Problem Set 8: Rotations, spin & spinors Graduate Quantum I Physics 6572 James Sethna Due Friday Oct. 17 Last correction at December 22, 2014, 10:24 am

Potentially useful reading

Sakurai and Napolitano, sections 3.1-3.3 (rotations & SU(2)), 3.5-3.6, 3.8 (angular momentum), 4.1 (infinitesimal symmetries, degeneracy), 5.3 (fine structure) Schumacher & Westmoreland section 6.3 (4π rotations), chapter 12 (spin) Weinberg, sections 4.1-3 (rotations)

Arfkin, Weber, and Harris, Mathematical Methods for Physicists, chapter 17 (Group theory)

8.1 Fine and hyperfine structure: Hydrogen and angular momentum addition. (Angular Momentum) ③

Symmetries have powerful implications for energy eigenstates of composite systems. They are ordinarily the only cause for degenerate states, for example. Here we use rotational symmetry, and the corresponding angular-momentum addition laws, to derive the degeneracies of the hydrogen n = 2 states.

Including the spin $\frac{1}{2}$ of the electron and the spin $\frac{1}{2}$ of the proton, and the four n = 2 states of hydrogen, there are sixteen degenerate energy eigenstates in Schrödinger's solution for hydrogen with n = 2. In this exercise, we shall follow how these energy eigenstates split up when we include the 'fine splitting' and 'hyperfine splitting'. We shall not need to do any calculations with Hamiltonians; we shall just use the rotational symmetry of the Hamiltonian and angular momentum addition rules.

(a) What is the energy of the n = 2 state of hydrogen, ignoring spin, relativity, and the nuclear spin? (Include the fact that the proton and electron have spin $\frac{1}{2}$ in the degeneracy calculation, but ignore their effects on the energy for now.)

The 2s and 2p states in hydrogen both have n = 2, and are degenerate to this order. This degeneracy is not due to a straightforward symmetry of the Hamiltonian.¹ It is split by terms of order α^2 , where $\alpha = e^2/\hbar c \approx 1/137$ is the fine structure constant, representing the importance of relativity.

The relativistic correction to the kinetic energy splits the 2s and 2p states, but does not couple to the electron or proton spin.

(b) Including these kinetic energy terms, how do the sixteen original states split up in energy?

¹It's peculiar to the $1/\mathbf{r}$ potential energy law, and an associated conserved Lenz's vector. The hydrogen problem can be mapped in an obscure way to the four-dimensional harmonic oscillator: see S&N sect. 4.1.

The spin-orbit coupling, also of order α^2 , is proportional to $\mathbf{L} \cdot \mathbf{S}$, where \mathbf{L} is the angular momentum of the electron and \mathbf{S} is the spin of the electron. Because it is a dot product, it maintains rotational symmetry.

(c) Using angular momentum addition rules, discuss what happens to the twelve 2p orbitals after incorporating the spin-orbit coupling. What values of j are are allowed, where J = L + S? What are the degeneracies of the coupled states? (Hint: The different energy eigenstates with the same J are related by rotations. You should not need the form of the interaction to solve this part or the next.)

The splitting due to the spin-orbit interaction is called *fine structure*, and also arises in heavier atoms. For example, the yellow light from sodium vapor lamps is comprised of two nearby spectral lines, split by the spin-orbit interaction.²

For states with L > 0 the coupling to the nuclear spin I is approximately given by $\hat{A}\mathbf{I} \cdot \mathbf{J}$. This is called the *hyperfine* splitting; it is smaller than the fine structure splittings because the nucleus is heavy compared to the electron. Again, this interaction maintains rotational symmetry (as it must).

(d) For each of your degenerate families of 2p states in part (c) ignoring the hyperfine splitting, what are the allowed values of F = I + J? What degeneracies in the final eigenvalues do you expect?

8.2 Identical Spin-1 Addition. (Sakurai & Napolitano 7.3) \bigcirc

It is obvious that two nonidentical spin 1 particles with no orbital angular momenta (that is, s-states for both) can form j = 0, j = 1, and j = 2. Suppose, however, that the two particles are *identical*. What restrictions do we get?

8.3 A Peculiar Unitary Matrix. (Adapted from Sakurai & Napolitano 3.3)

Consider the 2×2 matrix defined by

$$U = (a_0 \mathbb{1} + i\boldsymbol{\sigma} \cdot \mathbf{a}) (a_0 \mathbb{1} - i\boldsymbol{\sigma} \cdot \mathbf{a})^{-1}$$

where a_0 is a real number and **a** is a three-dimensional vector with real components. (a) *Prove that U is unitary and unimodular.* (Hint: This can be done without writing out the components.)

(b) In general, a 2×2 unitary unimodular matrix represents a rotation in three dimensions. Find the axis and angle of rotation appropriate for U in terms of a_0 , a_1 , a_2 , and a_3 . (Hint: I first did it in Mathematica, and then figured out that one can find the answer by rotating the coordinate system until $\mathbf{a} \propto \hat{z}$.)

²Wikipedia also calls the 2s-2p splitting in hydrogen a fine structure effect, but I'm not sure that's standard. In heavier atoms, the energies of these orbitals (quasiparticle resonance energies, not eigenstates) are shifted primarily not due to relativity, but due to the effects of the other electrons.

8.4 Minus Signs in 2π Rotations. (Adapted from Gottfried and Yan 3.9) (3)

The goal is to design, in concept, an experiment that demonstrates that a particle of spin $\frac{1}{2}$ has double-valued wave functions. Consider a neutral particle with magnetic moment $\boldsymbol{\mu} = g\mathbf{s}$, where s is a spin of arbitrary magnitude, placed in a homogeneous and static magnetic field **B**. Assume that as in classical physics the Hamiltonian is $\mathcal{H} = -\boldsymbol{\mu} \cdot \mathbf{B}$. Show first that the time evolution of $\mathbf{s}(t)$ in the Heisenberg picture is a rotation about **B** through the angle $\theta = -gBt/\hbar$. Hence, an appropriate choice of Bt can produce a net rotation difference of 2π , which supposedly produces the factor ± 1 multiplying the wave function depending on whether s is integer or half-integer.³

Allow a spin-polarized monochromatic beam to strike a screen with two holes, beyond which there are identical magnetic fields, but of opposite sign. Study the interference pattern it produces, and show that a measurement of the intensity (i.e. no measurement of spin as such) for the cases $s = \frac{1}{2}$ and s = 1 leads to a confirmation of the different signature after a net rotation difference of 2π . In the case of cold neutrons with momentum corresponding to a wavelength of one Å, in a field of 100 Gauss, how long a path through the field is required to produce a rotation through 2π ? Experiments of this type have been done; see S.A. Werner et al., Phys. Rev. Lett. **35**, 1053 (1975); and A.G. Klein and G.I. Opat, Phys. Rev. Lett. **37**, 238 (1976).

8.5 Triangle Of Spinless Bosons. (Sakurai and Napolitano, problem 7.5, red version 6.4.) ②



Fig. 1 Triangle of spinless bosons

³Make sure you get the number of \hbar right! Use dimensional analysis. There are two conventions for the spin operator, $\mathbf{s} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$ and $\mathbf{s} = \begin{pmatrix} \frac{\hbar/2}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}$. In this notation, the factor $g = -1.930427\mu_N$, where the nuclear magneton $\mu_N = (e\hbar/2m_pc)$ in CGS units has units of erg/gm, and $\mu_N = (e\hbar/2m_p)$ in SI units has units of Joule/Tesla. Note that m_p is the proton mass, not the electron mass.

Three spin 0 particles are situated at the corners of an equilateral triangle (see the accompanying figure). Let us define the z-axis to go through the center and in the direction normal to the plane of the triangle. The whole system is free to rotate about the z-axis. Using statistics considerations, obtain restrictions on the magnetic quantum numbers corresponding to J_z .

8.6 Mystery: Properties of the group character table. (Group Reps) ③

In the week following this assignment, we shall learn about representations of finite groups. Group representation theory involves new conceptual ideas, new mathematical theorems, and some new calculational methods. Even knowing the ideas and the theorems, I find the calculational methods seem mysterious, almost magical. Let's try to introduce these tools first, to motivate the lectures to come. I am not pretending to introduce why we do these manipulations – this is an experiment, giving you the mechanics of the calculation before we explain the context in order to motivate your interest.

Consider the following table. It is an expanded version of the character table for the group representations of C_3v , the symmetry group of a triangle. But just treat it as a list of row vectors A_1 , A_2 , and E, along the six 'directions' labeled by the six symmetry group elements $g = e, r, r^2, v, rv$, and r^2v in the group G.

C_{3v}	е	r	r^2	V	r v	$r^2 v$
A_1	1	1	1	1	1	1
A_2	1	1	1	-1	-1	-1
E	2	-1	-1	0	0	0

Table 1: Expanded character table for C_{3v} . The group elements $g = e, r, \ldots$ label the columns; the representations $R = A_1, A_2, \ldots$ label the rows, and the entries are the characters $\chi_R(g)$.

(a) Orthogonality Show that the three character row vectors are orthogonal to one another. Show that the naive 'dot product' of a row vector with itself is equal to the number of group elements (called O(G).

Thus the three representations A_1 , A_2 , and E are orthonormal using the *inner product* given by the naive dot product divided by the order of the group:

$$\chi_1 * \chi_2 = (1/O(g)) \sum_{g \in G} \chi_1(g) \chi_2(g).$$
(1)

Group representations give one matrix R(g) for each abstract symmetry operation g. So rotation matrices form a representation of the rotation group. (Mathematicians carefully distinguish between the abstract multiplication table G for a group, and the implementation R(g) of that group in matrix form.) The *characters* of the group $\chi(g)$ are the traces of these matrices. (Much more about groups and characters will in lecture.)

For example, we can write a representation of the triangle symmetry group C_{3v} by thinking of how each symmetry operation permutes the three vertices of the triangle. Label the three vertices of the triangle by the three unit vectors. Let $R(g)_{ij}$ be one if vertex j shifts to vertex i under the symmetry operation g.

What triangle symmetry corresponds to the six group elements e, r, \ldots ? We always use e to represent the 'do-nothing' symmetry, so $R(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. The matrix r rotates the triangle 180°, so $R(r) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$. The matrix v flips the triangle around the first vertex, so $R(v) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$.

(b) What are the characters $\chi(e)$, $\chi(r)$, and $\chi(v)$?

We define the product of two symmetries (say rv) as performing the symmetry operations from left to right (so, flipping by v and then rotating by r).

(c) What is the matrix R(rv)? Do this two ways. Figure out how the symmetry rv permutes the vertices. Or use the property R(rv) = R(r)R(v); the matrices have the same multiplication table as the group. What is $\chi(rv)$? Is it the same as that of e, r, or v?

Notice in Table (1) that the column vectors labeled by r and r^2 are the same, while v, rv, and r^2v also share the same characters. This is generally true: the characters of two elements in the same conjugacy class are always the same. Use this to check your character for rv in section (c). [We will explain why this is true in lecture.] We put the two rotations r and r^2 into the conjugacy class C_3 , and we put the three reflections v, rv, and r^2v into the conjugacy class σ_v ; the identity e is put into the one-element class E. This allows us to make a more efficient character table (Table 2), where the number of elements in multiply-occupied conjugacy classes is included in the column heading (hence $3\sigma_v$, because there are three σ_v rotations). Now, to find the character of a representation, you only need to compute the trace of one element of each conjugacy classes but multiply by the multiplicity (number of elements in the class).

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Table 2: Traditional character table for C_{3v}

One of the main uses for character tables is for finding *decompositions* of representations into *irreducible* representations. This turns out to be related to Fourier transforms, to angular momentum addition rules, and to many other standard problems in mathematics and quantum mechanics. We shall leave what this means mysterious until lecture, but let us perform a decomposition of the representation R we have described in parts (b) and (c).

(d) What would the character row for our representation R look like in Table 2? Show that the inner product (eqn 1) of the representation with itself is an integer, but not one. Irreducible representations have norm one. Take the inner product of χ_R with the three irreducible representations, and show that they are integers. Any reducible representation can be decomposed into integer numbers of the irreducible representations.

I always find it surprising when my naive dot products work out to be multiples of the size of the group. In more complicated cases, it seems magical.

8.7 White dwarfs, neutron stars, and black holes. (Astrophysics, Quantum) ③

As the energy sources in large stars are consumed, and the temperature approaches zero, the final state is determined by the competition between gravity and the chemical or nuclear energy needed to compress the material.

A simplified model of ordinary stellar matter is a Fermi sea of non-interacting electrons, with enough nuclei to balance the charge. Let us model a white dwarf (or black dwarf, since we assume zero temperature) as a uniform density of He⁴ nuclei and a compensating uniform density of electrons.⁴ Assume Newtonian gravity. Assume the chemical energy is given solely by the energy of a gas of non-interacting electrons (filling the levels to the Fermi energy).

(a) Assuming non-relativistic electrons, calculate the energy of a sphere with N zerotemperature non-interacting electrons and radius R^{5} Calculate the Newtonian gravitational energy of a sphere of He⁴ nuclei of equal and opposite charge density. At what radius is the total energy minimized?

A more detailed version of this model was studied by Chandrasekhar and others as a model for white dwarf stars. Useful numbers: $m_p = 1.6726 \times 10^{-24}$ g, $m_n = 1.6749 \times 10^{-24}$ g, $m_e = 9.1095 \times 10^{-28}$ g, $\hbar = 1.05459 \times 10^{-27}$ erg s, $G = 6.672 \times 10^{-8}$ cm³/(g s²), $1 \text{ eV} = 1.60219 \times 10^{-12}$ erg, $k_B = 1.3807 \times 10^{-16}$ erg/K, and $c = 3 \times 10^{10}$ cm/s.

(b) Using the non-relativistic model in part (a), calculate the Fermi energy of the electrons in a white dwarf star of the mass of the Sun, 2×10^{33} g, assuming that it is composed of helium. (i) Compare it to a typical chemical binding energy of an atom. Are we justified in ignoring the electron-electron and electron-nuclear interactions (i.e., chemistry)? (ii) Compare it to the temperature inside the star, say 10^7 K. Are we justified in assuming that the electron gas is degenerate (roughly zero temperature)? (iii) Compare

⁴This exercise involves a fair amount of algebra. You might consider using a symbolic maniplulation package like Mathematica or Sympy.

⁵You may assume that the single-particle eigenstates have the same energies and **k**-space density in a sphere of volume V as they do for a cube of volume V; just like fixed versus periodic boundary conditions, the boundary does not matter to bulk properties.

it to the mass of the electron. Are we roughly justified in using a non-relativistic theory? (iv) Compare it to the mass difference between a proton and a neutron.

The electrons in large white dwarf stars are relativistic. This leads to an energy which grows more slowly with radius, and eventually to an upper bound on their mass.

(c) Assuming extremely relativistic electrons with $\varepsilon = pc$, calculate the energy of a sphere of non-interacting electrons. Notice that this energy cannot balance against the gravitational energy of the nuclei except for a special value of the mass, M_0 . Calculate M_0 . How does your M_0 compare with the mass of the Sun, above?

A star with mass larger than M_0 continues to shrink as it cools. The electrons (see (iv) in part (b) above) combine with the protons, staying at a constant density as the star shrinks into a ball of almost pure neutrons (a *neutron star*, often forming a *pulsar* because of trapped magnetic flux). Recent speculations suggest that the 'neutronium' will further transform into a kind of quark soup with many strange quarks, forming a transparent insulating material.

For an even higher mass, the Fermi repulsion between quarks cannot survive the gravitational pressure (the quarks become relativistic), and the star collapses into a black hole. At these masses, general relativity is important, going beyond the purview of this text. But the basic competition, between degeneracy pressure and gravity, is the same.