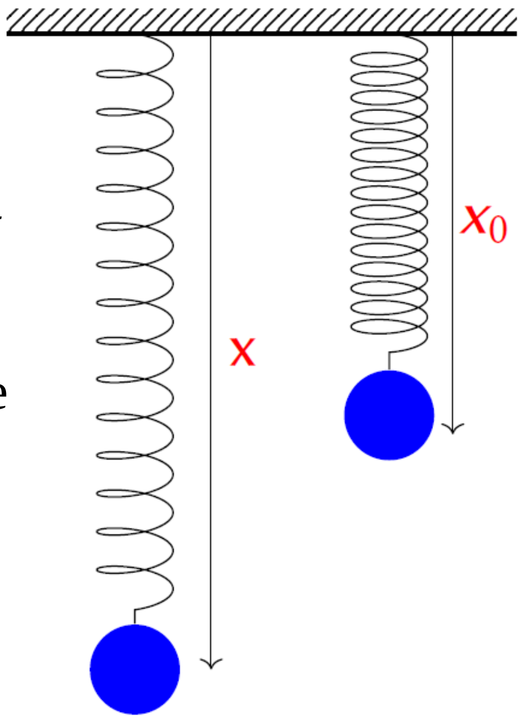
One-dimensional harmonic oscillator potential

One-dimensional Simple harmonic oscillator (SHO)

- In classical mechanics, SHO is a system or a particle that under goes harmonic motion about an equilibrium point. The eq of motion is

$$F = m\frac{d^2x}{dt^2} = -kx\,;k\ is\ spring\ constant$$

- The RHS is the restoring force $\left(F = -\frac{dV(x)}{dx}\right)$ that acts in the direction opposite to the displacement .



k is spring constant
m is mass of the ball
spring is massless

- Solution to Newton's equation is,

$$x(t) = A\sin(\omega t + \phi_o)\ and\ \omega^2 = \frac{k}{m}$$

- Work done by the restoring force,

$$\Delta W = \int_x^{x_o} F.x = -\frac{k\,(x - x_o)^2}{2}$$

- The potential energy of the oscillator is, $V(x) = -\Delta W = \frac{k\,(x - x_o)}{2}$

- If $x_o = 0$ then $V(x) = \frac{kx^2}{2}$

One-dimensional Simple harmonic oscillator (SHO)

Solution: $x(t) = A\sin(\omega t + \phi)$ $\quad v(t) = \omega A\cos(\omega t + \phi)$

Total Energy $E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$

$$= \frac{1}{2}m\omega^2 A^2\cos^2(\omega t + \phi) + \frac{1}{2}kA^2\sin^2(\omega t + \phi)$$

$$= \frac{1}{2}m\omega^2 A^2$$

The total energy of the oscillator is constant.

$$\Longrightarrow A = \pm\sqrt{\frac{2E}{m\omega^2}} = \pm\sqrt{\frac{2E}{k}}$$

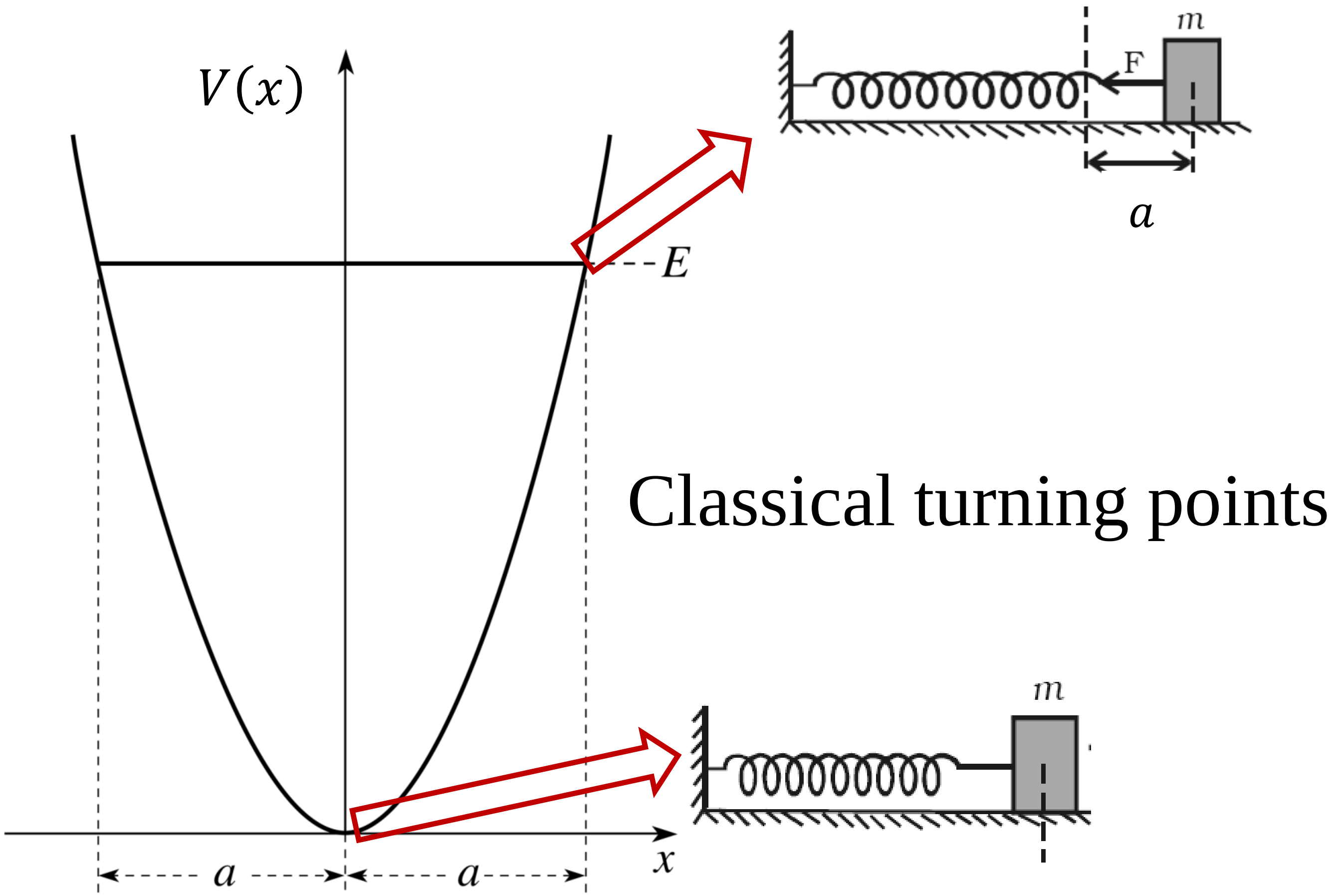
One-dimensional harmonic oscillator potential

Classical turning point: When total energy = potential energy

$$V(x) = \frac{kx^2}{2}$$

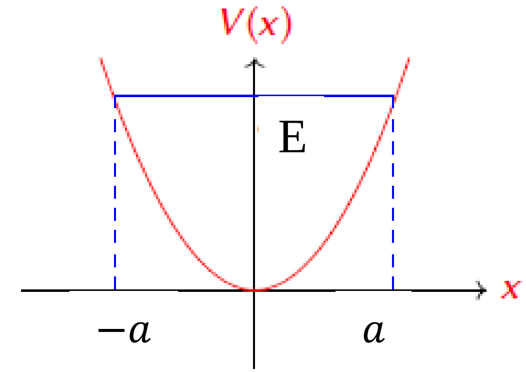
$$E = \frac{1}{2}ka^2$$

$$\Longrightarrow \; a = \pm\sqrt{\frac{2E}{k}}$$



Classical SHO : Properties

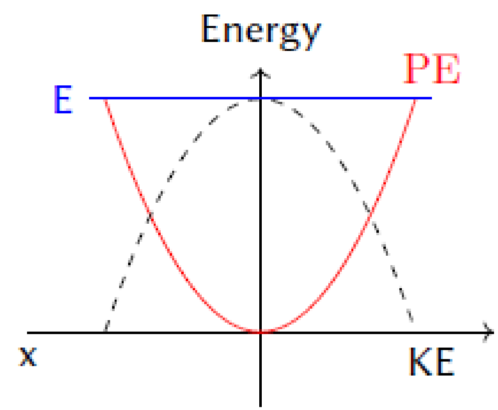
- Velocity at turning point is zero, $v_{\pm a} = 0$ and Potential Energy $PE_{\pm a} = E$.
- The motion of the HO is confined to the region where $KE \geq 0$. CHO can never be found beyond the turning points.



X = 0 is equilibrium point

X= ±a are turning points

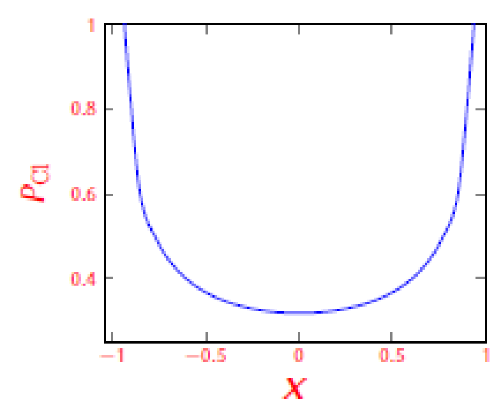
- The energy of the CHO changes in a continuous way.
- HO is at rest in its equilibrium position: $PE = 0$



- The classical probability to find the object in the region x and $x + dx$:

$$P_{Cl}(x)dx = 2 \times \frac{dt}{T} = \frac{\omega}{\pi}\frac{dx}{v(t)} = \frac{1}{pi}\frac{1}{\sqrt{A^2 - x^2(t)}}$$

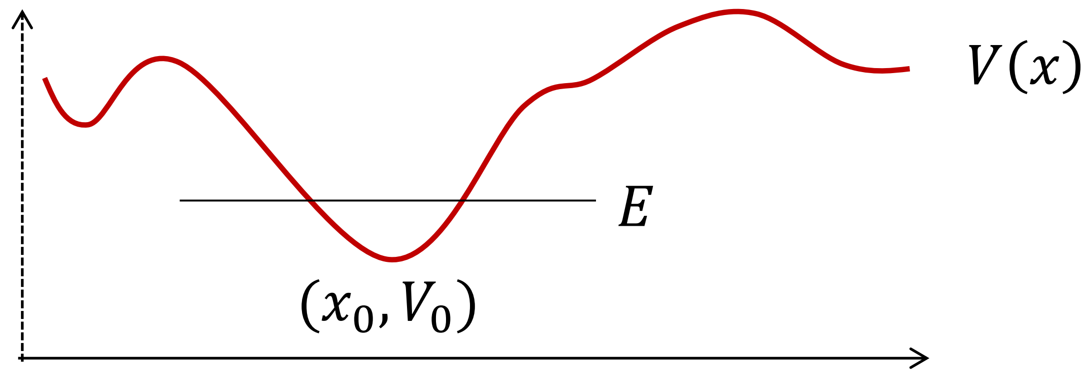
$$v(t) = A\omega\cos(\omega t + \phi_0) = A\omega\sqrt{1 - \sin^2(\omega t + \phi_0)} = \omega\sqrt{A^2 - x^2(t)}$$



- Factor 2 appears above because HO is in the region x and $x + dx$ twice in one time-period T.

Importance of the Harmonic Oscillator potential

Consider any arbitrary potential. Close to the equilibrium point, most potentials look like HO:



Taylor expansion of $V(x)$ about the minimum V_0 is

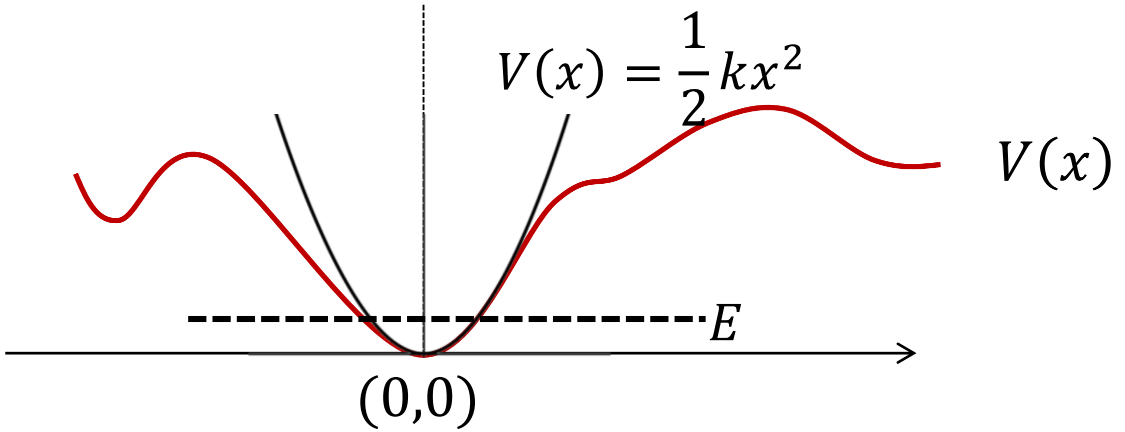
$$V(x) = V_0 + \left.\frac{dV(x)}{dx}\right|_{V_0} (x - x_0) + \left.\frac{d^2V(x)}{dx^2}\right|_{V_0} (x - x_0)^2 + \cdots$$

Since $\left.\frac{dV(x)}{dx}\right|_{V_0} = 0$ and noting that $\mathrm{k} = \left.\frac{d^2V(x)}{dx^2}\right|_{V_0} > 0$

$$V(x) = V_0 + \frac{1}{2}k(x - x_0)^2$$

By suitably shifting the origin to (x_0, V_0), we get , $V(x) = \frac{1}{2}kx^2$

Importance of the Harmonic Oscillator potential



- For small excursions of the particle away from the minimum, the arbitrary potential can be approximated to be simple harmonic.

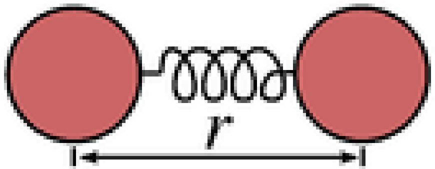
- Harmonic oscillator is one of the favourite systems a physicist uses to understand many complex phenomenon.

- Oscillations are found throughout in the nature. Examples: Water waves, Vibration of a string, Vibrations of crystals, Light.

- HO serves as a prototype in the mathematical treatment of such diverse systems.

Example 1: Vibration of a diatomic molecule

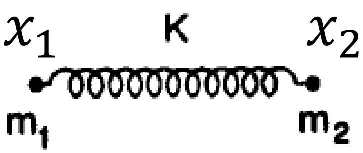
- Consider a molecule consisting of two atoms.



- Atoms attract each other via a potential — Morse potential

$$V(r) = D_e\left([1 - e^{-a(r-r_e)}]^2 - 1\right)$$

Example1 : Vibration of a diatomic molecule



Eq. length of the spring : x_0

Displacement from equilibrium position: $x = x_1 - x_2$

Classical equations of motion

$$m_1\ddot{x}_1 = k(x - x_0)$$

$$m_2\ddot{x}_2 = k(x - x_0)$$

$$\ddot{x}_1 - \ddot{x}_2 = \ddot{x} = -\frac{k}{\mu}(x - x_0);\ \mu = \frac{m_1 m_2}{m_1 + m_1}\text{: Reduced mass}$$

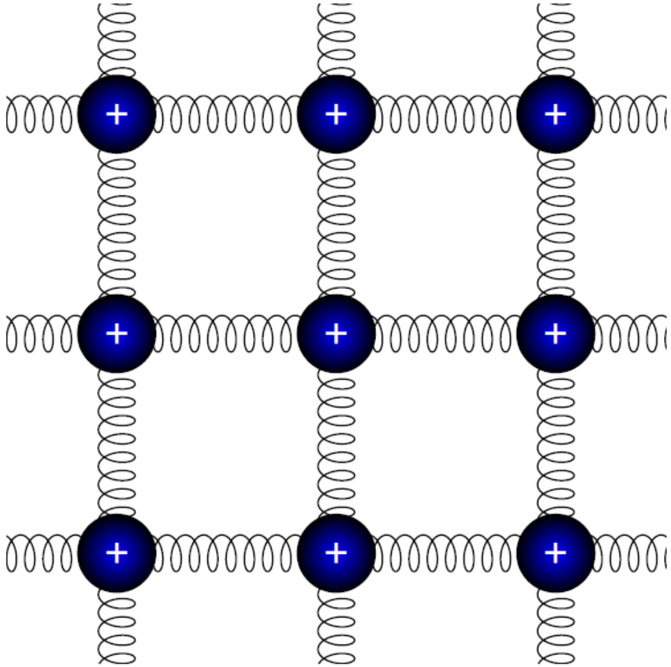
Example 2: Vibration of Solid

- A solid can be thought of a spheres connected by springs in all the 3 directions.

- Along each direction, motion can be analyzed in terms normal modes

- Each mode can be treated as a set of independent oscillator.

- Quantization of the crystal oscillators leads to the concept of phonons (sound quanta), which are analogous to photons.

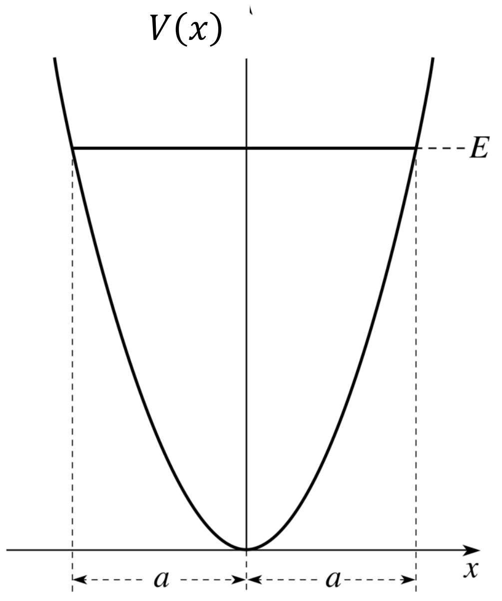


Quantum One-dimensional harmonic oscillator

Quantum harmonic oscillator

Two important features about the potential:

- $V(x)$ is a symmetric potential.
- $V(x)$ increases without limit as $x \longrightarrow$ **± infinity**



For the quantum mechanical behavior of a particle subject to such a potential, one should solve,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}kx^2\right)\psi(x)=E\psi(x)$$

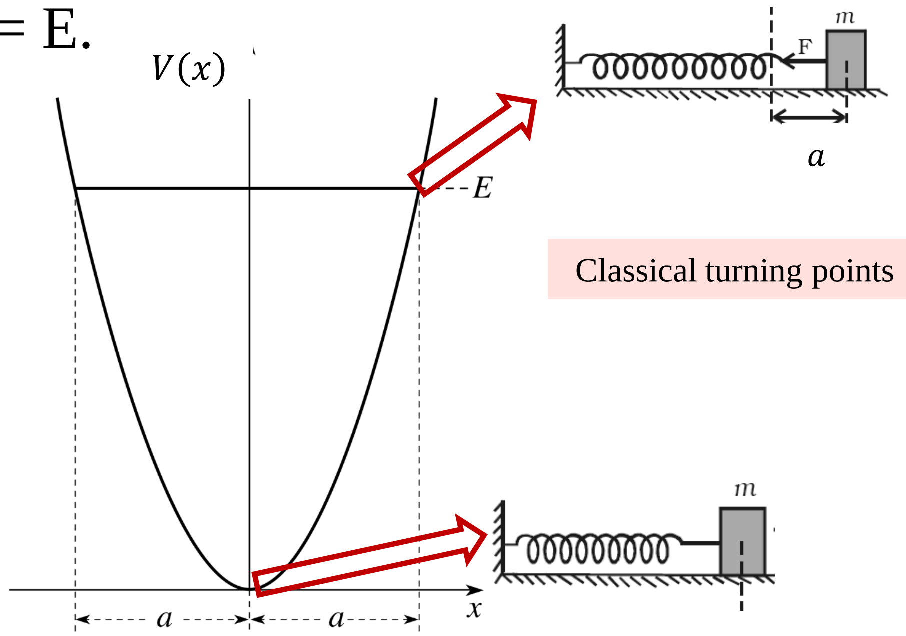
where E is the energy eigen value.

Quantum harmonic oscillator

Turning points are points at which V(x) = E.

Since, $\omega = \sqrt{k/m}$ the equation can be written as

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\psi(x) = E\psi(x)$$



Hamiltonian : K.E + P.E

At turning points,

$$\boldsymbol{Since}, V(x) = \frac{kx^2}{2} \Rightarrow E = \frac{1}{2}ka^2$$

Heuristic way to find solution, $\psi(x)$

The exponential and trigonometric solutions of $\psi(x)$ will not work due to x^2 form of the potential.

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi(x)=E\psi(x)$$

- $e^{\pm ix}$: Donot fall off for large $|x|$. We need a function that falls off faster than $1/x^2$

- $\mathrm{e}^{-\mathrm{x}}$: Works only for positive x.

- $\mathrm{e}^{-|x|}$: Derivative not smooth at $\mathrm{x}=0$

Solution for HO

Ground state wave function $\psi(x)$ should be

- *Symmetric* around symmetric around x = 0
- *Nodeless* but approaching zero for large $|x|$

Let's choose Gaussian function, $\boldsymbol{\psi_o(x) = C_o\, e^{-\alpha x^2}}$

Second derivative;

$$\frac{d^2\psi_o(x)}{dx^2} = \{4\alpha^2x^2 - 2\alpha\}\, C_o\, e^{-\alpha x^2}$$

$$= \{4\alpha^2x^2 - 2\alpha\}\psi_o(x)$$

Since $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\psi_o(x) = E\psi_o(x)$

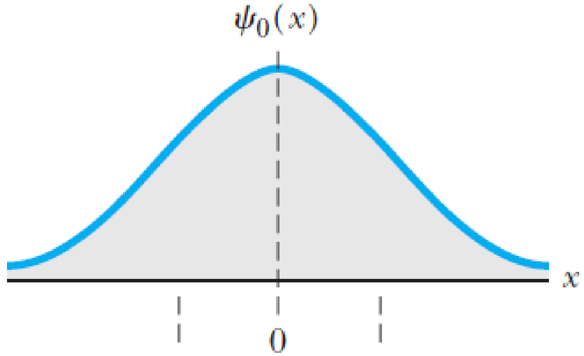
$$\frac{d^2\psi_o(x)}{dx^2} = \frac{2m}{\hbar^2}\left(\frac{1}{2}m\omega^2x^2 - E\right)\psi_o(x)$$

$$4\alpha^2 = \frac{2m}{\hbar^2}\frac{1}{2}\, m\omega^2 \quad \Longrightarrow \quad \alpha^2 = \frac{m\omega}{2\hbar}$$

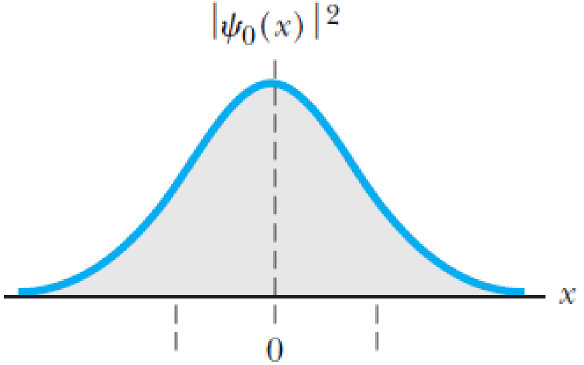
$$\frac{2mE}{\hbar^2} = 2\alpha \quad \Longrightarrow \quad E = \frac{1\hbar\omega}{2}$$

The ground state wave function,

$$\psi_o(x) = C_o\, e^{-m\omega x^2/2\hbar}$$

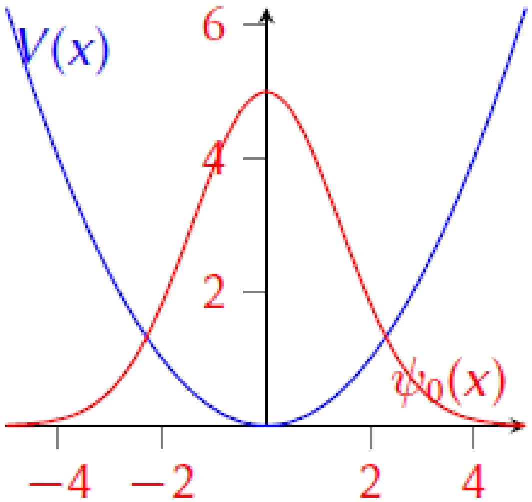


(a)



(b)

Properties of the solution



- Energy of the oscillator is not zero. It is a positive and depends on the frequency of the oscillator.

$$E = \frac{1\hbar\omega}{2}$$

- At the classical turning points are

$$E = \frac{1}{2}ka^2$$

$$a = \sqrt{\frac{\boldsymbol{2E}}{\boldsymbol{m}\omega^2}}$$

- For x > a, $\psi(x) \neq 0$. However this is classically forbidden.

Classical vs Quantum- Harmonic Oscillator

Key differences between classical SHO and quantum SHO are:

- Classical HO cannot penetrate into forbidden region , $x > \pm a$.
- Quantum HO does penetrate into forbidden region

- For classical HO, probability density maximum at turning points.
- Quantum HO are most likely to be found in the center of potential region.