Lecture 9: Physics 212

Monday, February 22, 1999
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1 Reading

For today's and Thursday's lectures, please concentrate on understanding the handouts on NMR and on Section 4.4.3 of Griffiths (how to add angular momenta vectors in quantum mechanics).

Further discussion of the quantum mechanics of NMR is available on pages 443-450 in the book "Quantum Mechanics, Vol. I" by Claude Cohen-Tannoudji et al (on reserve in the Math-Physics library). A more complete treatment is available in the classic, "Principles of Magnetic Resonance, 2nd Edition" by Charles Slichter, which is likely too much information unless you become especially interested in magnetic resonance.

2 Appointment for Course Project

During the next two weeks, I would like to meet with each one of you one-on-one to help you identify a suitable topic for the course project. Please send me e-mail by Thursday of this week (2/25/99) to set up a 15-minute appointment no later than March 5.

As mentioned earlier in the semester, the project will consist of a 1/2-hour oral presentation to the class in the style of an American Physical Society (APS) talk using overhead transparencies, together with a 15-page double-space project report (corresponding to about 3 journal pages) done in the style of an article submitted to Physical Review. We will spend a lecture in March discussing how to prepare such a talk and article using software tools widely used by many scientists: LaTeX, bibtex, and the APS REVTEX macros. We will also discuss how to present a good scientific talk and how to write a clear readable scientific paper.

3 Thought Questions

1. Here is a challenge for which there are just enough clues in Griffiths for you to solve: with a Stern-Gerlach device oriented in the vertical direction, one can create beams of up or down-spin states (assuming an input of neutral spin-1/2 atoms, like Ag atoms). If we follow Griffiths and denote these two states by $\chi_\pm$, how could you use a Stern-Gerlach device (or several such devices) to create a beam that is *an arbitrary specified superposition of up and down states*, say

$$\chi = a\chi_+ + b\chi_-, \tag{1}$$

   where a and b are specified arbitrary complex coefficients satisfying $|a|^2 + |b|^2 = 1$? Hint: Equation [4.155] on page 160.

   Solving this problem should convince you that one can really physically prepare arbitrary superpositions of quantum states with which one can then carry out various experiments. As a future challenge for ourselves, let's see if we can figure out how to prepare a beam of particles experimentally that is an arbitrary superposition of energy states, e.g., a superposition of the 1s ground state and 2s excited state of the hydrogen atom, $|\psi\rangle = a|1\text{s}\rangle + b|2\text{s}\rangle$.

4 Concepts to Understand

1. You should appreciate that the average angular momentum vector $\langle\psi|\mathbf{L}|\psi\rangle$ often behaves like a classical vector when a magnetic field is turned on; this is helpful when trying to anticipate the behavior of a quantum mechanical system. E.g., for a bound particle moving in a potential $V(\mathbf{r})$, the time derivative of the average angular momentum is given by the average of the quantum mechanical torque operator $\mathbf{N}$ as follows:

$$\frac{d}{dt}\langle\mathbf{L}\rangle = \langle\mathbf{N}\rangle, \tag{2}$$

where the torque operator is given by:

$$\mathbf{N} = \mathbf{r} \times (-\nabla V). \tag{3}$$

The quantity $-\nabla V$ is classically just the force acting on a particle.

Let me show you how one would start to derive Eq. (2). One of your midterm questions from Physics 211 asked you to derive the following formula for the time derivative of a general operator $Q(t)$:

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[H,Q]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle, \tag{4}$$

where H is the Hamiltonian of the system. (This is Eq. [3.148] on page 113 of the Griffiths book). In this formula, let's choose

$$Q = \mathbf{L} = \mathbf{r} \times \mathbf{p}. \tag{5}$$

This is time independent so $\partial_t Q = 0$ and Eq. (4) tells us that

$$\frac{d}{dt}\langle\mathbf{L}\rangle = \frac{i}{\hbar}\langle[H,\mathbf{L}]\rangle; \tag{6}$$

the time dependence of the average angular momentum is determined by the commutator of the Hamiltonian $H = \mathbf{P}^2/2m + V$ with $\mathbf{L}$.

Let's look at the x-component of the vector relation Eq. (6), since we can deduce the other components by an appropriate cyclic permutations of symbols. We have:

$$[H, L_x] = [H, yp_z - zp_y] = y[V, p_z] - z[V, p_y], \tag{7}$$

using $[A, BC] = [A, B]C + B[A, C]$, $[p_y^2, y] = -2i\hbar p_y$, and $[\mathbf{p}^2, p_i] = 0$ for $i = x, y, z$. But in an earlier homework exercise, you showed that

$$[f(x), p_x] = i\hbar\partial_x f, \tag{8}$$

and generalizing this to several variables we see that:

$$[V, p_z] = i\hbar\partial_z V, \qquad [V, p_y] = i\hbar\partial_y V, \tag{9}$$

and so:

$$[H, L_x] = y[V, p_z] - z[V, p_y] = i\hbar\left(y\partial_z V - z\partial_y V\right) = i\hbar\big[\mathbf{r} \times (-\nabla V)\big]_x, \tag{10}$$

which shows that:

$$\frac{d}{dt}\langle L_x\rangle = \langle[\mathbf{r} \times (-\nabla V)]_x\rangle, \tag{11}$$

and so Eq. (2) follows.

A neat consequence of Eq. (2) is a statement of conservation of angular momentum in the absence of an external torque. In particular, if one has a central potential that is a function of radius only, $V(x, y, z) = V(r)$, then ∇V is parallel to $\mathbf{r}$, the average $\langle\mathbf{N}\rangle$ of the torque operator vanishes, and we have $d\langle\mathbf{L}\rangle/\mathbf{dt} = \mathbf{0}$.

Eq. (2) also tells us that the average of a spin vector $\langle\mathbf{S}\rangle$ precesses in a constant homogeneous magnetic field $\mathbf{B}$ since a magnetic moment $\mu = \gamma\mathbf{S}$ feels a torque $\mathbf{N} = \mu \times \mathbf{B}$. To get a sense of the order of magnitude, the angular frequency of rotation of a spin 1/2 electron in a strong magnetic field of 1 Tesla (10^4 Gauss) would be:

$$\omega = \gamma B_0 = \frac{e}{cm_e} 10^4 = \frac{4.8 \times 10^{-10}}{(3 \times 10^{10})(9.1 \times 10^{-28})} 10^4 \approx 2 \times 10^{11}\,\mathrm{sec}^{-1}, \tag{12}$$

i.e., a frequency in the 100 GHz range. The magnetic moment of a nucleus would be down by a factor of about 2000 and so the Larmor frequency in the same field would be about 100 MHz.

2. Nuclear magnetic resonance or NMR is an ingenious and valuable way to explore the magnetic properties of atomic nuclei. One way to think about it is to first consider that a nucleus with a magnetic moment with spin number s has $2s+1$ energy levels in the presence of a magnetic field, representing the possible eigenstates of S_z. One could then imagine photons being absorbed or emitted with energies corresponding to the differences in energy levels $\triangle E = -\gamma\hbar B_0 \triangle m$ and a study of these photons would give information about the magnetic moment. (Conservation of angular momentum requires that $\triangle m = \pm 1$ when a photon is emitted or absorbed so, in fact, transitions can only occur between adjacent levels.) In the 1950's, Edward Purcell and independently Felix Bloch hit upon the idea (and demonstrated the idea in the laboratory) of using an oscillatory magnetic field, perpendicular to a given large magnetic field $B_0\mathbf{z}$, to stimulate transitions between these levels and so measure the tiny and otherwise inaccessible nuclear magnetic moments.

   A humorous note: NMR is used heavily in the medical community but has been renamed "magnetic resonance" because many patients were scared by the "nuclear" part of this name, mistakingly thinking that radioactive materials were involved.

3. The quantum dynamics of a spin 1/2 particle in a field of the form

$$\mathbf{B} = (b\cos(\omega t), b\sin(\omega t), B_0), \qquad B_0 \gg b, \tag{13}$$

   provides the foundation for NMR and we will solve this in lecture, following the handout from Park's 3rd edition on quantum mechanics. A key conclusion from this analysis is that a beam of up-spin particles (say the output from a Stern-Gerlach device) subjected to the above magnetic field will be partially converted to a mixture of spin-up and spin-down particles, with the fraction of the spin-down beam varying in time according to the relation

$$|\chi_-|^2 = \left(\frac{\beta}{\triangle}\right)^2 \sin^2(\triangle t), \tag{14}$$

   where

$$\beta = \frac{1}{2}\gamma b, \qquad \triangle = \left(\frac{1}{4}(\omega-\omega_0)^2 + \beta^2\right)^{1/2}, \qquad \omega_0 = \text{Larmor freq} = \gamma B. \tag{15}$$

   Since the amplitude of the oscillations in Eq. (14) can be written as:

$$|\chi_-|_{\max} = \frac{\beta}{\triangle} = \frac{1}{\sqrt{1+\left(\frac{\omega-\omega_0}{\gamma b}\right)^2}}, \tag{16}$$

   we see that there is indeed a resonance effect: as the frequency ω of the horizontal magnetic field is swept through resonance with the Larmor frequency ω_0, the probability of spin-up particles converting to spin-down particles attains the value of certainty periodically in time.

   This result was tested experimentally in a wonderfully clever apparatus invented by Isadore Rabi, an experimental physicist at Columbia University who later won the Physics Nobel Prize for the incredible precisions that his insight permitted. The idea is to set up an atomic beam apparatus consisting of a Stern-Gerlach device with dB_z/dz positive, followed by a narrow horizontal slit, followed by magnets that impose the field Eq. (13), then followed by a Stern-Gerlach device that is flipped upside down, followed by another narrow horizontal slit, followed finally by a detector that measures the magnitude of an atom current (e.g., by ionizing the atoms and measuring the resulting current of released electrons). The first Stern-Gerlach device splits a spin-1/2 beam into positive and negative magnetic moment components (of angular momentum $\mp\hbar/2$ respectively since electrons with their negative charge have a magnetic moment vector opposite to their angular momentum vector). Particles of both spin-up and spin-down are then passed through the oscillating magnetic field Eq. (13) where some of them are converted to the opposite spin. When these flipped particles enter the upside-down Stern-Gerlach device, they are further accelerated and can't make the slit at the far end. So one sees a sharp drop in final atom current when $\omega \approx \omega_0$ and one can measure with enormous precision the gyromagnetic ratio of particles in the beam.

4. The Rabi experiment is our first example of a quantum mechanical problem that involves a *time dependent* Hamiltonian. The conclusions generalize: a time-dependent Hamiltonian $H = H_0 + H'(t)$ defined by a weak time-dependent perturbation H' of a time-independent Hamiltonian H_0 can be understood as the absorption or emission of photons between the levels defined by H_0 by itself. The more general theory is discussed in Chapter 9 of Griffiths, where the climactic insight is something called "Fermi's golden rule", which tells us how to calculate the probability of transition per unit time from some initial stationary state $|\psi_i\rangle$ to some other state $|\psi_f\rangle$ because of some small time-dependent perturbation H' in the Hamiltonian. Just to give you something to ponder until we derive this later in the semester, the golden rule is mathematically stated as follows:

$$P_{i\to f}(t) = \frac{2\pi}{\hbar}|\langle\psi_f|H'|\psi_i\rangle|^2\delta(E_i - E_f - \hbar\omega). \tag{17}$$

   The probability of transition is proportional to the magnitude squared of the amplitude to go from state i to state f via the time-dependent perturbation H'; it is symmetric between i and f. The delta function makes sure that energy is conserved in the transition, where ω is the frequency of the photon absorbed or emitted during the transition. For the Rabi experiment, $H' = -\mu \cdot (b\cos(\omega t), b\sin(\omega t), 0)$ and I'll let you test the golden rule by calculating the appropriate amplitude.

5. If you have N spin-1/2 particles in a volume V sitting in an external magnetic field $\mathbf{B} = B_0\hat{\mathbf{z}}$, what is the magnetic moment of the entire volume? Actually, the magnetic moment will be proportional to the number of spins and so the more interesting question is what is the *density* of magnetic moments which is called the *magnetization* $\mathbf{M}$? The answer turns out to depend on the temperature T of the particles since, if the temperature is sufficiently high, collisions will keep knocking the spins into different directions and they will no longer be aligned with the magnetic field. If the temperature is sufficiently low, the spins all align and one gets a magnetic moment proportional to the actual magnitude of the atomic spins.

   You have hopefully seen in a previous statistical mechanics course that, for a system of particles in thermal equilibrium at temperature $T > 0$, the probability of observing the system with total energy E is proportional to $\exp(-E/kT)$ where k is the Boltzmann constant and T is the temperature measured in degrees Kelvin. (This is called a "Gibbs' probability" after the American scientist Gibbs' who was the Einstein of thermodynamics and statistical physics.) For a single spin-1/2 particle, there are two possible energy values in an external magnetic field, $E_\pm = \pm\gamma\hbar B_0/2$, and a little work shows that the total magnetization is given by the formula:

$$M = N\mu_0 \tanh\left(\frac{\mu_0 B}{kT}\right), \tag{18}$$

   where $\mu_0 = g(e\hbar/4m_e)$ is the z-component of the magnetic moment of a spin-1/2 particle with charge e. For magnetic fields of a tesla or less and near room temperature, the ratio $\mu_0 B/kT$ is rather small (a few percent) and we can approximate $\tanh(x) \approx x$ in which case we get the approximate formula:

$$M \approx \frac{N\mu_0^2 B}{kT}, \qquad \text{for } \mu_0 B \ll kT, \tag{19}$$

   which predicts that the magnetization is proportional to the magnetic field strength (this defines the phenomenon of *paramagnetism*) and further, that the magnetization of a bunch of spins in an external field at finite temperature is proportional to the *square* of the individual spin's magnetic moment, i.e., it is substantially smaller than what one would expect based on a single isolated spin.