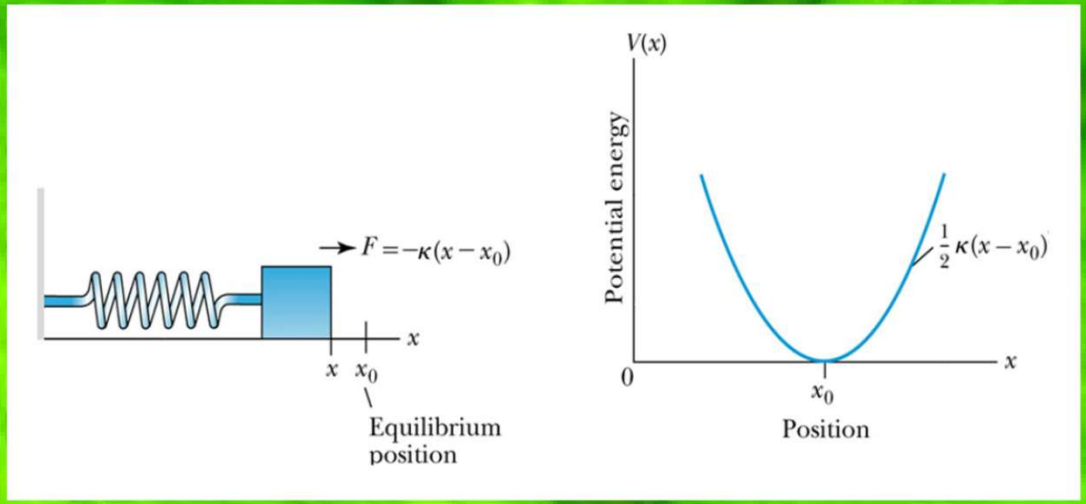
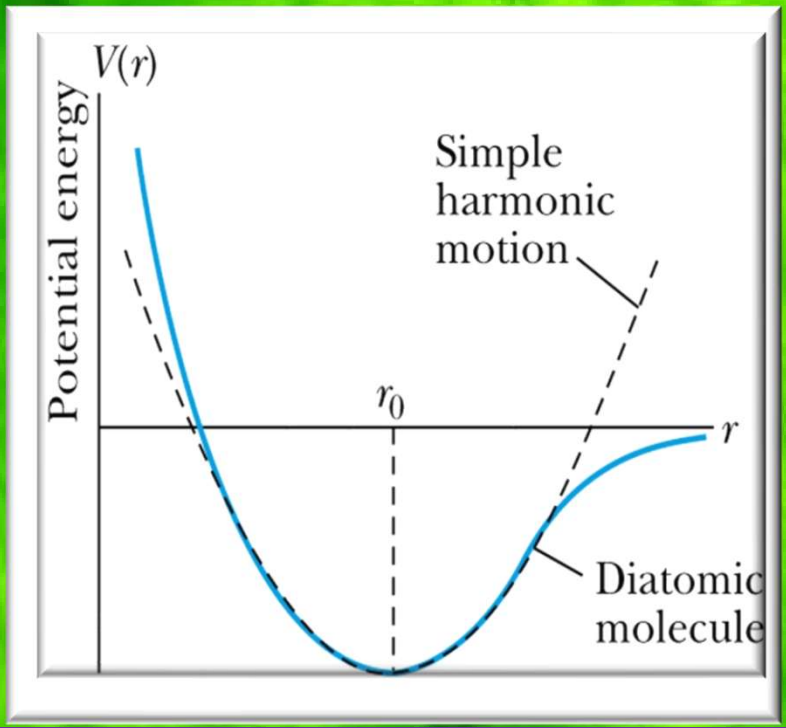
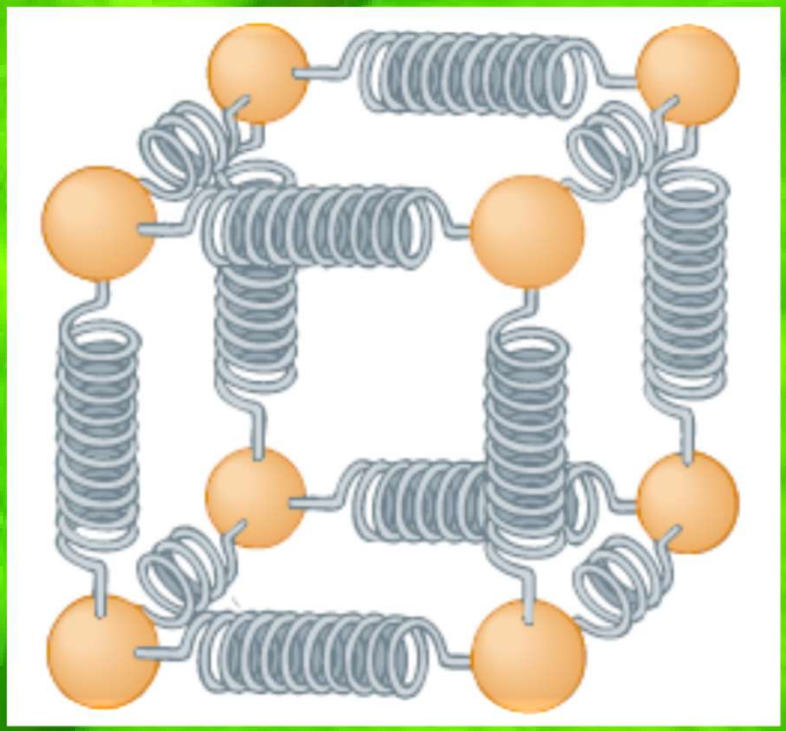
Simple Harmonic Oscillator

•Simple harmonic oscillators describe many physical situations: springs, diatomic molecules and atomic lattices.







Consider the Taylor expansion of a potential function:

$$V(x) = V_0 + V_1(x - x_0) + \frac{1}{2}V_2(x - x_0)^2 + \ldots$$

Energy Eigenkets and Energy Eigenvalues

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$$

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right)$$

annihilation operator

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

creation operator

$$H = \hbar\omega\left(N + \tfrac{1}{2}\right)$$

$$[a, a^\dagger] = \left(\frac{1}{2\hbar}\right)(-i[x, p] + i[p, x]) = 1$$

$$N = a^\dagger a$$

$$a^\dagger a = \left(\frac{m\omega}{2\hbar}\right)\left(x^2 + \frac{p^2}{m^2\omega^2}\right) + \left(\frac{i}{2\hbar}\right)[x, p]$$

$$= \frac{H}{\hbar\omega} - \frac{1}{2}$$

$$N|n\rangle = n|n\rangle$$

$$H|n\rangle = \left(n+\tfrac{1}{2}\right)\hbar\omega|n\rangle$$

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

$$[N,a] = [a^\dagger a, a] = a^\dagger[a,a] + [a^\dagger,a]a = -a$$

$$[N,a^\dagger] = a^\dagger$$

$$Na^\dagger|n\rangle = \left([N,a^\dagger] + a^\dagger N\right)|n\rangle = (n+1)a^\dagger|n\rangle$$

$$Na|n\rangle = \left([N,a] + aN\right)|n\rangle = (n-1)a|n\rangle$$

$$a|n\rangle = c|n-1\rangle$$

$$< n | a^{\dagger} = c^{*} < n-1 |$$

$$\langle n|a^{\dagger}a|n\rangle = |c|^{2}$$

$$N = a^{\dagger}a$$

$$n = |c|^{2}$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$a^{\dagger}\,|\,n>=c'\,|\,n+1>$$

$$< n | a = c'^{*} < 1+n |$$

$$< n | aa^{\dagger} | n >=| c' |^{2}$$

$$< n | 1+a^{\dagger}a | n >= 1+n =| c' |^{2}$$

$$[a, a^{\dagger}] = 1$$

$$a^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$a^2|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle$$

$$a^3|n\rangle = \sqrt{n(n-1)(n-2)}\,|n-3\rangle$$

$$\vdots$$

n can never be negative, because:

$$n = \langle n|N|n\rangle = \left(\langle n|a^\dagger\right)\cdot\left(a|n\rangle\right) \geq 0$$

Because the smallest possible value of n is zero, the ground state of the harmonic oscillator has

$$E_0 = \tfrac{1}{2}\hbar\omega$$

So we conclude that the sequence must terminate with n = 0 and that the allowed values of n are nonnegative integers.

$$|1\rangle = a^\dagger |0\rangle$$

$$|2\rangle = \left(\frac{a^\dagger}{\sqrt{2}}\right)|1\rangle = \left[\frac{(a^\dagger)^2}{\sqrt{2}}\right]|0\rangle$$

$$|3\rangle = \left(\frac{a^\dagger}{\sqrt{3}}\right)|2\rangle = \left[\frac{(a^\dagger)^3}{\sqrt{3!}}\right]|0\rangle$$

$$\vdots$$

$$|n\rangle = \left[\frac{(a^\dagger)^n}{\sqrt{n!}}\right]|0\rangle$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$\langle n'|a|n\rangle = \sqrt{n}\,\delta_{n',\,n-1}$$

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$\langle n'|a^\dagger|n\rangle = \sqrt{n+1}\,\delta_{n',\,n+1}$$

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right)$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^\dagger)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

$$p = i\sqrt{\frac{m\hbar\omega}{2}}\,(-a + a^\dagger)$$

$$\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{n',\,n-1} + \sqrt{n+1}\,\delta_{n',\,n+1}\right)$$

$$\langle n'|p|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left(-\sqrt{n}\,\delta_{n',\,n-1} + \sqrt{n+1}\,\delta_{n',\,n+1}\right)$$

$$a|0\rangle = 0$$

$$\langle x'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\,\langle x'|\left(x + \frac{ip}{m\omega}\right)|0\rangle = 0$$

$$\left(x' + x_0^2\frac{d}{dx'}\right)\langle x'|0\rangle = 0$$

$$x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$$

$$\langle x'|0\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{x_0}}\right)\exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]$$

$$\langle x'|1\rangle = \langle x'|a^\dagger|0\rangle = \left(\frac{1}{\sqrt{2}\,x_0}\right)\left(x' - x_0^2\frac{d}{dx'}\right)\langle x'|0\rangle$$

$$\langle x'|2\rangle = \left(\frac{1}{\sqrt{2}}\right)\langle x'|(a^\dagger)^2|0\rangle = \left(\frac{1}{\sqrt{2!}}\right)\left(\frac{1}{\sqrt{2}\,x_0}\right)^2\left(x' - x_0^2\frac{d}{dx'}\right)^2\langle x'|0\rangle, \ldots$$

$$\langle x'|n\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{2^n n!}}\right)\left(\frac{1}{x_0^{n+1/2}}\right)\left(x' - x_0^2\frac{d}{dx'}\right)^n \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]$$

$$x^2 = \left(\frac{\hbar}{2m\omega}\right)(a^2 + a^{\dagger 2} + a^\dagger a + aa^\dagger)$$

$$\langle x^2\rangle = \frac{\hbar}{2m\omega} = \frac{x_0^2}{2}$$

$$\langle p^2\rangle = \frac{\hbar m\omega}{2}$$

When we take the expectation value of x^2 under ground state, $\langle 0|x^2|0\rangle$, only the last term in this relation yields a nonvanishing contribution:

It follows that the expectation values of the kinetic and the potential energies are, respectively, as expected from the virial theorem.

$$\left\langle \frac{p^2}{2m}\right\rangle = \frac{\hbar\omega}{4} = \frac{\langle H\rangle}{2}$$

$$\left\langle \frac{m\omega^2 x^2}{2}\right\rangle = \frac{\hbar\omega}{4} = \frac{\langle H\rangle}{2}$$

The virial theorem

$$\sum_i q_i \dot{p}_i = \mathcal{V} = -3NkT$$

$$\left\langle \sum_i p_i \frac{\partial H}{\partial p_i} \right\rangle = \left\langle \sum_i p_i \dot{q}_i \right\rangle = 3NkT$$

$$\left\langle \sum_i q_i \frac{\partial H}{\partial q_i} \right\rangle = -\left\langle \sum_i q_i \dot{p}_i \right\rangle = 3NkT$$

$$H = \sum_j A_j P_j^2 + \sum_j B_j Q_j^2$$

$$\sum_j \left(P_j \frac{\partial H}{\partial P_j} + Q_j \frac{\partial H}{\partial Q_j} \right) = \sum_j \left(P_j \left(2 A_j P_j \right) + Q_j \left(2 B_j Q_j \right) \right) =$$

$$= 2 \sum_j \left(A_j P_j^2 + B_j Q_j^2 \right) = \ 2H$$

$$\langle 2H \rangle = \left\langle \sum_j \left(P_j \frac{\partial H}{\partial P_j} + Q_j \frac{\partial H}{\partial Q_j} \right) \right\rangle$$

$$\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \delta_{ij} kT$$

$$\langle 2H \rangle = \left\langle \sum_j \left(P_j \frac{\partial H}{\partial P_j} + Q_j \frac{\partial H}{\partial Q_j} \right) \right\rangle$$

$$\langle 2H \rangle = 3NkT + 3NkT = 6NkT = fkT$$

$$\langle H \rangle = 3NkT = \frac{1}{2} fkT$$

$$\langle x \rangle = \langle p \rangle = 0$$

$$\langle (\Delta x)^2 \rangle = \langle x^2 \rangle = \frac{\hbar}{2m\omega}$$

$$\langle (\Delta p)^2 \rangle = \langle p^2 \rangle = \frac{\hbar m\omega}{2}$$

and we see that the uncertainty relation is satisfied in the minimum uncertainty product form:

$$\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \frac{\hbar^2}{4}$$

This is not surprising because the ground-state wave function has a Gaussian shape.

In contrast, the uncertainty products for the excited states are larger

$$\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \left(n + \tfrac{1}{2}\right)^2 \hbar^2$$

The Parabolic Potential Well

$$\psi_n(x) = \frac{1}{\sqrt{n!\sqrt{\pi}\,2^n}} e^{-x^2/2} H_n(x)$$

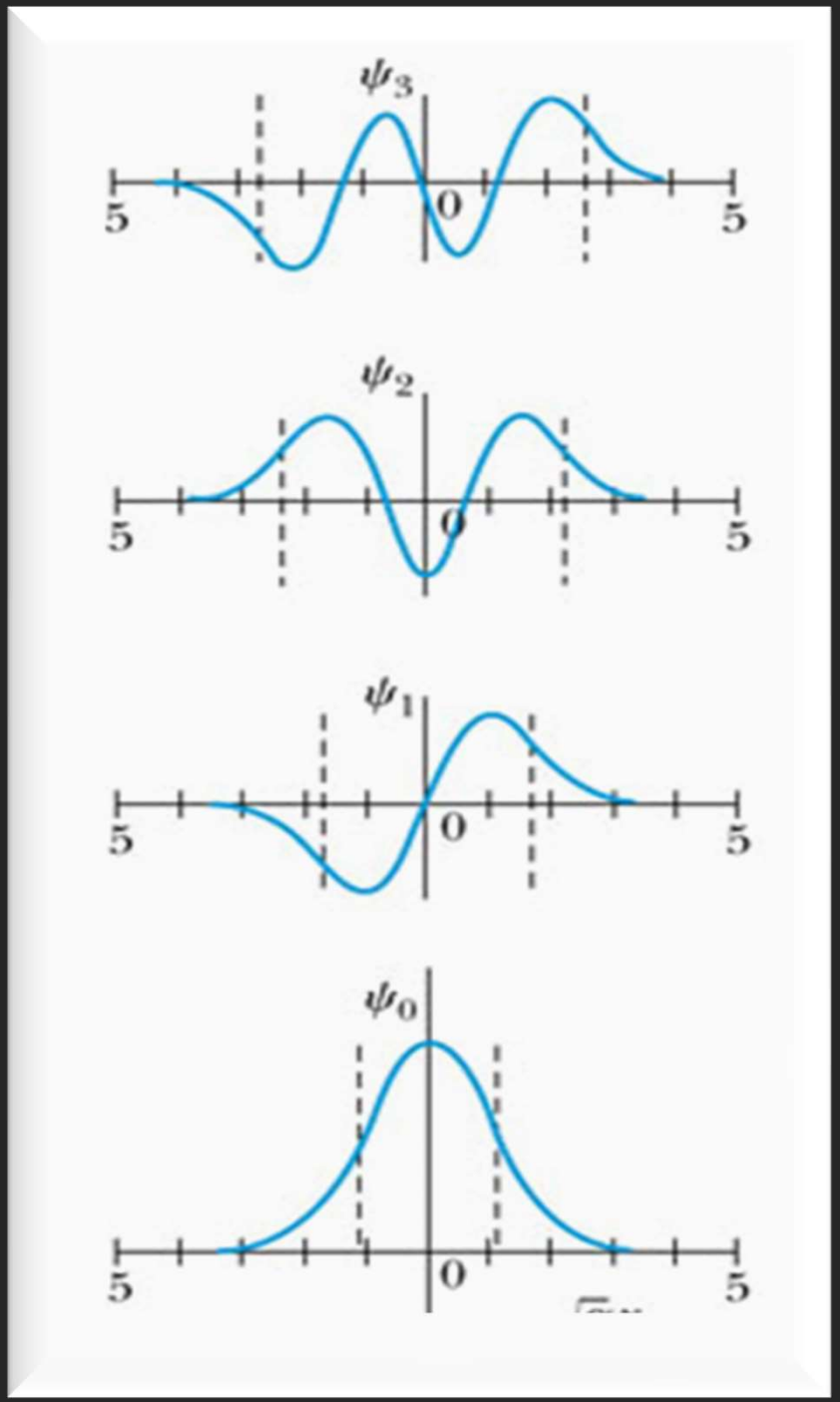
Wave functions

$$\psi_3(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} (\sqrt{\alpha}x)(2\alpha x^2 - 3) e^{-\alpha x^2/2}$$

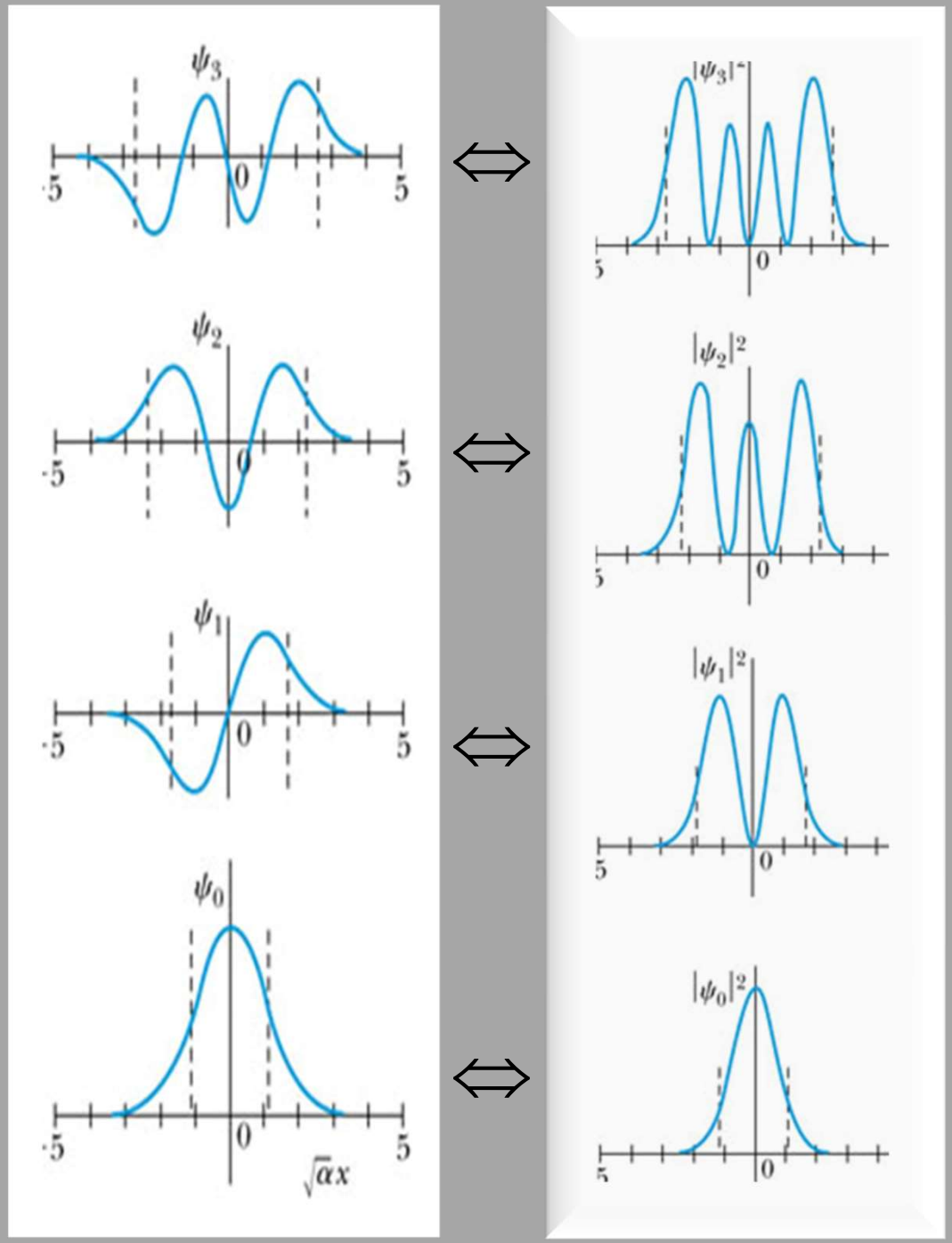
$$\psi_2(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} (2\alpha x^2 - 1) e^{-\alpha x^2/2}$$

$$\psi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}\, x e^{-\alpha x^2/2}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$



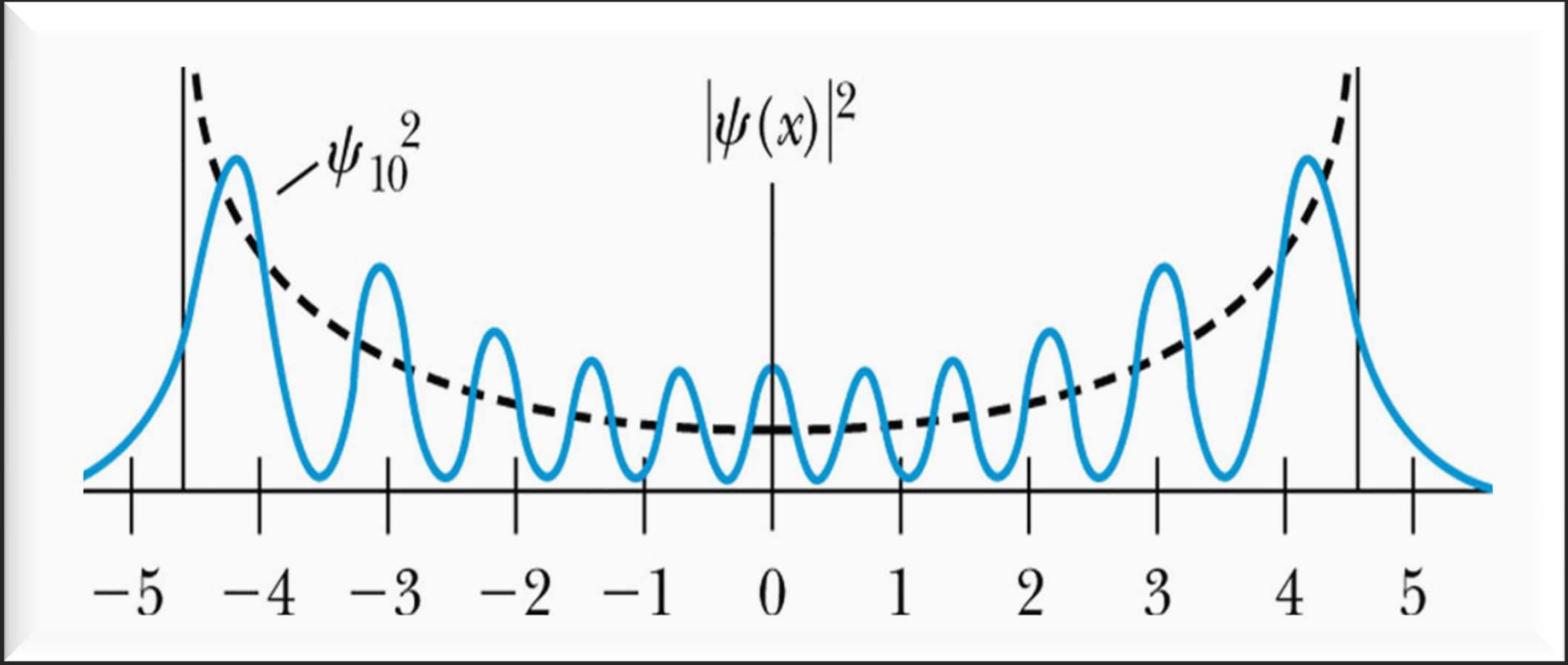
The Parabolic Potential Well



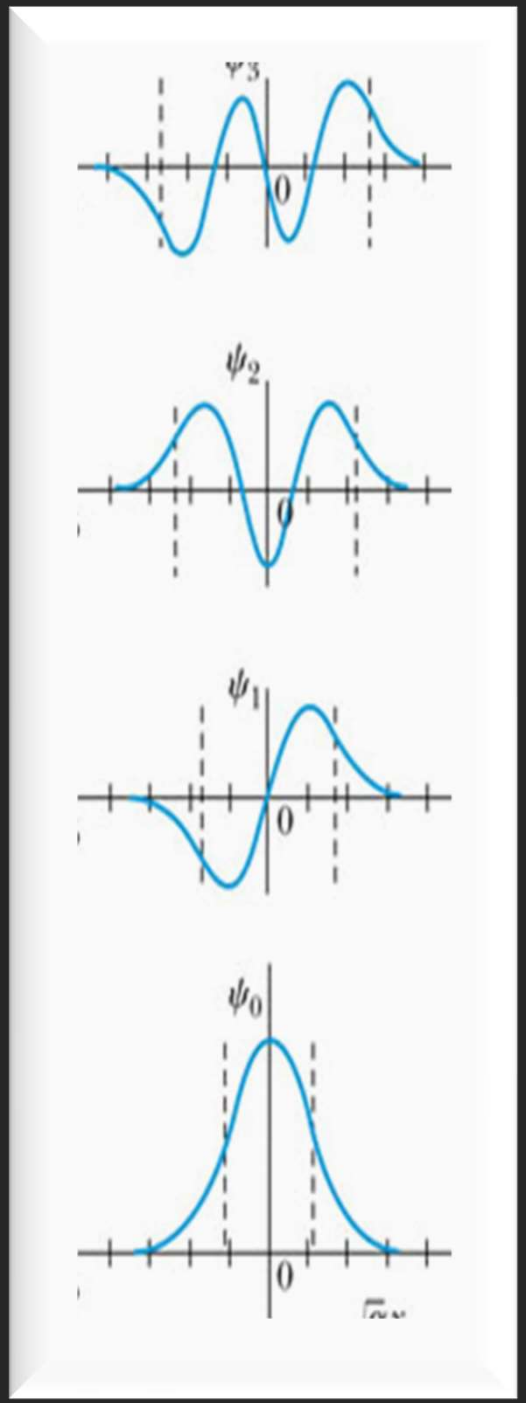
- Classically, the probability of finding the mass is greatest at the ends of motion and smallest at the center.
- Contrary to the classical one, the largest probability for this lowest energy state is for the particle to be at the center.

Analysis of the Parabolic Potential Well

As the quantum number increases, however, the solution approaches the classical result.

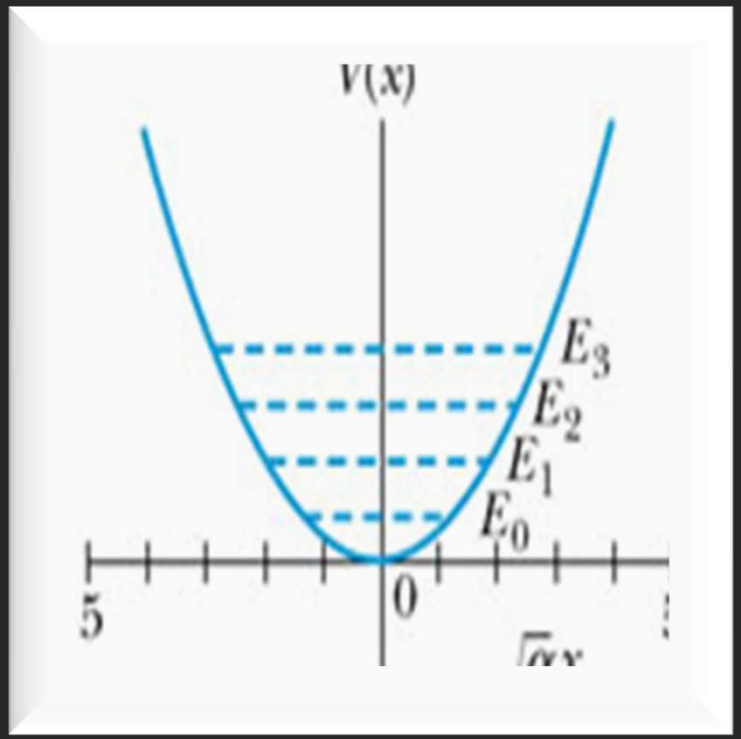


The Parabolic Potential Well



- The energy levels are given by:

$$E_n = (n + \tfrac{1}{2})\hbar\sqrt{\kappa / m} = (n + \tfrac{1}{2})\hbar\omega$$



The zero point energy is called the Heisenberg limit:

$$E_0 = \frac{1}{2}\hbar\omega$$

Time Development of the Oscillator

So far we have not discussed the time evolution of oscillator state kets nor of observables like x and p.

Everything we have done is supposed to hold at some instant of time, say at t = 0; the operators x, a, p, and a^+ are to be regarded either as Schrodinger-picture operators (at all t) or as Heisenberg-picture operators at t = 0.

In the remaining part of this section, we work exclusively in the Heisenberg picture, which means that x, p, a, and a^+ are all time-dependent even though we do not explicitly write $x^{(H)}(t)$, and so forth.

The Heisenberg equations of motion for p and x are,

$$\frac{dp}{dt} = -m\omega^2 x$$

$$\frac{dx}{dt} = \frac{p}{m}$$

This pair of coupled differential equations is equivalent to two uncoupled differential equations for a and a^{+}, namely,

$$\frac{da}{dt} = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{p}{m} - i\omega x\right) = -i\omega a$$

$$\frac{da^{\dagger}}{dt} = i\omega a^{\dagger}$$

$$a(t) = a(0)\exp(-i\omega t)$$

$$a^{\dagger}(t) = a^{\dagger}(0)\exp(i\omega t)$$

Incidentally, these relations explicitly show that N and H are time-independent operators even in the Heisenberg picture, as they must be.

$$x(t) + \frac{ip(t)}{m\omega} = x(0)\exp(-i\omega t) + i\left[\frac{p(0)}{m\omega}\right]\exp(-i\omega t)$$

$$x(t) - \frac{ip(t)}{m\omega} = x(0)\exp(i\omega t) - i\left[\frac{p(0)}{m\omega}\right]\exp(i\omega t)$$

$$x(t) = x(0)\cos\omega t + \left[\frac{p(0)}{m\omega}\right]\sin\omega t$$

$$p(t) = -m\omega x(0)\sin\omega t + p(0)\cos\omega t$$

These look the same as the classical equations of motion. We see that the x and p operators "oscillate" just like their classical analogues.

For pedagogical reasons we now present an alternative derivation of the above relation for x(t).

Instead of solving the Heisenberg equation of motion, we attempt to evaluate

$$x(t) = \exp\left(\frac{iHt}{\hbar}\right)x(0)\exp\left(\frac{-iHt}{\hbar}\right)$$

$$\exp(iG\lambda)A\exp(-iG\lambda) = A + i\lambda[G,A] + \left(\frac{i^2\lambda^2}{2!}\right)[G,[G,A]] + \cdots + \left(\frac{i^n\lambda^n}{n!}\right)[G,[G,[G,\ldots[G,A]]]\ldots] + \cdots,$$

$$\exp\left(\frac{iHt}{\hbar}\right)x(0)\exp\left(\frac{-iHt}{\hbar}\right)$$

Baker-Hausdorff lemma

$$= x(0) + \left(\frac{it}{\hbar}\right)[H, x(0)] + \left(\frac{i^2t^2}{2!\hbar^2}\right)[H, [H, x(0)]] + \cdots$$

Each term on the right-hand side can be reduced to either x or p by repeatedly using

$$[H, x(0)] = \frac{-i\hbar p(0)}{m}$$

$$[H, p(0)] = i\hbar m\omega^2 x(0)$$

Thus

$$\exp\left(\frac{iHt}{\hbar}\right)x(0)\exp\left(\frac{-iHt}{\hbar}\right) = x(0) + \left[\frac{p(0)}{m}\right]t - \left(\frac{1}{2!}\right)t^2\omega^2 x(0) - \left(\frac{1}{3!}\right)\frac{t^3\omega^2 p(0)}{m} + \cdots$$

$$= x(0)\cos\omega t + \left[\frac{p(0)}{m\omega}\right]\sin\omega t$$

Ok

From the following relations:

$$x(t) = x(0)\cos\omega t + \left[\frac{p(0)}{m\omega}\right]\sin\omega t$$

$$p(t) = -m\omega x(0)\sin\omega t + p(0)\cos\omega t$$

one may be tempted to conclude that (x) and (p) always oscillate with angular frequency ω.

However, this inference is not correct.

Take any energy eigenstate characterized by a definite value of n; the expectation value $\langle n|x(t)|n\rangle$ vanishes because the operators x(0) and p(0) change n by ±1 and $|n\rangle$ and $|n+1\rangle$ are orthogonal.

This point is also obvious from our earlier conclusion that the expectation value of an observable taken with respect to a stationary state does not vary with time.

To observe oscillations reminiscent of the classical oscillator, we must look at a superposition of energy eigenstates such as

$$|\alpha\rangle = c_0|0\rangle + c_1|1\rangle$$

The expectation value of x(t) taken with respect to the above ket does oscillate, as the reader may readily verify.

We have seen that an energy eigenstate does not behave like the classical oscillator—in the sense of oscillating expectation values for x and p—no matter how large n may be.

We may logically ask, How can we construct a superposition of energy eigenstates that most closely imitates the classical oscillator?

In wave-function language, we want a wave packet that bounces back and forth without spreading in shape.

It turns out that a coherent state defined by the eigenvalue equation for the non-Hermitian annihilation operator a,

$$a|\lambda\rangle = \lambda|\lambda\rangle$$

with, in general, a complex eigenvalue λ does the desired job.

The coherent state has many other remarkable properties:

1. When expressed as a superposition of energy (or N) eigenstates,

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle$$

the distribution of $|f(n)|^2$ with respect to n is of the Poisson type about some mean value n:

$$|f(n)|^2 = \left(\frac{\bar{n}^n}{n!}\right)\exp(-\bar{n})$$

2. It can be obtained by translating the oscillator ground state by some finite distance.

3. It satisfies the minimum uncertainty product relation at all times.

A systematic study of coherent states, pioneered by R. Glauber, is very rewarding; the reader is urged to work out an exercise on this subject at the end of this chapter.*