

Harmonic Oscillator

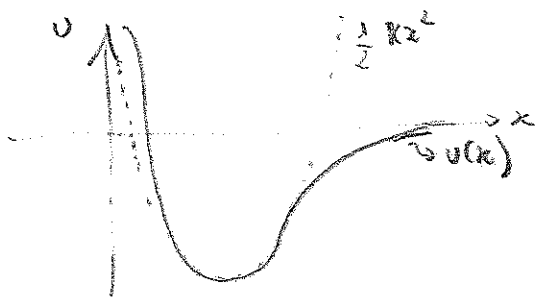
The harmonic oscillator is a particle subject to a linear force $F = -\kappa x$. This is a conservative force that can be derived from the potential energy $U = \frac{1}{2} \kappa x^2$. So we can easily write the Schrödinger Equation for the harmonic oscillator (and hence study how such a particle behaves in quantum mechanics).

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} \kappa x^2 \psi = i \hbar \frac{\partial \psi}{\partial t}$$

and the stationary states $\psi(x, t) = \psi_E(x) e^{-\frac{i}{\hbar} E t}$ satisfy

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_E}{\partial x^2} + \frac{1}{2} \kappa x^2 \psi_E = E \psi_E$$

This is a very important system because it can be used, as an approximation, to describe many real situations. In general the potential energy in the Schrödinger equation is a complicated function $U(x)$ and not just simply $\frac{1}{2} \kappa x^2$. But if $U(x)$ has a minimum for some x_m , around that value we can approximate it as $U(x) = U(x_m) + \frac{1}{2} \left. \frac{d^2 U}{dx^2} \right|_{x=x_m} (x-x_m)^2$



An example: the binding energy of diatomic molecules.

So we now want to solve the time-independent SE, which is a 2nd-order diff equation. So we expect that the solution

looks like $\psi_E(x) = A f(x) + B g(x)$. Let us check that the functions $e^{\pm 2ax^2}$ are both solutions if $a = \frac{\sqrt{\kappa m}}{2\hbar}$

$$\frac{d^2}{dx^2} e^{\pm 2ax^2} = \frac{d}{dx} (\pm 2a x e^{\pm 2ax^2}) = (\pm 2a + 4a^2 x^2) e^{\pm 2ax^2}$$

So the contribution of the kinetic energy is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_E}{dx^2} = \mp \frac{\hbar^2}{2m} 2a e^{\pm 2ax^2} - \frac{\hbar^2}{2m} 4a^2 x^2 e^{\pm 2ax^2}$$

Thus if $\frac{\hbar^2 4a^2}{m} = \kappa$ this second term just cancel the contribution of the potential energy $+\frac{1}{2} \kappa x^2 e^{\pm 2ax^2}$. So we get that $e^{\pm 2ax^2}$ solves the SE with $E = \mp \frac{\hbar^2 a}{m} = \mp \frac{\hbar}{2} \sqrt{\frac{\kappa}{m}}$

However the solution $e^{2ax^2} \rightarrow \infty$ as $x \rightarrow \pm\infty$ (since $a = \frac{\sqrt{\kappa m}}{2\hbar} > 0$)

and so we will never be able to impose the normalization condition $\int_{-\infty}^{+\infty} \psi^* \psi dx = 1$ on it... this solution must be neglected.

So we found a solution $f(x) = e^{-\frac{\sqrt{\kappa m}}{2\hbar} x^2}$ with energy $E = \frac{\hbar}{2} \sqrt{\frac{\kappa}{m}}$.

Of course there is a second solution $g(x)$ with the same energy which is not normalizable... thus we have to neglect it anyway

because $g(x) \rightarrow \infty$ as $x \rightarrow \pm \infty$ and would yield infinite probabilities - so we have that the only normalizable

solution of energy $\frac{\hbar}{2} \omega$ (with $\omega = \sqrt{\frac{k}{m}}$) is

$$\psi_0(x) = A e^{-\frac{\sqrt{km}}{2\hbar} x^2} \quad \text{with } A \text{ fixed by}$$

$$1 = A^* A \int_{-\infty}^{\infty} e^{-\frac{\sqrt{km}}{\hbar} x^2} = |A|^2 \left(\frac{\pi \hbar}{\sqrt{km}} \right)^{1/2} \Rightarrow A = \left(\frac{\sqrt{km}}{\pi \hbar} \right)^{1/2}$$

There are 2 important properties of the harmonic oscillator (stated but not proof):

1) $\psi_0(x)$ is the (normalizable) solution with lowest possible energy

2) All other (normalizable) solutions can be derived from $\psi_0(x)$

by acting with the operator $\left(-\frac{d}{dx} + 2ax\right)$ many times.

Example $\psi_1(x) \sim \left(\frac{d}{dx} + 2ax\right) = +4ax e^{-ax^2}$

$$\psi_2(x) \sim \left(-\frac{d}{dx} + 2ax\right) = (-4a + 16a^2 x^2) e^{-ax^2}$$

and $\psi_1(x)$ has energy $E_1 = \frac{3}{2} \hbar \omega$ and ψ_2 has $E = \frac{5}{2} \hbar \omega$.

In general $\left(-\frac{d}{dx} + 2ax\right)^n \psi_0(x)$ has energy $E_n = \hbar \omega \left(\frac{1}{2} + n\right)$.

So in a nut-shell: the harmonic oscillator has discrete energy

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

→ Go through the example 40.6
p. 1535 $\sqrt{9.3}$

B1.

(i) According to Newtonian mechanics the energy of an oxygen molecule in the harmonic oscillator approximation is

$$\frac{1}{2} m_0 v_1^2 + \frac{1}{2} m_0 v_2^2 + \frac{1}{2} k [(x_1 - x_2) - x_e]^2 = E$$

where $m_0 = 2.66 \times 10^{-26} \text{ Kg}$, $k = 1.1 \times 10^3 \frac{\text{N}}{\text{m}}$ and x_e is the equilibrium position.

We can rewrite E as follows

$$E = \frac{1}{2} M \left(\frac{v_1 + v_2}{2} \right)^2 + \frac{1}{2} M \left(\frac{v_1 - v_2}{2} \right)^2 + \frac{1}{2} k [(x_1 - x_2) - x_e]^2$$

where $M = 2 m_0$ is the total mass of the molecule, $\frac{v_1 + v_2}{2}$ is the velocity of the center of mass and $\frac{v_1 - v_2}{2} = \frac{d}{dt} (x_1 - x_2)$ represents the vibration. So the vibration

energy is $\frac{1}{2} \left(\frac{m_0}{2} \right) \left(\frac{d}{dt} (x_1 - x_2) \right)^2 + \frac{1}{2} k [(x_1 - x_2) - x_e]^2$ where $\frac{m_0}{2} = \mu$ is

called the reduced mass. Then the frequency is $\omega = \sqrt{\frac{k}{\mu}} = 2.9 \times 10^{14} \text{ /sec}$.

(ii) The energy level of a quantum harmonic oscillator are $\hbar \omega (n + \frac{1}{2})$ with

$$n = 1, 2, \dots \quad \text{so} \quad E_{n+1} - E_n = \hbar \omega = 3.06 \times 10^{-20} \text{ J}$$

(iii) In order to excite the vibration modes, we need to have a thermal energy of at least $\hbar \omega = 3.06 \times 10^{-20} \text{ J}$ for each molecule. This is

equivalent to a temperature $T = \frac{\hbar \omega}{k} = 2.22 \times 10^3 \text{ K}$ almost 10

times bigger than the room temperature $\sim 300 \text{ K}$.