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

Plan for Lecture 14:
Reading in Shankar: Read Chapter 12

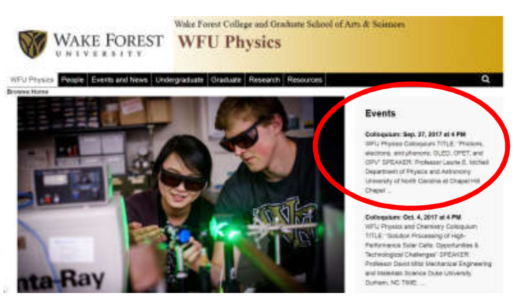
Quantum mechanics of angular momentum

1. **Review of commutation relations**
2. **Eigenvalues and eigenvectors of angular momentum**
3. **Generalization to spin angular momentum**
4. **Finite rotations**

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/28/2017	Chap. 1	Review of basic principles	#1	9/6/2017
2	Wed, 8/30/2017	Chap. 1	Linear vector spaces	#2	9/6/2017
3	Fri, 9/01/2017	Chap. 1	Linear vector spaces	#3	9/6/2017
4	Mon, 9/04/2017	Chap. 4	Principles of Quantum Mechanics	#4	9/8/2017
5	Wed, 9/06/2017	Chap. 5	Examples in 1 dimension		
6	Fri, 9/08/2017	Chap. 5	Schrödinger equation in one-dimension	#5	9/13/2017
7	Mon, 9/11/2017	Chap. 5	Schrödinger equation in one-dimension		
8	Wed, 9/13/2017	Chap. 7	Schrödinger equation in one-dimension	#6	9/15/2017
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				



WFU Physics Colloquium

TITLE: "Photons, electrons, and phonons; OLED, OFET, and OPV"

SPEAKER: Professor Laurie E. McNeil
Department of Physics and Astronomy
University of North Carolina at Cha
Chapel Hill, NC

TIME: Wed. Sep. 27, 2017 at 4:00

PLACE: George P. Williams, Jr. Le
101)

ABSTRACT

First discovered at the beginning of the 20th century but still only partially understood today, organic semiconductors combine the electrical and optical properties typical of inorganic semiconductors with properties such as flexibility, low cost, and structural tunability via chemical modification. They are of significant interest due to their potential for opto-electronic applications such as displays, photosensors and solar cells. Charge transfer compounds, which are made of two or more organic molecules in which one species acts as a donor of electric charge and the other as an acceptor, could provide new properties or improved performance to increase the range of application of organic semiconductors. I will discuss how optical measurements such as resonant Raman scattering and transient absorption, when combined with numerical calculations, can elucidate the physics of the subtle interplay of interactions that is critical to applications of these materials in 21st-century opto-electronic devices.

Review of commutation relations for angular momentum

Angular momentum in three dimensions

$$L_x = YP_z - ZP_y$$
$$L_y = ZP_x - XP_z$$
$$L_z = XP_y - YP_x$$

Consider:

$$[L_x, Y] = [YP_z - ZP_y, Y] = -Z[P_y, Y] = i\hbar Z$$
$$[L_x, P_y] = [YP_z - ZP_y, P_y] = P_z[Y, P_y] = i\hbar P_z$$
$$[L_x, L_y] = [YP_z - ZP_y, ZP_x - XP_z] = i\hbar L_z$$

Summary:

$$[L_x, L_y] = i\hbar L_z \qquad [L_y, L_z] = i\hbar L_x \qquad [L_z, L_x] = i\hbar L_y$$

Summary:

$$[L_x, L_y] = i\hbar L_z \qquad [L_y, L_z] = i\hbar L_x \qquad [L_z, L_x] = i\hbar L_y$$

Consider $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$

$$\left[\mathbf{L}^2, L_z\right] = \left[L_x^2 + L_y^2, L_z\right]$$
$$= L_x[L_x, L_z] + [L_x, L_z]L_x + L_y[L_y, L_z] + [L_y, L_z]L_y$$
$$= -i\hbar L_x L_y - i\hbar L_y L_x + i\hbar L_y L_x + i\hbar L_x L_y$$
$$= 0$$

Since **L**^{2} and L_z commute, it is possible to simultaneous eigenvectors

Using α and β to denote the eigenvalues, assume:

$$L^2|\alpha\beta\rangle = \alpha|\alpha\beta\rangle$$

$$L_z|\alpha\beta\rangle = \beta|\alpha\beta\rangle$$

Let: $L_\pm = L_x \pm iL_y$

Note that: $[L_z, L_\pm] = \pm\hbar L_\pm$ and $[L^2, L_\pm] = 0$

Consider $L_\pm|\alpha\beta\rangle = C|\alpha(\beta\pm\hbar)\rangle$

Since $\mathbf{L}^2\left(L_\pm|\alpha\beta\rangle\right) = \alpha\left(L_\pm|\alpha\beta\rangle\right)$

$$L_z\left(L_\pm|\alpha\beta\rangle\right) = (\beta\pm\hbar)\left(L_\pm|\alpha\beta\rangle\right)$$

Eigenvalues and eigenvectors of **L**^{2} and L_z -- continued

Consider $L_\pm|\alpha\beta\rangle = C|\alpha(\beta\pm\hbar)\rangle$

Since $\mathbf{L}^2\left(L_\pm|\alpha\beta\rangle\right) = \alpha\left(L_\pm|\alpha\beta\rangle\right)$

$$L_z\left(L_\pm|\alpha\beta\rangle\right) = (\beta\pm\hbar)\left(L_\pm|\alpha\beta\rangle\right)$$

$$|C|^2 = \langle L_\pm\alpha\beta|L_\pm\alpha\beta\rangle = \langle\alpha\beta|L_\pm^\dagger L_\pm|\alpha\beta\rangle = \langle\alpha\beta|\mathbf{L}^2 - L_z^2 \mp \hbar L_z|\alpha\beta\rangle$$
$$= \alpha - \beta^2 \mp \hbar\beta$$

Summary of results (with simple choice of phase)

$$L_+|\alpha\beta\rangle = \sqrt{\alpha-\beta^2-\hbar\beta}\,|\alpha(\beta+\hbar)\rangle$$

$$L_-|\alpha\beta\rangle = \sqrt{\alpha-\beta^2+\hbar\beta}\,|\alpha(\beta-\hbar)\rangle$$

Eigenvalues and eigenvectors of **L**^{2} and L_z -- continued

Also note that:

$$\langle\alpha\beta|L_x^2 + L_y^2|\alpha\beta\rangle = \langle\alpha\beta|\mathbf{L}^2 - L_z^2|\alpha\beta\rangle = \alpha - \beta^2 \geq 0$$
$$\Rightarrow \alpha \geq \beta^2$$

Suppose that there is a maximum value of β

$$L_+|\alpha\beta_{max}\rangle = \sqrt{\alpha-\beta_{\max}{}^2-\hbar\beta_{\max}}\,|\alpha(\beta_{\max}+\hbar)\rangle = 0$$
$$\Rightarrow \alpha - \beta_{\max}{}^2 - \hbar\beta_{\max} = 0$$
$$\Rightarrow \alpha = \beta_{\max}(\beta_{\max}+\hbar)$$

Now suppose that there is a minimum value of β

$$L_-|\alpha\beta_{\min}\rangle = \sqrt{\alpha-\beta_{\min}{}^2+\hbar\beta_{\min}}\,|\alpha(\beta_{\min}-\hbar)\rangle = 0$$
$$\Rightarrow \alpha - \beta_{\min}{}^2 + \hbar\beta_{\min} = 0$$
$$\Rightarrow \alpha = \beta_{\min}(\beta_{\min}-\hbar)$$

Eigenvalues and eigenvectors of $\mathbf{L}^2$ and L_z -- continued

$$\alpha = \beta_{\max}\left(\beta_{\max} + \hbar\right) = \beta_{\min}\left(\beta_{\min} - \hbar\right)$$
$$\Rightarrow \beta_{\max} = -\beta_{\min}$$

Possible values of β :

$$\beta_{\min}, \beta_{\min} + \hbar, \beta_{\min} + 2\hbar, \ldots \beta_{\max} - \hbar, \beta_{\max}$$

Note that $\beta_{\max} - \beta_{\min} = 2\beta_{\max} = \hbar\nu \quad (\nu \equiv \text{integer})$

$$\frac{\beta_{\max}}{\hbar} = \frac{\nu}{2} \quad \text{(integer or half-integer)}$$

Typical notation:

$$\beta_{max} = \hbar j \qquad \beta = \hbar m \ \text{ for } m = -j, -j+1 \ldots j-1, j$$
$$\alpha = \hbar^2 j(j+1)$$

Eigenvalues and eigenvectors of $\mathbf{J}^2$ and J_z -- continued

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

Matrix representations of angular momentum operators:

$J^2 \rightarrow$

$j'm'$ \ jm	(0, 0)	$(\frac{1}{2}, \frac{1}{2})$	$(\frac{1}{2}, -\frac{1}{2})$	(1, 1)	(1, 0)	(1, −1)	⋯
(0, 0)	0	0	0	0	0	0	⋯
$(\frac{1}{2}, \frac{1}{2})$	0	$\frac{3}{4}\hbar^2$	0	0	0	0	
$(\frac{1}{2}, -\frac{1}{2})$	0	0	$\frac{3}{4}\hbar^2$	0	0	0	
(1, 1)	0	0	0	$2\hbar^2$	0	0	
(1, 0)	0	0	0	0	$2\hbar^2$	0	
(1, −1)	0	0	0	0	0	$2\hbar^2$	
	⋮						⋱

$J_z \rightarrow$

$j'm'$ \ jm	(0, 0)	$(\frac{1}{2}, \frac{1}{2})$	$(\frac{1}{2}, -\frac{1}{2})$	(1, 1)	(1, 0)	(1, −1)	⋯
(0, 0)	0	0	0	0	0	0	⋯
$(\frac{1}{2}, \frac{1}{2})$	0	$\frac{1}{2}\hbar$	0	0	0	0	
$(\frac{1}{2}, -\frac{1}{2})$	0	0	$-\frac{1}{2}\hbar$	0	0	0	
(1, 1)	0	0	0	$\hbar$	0	0	
(1, 0)	0	0	0	0	0	0	
(1, −1)	0	0	0	0	0	$-\hbar$	
	⋮						⋱

Matrix representations of angular momentum operators:
(block diagonal form)

$$J_x \rightarrow \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & \hbar/2 & 0 & 0 & 0 & \\ 0 & \hbar/2 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & \hbar/2^{1/2} & 0 & \\ 0 & 0 & 0 & \hbar/2^{1/2} & 0 & \hbar/2^{1/2} & \\ 0 & 0 & 0 & 0 & \hbar/2^{1/2} & 0 & \\ \vdots & & & & & & \ddots \end{bmatrix}$$

$$J_y \rightarrow \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & -i\hbar/2 & 0 & 0 & 0 & \\ 0 & i\hbar/2 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & -i\hbar/2^{1/2} & 0 & \\ 0 & 0 & 0 & i\hbar/2^{1/2} & 0 & -i\hbar/2^{1/2} & \\ 0 & 0 & 0 & 0 & i\hbar/2^{1/2} & 0 & \\ \vdots & & & & & & \ddots \end{bmatrix}$$

Note that each *j* block is typically considered separately

Example -- for $j = \frac{1}{2}$

$$\mathbf{J} = \frac{\hbar}{2}\left(\sigma_x \hat{\mathbf{x}} + \sigma_y \hat{\mathbf{y}} + \sigma_z \hat{\mathbf{z}}\right)$$

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

$$\mathbf{J}^2 = \frac{\hbar^2}{4}\left(\sigma_x^2 + \sigma_y^2 + \sigma_z^2\right) = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

For integer values of *j*, it is also possible to find special representations of the operators L^2 and L_z

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

$$L_z \rightarrow -i\hbar\frac{\partial}{\partial\phi}$$

$$\left|lm\right\rangle = Y_{lm}(\theta,\phi)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \, Y_{lm}^*(\theta,\phi) Y_{l'm'}(\theta,\phi) = \delta_{ll'}\delta_{mm'}$$

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}^*(\theta,\phi) Y_{lm}(\theta',\phi') = \delta(\phi-\phi')\delta(\cos\theta - \cos\theta')$$

Some spherical harmonic functions:

$$Y_{00}(\hat{\mathbf{r}}) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1(\pm1)}(\hat{\mathbf{r}}) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

$$Y_{10}(\hat{\mathbf{r}}) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{2(\pm2)}(\hat{\mathbf{r}}) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}$$

$$Y_{2(\pm1)}(\hat{\mathbf{r}}) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi}$$

$$Y_{20}(\hat{\mathbf{r}}) = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

Note that:

$Y_{lm}^*(\hat{\mathbf{r}}) = (-1)^m Y_{l-m}(\hat{\mathbf{r}})$

(Condon & Shortley convention)

$Y_{lm}(-\hat{\mathbf{r}}) = (-1)^l Y_{lm}(\hat{\mathbf{r}})$

Relationship of angular momentum to rotations

$$\psi(\theta,\varphi+\alpha) = \psi(\theta,\varphi) + \alpha\frac{\partial\psi(\theta,\varphi)}{\partial\varphi} + \frac{\alpha^2}{2!}\frac{\partial^2\psi(\theta,\varphi)}{\partial\varphi^2} + \ldots$$

Note that: $L_z = -i\hbar\frac{\partial}{\partial\varphi}$

$$\Rightarrow \psi(\theta,\varphi+\alpha) = \psi(\theta,\varphi) + \alpha\left(\frac{i}{\hbar}L_z\right)\psi(\theta,\varphi) + \frac{\alpha^2}{2!}\left(\frac{i}{\hbar}L_z\right)^2\psi(\theta,\varphi) + \ldots$$

$$= e^{i\alpha L_z/\hbar}\psi(\theta,\varphi)$$

Generator of rotation by α about the z-axis:

$e^{i\alpha J_z/\hbar}$

Generator of rotation by α about the α-axis:

$e^{i\boldsymbol{\alpha}\cdot\mathbf{J}/\hbar}$

Rotation transformations

$$D^j_{mm'}(\boldsymbol{\alpha}) = \langle jm | e^{i\boldsymbol{\alpha}\cdot\mathbf{J}/\hbar} | jm'\rangle$$

Rotation about the z-axis

$$D^j_{mm'}(\alpha\hat{\mathbf{z}}) = \langle jm | e^{i\alpha J_z/\hbar} | jm'\rangle = e^{i\alpha m}\delta_{mm'}$$

Rotation about the y-axis for *j=1/2*

$$D^j_{mm'}(\beta\hat{\mathbf{y}}) = \langle jm | e^{i\beta J_y/\hbar} | jm'\rangle = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}$$

Rotation about the y-axis for *j=1*

$$D^j_{mm'}(\beta\hat{\mathbf{y}}) = \langle jm | e^{i\beta J_y/\hbar} | jm'\rangle = \frac{1}{2}\begin{pmatrix} 1+\cos\beta & -\sqrt{2}\sin\beta & 1-\cos\beta \\ \sqrt{2}\sin\beta & 2\cos\beta & -\sqrt{2}\sin\beta \\ 1-\cos\beta & \sqrt{2}\sin\beta & 1+\cos\beta \end{pmatrix}$$