Lecture 8 Basic of Quantum Mechanics and the Angular Momentum

SCPY152, Second Semester 2021-22

Udom Robkob, Physics-MUSC

February 9, 2022

Topics

1. Basic of quantum mechanics, quantum states and operators
2. Interactions
3. Transitions
4. The angular momentum
5. Electron spin
6. Spin resonance

Basic of quantum mechanics

As we have learn some of simple quantum systems from solving Schrodinger's equation. Here we want to make a general statement for constructing quantum operators from their corresponding classical variables. This will be called *corresponding principle*
For any classical system identify with its position x and momentum p, its corresponding quantum behavior can be determined from quantum operators $\hat{x}$ and $\hat{p}$ with the following corresponding relations

	Classical variables	Quantum operators
Dynamics	x, p	$\hat{x} = x, \hat{p} = -i\hbar\frac{d}{dx}$
Energy	$E = \frac{p^2}{2m} + U(x)$	$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)$
EOM	$F = \frac{dp}{dt}$	$\hat{H}\varphi_E(x) = E\varphi_E(x)$

Quantum EOM is always called *Schrodinger equation*.

Interactions

Interaction of quantum system may be come from internal interaction and external field interaction. All of these will be determined in term of interaction potential energy $V(x,p)$. Effect of interaction to quantum energy E will be calculated from *quantum expectation value* as

$$E_n \mapsto E_n + \delta E_n,\ \delta E_n = \int_a^b \varphi_n^*(x) V(x, -i\hbar \frac{d}{dx}) \varphi_n(x) dx$$

with $x \in [a,b]$. Actually $\varphi_E(x)$ is also effected by $V(x,p)$ but we will not determine it here.

Interaction with uniform electric field:

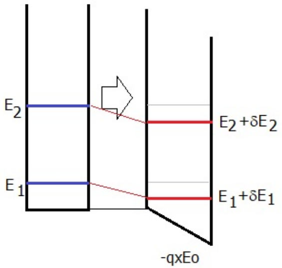
Interaction energy is

$$V(x) = -qxE_0 \ (F_x = -\frac{dV}{dx} = qE) \tag{1}$$

$$\mapsto \delta E_n = -qE_0 \int \varphi_n^*(x) x \varphi_n(x) dx \tag{2}$$

Example of infinite potential well

$$
\begin{aligned}
E_n &= \frac{\hbar^2\pi^2 n^2}{2ma^2},\ \varphi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a}) \\
\delta E_n &= -qE_0\frac{2}{a}\int_0^a x\sin^2(\frac{n\pi x}{a})dx = -\frac{qaE_0}{2} \\
&\mapsto E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2} - \frac{qaE_0}{2}
\end{aligned} \tag{3}
$$

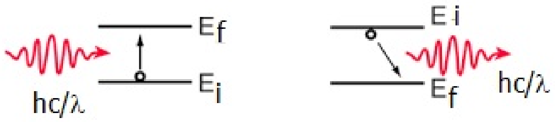


Transitions

Change of energy level of quantum system can occur by absorption or emission of photon, with photon energy equal to the different of energy levels

$$|E_f - E_i| = hf = \frac{hc}{\lambda}$$

when $E_f > E_i$ the photon is absorbed by a system, while $E_f < E_i$ the photon is emitted by a system.



The angular momentum

One more interesting quantity of mechanical system is the *angular momentum*

$$\vec{L} = \vec{r} \times \vec{p}$$

In Cartesian system with $\vec{r} = (x, y, z), \vec{p} = (p_x, p_y, p_z)$, we will have $\vec{L} = (L_x, L_y, L_z)$ in which

$$L_x = yp_x - zp_y,\ L_y = zp_x - xp_z,\ L_z = xp_y - yp_x \tag{4}$$

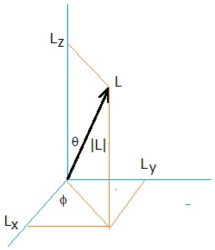
Its corresponding quantum operators are

$$\hat{L}_x = -i\hbar(y\frac{d}{dz} - z\frac{d}{dy}) \tag{5}$$

$$\hat{L}_y = -i\hbar(z\frac{d}{dx} - x\frac{d}{dz}) \tag{6}$$

$$\hat{L}_z = -i\hbar(x\frac{d}{dy} - y\frac{d}{dx}) \tag{7}$$

The quantum value of $\hat{L}$ is determined from $\hat{L}^2 = L_x^2 + L_y^2 + L_z^2$ (its length) and $\hat{L}_z$ (its orientation)



In spherical system, one can write

$$L_x = i\hbar(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}) \tag{8}$$

$$L_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}) \tag{9}$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi} \tag{10}$$

$$L^2 = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\} \tag{11}$$

Quantum equations for L_z and L^2 are

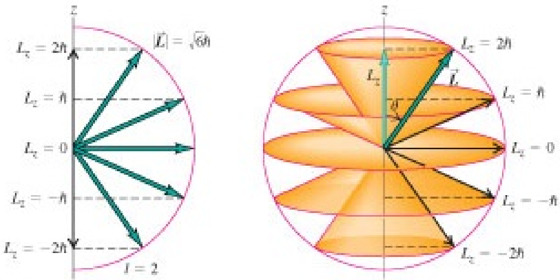
$$\hat{L}_Z Y_{lm}(\theta,\phi) = -i\hbar \frac{d}{d\phi} Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi) \quad (12)$$

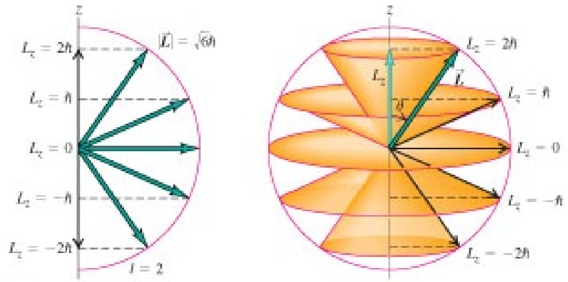
with $m = 0, \pm 1, \pm 2, ..., \pm l$ and

$$\frac{L^2}{\hbar^2} Y_{lm}(\theta,\phi) = -\left\{ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right\} Y_{lm}(\theta,\phi)$$
$$= l(l+1) Y_{lm}(\theta,\phi)$$
$$\mapsto L^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi) \quad (13)$$

with $l = 0, 1, 2, ..., \infty$

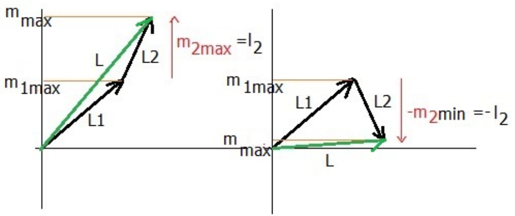
l	$L^2(\hbar^2)$	$L_z(\hbar), (m)$
0	0	0
1	2	$0, \pm 1$
2	6	$0, \pm 1, \pm 2$
3	12	$0, \pm 1, \pm 2, \pm 3$


z
$L_z = 2\hbar$
$|\vec{L}| = \sqrt{6}\hbar$
$L_z = \hbar$
$L_z = 0$
$L_z = -\hbar$
$L_z = -2\hbar$
$l = 2$
z
$L_z = 2\hbar$
L_z
$\vec{L}$
θ
$L_z = \hbar$
$L_z = 0$
$L_z = -\hbar$
$L_z = -2\hbar$



Addition of two angular momenta: Let

$$\vec{L} = \vec{L}_1 + \vec{L}_2, \text{ with } L_1^2 = l_1(l_1+1)\hbar^2, L_{1z} = m_1\hbar$$
$$L_2^2 = l_2(l_2+1)\hbar^2, L_{2z} = m_2\hbar$$
$$\text{Since } \; L^2 = l(l+1)\hbar^2, L_z = m\hbar, \quad (14)$$
$$\text{From graphical sum below : } \; l = l_1 + l_2, l_1 + l_2 - 1, ..., |l_1 - l_2| \quad (15)$$



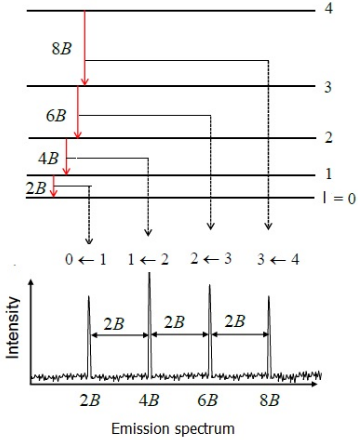
For example: $l_1 = 1, l_2 = 1 \mapsto l = 2, 1, 0.$
For example: $l_1 = 1, l_2 = 2$

$$\mapsto l = 3, 2, 1; \qquad \begin{aligned} l &= 1, m = 0, \pm 1 \\ l &= 2, m = 0, \pm 1, \pm 2 \\ l &= 3, m = 0, \pm 1, \pm 2, \pm 3 \end{aligned}$$

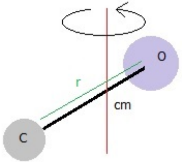
For example of *rigid rotator*, with the Hamiltonian operator

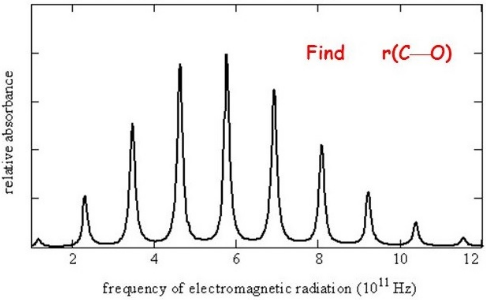
$$H = \frac{1}{2I_0}L^2 \mapsto E_l = \frac{\hbar^2}{2I_0}l(l+1), \;\; l = 0, 1, 2, ... \tag{16}$$

Let $B = \hbar^2/2I_0$, the E_l will appear with the emission spectrum as



Rigid rotator model of diatomic molecule: CO





Mass of C
= 19.92168×10^{-27} kg

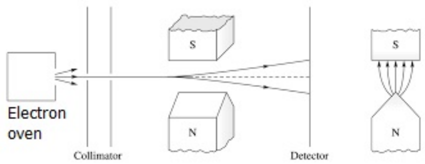
Mass of O
= 26.561×10^{-27} kg

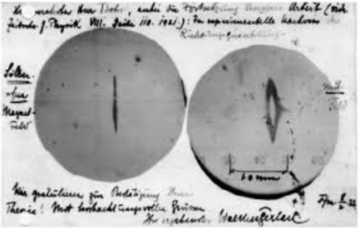
First line (J = 0 to J=1 transition) in the rotation spectrum of CO is 3.84235 cm^{-1}.

Calculate the moment of inertia (I) and bond length (r) of CO.

Electron spin

From Stern-Gerlach experiment





Magnetic interaction with non-uniform magnetic field, assumed in z-direction, is

$$U(z) = -\vec{\mu} \cdot \vec{B}(z) = -\mu_z B_z(z)$$

where $\vec{\mu}$ is magnetic (dipole) moment of an electron, here we may determine from a current loop, so that

$$\vec{\mu} = i\vec{A} = \frac{-ev}{2\pi r}(\pi r^2)\hat{n} = -\frac{e}{2m}(mvr)\hat{n} = -\frac{e}{2m}\vec{L}$$

From above we will have

$$U(x) = \frac{e}{2m} L_z B(z) \mapsto F_z = -\frac{dU(z)}{dz} = -\frac{e}{2m} L_z \frac{dB(z)}{dz} \qquad (17)$$

With the double lines splitting, and quantization of $L_z = m\hbar$, we have to have $m = \pm\frac{1}{2}$

$$F_z = \mp \frac{e\hbar}{4m} \frac{dB(z)}{dz}$$

This also corresponds to the quantum of the angular momentum with the quantum number of $l = \frac{1}{2}$. This is later known as *spin angular momentum* of an electron and denote by $\vec{S}$ with its quantum value of

$$S^2 \chi_{s,m_s} = s(s+1)\hbar^2 \chi_{s,m_s}, \; S_z \chi_{s,m_s} = m_s \hbar \chi_{s,m_s} \qquad (18)$$

when $s = \frac{1}{2}, \; m_s = \pm\frac{1}{2}$ for electron (e), proton (p) and neutron (n).

From above the magnetic moment is related to spin angular momentum in the form

$$\vec{\mu} = g\frac{q}{2m}\vec{S}$$

where g is called g-factor, it is relativistic correction of the relation above, q is charge and m is mass of particle.

Particle	Mass	Charge	g-factor
Electron	m_e	$-e$	$2.003 \simeq 2$
Proton	m_p	$+e$	5.586
Neutron	m_n	$0(+e)$	-3.826

Spin resonance

Magnetic interaction of particle spin in uniform magnetic field, assume in z-direction, is

$$U = -\vec{\mu} \cdot \vec{B} = -g \frac{q}{2m} S_Z B = -m_s \frac{q\hbar B}{2m} \tag{19}$$

Spin resonance

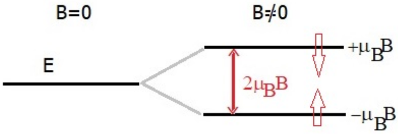
Magnetic interaction of particle spin in uniform magnetic field, assume in z-direction, is

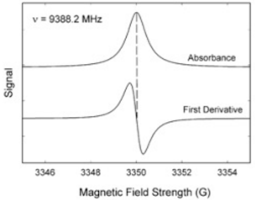
$$U = -\vec{\mu} \cdot \vec{B} = -g \frac{q}{2m} S_Z B = -m_s \frac{q\hbar B}{2m} \tag{19}$$

Electron Spin Resonance (ESR):

$$U = \pm \frac{e\hbar}{2m_e} B = \pm \mu_B B \tag{20}$$

where $\mu_B = 5.7885 \times 10^{-5} [eV/T]$ is called *Bohr magneton*





For example, let $B = 0.001\,T$

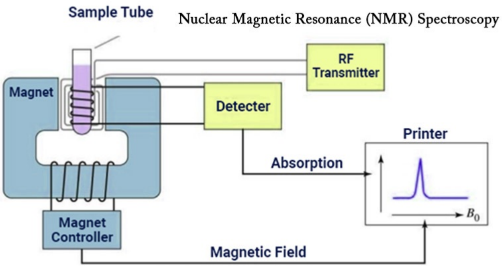
$$hf = 2\mu_B B \mapsto f = \frac{2\mu_B B}{h} = \frac{2(5.7885 \times 10^{-5} eV/T)(0.001\,T)}{4.136 \times 10^{-15} eV \cdot s}$$
$$= 2.7 \times 10^{7} Hz = 27\,MHz$$

Nuclear magnetic resonance (NMR): for proton

$$U = \mp\frac{g_p}{2}\frac{e\hbar}{2m_p}B = \mp\frac{g_p}{2}\mu_N B \tag{21}$$

where $\mu_N = 3.153 \times 10^{-8}[eV/T]$ is called *nuclear magneton*. For example, let $B = 10T$

$$hf = g_p\mu_N B \mapsto f = \frac{g\mu_N B}{h} = \frac{5.586(3.153 \times 10^{-8}eV/T)(10T)}{4.136 \times 10^{-15}eV \cdot s}$$
$$= 4.26 \times 10^{-8}Hz = 426MHz$$



Magnetic resonance imaging: MRI

Image reconstruction by back projection technique