PHY662, Spring 2004
Outline for Tues. Feb. 3, 2004
NMR, MRI, C-G

3rd February 2004

1 Miscellaneous

1. Homework #4 handed out.
2. Note Exam on Feb. 12 - I will hand out review information on Thursday Feb. 5.
3. Questions about HWK #3?
4. Colloquium today - quantum computing. *Very relevant*. Hand out abstract - discuss qubit, superposition, entanglement. [If interested, see also http://arxiv.org/abs/cond-mat/0305461 by Mooij group.]

2 NMR, MRI

NMR: Consider the H-atom, which is *essentially* a proton, immersed in a relatively strong (few Tesla) magnetic field. Expose the atom to a $\frac{\pi}{2}$-pulse. Then $\langle\vec{\mu}\rangle$ rotates at frequency γB_0. This rotating magnetic dipole *radiates energy* (or creates an oscillating electric field, due to the rotating magnetic moment, in a coil). With enough rotating protons, you can pick up a signal. Note that this signal is safe as it is low energy, radio frequency (RF, 10's of MHz). This radiation/emf provides the basis of a method to detect atoms and the effects of their chemical environment (homework problem #3, set #3). People can even reconstruct the structure of proteins!

MRI: One gets chemical information, in a somewhat different fashion, but more importantly, one can get the spatial location of different types of tissue, where the characteristics of the relaxation of the radiation varies.

The tricky part is how to encode spatial information at the sub-mm scale in the long wavelength (meters) radio signal that the rotating protons generate.

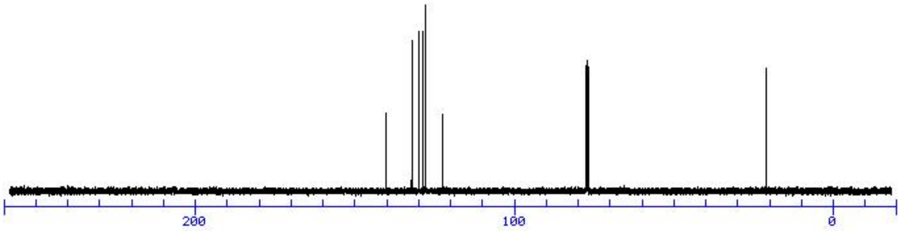


Figure 1: NMR spectrum, showing the chemical shifts of the protons sitting in distinct parts of a molecule. This “fingerprint” is a plot of intensity of signal vs. frequency for C_7H_7Br from http://www.chem.ucla.edu/cgi-bin/webspectra.cgi?Problem=bp15&Type=C.

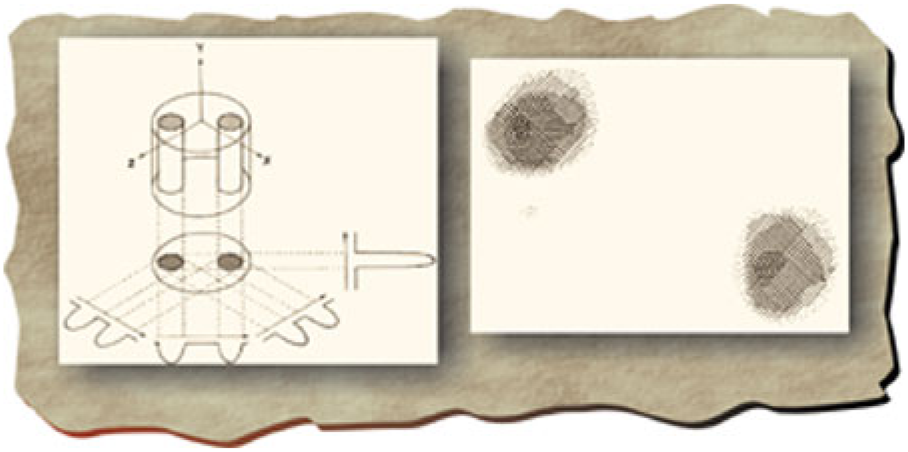
2.1 MRI - One dimension (1D) - frequency encoding

The signal (picked up in a detection coil) from the excited protons has a frequency that depends on B_0. So by making B_0 depend on, say, the x-position, ***after*** applying a $\frac{\pi}{2}$-pulse, one gets a signal composed of different frequencies, with the magnitude of the signal at a particular frequency dependent on the magnitude of excited protons at a given location. The spatial information is encoded in the frequency. Something like

$$S(t) \sim \int d\omega\, S(\omega) \sim \int d\omega\, n(x)\,,$$

where S is the signal in time or frequency space and $n(x)$ is the total density of protons in the plane defined by x.

Here is an early MRI image from 1973 that helped win a Nobel prize in 2003, based upon frequency encoding. Paul Lauterbur used an NMR machine with controllable linear field gradients to measure the projection of the density of water along four directions. These four projections, each using frequency encoding, were combined to estimate the location of the water tubes.



[From Physics Today, December 2003 - excerpted from *Nature*, 1973].

2.2 MRI - Slice selection

Before applying the gradient in the $\hat{x}$-direction, you can select a *slice* to excite. This can be done by applying a $\hat{z}$-gradient in the magnetic field so that B_0 depends on z. Then the resonance condition $\omega = \omega_0$ is satisfied only near a selected z. The $\frac{\pi}{2}$-pulse only excites a *2D layer* of protons, the "slice". An x-gradient in B_0 can then be applied to obtain information along one axis of the slice.

2.3 MRI - 3D imaging - phase encoding

To obtaine 3D information, one combines (i) slice selection using a $\hat{z}$-gradient and a $\frac{\pi}{2}$-pulse followed by (ii) "phase encoding" and then (iii) frequency encoding. To implement phase encoding, a gradient in B_0 along a third direction (y) is applied for a short time after the $\frac{\pi}{2}$-pulse. During the application of this gradient, the spins that are precessing in the xy plane rotate at a rate that is linear in their y position. This leads to y-dependent phase differences in the emf generated by a volume element, which can be detected by having two detection coils. After many slice selections, with repetitions of $\frac{\pi}{2}$-pulses and applied field gradients, one can reconstruct the characteristics of volume elements in 3D space. The field gradients are changed at frequencies of 100's of Hz and the magnetic coils move each time they turn on, so lots of noise is made.

There are *many* other tricks, like spin echo, etc., that get rather clever, but quite technical. The results are incredibly impressive, though, and even allow for real-time imaging of such things beating hearts and flowing chemical activity in the brain, as well as the usual static 3D pictures.

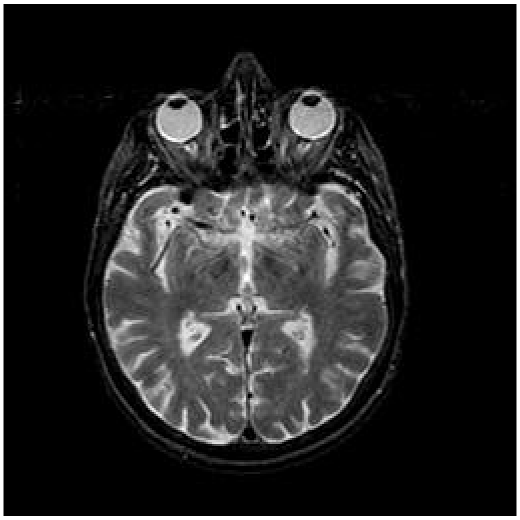


Figure 2: MRI image of a brain from The Whole Brain Atalas at www.med.harvard.edu. The image is a T_2-image, which plots, in space, how quickly the phase (xy-coherence) decays after a $\frac{\pi}{2}$-pulse.

3 Addition of angular momentum and Clebsch-Gordon coefficients

Adding together angular momenta is a specific case of a general problem. This general problem is understanding combinations representations of a given symmetry. Representation theory studies how group operations can be expressed using linear operators (matrices). [Here, we will use “representation” to mean both the representation for the symmetry group operators (rotation matrices) and for the generators of the rotations (J_x, J_y, J_z).] An irreducible representation of a symmetry is one that can not be broken down into subrepresentations. For linear matrices, this means that the operators cannot be transformed to a block-diagonal form.

General question: When you take the *direct product* of two irreducible representations, how can you decompose this product into a *direct sum* of irreducible representations?

Specific example: If you consider two spin-1/2 particles, what values can their total spin have and what is the amplitude to be in each of these total-spin states?

Clebsch-Gordon coefficients are used not just for combining angular momenta, but also for isospin (another $SU(2)$ group), $SU(3)$ in particle physics, etc. Clebsch-Gordon coefficients give ratios, for example, between rates of possible processes.

When adding angular momenta, representations of $SU(2)$, we are asking: what are the possible total angular momenta states and how are they related to the component states? [See p. 331 in Shankar for discussion of irreducible representations.]

3.1 Why add together angular momenta?

Sample motivations:

- An electron in an atom has total angular momentum given by the sum of spin and orbital angular momentum. It can be that this total is conserved, though spin and orbital are not, separately. So the state of the electron may be given by j, not l and s. But you might measure l_z or s_z. To find out the probability of measuring a particular value of s_z, you need to be able to relate the total to the parts.
- When you combine two particles together, you add their angular momenta. Or when a particle decays into two other particles, you split the angular momentum between the two particles (and their relative angular momentum). So you need to know the possible combinations and their probabilities.
- Composite particles, like Cooper pairs in superconductors, nuclei, or particles composed of quarks, have total angular momentum given by summing the parts and their orbital motion.

3.2 Combining representations

Let a representation of a symmetry be given by a set of matrices. If the matrices can be simultaneously written in block-diagonal form, the representation is decomposed into sub-representations. That is, the vector space operated on by the sub-representations are not mixed together by the symmetry operations.

3.3 Review of effects of raising and lowering operators

[This material is also presented in Sec. 12.5 in Shankar, p. 321 and following.]

A sample question for *one spin* is: how is $J_-|j,m\rangle$ related to $|j,m-1\rangle$? (Here $|j,m\rangle$ is the state with $J^2 = j(j+1)\hbar^2$ and an eigenstate of J_z, with eigenvalue $m\hbar$.) Note that $J_zJ_- = J_z(J_x - iJ_y) = J_xJ_z + i\hbar J_y - iJ_yJ_z - i\hbar J_x = J_-(J_z - \hbar)$, so $J_z(J_-|j,m\rangle) = (m-1)\hbar J_-|j,m\rangle$, so J_- does lower the eigenvalue of J_z by $\hbar$.

To find the proportionality coefficient between $J_-|j,m\rangle$ and $|j,m-1\rangle$, note $J_-^\dagger = J_+$ and $J_+J_- = (J_x + iJ_y)(J_x - iJ_y) = J_x^2 + J_y^2 - i(J_xJ_y - J_yJ_x) = J^2 - J_z^2 + \hbar J_z$. So, if $|\psi\rangle = J_-|j,m\rangle$,

$$\begin{aligned}
\langle\psi|\psi\rangle &= \langle j,m|J_-J_+|j,m\rangle \\
&= \langle j,m|(J^2 - J_z^2 + \hbar J_z|j,m \\
rangle \\
&= [j(j+1) - m^2 + m]\hbar^2 \,.
\end{aligned}$$

This gives $J_-|j,m\rangle = e^{i\theta(j,m)}\sqrt{j(j+1) - m(m-1)}|j,m-1\rangle$. By convention, set $\theta(j,m) = 0$, so

$$\begin{aligned}
J_-|j,m\rangle &= \sqrt{j(j+1) - m(m-1)}|j,m-1\rangle \\
&= \sqrt{(j+m)(j-m+1)}|j,m-1\rangle
\end{aligned}$$

and, similarly,

$$\begin{aligned} J_+|j,m\rangle &= \sqrt{j(j+1)-m(m+1)}|j,m+1\rangle \\ &= \sqrt{(j-m)(j+m+1)}|j,m+1\rangle \,. \end{aligned}$$

(Note there are two standard ways to write the coefficient.)

3.4 Combining particles

Take particles with spin. Let $\vec{J}_1$ and $\vec{J}_2$ be the operators that rotate particles 1 and 2, respectively. Define total spin $\vec{J} = \vec{J}_1 + \vec{J}_2$ and total $J_z = J_{1,z} + J_{2,z}$ operators. [More completely, this notation is understood to mean $\vec{J} = \vec{J}_1 I_2 + I_1 \vec{J}_2$, e.g., where $I_{1,2}$ are the identity matrices for particles 1 and 2.] Note that $J_{1,i}$ and $J_{2,j}$ commute for all $i,j = x,y,z$ as the operators work on the particles separately. Hence, $[J_i, J_j] = i\epsilon_{ijk}J_k$, so the total angular momentum components obeys the same algebra as any rotation operator. So what representation does the total angular momentum together follow???

Phrased another way, this question says “how can we relate states of given individual angular momenta and z-components, $|j_1, m_1; j_2, m_2\rangle$ to total angular momenta states $|j, m; j_1, j_2\rangle$?”

First note that, in general, $J_z|j_1, m_1; j_2, m_2\rangle = (m_1 + m_2)|j_1, m_1; j_2, m_2\rangle$, so J_z, the total z-component, is diagonal in the $|j_1, m_1; j_2, m_2\rangle$ basis.

3.5 Example: Two spin-1/2 particles

This is the most important case to know and is also the simplest! Answer: $\frac{1}{2}\otimes\frac{1}{2} = 1\otimes 0$.

3.5.1 Approach #1 (as in Shankar)

Each spin-1/2 particle can have spin up or down: $+$,- . So let’s write the states for two particles as $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$. Then

$$S_z^{\rm tot} = S_{1,z} + S_{2,z} = \hbar \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

and

$$S^2 = (\vec{S}_1^2 + \vec{S}_2^2) = S_1^2 + S_2^2 + 2\vec{S}_1\cdot\vec{S}_2 = S_1^2 + S_2^2 + S_{1,+}S_{2,-} + S_{1,-}S_{2,+} = \hbar^2 \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

Note that

$$S_+ = S_{1,+}I_2 + I_1 S_{2,+} = \hbar \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \hbar \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Now the central part of that matrix can be diagonalized from $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ to $\begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$. The eigenvectors are $\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$ and $\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$. This means there is a transformation so that

$$S_z = \hbar \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \; ; \; S^2 = \hbar^2 \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} .$$

This shows there are 3 spin-1 states and 1 spin-0 state here. Rearranging the rows and columns to reflect the matrix elements between $|++\rangle$, $\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$, $|--\rangle$ and $\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$ gives

$$S_z = \hbar \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \; ; \; S^2 = \hbar \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} ,$$

and carrying out the details of the transformation $S_+ \rightarrow U S_+ U^\dagger$ with

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

gives

$$S_+ = S_{1,+}I_2 + I_1 S_{2,+} = \hbar \begin{bmatrix} 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} ,$$

which in the upper left 3×3 block raises the triplet states. A similar result is found for S_-,

$$U S\_ U^\dagger \;=\; \hbar \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

$$
\begin{aligned}
& \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \\
= \; & \hbar \begin{bmatrix} 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} .
\end{aligned}
$$

Now S_x and S_y are combinations of S_+ and S_-, so all S_i components of $\vec{S}$ are of the block-diagonal form

$$
\begin{bmatrix} t & t & t & 0 \\ t & t & t & 0 \\ t & t & t & 0 \\ 0 & 0 & 0 & s \end{bmatrix} ,
$$

where t are the triplet (spin-1) matrix elements for spin and s is always 0 (singlet representation). This shows in detail how the 2 spin-1/2 representations combine to form 2 subrepresentations.

3.5.2 Approach #2 (preview of the general procedure)

With two spin-1/2 particles, there are 4 states in the $|s_1, m_1; s_2, m_2\rangle$ basis, given just by $m_1, m_2 = \pm\frac{1}{2}, \pm\frac{1}{2}$. There is only one state with $S_z = 1$: $|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle$. This implies that we must have an integer subrepresentation buried in $\frac{1}{2} \otimes \frac{1}{2}$. As there is no higher S_z, the J for this representation must be 1, so

$$
|1,1\rangle = |\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle .
$$

By the same argument,

$$
|1,-1\rangle = |\frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle .
$$

To find the other state that makes up the $J = 1$ representation, apply J_-^{tot} to $|1,1\rangle$:

$$
\begin{aligned}
J_-|1,1\rangle &= \sqrt{2-0}\hbar|1,0 \\
rangle & \\
&= (J_-^1 + J_-^2)|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle \\
&= \hbar|\frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + \hbar|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle .
\end{aligned}
$$

The state $\frac{1}{\sqrt{2}}(\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle + |\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle) = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$ is the $m = 0$ state of the $J = 1$ representation. This triplet of states, $|++\rangle$, $\frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$, $|--\rangle$ makes up a representation of $J = 1$.

What is remaining? One more state. This must be a $J = 0$ singlet, orthogonal to $|1, 0\rangle$. This gives $\frac{1}{\sqrt{2}}(| + -\rangle + | - +\rangle)$.

This combination of a triplet and a singlet resulting from two spin-1/2 particles and the *symmetry* of these states is a primary example in quantum mechanics.

3.6 General case: Clebsch-Gordon coefficients

We wish to write the state $|j, m; j_1 j_2\rangle$ as a sum over states $|j_1, m_1; j_2, m_2\rangle$. There is a well defined procedure for doing this:

1. Write the maximal j_z^{tot} state as $|j_1, j_1; j_2, j_2\rangle$. This is $|j, j; j_1, j_2\rangle$.
2. Find all other states with total angular momentum j by repeatedly applying the J_-^{tot} operator.
3. Find the states with total angular momentum $j-1$ by finding the state orthogonal to $|j, j-1; j_1 j_2\rangle$ and then again repeatedly applying J_-^{tot}.
4. Repeat step 3 for the $j-2$ states, etc., where $|j-k, j-k\rangle$ is the state orthogonal to all of $|j, j-k\rangle, |j-1, j-k\rangle, \ldots, |j-k+1, j-k\rangle$.