The Schrodinger equation in three dimensions

I- Separation of the Schrodinger equation in Cartesian coordinates:

We generalize our treatment, to study, in three dimension the non-relativistic Motion of a particle in a time-independent potential V(r) where r represent The position vector of the particle.

The time-independent Schrodinger equation that we want to solve is

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\psi(r) = E\psi(r)$$

The solution of the above equation in three dimension can only be obtain Exactly in a few simple cases. In these cases the potential such that the technique of separation of variable may be used.

We consider

$$V(r) = V_1(x) + V_2(y) + V_3(z)$$

The Schrodinger equation become

$$\left\{\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V_1(x)\right] + \left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial y^2} + V_2(y)\right] + \left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + V_3(z)\right]\right\}\psi(x,y,z) = E\psi(x,y,z)$$

We assume

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

$$\left\{\left[-\frac{\hbar^2}{2\mu}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + V_1(x)\right] + \left[-\frac{\hbar^2}{2\mu}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + V_2(y)\right] + \left[-\frac{\hbar^2}{2\mu}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} + V_3(z)\right]\right\} = E$$

Therefore we obtain the three ordinary differential equations

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}+V_1(x)\right]X(x)=E_xX(x)$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial y^2}+V_2(y)\right]Y(y)=E_yY(y)$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}+V_3(z)\right]Z(z)=E_zZ(z)$$

Each one is similar to that
We have solved in our previous
Work.

With the condition

$$E = E_x + E_y + E_z$$

Free particle: as you will see in the home work the wave function and the energy Of the free particle in three dimension is given by

$$\psi_k(\vec{r}) = \frac{1}{(2\pi)^{2/3}} \exp[i\vec{k}\cdot\vec{r}]$$

$$E = E_x + E_y + E_z = \frac{\hbar^2}{2\mu}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{\hbar^2 k^2}{2\mu} = \frac{p^2}{2\mu}$$

The wave function satisfy

$$\int \psi_{k'}^*(r)\psi_k(r)d\vec{r} = \delta\left(\vec{k} - \vec{k}'\right)$$

$$\delta\left(\vec{k} - \vec{k}'\right) = \delta(k_x - k_x')\delta(k_y - k_y')\delta(k_z - k_z')$$

$$\delta(k_x - k_x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp[i(k_x - k_x')x]dx$$

The three dimensional Box

As you will see in the H.W

$$\psi_{n_1,n_2,n_3}(x,y,z) = \sqrt{\frac{8}{V}}\sin\left(\frac{n_1\pi}{a}x\right)\sin\left(\frac{n_2\pi}{b}y\right)\sin\left(\frac{n_3\pi}{c}z\right)$$

$V = abc$ → Volume of the Box

$n_1, n_2,$ and n_3 are postive integers

$$E_{n_1,n_2,n_3} = \frac{\hbar^2\pi^2}{2\mu}\left(\frac{n_1^2}{a^2}+\frac{n_2^2}{b^2}+\frac{n_3^2}{c^2}\right)$$

As the dimension of the box increase the spacing of the energy levels decreases, so that for a macroscopic box the spectrum is Nearly continuous.

For a=b=c

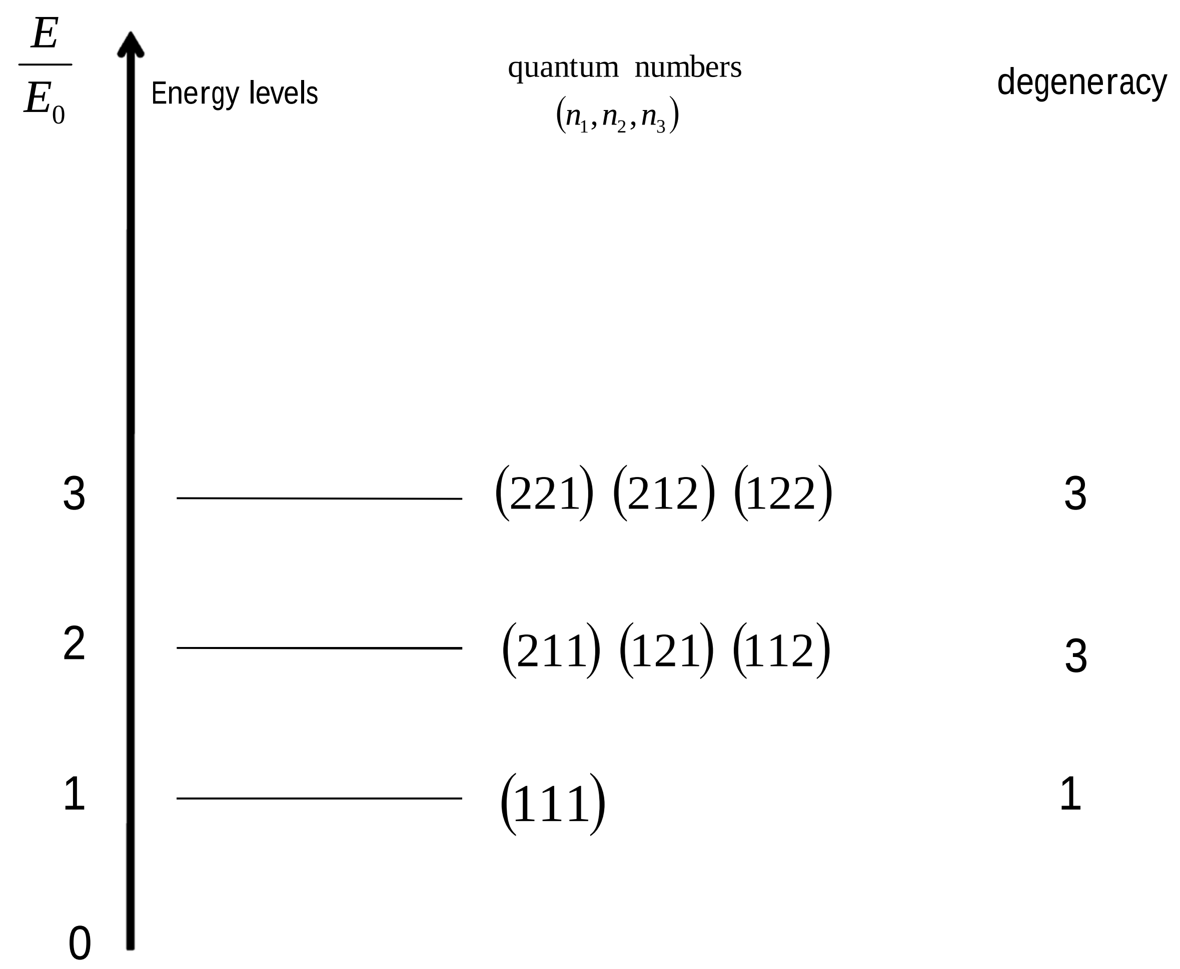
$$E_n = \frac{\hbar^2 \pi^2}{2\mu a^2} n^2$$

$$n^2 = n_1^2 + n_2^2 + n_3^2$$

if n_1 or n_2 or n_3 equal zero then $\psi = 0$, non-physical solution,so the ground state is such that

$$n_1 = n_2 = n_3 = 1$$

$$E_0 = 3\frac{\hbar^2 \pi^2}{2\mu a^2}$$



The existence of degeneracy is directly related to the symmetry of the potential

The three dimension harmonic oscillator

We consider a potential corresponding to a three dimensional harmonic oscillator

$$V(r)=\frac{1}{2}k_1x^2+\frac{1}{2}k_2y^2+\frac{1}{2}k_3z^2$$

As you will see in the H.W the normalized wave functions for a particle move
In such potential is given by

$$\psi_{n_1,n_2,n_3}(x,y,z)=\left(\frac{\alpha_1}{\sqrt{\pi}2^{n_1}n_1!}\right)\left(\frac{\alpha_2}{\sqrt{\pi}2^{n_2}n_2!}\right)\left(\frac{\alpha_3}{\sqrt{\pi}2^{n_3}n_3!}\right)\exp\left[-\frac{1}{2}\left(\alpha_1^2x^2+\alpha_2^2y^2+\alpha_3^2z^2\right)\right]\times$$
$$H_{n_1}(\alpha_1x)H_{n_2}(\alpha_2y)H_{n_3}(\alpha_3z)$$

where $H_n(\eta)$ is the Hermite polynomial defined before.

$$\alpha_1=\left(\frac{\mu k_1}{\hbar^2}\right)^{1/4}$$

The energy level is defined by

$$E_{n_1,n_2,n_3} = \left(n_1 + \frac{1}{2}\right)\hbar\omega_1 + \left(n_2 + \frac{1}{2}\right)\hbar\omega_2 + \left(n_3 + \frac{1}{2}\right)\hbar\omega_3$$

$$\omega_1 = \sqrt{\frac{k_1}{\mu}}, \ \omega_2 = \sqrt{\frac{k_2}{\mu}}, \ \omega_3 = \sqrt{\frac{k_3}{\mu}}$$

where n_1 , n_2 , and n_3 are positive integers or zero.

In this case the energy levels are not degenerate

An isotropic three dimensional harmonic oscillator

$$k_1 = k_2 = k_3 = k$$

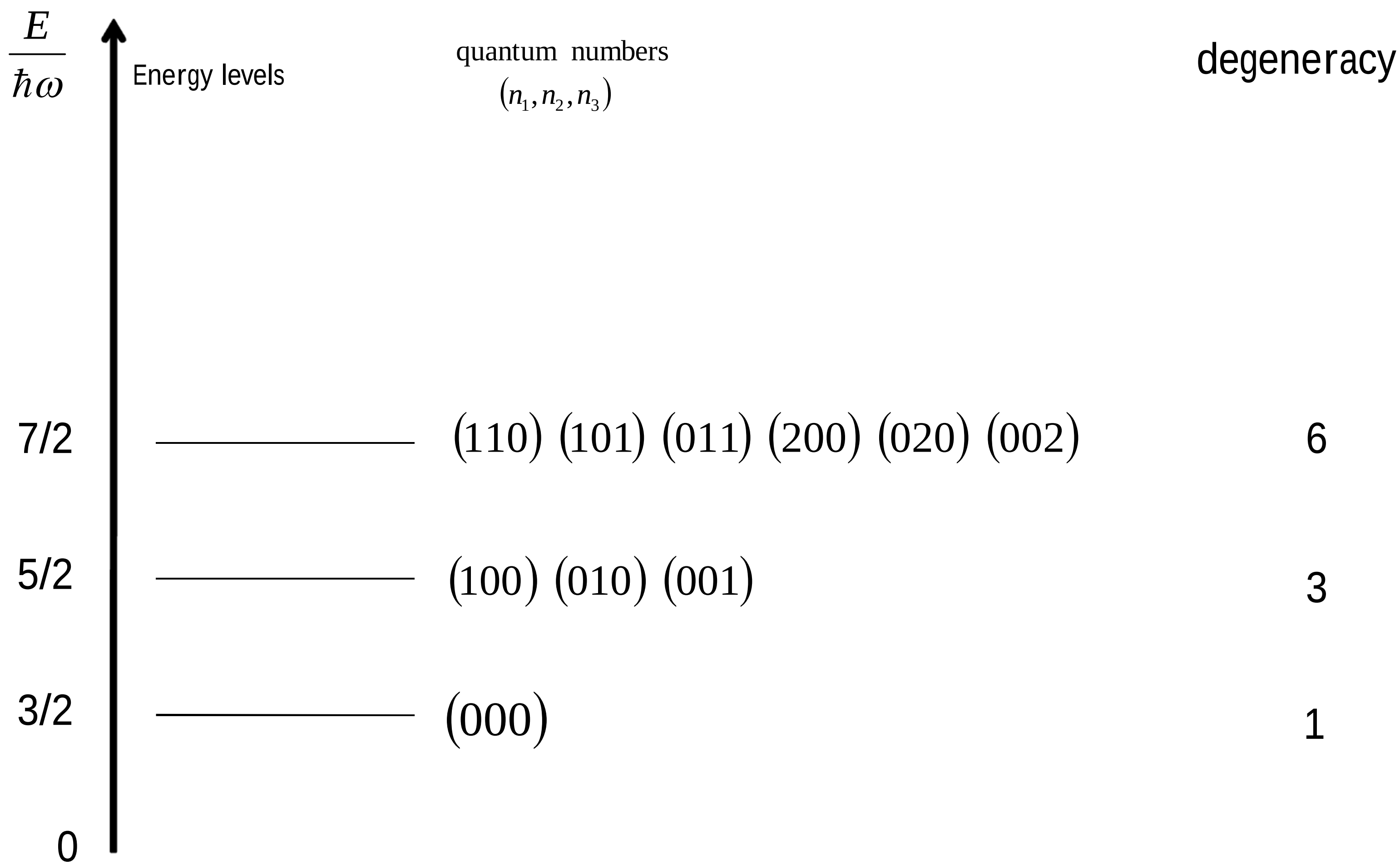
$$V(r) = \frac{1}{2}k\left(x^2 + y^2 + z^2\right) = \frac{1}{2}kr^2$$

The energy levels become

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega$$

$$n = n_1 + n_2 + n_3$$

$$E_0 = \frac{3}{2}\hbar\omega$$



This another example of how the symmetry of the potential results in degeneracies

II- Separation of the Schrodinger equation in spherical polar coordinates: (Central potentials)

Here we study the non-relativistic motion of a spinless particle of mass m in A central potential (that is a potential V (r) which depends only on the magnitude r of the position vector). Since V(r) is spherically symmetry, It is natural to use the spherical polar coordinates.

$$H=-\frac{\hbar^2}{2\mu}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right\}+V(r)$$

$$H=-\frac{\hbar^2}{2\mu}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{L^2}{\hbar^2 r^2}\right\}+V(r)$$

$$\left\{-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{L^2}{\hbar^2 r^2}\right]+V(r)\right\}\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$ Eq. I

Since the spherical harmonics Y_{lm} are simultaneous eigenfunctions of L^2 and L_z we look for a solution of the above equation having the form

$$\psi_{Elm}(r,\theta,\phi)=R_{El}(r)Y_{lm}(\theta,\phi)$$ Eq. II

ψ_{Elm} is a simultaneous eigenfunctions for H, L^2, L_z

$$\left[H,L^2\right]=\left[H,L_z\right]=\left[L^2,L_z\right]=0$$

Since for spherically symmetric potential (the potential does not depend on θ and ϕ)

$$\left[V(r),L\right]=\left[V(r),L^2\right]=0$$

Eq. I is separable

$$\left\{-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{L^2}{\hbar^2 r^2}\right]+V(r)\right\}\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

$$\left\{-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-\frac{L^2}{\hbar^2 r^2}\right]+V(r)\right\}\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

$$\left\{\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{L^2}{\hbar^2 r^2}-\frac{2\mu V(r)}{\hbar^2}+\frac{2\mu E}{\hbar^2}\right\}\psi(r,\theta,\phi)=0$$

$$\left\{\left[r^2\frac{\partial^2}{\partial r^2}+2r\frac{\partial}{\partial r}-\frac{2\mu V(r)}{\hbar^2}r^2+\frac{2\mu E}{\hbar^2}r^2\right]-\frac{L^2}{\hbar^2}\right\}\psi(r,\theta,\phi)=0$$

Insert Eq. II in the above equation and divided by it, we get

$$\frac{1}{R(r)}\left[r^2\frac{\partial^2}{\partial r^2}+2r\frac{\partial}{\partial r}-\frac{2\mu V(r)}{\hbar^2}r^2+\frac{2\mu E}{\hbar^2}r^2\right]R(r)-\frac{1}{Y_{lm}(\theta,\phi)}L^2Y_{lm}(\theta,\phi)=0$$

depend only on r

depend only on θ,ϕ

This means

$$\frac{1}{Y_{lm}(\theta,\phi)}L^2Y_{lm}(\theta,\phi)=C$$

→ We have solved this problem before
And we know the wave functions
And the eigenvalues C.

$$\frac{1}{R(r)}\left[r^2\frac{\partial^2}{\partial r^2}+2r\frac{\partial}{\partial r}-\frac{2\mu V(r)}{\hbar^2}r^2+\frac{2\mu E}{\hbar^2}r^2\right]R(r)=C$$

From our previous study we know the value of C.

$$C=l(l+1)$$

The remaining wave equation that we have to solve to obtain R(r) is

$$\frac{1}{R(r)}\left[r^2\frac{\partial^2}{\partial r^2}+2r\frac{\partial}{\partial r}-\frac{2\mu V(r)}{\hbar^2}r^2+\frac{2\mu E}{\hbar^2}r^2\right]R(r)=l(l+1)$$

or

$$\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{2\mu V(r)}{\hbar^2}+\frac{2\mu E}{\hbar^2}-\frac{l(l+1)}{r^2}\right]R(r)=0$$

or

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)+\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)\right]R(r)=ER(r)$$

R_{El} is a radial function which remain to be found

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)+\underbrace{\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)}_{V_{eff}}\right]R_{El}(r)=ER_{El}(r)$$

The magnetic quantum number, m, does not appear in the above equation, So the radial function is independent of this quantum number. Similarly the Energy will independent of m.