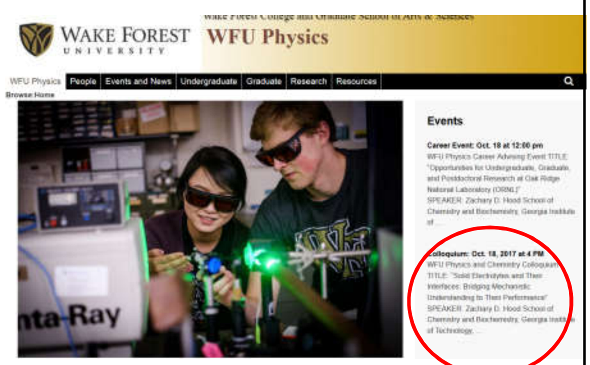
PHY 741 Quantum Mechanics
12-12:50 AM MWF Olin 103

Plan for Lecture 20:

Preparation for studying multi-electron atoms; notions of spin and "addition" of angular momenta – Chap. 14-15

1. **Internal spin**
2. **Spin interactions**



11	Wed, 9/20/2017	Chap. 9	Commutator formalism	#8	9/22/2017
12	Fri, 9/22/2017	Chap. 10	Quantum mechanics of multiparticle systems	#9	9/25/2017
13	Mon, 9/25/2017	Chap. 10-12	Multiparticle systems and angular momentum		
14	Wed, 9/27/2017	Chap. 12	Eigenstates of angular momentum		
15	Fri, 9/29/2017	Chap. 1,4,5,7,9,10,12	Review		
	Mon, 10/02/2017		*Take-home exam -- No class*		
	Wed, 10/04/2017		*Take-home exam -- No class*		
16	Fri, 10/06/2017	Chap. 12-13	Spherically symmetric systems		
17	Mon, 10/09/2017	Chap. 13	Quantum mechanics of a hydrogen atom	#10	10/16/2017
18	Wed, 10/11/2017	Chap. 13	Quantum mechanics of multi-electron atoms		
	Fri, 10/13/2017		*Fall break -- No class*		
19	Mon, 10/16/2017		Discuss exam questions and topics for presentations	Topic	10/18/2017
20	Wed, 10/18/2017	Chap. 14	Intrinsic spin	#11	10/20/2017
21	Fri, 10/20/2017				
22	Mon, 10/23/2017				
23	Wed, 10/25/2017				
24	Fri, 10/27/2017				
25	Mon, 10/30/2017				

Recall that, we analyzed the general eignstates of angular momentum, especially finding eigenvalues and eigenvectors of $\mathbf{J}^2$ and J_z

→ *j*=integer or *half integer*

$$|\alpha\beta\rangle \Rightarrow |jm\rangle$$
$$\mathbf{J}^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle$$
$$J_z|jm\rangle = \hbar m|jm\rangle$$
$$J_+|jm\rangle = \hbar\sqrt{j(j+1)-m^2-m}\,|j(m+1)\rangle$$
$$J_-|jm\rangle = \hbar\sqrt{j(j+1)-m^2+m}\,|j(m-1)\rangle$$

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Particles can have intrinsic spin angular momentum, related to their magnetic dipole moments

$$\boldsymbol{\mu} = g\frac{q}{Mc}\mathbf{S}$$

	g
electron	-2.0023
proton	5.586
neutron	-3.826

Bohr magnetron for electron: $\mu_B = \mathbf{927.4009994\,x\,10^{-26}\,J\,T^{-1}}$

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Spin ½ systems –

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} \quad \text{where } \boldsymbol{\sigma} = \sigma_x\hat{\mathbf{x}} + \sigma_y\hat{\mathbf{y}} + \sigma_z\hat{\mathbf{z}}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Properties of Pauli spin matrices

$$\sigma_x\sigma_y = i\sigma_z \quad \text{(and all cyclic permutations)}$$
$$[\sigma_x, \sigma_y] = 2i\sigma_z \quad \text{(and all cyclic permutations)}$$

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Rotation of angular momentum

Previously we showed that the operator that represents rotation about the $\hat{\mathbf{n}}$ axis by the angle θ is given by

$$R(\hat{\mathbf{n}},\theta) = e^{-i\theta\hat{\mathbf{n}}\cdot\mathbf{S}/\hbar} = e^{-i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}/2}$$

$$= 1 - \frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2} + \frac{1}{2!}\left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2}\right)^2 + \frac{1}{3!}\left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2}\right)^3 + \frac{1}{4!}\left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2}\right)^4 + \ldots$$

$$= \left(1 + \frac{1}{2!}\left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2}\right)^2 + \frac{1}{4!}\left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2}\right)^4 + \ldots\right) + \left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2} + \frac{1}{3!}\left(-\frac{i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}{2}\right)^3 + \ldots\right)$$

Note that: $(\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})^2 = I$

$$\Rightarrow R(\hat{\mathbf{n}},\theta) = e^{-i\theta\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}/2}$$

$$= I\cos\left(\frac{\theta}{2}\right) - \hat{\mathbf{n}}\cdot\boldsymbol{\sigma}\; i\sin\left(\frac{\theta}{2}\right)$$

Response of magnetic moment to an applied magnetic field

$$\mathcal{H} = -\vec{\mu}\cdot\mathbf{B}.$$

In magnetic resonance experiments, the magnetic field is generally composed of a constant component (B_0) taken to be in the $\hat{\mathbf{z}}$ direction and a rotating component (B_1) in the perpendicular direction taken to be in the $x-y$ plane. Suppose that the rotation frequency is denoted by Ω, the magnetic field can be written:

$$\mathbf{B} = B_1(\cos(\Omega t)\hat{\mathbf{x}} + \sin(\Omega t)\hat{\mathbf{y}}) + B_0\hat{\mathbf{z}}, \tag{4}$$

where it is generally assumed that $B_0 >> B_1$. For this field, the interaction Hamiltonian can be written:

$$\mathcal{H} = -\mu_e\mathbf{B}\cdot\vec{\sigma} \equiv -\mu_e\begin{pmatrix} B_0 & B_1 e^{-i\Omega t} \\ B_1 e^{i\Omega t} & -B_0 \end{pmatrix}. \tag{5}$$

We would like to solve the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi(t)}{\partial t} = \mathcal{H}(t)\Psi(t). \tag{6}$$

It turns out to be simpler to solve the equation by transforming it into the form of a time-independent Hamiltonian:

$$i\hbar\frac{\partial\Psi'(t)}{\partial t} = \begin{pmatrix} -\mu_e B_0 - \frac{\hbar\Omega}{2} & -\mu_e B_1 \\ -\mu_e B_1 & -(-\mu_e B_0 - \frac{\hbar\Omega}{2}) \end{pmatrix}\Psi'(t) \equiv \mathcal{H}_{\text{eff}}\Psi'(t). \tag{7}$$

Here, the transformed wavefunction Ψ' is defined to be

$$\Psi'(t) \equiv \begin{pmatrix} e^{i\Omega t/2} & 0 \\ 0 & e^{-i\Omega t/2} \end{pmatrix}\Psi(t),$$

and the time independent effective Hamiltonian is given by

$$\mathcal{H}_{\text{eff}} \equiv \begin{pmatrix} -\mu_e B_0 - \frac{\hbar\Omega}{2} & -\mu_e B_1 \\ -\mu_e B_1 & -(-\mu_e B_0 - \frac{\hbar\Omega}{2}) \end{pmatrix}.$$

The derivation of this result depends on the following identities:

$$\begin{pmatrix} B_0 & B_1 e^{-i\Omega t} \\ B_1 e^{i\Omega t} & -B_0 \end{pmatrix} = \begin{pmatrix} e^{-i\Omega t/2} & 0 \\ 0 & e^{i\Omega t/2} \end{pmatrix} \begin{pmatrix} B_0 & B_1 \\ B_1 & -B_0 \end{pmatrix} \begin{pmatrix} e^{i\Omega t/2} & 0 \\ 0 & e^{-i\Omega t/2} \end{pmatrix},$$

and

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = \begin{pmatrix} e^{-i\Omega t/2} & 0 \\ 0 & e^{i\Omega t/2} \end{pmatrix} \left\{ i\hbar \frac{\partial}{\partial t} - \begin{pmatrix} \frac{-\hbar\Omega}{2} & 0 \\ 0 & \frac{\hbar\Omega}{2} \end{pmatrix} \right\} \begin{pmatrix} e^{i\Omega t/2} & 0 \\ 0 & e^{-i\Omega t/2} \end{pmatrix} \Psi(t).$$

The transformed wave function Ψ' can be interpreted as representing the spin in a rotating coordinate system in which the effective Hamiltonian is now independent of time. Solving the differential equation (7), we find

$$\Psi'(t) = e^{-i\mathcal{H}_{eff}t/\hbar}\Psi'(0), \tag{12}$$

where $\Psi'(0)$ denotes the initial value of the transformed wave function and where the exponential function must be evaluated by taking its Taylor series expansion.

From this result, we obtain the full solution

$$\Psi(t) = \begin{pmatrix} e^{-i\Omega t/2} & 0 \\ 0 & e^{i\Omega t/2} \end{pmatrix} \left\{ \cos(\Omega_T t/2) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\sin(\Omega_T t/2) \begin{pmatrix} \cos(\theta_0) & \sin(\theta_0) \\ \sin(\theta_0) & -\cos(\theta_0) \end{pmatrix} \right\} \Psi(0) \tag{17}$$

Some details: $e^{-i\mathcal{H}_{eff}t} \Leftrightarrow e^{-im}$

$$m \equiv \begin{pmatrix} a & b \\ b & -a \end{pmatrix}. \tag{13}$$

The exponential of m can be evaluated:

$$e^{-im} \equiv 1 - im - \frac{1}{2!}m^2 - \frac{1}{3!}m^2(-im) + \frac{1}{4!}(m^2)^2 \cdots \tag{14}$$

For our form of m, all even terms are diagonal,

$$m^2 = \begin{pmatrix} a^2+b^2 & 0 \\ 0 & a^2+b^2 \end{pmatrix} \equiv (a^2+b^2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{15}$$

and all odd terms are proportional to m itself, so that we can simplify the expansion by summing the odd and even terms separately:

$$e^{-im} = \cos(\sqrt{a^2+b^2})\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\frac{\sin(\sqrt{a^2+b^2})}{\sqrt{a^2+b^2}}\begin{pmatrix} a & b \\ b & -a \end{pmatrix}. \tag{16}$$

In our case --

$$m = \mathcal{H}_{eff}t = \begin{pmatrix} -\mu_e B_0 t - \frac{\hbar\Omega t}{2} & -\mu_e B_1 t \\ -\mu_e B_1 t & -\left(-\mu_e B_0 t - \frac{\hbar\Omega t}{2}\right) \end{pmatrix}$$

$$= \begin{pmatrix} a & b \\ b & -a \end{pmatrix}$$

The results can be put in a more convienient form by defining the simplifying notation, $\Omega_0 \equiv -2\mu_e B_0/\hbar$, $\Omega_1 \equiv -2\mu_e B_1/\hbar$, $\Omega_T \equiv \sqrt{(\Omega_0-\Omega)^2+\Omega_1^2}$, $\cos(\theta_0) \equiv (\Omega_0 - \Omega)/\Omega_T$, and $\sin(\theta_0) \equiv \Omega_1/\Omega_T$. In these terms, the full solution to the Schrödinger equation in the form

$$\Psi(t) = \begin{pmatrix} e^{-i\Omega t/2} & 0 \\ 0 & e^{i\Omega t/2} \end{pmatrix} \left\{ \cos(\Omega_T t/2) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\sin(\Omega_T t/2) \begin{pmatrix} \cos(\theta_0) & \sin(\theta_0) \\ \sin(\theta_0) & -\cos(\theta_0) \end{pmatrix} \right\} \Psi(0) \tag{17}$$

For the special value of the rotational frequency $\Omega = \Omega_0$, the general result 17 simplifies to

$$\Psi(t) = \begin{pmatrix} e^{-i\Omega_0 t/2} & 0 \\ 0 & e^{i\Omega_0 t/2} \end{pmatrix} \begin{pmatrix} \cos(\Omega_1 t/2) & -i\sin(\Omega_1 t/2) \\ -i\sin(\Omega_1 t/2) & \cos(\Omega_1 t/2) \end{pmatrix} \Psi(0). \tag{18}$$

$$\Psi(t) = \begin{pmatrix} e^{-i\Omega_0 t/2} & 0 \\ 0 & e^{i\Omega_0 t/2} \end{pmatrix} \begin{pmatrix} \cos(\Omega_1 t/2) & -i\sin(\Omega_1 t/2) \\ -i\sin(\Omega_1 t/2) & \cos(\Omega_1 t/2) \end{pmatrix} \Psi(0).$$

For $\psi(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$,

$$\psi(t) = \begin{pmatrix} e^{-i\Omega_0 t/2}\cos(\Omega_1 t/2) \\ -ie^{i\Omega_0 t/2}\sin(\Omega_1 t/2) \end{pmatrix}.$$

Physical effects of intrinsic spin and orbital angular momentum:

Because both are associated with magnetic fields, there is an interaction energy of the form

$$\mathcal{H} = -\vec{\mu}\cdot\mathbf{B}.$$

Hyperfine interaction between nuclear spin and electronic spin and angular momentum:

$$\mathcal{H}_{\rm HF} = -\mu_{\mathbf{N}}\cdot(\mathbf{B}_{\mu_e} + \mathbf{B}_o(0))\,. \qquad (51)$$

$$\mathcal{H}_{\rm HF} = -\frac{\mu_0}{4\pi}\left(\frac{3(\mu_{\mathbf{N}}\cdot\hat{\mathbf{r}})(\mu_{\mathbf{e}}\cdot\hat{\mathbf{r}}) - \mu_{\mathbf{N}}\cdot\mu_{\mathbf{e}}}{r^3} + \frac{8\pi}{3}\mu_{\mathbf{N}}\cdot\mu_{\mathbf{e}}\delta^3(\mathbf{r}) + \frac{e}{m_e}\left\langle\frac{\mathbf{L}\cdot\mu_{\mathbf{N}}}{r^3}\right\rangle\right). \qquad (52)$$

In the absence of external magnetic fields, the internal magnetic dipoles cause spin interactions within each system, however, the total angular momentum of the system should be conserved.

Clebsch-Gordon coefficients

$$|JM, j_1 j_2\rangle = \sum_{m_1 m_2} |j_1 m_1, j_2 m_2\rangle\langle j_1 m_1, j_2 m_2 | JM, j_1 j_2\rangle$$

Finding the total angular momentum – "addition" of angular momentum.

$$\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2$$

$$\mathbf{J}^2|JM\rangle = \hbar^2 J(J+1)|JM\rangle$$

$$J_z|JM\rangle = \hbar M|JM\rangle$$

$$\mathbf{j}_1{}^2|j_1 m_1\rangle = \hbar^2 j_1(j_1+1)|j_1 m_1\rangle$$

$$j_{1z}|j_1 m_1\rangle = \hbar m_1|j_1 m_1\rangle$$

"Addition" of angular momentum

Clebsch-Gordon coefficients

$$\left|JM, j_1 j_2\right\rangle = \sum_{m_1, m_2} \left|j_1 m_1, j_2 m_2\right\rangle \left\langle j_1 m_1, j_2 m_2 \middle| JM, j_1 j_2\right\rangle$$