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

Plan for Lecture 21:

"Addition" of angular momenta – Chap. 15

1. **Total spin due to two spin-1/2 particles**
2. **Clebsch-Gordon coefficients**

9	Fri, 9/15/2017	Chap. 7	Schrödinger equation in one-dimension	#7	9/20/2017
10	Mon, 9/18/2017	Chap. 5 and 7	Schrödinger equation in one-dimension		
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	Chap. 15	Addition of Angular Momentum	#12	10/23/2017
22	Mon, 10/23/2017				
23	Wed, 10/25/2017				
24	Fri, 10/27/2017				
25	Mon, 10/30/2017				
26	Wed, 11/01/2017				

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

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

Finding the total angular momentum – "addition" of angular momentum. $\mathbf{J} = \mathbf{j}_1 + \mathbf{j}_2$

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

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

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

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

“Addition” of angular momentum

Clebsch-Gordon coefficients

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

Explicit formula for Clebsch-Gordon coefficients:

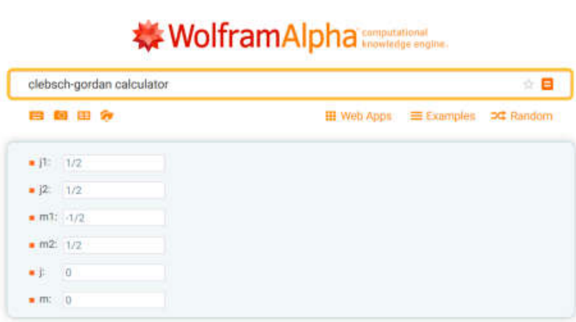
Reference: Abramowitz & Stegum – pg. 1006

Original formula:

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle = \delta_{m, m_1+m_2} \sqrt{\frac{(j_1+j_2-j)!(j_1-j_2+j)!(-j_1+j_2+j)!(2j+1)}{(j_1+j_2+j+1)!}}$$
$$\times \sum_k \frac{(-1)^k \sqrt{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j+m)!(j-m)!}}{k!(j_1+j_2-j-k)!(j_1-m_1-k)!(j_2+m_2-k)!(j-j_2+m_1+k)!(j-j_1-m_2+k)!}$$

Working formula:

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle = \delta_{m, m_1+m_2} \sqrt{\frac{(j_1-j_2+j)!(-j_1+j_2+j)!(2j+1)}{(j_1+j_2-j)!(j_1+j_2+j+1)!}}$$
$$\times \sqrt{\frac{(j_1+m1)!(j_2-m_2)!(j+m)!}{(j_1-m1)!(j_2+m_2)!(j-m)!}}$$
$$\times \sum_k \frac{(-1)^k}{k!} \frac{(j_1+j_2-j)!}{(j_1+j_2-j-k)!} \frac{(j_1-m_1)!}{(j_1-m_1-k)!} \frac{(j_2+m_2)!}{(j_2+m_2-k)!} \frac{(j-m)!}{(j-j_2+m_1+k)!(j-j_1-m_2+k)!}$$



- j1: 1/2
- j2: 1/2
- m1: -1/2
- m2: 1/2
- j: 0
- m: 0

Input:

$$\left\langle \frac{1}{2}\, \frac{1}{2}\, -\frac{1}{2}\, \frac{1}{2} \;\middle|\; \frac{1}{2}\, \frac{1}{2}\, 0\, 0 \right\rangle$$

Open code

$\langle j_1\, j_2\, m_1\, m_2 \mid j_1\, j_2\, j\, m\rangle$ is the Clebsch-Gordan coefficient

Result: More digits

$$-\frac{1}{\sqrt{2}} \approx -0.707107$$

Details for a simple case:

Clebsch-Gordon coefficients

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

Recall that:

$$J_{\pm}\left|JM\right\rangle = \hbar\sqrt{J^2 - M^2 + J \mp M}\left|J(M \pm 1)\right\rangle$$

$$J_{\pm} = j_{1\pm} + j_{2\pm}$$

$$\left|11; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\right\rangle$$

$$J_{-}\left|11; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \hbar\sqrt{2}\left|10; \tfrac{1}{2}\tfrac{1}{2}\right\rangle$$

$$\left(j_{1-} + j_{2-}\right)\left|\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \hbar\left|\tfrac{1}{2} - \tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\right\rangle + \hbar\left|\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2} - \tfrac{1}{2}\right\rangle$$

$$\Rightarrow \left|10; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\tfrac{1}{2} - \tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\right\rangle + \left|\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2} - \tfrac{1}{2}\right\rangle\right)$$

$$\left|1-1; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2} - \tfrac{1}{2}, \tfrac{1}{2} - \tfrac{1}{2}\right\rangle$$

Summary of results:

$$\left|11; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\right\rangle$$

$$\left|10; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\tfrac{1}{2} - \tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\right\rangle + \left|\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2} - \tfrac{1}{2}\right\rangle\right)$$

$$\left|1-1; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2} - \tfrac{1}{2}, \tfrac{1}{2} - \tfrac{1}{2}\right\rangle$$

J=1
degeneracy:
2J+1=3

$$\left|00; \tfrac{1}{2}\tfrac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\tfrac{1}{2} - \tfrac{1}{2}, \tfrac{1}{2}\tfrac{1}{2}\right\rangle - \left|\tfrac{1}{2}\tfrac{1}{2}, \tfrac{1}{2} - \tfrac{1}{2}\right\rangle\right)$$

J=0
degeneracy:
2J+1=1

Note that these eigenstates have different behaviors wrt to particle exchange:

$\left|1M; \tfrac{1}{2}\tfrac{1}{2}\right\rangle \Rightarrow$ even under particle exchange

$\left|00; \tfrac{1}{2}\tfrac{1}{2}\right\rangle \Rightarrow$ odd under particle exchange

General accounting:

Total number of states:

$$(2j_1+1)(2j_2+1)=\sum_{J=|j_1-j_2|}^{j_1+j_2}(2J+1)$$

Case of "addition" of spin and orbital angular momentum

$j_1 = l \qquad j_2 = s = \frac{1}{2}$

$$\left|\left(l+\tfrac{1}{2}\right)M;l\tfrac{1}{2}\right\rangle=\sqrt{\frac{l+M+\frac{1}{2}}{2l+1}}\left|l\left(M-\tfrac{1}{2}\right);\tfrac{1}{2}\tfrac{1}{2}\right\rangle+\sqrt{\frac{l-M+\frac{1}{2}}{2l+1}}\left|l\left(M+\tfrac{1}{2}\right);\tfrac{1}{2}-\tfrac{1}{2}\right\rangle$$

$$\left|\left(l-\tfrac{1}{2}\right)M;l\tfrac{1}{2}\right\rangle=-\sqrt{\frac{l-M+\frac{1}{2}}{2l+1}}\left|l\left(M-\tfrac{1}{2}\right);\tfrac{1}{2}\tfrac{1}{2}\right\rangle+\sqrt{\frac{l+M+\frac{1}{2}}{2l+1}}\left|l\left(M+\tfrac{1}{2}\right);\tfrac{1}{2}-\tfrac{1}{2}\right\rangle$$

Spin-orbit interaction due to spin alignment in magnetic field generated by orbital motion

$$H_{SO} = G(r)\mathbf{S}\cdot\mathbf{L}$$

Note that: $\mathbf{J}=\mathbf{S}+\mathbf{L}$

$$\mathbf{J}^2=\mathbf{S}^2+\mathbf{L}^2+2\mathbf{S}\cdot\mathbf{L}$$

$$\langle JM;ls|H_{SO}|JM;ls\rangle = G(r)\langle JM;ls|\mathbf{S}\cdot\mathbf{L}|JM;ls\rangle$$

$$=\frac{\hbar^2 G(r)}{2}\left(j(j+1)-s(s+1)-l(l+1)\right)$$

$$\left\langle\left(l+\tfrac{1}{2}\right)M;ls\right|H_{SO}\left|\left(l+\tfrac{1}{2}\right)M;ls\right\rangle=\frac{\hbar^2G(r)}{2}l$$

$$\left\langle\left(l-\tfrac{1}{2}\right)M;ls\right|H_{SO}\left|\left(l-\tfrac{1}{2}\right)M;ls\right\rangle=-\frac{\hbar^2G(r)}{2}(l+1)$$

Coupling of orbital angular momenta of multiple electrons

$$\mathbf{J}=\mathbf{L_1}+\mathbf{L_2}$$

$$J=|l_1-l_2|,|l_1-l_2|+1,....,(l_1+l_2)$$

Example: $l_1 = l_2 = 1$ total of 9 orbital states

$J=0$ 1 state

$J=1$ 3 states

$J=2$ 5 states

Consequences of orbital coupling on energies of multi-electron atoms

Example C $1s^2\ 2s^2\ 2p^2$

https://physics.nist.gov/PhysRefData/ASD/levels_form.html

Primary data source	Query NIST Bibliographic Database for **C I** (new window)
Moore 1993	Literature on C I Energy Levels

Configuration	Term	J	Level (eV)	Reference
$2s^22p^2$	^3P	0	0.00000	L7288
		1	0.002033	
		2	0.005381	
$2s^22p^2$	^1D	2	1.263725	
$2s^22p^2$	^1S	0	2.684011	

Atomic term notation: $^{(2S+1)}L_J$

L	*symbol*	*spin*
0	*S*	*S=0*
1	*P*	*S=1*
2	*D*	*S=0*
3	*F*	*S=1*

Example for C $1s^2\ 2s^2\ 2p^2$

States of total orbital momentum: $(2l_1+1)(2l_2+1)=9$

Total number of orbital and spin configurations: $6\cdot 5/2=15$

$^1D \Rightarrow 5$ states

$^1S \Rightarrow 1$ states

$^3P \Rightarrow 9$ states

Energetic differences are due to the electron-electron Coulomb repulsion:

$$V_{ee}=\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}=\sum_{\lambda\mu}\frac{4\pi}{2\lambda+1}\frac{r_<^\lambda}{r_>^{\lambda+1}}Y_{\lambda\mu}(\hat{\mathbf{r}}_1)Y_{\lambda\mu}^*(\hat{\mathbf{r}}_2)$$

Example for ^{1}D state

$$\left|JM;l_1l_2\right\rangle = \left|22;11\right\rangle = \sum_{m_1,m_2} \left|l_1m_1,l_2m_2\right\rangle \left\langle l_1m_1,l_2m_2\right|JM;l_1l_2\rangle$$
$$= \left|11,11\right\rangle = R_{2p}(r_1)R_{2p}(r_2)Y_{11}(\hat{\mathbf{r}}_1)Y_{11}(\hat{\mathbf{r}}_2)$$

$$\left\langle 11,11\right|V_{ee}\left|11,11\right\rangle$$

10/20/2017 PHY 741 Fall 2017 -- Lecture 21 16