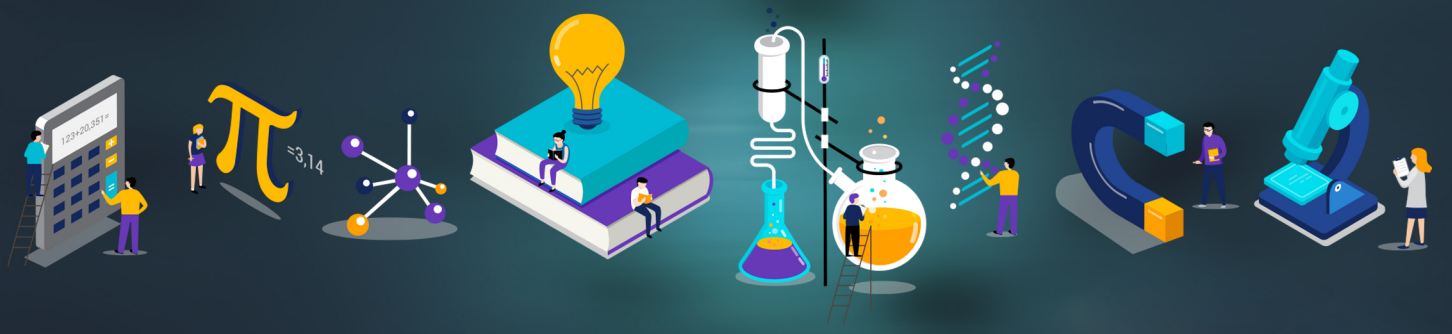


1. Hydrogen atom

1.1 Central potential

We are going to study the structure of the schrodinger equation for the particle of mass M moving in a spherically symmetric potential
$V(\vec{r}) = V(r)$,
which is also known as the central potential.
The time-independent Schrödinger equation for this particle, of momentum $-i\hbar\vec{\nabla}$ and position vector r, is

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

Since the Hamiltonian is spherically symmetric, we are going to use the spherical coordinates (r,θ,φ) which are related to their Cartesian counterparts by

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta.$$

The Laplacian ∇^2 separates into a radial part ∇_r^2 and an angular part ∇_Ω^2 as follows:

$$\nabla^2 = \nabla_r^2 - \frac{1}{\hbar^2 r^2}$$

$$\nabla_\Omega^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}$$

$$\hat{L}^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{1}{\hbar^2 r^2}\hat{L}^2$$

where $\hat{L}$ is the orbital angular momentum with

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

In spherical coordinates the Schrödinger equation therefore takes the form

$$\left[-\frac{\hbar^2}{2M}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{2Mr^2}\hat{L}^2 + V(r)\right]\psi(\vec{r}) = E\psi(\vec{r}).$$

The first term of this equation can be viewed as the radial kinetic energy

$$-\frac{\hbar^2}{2M}\frac{1}{r}\frac{\partial^2}{\partial r^2}r=\frac{\hat{P}_r^2}{2M},$$

Now $\hat{\vec{L}}^2$ does not depends on r, it commute with both $\vec{V}(r)$ and the radial KE.Hence it also commute with the Hamiltonian H . In addition since L_z commute with $\hat{\vec{L}}^2$, the three operators H,$\hat{\vec{L}}^2$, and L_z mutually commute:

$$\left[\hat{H},\hat{\vec{L}}^2\right]=\left[\hat{H},\hat{L}_z\right]=0.$$

Thus $\hat{H},\hat{\vec{L}}^2$, and $\hat{L}_z$ have common eigenfunctions. We know that the simultaneous eigenfunctions of $\hat{\vec{L}}^2$ and $\hat{L}_z$ are given by the spherical harmonics $Y_{lm}(\theta,\varphi)$:

$$\hat{\vec{L}}^2Y_{lm}(\theta,\varphi)=l(l+1)\hbar^2Y_{lm}(\theta,\varphi),$$
$$\hat{L}_zY_{lm}(\theta,\varphi)=m\hbar Y_{lm}(\theta,\varphi).$$

Since the Hamiltonian is a sum of a radial part and an angular part, we can look for solutions that are products of a radial part and an angular part, where the angular part is simply the spherical harmonic $Y_{lm}(\theta,\varphi)$:

$$\psi(\vec{r})=\langle\vec{r}\mid nlm\rangle=\psi_{nlm}(r,\theta,\varphi)=R_{nl}(r)Y_{lm}(\theta,\varphi).$$

Note that the orbital angular momentum of a system moving in a central potential is conserved,it commutes with the Hamiltonian.

The radial wave function $R_{nl}(r)$ has yet to be found. The quantum number n is introduced to identify the eigenvalues of $\hat{H}$:

$$\hat{H}|nlm\rangle=E_n|nlm\rangle$$

Substituting $\psi_{nlm}(r,\theta,\varphi)$ into schrodinger equation and using the fact that $\psi_{nlm}(r,\theta,\varphi)$ is an eigenfunction of $\hat{\vec{L}}^2$ with eigenvalue $l(l+1)\hbar^2$, then dividing through by $R_{nl}(r)Y_{lm}(\theta,\varphi)$ and multiplying by $2Mr^2$, we end up with an equation where the radial and angular degrees of freedom are separated:

$$\left[-\hbar^2\frac{r}{R_{nl}}\frac{\partial^2}{\partial r^2}(rR_{nl})+2Mr^2(V(r)-E)\right]+\left[\frac{\hat{\vec{L}}^2Y_{lm}(\theta,\varphi)}{Y_{lm}(\theta,\varphi)}\right]=0$$

The terms inside the first square bracket are independent of θ and φ and those of the second are independent of r. They must then be separately equal to constants and their sum equal to zero. The second square bracket is the the eigenvalue equation of $\hat{\vec{L}}^2$; hence it is equal to $l(l+1)\hbar^2$. As for the first bracket, it must be equal to $-l(l+1)\hbar^2$; this leads to an equation known as the radial equation for a central potential:

$$-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}(rR_{nl}(r))+\left[V(r)+\frac{l(l+1)\hbar^2}{2Mr^2}\right](rR_{nl}(r))=E_n(rR_{nl}(r)).$$

Note that the above equation, which gives the energy levels of the system, does not depend on the azimuthal quantum number m. Thus, the energy E_n is $(2l+1)$-fold degenerate.

1.2 Hydrogen atom

Schrödinger's equation for the electron in three dimensions, which is what we must use for the hydrogen atom, is

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2m}{\hbar^2}(E-U)\psi=0$$

The potential energy U here is the electric potential energy Electric potential

$$U=-\frac{e^2}{4\pi\varepsilon_0 r}$$

of a charge $-e$ when it is the distance r from another charge $+e$.
In spherical polar coordinates Schrödinger's equation is written

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2m}{\hbar^2}(E-U)\psi=0$$

Substituting for the potential energy U and multiplying the entire equation by $r^2\sin^2\theta$, we obtain

Hydrogen atom

$$\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{\partial^2\psi}{\partial\phi^2}+\frac{2mr^2\sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)\psi=0$$

Equation is the partial differential equation for the wave function ψ of the electron in a hydrogen atom. Together with the various conditions ψ must obey, namely that ψ be normalizable and that ψ and its derivatives be continuous and single-valued at each point r,θ,ϕ, this equation completely specifies the behavior of the electron.

1.2.1 Seperation of variables

The advantage of writing Schrödinger's equation in spherical polar coordinates for the problem of the hydrogen atom is that in this form it may be separated into three independent equations, each involving only a single coordinate. Such a separation is possible here because the wave function $\psi(r,\theta,\phi)$ has the form of a product of three different functions: $R(r)$, which depends on r alone; $\Theta(\theta)$ which depends on θ alone; and $\Phi(\phi)$, which depends on ϕ alone. Of course, we do not really know that this separation is possible yet, but we can proceed by assuming that

$$\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$$

which we may write more simply as

$$\psi=R\Theta\Phi$$

we see that

$$\frac{\partial\psi}{\partial r}=\Theta\Phi\frac{\partial R}{\partial r}=\Theta\Phi\frac{dR}{dr}$$
$$\frac{\partial\psi}{\partial\theta}=R\Phi\frac{\partial\Theta}{\partial\theta}=R\Phi\frac{d\Theta}{d\theta}$$
$$\frac{\partial^2\psi}{\partial\phi^2}=R\Theta\frac{\partial^2\Phi}{\partial\phi^2}=R\Theta\frac{d^2\Phi}{d\phi^2}$$

When we substitute $R\Theta\Phi$ for ψ in Schrödinger's equation for the hydrogen atom and divide the entire equation by $R\Theta\Phi$, we find that

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}+\frac{2mr^2\sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)=0$$

The third term is a function of azimuth angle ϕ only, whereas the other terms are functions of r and θ only. Let us rearrange the equation to read

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{2mr^2\sin^2\theta}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)=-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

This equation can be correct only if both sides of it are equal to the same constant, since they are functions of different variables. As we shall see, it is convenient to call this constant m_l^2. The differential equation for the function ϕ is the refore

$$-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=m_l^2$$

Next we substitute m_l^2 for the right-hand side the last equation and divide the entire equation by $\sin^2\theta$, and rearrange the various terms, which yields

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)=\frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)$$

Again we have an equation in which different variables appear on each side, requiring that both sides be equal to the same constant. This constant is called $l(l+1)$, once more for reasons that will be apparent later. The equations for the functions Θ and R are therefore

$$\frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=l(l+1)$$
$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)=l(l+1)$$

Equation for Φ

$$\frac{d^2\Phi}{d\phi^2}+m_l^2\Phi=0$$

Equation for θ

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m_l^2}{\sin^2\theta}\right]\Theta=0$$

Equation for R

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left[\frac{2m}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)-\frac{l(l+1)}{r^2}\right]R=0$$

1.2.2 Quantum numbers

magnetic quantum number

$$\Phi(\phi)=Ae^{im_l\phi}$$

As we know, one of the conditions that a wave function-and hence Φ, which is a component of the complete wave function ψ-must obey is that it have a single value at a given point in space.We konw that ϕ and $\phi+2\pi$ both identify the same meridian plane. Hence it must be true that $\Phi(\phi)=\Phi(\phi+2\pi)$, or

$$Ae^{im_l\phi}=Ae^{im_l(\phi+2\pi)}$$

which can happen only when m_l is 0 or a positive or negative integer (±1, $\pm2,\pm3$....). The constant m_l is known as the magnetic quantum number of the hydrogen atom.
The differential equation for $\Theta(\theta)$, has a solution provided that the constant l is an integer equal to or greater than $|m_l|$, the absolute value of m_l. This requirement can be expressed as a condition on m_l in the form

$$m_l=0,\pm1,\pm2,\ldots,\pm l$$

The constant l is known as the **orbital quantum number**
An atomic electron that possesses angular momentum interacts with an external magnetic field **B**. The magnetic quantum number m_l specifies the direction of **L** by determining the component of **L** in the field direction. This phenomenon is often referred to as space quantization.

If we let the magnetic-field direction be parallel to the z axis, the component of **L** in this direction is Space quantization

$$L_z=m_l\hbar\quad m_l=0,\pm1,\pm2,\ldots,\pm l$$

The possible values of m_l for a given value of l range from $+l$ through 0 to $-l$, so that the number of possible orientations of the angular-momentum vector **L** in a magnetic field is $2l+1$. When $l=0,L_z$ can have only the single value of 0 ; when $l=1,L_z$ may be $\hbar,0$, or $-\hbar$; when $l=2,L_z$ may be $2\hbar,\hbar,0,-\hbar$, or $-2\hbar$; and so on.

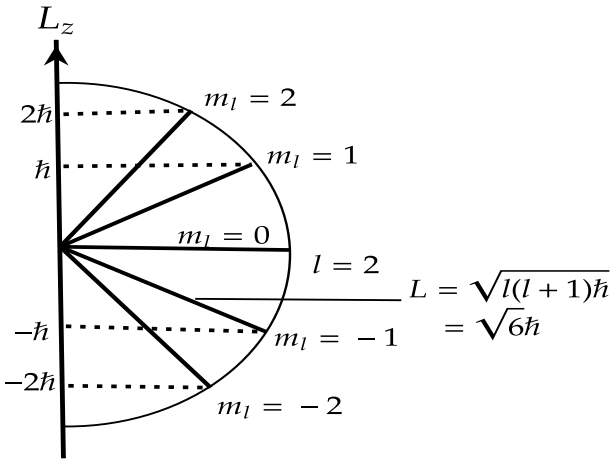


Figure 1.1: Space quantization of orbital angular momentum with (l=2)

Orbital quantum number

Electron angular momenta

$$L = \sqrt{l(l+1)}\hbar$$

momentum With the orbital quantum number l restricted to the values

$$l = 0, 1, 2, \ldots, (n-1)$$

The electron can have only the angular momenta L specified by $L = \sqrt{l(l+1)}\hbar$, Like total energy E, angular momentum is both conserved and quantized. The quantity

$$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34}\ \mathrm{J \cdot s}$$

is thus the natural unit of angular momentum.

Designation of Angular-Momentum States

It is customary to specify electron angular-momentum states by a letter, with s corresponding to $l = 0$, p to $l = 1$, and so on, according to the following scheme:

$l = 0$	1	2	3	4	5	6	…
s	p	d	f	g	h	i	…

Table of Atomic Electron States

	$I = 0$	$I = 1$	$I = 2$	$I = 3$	$I = 4$	$I = 5$
$n = 1$	$1s$					
$n = 2$	$2s$	$2p$				
$n = 3$	$3s$	$3p$	$3d$			
$n = 4$	$4s$	$4p$	$4d$	$4f$		
$n = 5$	$5s$	$5p$	$5d$	$5f$	$5g$	
$n = 6$	$6s$	$6p$	$6d$	$6f$	$6g$	$6h$

Principal quantum number

For the radial part $R(r)$ of the hydrogenatom wave function ψ also requires that a certain condition be fulfilled. This condition is that E be positive or have one of the negative values E_n (signifying that the electron is bound to the atom) specified by

$$E_n = -\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}\left(\frac{1}{n^2}\right) = \frac{E_1}{n^2} \quad n = 1, 2, 3, \ldots$$

Another condition that must be obeyed in order to solve radial equation is that n, known as the principal quantum number, must be equal to or greater than $l + 1$. This requirement may be expressed as a condition on l in the form

$$l = 0, 1, 2, \ldots, (n-1)$$

Hence we may tabulate the three quantum numbers n, l, and m together with their permissible values as follows:

Principal quantum number	$n = 1, 2, 3, \ldots$
Orbital quantum number	$l = 0, 1, 2, \ldots, (n-1)$
Magnetic quantum number	$m_l = 0, \pm 1, \pm 2, \ldots, \pm l$

To exhibit the dependence of R, Θ, and Φ upon the quantum numbers n, l, m, we may write for the electron wave functions of the hydrogen atom

$$\psi = R_{nl}\Theta_{lm_l}\Phi_{m_l}$$

1.2.3 Normalized wavefunction of the Hydrogen atom for n=1,2,3.

n	l	m_l	$\Phi(\phi)$	$\theta(\theta)$	$R(r)$	$\psi(r,\theta,\phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}}e^{-r/a_0}$	$\frac{1}{\sqrt{\pi}a_0^{3/2}}e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}a_0^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}a_0^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\cos\theta$
2	1	± 1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}\sin\theta e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}a_0^{3/2}}\left(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2}\right)e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{4}{81\sqrt{6}a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}\cos\theta$
3	1	± 1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{4}{81\sqrt{6}a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}a_0^{3/2}}\left(6-\frac{r}{a_0}\right)\frac{r}{a_0}e^{-r/3a_0}\sin\theta e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4}\left(3\cos^2\theta-1\right)$	$\frac{4}{81\sqrt{30}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\left(3\cos^2\theta-1\right)$
3	2	± 1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{15}}{2}\sin\theta\cos\theta$	$\frac{4}{81\sqrt{30}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_o}\sin\theta\cos\theta e^{\pm i\phi}$
3	2	± 2	$\frac{1}{\sqrt{2\pi}}e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4}\sin^2\theta$	$\frac{4}{81\sqrt{30}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-r/3a_0}\sin^2\theta e^{\pm 2i\phi}$

1.2.4 Electron probability density

The probability density $|\psi|^2$ that corresponds to the electron wave function $\psi = R\Theta\Phi$ in the hydrogen atom is |

$$\psi|^2 = |\mathrm{R}|^2|\Theta|^2|\Phi|^2$$

we see that the azimuthal wave function is given by

$$\Phi(\phi) = Ae^{im_\ell\phi}$$

The azimuthal probability density $|\Phi|^2$ is therefore

$$|\Phi|^2 = \Phi^*\Phi = A^2e^{-im_1\phi}e^{im_1\phi} = A^2e^0 = A^2$$

The likelihood of finding the electron at a particular azimuth angle ϕ is a constant that does not depend upon ϕ at all. The electron's probability density is symmetrical about the z axis regardless of the quantum state it is in, and the electron has the same chance of being found at one angle ϕ as at another.

The probability density of the electron at the point r, θ, ϕ is proportional to $|\psi|^2$, but the actual probability of finding it in the infinitesimal volume element dV there is $|\psi|^2 dV$. In spherical polar coordinates $dV = (dr)(rd\theta)(r\sin\theta d\phi)$

$= r^2\sin\theta dr d\theta d\phi$

As Θ and Φ are normalized functions, the actual probability $P(r)dr$ of finding the electron in a hydrogen atom somewhere in the spherical shell between r and $r+dr$ from the nucleus is

$$\begin{aligned} P(r)dr &= r^2|R|^2dr\int_0^\pi|\Theta|^2\sin\theta d\theta\int_0^{2\pi}|\Phi|^2d\phi \\ &= r^2|R|^2dr \end{aligned}$$

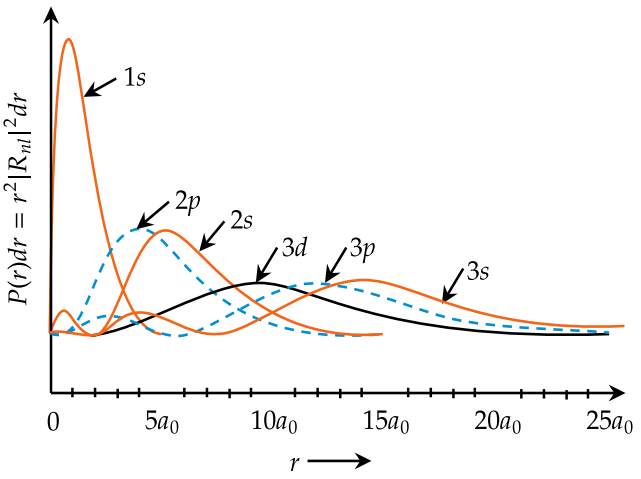


Figure 1.2: The probability of finding the electron in a hydrogen atom at a distance between r and $r+dr$ from the nucleus for the quantum states.

1.2.5 Degeneracy of Hydrogen atom

If spin of the electron is not included then degeneracy of atom is $\sum_{i=0}^{n-1}(2l+1) = n^2$
If spin of the electron is included then degeneracy of atom is $2\sum_{l=0}^{n-1}(2l+1) = 2n^2$

Exercise 1.1 Verify that the average value of $1/r$ for a 1 s electron in the hydrogen atom is $1/a_0$. ■

Solution: The wave function of a ls electron is,

$$\psi = \frac{e^{-r/a_0}}{\sqrt{\pi}a_0^{3/2}}$$

Since $dV = r^2 \sin\theta dr d\theta d\phi$ we have for the expectation value of $1/r$

$$\left\langle \frac{1}{r} \right\rangle = \int_0^\infty \left(\frac{1}{r}\right)|\psi|^2 dV$$
$$= \frac{1}{\pi a_0^3}\int_0^\infty re^{-2r/a_0}dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi$$

The integrals have the respective values

$$\int_0^\infty re^{-2r/a_0}dr = \left[\frac{a_0^2}{4}e^{-2r/a_0} - \frac{r}{2}e^{-2r/a_0}\right]_0^\infty = \frac{a_0^2}{4}$$
$$\int_0^\pi \sin\theta d\theta = [-\cos\theta]_0^\pi = 2$$
$$\int_0^{2\pi} d\phi = [\phi]_0^{2\pi} = 2\pi$$
$$\left\langle \frac{1}{r} \right\rangle = \left(\frac{1}{\pi a_0^3}\right)\left(\frac{a_0^2}{4}\right)(2)(2\pi) = \frac{1}{a_0}$$

Exercise 1.2 Show that the most probable distance by the electron from the nucleus in the ground state of hydrogen atom is equal to the Bohr's radius. ■

Solution: For the ground state of hydrogen atom, $n = 1, \ell = 0$ and $m = 0$. Hence the ground state wave function is,

$$\psi_{1,0,0} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

Since, the wave function is independent of θ and ϕ, therefore,
Radial probability density $= P(r) = |\psi_{100}|^2 4\pi r^2 = \frac{4}{a_0^3} e^{-2r/a_0} r^2$ For most probable distance, $P(r)$ is to be the maximum

$$\frac{dP}{dr} = \frac{4}{a_0^3}\left[r^2\left(-\frac{2}{a_0}\right)e^{-2r/a_0} + 2re^{-2r/a_0}\right] = 0 \Rightarrow r = a_0$$

Thus the most probable distance of the electron from the nucleus of hydrogen atom in the ground state is equal tothe Bohr radius (a_0).

Exercise 1.3 If the ground state wave function for the hydrogen atom is

$$\psi = \frac{1}{\sqrt{\pi}}\frac{1}{a_0^{3/2}} e^{-r/a_0}$$

show that average distance of the electron from the nucleus is $1.5a_0$. ■

Solution: We have the average distance of the electron from the hydrogen nucleus in the ground state is,

$$\langle r\rangle = \int_0^\infty \psi^* \hat{r}\psi dr = \int_0^\infty \frac{1}{\sqrt{\pi}}\frac{1}{a_0^{3/2}} e^{-r/a_0} r \frac{1}{\sqrt{\pi}}\frac{1}{a_0^{3/2}} e^{-r/a_0} d\tau$$

$$= \frac{1}{\pi a_0^3}\int_0^\infty r e^{-2r/a_0} r^2 \sin\theta dr d\theta d\phi$$

Using the standard integral $\int_0^\infty e^{-ax} x^n dx = \frac{n!}{a^{n+1}}$, we get

$$\langle r\rangle = \frac{1}{\pi a_0^3}\int_0^\infty r^3 e^{-2r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = \frac{1}{\pi a_0^3} \times \frac{3!}{(2/a_0)^4} \times 2 \times 2\pi$$

Therefore, $\langle r\rangle = \frac{3}{2}a_0 = 1.5a_0$

Exercise 1.4 What is the expectation value of the knetice nergy $\left(E^2\right)$ of the electron in the 1s state of the hydrogen atom? ■

Solution: The expectation value of the kinetic energy is,

$$\langle E_k\rangle = \int_\tau \psi^*_{1,0,0}\hat{E}_k\psi_{1,0,0} d\tau = \int_0^\infty\int_0^\pi\int_0^{2\pi} \psi_{1,0,0}\hat{E}_k\psi_{1,0,0} r^2 \sin\theta dr d\theta d\phi$$

But, $\vec{E}_k = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$
Since $\psi_{1,0,0}$ depends on r only, the terms in $\frac{\partial}{\partial\theta}$ and $\frac{\partial}{\partial\phi}$ are zero.

$$\langle E_k\rangle = -\frac{\hbar^2}{2m}\cdot 4\pi\left(\frac{1}{\sqrt{\pi}a_0^3}\right)^2\int_0^\infty e^{-r/a_0} \times \left\{\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)e^{-r/a_0}\right\} r^2 dr$$

$$= -\frac{\hbar^2}{2m}\frac{4}{a_0^3}\int_0^\infty \left(\frac{1}{a_0^2} - \frac{2}{ra_0}\right) e^{-2r/a_0} r^2 dr$$
$$= -\frac{2\hbar^2}{ma_0^3}\left[\frac{1}{a_0^2}\int_0^\infty r^2 e^{-2r/a_0} dr - \frac{2}{a_0}\int_0^\infty r e^{-2r/a_0} dr\right]$$
$$= -\frac{2\hbar^2}{ma_0^3}\left[\frac{1}{a_0^2}\frac{2}{(2/a_0)^3} - \frac{2}{a_0}\frac{1}{(2/a_0)^2}\right] = \frac{2\hbar^2}{ma_0^3}\cdot\frac{a_0}{4}$$

Therefore, $\langle E_k\rangle = \frac{\hbar^2}{2ma_0^3} = \frac{\hbar^2}{2m}\left(\frac{me^2}{\hbar^2}\right) = \frac{me^4}{2\hbar^2}$

Exercise 1.5 Estimate the uncertainity in the radial position of the electron in the ground state of hydrogen atom. ■

Solution: For ground state

$$\langle r\rangle = \frac{4}{a_0^3}\int_0^\infty r^3 e^{\frac{-2r}{a_0}} dr = \frac{3a_0}{2}$$
$$\langle r^2\rangle = \frac{4}{a_0^3}\int_0^\infty r^4 e^{\frac{-2r}{a_0}} dr = 3a_0^2$$

uncertainity in the radial position of the particle will be

$$\Delta r = \sqrt{\langle r^2\rangle - \langle r\rangle^2} = \frac{\sqrt{3}}{2}a_0$$

Exercise 1.6 Find the positions of maxima of the radial probability curves for 1s,2s,2p and 3d orbitals of the hydrogen like atom ■

Solution: The radial probability density

$$P_{nl} = r^2|R_{nl}|^2$$
$$R_{10} = Constant \times e^{-Zr/a_0}$$
$$R_{21} = Constant \times e^{-Zr/2a_0}$$
$$R_{32} = Constant \times e^{-Zr/3a_0}$$

P_{nl} will be maximum when $\frac{dP_{nl}}{dr} = 0$ hence

$$\frac{dP_{10}}{dr} = 0 \implies C(2r - \frac{2Zr^2}{a_0})e^{\frac{-2Zr}{a_0}} = 0$$
$$\implies r = \frac{a_0}{Z}$$
$$\frac{dP21}{dr} = 0 \implies C(4r^3 - \frac{Zr^4}{a_0})e^{\frac{-Zr}{a_0}} = 0$$
$$\implies r = \frac{4a_0}{Z}$$

Similarly $\frac{dP_{32}}{dr} = 0 \implies r = \frac{9a_0}{2}$
In general $r_{max} = \frac{n^2 a_0}{2}$

Exercise 1.7 At time $t = 0$, the wave function for the hydrogen atom is

$$\psi(r,0) = \frac{1}{\sqrt{10}}\left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right)$$

where the subscripts are values of the quantum numbers n, l, m. (i) What is the expectation value for the energy of the system? (ii) What is the probability of finding the system with $l = 1, m = 1$? . ■

Solution: Expectation value $= \langle E \rangle = \langle \psi | H | \psi \rangle$

$$= \frac{1}{10}\left\langle \left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right) |H| \left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right) \right\rangle$$

$$= \frac{1}{10}\left\langle \left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right) | \left(2E_1\psi_{100} + E_2\psi_{210} + \sqrt{2}E_2\psi_{211} + \sqrt{3}E_2\psi_{21,-1}\right) \right\rangle$$

$$= \frac{1}{10}(4E_1 + E_2 + 2E_2 + 3E_2) = \frac{1}{10}[4E_1 + 6E_2]$$

$$E_1 = -13.6eV \quad E_2 = -3.4eV$$

$$\langle E \rangle = -74.8eV$$

Practice set 1

1. The energy levels of the non-relativistic electron in a hydrogen atom (i.e. in a Coulomb potential $V(r) \propto -1/r$) are given by $E_{nlm} \propto -1/n^2$, where n is the principal quantum number, and the corresponding wave functions are given by ψ_{nlm}, where l is the orbital angular momentum quantum number and m is the magnetic quantum number. The spin of the electron is not considered. Which of the following is a correct statement?

[NET JUNE 2011]

A. There are exactly $(2l+1)$ different wave functions ψ_{nlm}, for each E_{nlm}.

B. There are $l(l+1)$ different wave functions ψ_{nlm}, for each E_{nlm}.

C. E_{nlm} does not depend on l and m for the Coulomb potential.

D. There is a unique wave function ψ_{nlm} for each E_{nlm}.

2. Let ψ_{nlm_l} denote the eigenfunctions of a Hamiltonian for a spherically symmetric potential $V(r)$. The wavefunction $\psi = \frac{1}{4}\left[\psi_{210} + \sqrt{5}\psi_{21-1} + \sqrt{10}\psi_{211}\right]$ is an eigenfunction only of

[NET JUNE 2012]

A. H, L^2 and L_2

B. H and L_z

C. H and L^2

D. L^2 and L_z

3. The wave function of a state of the Hydrogen atom is given by,

$$\psi = \psi_{200} + 2\psi_{211} + 3\psi_{210} + \sqrt{2}\psi_{21-1}$$

where ψ_{nlm} is the normalized eigen function of the state with quantum numbers n, l, m in the usual notation. The expectation value of L_z in the state ψ is

[NET DEC 2012]

A. $\frac{15\hbar}{6}$

B. $\frac{11\hbar}{6}$

C. $\frac{3\hbar}{8}$

D. $\frac{\hbar}{8}$

4. Let ψ_{nlm} denote the eigenfunctions of a Hamiltonian for a spherically symmetric potential $V(r)$. The expectation value of L_z in the state

$$\psi = \frac{1}{6}\left[\psi_{200} + \sqrt{5}\psi_{210} + \sqrt{10}\psi_{21-1} + \sqrt{20}\psi_{211}\right] \text{ is}$$

[NET DEC 2013]

A. $-\frac{5}{18}\hbar$

B. $\frac{5}{6}\hbar$

C. $\hbar$

D. $\frac{5}{18}\hbar$

5. An electron is in the ground state of a hydrogen atom. The probability that it is within the Bohr radius is approximately equal to

[NET JUNE 2014]

A. 0.60

B. 0.90

C. 0.16

D. 0.32

6. Let ψ_{nlm} denote the eigenstates of a hydrogen atom in the usual notation. The state

$$\frac{1}{5}\left[2\psi_{200} - 3\psi_{211} + \sqrt{7}\psi_{210} - \sqrt{5}\psi_{21-1}\right]$$

is an eigenstate of

[NET DEC 2015]

A. L^2, but not of the Hamiltonian or L_z

B. the Hamiltonian, but not of L^2 or L_z

C. the Hamiltonian, L^2 and L_z

D. L^2 and L_z, but not of the Hamiltonian

7. If the position of the electron in the ground state of a Hydrogen atom is measured, the probability that it will be found at a distance $r \geq a_0$ (a_0 being Bohr radius) is nearest to

[NET DEC 2018]

A. 0.91

B. 0.66

C. 0.32

D. 0.13

Answer key			
Q.No.	Answer	Q.No.	Answer
1	**c**	2	**c**
3	**d**	4	**d**
5	**d**	6	**b**
7	**b**		

Practice set 2

1. The normalized ground state wavefunciton of a hydrogen atom is given by $\psi(r) = \frac{1}{\sqrt{4\pi}} \frac{2}{a^{3/2}} e^{-r/a}$, where a is the Bohr radius and r is the distance of the electron from the nucleus, located at the origin. The expectation value $\left\langle \frac{1}{r^2} \right\rangle$ is

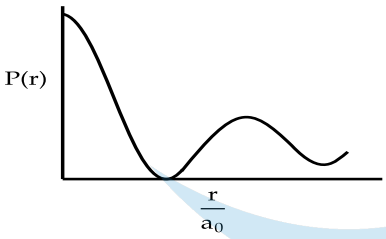
[GATE 2011]

A. $\frac{8\pi}{a^2}$ **B.** $\frac{4\pi}{a^2}$
C. $\frac{4}{a^2}$ **D.** $\frac{2}{a^2}$

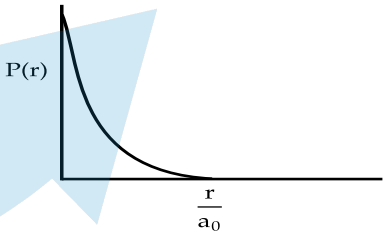
2. The ground state wavefunction for the hydrogen atom is given by $\psi_{100} = \frac{1}{\sqrt{4\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$, where a_0 is the Bohr radius. The plot of the radial probability density, $P(r)$ for the hydrogen atom in the ground state is

[GATE 2012]

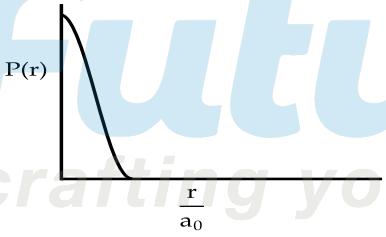
A.



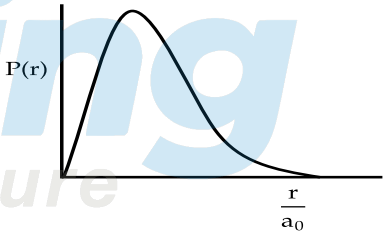
B.



C.



D.



3. An electron in the ground state of the hydrogen atom has the wave function $\psi(\vec{r}) = \frac{1}{\sqrt{\pi a_0^3}} e^{-\left(\frac{r}{a_0}\right)}$, where a_0 is constant. The expectation value of the operator $\hat{Q} = z^2 - r^2$, where $z = r\cos\theta$ is (Hint: $\int_0^\infty e^{-ar} r^n dr = \frac{\sqrt{n}}{a^{n+1}} = \frac{(n-1)!}{a^{n+1}}$)

[GATE 2014]

A. $\frac{-a_0^2}{2}$ **B.** $-a_0^2$
C. $\frac{-3a_0^2}{2}$ **D.** $-2a_0^2$

4. A hydrogen atom is in the state

$$\psi = \sqrt{\frac{8}{21}}\psi_{200} - \sqrt{\frac{3}{7}}\psi_{310} + \sqrt{\frac{4}{21}}\psi_{321},$$

where n, l, m in ψ_{nlm} denote the principal, orbital and magnetic quantum numbers, respectively. If $\vec{L}$ is the angular momentum operator, then the average value of L^2 is $\cdots$ $\hbar^2$

[GATE 2014]

5. An electric field $\vec{E} = E_0\hat{z}$ is applied to a Hydrogen atom in $n = 2$ excited state. Ignoring spin the $n = 2$ state is fourfold degenerate, which in the $|l, m\rangle$ basis are given by $|0,0\rangle, |1,1\rangle, |1,0\rangle$ and $|1,-1\rangle$. If H' is the interaction Hamiltonian corresponding to the applied electric field, which of the following matrix elements is nonzero?

[GATE 2019]

Answer key			
Q.No.	Answer	Q.No.	Answer
1	**d**	2	**d**
3	**d**	4	**2**
5	**c**		

Practice set 3

1. Verify that the average value of $1/r$ for a 1 s electron in the hydrogen atom is $1/a_0$.

Solution: The wave function of a ls electron is,

$$\psi = \frac{e^{-r/a_0}}{\sqrt{\pi} a_0^{3/2}}$$

Since $dV = r^2 \sin\theta dr d\theta d\phi$ we have for the expectation value of $1/r$

$$\left\langle \frac{1}{r} \right\rangle = \int_0^\infty \left(\frac{1}{r}\right) |\psi|^2 dV$$
$$= \frac{1}{\pi a_0^3} \int_0^\infty r e^{-2r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi$$

The integrals have the respective values

$$\int_0^\infty r e^{-2r/a_0} dr = \left[\frac{a_0^2}{4} e^{-2r/a_0} - \frac{r}{2} e^{-2r/a_0}\right]_0^\infty = \frac{a_0^2}{4}$$
$$\int_0^\pi \sin\theta d\theta = [-\cos\theta]_0^\pi = 2$$
$$\int_0^{2\pi} d\phi = [\phi]_0^{2\pi} = 2\pi$$
$$\left\langle \frac{1}{r} \right\rangle = \left(\frac{1}{\pi a_0^3}\right)\left(\frac{a_0^2}{4}\right)(2)(2\pi) = \frac{1}{a_0}$$

2. Show that the most probable distance by the electron from the nucleus in the ground state of hydrogen atom is equal to the Bohr's radius.

Solution: For the ground state of hydrogen atom, $n = 1, \ell = 0$ and $m = 0$. Hence the ground state wave function is,

$$\psi_{1,0,0} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

Since, the wave function is independent of θ and ϕ, therefore,
Radial probability density $= P(r) = |\psi_{100}|^2 4\pi r^2 = \frac{4}{a_0^3} e^{-2r/a_0} r^2$ For most probable distance, $P(r)$ is to be the maximum

$$\frac{dP}{dr} = \frac{4}{a_0^3}\left[r^2\left(-\frac{2}{a_0}\right)e^{-2r/a_0} + 2re^{-2r/a_0}\right] = 0 \Rightarrow r = a_0$$

Thus the most probable distance of the electron from the nucleus of hydrogen atom in the ground state is equal tothe Bohr radius (a_0).

3. If the ground state wave function for the hydrogen atom is

$$\psi = \frac{1}{\sqrt{\pi}} \frac{1}{a_0^{3/2}} e^{-r/a_0}$$

show that average distance of the electron from the nucleus is $1.5a_0$.

Solution: We have the average distance of the electron from the hydrogen nucleus in the ground state is,

$$\langle r\rangle = \int_0^\infty \psi^* \hat{r}\psi dr = \int_0^\infty \frac{1}{\sqrt{\pi}}\frac{1}{a_0^{3/2}} e^{-r/a_0} r \frac{1}{\sqrt{\pi}}\frac{1}{a_0^{3/2}} e^{-r/a_0} d\tau$$
$$= \frac{1}{\pi a_0^3}\int_0^\infty r e^{-2r/a_0} r^2 \sin\theta dr d\theta d\phi$$

Using the standard integral $\int_0^\infty e^{-ax}x^n dx = \frac{n!}{a^{n+1}}$, we get

$$\langle r\rangle = \frac{1}{\pi a_0^3}\int_0^\infty r^3 e^{-2r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = \frac{1}{\pi a_0^3} \times \frac{3!}{(2/a_0)^4} \times 2 \times 2\pi$$

Therefore, $\langle r\rangle = \frac{3}{2}a_0 = 1.5a_0$

4. What is the expectation value of the knetice nergy $\left(E^2\right)$ of the electron in the 1s state of the hydrogen atom?

Solution: The expectation value of the kinetic energy is,

$$\langle E_k\rangle = \int_\tau \psi^*_{1,0,0}\hat{E}_k\psi_{1,0,0}d\tau = \int_0^\infty\int_0^\pi\int_0^{2\pi} \psi_{1,0,0}\hat{E}_k\psi_{1,0,0} r^2\sin\theta dr d\theta d\phi$$

But, $\vec{E}_k = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

Since $\psi_{1,0,0}$ depends on r only, the terms in $\frac{\partial}{\partial\theta}$ and $\frac{\partial}{\partial\phi}$ are zero.

$$\langle E_k\rangle = -\frac{\hbar^2}{2m}\cdot 4\pi\left(\frac{1}{\sqrt{\pi}a_0^3}\right)^2\int_0^\infty e^{-r/a_0}\times\left\{\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)e^{-r/a_0}\right\}r^2 dr$$
$$= -\frac{\hbar^2}{2m}\frac{4}{a_0^3}\int_0^\infty\left(\frac{1}{a_0^2}-\frac{2}{ra_0}\right)e^{-2r/a_0}r^2 dr$$
$$= -\frac{2\hbar^2}{ma_0^3}\left[\frac{1}{a_0^2}\int_0^\infty r^2 e^{-2r/a_0}dr - \frac{2}{a_0}\int_0^\infty r e^{-2r/a_0}dr\right]$$
$$= -\frac{2\hbar^2}{ma_0^3}\left[\frac{1}{a_0^2}\frac{2}{(2/a_0)^3} - \frac{2}{a_0}\frac{1}{(2/a_0)^2}\right] = \frac{2\hbar^2}{ma_0^3}\cdot\frac{a_0}{4}$$

Therefore, $\langle E_k\rangle = \frac{\hbar^2}{2ma_0^3} = \frac{\hbar^2}{2m}\left(\frac{me^2}{\hbar^2}\right) = \frac{me^4}{2\hbar^2}$

5. Estimate the uncertainity in the radial position of the electron in the ground state of hydrogen atom.

Solution: For ground state

$$\langle r\rangle = \frac{4}{a_0^3}\int_0^\infty r^3 e^{\frac{-2r}{a_0}}dr = \frac{3a_0}{2}$$
$$\langle r^2\rangle = \frac{4}{a_0^3}\int_0^\infty r^4 e^{\frac{-2r}{a_0}}dr = 3a_0^2$$

uncertainity in the radial position of the particle will be

$$\Delta r = \sqrt{\langle r^2\rangle - \langle r\rangle^2} = \frac{\sqrt{3}}{2}a_0$$

6. Find the positions of maxima of the radial probability curves for 1s,2s,2p and 3d orbitals of the hydrogen like atom

Solution: The radial probability density

$$P_{nl} = r^2 |R_{nl}|^2$$
$$R_{10} = Constant \times e^{-Zr/a_0}$$
$$R_{21} = Constant \times e^{-Zr/2a_0}$$
$$R_{32} = Constant \times e^{-Zr/3a_0}$$

P_{nl} will be maximum when $\frac{dP_{nl}}{dr} = 0$ hence

$$\frac{dP_{10}}{dr} = 0 \implies C(2r - \frac{2Zr^2}{a_0})e^{\frac{-2Zr}{a_0}} = 0$$
$$\implies r = \frac{a_0}{Z}$$
$$\frac{dP21}{dr} = 0 \implies C(4r^3 - \frac{Zr^4}{a_0})e^{\frac{-Zr}{a_0}} = 0$$
$$\implies r = \frac{4a_0}{Z}$$

Similarly $\frac{dP_{32}}{dr} = 0 \implies r = \frac{9a_0}{2}$
In general $r_{max} = \frac{n^2 a_0}{2}$

7. At time $t = 0$, the wave function for the hydrogen atom is

$$\psi(r,0) = \frac{1}{\sqrt{10}}\left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right)$$

where the subscripts are values of the quantum numbers n, l, m. (i) What is the expectation value for the energy of the system? (ii) What is the probability of finding the system with $l = 1, m = 1$? .

Solution: Expectation value $= \langle E \rangle = \langle \psi | H | \psi \rangle$

$$= \frac{1}{10}\left\langle \left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right) |H| \left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right) \right\rangle$$
$$= \frac{1}{10}\left\langle \left(2\psi_{100} + \psi_{210} + \sqrt{2}\psi_{211} + \sqrt{3}\psi_{21,-1}\right) | \left(2E_1\psi_{100} + E_2\psi_{210} + \sqrt{2}E_2\psi_{211} + \sqrt{3}E_2\psi_{21,-1}\right) \right\rangle$$
$$= \frac{1}{10}(4E_1 + E_2 + 2E_2 + 3E_2) = \frac{1}{10}[4E_1 + 6E_2]$$
$$E_1 = -13.6eV \quad E_2 = -3.4eV$$
$$\langle E \rangle = -74.8eV$$

8. Let ψ_{nlm} denote the eigenfunctions of a Hamiltonian for a spherically symmetric potential $V(r)$

$$\psi_{n,l,m} = \frac{1}{6}\left[\psi_{200} + \sqrt{5}\psi_{210} + \sqrt{10}\psi_{21-1} + \sqrt{20}\psi_{211}\right]$$

Then find (a) the expectation value of L_z
(b) the expectation value of L^2 in the state
(c) the expectation value of L_y

Solution: $\psi_{nmm} = \frac{1}{6}\left[\psi_{200} + \sqrt{5}\psi_{210} + \sqrt{10}\psi_{21-1} + \sqrt{20}\psi_{211}\right]$

(a)

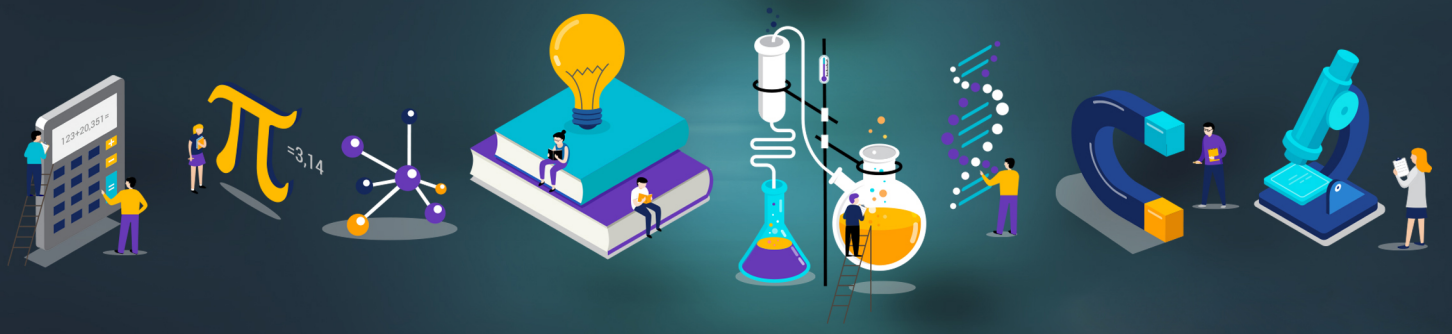
$$\langle L_z\rangle = \frac{1}{36}0\hbar + \frac{5}{36}\times 0\hbar + \frac{10}{36}\times(-1\hbar) + \frac{20}{36}(1\hbar)$$
$$= \frac{10}{36}\hbar = \frac{5}{18}\hbar$$

(b) $\left\langle L^2\right\rangle = \frac{1}{36}\times 0\hbar^2 + \frac{5}{36}\times\left(2\hbar^2\right) + \frac{10}{36}\times\left(2\hbar^2\right) + \frac{20}{36}\left(2\hbar^2\right)$

$$= \frac{35}{36}\left(2\hbar^2\right) = \frac{35}{18}\hbar^2$$

(c) $L_y = \frac{L_+ - L_-}{2i}$

$$\therefore \langle L_y\rangle = \frac{1}{2i}\{\langle L_+\rangle - \langle L_-\rangle\}$$
$$L_+|\psi\rangle = \frac{\sqrt{5}}{6}\times\sqrt{2}\hbar\psi_{211} + \frac{\sqrt{10}}{6}\times\sqrt{2}\hbar\psi_{210}$$
$$\langle\psi|L_+|\psi\rangle = \frac{\sqrt{20}\times\sqrt{5}\times\sqrt{2}\hbar}{36} + \frac{\sqrt{10}\times\sqrt{5}\times\sqrt{2}\hbar}{36}$$
$$L_-|\psi\rangle = \frac{\sqrt{5}}{6}\times\sqrt{2}\hbar\psi_{21-1} + \frac{\sqrt{20}}{6}\times\sqrt{2}\hbar\psi_{210}$$
$$\langle\psi|L_-|\psi\rangle = \frac{\sqrt{10}\times\sqrt{5}\times\sqrt{2}\hbar}{36} + \frac{\sqrt{20}\times\sqrt{5}\times\sqrt{2}\hbar}{36} \qquad \therefore \langle L_y\rangle = 0$$



2. Angular momentum

2.1 Angular momentum

The angular momentum of a particle about a point is defined in position vector of a particle with the given point as the origin of the co-ordinate system and p is the linear momentum.

Analogically in quantum mechanics there exist quantum mechanically orbital angular momentum is defined as

$$L = L_x\hat{i} + L_y\hat{j} + L_z\hat{k}$$

where

$$L_x = YP_z - ZP_y$$

$$L_y = ZP_x - XP_z$$

$$L_z = XP_y - YP_x$$

where X, Y, Z are position operator in x, y, z direction
and p_1, p_y, p_z momentum in respective x, y, z direction it is given that

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

$$P_v = -i\hbar\frac{\partial}{\partial y}$$

$$P_z = -i\hbar\frac{\partial}{\partial z}$$

In quantum mechanics one can defined the Hermitian operator

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

Commutation relation

$$\begin{matrix}[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \\ [\hat{L}_y, \hat{L}_x] = -i\hbar\hat{L}_z\end{matrix} \quad \begin{matrix}[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \\ [\hat{L}_z, \hat{L}_y] = -i\hbar\hat{L}_x\end{matrix} \quad \begin{matrix}[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y \\ [\hat{L}_x, \hat{L}_z] = -i\hbar\hat{L}_y\end{matrix}$$

i.e. the components of the orbital angular momentums cannot be measured simultaneously accurately.

$$[\hat{L}^2, \hat{L}_x] = 0$$

$$\left[\hat{L}^2,\hat{L}_y\right]=0 \quad \left[\hat{L}^2,\hat{L}_z\right]=0$$

i.e. square of the orbital angular momentum commutes with any one of components of the orbital angular momentum.

$$\left[\hat{L}_x,\hat{p}_x\right]=0$$
$$\left[\hat{L}_y,\hat{p}_y\right]=0 \quad \left[\hat{L}_z,\hat{p}_z\right]=0$$
$$\begin{array}{lll}\left[\hat{L}_x,\hat{p}_y\right]=i\hbar\hat{p}_z & \left[\hat{L}_y,\hat{p}_z\right]=i\hbar\hat{p}_x & \left[\hat{L}_z,\hat{p}_x\right]=i\hbar\hat{p}_y\\ \left[\hat{L}_x,\hat{x}\right]=0 & \left[\hat{L}_y,\hat{y}\right]=0 & \left[\hat{L}_z,\hat{z}\right]=0\\ \left[\hat{L}_x,\hat{y}\right]=i\hbar\hat{z} & \left[\hat{L}_y,\hat{z}\right]=i\hbar\hat{x} & \left[\hat{L}_z,\hat{x}\right]=i\hbar\hat{y}\end{array}$$

2.1.1 Orbital angular momentum in sperical polar coordinates

$$L_x=i\hbar\left(\sin\phi\frac{\partial}{\partial\theta}+\cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$
$$L_y=i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta}+\sin\phi\cot\theta\frac{\partial}{\partial\phi}\right) \text{ and}$$
$$L_z=-i\hbar\frac{\partial}{\partial\phi}$$

2.1.2 eigen value and eigen vector of L^2 and L_z

Since,the commutator bracket $\left[L^2,L_z\right]=0$ therefore L^2 and L_z can be measured simultaneously accurately and both have simultaneous eigenfunctions and eigenkets.Denoting the simultaneous eigen kets $|l,m_l\rangle$ (Where l and m_l are the orbital quantum number magnetic quantum number respectevely),the eigen value equation for L^2 and L_z can be written as

$$\hat{L}^2|l,m_l\rangle=l(l+1)\hbar^2|l,m_l\rangle$$
$$\hat{L}_z|l,m_l\rangle=m_l\hbar|l,m_l\rangle$$

Alternate form: Since, $\hat{L}^2$ and $\hat{L}_z$ depends on θ,ϕ then their eigen function is function of θ,ϕ i.e.

$$\hat{L}^2Y_{\ell,m_l}(\theta,\phi)=\ell(\ell+1)\hbar^2Y_{\ell,m_l}(\theta,\phi)$$
$$\hat{L}_zY_{\ell,m_l}(\theta,\phi)=m_l\hbar Y_{\ell,m_l}(\theta,\phi)$$

where $Y_{\ell,m}(\theta,\phi)$ is said to be Spherical Harmonics and defined as

$$Y_{l,m_l}(\theta,\varphi)=\varepsilon\sqrt{\left(\frac{2\ell+1}{4\pi}\right)\frac{(\ell-|m_l|)!}{(\ell+|m_l|)!}}P_\ell^{|m_l|}(\cos\theta)e^{im_l\phi}$$

where $\varepsilon=(-1)^{m_l}$ for $m_l>0$ and $\varepsilon=1$ for $m_l\leq 0$.

2.1.3 Lowering and raising operators

Raising Operator: $\hat{L}_+=\hat{L}_x+i\hat{L}_y$

Lowering Operator: $\hat{L}_-=\hat{L}_x-i\hat{L}_y$

Important relations:

$$\begin{array}{llll}\left[\hat{L}_z,\hat{L}_+\right]=\hbar\hat{L}_+ & \left[\hat{L}_z,\hat{L}_-\right]=-\hbar\hat{L}_- & \left[\hat{L}_x,\hat{L}_+\right]=-\hbar\hat{L}_z & \left[\hat{L}_x,\hat{L}_-\right]=\hbar\hat{L}_z\\ \left[\hat{L}_y,\hat{L}_+\right]=-i\hbar\hat{L}_z & \left[\hat{L}_y,\hat{L}_-\right]=i\hbar\hat{L}_z & \left[\hat{L}_+,\hat{L}_-\right]=2\hbar\hat{L}_z & \\ \hat{L}_+\hat{L}_-=\hat{L}^2-\hat{L}_z^2+\hbar\hat{L}_z & \hat{L}_-\hat{L}_+=\hat{L}^2-\hat{L}_z^2-\hbar\hat{L}_z & & \end{array}$$

Action of $\hat{L}_+$and $\hat{L}_-$:

$$\hat{L}_+|l,m_l\rangle=\sqrt{(\ell-m_l)(l+m_l+1)}\hbar|l,m_l+1\rangle$$
$$\hat{L}_+Y_{\ell,m_l}(\theta,\phi)=\sqrt{(\ell-m_l)(l+m_l+1)}\hbar Y_{i,m_i+1}(\theta,\phi)$$
$$\hat{L}_-|l,m_l\rangle=\sqrt{(\ell+m_l)(l-m_l+1)}\hbar|l,m_l-1\rangle$$
$$\hat{L}_-Y_{(,m_l}(\theta,\phi)=\sqrt{(\ell+m_l)(l-m_l+1)}\hbar Y_{\ell,m_l-1}(\theta,\phi)$$

2.1.4 Matrix Representation of the operators:

Elements of $\hat{L}^2 = \langle \ell', m_l' | \hat{L}^2 | \ell, m_l \rangle = \ell(\ell+1)\hbar^2 \delta_{\ell\ell'} \delta_{m_l m_l'}$, will be non-zero for $l = l'$ and $m_l = m_{l'}$ is

$$\hat{L}^2 = \begin{bmatrix} 2\hbar^2 & 0 & 0 \\ 0 & 2\hbar^2 & 0 \\ 0 & 0 & 2\hbar^2 \end{bmatrix} = 2\hbar^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ (for } l = 1)$$

Elements of $\hat{L}_z = \langle \ell', m_l' | \hat{L}_z | \ell, m_l \rangle = m_l \hbar \delta_{\ell\ell'} \delta_{m_l m_l'}$, will be non-zero for $l = l'$ and $m_l = m_l'$ i.e.

$$\hat{L}_z = \begin{bmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{bmatrix} = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \text{ (for } l = 1)$$

Elements of $\hat{L}_+ = \langle \ell', m_l' | \hat{L}_+ | \ell, m_l \rangle = \hbar\sqrt{(\ell - m_l)(\ell + m_l + 1)}\,\delta_{\ell\ell'} \delta_{m_l', m_l+1}$, will be non-zero for $l = l'$ and $m_l = m_l' + 1$ i.e.

$$\hat{L}_+ = \begin{bmatrix} 0 & \sqrt{2}\hbar & 0 \\ 0 & 0 & \sqrt{2}\hbar \\ 0 & 0 & 0 \end{bmatrix} = \sqrt{2}\hbar \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{(for } l = 1)$$

Elements of $\hat{L}_+ = \langle \ell', m_l' | \hat{L}_- | \ell, m_l \rangle = \hbar\sqrt{(\ell + m_l)(\ell - m_l + 1)}\,\delta_{\ell\ell}, \delta_{m_l, m_l} - 1$, will be non-zero for $l = l'$ and $m_l = m_l' - 1$ i.e.

$$\hat{L}_- = \sqrt{2}\hbar \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad \text{(for } l = 1)$$

Expectation values in the state $|\ell, \mathbf{m}_\ell\rangle$:

$$\langle \hat{L}_x \rangle = 0, \langle \hat{L}_y \rangle = 0, \langle \hat{L}_z \rangle = m_l \hbar$$

$$\langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle = \frac{\hbar^2}{2}\left[\ell(\ell+1) - m_l^2\right], \langle \hat{L}_z^2 \rangle = m_l^2 \hbar^2$$

Exercise 2.1 The expectation value of the operator $\hat{L}_+$in the state $|\psi\rangle = \frac{1}{\sqrt{3}}[|1,1\rangle + |1,0\rangle + |1,-1\rangle]$ is ■

Solution: $\langle L_+ \rangle = \frac{1}{3}[\langle 11|L_+|11\rangle + \langle 11|L_+|10\rangle + \langle 11|L_+|1-1\rangle + \langle 10|L_+|11\rangle + \langle 10|L_+|10\rangle + \langle 10|L_+|1-1\rangle + \langle 1-1|L_+|11\rangle + \langle 1-1|L_+|10\rangle + \langle 1-1|L_+|1-1\rangle]$

L_+ will raise the value of m to $m+1$ .Only those terms will survive in which this raised values of min the ket is equal to the value of m in the bra. Thus ,

$\langle L_+ \rangle = \frac{1}{3}[\langle 11|L_+|10\rangle + \langle 10|L_+|1-1\rangle] = \frac{1}{3}[\langle 11|\sqrt{2}\hbar|11\rangle + \langle 10|\sqrt{2}\hbar|10\rangle] = \frac{2\sqrt{2}\hbar}{3}$

2.2 Angular momentum algebra

Generalised angular momentum is defined as $J = J_x\hat{i} + J_y\hat{j} + J_z\hat{k}$

The commutation $[J_x J_y] = i\hbar J_z$ $[J_y, J_z] = i\hbar J_x$ $[J_z J_x] = i\hbar J_y$

The state $|j,m\rangle$ make complete basis so

$$J^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle \quad j = 0,1,2,3,\ldots$$

$$J_z|j,m\rangle = m\hbar|j,m\rangle \qquad -j < m < j$$

It is also given that

$$[J^2, J_x] = 0, \quad [J^2, J_y] = 0 \quad [J^2, J_z] = 0$$

The completeness relation is given as

$$\sum_{m=-j}^{j} \sum_{j=0}^{j} |j,m\rangle\langle j,m| = 1$$

The raising and lowering operators.

$$J_+ = J_x + iJ_y$$
$$J_- = J_x - iJ_y$$

One can calculate

$$[J_z, J_+] = \hbar J_+ \quad [J_z, J_-] = -\hbar J_- \quad [J^2, J_+] = 0 \quad [J^2, J_-] = 0$$

So J^2, and $J_+$and J - can be simultaneously measured.

The state $J_+|j,m\rangle$

$$[J_z, J_+] = \hbar J_+ \qquad J_z, J_+ - J_+ J_z = \hbar J_+$$
$$J_z J_+|j,m\rangle - J_+ J_z|j,m\rangle = \hbar J_+ \quad J_z(J_+|j,m\rangle) = (m+1)\hbar J_+|j,m\rangle$$

So $J_+|jm\rangle$ is eigen vector of J_z with the eigen value $(m+1)\hbar$ i.e., $J+|jm\rangle$ can be represented as

$$J_+|j,m\rangle \equiv C_+|j,m+1\rangle$$

Now one can find the value of $C_+$with orthonormal condition.

$$\langle j,m|J_-J_+|j,m\rangle = |C_+^*|^2 \quad \langle m+1, j \mid j,m+1\rangle$$

$$|C_+^*|^2 = \sqrt{j(j+1) - m(m+1)}$$
$$J_+|j,m\rangle = \sqrt{j(j+1) - m(m+1)}\hbar|j,m+1\rangle$$

For $j = m \qquad J_+|jm\rangle = 0 \qquad m \leq j$

The state $J_-|j,m\rangle$

Similarly one can find from the relation

$$[J_z, J_-] = -\hbar J_-$$

And

$$J_z(J_-|j,m\rangle = (m-1)\hbar J_-|j,m\rangle$$
$$J_-|j,m\rangle = C_-|j,m-1\rangle$$

Again C_-can be found with the relation

$$\langle m, j|J_+J_-|j,m\rangle = |C_-^*|^2$$

$$|C_-^*|^2 = \sqrt{j(j+1) - m(m-1)}\hbar|j,m-1\rangle$$
$$J_-|j,m\rangle = \sqrt{j(j+1) - m(m-1)}\hbar|j,\dot{m}-1\rangle$$

If $m=-j, J_-|j,-j\rangle=0$ So again the $m\geq -j$.
So the value of $-j<m<j$ the $J_+$and J_-can be named as ladder operator where

$J_+|j,m\rangle=\sqrt{j(j+1)-m(m+1)}\hbar|j,m+1\rangle$, which raise the state by $|j,m\rangle$ to $|j,m+1\rangle$ and

$J_-|j,m\rangle=\sqrt{j(j+1)-m(m-1)}\hbar|j,m+1\rangle$ who lower the state $|j,m\rangle$ to $|j,m-1\rangle$.

Exercise 2.2 Find the matrix representation of operator for $j=1$
(a) J^2 and J_z
(b) $J_+$and J_-
(c) J_x and J_y ■

Solution: (a) For $j=1m=-1,01$

$$J^2=\begin{vmatrix} \langle 1,1|J^2|1,1\rangle & \langle 1,1|J^2|1,0\rangle & \langle 1,1|J^2|1,-1\rangle \\ \langle 1,0|J^2|1,1\rangle & \langle 1,0|J^2|1,0\rangle & \langle 1,0|J^2|1,-1\rangle \\ \langle 1,-1|J^2|1,1\rangle & \langle 1,-1|J^2|1,0\rangle & \langle 1,-1|J^2|1,-1\rangle \end{vmatrix}=2\hbar^2\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$$

Similarly,

$$J_z=\hbar\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}$$

$$J_+=h\sqrt{2}\begin{pmatrix}0&1&0\\0&0&1\\0&0&0\end{pmatrix},J_-=\hbar\sqrt{2}\begin{pmatrix}0&0&0\\1&0&0\\0&1&0\end{pmatrix}$$

$$J_x=\frac{J_++J_-}{2}=\frac{h}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix},$$

$$j_y=\frac{1}{2i}(J_+-J_-)=\frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}$$

Exercise 2.3 (a) Find $\langle J_x\rangle,\langle J_y\rangle$ (b) Find $\langle J_x^2\rangle,\langle J_y^2\rangle$ (c) Find $\Delta J_x\cdot\Delta J_y$ ■

Solution:

$$\text{(a) } \langle J_x\rangle=\frac{1}{2}(\langle J_+\rangle+\langle J_-\rangle)$$

$$J_x|j,m\rangle=\frac{1}{2}(J_+|j,m\rangle+J_-|j,m\rangle)$$

$$=\frac{\hbar}{2}(\sqrt{j,(j+1)-m(m+1)}|j,m+1\rangle+\sqrt{j(j+1)-m(m-1)}|j,m-1\rangle)$$

$$\langle j,m|J_,|j,m\rangle=\frac{h}{2}\sqrt{j(j+1)-m(m+1)}\langle j,m\mid j,m+1\rangle$$

$$\frac{\hbar}{2}\sqrt{j(j+1)-m(m-1)\langle j,m\mid j,m-1\rangle}=0$$

Similarly $\langle J_y\rangle=0$

$$(b)\left\langle J_x^2\right\rangle = \left\langle \frac{1}{2}\left(J_+ + J_-\right)\left(J_+ + J_-\right)\right\rangle$$

$$= \frac{1}{4}\left\langle J_+^2 + J_+J_- + J_-J_+ + J_-^2\right\rangle = \frac{1}{4}\left\langle J_+^2\right\rangle + \frac{1}{4}\left\langle J_+J_- + J_-J_+\right\rangle + \frac{1}{4}\left\langle J_-^2\right\rangle$$

$$= \frac{1}{4}\left\langle J_+^2\right\rangle + \frac{2}{4}\left(J^2 - J_=^2\right) + \frac{1}{4}\left\langle J_-^2\right\rangle = 0 + \frac{\hbar^2}{2}\left(j(j+1) - m^2\right) + 0\cdot\hbar^2$$

$$\Rightarrow \left\langle J_x^2\right\rangle = \frac{1}{2}\left[j(j+1) - m^2\right]\cdot\hbar^2$$

Similarly $\left\langle J_y^2\right\rangle = \frac{1}{2}\left[j(j+1) - m^2\right]\cdot\hbar^2 \quad \left\langle J_x^2\right\rangle = \left\langle J_y^2\right\rangle$

(c) $\Delta J_x = \sqrt{\left\langle J_x^2\right\rangle - \left\langle J_x\right\rangle^2} = \sqrt{\frac{1}{2}\left(j(j+1) - m^2\right)\hbar}$

$$\Delta J_y = \sqrt{\left\langle J_y^2\right\rangle - \left\langle J_y\right\rangle^2} = \sqrt{\frac{1}{2}\left(j(j+1) - m^2\right)\hbar} \text{ so } \Delta J_x \Delta J_y = \frac{1}{2}\left(j(j+1) - m^2\right)\hbar^2$$

2.3 Concepts of spin in quantum mechanics

2.3.1 The stern-Gerlach experiment

The existance of spin is first confirmed experimentally by stern and Gerlack in 1922. Using silver (Ag) atoms. Silver has 47 electrons, out of which 46 electrons form a spherically symmetric charge distribution and 47^{th} . electron occupies a ' 5 s' orbital ($l = 0$). If the silver atom is its ground state, then its total orbital angular momentum will be zero.

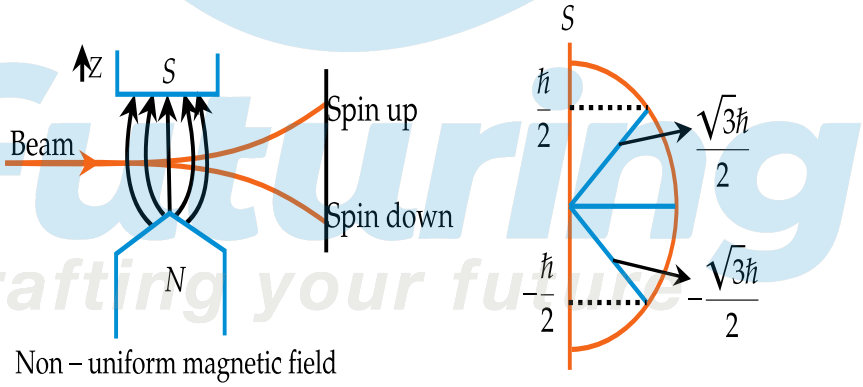


Figure 2.1

If a beam of silver atoms passes through an in homogeneous (non-uniform) magnetic field (along z-direction), we would expect the following results:

(i) Classically, there will be a continuous band on the screen and the band will be symmetric about theundeflected direction z = 0.

(ii) Accordinh to Schrodinger's wave theory, if the atom has an orbital angular momentum ' l ' then the beam will split into discrete $(2l+1)$ components. Since, the silver atom is in ground state $(l = 0)$, there will be only spot on the screen. But, in experiments the beam splits into two distinct components.

To solve this problem, Goudsmith and Unlenbeck postulated that in addition to its orbital angular momentum the electron possesses an intrinsic angular momentum. This angular momentum has no connection with the spaial degrees of freedom but it can be related with the internal rotational or spinning mation of the electron about its own axis. This is known as spin angular momentum which is connected with an intrinsic degree of freedom i.e. spin. Spin is a purely quantum mechanical concept with classical analog. Unlike orbital angular momentum, the spin cannot be described by a differential operator. Consider a particle of mass 'm' and charge ' q ' is moving in a circle of radius ' r '. The magnetic dipole moment due to the orbital motion of the particle will be

$$\vec{\mu}_L = \frac{q}{2m}\vec{L}$$

where $\vec{L}$ is the orbital angular momentum of the particle and z-components of magnetic moment will be

$$\mu_z = \frac{q}{2m} L_z$$

For an electron the relation will be $\mu_z = -\frac{e}{2m_e} L_z$
If the electron is the eigenstates of $\hat{L}_z$, then

$$(\mu_L)_z = -\left(\frac{e}{2m_e}\right) m_l \hbar = -\mu_B m_l$$

where $\left(\frac{e\hbar}{2m_e}\right) = \mu_B =$ Bohr magneton and m_l is the orbital magnetic quantum number.
Eor a narticular value of l, we will get $(2\ell+1)$ values of ' m_l ' i.e $m_l = -l, -l+1, \ldots\ldots\ldots\ldots, 0, \ldots\ldots, l-1, l$
Similarly, if we take electron as spinning charged sphere, then the magnetic dipole moment due to the motion of the particle will be

$$\vec{\mu}_S = -g_s \frac{e}{2m} \vec{S}$$

where $\vec{S}$ is the spin angular momentum of the electron and g_S is the spin g-iactor. Therefore, z-components of magnetic dipole moment will be

$$(\mu_S)_z = -g_S \frac{e}{2m} S_z$$

If the electron is in an eigenstate of S_z, then

$$(\mu_S)_z = -g_s \mu_B m_s$$

where $\left(\frac{e\hbar}{2m_e}\right) = \mu_B =$ Bohr magneton and m_s is the spin magnetic quantum number.
For a particular value of s, we will get $(2s+1)$ values of ' m ' i.e. $m_s = -s, -s+1, \ldots\ldots, 0, \ldots\ldots..s-1, s$
Every fundamental particle has a specific spin $(s = 0, 1, 2, \ldots\ldots\ldots\ldots\ldots)$
Fermions: Particle having half-integer spins. Examples: quarks, electrons, protons, neutrons etc.
Bosons: Particles having integer spins. Example: Photons, pions, gravitons etc.
Therefore, there are two kinds of angular momentum of the particle i.e.
(i) Orbital angular momentum $(\vec{L})$ due to particle's orbital motion and it is characterized by two quantro numbers i.e. ℓ and its projection of z-axis ' m_ℓ ' which can take values from $-\ell$ to $+\ell$.
(ii) Spin angular momentum $(\vec{S})$ due to some intrinsic motion of the particle and it is characterised by two quantum numbers i.e. s and its projection on z-axis m_s ' which can take values from $-s$ to $+s$. Thus, the total angular momentum can be written as

$$\vec{J} = \vec{L} + \vec{S}$$

and it is characterised by two quantum numbers i.e. j and its projection on z-axis i.e. ' m_j ' which can take values from $-j$ to $+j$.
In the Stern-Gerlach experiment, the silver atom has orbital angular momentum to be zero i.e $l = 0$ but spin angular momentum to be $1/2$ i.e. $s = 1/2$. Therefore, total angular momentum will be

$$j = |l - s| \text{ to } |l + s| = -\frac{1}{2}, \frac{1}{2}$$

For thiis, we are getting two spots on the screen.

2.3.2 spin angular momentum

- Spin angular momentum has components S_x, S_y, S_z and the corresponding operators satisfy the following commutation relation:

$$\left[\hat{S}_x, \hat{S}_y\right] = ih\hat{S}_z \quad \left[\hat{S}_y, \hat{S}_z\right] = i\hbar\hat{S}_x \quad \left[\hat{S}_z, \hat{S}_x\right] = i\hbar\hat{S}_y$$

- $\left[\hat{S}^2, \hat{S}_z\right] = 0$ i.e. they have simultaneous eigenstate as following:

$$\hat{S}^2 |s, m_s\rangle = s(s+1)\hbar^2 |s, m_s\rangle$$
$$\hat{S}_z |s, m_s\rangle = m_s \hbar |s, m_s\rangle$$

- Raising and lowering operators are defined as following:

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$$
$$\hat{S}_+ |s,m_s\rangle = \hbar\sqrt{(s-m_s)(s+m_s+1)}\,|s,m_s+1\rangle$$
$$\hat{S}_- |s,m_s\rangle = \hbar\sqrt{(s+m_s)(s-m_s+1)}\,|s,m_s-1\rangle$$

- - For a spin $\frac{1}{2}$ particles like electrons, m_s can take values $\frac{1}{2}$ and $-\frac{1}{2}$, so the possible spin states are
Spin-up state: $\chi_{1/2} = |\uparrow\rangle = \left|\frac{1}{2},\frac{1}{2}\right\rangle$
Spin-down state: $\chi_{-1/2} = |\downarrow\rangle = \left|\frac{1}{2},-\frac{1}{2}\right\rangle$ such that

$$\hat{S}^2\chi_{1/2} = \frac{3}{4}\hbar^2\chi_{1/2}, \quad \hat{S}^2\chi_{-1/2} = \frac{3}{4}\hbar^2\chi_{-1/2}$$
$$\hat{S}_z\chi_{1/2} = \frac{\hbar}{2}\chi_{1/2}, \quad \hat{S}_z\chi_{-1/2} = \frac{\hbar}{2}\chi_{-1/2}$$
$$\hat{S}_+\chi_{1/2} = 0, \quad \hat{S}_+\chi_{-1/2} = \hbar\chi_{1/2}$$
$$\hat{S}_-\chi_{1/2} = \hbar\chi_{-1/2}, \quad \hat{S}_-\chi_{-1/2} = 0$$

Matrix representation of the various spin operators for a spin-1/2 particle:

$$\hat{S}^2 = \begin{bmatrix} \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}^2\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}^2\left|\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}^2\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}^2\left|\frac{1}{2},-\frac{1}{2}\right\rangle \end{bmatrix} = \frac{3}{4}\hbar^2\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\hat{S}_z = \begin{bmatrix} \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}_z\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}_z\left|\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}_z\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}_z\left|\frac{1}{2},-\frac{1}{2}\right\rangle \end{bmatrix} = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\hat{S}_+ = \begin{bmatrix} \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}_+\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}_+\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle \end{bmatrix} = \begin{bmatrix} 0 & \hbar \\ 0 & 0 \end{bmatrix} = \hbar\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$\hat{S}_- = \begin{bmatrix} \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}_-\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},\frac{1}{2}\right|\hat{S}_-\left|\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}_-\left|\frac{1}{2},\frac{1}{2}\right\rangle & \left\langle\frac{1}{2},-\frac{1}{2}\right|\hat{S}_-\left|\frac{1}{2},-\frac{1}{2}\right\rangle \end{bmatrix} = \hbar\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\hat{S}_x = \frac{1}{2}\left[\hat{S}_+ + \hat{S}_-\right] = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
$$\hat{S}_y = \frac{1}{2i}\left[\hat{S}_+ - \hat{S}_-\right] = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Eigenvalues and eigenvectors of $\hat{S}_z$:

Eigenvalues: $\lambda = \pm\frac{\hbar}{2}$

Eigenvectors: $\chi_{1/2} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ for $\lambda = \frac{\hbar}{2}$ and $\chi_{-1/2} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ for $\lambda = -\frac{\hbar}{2}$

Eigenvalues and eigenvectors of $\hat{S}_x$:

Eigenvalues: $\lambda = \pm\frac{\hbar}{2}$

Eigenvectors: $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} + \chi_{-1/2}\right]$ for $\lambda = \frac{\hbar}{2}$
and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} - \chi_{-1/2}\right]$ for $\lambda = -\frac{\hbar}{2}$

Eigenvalues and eigenvectors of $\hat{S}_y$:

Eigenvalues: $\lambda = \pm\frac{\hbar}{2}$

Eigenvectors: $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} + i\chi_{-1/2}\right]$ for $\lambda = \frac{\hbar}{2}$

and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix} = \frac{1}{\sqrt{2}}\left[\chi_{1/2} - i\chi_{-1/2}\right]$ for $\lambda = -\frac{\hbar}{2}$

2.3.3 Pauli spin matrices

Spin angular momentum can be related with Pauli spin vector as follows:

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are components of the Pauli spin vectors and known as Pauli spin matrices. These matrices satisfies the following conditions:

(i) $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$

(ii) $\sigma_j\sigma_k + \sigma_k\sigma_j = \{\sigma_j, \sigma_k\} = 2I\delta_{jk}$

(iii) $[\sigma_j, \sigma_k] = 2i\varepsilon_{jkl}\sigma_l$

(iv) Pauli spin matrices are hermitian, traceless and determinant is -1.

(v) $\sigma_x\sigma_y\sigma_z = iI$

(vi) Since spin does not depend on spatial degrees of freedom then the components of spin S_x, S_y, S_z commute with all spatial operators i.e. momentum, position, orbital angular momentum.

(vii) $e^{i\alpha\sigma_j} = I\cos\alpha + i\sigma_j\sin\alpha$

(viii) For any two vectors $\vec{A}$ and $\vec{B}, (\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = (\vec{A}\cdot\vec{B})I + i\sigma\cdot(\vec{A}\times\vec{B})$

2.4 Addition of Angular Momenta

Let J_1 and J_2 be two independent commuting angularmomenta vectors ie.

$$[J_1, J_2] = 0$$

For example J_1 may be the orbital angular momentum L and J_2 the spin S of the same particle. Basis for the system is the set of simultaneous eigen states $|j_1m_1; j_2m_2>$ of the four commuting operators J_1^2, J_1z, J_2^2, J_2z which form a complete commuting set of observables. Let us consider the set of $(2j,+1)$ $(2j_2+11)$ states for fixed j_1 and $j_2(m_1 = j_1, j_1-1 ..... -j_1; m_2 = j_2, j_2-1, ... -j_2)$. So we suppress the fixed values of j_1 and j_2 from the notation for the basis state and write simple $|j_1m_1; j_2m_2>$ leaving it to be understood that

$$J_1^2\ |m_1; m_2> = j_1(j_1+1)\hbar^2|m_1; m_2>$$

$$J_2^2\ |m_1; m_2> = j_2(j_2+1)\hbar^2|m_1; m_2>$$

For J_z

$$J_1z|m_1; m_2> = m_1\hbar|m_1; m_2>, J_2z|m_1; m_2> = m_2\hbar|m_1; m_2>$$

Noting that $J_{1\pm}$ are ladder operators on m_1 and $J_2\pm$ on m_2, Then

$$J_{1\pm}|m_1;m_2>=[(j_1\mp m_1)(j_1\pm m_1+1)]^{\frac{1}{2}}|m_1\pm 1;m_2>$$

$$J_{2\pm}|m_1;m_2>=[(j_2\mp m_2)(j_2\pm m_2+1)]^{\frac{1}{2}}|m_1;m_2\pm 1>$$

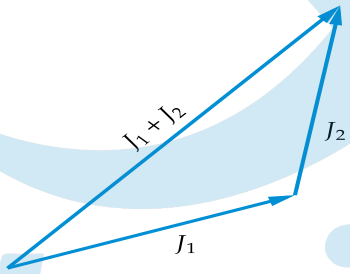
Suppose the interaction between the two system is such as to couple J_1 and J_2 then J_1z and J_2z are no longer constant of motion. It would be more advantageous to use other operators which commute with such an interactions for defining a basis. It is natural to use for this prupose J^2 and J_z where J is the total angular momentum operator for the composite system made up of J_1 and J_2.

$$J=J_1+J_2 \quad J^2=J_1^2+J_2^2+2J_1J_2$$

J_1^2 and J_2^2 do commute with J^2 and J_z, the simultaneous eigen state of these four operators will be taken as a new basis. We denote these by $|jm>$ is the abbreviation for $|j_1j_2j_m>$. The quantum numbers j,m are of course defined by

$$J^2|jm>=j(j+1)\hbar^2|jm> \quad J_z|jm>=m\hbar|jm>$$

The possible vlue of j for the composite system can be obtained by stating in terms of the vector model. If J_1 and J_2 thought of as two ordinary vectors of length j_1 and j_2 respectively, these vector together with J_1+J_2 form a triangle. The values of j_1,j_2,j must be then such that a triangle with these sides can be constructed.



This triangle rule or triangle condition immedietly set the maximum and minimum limits for j as (j_1+j_2) and $|j_1-j_2|$ (corresponding J_1 and J_2 are being parallel and antiparallel raspectively). Since angular momentum is quandized, the only allowed values between these limits are $j_1+j_2-1, j_1+j_2-2....|j_1-j_2|+1$
We shall now see that the same conclusion follow from quantum mechanics.

The states $|jm>$ and the sets $|m_1;m_2>$ are simple different bases for the same space. So any $|jm>$ can be written as a linear combination of the states $|m_;m_2>$

$$|jm>=\sum_{m_1m_2}|m_1;m_2><m_1;m_2|jm>$$

The matrix formed by the elements $<m_1;m_2|jm>$ where in m_1,m_2 together label the rows and j,m label the columns, must be unitary.

Since $J_z=J_1z+J_2z$ it is evident that

$$m=m_1+m_2$$

ie $<m_1;m_2|jm>=0$ unless $m_2=m-m_1$

Then $|jm>$ reduces to a single sum.

$$|jm>=\sum_{m_1}|m_1;m-m_1><m_1;m-m_1|jm>$$

Since the maximum value of m_1 and m_2 are j_1 and j_2 which is then necessarly the maximum value of j too. Since this value of m occurs only once (when $m_1=j_1$ and $m_2=j_2$), j_1+j_2 occurs only once.

Consider now the next lower value of m namely $m=j_1+j_2-1$ There are two states with this m one has

$m_1 = j_1, m_2 = j_2 - 1$ and the other $m - 1 = j_1 - 1, m_2 = j_2$ one of these or rather a linear combination of these must belongs to the value $j = j_1 + j_2$ already found, since one state with each value of m from $j_1 + j_2$ down to $-(j_1 + j_2)$ must go with this j

We have other state with $m = j_1 + j_2 - 1$ which must belong to a new value of $J, j = j_1 + j_2 - 1$

By extending this procedure $m = j_1 + j_2 - 2$ and so on we find new values $j_1 + j_2 - 2$ for j

This process ends when all the available states are exhausted. The total number of independent states is $(2j_1 + 1)(2j_2 + 1)$ as observed at the begining of this section on the other hand each value of j has $2j + 1$ states associated with it

So the minimum value of j_{min} of j is reached when

$$\sum_{j=J_{min}}^{j_1+j_2} (2j+1) = (2j+1)(2j_2+1)$$

After the summation of left had side we ger J_{min} as $J_{min} = |j_1 - j_2|$ as expected.
To sum up, the possible values j of the total angular momentum,, resulting from the addition of two given angular momenta j_1, j_2 are.

$$(j_1 + j_2)(j_1 + j_2 - 1), ..., |j_1 - j_2|$$

Practice set 1

1. The Hamiltonian of an electron in a constant magnetic field $\vec{B}$ is given by $H = \mu\vec{\sigma}\cdot\vec{B}$. where μ is a positive constant and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ denotes the Pauli matrices. Let $\omega = \mu B/\hbar$ and I be the 2×2 unit matrix. Then the operator $e^{iHt/\hbar}$ simplifies to

[NET JUNE 2011]

A. $I\cos\frac{\omega t}{2} + \frac{i\vec{\sigma}\cdot\vec{B}}{B}\sin\frac{\omega t}{2}$

B. $I\cos\omega t + \frac{i\vec{\sigma}\cdot\vec{B}}{B}\sin\omega t$

C. $I\sin\omega t + \frac{i\vec{\sigma}\cdot\vec{B}}{B}\cos\omega t$

D. $I\sin 2\omega t + \frac{i\vec{\sigma}\cdot\vec{B}}{B}\cos 2\omega t$

2. In a system consisting of two spin $\frac{1}{2}$ particles labeled 1 and 2, let $\vec{S}^{(1)} = \frac{\hbar}{2}\vec{\sigma}^{(1)}$ and $\vec{S}^{(2)} = \frac{\hbar}{2}\vec{\sigma}^{(2)}$ denote the corresponding spin operators. Here $\vec{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ and $\sigma_x, \sigma_y, \sigma_z$ are the three Pauli matrices.
In the standard basis the matrices for the operators $S_x^{(1)}S_y^{(2)}$ and $S_y^{(1)}S_x^{(2)}$ are respectively,

[NET JUNE 2011]

A. $\frac{\hbar^2}{4}\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

B. $\frac{\hbar^2}{4}\begin{pmatrix}i&0\\0&-i\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}-i&0\\0&i\end{pmatrix}$

C. $\frac{\hbar^2}{4}\begin{pmatrix}0&0&0&-i\\0&0&i&0\\0&-i&0&0\\i&0&0&0\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}0&0&0&-i\\0&0&-i&0\\0&i&0&0\\i&0&0&0\end{pmatrix}$

D. $\frac{\hbar^2}{4}\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&-i\\0&0&i&0\end{pmatrix}, \frac{\hbar^2}{4}\begin{pmatrix}0&-i&0&0\\i&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$

3. These two operators of above QUESTION satisfy the relation

[NET JUNE 2011]

A. $\left\{S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right\} = S_z^{(1)}S_z^{(2)}$

B. $\left\{S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right\} = 0$

C. $\left[S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right] = iS_z^{(1)}S_z^{(2)}$

D. $\left[S_x^{(1)}S_y^{(2)}, S_y^{(1)}S_x^{(2)}\right] = 0$

4. The component along an arbitrary direction $\hat{n}$, with direction cosines (n_x, n_y, n_z), of the spin of a spin $-\frac{1}{2}$ particle is measured. The result is

[NET JUNE 2012]

A. 0

B. $\pm\frac{\hbar}{2}n_z$

C. $\pm\frac{\hbar}{2}(n_x+n_y+n_z)$

D. $\pm\frac{\hbar}{2}$

5. In a basis in which the z - component S_z of the spin is diagonal, an electron is in a spin state $\psi = \begin{pmatrix}(1+i)/\sqrt{6}\\ \sqrt{2/3}\end{pmatrix}$.
The probabilities that a measurement of S_2 will yield the values $\hbar/2$ and $-\hbar/2$ are, respectively,

[NET JUNE 2013]

A. $1/2$ and $1/2$

B. $2/3$ and $1/3$

C. $1/4$ and $3/4$

D. $1/3$ and $2/3$

6. A spin $-\frac{1}{2}$ particle is in the state $\chi = \frac{1}{\sqrt{11}}\begin{pmatrix} 1+i \\ 3 \end{pmatrix}$ in the eigenbasis of S^2 and S_2. If we measure S_z, the probabilities of getting $+\frac{h}{2}$ and $-\frac{h}{2}$, respectively are

[NET DEC 2013]

A. $\frac{1}{2}$ and $\frac{1}{2}$ **B.** $\frac{2}{11}$ and $\frac{9}{11}$

C. 0 and 1 **D.** $\frac{1}{11}$ and $\frac{3}{11}$

7. Let $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, where $\sigma_1, \sigma_2, \sigma_3$ are the Pauli matrices. If $\vec{a}$ and $\vec{b}$ are two arbitrary constant vectors in three dimensions, the commutator $[\vec{a}\cdot\vec{\sigma}, \vec{b}\cdot\vec{\sigma}]$ is equal to (in the following I is the identity matrix)

[NET DEC 2014]

A. $(\vec{a}\cdot\vec{b})(\sigma_1+\sigma_2+\sigma_3)$ **B.** $2i(\vec{a}\times\vec{b})\cdot\vec{\sigma}$

C. $(\vec{a}\cdot\vec{b})I$ **D.** $|\vec{a}||\vec{b}|I$

8. If L_i are the components of the angular momentum operator $\vec{L}$, then the operator $\sum_{i=1,2,3}\left[\vec{L}, L_i\right]$ equals

[NET JUNE 2015]

A. $\vec{L}$ **B.** $2\vec{L}$

C. $3\vec{L}$ **D.** $-\vec{L}$

9. The Hamiltonian for a spin- $\frac{1}{2}$ particle at rest is given by $H = E_0(\sigma_z + \alpha\sigma_x)$, where σ_x and σ_z are Pauli spin matrices and E_0 and α are constants. The eigenvalues of this Hamiltonian are

[NET DEC 2015]

A. $\pm E_0\sqrt{1+\alpha^2}$ **B.** $\pm E_0\sqrt{1-\alpha^2}$

C. E_0 (doubly degenerate) **D.** $E_0\left(1 \pm \frac{1}{2}\alpha^2\right)$

10. If $\hat{L}_x, \hat{L}_y, \hat{L}_z$ are the components of the angular momentum operator in three dimensions the commutator $\left[\hat{L}_x, \hat{L}_x\hat{L}_y\hat{L}_z\right]$ may be simplified to

[NET JUNE 2016]

A. $i\hbar L_x\left(\hat{L}_z^2 - \hat{L}_y^2\right)$ **B.** $i\hbar\hat{L}_z\hat{L}_y\hat{L}_x$

C. $i\hbar L_x\left(2\hat{L}_z^2 - \hat{L}_y^2\right)$ **D.** 0

11. The Hamiltonian of a spin $\frac{1}{2}$ particle in a magnetic field $\vec{B}$ is given by $H = -\mu\cdot\vec{B}\cdot\vec{\sigma}$, where μ is a real constant and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices. If $\vec{B} = (B_0, B_0, 0)$ and the spin state at time $t = 0$ is an eigenstate of σ_x, then of the expectation values $\langle\sigma_x\rangle, \langle\sigma_y\rangle$ and $\langle\sigma_z\rangle$

[NET JUNE 2018]

A. only $\langle\sigma_x\rangle$ changes with time **B.** only $\langle\sigma_y\rangle$ changes with time

C. only $\langle\sigma_z\rangle$ changes with time **D.** all three change with time

Answer key

Q.No.	Answer	Q.No.	Answer
1	**b**	2	**c**
3	**d**	4	**d**
5	**d**	6	**b**
7	**b**	8	**b**
9	**a**	10	**a**
11	**d**		

Practice set 2

1. For a spin-s particle, in the eigen basis of $\vec{S}^2, S_x$ the expectation value $\langle sm|S_x^2|sm\rangle$ is
[GATE 2010]

A. $\frac{\hbar^2\{s(s+1)-m^2\}}{2}$ **B.** $\hbar^2\{s(s+1)-2m^2\}$

C. $\hbar^2\{s(s+1)-m^2\}$ **D.** $\hbar^2 m^2$

2. If L_x, L_y and L_z are respectively the x, y and z components of angular momentum operator L. The commutator $[L_xL_y, L_z]$ is equal to
[GATE 2011]

A. $i\hbar\left(L_x^2+L_y^2\right)$ **B.** $2i\hbar L_z$

C. $i\hbar\left(L_x^2-L_y^2\right)$ **D.** 0

3. Which one of the following commutation relations is NOT CORRECT? Here, symbols have their usual meanings.
[GATE 2013]

A. $\left[L^2, L_z\right]=0$ **B.** $\left[L_x, L_y\right]=i\hbar L_z$

C. $[L_z, L_+]=\hbar L_+$ **D.** $[L_z, L_-]=\hbar L_-$

4. A spin-half particle is in a linear superposition $0.8|\uparrow\rangle+0.6|\downarrow\rangle$ of its spin-up and spindown states. If $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of σ_z, then what is the expectation value up to one decimal place, of the operator $10\sigma_z+5\sigma_x$? Here, symbols have their usual meanings.
[GATE 2013]

5. If $\vec{L}$ is the orbital angular momentum and $\vec{S}$ is the spin angular momentum, then $\vec{L}\cdot\vec{S}$ does not commute with
[GATE 2014]

A. S_z **B.** L^2

C. S^2 **D.** $(\vec{L}+\vec{S})^2$

6. If $L_+$and $L_-$are the angular momentum ladder operators then the expectation value of $(L_+L_-+L_-L_+)$in the state $|l=1, m=1\rangle$ of an atom is $\hbar^2$
[GATE 2014]

7. The Pauli matrices for three spin $-\frac{1}{2}$ particles are $\vec{\sigma}_1, \vec{\sigma}_2$ and $\vec{\sigma}_3$, respectively. The dimension of the Hilbert space required to define an operator $\hat{O}=\vec{\sigma}_1\cdot\vec{\sigma}_2\times\vec{\sigma}_3$ is
[GATE 2015]

8. Let the Hamiltonian for two spin-1/2 particles of equal masses m, momenta $\vec{p}_1$ and $\vec{p}_2$ and positions $\vec{r}_1$ and $\vec{r}_2$ be $H=\frac{1}{2m}p_1^2+\frac{1}{2m}p_2^2+\frac{1}{2}m\omega^2\left(r_1^2+r_2^2\right)+k\vec{\sigma}_1\cdot\vec{\sigma}_2$, where $\vec{\sigma}_1$ and $\vec{\sigma}_2$ denote the corresponding Pauli matrices, $\hbar\omega=0.1$eV and $k=0.2$eV. If the ground state has net spin zero, then the energy (in eV) is
[GATE 2015]

9. If $\vec{s}_1$ and $\vec{s}_2$ are the spin operators of the two electrons of a He atom, the value o $\langle\vec{s}_1\cdot\vec{s}_2\rangle$ for the ground state is
[GATE 2016]

A. $-\frac{3}{2}\hbar^2$ **B.** $-\frac{3}{4}\hbar^2$

C. 0 **D.** $\frac{1}{4}\hbar^2$

10. The Hamiltonian of a spin $\frac{1}{2}$ particle in a magnetic field $\vec{B}$ is given by $H=-\mu\cdot\vec{B}\cdot\vec{\sigma}$, where μ is a real constant and $\vec{\sigma}=(\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices. If $\vec{B}=(B_0, B_0, 0)$ and the spin state at time $t=0$ is an eigenstate of σ_x, then of the expectation values $\langle\sigma_x\rangle, \langle\sigma_y\rangle$ and $\langle\sigma_z\rangle$
[NET JUNE 2018]

A. only $\langle \sigma_x \rangle$ changes with time

B. only $\langle \sigma_y \rangle$ changes with time

C. only $\langle \sigma_z \rangle$ changes with time

D. all three change with time

11. For the Hamiltonian $H = a_0 I + \vec{b} \cdot \vec{\sigma}$ where $a_0 \in R, \vec{b}$ is a real vector, I is the 2×2 identity matrix, and $\vec{\sigma}$ are the Pauli matrices, the ground state energy is

[GATE 2017]

A. $|b|$

B. $2a_0 - |b|$

C. $a_0 - |b|$

D. a_0

Answer key			
Q.No.	Answer	Q.No.	Answer
1	**a**	2	**c**
3	**d**	4	**7.6**
5	**d**	6	**2**
7	**8**	8	**-0.3**
9	**b**	10	**c**
11	**c**		

Practice set 3

1. Two spin half particle identified as $\vec{S}_1$ and $\vec{S}_2$ and θ is angle between them. If they are in singlet configuration, then find the value of $\left\langle \vec{S}_1 \cdot \vec{S}_2 \right\rangle$.

Solution: $\vec{S} = \vec{S}_1 + \vec{S}_2$

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{S^2 - S_1^2 - S_2^2}{2}$$
$$\therefore S_1 = \frac{1}{2}, S_2 = \frac{1}{2} \Rightarrow S = 0 \text{ (singlet) } S = 1 \text{ (Triplet)}$$
$$\langle S_1^2 \rangle = \frac{3}{4}\hbar^2 \quad \langle S_2^2 \rangle = \frac{3}{4}\hbar^2$$
$$\langle S \rangle = 0\hbar^2 (\text{ for singlet }) \therefore \left\langle \vec{S}_1 \cdot \vec{S}_2 \right\rangle = \frac{\langle S \rangle^2 - \langle S_1 \rangle^2 - \langle S_2 \rangle^2}{2} = \frac{0 - \frac{3}{4}\hbar^2 - \frac{3}{4}\hbar^2}{2}.$$
$$\left\langle \vec{S}_1 \cdot \vec{S}_2 \right\rangle = \frac{-3}{4}\hbar^2$$

2. The components of arbitrary vectors A and B commute with those of σ. Show that $(\sigma \cdot A)(\sigma \cdot B) = A \cdot B + i\sigma \cdot (A \times B)$.

Solution: $(\sigma.A)(\sigma.B) = (\sigma_x A_x + \sigma_y A_y + \sigma_z A_z)(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z)$

$$= \sigma_x^2 A_x B_x + \sigma_y^2 A_y B_y + \sigma_z^2 A_z B_z + \sigma_x \sigma_y A_x B_y + \sigma_y \sigma_x A_y B_x$$
$$+ \sigma_x \sigma_z A_x B_z + \sigma_y \sigma_z A_y B_z + \sigma_z \sigma_y A_z B_y + \sigma_z \sigma_x A_z B_x$$

Using the relations $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1, \sigma_x \sigma_y = i\sigma_z, \sigma_y \sigma_z = i\sigma_x, \sigma_z \sigma_x = i\sigma_y,$
$\sigma_x \sigma_y + \sigma_y \sigma_x = \sigma_y \sigma_z + \sigma_z \sigma_y = \sigma_z \sigma_x + \sigma_x \sigma_z = 0$

$$\text{We get } (\sigma \cdot A)(\sigma \cdot B) = (A \cdot B) + i\sigma_z (A_x B_y - A_y B_x) + i\sigma_y (A_z B_x - A_x B_z) + i\sigma_x (A_y B_z - A_z B_y)$$
$$= (A \cdot B) + i\sigma \cdot (A \times B)$$

3. Find the equivalence of the following operators:

(i) $S_x^2 S_y S_z^2$;

(ii) $S_x^2 S_y^2 S_z^2$;

(iii) $S_x S_y S_z^3$

Solution: (i) $S_x^2 S_y S_z^2 = \left(\frac{\hbar}{2}\right)^2 \sigma_x^2 \frac{\hbar}{2} \sigma_y \left(\frac{\hbar}{2}\right)^2 \sigma_z^2 = \left(\frac{\hbar}{2}\right)^5 \sigma_y$

(ii) $S_x^2 S_y^2 S_z^2 = \left(\frac{\hbar}{2}\right)^2 \sigma_x^2 \left(\frac{\hbar}{2}\right)^2 \sigma_y^2 \left(\frac{\hbar}{2}\right)^2 \sigma_z^2 = \left(\frac{\hbar}{2}\right)^6$

(iii) $S_x S_y S_z^3 = \frac{\hbar}{2} \sigma_x \frac{\hbar}{2} \sigma_y \left(\frac{\hbar}{2}\right)^3 \sigma_x^3 = \left(\frac{\hbar}{2}\right)^5 \sigma_x \sigma_y \sigma_z = \left(\frac{\hbar}{2}\right)^5 i$

4. $\vec{J} = \vec{L} + \vec{S}$ where $\vec{J}$ is total angular momentum and $\vec{L}$ and $\vec{S}$ are orbital angl momentum and spin angular momentum respectively. Find the value of $a < L.S >$.

Solution: $J = L+S$

$$J^2 = (L+S)(L+S) = L^2 + L\cdot S + S\cdot L + S^2$$
$$= L^2 + S^2 + 2L\cdot S \quad \because S\cdot L = L\cdot S$$
$$L\cdot S = \frac{1}{2}\left(J^2 - L^2 - S^2\right) \Rightarrow \langle L\cdot S\rangle = \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - s(s+1)\right]$$

5. Find the energy level of spin $s = 1/2$ particle whose Hamiltonion is given by

$$\hat{H} = \frac{\alpha}{\hbar^2}\left(S_x^2 + S_y^2 - 2S_z^2\right) - \frac{\beta}{\hbar}S_z$$

where α and β are constants. What is degeneracy of the energy?

Solution: $\mathrm{H} = \frac{\alpha}{\hbar^2}\left(S_x^2 + S_y^2 - 2S_z^2\right) - \frac{\beta}{\hbar}S_z \Rightarrow S^2 = S_x^2 + S_y^2 + S_z^2, S_x^2 + S_y^2 = S^2 - S_z^2$
$\Rightarrow H = \frac{\alpha}{\hbar^2}\left(S^2 - S_z^2 - 2S_z^2\right) - \frac{\beta}{\hbar}S_z$
$= \frac{\alpha}{\hbar^2}\left(S^2 - 3S_z^2\right) - \frac{\beta}{\hbar}S_z = \frac{\alpha}{\hbar^2}\left(s(s+1)\hbar^2 - 3m^2\hbar^2\right) - \frac{\beta}{\hbar}m\hbar = \frac{3\alpha}{4} - m(3m+\beta)$
The degeneracy of the system is $(2s+1)$ i.e. $\left[2\left(\frac{1}{2}\right)+1\right] = 2$

6. Consider a system which is initially in the state

$$\psi(\theta,\phi) = \frac{1}{\sqrt{5}}Y_{1,-1}(\theta,\phi) + \sqrt{\frac{3}{5}}Y_{1,0}(\theta,\phi) + \frac{1}{\sqrt{5}}Y_{1,1}(\theta,\phi)$$

(i) If L^2 is measured $\psi(\theta,\phi)$ then what is the measured with what probability?
(ii) If L_z is measured $\psi(\theta,\phi)$ then what is the measured with what probability?
(iii) What is the expectation value of L^2 and L_z

Solution: (i) If L^2 measured $\psi(\theta,\phi)$ then it will measured either $Y_{1,-1}$ or $Y_{1,0}$ or $Y_{1,1}$ each time. The measurement is $l(l+1)\hbar^2$ i.e. $2\hbar^2$ and the probability of measurement is $\left(\frac{1}{\sqrt{5}}\right)^2 + \left(\sqrt{\frac{3}{5}}\right)^2 + \left(\frac{1}{\sqrt{5}}\right)^2$ i.e. 1 .
(ii) If L_z measured on $\psi(\theta,\phi)$ then it will measured either $Y_{1,-1}$ or $Y_{1,0}$ or $Y_{1,1}$.
The measurement of L_2 on $Y_{1,1}$ yields $1\hbar$ with probability $1/5$.
The measurement of L_z on $Y_{1,0}$ yields $0\hbar$ with probability $3/5$.
The measurement of L_z on $Y_{1,-1}$ yields $-1\hbar$ with probability $1/5$.
(iii) The expectation value of L^2 is given as

$$2\hbar^2\cdot\frac{1}{5} + 2\hbar^2\cdot\frac{3}{5} + 2\hbar^2\cdot\frac{1}{5} = 2\hbar^2$$

The expectation value of L_z is given as $1\hbar\cdot\frac{1}{5} + 0\hbar\cdot\frac{3}{5} + (-1\hbar)\cdot\frac{1}{5} = 0$

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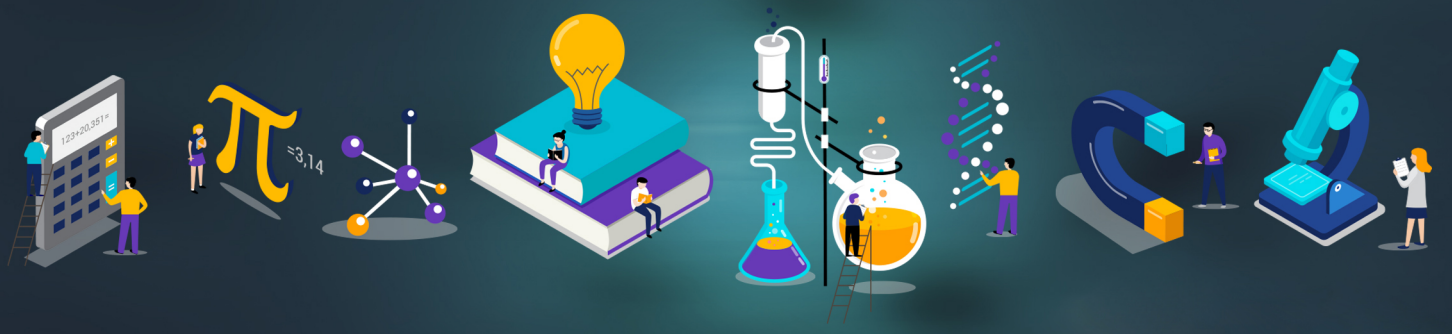

3. Identical particles

3.1 Introduction

Identical particles

Particle having same intrinsic properties (mass, charge, spin) as known as identical particles. There are two types of identical particles i.e.

1. Classical identical particle(Distiquishable particles)
   Volume available for a gas molecule at NTP is $\sim 10^{-25}$ m^3 and volume of single gas molecule $\sim 10^{-30}$ m^3
   So, we can identify every molecule of the gas. Hence, gas molecules are distinguishable.
2. Quantum identical particle(indistiquishable) Volume available for each electron taking part in conduction within the metals is $\sim 10^{-28}$ m^3 but the volume of a single electron is $\sim 10^{-27}$ m^3. This shows that the electron wave functions overlap considerably and hence cannot be identified separately, i.e. they are indistinguishable.

Note For a system of 'n' indistinguishable particles say electrons, we may be able to specify their positions, but it is not possible to say which electron is at a particular position. Therfore, interchanging the coordinates of any two electrons does not change the Hamiltonian. In other words, the Hamiltonian of the system is symmetric in coordinates of the particles i.e.

$$\hat{H}(x_1, x_2, x_3 \ldots\ldots x_i, x_{i+1}, \ldots x_n) = \hat{H}(x_1, x_2, x_3 \ldots\ldots x_{i+1}, x_i, \ldots x_n)$$

Particle exchange operator

This operator exchanges the particle in pair (both position and spin co-ordinates).

Note (i) Particle exchange operator is a hermitian operator.
(ii) Since particles are indistinguishable, any operator representing a physical property of the system must be symmetric w.r.t the particle exchange. Therefore, any operator representing a physical property commute with the particle exchange operator.

3.1.1 Symmetric wave function:

A wave function is said to be symmetric if interchange of any pair of particles leaves the wave function unchanged.

$$\psi_s(1, 2, \ldots . \text{i}, \text{j} \ldots \text{N}) = \psi_s(1, 2 \ldots\ldots . \text{j}, \text{i}, \ldots . . \text{N})$$

The particles having symmetric wave function obey BE statistics and known as bosons. Example: Photons (spin 1), neutral helium (spin 0), α-particle (spin 0), deutron (spin 1)

3.1.2 Anti-symmetric wave function:

A wave function is said to be anti-symmetric if interchange of any pair of particle changes the signof the wave function.

$$\psi_a(1,2,.....i,j,.....N) = -\psi_a(1,2,.....j,i.....N)$$

The particles having anti-symmetric wave functions are known as fermions and follow FD statistics. Example: Electron, protons, neutrons, muons (spin $1/2$), Ω particle (spin $3/2$)

3.2 Symmetrization postulate

The state of the system containing N identical particles, are either totally symmetric or totally anti symmetric under the exchange of any pair of particles and the states with mixed symmetry do not exist.

Note (i) Bosons have symmetric wave functions and Fermions have anti-symmetric wave functions
(ii) Wave function of a system of identical bosons is totally symmetric and of a system of identical fermions is totally anti-symmetric.

The total wave function corresponding to a system containing of N identical particles consisting of two parts (a) space part and (b) spin part, i.e. Therefore,

$$\psi_{\text{total}} = \psi_{\text{space}} \times \chi_{\text{spin}}$$

Therefore
(i) Both space part and spin part of total wave function of a system of identical bosons will be either symmetric or anti-symmetric.

$$\psi_{s,fermion} = \begin{cases} \psi_s(\text{ space }) \times \chi_a(\text{ spin }) \\ \psi_a(\text{ space }) \times \chi_s(\text{ spin }) \end{cases}$$

(ii) any one of the space part and spin part of total wave function of a system of identical fermions will be symmetric and other one is anti-symmetric.

$$\psi_{s,jermion} = \begin{cases} \psi_s(\text{ space }) \times \chi_a(\text{ spin }) \\ \psi_a(\text{ space }) \times \chi_s(\text{ spin }) \end{cases}$$

Composite particle:
Consider a system of identical composite particles where each particle is composed of two or more identical particles. Spin of each composite particles can be obtained by adding the spin of its constituents. If total spin of the composite particles is half-integer, then the particle will behave as a fermion. If total spin of the composite particles is integer, then the particle will behave as a boson.
example
(i) A system of N identical H atoms. Each H atom consists of 1 proton and 1 electron (spin $I/2$) Therefore each H atom has spin 1 and it will behave as a boson.So the system of N identical H atoms will have symmetric wavefunction
(ii) ^{4}He (two protons and two meutrons) has integer spin and will behave as boson.
(iii)^3He(2 proton and 1 neutron) has half integral spin and will behave as fermion

3.3 Symmetric and anti symmetric wavefunction(space part)

For a system of ' n ' non-interacting distinguishable particles, the wave function can be written as

$$\psi(\vec{r}_1,\vec{r}_2,\vec{r}_3 \ldots\ldots\ldots \vec{r}_n) = \psi_1(\vec{r}_1) \cdot \psi_2(\vec{r}_2) \cdot \psi_3(\vec{r}_3) \ldots\ldots\ldots \psi_n(\vec{r}_n)$$

But, for a system of ' n ' non-interacting indistinguishable particles, the wave function will be different. Example: Consider a system of 2 non-interacting indistinguishable particles, in which one particle is in state 1 and the

other particle is in state 2. Since, the particles are distinguishable, therefore the possible eigenfunctions are $\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)$ and $\psi_1(\vec{r}_2)\psi_2(\vec{r}_1)$ and both are equal probable. The symmetric and anti-symmetric combinations for the wave function of the system of 2 particles will be

$$\psi_s(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)]$$
$$\psi_a(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)]$$

If both the particles are in the same state, then $\psi_a(\vec{r}_1,\vec{r}_2) = 0$ i.e. two identical fermions cannot occupy the same state. This is known as 'Pauli's exclusion principle'.
In general, if we take a system of N identical non-interacting indistinguishable particles and each particle is in a different state, then there will be $N!$ different type possible eiegenfunctions having same value of energy. The degenaracy arises due to the exchange of indistingushable particles and known as exchange degenaracy. The symmetric and anti-symmetric combinations for the wave function of the system of N particles will be

$$\psi_S(\vec{r}_1,\vec{r}_2,.....\vec{r}_N) = \frac{1}{\sqrt{N!}}\sum_P \hat{P}[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)\psi_3(\vec{r}_3).....\psi_n(\vec{r}_N)]$$
$$\psi_a(\vec{r}_1,\vec{r}_2,.....\vec{r}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(\vec{r}_1) & \psi_1(\vec{r}_2) & ..... & \psi_1(\vec{r}_N) \\ \psi_2(\vec{r}_1) & \psi_2(\vec{r}_2) & ..... & \psi_2(\vec{r}_N) \\ \vdots & & & \\ \psi_N(\vec{r}_1) & \psi_N(\vec{r}_2) & ..... & \psi_N(\vec{r}_N) \end{vmatrix}$$

3.4 Symmetric and anti symmetric wavefunction(spin part)

Spin functions for two-electron system: Two electrons each having spin $1/2$ i.e. $s_1 = \frac{1}{2}, s_2 = \frac{1}{2}$, then the total spin of two electrons will be

$$s = |s_1 + s_2|.....|s_1 - s_2| = 1,0$$

and corresponding magnetic spin quantum number will be $m_s = 1,0,-1,0$ Therefore, the possible spin states will be $|s,m_s\rangle \equiv |0,0\rangle, |1,1\rangle, |1,0\rangle, |1,-1\rangle$ and given as follows:
Symmetric Triplet state:

$$|1,1\rangle = |\uparrow\uparrow\rangle = |\alpha\alpha\rangle = \left|\frac{1}{2},\frac{1}{2}\right\rangle\left|\frac{1}{2},\frac{1}{2}\right\rangle$$
$$|1,-1\rangle = |\downarrow\downarrow\rangle = |\beta\beta\rangle = \left|\frac{1}{2},-\frac{1}{2}\right\rangle\left(\frac{1}{2},-\frac{1}{2}\right\rangle$$
$$|1,0\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] = \frac{1}{\sqrt{2}}[|\alpha\beta\rangle + |\beta\alpha\rangle]$$
$$= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{1}{2}\right\rangle\left\langle\frac{1}{2},-\frac{1}{2}\right| + \left|\frac{1}{2},-\frac{1}{2}\right\rangle\left\langle\frac{1}{2},\frac{1}{2}\right|\right]$$

Anti-symmetric Singlet state:

$$|0,0\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] = \frac{1}{\sqrt{2}}[|\alpha\beta\rangle - |\beta\alpha\rangle]$$
$$= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{1}{2}\right\rangle\left|\frac{1}{2},-\frac{1}{2}\right\rangle - \left|\frac{1}{2},-\frac{1}{2}\right\rangle\left|\frac{1}{2},\frac{1}{2}\right\rangle\right]$$

For a system of N identical non-interacting indistinguishable particles each having spin 's', total number of possible spin states is $(2s+1)^N$.

Exercise 3.1 Example 1. N non interacting bosons are in an infinite potential well defined by $V(x) = 0$ for $0 < x < a$; $V(x) = \infty$ for $x < 0$ and for $x > a$. Find the ground state energy of the system. What would be the ground state energy if the particles are fermions. ■

Solution: The energy eigenvalue of a particle in the infinite square well is given by

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}, \quad n = 1,2,3,\ldots$$

As the particles are bosons, all the N particles will be in the $n = 1$ state in the ground state configuration. Hence, the ground state energy of the configuration will be

$$E = \frac{N\pi^2\hbar^2}{2ma^2}$$

If the particles are fermions, a state can have only two of them, one spin up and the other spin down.
xilaal Part Therefore, the lowest N/2 states will be filled. The total ground state energy will be

$$\begin{aligned} E &= 2\frac{\pi^2\hbar^2}{2ma^2}\left[1^2+2^2+3^3+\ldots+(N/2)^2\right] \\ &= \frac{\pi^2\hbar^2}{ma^2}\frac{1}{6}\left[\frac{N}{2}\left(\frac{N}{2}+1\right)\left(2\frac{N}{2}+1\right)\right] \\ &= \frac{\pi^2\hbar^2}{24ma^2}N(N+1)(N+2) \end{aligned}$$

Exercise 3.2 Consider two noninteracting electrons described by the Hamiltonian

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1) + V(x_2)$$

where $V(x) = 0$ for $0 < x < a; V(x) = \infty$ for $x < 0$ and for $x > a$. If both the electrons are in the same spin state, what is the lowest energy and eigenfunction of the two-electron system? ■

Solution: As both the electrons are in the same spin state, the possible combinations of spin part of the wave functions will be $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$, both being symmetric. Since, the system contains two electrons (fermions), then the total wave function of the sytem will be anti-symmetric. Hence the space function must be antisymmetric. Therefore, both electrons cannot be in the same state. So, ground state energy will corresponds to $n_1 = 1, n_2 = 2$
Ground state energy $(n_1 = 1, n_2 = 2) = \frac{\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{2ma^2}$
Since, the electrons are indistinguishable, therefore the antisymmetric combination for the space part is

$$\frac{1}{\sqrt{2}}\left[\psi_1(\vec{r}_1)\,\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\,\psi_2(\vec{r}_1)\right]$$

Exercise 3.3 Example 3. Sixteen noninteracting electrons are confined in a potential $V(x) = \infty$ for $x < 0$ and $x > 0; V(x) = 0$, for $0 < x < a$.
(i) What is the energy of the least energetic electron in the ground state?
(ii) What is the energy of the most energetic electron in the ground state?
(iii) What is the Fermi energy E_f of the system? ■

Solution: (i) The least energetic electron in the ground state is given by $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$.
(ii) In the given potential, the energy eigenvalue

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}, \quad n = 1,2,3,\ldots$$

As two electrons can go into each of the states $n = 1, 2, 3, \ldots$, the highest filled level will have $n = 8$ and its energy will be

$$E_8 = \frac{\pi^2\hbar^2 8^2}{2ma^2} = \frac{32\pi^2\hbar^2}{ma^2}$$

(iii)The energy of the highest filled state is the Fermi energy E_F Hence,

$$E_F = \frac{32\pi^2\hbar^2}{ma^2}$$

Practice set 1

1. Consider a particle in a one dimensional potential that satisfies $V(x) = V(-x)$. Let $|\psi_0\rangle$ and $|\psi_1\rangle$ denote the ground and the first excited states, respectively, and let $|\psi\rangle = \alpha_0 |\psi_0\rangle + \alpha_1 |\psi_1\rangle$ be a normalized state with α_0 and α_1 being real constants. The expectation value $\langle x\rangle$ of the position operator x in the state $|\psi\rangle$ is given by **[NET DEC 2011]**

   A. $\alpha_0^2 \langle\psi_0|x|\psi_0\rangle + \alpha_1^2 \langle\psi_1|x|\psi_1\rangle$
   B. $\alpha_0\alpha_1 [\langle\psi_0|x|\psi_1\rangle + \langle\psi_1|x|\psi_0\rangle]$
   C. $\alpha_0^2 + \alpha_1^2$
   D. $2\alpha_0\alpha_1$

2. Consider a system of two non-interacting identical fermions, each of mass m in an infinite square well potential of width a. (Take the potential inside the well to be zero and ignore spin). The composite wavefunction for the system with total energy $E = \frac{5\pi^2\hbar^2}{2ma^2}$ is **[NET JUNE 2014]**

   A. $\frac{2}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) - \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$
   B. $\frac{2}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) + \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$
   C. $\frac{2}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{2a}\right) - \sin\left(\frac{3\pi x_1}{2a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$
   D. $\frac{2}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{a}\right) - \sin\left(\frac{\pi x_2}{a}\right)\cos\left(\frac{\pi x_2}{a}\right)\right]$

3. The state vector of a one-dimensional simple harmonic oscillator of angular frequency ω, at time $t = 0$, is given by $|\psi(0)\rangle = \frac{1}{\sqrt{2}}[|0\rangle + |2\rangle]$, where $|0\rangle$ and $|2\rangle$ are the normalized ground state and the second excited state, respectively. The minimum time t after which the state vector $|\psi(t)\rangle$ is orthogonal to $|\psi(0)\rangle$, is **[NET DEC 2017]**

   A. $\frac{\pi}{2\omega}$
   B. $\frac{2\pi}{\omega}$
   C. $\frac{\pi}{\omega}$
   D. $\frac{4\pi}{\omega}$

Answer key

Q.No.	Answer	Q.No.	Answer
1	**b**	2	**a**
3	**a**		

Practice set 2

1. Consider the wavefunction $\psi = \psi(\vec{r}_1, \vec{r}_2)\chi_s$ for a fermionic system consisting of two spinhalf particles. The spatial part of the wavefunction is given by

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) + \phi_2(\vec{r}_1)\phi_1(\vec{r}_2)]$$

where ϕ_1 and ϕ_2 are single particle states. The spin part χ_s of the wavefunction with spin states $\alpha(+1/2)$ and $\beta(-1/2)$ should be

[GATE 2013]

A. $\frac{1}{\sqrt{2}}(\alpha\beta + \beta\alpha)$ **B.** $\frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$

C. $\alpha\alpha$ **D.** $\beta\beta$

2. The ground state and first excited state wave function of a one dimensional infinite potential well are ψ_1 and ψ_2 respectively. When two spin-up electrons are placed in this potential which one of the following with x_1 and x_2 denoting the position of the two electrons correctly represents the space part of the ground state wave function of the system?

[GATE 2014]

A. $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_1) - \psi_1(x_2)\psi_2(x_2)]$ **B.** $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)]$

C. $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_1) + \psi_1(x_2)\psi_2(x_2)]$ **D.** $\frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)]$

3. ψ_1 and ψ_2 are two orthogonal states of a spin $\frac{1}{2}$ system. It is given that $\psi_1 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\0\end{pmatrix} + \sqrt{\frac{2}{3}}\begin{pmatrix}0\\1\end{pmatrix}$, where $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$ represent the spin-up and spin-down states, respectively. When the system is in the state ψ_2 its probability to be in the spin-up state is

[GATE 2014]

4. For a spin $\frac{1}{2}$ particle, let $|\uparrow\rangle$ and $|\downarrow\rangle$ denote its spin up and spin down states respectively. If $|a\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle)$ and $|b\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$ are composite states of two such particles, which of the following statements is true for their total spin S?

[GATE 2018]

A. $S = 1$ for $|a\rangle$ and $|b\rangle$ is not an eigenstate of the operator $\hat{S}^2$

B. $|a\rangle$ is not an eigenstate of the operator $\hat{S}^2$ and $S = 0$ for $|b\rangle$

C. $S = 0$ for $|a\rangle$, and $S = 1$ for $|b\rangle$

D. $S = 1$ for $|a\rangle$, and $S = 0$ for $|b\rangle$

5. Let $|\psi_2\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |\psi_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ represent two possible states of a two-level quantum system. The state obtained by the incoherent superposition of $|\psi_1\rangle$ and $|\psi_2\rangle$ is given by a density matrix that is defined as $\rho \equiv c_1|\psi_1\rangle\langle\psi_1| + c_2|\psi_2\rangle\langle\psi_2|$. If $c_1 = 0.4$ and $c_2 = 0.6$, the matrix element ρ_{22} (rounded off to one decimal place) is

[GATE 2018]

Answer key			
Q.No.	Answer	Q.No.	Answer
1	**b**	2	**d**
3	**2/3**	4	**d**
5	**0.6**		

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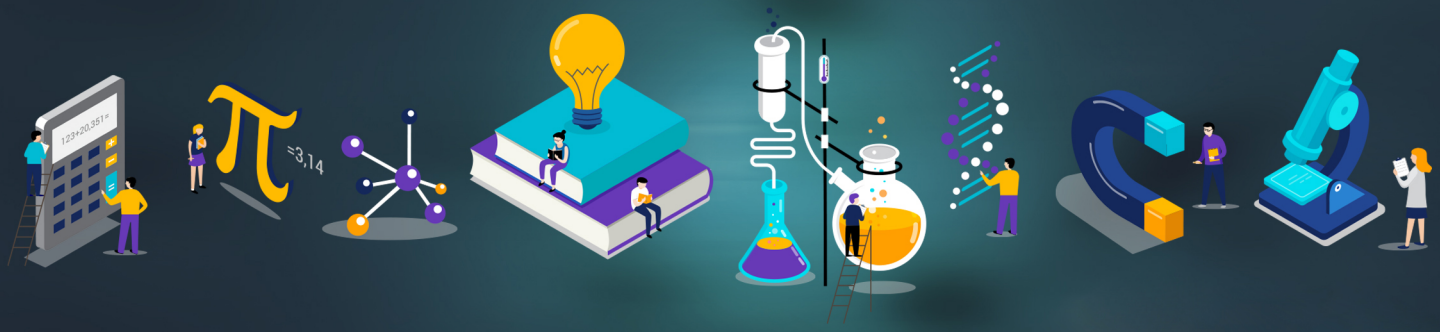


4. Scattering theory

4.1 The scattering cross section

A parallel beam of particle of given momentum is directed towards a target which deflects or scatters the particle in various directions.The scattered particles diverge. Eventually at large distance from the target, their motion is directed radially outwards.It is convenient to choose a system with the origin at the position of the target or scattering center. and with Z-axis in the direction of the incident beam .The direction of any scattered particle is indicated by polar angles (θ, ϕ) with the z-axis taken as the polar axis.Then θ is the angle of scattering ie the angle between the scattered and the incident direction .These two directions together define the plane of scattering .The azimuthal angle ϕ specifies the orientation of the this plane with respect to some reference plane containing z-axis.

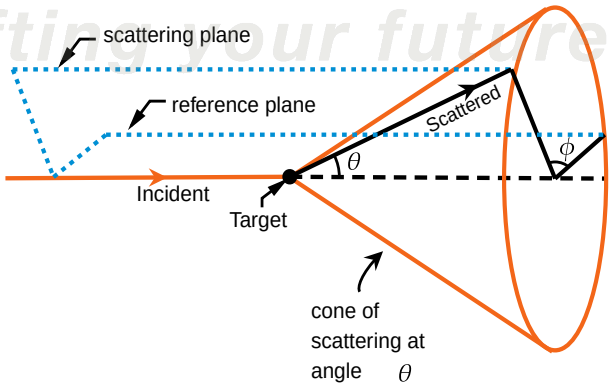


Figure 4.1

Let the incident flux F is independent of time.There will then be steady stream of particles too.Let ΔN be the number of particles scattered in to a small solid angle $\Delta\Omega$ about the direction $(\theta\phi)$ in time Δt.Evidently ΔN must be proportional to $\Delta\Omega\Delta t$ and to the incident flux F.The proportionality factor which depends in general on θ and ϕ is called the differential scattering cross section, and is denoted by $(\frac{d\sigma}{d\Omega})$

$$\Delta N = \frac{d\sigma(\theta,\phi)}{d\Omega}\Delta t\Delta\Omega F$$

$\frac{d\sigma}{d\Omega}$ has a dimension of area,it depends only on the parameters of the incident particle and nature of the target. The total scattering crosssection σ may be obtained from it by integration over all directions:

$$\sigma = \int (\frac{d\sigma}{d\Omega}) d\Omega = \int_0^{2\pi} \int_0^{\pi} (\frac{d\sigma}{d\Omega}) \sin\theta d\theta d\phi$$

In most cases we consider $(\frac{d\sigma}{d\Omega})$ is independent of ϕ
Then

$$\sigma = \int (\frac{d\sigma}{d\Omega}) 2\pi \sin\theta d\theta$$

4.1.1 The scattering amplitude

When the particle involved in the scattering process are quantum mechanical objects ,we must describe them by a wave function.At large distance from the scattering centre ($r \to \infty$) the form of the wavefunction must consist of a part u_{inc} corresponding to the parallel beam of incident particles and the other part u_{sc} representing the scattered particle moving radially outwards from the center.

$$u(\mathbf{x}) \underset{r\to\infty}{\longrightarrow} u_{inc} + u_{sc}$$

The beam of incident particles with momentum $p = \hbar k$ along the z-axis must evidently be described by the plane wave (momentum eigenfunction) $u_{inc} = e^{ikz}$.
$|u_{\text{inc}}|^2$ is to be understood as the number of incident particles per unit volume. The incident flux is obtained by multiplying this quantity by the particle velocity v.

$$F = |u_{\text{inc}}|^2 v = \hbar k/m$$

Suppose that the scattering is elastic. Then the wave u_{sc} representing them must have the same propagation constant k_i but it must be a spherical wave since these particles move radially. The only such waves are e^{ikr} and e^{-ikr}; the latter is an incoming wave (contracting towards the origin). Since the scattercd particles move outwards, we must choose the outgoing wave ${}_2u_{sc} \propto e^{ikr}$. Further, the flux of scattered particles, $|u_{sc}|^2 (\hbar k/m)$ must evidently decrease as $(1/r^2)$ as r increases. Hence $u_{sc} \propto (1/r)$ also, and we writê

$$u_{sc} = f(\theta, \varphi) \frac{e^{ikr}}{r}$$

The dependence of the proportionality factor f on θ, φ allows for the fact that the scattered flux is, in gencral, direction-dependent. We observe now that $\triangle\mathcal{N}$ is nothing but the radial flux times $\triangle S\Delta t$, where $\Delta S \equiv r^2 d\Omega$ is the element of area (normal to the radial direction) covered by the solid angle $\Delta\Omega$. Thus

$$\begin{aligned}\Delta\mathcal{N} &= |u_{sc}|^2 (\hbar k/m) \cdot r^2 \Delta\Omega\Delta t \\ &= |f(\theta,\varphi)|_0^2 (\hbar k/m)\Delta\Omega\Delta t\end{aligned}$$

On substituting this together with $F = \frac{\hbar k}{m}$ in $\Delta N = \frac{d\sigma(\theta,\phi)}{d\Omega}\Delta t\Delta\Omega F$, we obtain

$$\frac{d\sigma(\theta,\varphi)}{d\Omega} = |f(\theta,\varphi)|^2$$

$f(\theta,\varphi)$ is called the scattering amplitude.
The particular stationary wavefunction can be written as

$$u(\mathbf{x}) \underset{r\to\infty}{\longrightarrow} e^{ikz} + f(\theta,\varphi)\frac{e^{ikr}}{r}$$

Since any stationary wave function must satisfy the time independent Schrcdinger equation, we must have

$$-\frac{\hbar^2}{2m}\nabla^2 u(\mathbf{x}) + V(\mathbf{x})u(\mathbf{x}) = Eu(\mathbf{x}), \quad E = \frac{\hbar^2 k^2}{2m}$$

Here $V(\mathbf{x})$ is the potential energy function for the projectile particle in the force field of the scattering centre.
Formal expression for scattering amplitude

$$\begin{aligned}f(\theta,\varphi) &= -\frac{1}{4\pi}\int e^{-i\mathbf{k}\cdot\mathbf{x}} U(\mathbf{x}) u(\mathbf{x}) d\tau, \\ &= -\frac{m}{2\pi\hbar^2}\int e^{-i\mathbf{k}\cdot\mathbf{x}} V(\mathbf{x}) u(\mathbf{x}) d\tau\end{aligned}$$

4.1.2 First Born approximation

$$f(\theta,\varphi) = -\frac{1}{4\pi}\int e^{-i\mathbf{k}\cdot\mathbf{x}}U(\mathbf{x})u(\mathbf{x})d\tau$$

Suppose that $\left|u(\mathbf{x}) - e^{ikz}\right| < \left|e^{ikz}\right| = 1$
Then we can replace the unknown $u(\mathbf{x})$ in $f(\theta,\varphi)$ to a good approximation, by $e^{ikz} \equiv e^{i\mathbf{k}_0\cdot\mathbf{x}}$ where k_0 is the vector of magnitude k in the incident direction. The resulting expression is called the **first Born approximation** to $f(\theta,\varphi)$ and is given by

$$f_{\mathrm{H}}(\theta,\varphi) = -(4\pi)^{-1}\int e^{-i\mathbf{K}\cdot\mathbf{x}}U(\mathbf{x})d\tau.$$

The scattering. cross-scction in this approximation is

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{B}} = (4\pi)^{-2}\left|\int e^{-i}\mathbf{K}\cdot\mathbf{x}U(\mathbf{x})d\tau\right|^2.$$

In equation $f_{\mathrm{H}}(\theta,\varphi)$ $\mathbf{K} = \mathbf{k} - \mathbf{k}_0$. It may be noted that $\hbar\mathbf{K}$ is the momentum transferred to the particle in its encounter with the potential. Since $|k_0| = |\mathbf{k}| = k$, it follows (from the figure)that

$$K \equiv |\mathbf{K}| = 2k\sin\frac{1}{2}\theta$$

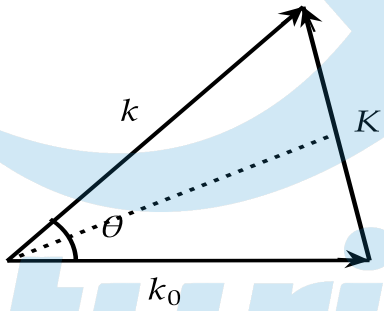


Figure 4.2

The scattcring amplitude in the Born approximation, considered as ifunction of K : is the Fourier transform of the potcntial (apart from constant facturs;)
In the most important special case when V is sphcrically symmetric, $V(\mathbf{x})$ - V (r), we can reduce $f_{\mathrm{H}}(\theta,\varphi)$ to an integral over r alone, by going over to spherical polar coordinates (r,α,β) with the direction of $\mathbf{K}$ chosen as the polar axis. Then $\mathbf{K}.\mathbf{x} = K_r\cos\alpha$ and on carrying out the angular integrations one gcts

$$f_B(\theta) = -K^{-1}\int_0^\infty r\sin KrU(r)dr$$

4.1.3 Partial wave analysis

While the Born approximation is basically a truncation of a perturbation expansion of $u(x)$, the method of partial waves is based upon an expansion of $u(\mathbf{x})$ in terms of angular momentum eigenfunctions. It is applicable if the potential is spherically symmetric. one gets a fornial expression for the scattering amplitude as an infinite scries; cach term of the series is the contribution to $f(\theta,\varphi)$ from a partial wave characterized by a particular angular momentum. We shall see that the first few terms in the series approximate $f(\theta,\varphi)$ if the incident particle is of low energy. Thus the partial wave method leads to a low energy approximation which complements the Born approximation (good at high energies).

Partial waves

If the potential has sphencal symmetry we can separate the Schrödinger equation into radial and angular parts, and obtain solutions in the form $R_l(r)Y_{lm}(\theta,\varphi)$, where the radial wave functions $R_l(r)$ satisfy the equation

$$1/r^2\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \frac{2\mu}{\hbar^2}\left[E - V - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]R_l = 0$$

The general solution of the Schrödinger equation can be written as a linear combination of such solutions. In the scattering problem which we are considering, only the function $R_l(r)\bar{\gamma}_{lo}(\theta,\varphi) \propto R_l(r)P_l(\cos\theta)$ appears in the linear combination. This is because we have assumed the particle to be travelling in the z-direction initially, so that the z-component of its angular momentum is zero; it continues to be zero because a spherically symmetric potential does not disturb the angular momentum. Thus we can write

$$u(\mathbf{x}) = \sum_{l=0}^{\infty} R_l(r)P_l(\cos\theta)$$

The term corresponding to a particular l in this series is called the lth partial wave.

Asymptotic form of radial function

We must now require that $u(\mathbf{x})$ should have the asymptotic form of$u(\mathbf{x}) \underset{r\to\infty}{\longrightarrow} e^{ikz} + f(\theta,\varphi)\frac{e^{ikr}}{r}$

This condition places constraints on the radial wave functions $Rl(r)$. To see what they are, we need to have the asymptotic $(r \to \infty)$ form of $R_l(r)$. We can infer it from the radial wave equation which we rewrite as

$$\left.\begin{array}{l} \frac{d^2\chi_l}{dr^2} + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right]\chi_l = 0, \\ \chi_l = rR_l(r), k^2 = \left(2mE/\hbar^2\right), U(r) = 2mV/\hbar^2 \end{array}\right\}$$

In the asymptotic region, both $U(r)$ and the centrifugal potential $\left(\propto 1/r^2\right)$ are very small. On neglecting these, in comparison with k^2, we obtain the approximate asymptotic solution $\chi_l(r) \propto e^{\pm ikr}$. To improve this approximation, let us suppose that

$$\chi_l(r) = v_l(r)e^{\pm ikr}$$

where $v_l(r)$ is expected to be very slowly varying in the asymptotic region. On introducing this into Eq in to new radial equation we get

$$d^2v_l/dr^2 \pm 2ikdv_l/dr - \left[U + l(l+1)/r^2\right]v_l = 0$$

on solving this we will get

$$\ln v_l \approx \mp\frac{i}{2k}\int^r \left[U + \frac{l(l+1)}{r^2}\right]dr$$

some text missing if $1/r$ is large enough the value of the integral is effectively independent of r and hence $v_l(r)$ is a constant in the asymptotic region. In the following, we will confine our attention to such potentials, leaving the Coulomb case to be dealt with later. Then the asymptotic form of $\chi_l(r)$ is, in general, some linear combination of the two solutions with v_l constant, i.e. of e^{ikr} and e^{-ikr}. Without loss of generality, we can write any such combination in the form

$$\chi_l \to C_l \sin(kr + \Delta_l)$$

where C_l, Δ_l are constants.

Phase shift

Let us compare the above asymptotic behaviour with that of the partial waves for a free particle $(V'(r) = 0)$. We have already seen that in any range of r over which $V(r)$ is constant, the solutions of the radial wave equation are the spherical Bessel functions j_l or n_l. In particular, if $V = 0$ everywhere, the only admissible solution is $j_l(kr); n_l$ is ruled out because it becomes infinite at $r = 0$. Thus $R_l(r) = \text{const. } j_l(kr)$ in the free-particle case. Since the asymptotic forms of the spherical Bessel functions are known to be given by

$$j_l(kr) \to (kr)^{-1}\sin\left(kr - \frac{1}{2}l\pi\right)$$
$$n_l(kr) \to -(kr)^{-1}\cos\left(kr - \frac{1}{2}l\pi\right)$$

(as $r \to \infty$), it follows tha $\chi_l(r) = rR_l(r) \to \text{const. } \sin\left(kr - \frac{1}{2}l\pi\right)$. Hence χ_l in this case has the asymptotic form $\chi_l \to C_l \sin(kr + \Delta_l)$ with the particular value $-\frac{1}{2}l\pi$ for Δ_l.

The effect of the potential on the partial waves in the asymptotic region is, therefore, simply to change the phase from - $\frac{1}{2}\pi l$ to some other value $\triangle_l$. This change,

$$\delta_l = \Delta_l + \frac{1}{2} l\pi$$

is called the phase shift in the lth partial wave.

Practice set 1

1. A free particle described by a plane wave and moving in the positive z-direction undergoes scattering by a potential

$$V(r) = \begin{cases} V_0, & \text{if } r \le R \\ 0, & \text{if } r > R \end{cases}$$

If V_0 is changed to $2V_0$, keeping R fixed, then the differential scattering cross-section, in the Born approximation.

[NET JUNE 2012]

A. increases to four times the original value
B. increases to twice the original value
C. decreases to half the original value
D. decreases to one fourth the original value

2. The differential cross-section for scattering by a target is given by

$$\frac{d\sigma}{d\Omega}(\theta,\phi) = a^2 + b^2\cos^2\theta$$

If N is the flux of the incoming particles, the number of particles scattered per unit time is

[NET JUNE 2015]

A. $\frac{4\pi}{3}N\left(a^2+b^2\right)$
B. $4\pi N\left(a^2+\frac{1}{6}b^2\right)$
C. $4\pi N\left(\frac{1}{2}a^2+\frac{1}{3}b^2\right)$
D. $4\pi N\left(a^2+\frac{1}{3}b^2\right)$

3. A particle of energy E scatters off a repulsive spherical potential

$$V(r) = \begin{cases} V_0 & \text{for} \quad r < a \\ 0 & \text{for} \quad r \le a \end{cases}$$

where V_0 and a are positive constants. In the low energy limit, the total scattering crosssection is $\sigma = 4\pi a^2\left(\frac{1}{ka}\tanh ka - 1\right)^2$, where $k^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0$. In the limit $V_0 \to \infty$ the ratio of σ to the classical scattering cross-section off a sphere of radius a is

[NET JUNE 2015]

A. 4
B. 3
C. 1
D. $\frac{1}{2}$

4. A particle is scattered by a central potential $V(r) = V_0 re^{-\mu r}$, where V_0 and μ are positive constants. If the momentum transfer $\vec{q}$ is such that $q = |\vec{q}| \gg \mu$, the scattering crosssection in the Born approximation, as $q \to \infty$, depends on q as [You may use $\int x^n e^{ax}dx = \frac{d^n}{da^n}\int e^{ax}dx$]

[NET DEC 2016]

A. q^{-8}
B. q^{-2}
C. q^2
D. q^6

5. Consider the potential

$$V(\vec{r}) = \sum_i V_0 a^3 \delta^{(3)}(\vec{r} - \vec{r}_i)$$

where $\vec{r}_i$ are the position vectors of the vertices of a cube of length a centered at the origin and V_0 is a constant. If $V_0 a^2 << \frac{\hbar^2}{m}$, the total scattering cross-section, in the lowenergy limit, is

[NET JUNE 2017]

A. $16a^2\left(\frac{mV_0a^2}{\hbar^2}\right)$
B. $\frac{16a^2}{\pi^2}\left(\frac{mV_0a^2}{\hbar^2}\right)^2$
C. $\frac{64a^2}{\pi}\left(\frac{mV_0a^2}{\hbar^2}\right)^2$
D. $\frac{64a^2}{\pi^2}\left(\frac{mV_0a^2}{\hbar^2}\right)$

6. A phase shift of 30° is observed when a beam of particles of energy 0.1MeV is scattered by a target. When the beam energy is changed, the observed phase shift is 60°. Assuming that only s-wave scattering is relevant and that the cross-section does not change with energy, the beam energy is

[NET DEC 2017]

A. 0.4MeV **B.** 0.3MeV

C. 0.2MeV **D.** 0.15MeV

7. The differential scattering cross-section $\frac{d\sigma}{d\Omega}$ for the central potential $V(r) = \frac{\beta}{r}e^{-\mu r}$, where β and μ are positive constants, is calculated in thee first Born approximation. Its dependence on the scattering angle θ is proportional to (A is a constant below)

[NET JUNE 2018]

A. $\left(A^2+\sin^2\frac{\theta}{2}\right)$ **B.** $\left(A^2+\sin^2\frac{\theta}{2}\right)^{-1}$

C. $\left(A^2+\sin^2\frac{\theta}{2}\right)^{-2}$ **D.** $\left(A^2+\sin^2\frac{\theta}{2}\right)^{2}$

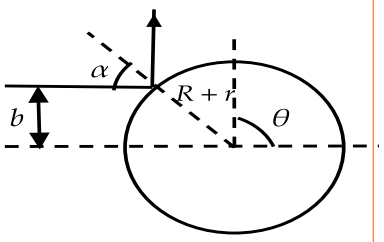
Answer key

Q.No.	Answer	Q.No.	Answer
1	**a**	2	**d**
3	**a**	4	**a**
5	**c**	6	**b**
7	**c**		

Practice set 2

1. Find the angular distribution and total cross section for the scattering of small marbles of mass m and radius r from a massive billiard ball of mass M and radius $R(m << M)$. You should treat the scattering as elastic involving no frictional forces.

Solution: As $m \ll M$, the massive billiard ball will remain stationary during scattering. As the scattering is elastic (see figure), the scattering angle Θ is related to the angle of incidence by
$\theta = \pi - 2\alpha \Rightarrow \alpha = \frac{\pi}{2} - \frac{\theta}{2}$



where θ is given by $(R+r)\sin\alpha = b \Rightarrow b = (R+r)\sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right) \Rightarrow b = (R+r)\cos\frac{\theta}{2}$

The differential scattering cross section is

$$D(\theta) = \frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \frac{(R+r)\cos\frac{\theta}{2}}{\sin\theta}\cdot(R+r)\sin\frac{\theta}{2}\cdot\frac{1}{2} = \frac{(R+r)^2}{4}$$

$$\Rightarrow D(\theta) = \frac{d\sigma}{d\Omega} = \frac{(R+r)^2}{4}$$

$$\sigma = \int_0^{\pi}\int_0^{2\pi} D(\theta)\sin\theta d\theta d\phi \Rightarrow \int_0^{\pi}\int_0^{2\pi}\frac{(R+r)^2}{4}\sin\theta d\theta d\phi = \pi(R+r)^2$$

2. If differential scattering cross-section is given by $D(\theta) = a^2\sin^2\theta + b^2\cos^2\theta$. If N is the flux of incoming particle then find the number of scattered particle per unit time.

Solution:

$$\sigma = \int_0^{\pi}\int_0^{2\pi} D(\theta)\sin\theta d\theta d\phi$$

$$\sigma = \int_0^{\pi}\int_0^{2\pi} a^2\sin^2\theta\sin\theta d\theta d\phi + \int_0^{\pi}\int_0^{2\pi} b^2\cos^2\theta\sin\theta d\theta d\phi$$

$$= 2\pi\left(a^2\int_0^{\pi}\sin^3\theta d\theta + b^2\int_0^{\pi}\cos^2\theta\sin\theta d\theta\right)$$

$$\sigma = 2\pi\left(\frac{4}{3}a^2 + \frac{2}{3}b^2\right) \Rightarrow \sigma = \frac{4\pi}{3}\left(2a^2 + b^2\right)$$

Number of scattered particle $N_{SC} = N\sigma \Rightarrow N_{SC} = N\frac{4\pi}{3}\left(2a^2 + b^2\right)$

3. Yukawa potential is defined as $V(r) = \beta\frac{e^{-\mu r}}{r}$ where $\beta > 0$ and $\mu > 0$.
(a) Using born approximation for for high energy $k = \sqrt{\frac{2mE}{\hbar^2}}$ if θ is scattering angle with parameter $q = 2k\sin\theta/2$ find differential scattering cross section
(b) Discuss the differential scattering cross section for case $q \gg \mu$

Solution: (a) $f(\theta) = -\frac{2m}{\hbar^2 q}\int_0^\infty rV(r)\sin(qr)dr$

$$= \frac{-2m\beta}{\hbar^2 q}\int_0^\infty e^{-\mu r}\sin(qr)dr = \frac{-2m\beta}{\hbar^2 q}\frac{1}{2i}\int_0^\infty e^{-\mu r}\exp iqr - \exp(-iqr)dr$$

$$\frac{-2m\beta}{\hbar^2 q}\frac{1}{2i}\left(\int_0^\infty \exp -r(\mu - iq)dr - \int_0^\infty \exp -r(\mu + iq)dr\right) = -\frac{m\beta}{i\hbar^2 q}\left(\frac{1}{\mu - iq} - \frac{1}{\mu + iq}\right)$$

$$= -\frac{m\beta}{i\hbar^2 q}\left(\frac{(\mu + iq) - (\mu - iq)}{\mu^2 + q^2}\right) = -\frac{2m\beta q}{\hbar^2 q}\cdot\frac{1}{\mu^2+q^2} = -\frac{2m\beta}{\hbar^2}\cdot\frac{1}{\mu^2+q^2}$$

$$D(\theta) = |f(\theta)|^2 = \left|-\frac{2m\beta}{\hbar^2}\cdot\frac{1}{\mu^2+q^2}\right|^2 = \frac{4m^2\beta^2}{\hbar^4}\cdot\left(\frac{1}{\mu^2+q^2}\right)^2$$

(b) for case $q >> \mu$

$$D(\theta) = \frac{4m^2\beta^2}{\hbar^4}\cdot\frac{1}{q^4}\left(\frac{1}{(\mu/q)^2+1}\right)^2 = \frac{4m^2\beta^2}{\hbar^4}\cdot\frac{1}{q^4}$$

4. A particle of energy E scatters off a repulsive spherical potential

$$V(r) = \begin{cases} V_0 & \text{for} \quad r < a \\ 0 & \text{for} \quad r \le a \end{cases}$$

where V_0 and a are positive constants. In the low energy limit, the total scattering crosssection is $\sigma = 4\pi a^2\left(\frac{1}{ka}\tanh ka - 1\right)^2$, where $k^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0$.
(a) In the limit $V_0 \to \infty$ find the total scattering cross section.
(b) Compare the total scattering cross section from (a) to classical scattering cross section Consider the notentiol

Solution: (a) $\sigma = 4\pi a^2\left[\frac{1}{ka}\tanh ka - 1\right]^2$
$V_0 \to \infty, ka \to \infty, \tanh ka \to 1 \Rightarrow \sigma = 4\pi a^2\left(\frac{1}{ka} - 1\right)^2$ and $ka \to \infty, \lim_{ka\to\infty}\sigma = 4\pi a^2$
(b) Classically $\sigma_c = \pi a^2, \frac{\sigma}{\sigma_c} = 4$

5. Consider the potential

$$V(x,y,z) = \sum_i V_0 a^3 \delta(x - x_i)\,\delta(y - y_i)\,\delta(z - z_i)$$

where x_i, y_i, z_i are the position vectors of the vertices of a cube of length a centered at the origin and V_0 is a constant. If $V_0 a^2 << \frac{\hbar^2}{m}$ for low energy limit
(a) Find differential cross section .
(b) The total scattering cross-section

Solution: $\sum_i V_0 a^3 \delta(x - x_i)\,\delta(y - y_i)\,\delta(z - z_i)$, where x_i, y_i, z_i are co-ordinate at 8 corner cube whose center is at origin.

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int V(r)d^3r$$

$$= \frac{-m}{2\pi\hbar^2}V_0 a^3 \iint_{-\infty}^{\infty}\int \sum_{i=1}^{8}\delta(x - x_i)\,\delta(y - y_i)\,\delta(z - z_i)\,dxdydz$$

$$= \frac{-m}{2\pi\hbar^2}V_0 a^3[1+1+1+1+1+1+1+1]$$

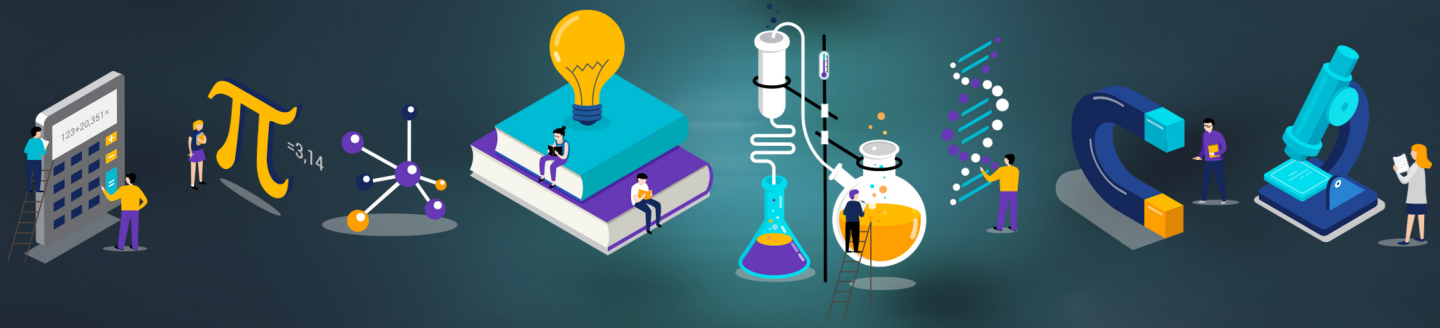
$$= \frac{-8mV_0 a^3}{2\pi\hbar^2} = \frac{-4mV_0 a^3}{\pi\hbar^2}$$

Differential scattering cross section $D(\theta) = |f(\theta)|^2 = \frac{16m^2V_0^2a^6}{\pi^2\hbar^4}$

(b) Total scattering cross section $\sigma = \int |f(\theta)|^2 \sin\theta d\theta d\phi$.

$$= \frac{16m^2V_0^2a^6}{\pi^2\hbar^4 \cdot 4\pi} = \frac{64a^2}{\pi}\left(\frac{m^2V_0^2a^4}{h^4}\right)$$

$$\sigma = \frac{64a^2}{\pi}\left(\frac{mV_0a^2}{\hbar^2}\right)^2$$



5. Relativistic quantum mechanism

5.1 Klein Gordon equation

In this chapter we consider two types of wave equations which have been proposed for the description of particles traveliing at speeds-close to that of light.At these speeds, the Iamiltonian of the (free) particle is no longer given by $(\mathbf{p}^2/2m)$; hence Schrödinger's equation, obtained from such a Hamiltonian by the prescription of Sec. 2.1, is not applicable to relativistic particles. One could try to generalize the equation by using, instead of $(\mathbf{p}^2/2m)$, the relativistic expression for the energy, namely $E = \left(c^2\mathbf{p}^2 + m^2c^4\right)^{1/2}$. The operator replacement $E \to i\hbar\partial_i t, \mathbf{p} \to -i\hbar\nabla$ would then lead to $i\hbar\partial\psi/\partial t = \left(-\hbar^2 i^2\nabla^2 + m^2c^4\right)^{1/2}\psi$ This equation has some obviously unattractive features. The space and time differential operators enter in it in very different ways. This is in contrast with the quite symmetric role of the space and time coordinates (as different components of a single four-vector) in relativity theory. The meaning of the operator $\left(-\hbar^2c^2\nabla^2 + m^2c^4\right)^{1/2}$ is itself unclear. One could get around this by passing to the momentum representation. But even this possibility would disappear if the quantity under the square root were to be modified to include functions of $\mathbf{x}$: for example, through the replacement $\mathbf{p} \to (\mathbf{p} - e\mathbf{A}/c)$ which becomes necessary when electromagnetic fields are present (assuming that the particle has charge e). Schrodinger suggested (immediately after his formulation of nonrelativistic quantum mechanics) that in order to avoid the difficulties arising from the square root, the operator replacement of $\mathbf{p}$ and E be made in the relativistic expression for E^2 :

$$E^2 = c^2p^2 + m^2c^4$$

The resulting equation is

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = -\hbar^2c^2\nabla^2\psi + m^2c^4\psi$$

or

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi + \left(\frac{mc}{\hbar}\right)^2\psi = 0$$

This equation is konwn is as Klein Gordon equation .
Meanwhile Dirac succeeded in constructing another equation which is of the first order in $(\partial/\partial t)$ and ∇, unlike Eq. 10.2, and yet involves these operators in a fully symmetric way. The Dirac equation constrains the spin of the particle to be $\frac{1}{2}$. Its application to the electron was phenomenally successful, not only in helping to understand its propertics in a natural way, but more spectacularly, in the prediction of its anti-particle, the positron (which was later discovered in cosmic rays). The Klein-Gordon equation has nothing to say about the spin of the particle; it is ribe ane to be used for particles of spin 0 , like the π-and K-mesons.

plane wave Solution

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}-\nabla^2\psi+\left(\frac{mc}{\hbar}\right)^2\psi=0$$

Solutions to this equation corresponding to particles of definite momentum $\mathbf{p}=\hbar\mathbf{k}$ may be obtained by substituting $\psi(\mathbf{x},t)=f(t)e^{i\mathbf{k}\cdot\mathbf{x}}$. This leads to $d^2f\mid dt^2=\left[c^2\mathbf{k}^2+\left(mc^2/\hbar\right)^2\right]f$. Solving this we obtain (apart from a constant normalization factor), the plane wave solutions:

$$\psi(\mathbf{x},t)=e^{i(\mathbf{k_x}\mathbf{x}\mp\omega t)}=e^{i(\mathbf{p}\cdot\mathbf{x}-Et)/\hbar}$$
$$E=\pm\hbar\omega=\pm\left(c^2\mathbf{p}^2+m^2c^4\right)^{1/2}$$

In contrast to the nonrelativistic case where the coefficient $(E/\hbar)$ of $(-it)$ in the exponent is the positive quantity $\left(\mathbf{p}^2/2m\hbar\right)$, here we have solutions with - ω as well as with $+\omega$. The appearance of the 'negative energy' solutions (characterized by $+\omega t$ in the exponent) is typical of relativistic wave equations;

Charge and current densities

Another difference from the nonrelativistic case is that $\psi^*\psi$ cannot be interpreted as the probability density $P(\mathbf{x},t)$. We expect $P(\mathbf{x},\bar{t})$ to satisfy a continuity equation of the form namely $\partial P\mid\partial t+\operatorname{div}\mathbf{S}=0$, which would ensure that $\int P(\mathbf{x},t)d^2x$ is time-independent. To obtain such an equation we multiply klein gordon equation on the left by ψ^*, its complex conjugate equation by ψ, and subtract. The resulting equation can be written as

$$\frac{1}{c^2}\frac{\partial}{\partial t}\left(\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right)-\nabla\cdot\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)=0$$

This is a continuity equation, with

$$P(\mathbf{x},t)=\frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right)$$
$$\mathbf{S}(\mathbf{x},t)=-\frac{i\hbar}{2m}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)$$

A convenient choice of a common constant factor in P and S has been made here. With this choice, S coincides exactly with the corresponding nonrelativistic expression. However, P is quite different. It vanishes identically if ψ is real, and in the case of complex wave functions, P can even be made negative by choosing $\partial\psi/\partial t$ appropriately. Clearly, P cannot be a probability density. One could multiply P by a charge e and then interpret it as a charge density (which can be positive or negative) and S as the corresponding electric current density.

5.2 Dirac equation

The occurance of negative probability density is due to the presence of time derivatives in the expression for $P(r,t)$. This can be avoided by not allowing any time derivative other than the first order to appear in the wave equation. When the wave equation is of first order in time, it must be first order in space coordinates too. Dirac was probably influenced by the Maxwell's equations as they are first order equations in both space and time coordinates.

As in Klein-Gordon equation, we can start from the basic energy equation, equation Replacing E by $i\hbar\partial/\partial t$ and p by $-i\hbar\nabla$ and allowing the

$$E=\pm\left(c^2p^2+m^2c^4\right)^{1/2}$$

Replacing E by $i\hbar\partial/\partial t$ and p by $-i\hbar\nabla$ and allowing the resulting operator equation to operate on the wavefunction $\Psi(r,t)$, we get

$$i\hbar\frac{\partial\Psi(r,t)}{\partial t}=\pm\left(-c^2\hbar^2\nabla^2+m^2c^4\right)^{1/2}\Psi(r,t)$$

To proceed further, we have to define the square root of an operator which is not yet defined. However, Dirac boldly wrote

$$c^2p^2+m^2c^4=\left[c\left(\alpha_xp_x+\alpha_yp_y+\alpha_zp_z+\beta mc\right)\right]^2$$

and then searched for conditions to be placed on the α 's and β so that the equation is valid. For equation above to hold true, we must have

$$\left.\begin{aligned} \alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1 \\ \alpha_x\alpha_y + \alpha_y\alpha_x = \alpha_y\alpha_z + \alpha_z\alpha_y = \alpha_z\alpha_x + \alpha_x\alpha_z = 0 \\ \alpha_x\beta + \beta\alpha_x = \alpha_y\beta + \beta\alpha_y = \alpha_z\beta + \beta\alpha_2 = 0 \end{aligned}\right\}$$

That is, the α 's and β anticommute in pairs and their squares are unity. These properties immediately suggest that they cannot be numbers. Already, we have a set of anticommuniting matrices, the Pauli's spin matrices. Hence, it is convenient to express them in terms of matrices. The energy can now be written as

$$E = \pm c\left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta_{mc}\right)$$

The positive or negative sign can be taken since replacement of α by $-\alpha$ and β by $-\beta$ does not change the relationships between α 's and β. Hence the relativistic Hamiltonian of a particle can be taken as

$$E = H = c\alpha \cdot p + \beta mc^2$$

Replacing E and p by their operators and allowing the resulting operator equation to operate on $\Psi(r,t)$, we

$$i\hbar\frac{\partial\Psi(r,t)}{\partial t} = -ic\hbar\left(\alpha_x\frac{\partial}{\partial x} + \alpha_y\frac{\partial}{\partial y} + \alpha_z\frac{\partial}{\partial z}\right)\Psi(r,t) + \beta mc^2\Psi(r,t)$$

which is Dirac's relativistic equation for a free particle.

Practice set 1

1. The Dirac Hamiltonian $H = c\vec{\alpha}\cdot\vec{p} + \beta mc^2$ for a free electron corresponds to the classical relation $E^2 = p^2c^2 + m^2c^4$. The classical energy-momentum relation of a piratical of charge q in a electromagnetic potential $(\phi, \vec{A})$ is $(E - q\phi)^2 = c^2\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + m^2c^4$. Therefore, the Dirac Hamiltonian for an electron in an electromagnetic field is

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A. $c\vec{\alpha}\cdot p + \frac{e}{C}\vec{A}\cdot\vec{A} + \beta mc^2 - e\phi$

B. $c\vec{\alpha}\cdot\left(\vec{p} + \frac{e}{c}\vec{A}\right) + \beta mc^2 + e\phi$

C. $c\left(\vec{\alpha}\cdot\vec{p} + e\phi + \frac{e}{c}|\vec{A}|\right) + \beta mc^2$

D. $c\vec{\alpha}\cdot\left(\vec{p} + \frac{e}{c}\vec{A}\right) + \beta mc^2 - e\phi$

2. The dynamics of a free relativistic particle of mass m is governed by the Dirac Hamiltonian $H = c\vec{\alpha}\cdot\vec{p} + \beta mc^2$, where $\vec{p}$ is the momentum operator and $\vec{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$ and β are four 4×4 Dirac matrices. The acceleration operator can be expressed as

[NET DEC 2016]

A. $\frac{2ic}{\hbar}(c\vec{p} - \vec{\alpha}H)$

B. $2ic^2\vec{\alpha}\beta$

C. $\frac{ic}{\hbar}H\vec{\alpha}$

D. $-\frac{2ic}{\hbar}(c\vec{p} + \vec{\alpha}H)$

Answer key

Q.No.	Answer	Q.No.	Answer
1	**d**	2	**a**