PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Plan for Lecture 15

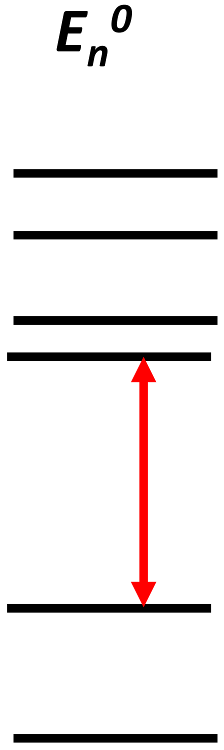
Matrix elements and selection rules
Ref: Chapter 15 and others in E. Carlson's textbook

1. Selection rules for electric dipole transitions between spherically symmetric states
2. Rotations of eigenstates of angular momentum
3. Other symmetry related issues

Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/10/2022	Chap. 12	Approximate solutions for stationary states -- The variational approach	#1	01/14/2022
2	Wed: 01/12/2022	Chap. 12 C	Approximate solutions for stationary states -- Perturbation theory	#2	01/19/2022
3	Fri: 01/14/2022	Chap. 12 D	Approximate solutions for stationary states -- Degenerate perturbation theory	#3	01/21/2022
	Mon: 01/17/2022		MLK Holiday -- no class		
4	Wed: 01/19/2022	Chap. 12 C & D	Approximate solutions for stationary states -- Additional tricks	#4	01/24/2022
5	Fri: 01/21/2022	Chap. 13	Examples of of the use of perturbation theory	#5	01/26/2022
6	Mon: 01/24/2022	Chap. 13 & 12 B	Hyperfine perturbation and also the WKB approximation	#6	01/28/2022
7	Wed: 01/26/2022	Chap. 14	Scattering theory		
8	Fri: 01/28/2022	Chap. 14	Scattering theory	#7	02/04/2022
9	Mon: 01/31/2022	Chap. 14	Scattering theory	#8	02/07/2022
	Wed: 02/02/2022	No class	Fire caution		
	Fri: 02/04/2022	No class	Fire caution		
10	Mon: 02/07/2022	Chap. 11 (A-C)	Time evolution and Feynman path integrals	#9	02/09/2022
11	Wed: 02/09/2022	Chap. 11 (A-C)	Time evolution and Feynman path integrals	#10	02/11/2022
12	Fri: 02/11/2022	Chap. 15 A	Approximation methods for time evolution of quantum systems	#11	02/14/2022
13	Mon: 02/14/2022	Chap. 15	Approximate time evolution	#12	02/16/2022
14	Wed: 02/16/2022	Chap. 15	Fermi Golden Rule	#13	02/18/2022
15	Fri: 02/18/2022	Chap. 15	Matrix elements and selection rules		
	Mon: 02/21/2022	Chaps. (11-15)	Homework review & presentations		



We will discuss "selection rules" for transitions between spherically symmetric states in due to interaction with an electromagnetic field in the dipole approximation --

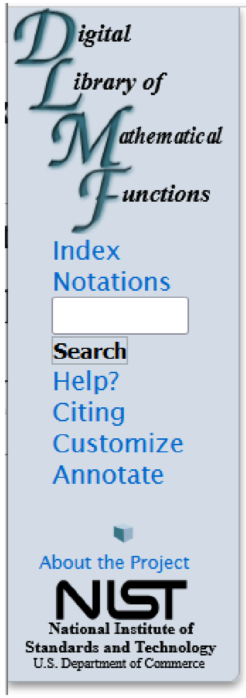
$$\left\langle f^0 \middle| \tilde{H}^1 \middle| I^0 \right\rangle = \left\langle f^0 \middle| -eF_0 r\cos\theta \middle| I^0 \right\rangle$$

Symmetry analysis of the matrix element finds non-trivial matrix elements for $\ell_f - \ell_I = \pm 1$ and $m_f - m_I = 0, \pm 1.$

Digression on matrix elements --

For transition matrix elements between states of spherically symmetric systems, we typically must evaluate "Gaunt" coefficents:

$$\left\langle f^0 \middle| \tilde{H}^1 \middle| I^0 \right\rangle \propto \int d\Omega \; Y^*_{l_1 m_1}(\theta,\phi) Y_{l_2 m_2}(\theta,\phi) Y_{l_3 m_3}(\theta,\phi)$$



34.3.22
$$\int_0^{2\pi}\int_0^{\pi} Y_{l_1,m_1}(\theta,\phi) Y_{l_2,m_2}(\theta,\phi) Y_{l_3,m_3}(\theta,\phi) \sin\theta \, d\theta \, d\phi = \left(\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right)^{\frac{1}{2}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}.$$

3j symbols

34.2.4
$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3}\Delta(j_1 j_2 j_3)\left((j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j_3+m_3)!(j_3-m_3)!\right)^{\frac{1}{2}}$$
$$\times \sum_s \frac{(-1)^s}{s!(j_1+j_2-j_3-s)!(j_1-m_1-s)!(j_2+m_2-s)!(j_3-j_2+m_1+s)!(j_3-j_1-m_2+s)!},$$

where

34.2.5
$$\Delta(j_1 j_2 j_3) = \left(\frac{(j_1+j_2-j_3)!(j_1-j_2+j_3)!(-j_1+j_2+j_3)!}{(j_1+j_2+j_3+1)!}\right)^{\frac{1}{2}},$$

The quantities j_1, j_2, j_3 in the $3j$ symbol are called *angular momenta*. Either all of them are nonnegative integers, or one is a nonnegative integer and the other two are half-odd positive integers. They must form the sides of a triangle (possibly degenerate). They therefore satisfy the *triangle conditions*

34.2.1
$$|j_r - j_s| \le j_t \le j_r + j_s,$$

where r, s, t is any permutation of $1, 2, 3$. The corresponding *projective quantum numbers* m_1, m_2, m_3 are given by

34.2.2
$$m_r = -j_r, -j_r+1, \ldots, j_r-1, j_r, \qquad r = 1, 2, 3,$$

and satisfy

34.2.3
$$m_1 + m_2 + m_3 = 0.$$

For transition matrix elements between states of spherically symmetric systems, we typically must evaluate "Gaunt" coefficents:

$$\left\langle f^0 \left| \tilde{H}^1 \right| I^0 \right\rangle = \left\langle f^0 \left| -e\mathbf{F}\cdot\mathbf{r} \right| I^0 \right\rangle \propto \int d\Omega \; Y^*_{l_f m_f}(\theta,\phi) Y_{1m}(\theta,\phi) Y_{l_i m_i}(\theta,\phi)$$

Recall that $\quad \hat{\mathbf{r}} = \hat{\mathbf{x}} \sin\theta \, \cos\phi + \hat{\mathbf{y}} \sin\theta \, \sin\phi + \hat{\mathbf{z}} \cos\theta$

$$= \sqrt{\frac{4\pi}{3}} \left(\hat{\mathbf{x}} \left(\frac{-Y_{11}(\theta,\phi) + Y_{1-1}(\theta,\phi)}{\sqrt{2}} \right) + \hat{\mathbf{y}} \left(i \frac{Y_{11}(\theta,\phi) + Y_{1-1}(\theta,\phi)}{\sqrt{2}} \right) + \hat{\mathbf{z}} Y_{10}(\theta,\phi) \right)$$

where $\quad Y_{11}(\theta,\phi) = -\sqrt{\frac{3}{8\pi}} \sin\theta \; e^{i\phi}, \quad Y_{1-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}} \sin\theta \; e^{-i\phi}, \quad Y_{10}(\theta,\phi) = \sqrt{\frac{3}{4\pi}} \cos\theta$

$$\left\langle f^0 \right| = R_f(r) Y^*_{l_f m_f}(\theta,\phi) \qquad\qquad \left| I^0 \right\rangle = R_i(r) Y_{l_i m_i}(\theta,\phi)$$

More details given in Chapter VIII of your textbook -- for example, from Pg. 131:

The coefficients $\langle j_1 j_2; m_1 m_2 | jm \rangle$ are called *Clebsch-Gordan coefficients*,[1] (CG coefficients for short) and are useful in a variety of settings. I have included a Maple routine called "Clebsch" that computes them on my web page if you ever need them. There are several constraints that they must satisfy to be non-zero:

(1) $-j \le m \le j$, $-j_1 \le m_1 \le j_1$, and $-j_2 \le m_2 \le j_2$, by integers;

(2) $|j_1 - j_2| \le j \le j_1 + j_2$, by integers; and

(3) $m = m_1 + m_2$.

Writing Clebsch-Gordan coefficients in terms of 3j symbols –
https://dlmf.nist.gov/search/search?q=Clebsch-Gordan

► … An often used alternative to the $3j$ symbol is the Clebsch–Gordan coefficient

34.1.1 $$\left(j_1\, m_1\, j_2\, m_2 \,|\, j_1\, j_2\, j_3\, m_3\right) = (-1)^{j_1 - j_2 + m_3}(2j_3+1)^{\frac{1}{2}}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix};$$

Gaunt coefficients in terms of Clebsch-Gordan coefficients (Pg. 139 of your textbook)

Substituting this back into Eq. (8.35), we have[1]

$$\int Y_l^m(\theta,\phi)^* Y_{l_1}^{m_1}(\theta,\phi) Y_{l_2}^{m_2}(\theta,\phi)\, d\Omega = \langle lm | l_1 l_2; m_1 m_2 \rangle \langle l_1 l_2; 00 | l0 \rangle \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}}. \quad (8.37)$$

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[1] Note that the matrix element $\langle lm | l_1 l_2; m_1 m_2 \rangle$ is often written as $\langle l_1 l_2; m_1 m_2 | lm \rangle$ in this expression. This is permissible since it is real.

Summary of results for dipole transition matrix elements --

$$\left\langle f^0 \left| \tilde{H}^1 \right| I^0 \right\rangle = \left\langle f^0 \left| -e\mathbf{F}\cdot\mathbf{r} \right| I^0 \right\rangle \propto \int d\Omega \; Y^*_{l_f m_f}(\theta,\phi) Y_{1m}(\theta,\phi) Y_{l_i m_i}(\theta,\phi)$$

$$\left\langle f^0 \right| = R_f(r) Y^*_{l_f m_f}(\theta,\phi) \qquad \left| I^0 \right\rangle = R_i(r) Y_{l_i m_i}(\theta,\phi)$$

$$\Rightarrow l_f = l_i \pm 1 \quad \text{and} \quad m_f = m_i + m$$

Depends on orientation of sample and polarization of EM field

Example -- Is the following transition between states of a H-like ion an "allowed" dipole transition?

$$\left| I^0 \right\rangle = \left| n_i l_i m_i \right\rangle = \left| 520 \right\rangle$$

$$\left| f^0 \right\rangle = \left| n_f l_f m_f \right\rangle = \left| 621 \right\rangle$$

(A) yes (B) no

Further abstraction of matrix element analysis using Group Theory

$$\text{Consider}\quad \left\langle f^0 \middle| O \middle| I^0 \right\rangle = \int d^3r \Psi^*_f(\mathbf{r}) O(\mathbf{r}) \Psi_i(\mathbf{r})$$

We want to find out which combinations give non-trivial results

Group theory enables the determination of the "distilled essence" of the initial and final states and of the operator to determine which transitions are non-trivial

$$\langle \Psi_1 | O | \Psi_2 \rangle = \int d^3r \Psi_1^*(\mathbf{r}) O \Psi_2(\mathbf{r})$$

$$= 0 \text{ if } \sum_R \left(\Gamma^i(R)\right)^* \Gamma^j(R) \Gamma^k(R) = 0$$

$$\text{or} \quad \sum_{\mathcal{C}} N_{\mathcal{C}} \left(\chi^i(\mathcal{C})\right)^* \chi^j(\mathcal{C}) \chi^k(\mathcal{C}) = 0$$

Initial state — Operator — Final state

***R* here represents symmetry rotations* of the system**

$\mathcal{C}$ represents "classes" of rotations of the system

***This can include the continuum of angles or discrete angles.**

Example of the use of a character table for the case of discrete angles

	E	A,B,C	D,F
χ^1	1	1	1
χ^2	1	-1	1
χ^3	2	0	-1

$\mathcal{C}$

Suppose $O \Rightarrow \chi^2$

Non-trivial matrix elements:

Initial state	$\Rightarrow$	Final state
χ^1	$\Rightarrow$	χ^2
χ^2	$\Rightarrow$	χ^1
χ^3	$\Rightarrow$	χ^3

For the spherical coordinates, we have used a particular coordinate system, standardized to the orientation of the z-axis. What happens if we want to use another orientation?

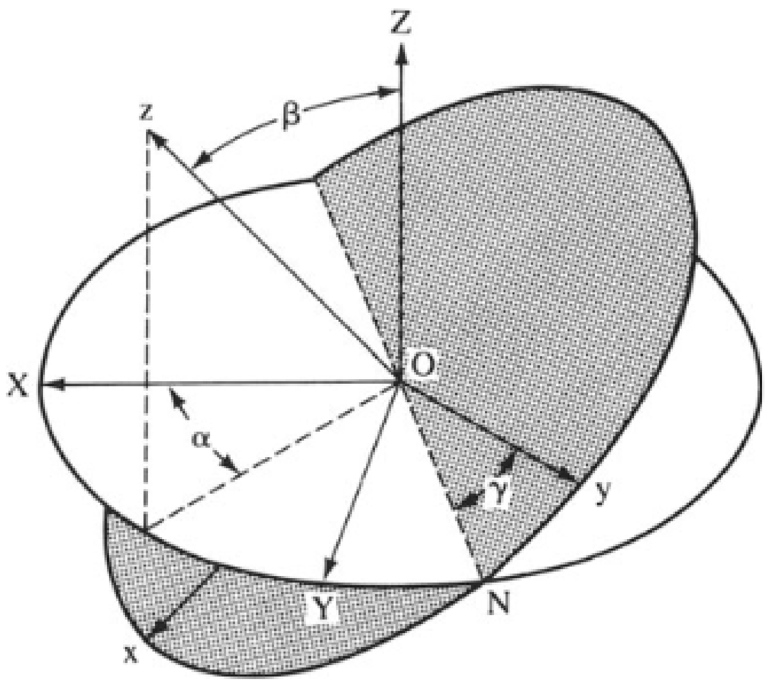

FIGURE A.1. Rotations used in the definition of the Euler angles.

Any rotation can be described by at most 3 successive rotations by α, β, and γ.

Note that, in Chap. 6, the notion of the rotation operator for angular moment L is presented as

A rotation by an arbitrary amount about an arbitrary axis $\hat{r}$ is then given by

$$R\left(\mathcal{R}\left(\hat{\mathbf{r}},\theta\right)\right)=\exp\left(-i\theta\hat{\mathbf{r}}\cdot\mathbf{L}/\hbar\right). \tag{6.44}$$

The angular momentum operators **L** do *not* commute with each other, which you can deduce directly from Eq. (6.43), or by noting that rotations around different axes do not commute.

More generally, it follows that the rotation operator for total angular momentum **J** is given by $R(\mathscr{R}(\hat{\mathbf{r}},\theta))=\exp(-i\theta\hat{\mathbf{r}}\cdot\mathbf{J}/\hbar)$

Even more generally, three successive Euler angle rotations is represented by:

$$R(\mathscr{R}(\hat{\mathbf{r}}_\alpha,\alpha))R(\mathscr{R}(\hat{\mathbf{r}}_\beta,\beta))R(\mathscr{R}(\hat{\mathbf{r}}_\gamma,\gamma))=\exp(-i\alpha\mathbf{J}_z/\hbar)\exp(-i\beta\mathbf{J}_y/\hbar)\exp(-i\gamma\mathbf{J}_z/\hbar)$$

What are the effects of rotation?

Typically, we are interested in the effects of rotation on the eigenstates of total angular momentum: $\left| jm \right\rangle$, where $\mathbf{J}^2 \left| jm \right\rangle = \hbar^2 j(j+1) \left| jm \right\rangle$ and $\mathbf{J}_z \left| jm \right\rangle = \hbar m \left| jm \right\rangle$

In general $R(\mathscr{R}(\hat{\mathbf{r}},\theta)) \left| jm \right\rangle = \sum_{m'=-j}^{j} \left\langle jm \right| R(\mathscr{R}(\hat{\mathbf{r}},\theta)) \left| jm' \right\rangle \left| jm' \right\rangle$

Note that $\left\langle jm \right| \exp(-i\theta J_z / \hbar) \left| jm' \right\rangle = \exp(-im\theta)\delta_{m,m'}$

$\Rightarrow \left\langle jm \right| \exp(-i\alpha J_z / \hbar) \exp(-i\beta J_y / \hbar) \exp(-i\gamma J_z / \hbar) \left| jm' \right\rangle = e^{-im\alpha} d^{j}_{m,m'}(\beta) e^{-im'\gamma}$

According to Eugene Wigner --

$$d^{j}_{m,m'}(\beta) = \sqrt{(j+m)!(j-m)!(j+m')!(j-m')!} \sum_{\mu} \frac{(-1)^{\mu} \left(\cos\left(\frac{\beta}{2}\right)\right)^{2j+m'-m-2\mu} \left(-\sin\left(\frac{\beta}{2}\right)\right)^{m-m'+2\mu}}{\mu!(j-m-\mu)!(j+m'-\mu)!(\mu+m-m')!}$$

For example *j=1/2*:

$$d^{1/2}(\beta)=\begin{pmatrix}\cos(\beta/2) & -\sin(\beta/2)\\ \sin(\beta/2) & \cos(\beta/2)\end{pmatrix}$$