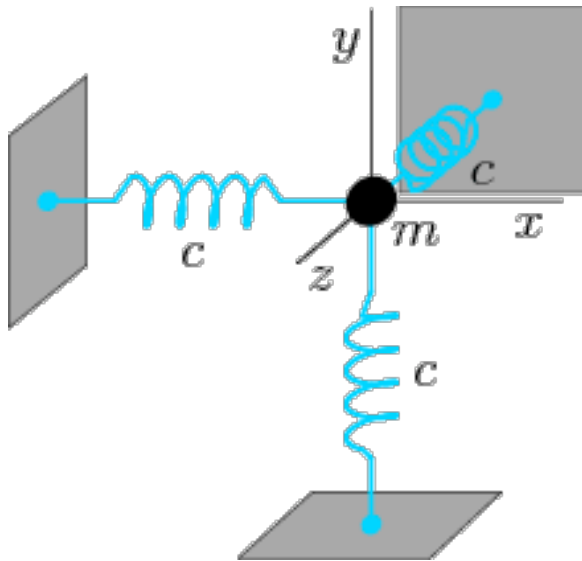


Simple Harmonic Oscillation (SHO)

- Homework set 10 is due today.
- Still have some midterms to return.
- Some Material Covered today is not in the book
- Homework Set #11 will be available later today



Classical picture of a Harmonic Oscillator

When should homework #11 be turned in? We have two more homework assignments this semester.

- A. Friday, Nov. 22
- B. Monday, Dec. 2

Friday Facts

- **Thomas Edison**

He invented the first electric light bulb.

He invented the movie camera.

He invented the fluoroscope.

He invented the re-chargeable battery.

He had more than 1300 patents in his lifetime.

Nicknamed his first two sons Dot and Dash.



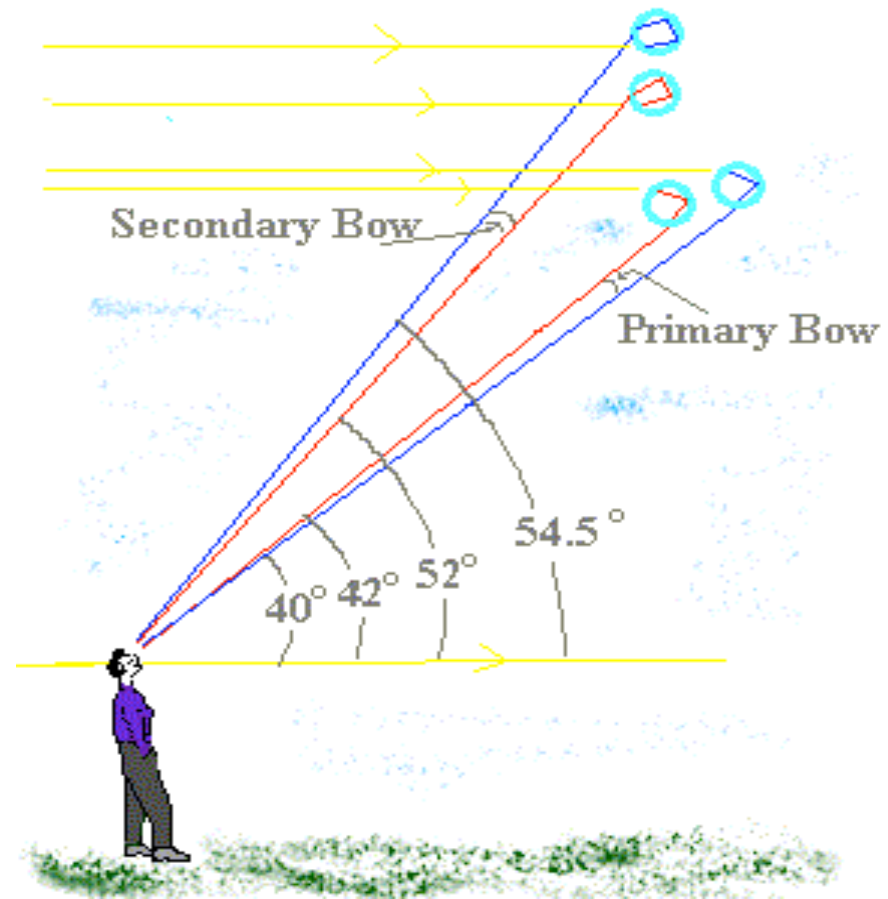
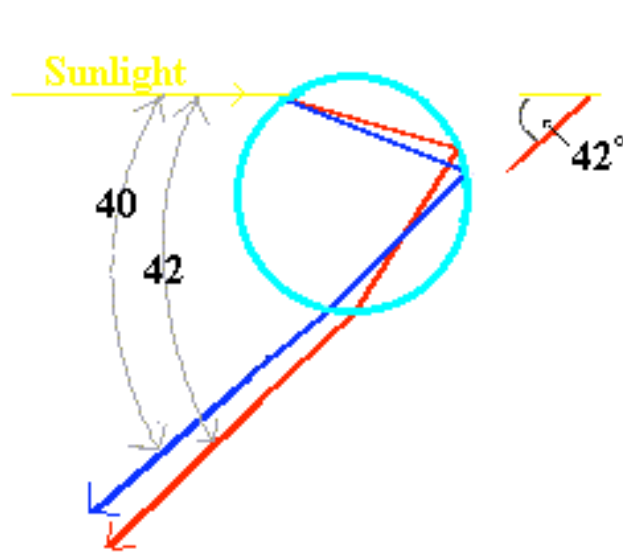
More facts

- **The first emails** could only be sent to someone using the same local host with two computers literally side by side. In late 1971 Raymond S Tomlinson sent the first useful email to a user separated from the same host by simply implementing a minor addition to the protocol that was being used and chose to use the @ sign in the email address

The Apple II had a hard drive of only 5 megabytes when it was launched.

A dentist is the inventor of the electric chair.

Description of Rainbow



Lunar Rainbow or Moonbow



A moonbow (also known as a lunar rainbow or white rainbow) is a rainbow that occurs at night. Moonbows are relatively faint, due to the smaller amount of light from the Moon. As with rainbows, they are in the **opposite part of the sky** from the moon. This picture was taken looking south, the Southern Cross can be seen to the left of center along with some of the brighter stars in the constellation of Centaurus. (Taken from Starry Night Skies Photography <http://www.colorado.edu/physics/phys2170/> Website)

Double Rainbow –over Lake Tahoe

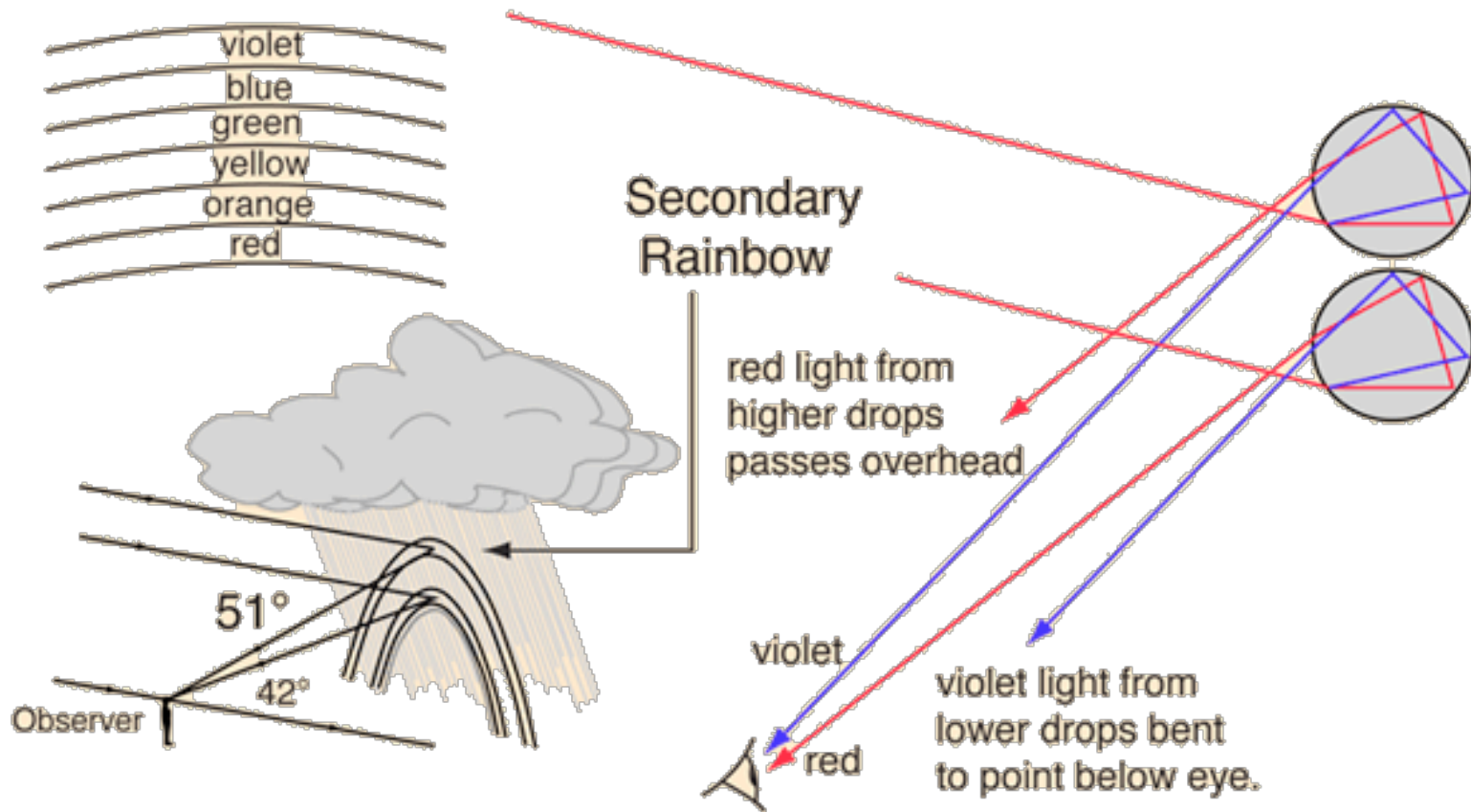


<http://www.colorado.edu/physics/phys2170/>

Double Rainbow



Secondary Rainbow



Double Rainbow Picture



<http://www.colorado.edu/physics/phys2170/>

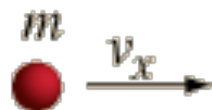
Level of Importance of states

- Have been talking about atoms, but want to say a few words about importance of energy levels and the physics behind them. Molecules have quantum energy levels. There are
- Electronic states ~ levels on order eV
- Vibrational states ~ levels on order $\sim .01 - 1$ eV
 $10^{12} - 10^{14}$ Hz
- Rotational states ~ levels on order $\sim .001$ eV –
 $10^{10} - 10^{11}$ Hz
- Let's tackle rotational states first ---

Rotational States

Linear momentum

$$p_x = mv_x$$

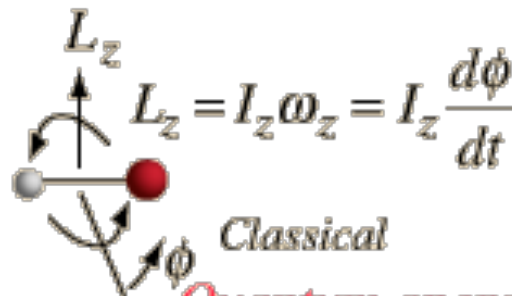


Classical

Quantum operator

$$P_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

Angular momentum



Classical

Quantum operator

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

Rotational kinetic energy $\frac{1}{2} I \omega^2 = \frac{L^2}{2I}$



Hamiltonian Operator

$$H_{op} = \frac{\hbar^2}{2I} \frac{\partial^2}{\partial \phi^2}$$

Schrodinger equation: $H_{op} \Psi = \frac{L_{op}^2}{2I} \Psi = \frac{J(J+1)\hbar^2}{2I} \Psi$

Energy eigenvalues: $E_J = J(J+1) \frac{\hbar^2}{2I}$

Rotational States

- Molecules can rotate like classical rigid bodies subject to the constraint that angular momentum is quantized in units of \hbar .

- We estimate the energy by $E = \frac{1}{2}I\omega^2; L = I\omega; E = \frac{1}{2}\frac{L^2}{I}$
- $$E_{rot} = \frac{1}{2}\frac{L^2}{I} = \frac{l(l+1)\hbar^2}{2I} \approx \frac{\hbar^2}{2Ma_0^2} = \frac{m}{M}\frac{\alpha^2 mc^2}{2} \approx \frac{m}{M}E \approx \frac{1}{1000}eV$$
- We use $I = Ma_0^2$ and $a_0 = \frac{\hbar}{\alpha mc} = \hbar^2/(ke^2m_e)$

- where M is mass of molecule and m is mass of the electron and $\alpha = ke^2/(\hbar c)$ called “fine structure-constant” $\approx 1/137$

Rotational States (cont.)

$$E = \frac{\ell(\ell + 1)\hbar^2}{2I}$$

Look at energy changes with $\Delta\ell = 1$ these states are strongly excited at room temperature

$$\Delta E = \frac{\hbar^2}{2I} [\ell(\ell + 1) - (\ell - 1)\ell] = \frac{\hbar^2}{2I} (2\ell) = \frac{\hbar^2 \ell}{I}$$

With identical nuclei ℓ has to be even or odd, so steps are $\frac{2\hbar^2 \ell}{I}$.

These states also have equal energy steps in emitted photon energy.

Rotational States

- A complex molecule will have three principal axes, and hence, three moments of inertia to use in our quantized formula.
- Counting degrees of freedom, which should be equal to the number of quantum numbers needed to describe the state, we have 3 coordinates to give the position of the center of mass, 3 for the rotational state, and $3N-6$ for vibrational. This formula should be modified if the molecule is too simple to have three principal axes.

Absorption Spectrum of Water

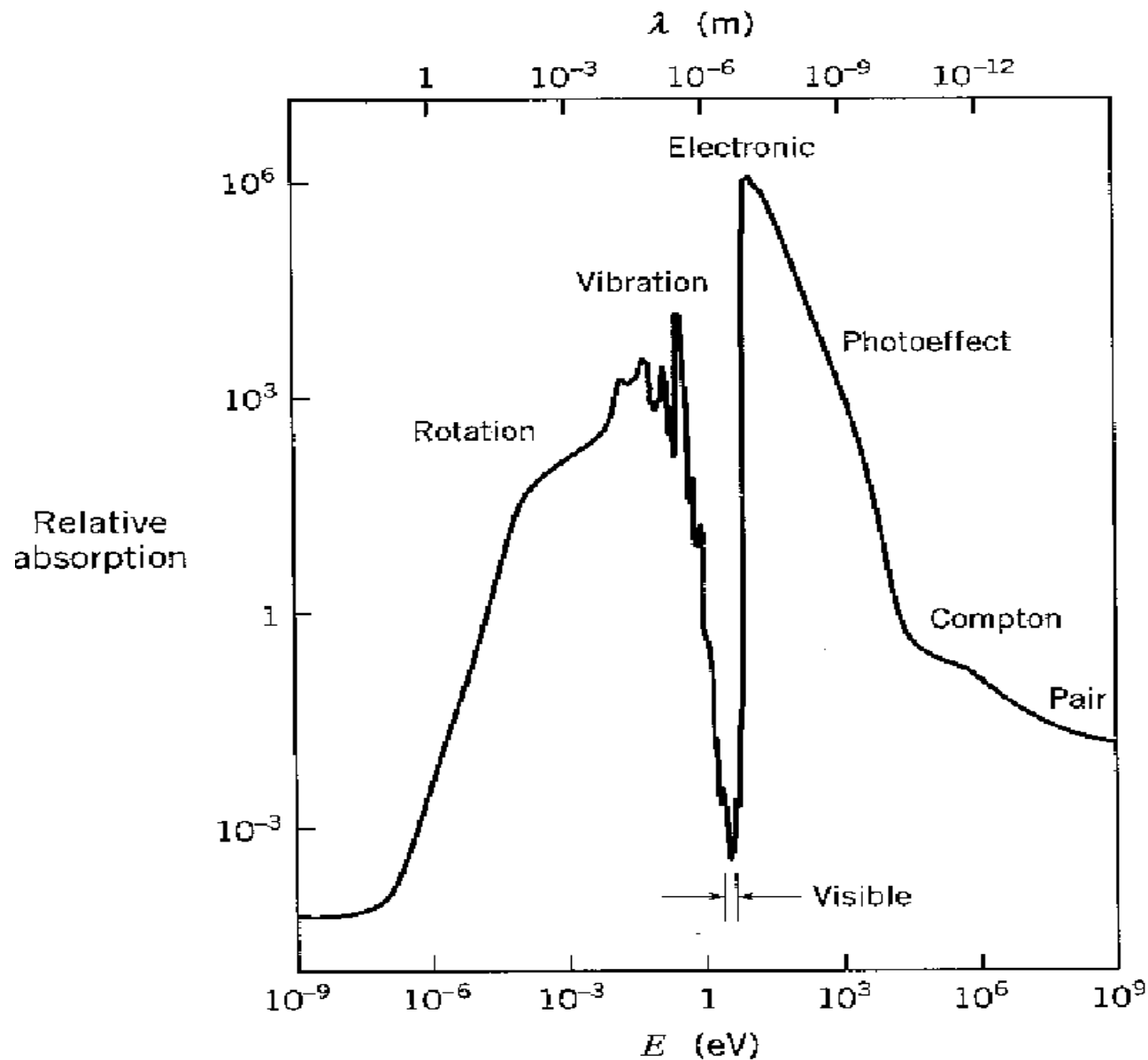


FIGURE 10-15 Absorption spectrum of water.

SHO Background – 1 dimension

- The simple harmonic oscillator potential is of great importance because it can be used to satisfy a broad class of problems in which a particle is oscillating about a position of stable equilibrium. At position of stable equilibrium, $V(x)$ must have a minimum.
- For any $V(x)$ which is continuous, the shape of the potential near the minimum can be approximated by a parabola.

$$U(x) = \frac{1}{2}kx^2$$

- If a particle of mass m is displaced by x_0 from equilibrium, it will oscillate with frequency

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

Harmonic Oscillator Potential

FIGURE 41.20 The potential energy of a harmonic oscillator.

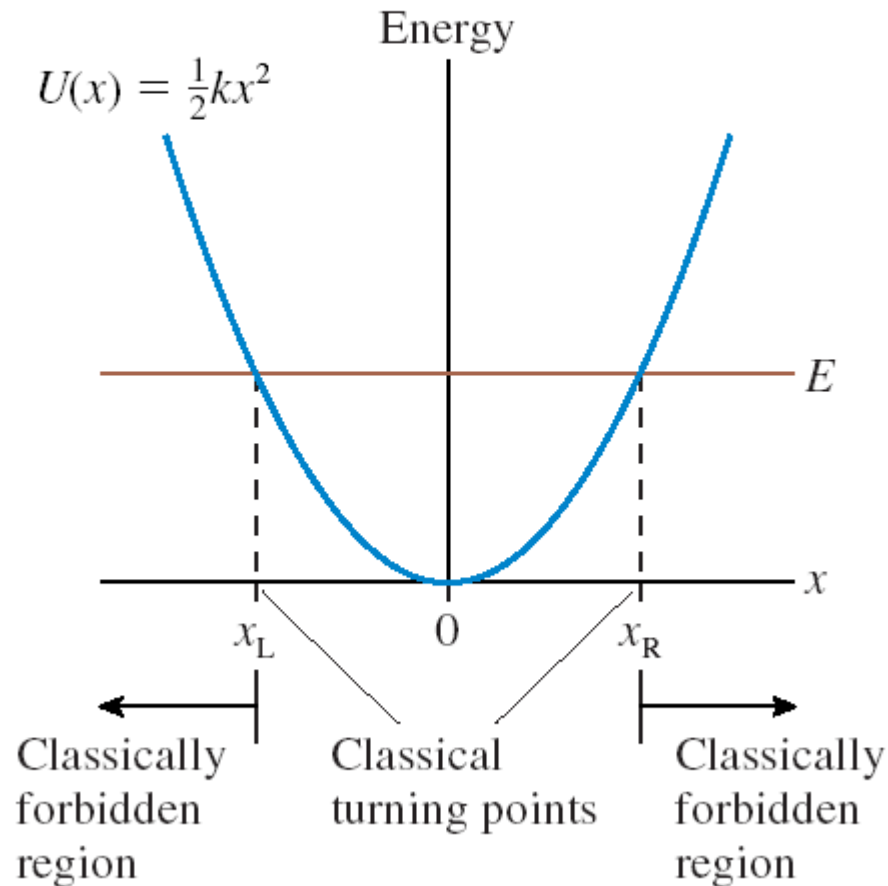
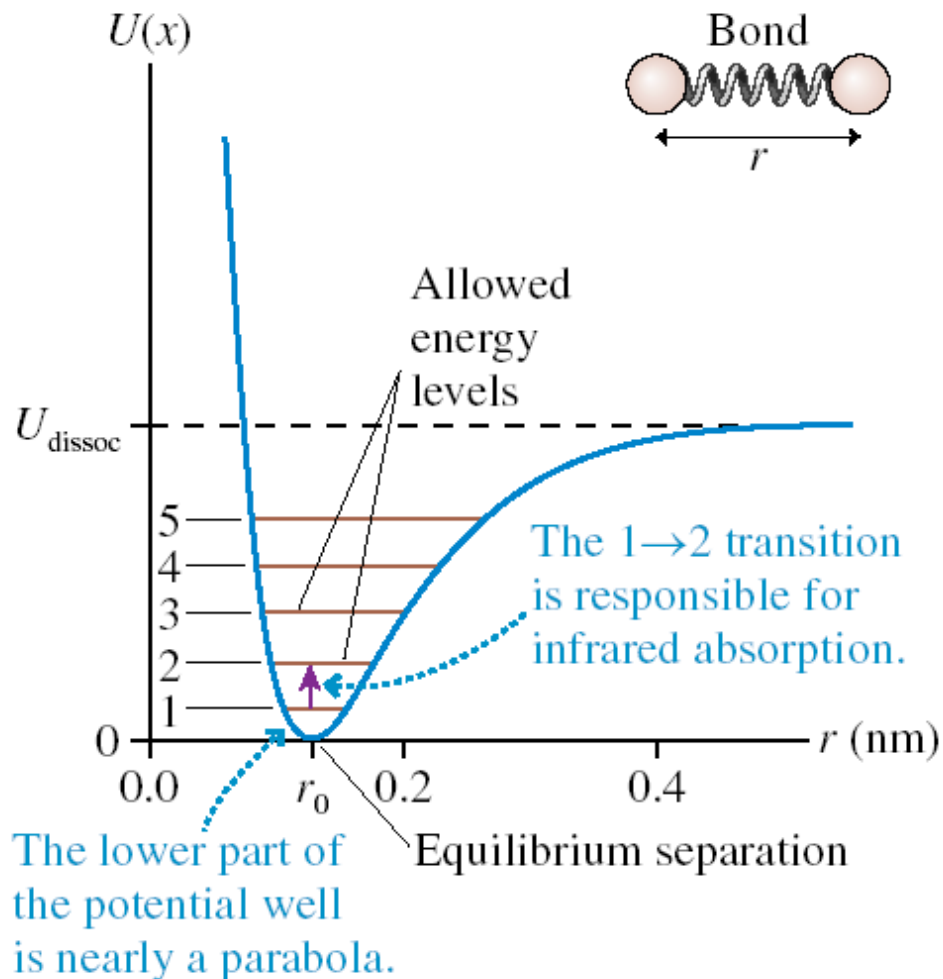


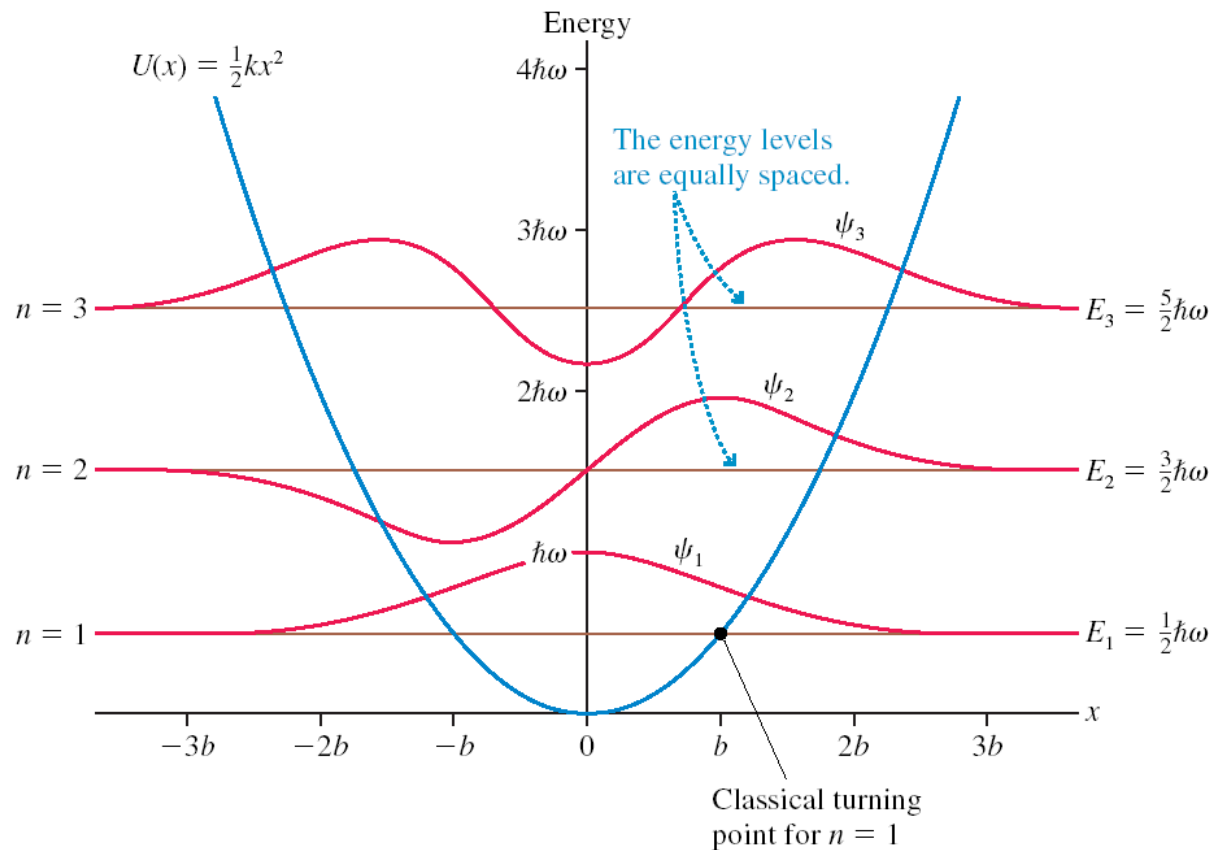
FIGURE 41.23 The potential energy of a molecular bond and a few of the allowed energies.



The energy-level spacing for the harmonic oscillator is constant. Expect the energy levels to diverge less rapidly than those for the square well because the higher energy states in the harmonic oscillator have effectively larger “boxes” than do the lower states (that is, the more energetic the oscillator, the more widely separated are its classical turning points).

The harmonic oscillator has finite zero-point energy.

FIGURE 41.21 The first three energy levels and wave functions of a quantum harmonic oscillator.



The wavefunctions for the harmonic oscillator are either symmetric or antisymmetric under reflection through $x=0$.

Harmonic Oscillator Potential

- The particle has a finite probability of being found beyond the classical turning points; it penetrates the barrier. This is to be expected on the basis of earlier considerations since the barrier is not infinite at the classical turning point.
- In the lowest-energy state the probability distribution favors the particle being in the low-potential central region of the well, while at higher energies the distribution approaches more nearly the classical result of favoring the higher potential regions .

The Quantum Harmonic Oscillator

The wave functions of the first three states are

$$\psi_1(x) = A_1 e^{-x^2/2b^2}$$

$$\psi_2(x) = A_2 \frac{x}{b} e^{-x^2/2b^2}$$

$$\psi_3(x) = A_3 \left(1 - \frac{2x^2}{b^2} \right) e^{-x^2/2b^2}$$

$$b = \sqrt{\frac{\hbar}{m\omega}}$$

$$E_n = \left(n - \frac{1}{2} \right) \hbar\omega \quad n = 1, 2, 3, \dots$$

Where $\omega = (k/m)^{1/2}$ is the classical angular frequency, and n is the quantum number

Simple Harmonic Oscillator

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

$$\psi_2(x) = A_2 \frac{x}{b} e^{-x^2/2b^2}; E = \frac{3}{2}\hbar\omega$$

$$\frac{d\psi_2(x)}{dx} = A_2 \left(\frac{1}{b} - \frac{x^2}{b^3} \right) e^{-x^2/2b^2}$$

$$\frac{d^2\psi_2(x)}{dx^2} = A_2 \left(-\frac{3x}{b^3} + \frac{x^3}{b^5} \right) e^{-x^2/2b^2} = A_2 \left(-\frac{3}{b^2} + \frac{x^2}{b^4} \right) \frac{x}{b} e^{-x^2/2b^2}$$

$$-\frac{2m}{\hbar^2} \left(E - \frac{1}{2}kx^2 \right) = -\frac{3}{b^2} + \frac{x^2}{b^4}$$

$$\frac{2m}{\hbar^2} E = \frac{3}{b^2}; \quad \frac{mk}{\hbar^2} = \frac{1}{b^4}$$

$$E = \frac{3\hbar^2}{2mb^2} = \frac{3\hbar^2}{2m} \frac{\sqrt{mk}}{\hbar} = \frac{3\hbar}{2} \sqrt{\frac{k}{m}} = \frac{3}{2}\hbar\omega$$

Light emission by an oscillating electron

The emitted photon has energy $E_{\text{photon}} = hf_{\text{ph}} = \Delta E$. Thus

$$\hbar\omega_e = \frac{h}{2\pi}\omega_e = hf_{\text{ph}} = \frac{hc}{\lambda}$$

The wavelength of the light is $\lambda = 600$ nm, so the classical angular frequency of the oscillating electron is

$$\omega_e = 2\pi\frac{c}{\lambda} = 3.14 \times 10^{15} \text{ rad/s}$$

The electron's angular frequency is related to the spring constant of the restoring force by

$$\omega_e = \sqrt{\frac{k}{m}}$$

Thus $k = m\omega_e^2 = 9.0$ N/m.

The Quantum Harmonic Oscillator

The time independent Schrödinger equation for a quantum harmonic oscillator is

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} \left(E - \frac{1}{2}kx^2 \right) \psi(x)$$
$$\frac{d^2\psi}{dx^2} + \left[\frac{2mE}{\hbar^2} - \left(\frac{\omega m}{\hbar} \right)^2 x^2 \right] \psi = 0$$

Define $\alpha \equiv \frac{m\omega}{\hbar}$ + $\beta \equiv \frac{2mE}{\hbar^2}$ $\frac{\beta}{\alpha} = \frac{2mE}{\hbar^2} \frac{\hbar}{m\omega} = \frac{2E}{\hbar\omega}$

$$\frac{d^2\psi}{dx^2} + [\beta - \alpha^2 x^2] \psi = 0$$

QHO solved

$$\frac{d^2\psi}{dx^2} + [\beta - \alpha^2 x^2]\psi = 0$$

Change variables to $\xi \equiv \sqrt{\alpha} x$

Then

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi} \frac{d\xi}{dx} = \sqrt{\alpha} \frac{d\psi}{d\xi} \quad \frac{d^2\psi}{dx^2} = \frac{d}{d\xi} \left(\frac{d\psi}{dx} \right) \frac{d\xi}{dx} = \alpha \frac{d^2\psi}{d\xi^2}$$

or

$$\frac{d^2\psi}{d\xi^2} + \left[\frac{\beta}{\alpha} - \xi^2 \right] \psi = 0 \quad \frac{\beta}{\alpha} = \frac{2mE}{\hbar^2} \frac{\hbar}{m\omega} = \frac{2E}{\hbar\omega}$$

For any finite value of E, the quantity β/α will be small compared to ξ^2 as ξ goes to ∞ , so

$$\psi(\xi) = B e^{-\xi^2/2}; \psi(\xi) = e^{-\xi^2/2} H(\xi)$$

QHO solved.....

$$\psi(\xi) = Be^{-\xi^2/2}; \psi(\xi) = e^{-\xi^2/2} H(\xi)$$

The $H(\xi)$ are functions which must at $|\xi| \rightarrow \infty$, be slowly Varying compared to $e^{-\xi^2/2}$. To evaluate these functions: We compute derivatives and factor out $e^{-\xi^2/2}$

$$e^{-\xi^2/2} \left[-H + \xi^2 H - 2\xi \frac{dH}{d\xi} + \frac{d^2 H}{d\xi^2} + \frac{\beta}{\alpha} H - \xi^2 H \right] = 0$$

$$\frac{d^2 H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + \left(\frac{\beta}{\alpha} - 1 \right) H = 0$$

Hermite's
Equation

QHO solved

$$\frac{d^2 H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + \left(\frac{\beta}{\alpha} - 1 \right) H = 0$$

$$H(\xi) = \sum_{k=0}^{\infty} a_k \xi^k \equiv a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 + \dots$$

$$\frac{dH}{d\xi} = \sum_{k=1}^{\infty} k a_k \xi^{k-1} \equiv a_1 + 2a_2 \xi + 3a_3 \xi^2 + \dots$$

$$\frac{d^2 H}{d\xi^2} = \sum_{k=2}^{\infty} (k-1) k a_k \xi^{k-2} \equiv 2a_2 + 2(3)a_3 \xi + 3(4)a_4 \xi^2 + \dots$$

For ξ power=0 $1 \cdot 2a_2 + (\beta/\alpha - 1)a_0 = 0$

For ξ power =1 $2 \cdot 3a_3 + (\beta/\alpha - 1 - 2 \cdot 1)a_1 = 0$

For ξ power =2 $3 \cdot 4a_4 + (\beta/\alpha - 1 - 2 \cdot 2)a_2 = 0$

For ξ power =3 $4 \cdot 5a_5 + (\beta/\alpha - 1 - 2 \cdot 3)a_3 = 0$

QHO solved

So we get

$$\frac{a_{k+2}}{a_k} = -\frac{\left(\frac{\beta}{\alpha} - 1 - 2k\right)}{(k+1)(k+2)}$$

If we wish to terminate the series, then $\frac{\beta}{\alpha} = 2k + 1$

This is our constraint which quantizes the energy

$$\frac{\beta}{\alpha} = \frac{2mE}{\hbar^2} \frac{\hbar}{m\omega} = \frac{2E}{\hbar\omega}$$

$$\text{or } E_n = (n+1/2)\hbar\omega$$