

**Problems:**

5.25, 6.29, 6.30, 6.24 (again), 6.32 (again), 6.33, 8.1, 8.5, 8.10, 8.12

Extend problems 6.32 (Hint problem 6.33 expects you to recall that for a particle attached to a spring the average kinetic energy equals the average potential energy. Below I ask you to show this directly.)

- Verify that the ground state wave function of the simple harmonic oscillator is a solution of the Schrödinger equation.
- Compute the average potential energy of the oscillator. Express your answer in terms of  $\hbar, \omega_o$  (Hint  $PE = \frac{1}{2}kx^2$ . (Answer  $\hbar\omega_o/4$ )
- (easy) Show that

$$\frac{\mathbb{P}^2}{2M} = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} \quad (1)$$

- (straight forward) Compute the following

$$\frac{\mathbb{P}^2}{2M} \psi(x) \quad (2)$$

which is the Kinetic energy operator acting on the wave function. Answer:

$$\frac{\hbar^2}{2ML^2} \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{y^2}{2}} (1 - y^2)$$

- Compute the average kinetic energy of the ground state wave function. (Answer  $\langle KE \rangle = \hbar\omega_o/4$ )
- Estimate using the uncertainty principle the typical momentum of an electron attached to a spring.
- In momentum space the ground wave function of the simple harmonic oscillator is

$$\hat{\psi}(p) = \pi^{1/4} \sqrt{2L} e^{-\frac{1}{2}\left(\frac{Lp}{\hbar}\right)^2} \quad (3)$$

Show this, if you can. You should see the typical momentum you estimated inside the argument of the exponential.

- Then since  $|\psi(p)|^2 \frac{dp}{2\pi\hbar}$  is the probability that the particle has momentum between  $p$  and  $p + dp$ ,  $\langle p^2 \rangle$  is

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} p^2 |\psi(p)|^2 \quad (4)$$

Compare  $\langle p^2 \rangle / (2M)$  to the average kinetic computed above. They should agree

**Time Dependent Schrödinger Equation**

1. The time dependent Schrödinger Equation is

$$\left[ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t) = +i\hbar \frac{\partial}{\partial t} \psi(x, t) \quad (5)$$

2. Stationary (probabilities don't change) wave functions are of the form

$$\psi(x, t) = e^{-iE_n t} \hbar \psi_n(x) \quad (6)$$

where  $\psi_n(x)$  satisfies the time independent Schrödinger equation

$$\left[ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi_n(x) = E_n \psi_n(x) \quad (7)$$

3. If the wave function is localized in time then its energy (or frequency) is not very well known.

$$\Delta E \Delta t \sim \hbar \quad (8)$$

## Finite Box

1. A particle can penetrate into the classically forbidden region where  $V(x) > E$ , i.e. the potential energy of the particle is greater than its energy. In this region the wave function typically decays exponentially,

$$\psi(x) \sim e^{-\frac{x}{\delta}} \quad (9)$$

where the penetration depth is  $\delta$

$$\delta = \sqrt{\frac{\hbar^2}{2M(V-E)}} \quad (10)$$

You should be able to show this from the time independent Schrödinger equation.

## The simple harmonic Oscillator

1. For a particle connected to a spring (e.g. a molecule stretching back and forth) the spring constant  $k$  determines the oscillation frequency

$$\omega_o = \sqrt{\frac{k}{M}} \quad (11)$$

where the potential energy is  $U_{\text{sp}} = \frac{1}{2} k x^2$ .

2. For a quantum particle attached to a spring the characteristic size of the wave function is

$$L = \sqrt{\frac{\hbar}{M\omega_o}} \quad (12)$$

At this point the kinetic energy balances the potential energy i.e. (remember  $(1/2)kx^2 = (1/2)m\omega_o^2x^2$ )

$$\frac{\hbar^2}{2ML^2} = \frac{1}{2}m\omega_o^2L^2 \quad (13)$$

3. The wave functions of the simple harmonic oscillator are given on the next page. In this figure

$$y = \frac{x}{L} \quad \text{with} \quad L = \sqrt{\frac{\hbar}{M\omega_o}} \quad \alpha = \frac{1}{L^2} \quad (14)$$

4. The energies of the simple harmonic oscillator are

$$E_n = \hbar\omega_o \left( n + \frac{1}{2} \right) \quad n = 0, 1, 2, \dots \quad (15)$$

## The 3D Particle in the Box

We will discuss a square box  $L_x = L_y = L_z = L$  but you should be able to generalize this to a rectangular box

1. The wave functions are described by three quantum numbers  $n_x, n_y, n_z$  and are

$$\psi_{n_x, n_y, n_z}(x, y, z) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n_x}{L}x\right) \times \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n_y}{L}y\right) \times \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n_z}{L}z\right) \times \quad (16)$$

with

$$n_x, n_y, n_z = 1, 2, 3, \dots \quad (17)$$

The Energies are

$$E_{n_x, n_y, n_z} = KE_x + KE_y + KE_z \quad (18)$$

$$= \frac{\hbar^2 k_x^2}{2M} + \frac{\hbar^2 k_y^2}{2M} + \frac{\hbar^2 k_z^2}{2M} \quad (19)$$

with

$$k_x = \frac{\pi n_x}{L} \quad k_y = \frac{\pi n_y}{L} \quad k_z = \frac{\pi n_z}{L} \quad (20)$$

## Quantum Harmonic Oscillator: Wavefunctions

The [Schrodinger equation](#) for a [harmonic oscillator](#) may be solved to give the wavefunctions illustrated below.

[Comparison of classical and quantum probabilities](#)

*First four harmonic oscillator normalized wavefunctions*

$$\Psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-y^2/2}$$

$$\Psi_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2}y e^{-y^2/2}$$

$$\Psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}}(2y^2 - 1)e^{-y^2/2}$$

$$\Psi_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}}(2y^3 - 3y)e^{-y^2/2}$$

$$\alpha = \frac{m\omega}{\hbar} \quad y = \sqrt{\alpha} x$$

The solution of the Shrodinger equation for the first four energy states gives the normalized wavefunctions at left. These functions are plotted at left in the above illustration. The probability of finding the oscillator at any given value of x is the square of the wavefunction, and those squares are shown at right above. Note that the wavefunctions for higher n have more "humps" within the potential well. This corresponds to a shorter wavelength and therefore by the [deBroglie relationship](#) they may be seen to have a higher momentum and therefore higher energy.

The most probable value of position for the lower states is very different from the classical harmonic oscillator where it spends more time near the end of its motion. But as the quantum number

[Index](#)

[Schrodinger equation concepts](#)

References

[Beiser, Perspectives](#)  
Sec 8-7

[Thornton & Rex](#)  
Sec 7-6

2. Some wave functions can have the same energy which is known as a degeneracy. For instance the following three states are degenerate for a square box

$$E_{211} = E_{121} = E_{112} = \frac{\hbar^2 \pi^2}{2ML^2} 6 \tag{21}$$

This is a consequence of the fact that the x direction is no different from the y (or z direction). There is a symmetry in the problem