$$\frac{d\,H_n(z)}{dz} = 2z\,H_n(z) - H_{n+1}(z)$$

$$\frac{d^2 H_n(z)}{dz^2} = 2(1+2z^2)\,H_n(z) - 4z\,H_{n+1}(z) + H_{n+2}(z)$$

$$H_{n+1}(z) - 2z\,H_n(z) + 2n\,H_{n-1}(z) = 0$$

$$\frac{d}{dz} H_n(z) = 2n\,H_{n-1}(z)$$

---

$$\int_{-\infty}^{\infty} \Psi_m^*(x)\, \Psi_n(x)\, dx = \delta_{m,n}$$

NOTICE THAT

$$\Psi_n(x) = \begin{cases} \text{IS EVEN IF } n \text{ IS EVEN} \\ \text{IS ODD IF } n \text{ IS ODD} \end{cases}$$

# EXPECTATION VALUES

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi_n^*(x) \; x \; \Psi_n(x) \; dx = 0$$

SINCE $\quad \Psi_n^*(x) \; x \; \Psi_n(x)$

is ODD.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \Psi_n^*(x) \; x^2 \; \Psi_n(x) \; dx$$

$$= \frac{\hbar}{\sqrt{\mu k}} \left(n + \frac{1}{2}\right) = \frac{1}{\alpha} (n + 1/2)$$

$$\boxed{\sigma_x^2 = \frac{1}{\alpha} (n + 1/2)}$$

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \Psi_n^*(x) \; \hat{p}_x \; \Psi_n(x) \; dx = 0$$

BECAUSE $\quad \hat{p}_x \Psi_n \sim \Psi_{n+1}, \; \Psi_{n-1}$

$$\langle \hat{p}^2 \rangle = \hbar \sqrt{\mu k} \left( n + \tfrac{1}{2} \right) = \hbar^2 \alpha (n + 1/2)$$

$$\sigma_p^{\,2} = \hbar^2 \alpha (n + 1/2)$$

$$\boxed{\sigma_x \sigma_p = \hbar (n + 1/2) \geq \frac{1}{2} \hbar}$$

$$\langle \hat{V} \rangle = \frac{1}{2} k \langle x^2 \rangle = \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} (n + 1/2)$$

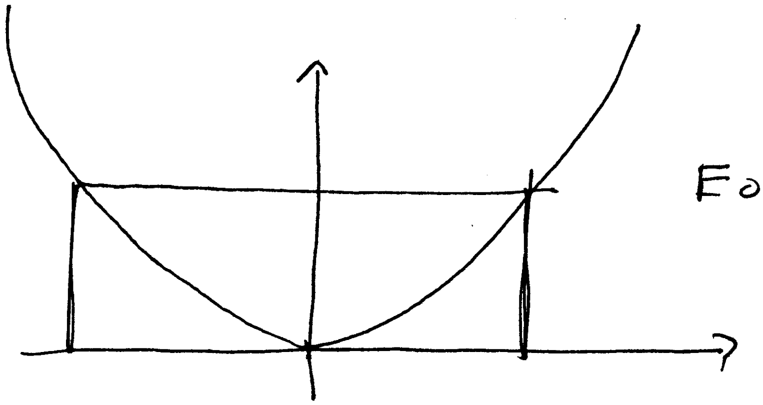
$$\boxed{\langle \hat{V} \rangle = \frac{1}{2} E_n}$$

$$\langle \hat{K} \rangle = \frac{1}{2\mu} \langle \hat{p}^2 \rangle = \frac{1}{2} \sqrt{\frac{k}{\mu}} (n + 1/2)$$

$$\boxed{\langle \hat{K} \rangle = \frac{1}{2} E_n}$$

$$\langle \hat{H} \rangle = \langle \hat{K} \rangle + \langle \hat{V} \rangle = E_n$$

CLASSICAL MAXIMUM DISPLACEMENT




CLASSICALLY

$$E_0 = \frac{1}{2} k A_{max}^2$$

$$A_{max} = \sqrt{\frac{2E_0}{k}}$$

$$= \sqrt{\frac{\cancel{2}}{k} \frac{1}{\cancel{2}} h \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}}$$

$$= \sqrt{\frac{\hbar}{\sqrt{k\mu}}}$$

$$\boxed{A_{max} = \frac{1}{\sqrt{\alpha}}} = 12.66 \text{ pm}$$

$$\mu = 8.5 \times 10^{-28} \text{ Kg}$$

$$\text{PROB}\left\{ x > \frac{1}{\sqrt{\alpha}} \; ; \; x < -\frac{1}{\sqrt{\alpha}} \right\} = P_{\text{FORBIDDEN}}$$

$$P_{\text{FORB}} = \int_{-\infty}^{-\frac{1}{\sqrt{\alpha}}} \Psi_0^*(x)\, \Psi_0(x)\, dx + \int_{\frac{1}{\sqrt{\alpha}}}^{\infty} \Psi_0^*(x)\, \Psi_0(x)\, dx$$

$$P_{\text{FORB}} = 0.16 \neq 0 \qquad n=0$$

# Chapter 1

# Three dimensional systems

In the case of three dimensions the momentum operator has three components {3d1}

$$\hat{p}_x = - i \hbar \frac{\partial}{\partial x} \tag{1.1}$$

$$\hat{p}_y = - i \hbar \frac{\partial}{\partial y} \tag{1.2}$$

$$\hat{p}_z = - i \hbar \frac{\partial}{\partial z} . \tag{1.3}$$

Using these expression we can construct the momentum square operator in cartesian coordinates as {3d2}

$$\begin{aligned} \hat{\vec{p}}^{\,2} &= \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 \\ &= - \hbar^2 \left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right\} && (1.4) \\ &= - \hbar^2 \nabla^2 , && (1.5) \end{aligned}$$

where $\nabla^2$ is the Laplacian. Therefore the kinetic energy operator in three dimension is given by the following expression: {3d3}

$$\hat{K} = - \frac{\hbar^2}{2 m} \nabla^2 . \tag{1.6}$$

Finally the time independent hamiltonian operator in three dimensions can be written as: {3d4}

$$\hat{H} = - \frac{\hbar^2}{2 m} \nabla^2 + \hat{V}(x, y, z) . \tag{1.7}$$

In many cases the potential has spherical symmetry in other words $\hat{V}$ is a
{3d5} function of the radius, e.g.,

$$\hat{V}(x,y,z) = \hat{V}(r) , \tag{1.8}$$

{3d6} where

$$r = \sqrt{x^2 + y^2 + z^2} . \tag{1.9}$$

For these systems we have to use spherical coordiantes, $(r, \theta, \phi)$,instead of cartesian coordinates, $(x, y, z)$. The relation between these coordinates are
{3d7} given by:

$$x = r \sin(\theta) \cos(\phi) \tag{1.10}$$

$$y = r \sin(\theta) \sin(\phi) \tag{1.11}$$

$$z = r \cos(\theta) . \tag{1.12}$$

{3d8a} In spherical coordinates the Laplacian is given by:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}. \tag{1.13}$$

In the following sections we will consider two important three dimensional problems. First we will consider a rigid rotator and the hydrogen atom.

## 1.1 Rigid rotator

A quantum mechanical rotator is simple model to study molecular rotations. In this case we consider two atoms separated a distance R apart. For this system we also use the reduced mass which reduces the two body problem to a one body problem. In contrast with the harmonic oscillator we consider a fixed distance between the atoms. In this way we are eliminating the molecular vibrations. In other words we consider a rigid rotator.

Recalling from classical mechanics the kinetic energy of a rigid rotator is given terms of the angular momentum. Using the angular momentum the
{3d8b} kinetic energy is given by:

$$K = \frac{1}{2\,I} L^2 , \tag{1.14}$$

{3d9} where I is the moment of inertia,

$$I = \mu R^2 , \qquad (1.15)$$

and L is the angular momentum.

Classically the angular momentum is a 3-dimensional vector. In cartesian coordinates the three components of the angular momentum are equal to: {3d10}

$$\begin{aligned} L_x &= y\, p_z - z\, p_y && (1.16)\\ L_y &= z\, p_x - x\, p_z && (1.17)\\ L_z &= x\, p_y - y\, p_x \,. && (1.18) \end{aligned}$$

Now we translate these expression into quantum operators we get {3d11}

$$\begin{aligned} \hat{L_x} &= -\, i\, \hbar \left( y\, \frac{\partial}{\partial z} - z\, \frac{\partial}{\partial y} \right) && (1.19)\\ \hat{L_y} &= -\, i\, \hbar \left( z\, \frac{\partial}{\partial x} - x\, \frac{\partial}{\partial z} \right) && (1.20)\\ \hat{L_z} &= -\, i\, \hbar \left( x\, \frac{\partial}{\partial y} - y\, \frac{\partial}{\partial x} \right) . && (1.21)\\ & && (1.22) \end{aligned}$$

Since the rigid rotator shows spherical symmetry we need to transform the angular momentum operator from cartesian to spherical coordinates. This transformation follows from Eqs. (1.10), and, after tedious but otherwise straightf forward algebra,we get the following expressions of the angular momentum operator in spherical coordinates: {3d12}

$$\begin{aligned} \hat{L_x} &= -i\, \hbar \left[ -\ \sin(\phi)\, \frac{\partial}{\partial \theta} - \cot(\theta)\, \cos(\phi)\, \frac{\partial}{\partial \phi} \right] && (1.23)\\ \hat{L_y} &= -i\, \hbar \left[ -\ \cos(\phi)\, \frac{\partial}{\partial \theta} - \cot(\theta)\, \sin(\phi)\, \frac{\partial}{\partial \phi} \right] && (1.24) \end{aligned}$$

{3d13}

$$\hat{L_z} = -\, i\, \hbar\, \frac{\partial}{\partial \phi} \qquad (1.25)$$

{3d14}

$$\hat{L^2} = -\, \hbar^2 \left[ \frac{1}{\sin(\theta)}\, \frac{\partial}{\partial \theta} \left( \sin(\theta)\, \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)}\, \frac{\partial^2}{\partial \phi^2} \right] . \qquad (1.26)$$

In the case of the rigid rotator no potential energy is present, which means that the Hamiltonian is given by {3d15}

$$\hat{H} \;=\; \frac{1}{2\mu R^2}\,\hat{L}^2\,. \tag{1.27}$$

{3d16} Thus the time-dependent Schrödinger reduces to

$$\hat{H}\psi_n \;=\; \frac{1}{2\mu R^2}\,\hat{L}^2\psi_n \;=\; E_n\psi_n\,. \tag{1.28}$$

Since the rigid rotator has spherical symmetry we will use spherical coordi-
{3d17} nates and find

$$-\,\frac{\hbar^2}{2\mu R^2}\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right]\psi_n = E_n\psi_n\,. \tag{1.29}$$

{3d18} The solution to a very similar equation has been found, namely

$$\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right]Y_\ell^m(\theta,\phi) = \;-\,\ell(\ell+1)Y_\ell^m(\theta,\phi), \tag{1.30}$$

where $Y_\ell^m$s are called the Spherical Harmonics. Therefore we can use this
{3d19} result to express $\psi$, i.e.,

$$\psi_n \;\longrightarrow\; Y_\ell^m(\theta,\phi)\;, \tag{1.31}$$

where $\ell = 0,1,2,3,\ldots$, and $m = 0,\pm1,\pm2,\pm3,\ldots,\pm\ell$. Also the spherical
{3d22} harmonics have the following estructure:

$$Y_\ell^m(\theta,\phi) \;=\; N_{\ell,m}\;P_\ell^{|m|}(\cos(\theta))\;\;\exp\{i\;m\phi\}\;, \tag{1.32}$$

where $P_\ell^{|m|}$ are the Legendre polynomyals. The first couple of Spherical
{3d22a} Harmonics are:

$$Y_0^0(\theta,\phi) \;=\; \frac{1}{\sqrt{4\;\pi}}\;, \tag{1.33}$$

{3d22b}

$$Y_1^0(\theta,\phi) \;=\; \sqrt{\frac{3}{4\;\pi}}\;\cos(\theta), \tag{1.34}$$

{3d22c}

$$Y_1^{-1}(\theta,\phi) \;=\; \sqrt{\frac{3}{8\;\pi}}\;\sin(\theta)\;\;\exp\{-\;i\phi\}\,, \tag{1.35}$$

{3d22d}

$$Y_1^{1}(\theta,\phi) \;=\; \sqrt{\frac{3}{8\;\pi}}\;\sin(\theta)\;\;\exp\{+\;i\phi\}\;. \tag{1.36}$$

{3d20} Using these results the energy levels for the rigid rotator are given by: