Physics 221A
Fall 2019
Notes 19
Irreducible Tensor Operators and the Wigner-Eckart Theorem†

1. Introduction

The Wigner-Eckart theorem concerns matrix elements of a type that is of frequent occurrence in all areas of quantum physics, especially in perturbation theory and in the theory of the emission and absorption of radiation. This theorem allows one to determine very quickly the selection rules for the matrix element that follow from rotational invariance. In addition, if matrix elements must be calculated, the Wigner-Eckart theorem frequently offers a way of significantly reducing the computational effort. We will make quite a few applications of the Wigner-Eckart theorem in this course.

The Wigner-Eckart theorem is based on an analysis of how operators transform under rotations. It turns out that operators of a certain type, the irreducible tensor operators, are associated with angular momentum quantum numbers and have transformation properties similar to those of kets with the same quantum numbers. An exploitation of these properties leads to the Wigner-Eckart theorem.

2. Definition of a Rotated Operator

We consider a quantum mechanical system with a ket space upon which rotation operators $U(\mathsf{R})$, forming a representation of the classical rotation group $SO(3)$, are defined. The representation will be double-valued if the angular momentum of the system is a half-integer. In these notes we consider only proper rotations R; improper rotations will be taken up later. The operators $U(\mathsf{R})$ map kets into new or rotated kets,

$$|\psi'\rangle = U(\mathsf{R})|\psi\rangle, \tag{1}$$

where $|\psi'\rangle$ is the rotated ket. We will also write this as

$$|\psi\rangle \xrightarrow{\mathsf{R}} U(\mathsf{R})|\psi\rangle. \tag{2}$$

In the case of half-integer angular momenta, the mapping above is only determined to within a sign by the classical rotation R.

† Links to the other sets of notes can be found at:
`http://bohr.physics.berkeley.edu/classes/221/1920/221.html`.

Now if A is an operator, we define the *rotated operator* A' by requiring that the expectation value of the original operator with respect to the initial state be equal to the expectation value of the rotated operator with respect to the rotated state, that is,

$$\langle\psi'|A'|\psi'\rangle = \langle\psi|A|\psi\rangle, \tag{3}$$

which is to hold for all initial states $|\psi\rangle$. But this implies

$$\langle\psi|U(\mathsf{R})^\dagger\, A'\, U(\mathsf{R})|\psi\rangle = \langle\psi|A|\psi\rangle, \tag{4}$$

or, since $|\psi\rangle$ is arbitrary [see Prob. 1.6(b)],

$$U(\mathsf{R})^\dagger\, A'\, U(\mathsf{R}) = A. \tag{5}$$

Solving for A', this becomes

$$A' = U(\mathsf{R})\, A\, U(\mathsf{R})^\dagger, \tag{6}$$

which is our definition of the rotated operator. We will also write this in the form,

$$A \xrightarrow{\mathsf{R}} U(\mathsf{R})\, A\, U(\mathsf{R})^\dagger. \tag{7}$$

Notice that in the case of half-integer angular momenta the rotated operator is specified by the $SO(3)$ rotation matrix R alone, since the sign of $U(\mathsf{R})$ cancels and the answer does not depend on which of the two rotation operators is used on the right hand side. This is unlike the case of rotating kets, where the sign does matter. Equation (7) defines the action of rotations on operators.

3. Scalar Operators

Now we classify operators by how they transform under rotations. First we define a *scalar operator* K to be an operator that is invariant under rotations, that is, that satisfies

$$\boxed{U(\mathsf{R})\, K\, U(\mathsf{R})^\dagger = K,} \tag{8}$$

for all operators $U(\mathsf{R})$. This terminology is obvious. Notice that it is equivalent to the statement that a scalar operator commutes with all rotations,

$$[U(\mathsf{R}), K] = 0. \tag{9}$$

If an operator commutes with all rotations, then it commutes in particular with infinitesimal rotations, and hence with the generators $\mathbf{J}$. See Eq. (12.13). Conversely, if an operator commutes with $\mathbf{J}$ (all three components), then it commutes with any function of $\mathbf{J}$, such as the rotation operators. Thus another equivalent definition of a scalar operator is one that satisfies

$$\boxed{[\mathbf{J}, K] = 0.} \tag{10}$$

The most important example of a scalar operator is the Hamiltonian for an isolated system, not interacting with any external fields. The consequences of this for the eigenvalues and eigenstates of the Hamiltonian are discussed in Secs. 7 and 10 below.

4. Vector Operators

In ordinary vector analysis in three-dimensional Euclidean space, a vector is defined as a collection of three numbers that have certain transformation properties under rotations. It is not sufficient just to have a collection of three numbers; they must in addition transform properly. Similarly, in quantum mechanics, we define a *vector operator* as a vector *of* operators (that is, a set of three operators) with certain transformation properties under rotations.

Our requirement shall be that the expectation value of a vector operator, which is a vector of ordinary or c-numbers, should transform as a vector in ordinary vector analysis. This means that if $|\psi\rangle$ is a state and $|\psi'\rangle$ is the rotated state as in Eq. (1), then

$$\langle\psi'|\mathbf{V}|\psi'\rangle = \mathsf{R}\langle\psi|\mathbf{V}|\psi\rangle, \tag{11}$$

where $\mathbf{V}$ is the vector of operators that qualify as a genuine vector operator. In case the notation in Eq. (11) is not clear, we write the same equation out in components,

$$\langle\psi'|V_i|\psi'\rangle = \sum_j R_{ij}\langle\psi|V_j|\psi\rangle. \tag{12}$$

Equation (11) or (12) is to hold for all $|\psi\rangle$, so by Eq. (1) they imply (after swapping R and R^{-1})

$$U(\mathsf{R})\,\mathbf{V}\,U(\mathsf{R})^\dagger = \mathsf{R}^{-1}\mathbf{V}, \tag{13}$$

or, in components,

$$\boxed{U(\mathsf{R})\,V_i\,U(\mathsf{R})^\dagger = \sum_j V_j\,R_{ji}.} \tag{14}$$

We will take Eq. (13) or (14) as the definition of a vector operator.

In the case of a scalar operator, we had one definition (8) involving its properties under conjugation by rotations, and another (10) involving its commutation relations with the angular momentum $\mathbf{J}$. The latter is in effect a version of the former, when the rotation is infinitesimal. Similarly, for vector operators there is a definition equivalent to Eq. (13) or (14) that involves commutation relations with $\mathbf{J}$. To derive it we let U and R in Eq. (13) have axis-angle form with an angle $\theta \ll 1$, so that

$$U(\mathsf{R}) = 1 - \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{J}, \tag{15}$$

and

$$\mathsf{R} = \mathsf{I} + \theta\hat{\mathbf{n}}\cdot\mathbf{J}. \tag{16}$$

See Eqs. (11.22) and (11.32) for the latter. Then the definition (13) becomes

$$\Big(1 - \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{J}\Big)\mathbf{V}\Big(1 + \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{J}\Big) = (\mathsf{I} - \theta\hat{\mathbf{n}}\cdot\mathbf{J})\mathbf{V}, \tag{17}$$

or

$$[\hat{\mathbf{n}}\cdot\mathbf{J}, \mathbf{V}] = -i\hbar\,\hat{\mathbf{n}}\times\mathbf{V}. \tag{18}$$

Taking the j-th component of this, we have

$$n_i[J_i, V_j] = -i\hbar\,\epsilon_{jik}\,n_i V_k, \tag{19}$$

or, since $\hat{\mathbf{n}}$ is an arbitrary unit vector,

$$\boxed{[J_i, V_j] = i\hbar\,\epsilon_{ijk}\,V_k.} \tag{20}$$

Any vector operator satisfies this commutation relation with the angular momentum of the system.

The converse is also true; if Eq. (20) is satisfied, then $\mathbf{V}$ is a vector operator. This follows since Eq. (20) implies Eq. (18) which implies Eq. (17), that is, it implies that the definition (13) is satisfied for infinitesimal rotations. But it is easy to show that if Eq. (13) is true for two rotations R_1 and R_2, then it is true for the product $\mathsf{R}_1\mathsf{R}_2$. Therefore, since finite rotations can be built up as the product of a large number of infinitesimal rotations (that is, as a limit), Eq. (20) implies Eq. (13) for all rotations. Equations (13) and (20) are equivalent ways of defining a vector operator.

We have now defined scalar and vector operators. Combining them, we can prove various theorems. For example, if $\mathbf{V}$ and $\mathbf{W}$ are vector operators, then $\mathbf{V}\cdot\mathbf{W}$ is a scalar operator, and $\mathbf{V}\times\mathbf{W}$ is a vector operator. This is of course just as in vector algebra, except that we must remember that operators do not commute, in general. For example, it is not generally true that $\mathbf{V}\cdot\mathbf{W} = \mathbf{W}\cdot\mathbf{V}$, or that $\mathbf{V}\times\mathbf{W} = -\mathbf{W}\times\mathbf{V}$.

If we wish to show that an operator is a scalar, we can compute its commutation relations with the angular momentum, as in Eq. (10). However, it may be easier to consider what happens when the operator is conjugated by rotations. For example, the central force Hamiltonian (16.1) is a scalar because it is a function of the dot products $\mathbf{p}\cdot\mathbf{p} = p^2$ and $\mathbf{x}\cdot\mathbf{x} = r^2$. See Sec. 16.2.

5. Examples of Vector Operators

Consider a system consisting of a single spinless particle moving in three-dimensional space, for which the wave functions are $\psi(\mathbf{x})$ and the angular momentum is $\mathbf{L} = \mathbf{x}\times\mathbf{p}$. To see whether $\mathbf{x}$ is a vector operator (we expect it is), we compute the commutation relations with $\mathbf{L}$, finding,

$$[L_i, x_j] = i\hbar\,\epsilon_{ijk}\,x_k. \tag{21}$$

According to Eq. (20), this confirms our expectation. Similarly, we find

$$[L_i, p_j] = i\hbar\,\epsilon_{ijk}\,p_k, \tag{22}$$

so that $\mathbf{p}$ is also a vector operator. Then $\mathbf{x}\times\mathbf{p}$ (see Sec. 4) must also be a vector operator, that is, we must have

$$[L_i, L_j] = i\hbar\,\epsilon_{ijk}\,L_k. \tag{23}$$

This last equation is of course just the angular momentum commutation relations, but here with a new interpretation. More generally, by comparing the adjoint formula (13.89) with the commutation relations (20), we see that the angular momentum $\mathbf{J}$ is always a vector operator.

6. Tensor Operators

Finally we define a *tensor operator* as a tensor *of* operators with certain transformation properties that we will illustrate in the case of a rank-2 tensor. In this case we have a set of 9 operators T_{ij}, where $i, j = 1, 2, 3$, which can be thought of as a 3×3 matrix of operators. These are required to transform under rotations according to

$$U(\mathsf{R})\, T_{ij}\, U(\mathsf{R})^\dagger = \sum_{k\ell} T_{k\ell}\, R_{ki} R_{\ell j}, \tag{24}$$

which is a generalization of Eq. (14) for vector operators. As with scalar and vector operators, a definition equivalent to Eq. (24) may be given that involves the commutation relations of T_{ij} with the components of angular momentum.

As an example of a tensor operator, let $\mathbf{V}$ and $\mathbf{W}$ be vector operators, and write

$$T_{ij} = V_i W_j. \tag{25}$$

Then T_{ij} is a tensor operator (it is the tensor product of $\mathbf{V}$ with $\mathbf{W}$). This is just an example; in general, a tensor operator cannot be written as the product of two vector operators as in Eq. (25).

Another example of a tensor operator is the quadrupole moment operator. In a system with a collection of particles with positions $\mathbf{x}_\alpha$ and charges q_α, where α indexes the particles, the quadrupole moment operator is

$$Q_{ij} = \sum_\alpha q_\alpha (3 x_{\alpha i}\, x_{\alpha j} - r_\alpha^2\, \delta_{ij}). \tag{26}$$

This is obtained from Eq. (15.88) by setting

$$\rho(\mathbf{x}) = \sum_\alpha q_\alpha\, \delta(\mathbf{x} - \mathbf{x}_\alpha). \tag{27}$$

The quadrupole moment operator is especially important in nuclear physics, in which the particles are the protons in a nucleus with charge $q = e$. Notice that the first term under the sum (26) is an operator of the form (25), with $\mathbf{V} = \mathbf{W} = \mathbf{x}_\alpha$.

Tensor operators of other ranks (besides 2) are possible; a scalar is considered a tensor operator of rank 0, and a vector is considered a tensor of rank 1. In the case of tensors of arbitrary rank, the transformation law involves one copy of the matrix $\mathsf{R}^{-1} = \mathsf{R}^t$ for each index of the tensor.

7. Energy Eigenstates in Isolated Systems

In this section we explore the consequences of rotational invariance for the eigenstates, eigenvalues and degeneracies of a scalar operator. The most important scalar operator in practice is the Hamiltonian for an isolated system, so for concreteness we will speak of such a Hamiltonian, but the following analysis applies to any scalar operator.

Let H be the Hamiltonian for an isolated system, and let $\mathcal{E}$ be the Hilbert space upon which it acts. Since H is a scalar it commutes with $\mathbf{J}$, and therefore with the commuting operators J^2

and J_3. Let us denote the simultaneous eigenspaces of J^2 and J_3 with quantum numbers j and m by $\mathcal{S}_{jm}$, as illustrated in Fig. 13.5. It was shown in Notes 13 that for a given system, j takes on certain values that must be either integers or half-integers. For example, in central force motion we have only integer values of j (which is called ℓ in that context), while for the ^{57}Fe nucleus, which is discussed in more detail in the next section, we have only half-integer values. For each value of j that occurs there is a collection of $2j+1$ eigenspaces $\mathcal{S}_{jm}$ of J^2 and J_3, for $m = -j, \ldots, +j$. These spaces are mapped invertibly into one another by J_+ and J_-, as illustrated in Fig. 13.5, and if they are finite-dimensional, then they all have the same dimension. As in Notes 13, we write $N_j = \dim \mathcal{S}_{jj}$, which we call the multiplicity of the given j value.

In Notes 13 we constructed a standard angular momentum basis by picking an arbitrary orthonormal basis in each stretched space $\mathcal{S}_{jj}$, with the basis vectors labeled by γ as in Fig. 13.5, where $\gamma = 1, \ldots, N_j$. We denote these basis vectors in $\mathcal{S}_{jj}$ by $|\gamma jj\rangle$. Then by applying lowering operators, we construct an orthonormal basis in each of the other $\mathcal{S}_{jm}$, for m running down to $-j$. In this way we construct a standard angular momentum basis $|\gamma jm\rangle$ on the whole Hilbert space $\mathcal{E}$. In this construction, it does not matter how the basis $|\gamma jj\rangle$ is chosen in $\mathcal{S}_{jj}$, as long as it is orthonormal.

Now, however, we have a Hamiltonian, and we would like a simultaneous eigenbasis of H, J^2 and J_3. To construct this we restrict H to $\mathcal{S}_{jj}$ for some j (see Sec. 1.23 for the concept of the restriction of an operator to a subspace, and how it is used in proving that commuting operators possess a simultaneous eigenbasis). This restricted H is a Hermitian operator on $\mathcal{S}_{jj}$ so it possesses an eigenbasis on that space.

The spectrum of H on $\mathcal{S}_{jj}$ can be either discrete, continuous, or mixed (in most problems we will consider in this course it has a continuous spectrum above a threshold energy, and may have discrete bound states below that). Let us focus on the bound states and assume that H possesses at least one bound eigenstate $|\psi\rangle$ on $\mathcal{S}_{jj}$ with corresponding eigenvalue E. Then $|\psi\rangle$ satisfies

$$J^2|\psi\rangle = j(j+1)\hbar^2\,|\psi\rangle, \qquad J_3|\psi\rangle = j\hbar\,|\psi\rangle, \qquad H|\psi\rangle = E|\psi\rangle. \tag{28}$$

Now by applying a lowering operator J_- we find

$$J_-H|\psi\rangle = HJ_-|\psi\rangle = EJ_-|\psi\rangle, \tag{29}$$

so that $J_-|\psi\rangle$ is an eigenstate of H, lying in the space $\mathcal{S}_{j,j-1}$, with the same eigenvalue E as $|\psi\rangle \in \mathcal{S}_{jj}$. Continuing to apply lowering operators, we generate a set of $2j+1$ linearly independent eigenstates of H with the same eigenvalue E, that is, E is independent of the quantum number m. These states span an irreducible, invariant subspace of $\mathcal{E}$.

There may be other irreducible subspaces with the same energy. This can occur in two ways. It could happen that there is another energy eigenstate in $\mathcal{S}_{jj}$, linearly independent of $|\psi\rangle$, with the same energy E. That is, it is possible that E is a degenerate eigenvalue of H restricted to $\mathcal{S}_{jj}$. In general, every discrete eigenvalue E of H restricted to $\mathcal{S}_{jj}$ corresponds to an eigenspace, a subspace of $\mathcal{S}_{jj}$ that may be multidimensional. Choosing an orthonormal basis in this subspace and applying

lowering operators, we obtain a set of orthogonal, irreducible subspaces of the same value of j, each with $2j+1$ dimensions and all having the same energy.

It could also happen that there is another bound energy eigenstate, in a different space $\mathcal{S}_{j'j'}$ for $j' \neq j$, with the same energy E as $|\psi\rangle \in \mathcal{S}_{jj}$. This would be a degeneracy of H that crosses j values. If such a degeneracy exists, then we have at least two irreducible subspaces of the same energy, one of dimension $2j+1$ and the other of dimension $2j'+1$. In other words, degeneracies can occur either within a given j value or across j values.

These facts that we have accumulated can be summarized by a theorem:

Theorem 1. *The discrete energy eigenspaces of an isolated system consist of one or more invariant, irreducible subspaces under rotations, each associated with a definite j value. The different irreducible subspaces can be chosen to be orthogonal.*

Let us look at two examples of how this theorem works out in practice, the first a simple one with a small number of degrees of freedom that is exactly solvable, and the other a complicated one with a large number of degrees of freedom, in which all we know about the Hamiltonian is that it is invariant under rotations.

8. Example: Central Force Motion

For the simple example we take the case of central force motion, for which we use the notation $\mathbf{L}$, ℓ etc. instead of $\mathbf{J}$, j etc.

In central force motion the stretched subspace $\mathcal{S}_{\ell\ell}$ consists of wave functions $R(r)Y_{\ell\ell}(\theta,\phi)$, where $R(r)$ is any radial wave function. To find the energy eigenstates in this stretched subspace we solve the radial Schrödinger equation for the given ℓ value, which produces in general a continuous and a discrete spectrum. We assume there is a discrete spectrum for the given ℓ value and denote the energy eigenvalues and corresponding radial wave functions by $E_{n\ell}$ and $R_{n\ell}(r)$, as in Notes 16. By applying lowering operators to the wave function $R_{n\ell}(r)\,Y_{\ell\ell}(\theta,\phi)$, we obtain an irreducible subspace of degenerate energy eigenfunctions, spanned by $\{R_{n\ell}(r)\,Y_{\ell m}(\theta,\phi), m = +\ell,\ldots,-\ell\}$.

Now we consider degeneracies. Is it possible, for a given value of ℓ in a central force problem, that a bound energy eigenvalue can be degenerate? That is, can there be more than one linearly independent bound energy eigenstate of a given energy in $\mathcal{S}_{\ell\ell}$? As discussed in Sec. 16.4, the answer is no, the boundary conditions on the radial wave functions guarantee that there can be no degeneracy of this type. In central force problems, we do not have degeneracies within a given ℓ value.

Then is it possible that there is a degeneracy between different values of ℓ? Again, as discussed in Notes 16, the answer is that in general it is not very likely, since the different radial equations for different values of ℓ are effectively different Schrödinger equations whose centrifugal potentials are different.

The fact is that systematic degeneracies require a non-Abelian symmetry. We are already taking into account the $SO(3)$ symmetry of proper rotations, which explains the degeneracy in the

magnetic quantum number m, so any additional degeneracy will require a larger symmetry group than $SO(3)$. In the absence of such extra symmetry, degeneracies between different ℓ values can occur only by "accident," that is, by fine tuning parameters in a Hamiltonian to force a degeneracy to happen. This is not likely in most practical situations. Therefore in central force problems we do not normally expect degeneracies that cross subspaces of different values of ℓ.

As explained in Notes 17, however, the electrostatic model of hydrogen is a notable exception, due to the symmetry group $SO(4)$ possessed by this model, which is larger than the rotation group $SO(3)$. The extra symmetry in this model of hydrogen explains why the energy levels $E_n = -1/2n^2$ (in the right units) are the same across the angular momentum values $\ell = 0, \ldots, n-1$. The isotropic harmonic oscillator in two or more dimensions is another example of a system with extra degeneracy; such oscillators are approximate models for certain types of molecular vibrations.

For a more complicated example of how Theorem 1 works out in practice we examine some energy levels of the nucleus ^{57}Fe, which is important in the Mössbauer effect. We use the opportunity to digress into some of the interesting physics connected with this effect. We begin with a general discussion of aspects of the emission and absorption of photons by quantum systems.

9. Emission and Absorpton of Photons

When an atom, nucleus or other quantum system is in an excited state B and emits a photon while dropping into the ground state A,

$$B \to A + \gamma, \tag{30}$$

then in a simple description of the process we say that the energy of the photon is given by

$$E_\gamma = E_B - E_A, \tag{31}$$

where E_B and E_A are the energies of the states B and A. If now there is another atom, nucleus or other system of the same type nearby in its ground state A, then it would appear that that photon has exactly the right energy to induce the inverse reaction,

$$A + \gamma \to B, \tag{32}$$

thereby lifting the second system into the excited state B.

Does this mean, for example, that when an atom in a gas emits a photon that the photon only travels as far as the nearest neighboring atom before being absorbed again? No, because there are several effects that complicate the basic picture just presented, modifying the energy E_γ of the photon so that is it not exactly given by Eq. (31). These include the natural line width of the transition $B \to A$; Doppler shifts; recoil; and, in the case of nuclei, what are called chemical shifts.

In quantum mechanics the energy of a system is only precisely defined in a process that takes place over an infinite amount of time. The excited state B of our system is unstable with some lifetime τ, so its energy E_B is only defined to within an uncertainty of order $\Delta E_B = \hbar/\tau$. Assuming

A is the ground state, it is stable and can exist over an infinite amount of time, so there is no uncertainty in its energy. Overall, the uncertainty in the energy E_B creates uncertainty of order $\hbar/\tau$ to the energy of the photon E_γ emitted in the process (30). This can be seen experimentally; if all other sources of broadening of the spectral line are eliminated, then the energy of photons emitted in an atomic or nuclear transition does not have a definite value, but rather there is a spread of order $\Delta E = \hbar/\tau$ about the nominal value $E_B - E_A$. This spread is called the *natural line width* of the spectral line. The natural line width of spectral lines is examined in some detail in Notes 43.

Similarly, if a photon of energy E_γ encounters a quantum system of the same type at rest in its ground state A, then if E_γ is roughly within the range $\Delta E = \hbar/\tau$ about the nominal energy $E_B - E_A$ it will be able to lift the second system into the excited state B, that is, the inverse reaction (32) will take place.

On the other hand, if the emitting atom, nucleus or other quantum system is in a state of motion, then the frequency $\omega_\gamma = E_\gamma/\hbar$ of the emitted photon will be Doppler shifted and may no longer be within the resonance needed to raise another such system into its excited state. Writing simply E for the nominal energy $E_B - E_A$ of the photon, the velocity v needed to shift the photon out of resonance is given by

$$\frac{v}{c} = \frac{\Delta E}{E} = \frac{\hbar}{E\tau}. \tag{33}$$

Whether or not the photon is shifted out of resonance depends on the velocity and other parameters, but in many practical circumstances one will find that thermal velocities do exceed the value given by Eq. (33). A similar logic applies in case the receiving system is in a state of motion (or both, as would be the case of a gas).

Even if the emitting atom or nucleus or other system is at rest, the energy E_γ is not given exactly by Eq. (31) because of the recoil of the emitting system when the photon is emitted. The photon has energy $E = \hbar\omega$ and momentum $\mathbf{p} = \hbar\mathbf{k}$ where $\omega = c|\mathbf{k}|$, so by conservation of momentum the emitting system suffers a recoil and has momentum $m\mathbf{v} = -\hbar\mathbf{k}$ after the photon of frequency ω is emitted, where m is the mass of the emitting system. Thus Eq. (31) should be replaced by

$$E_\gamma + \frac{1}{2}mv^2 = E_B - E_A, \tag{34}$$

where $\mathbf{v}$ is the recoil velocity. Some of the available energy goes into kinetic energy of the recoiling system, and the energy E_γ of the emitted photon is actually less than the nominal value (31). Again, whether this recoil shift is greater or less than the natural line width depends on the parameters of the problem.

10. The ^{57}Fe Nucleus and the Mössbauer Effect

The Mössbauer effect involves a transition $^{57}\mathrm{Fe}^* \to {}^{57}\mathrm{Fe} + \gamma$ between two energy levels of the ^{57}Fe nucleus, where the simple notation ^{57}Fe (or A) refers to the ground state and $^{57}\mathrm{Fe}^*$ (or B) refers to an excited state. These states are illustrated in the energy level diagram for the nucleus

given in Fig. 1. The photon emitted has energy 14.4 KeV, and the lifetime of the excited state $^{57}\text{Fe}^*$ is $\tau = 9.8 \times 10^{-8}$ sec. From these figures we find $\Delta\omega/\omega = \Delta E/E = 4.7 \times 10^{-13}$, where E and ω are the energy and frequency of the emitted photon. The spread in the energy is very small compared to the energy. For example, according to Eq. (33), to Doppler shift the photon out of resonance it would require a velocity of $v/c = 4.7 \times 10^{-13}$, or $v = 0.014\,\text{cm/sec}$.

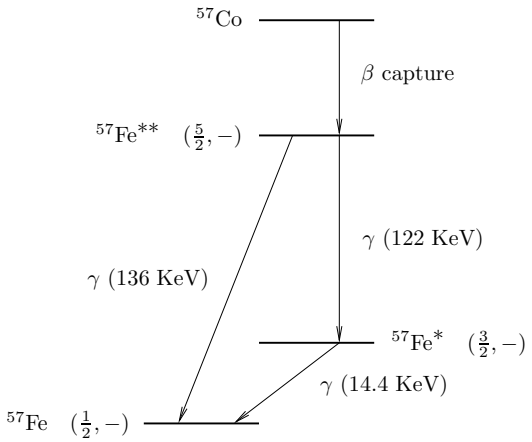

Fig. 1. Energy level diagram relevant for the Mössbauer effect in ^{57}Fe. ^{57}Fe is the ground state, $^{57}\text{Fe}^*$ is an excited state, and $^{57}\text{Fe}^{**}$ is a more highly excited state. Principal transitions via photon emission are shown.

The Mössbauer effect makes use of a source containing iron nuclei in the excited state $^{57}\text{Fe}^*$, which emits photons, and a receiver containing iron nuclei in the ground state which may absorb them by being lifted into the excited state $^{57}\text{Fe}^*$ via the reverse reaction. The receiver can be a block of natural iron, which contains the isotope ^{57}Fe at the 2% level, behind which a gamma-ray detector is placed. If the incident photons are within the narrow resonant range of energies, then they will be absorbed by the block of iron, and the detector will detect nothing. But if they are shifted out of resonance, the gamma rays will pass through the block of iron and the detector will detect them. If there is some effect that shifts the frequency of the gamma rays from their nominal energy (for example, the gravitational red shift in the Pound-Rebka experiment), then a compensating Doppler shift can be introduced by giving the source some velocity. By measuring the velocity of the source needed to shift the gamma rays back into resonance, one can measure the shift caused by the effect in question.

However, plugging in the numbers shows that the recoil shift described by Eq. (34), where m is the mass of an iron nucleus, is much greater than the natural line width, so the recoil would seem to spoil the whole idea. But the iron nucleus is not free, rather it is part of a crystal lattice, whose vibrations are described by a large number of harmonic oscillators, the normal modes of the lattice. (See the discussion in Sec. 8.2.) Thus the recoil kinetic energy $E = (1/2)mv^2$ in Eq. (34) is not free to take on any value, rather it must be some multiple of $\hbar\omega$, where ω is the frequency of a normal mode of the lattice. That is, when the photon is emitted by the nucleus, some number of phonons

are also emitted into the lattice, representing the recoil energy.

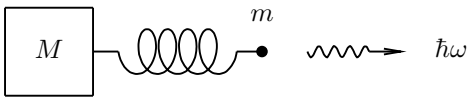

Fig. 2. A one dimensional model of an iron atom coupled to a normal mode of the lattice. The mass of the iron atom is m, the mass of the crystal is M. The iron atom emits a photon of energy $\hbar\omega$ and suffers a recoil (an impulse) as a result.

To model this situation in the simplest possible way, let us imagine an iron atom connected to a spring, forming a one-dimensional harmonic oscillator, as illustrated in Fig. 2. In the figure m is the mass of the iron atom while M is the mass of the crystal lattice to which it is coupled. When the atom emits a photon it suffers an an impulse, that is, a change Δp in its momentum. The emission takes place over a short time compared to the frequency of the harmonic oscillator (a normal mode of the lattice), so the position of the iron atom does not change much during the emission process. Classically we can model the impulse by the map,

$$x \mapsto x, \qquad p \mapsto p + \Delta p. \tag{35}$$

To model the effect of the recoil in quantum mechanics, we use the momentum displacement operator $S(b)$ introduced in Notes 8 [see Eqs. (8.64)–(8.66)]. That is, if $|\psi\rangle$ is the state of the oscillator before the photon is emitted, then the state after the emission is

$$|\psi'\rangle = e^{i\Delta p x/\hbar}|\psi\rangle. \tag{36}$$

The final state can be expanded in energy eigenstates,

$$|\psi'\rangle = \sum_n c_n |n\rangle, \tag{37}$$

so that the probability of finding the oscillator in state n after the photon has been emitted is $|c_n|^2$. In particular, if the initial state of the oscillator $|\psi\rangle = |n_i\rangle$ is an energy eigenstate, then the probability $|c_n|^2$ is the probability to make a transition $n_i \to n$ as a result of the recoil. As we say, $n - n_i$ phonons are emitted.

In fact, there is a certain probability that no phonons are emitted at all, that is $n = n_i$ and the oscillator remains in the initial state. Because of quantum mechanics, the recoil energy cannot take on any value, but rather is quantized, and the value zero is allowed. What makes the ^{57}Fe nucleus attractive for the Mössbauer effect is that it has a reasonable probability for this *recoilless emission*.

Of course there is not only a recoil energy but also a recoil momentum. In the Mössbauer effect, recoilless emission does not violate conservation of momentum because the entire crystal lattice, with an effectively infinite mass M (as in the figure) takes up the recoil momentum.

The excited state ^{57}Fe* has only a short lifetime but in practice a population of these excited states is maintained in the source as a part of the decay chain of ^{57}Co, as shown in Fig. 1. ^{57}Co has

a lifetime of 271 days, which is long enough to make it practical to use it as a source of $^{57}\text{Fe}^*$ in a real experiment. As shown in the figure, ^{57}Co transforms into an excited state $^{57}\text{Fe}^{**}$ by electron capture, after which $^{57}\text{Fe}^{**}$ decays by the emission of a photon into $^{57}\text{Fe}^*$, which is the source of the photons of interest in the Mössbauer effect.

Mössbauer was awarded the Nobel Prize in 1961 for his discovery of recoilless emission of gamma ray photons and some of its applications. A notable early application was the Pound-Rebka experiment, carried out in 1959, in which the Mössbauer effect was used to make the first measurement of the gravitational red shift. This is the red shift photons experience when climbing in a gravitational field, in accordance with the 1911 prediction of Einstein. The gravitational red shift is one of the physical cornerstones of general relativity.

11. Energy levels in ^{57}Fe

To return to the subject of Hamiltonians and their energy levels in isolated systems, let us draw attention to the three levels ^{57}Fe, $^{57}\text{Fe}^*$ and $^{57}\text{Fe}^{**}$, in Fig. 1. These are energy levels of the Hamiltonian for the ^{57}Fe nucleus, and, according to Theorem 1, each must consist of one or more irreducible subspaces under rotations. In fact, they each consist of precisely one such irreducible subspace, with a definite j value, which is indicated in the figure ($\frac{1}{2}$ for the ground state ^{57}Fe, and $\frac{3}{2}$ and $\frac{5}{2}$ for the two excited states $^{57}\text{Fe}^*$ and $^{57}\text{Fe}^{**}$, respectively). Also indicated are the parities of these states (all three have odd parity). The parity of energy eigenstates of isolated systems is discussed in Sec. 20.8.

A model for the Hamiltonian of the ^{57}Fe nucleus views it as a 57-particle system, that is, with 26 protons and 31 neutrons. The Hamiltonian is some function of the positions, momenta and spins of the particles,

$$H = H(\mathbf{x}_\alpha, \mathbf{p}_\alpha, \mathbf{S}_\alpha), \tag{38}$$

where $\alpha = 1, \ldots, 57$. In this model the total angular momentum of the system is the sum of the orbital and spin angular momenta of the nucleons,

$$\mathbf{J} = \sum_{\alpha=1}^{57} \mathbf{x}_\alpha \times \mathbf{p}_\alpha + \mathbf{S}_\alpha, \tag{39}$$

and the "spins" of the various nuclear states shown in Fig. 1 are actually the quantum numbers of J^2 (that is, we call $\mathbf{J}$ the "spin" and use the notation $\mathbf{S}$ etc. for it). For example, we say that the ground state ^{57}Fe has spin $s = \frac{1}{2}$.

This model is more or less crude, due to the fact that protons and neutrons are composite particles, each made up of three quarks, which interact with the quark and gluon fields via the strong interactions. For our purposes the only thing that matters is that rotations act upon the state space of the system by means of unitary operators, and that these commute with the Hamiltonian. The model (38) at least gives us something concrete to think about.

Each nuclear energy eigenstate consists of a single irreducible subspace under rotations for the same reasons discussed in connection with central force motion in Sec. 7. That is, extra degeneracy requires extra symmetry or else an unlikely accident, and neither of these is to be expected in nuclei. Therefore each energy level is characterized by a unique angular momentum value, as indicated in the figure.

We can summarize these accumulated facts by stating an addendum to Theorem 1.

Addendum to Theorem 1. *With a few exceptions, notably the electrostatic model of hydrogen, the bound state energy eigenspaces of isolated systems consist of a single invariant, irreducible subspace under rotations. Thus, the energy eigenvalues are characterized by an angular momentum quantum number, which is variously denoted ℓ, s, j, etc, depending on the system.*

We can now understand why the Hilbert space for spins in magnetic fields consists of a single irreducible subspace under rotations for a large class of particles, a question that was raised in Notes 14. For example, if we place the ^{57}Fe nucleus in a magnetic field that is strong by laboratory standards, say, 10T, then the energy splitting between the two magnetic substates $m = \pm\frac{1}{2}$ will be of the order of 100 MHz in frequency units, or about 4×10^{-7}eV, or roughly 3×10^{-11} times smaller than the energy separation from the first excited state $^{57}\text{Fe}^*$. Therefore it is an excellent approximation to ignore the state $^{57}\text{Fe}^*$ and all other excited states of the ^{57}Fe nucleus, and to treat the Hilbert space of the nucleus as if it were a single irreducible subspace with $s = \frac{1}{2}$, that is, the ground eigenspace. In other words, in the case of nuclei, the $2s + 1$-dimensional Hilbert space used in our study of spins in magnetic fields in Notes 14 is actually a subspace of a larger Hilbert space. It is, in fact, an energy eigenspace of an isolated system. This in turn explains why the magnetic moment is proportional to the spin [see Prob. 2(a)].

12. The Spherical Basis

We return to our development of the properties of operators under rotations. We take up the subject of the *spherical basis*, which is a basis of unit vectors in ordinary three-dimensional space that is alternative to the usual Cartesian basis. Initially we just present the definition of the spherical basis without motivation, and then we show how it can lead to some dramatic simplifications in certain problems. Then we explain its deeper significance. The spherical basis will play an important role in the development of later topics concerning operators and their transformation properties.

We denote the usual Cartesian basis by $\hat{\mathbf{c}}_i$, $i = 1, 2, 3$, so that

$$\hat{\mathbf{c}}_1 = \hat{\mathbf{x}}, \qquad \hat{\mathbf{c}}_2 = \hat{\mathbf{y}}, \qquad \hat{\mathbf{c}}_3 = \hat{\mathbf{z}}. \tag{40}$$

We have previously denoted this basis by $\hat{\mathbf{e}}_i$, but in these notes we reserve the symbol $\hat{\mathbf{e}}$ for the spherical basis.

The spherical basis is defined by

$$\hat{\mathbf{e}}_1 = -\frac{\hat{\mathbf{x}} + i\hat{\mathbf{y}}}{\sqrt{2}},$$

$$\hat{\mathbf{e}}_0 = \hat{\mathbf{z}},$$
$$\hat{\mathbf{e}}_{-1} = \frac{\hat{\mathbf{x}} - i\hat{\mathbf{y}}}{\sqrt{2}}. \tag{41}$$

This is a complex basis, so vectors with real components with respect to the Cartesian basis have complex components with respect to the spherical basis. We denote the spherical basis vectors collectively by $\hat{\mathbf{e}}_q$, $q = 1, 0, -1$.

The spherical basis vectors have the following properties. First, they are orthonormal, in the sense that

$$\hat{\mathbf{e}}_q^* \cdot \hat{\mathbf{e}}_{q'} = \delta_{qq'}. \tag{42}$$

Next, an arbitrary vector $\mathbf{X}$ can be expanded as a linear combination of the vectors $\hat{\mathbf{e}}_q^*$,

$$\mathbf{X} = \sum_q \hat{\mathbf{e}}_q^* X_q, \tag{43}$$

where the expansion coefficients are

$$X_q = \hat{\mathbf{e}}_q \cdot \mathbf{X}. \tag{44}$$

These equations are equivalent to a resolution of the identity in 3-dimensional space,

$$\mathsf{I} = \sum_q \hat{\mathbf{e}}_q^* \hat{\mathbf{e}}_q, \tag{45}$$

in which the juxtaposition of the two vectors represents a tensor product or dyad notation.

You may wonder why we expand $\mathbf{X}$ as a linear combination of $\hat{\mathbf{e}}_q^*$, instead of $\hat{\mathbf{e}}_q$. The latter type of expansion is possible too, that is, any vector $\mathbf{Y}$ can be written

$$\mathbf{Y} = \sum_q \hat{\mathbf{e}}_q Y_q, \tag{46}$$

where

$$Y_q = \hat{\mathbf{e}}_q^* \cdot \mathbf{Y}. \tag{47}$$

These relations correspond to a different resolution of the identity,

$$\mathsf{I} = \sum_q \hat{\mathbf{e}}_q \hat{\mathbf{e}}_q^*. \tag{48}$$

The two types of expansion give the contravariant and covariant components of a vector with respect to the spherical basis; in this course, however, we will only need the expansion indicated by Eq. (43).

13. An Application of the Spherical Basis

To show some of the utility of the spherical basis, we consider the problem of dipole radiative transitions in a single-electron atom such as hydrogen or an alkali. It is shown in Notes 41 that the transition amplitude for the emission of a photon is proportional to matrix elements of the dipole

operator between the initial and final states. We use an electrostatic, spinless model for the atom, as in Notes 16, and we consider the transition from initial energy level $E_{n\ell}$ to final level $E_{n'\ell'}$. These levels are degenerate, since the energy does not depend on the magnetic quantum number m or m'. The wave functions have the form,

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\Omega), \tag{49}$$

as in Eq. (16.15).

The dipole operator is proportional to the position operator of the electron, so we must evaluate matrix elements of the form,

$$\langle n\ell m|\mathbf{x}|n'\ell'm'\rangle, \tag{50}$$

where the initial state is on the left and the final one on the right. The position operator $\mathbf{x}$ has three components, and the initial and final levels consist of $2\ell+1$ and $2\ell'+1$ degenerate states, respectively. Therefore if we wish to evaluate the intensity of a spectral line as it would be observed, we really have to evaluate $3(2\ell'+1)(2\ell+1)$ matrix elements, for example, $3\times3\times5 = 45$ in a $3d \to 2p$ transition. This is actually an exaggeration, as we shall see, because many of the matrix elements vanish, but there are still many nonvanishing matrix elements to be calculated.

A great simplification can be achieved by expressing the components of $\mathbf{x}$, not with respect to the Cartesian basis, but with respect to the spherical basis. First we define

$$x_q = \hat{\mathbf{e}}_q \cdot \mathbf{x}, \tag{51}$$

exactly as in Eq.(44). Next, by inspecting a table of the $Y_{\ell m}$'s (see Sec. 15.7), we find that for $\ell = 1$ we have

$$\begin{aligned}
rY_{11}(\theta,\phi) &= -r\sqrt{\frac{3}{8\pi}}\,\sin\theta e^{i\phi} = \sqrt{\frac{3}{4\pi}}\Big(-\frac{x+iy}{\sqrt{2}}\Big),\\
rY_{10}(\theta,\phi) &= r\sqrt{\frac{3}{4\pi}}\,\cos\theta = \sqrt{\frac{3}{4\pi}}(z),\\
rY_{1,-1}(\theta,\phi) &= r\sqrt{\frac{3}{8\pi}}\,\sin\theta e^{-i\phi} = \sqrt{\frac{3}{4\pi}}\Big(\frac{x-iy}{\sqrt{2}}\Big),
\end{aligned} \tag{52}$$

where we have multiplied each Y_{1m} by the radius r. On the right hand side we see the spherical components x_q of the position vector $\mathbf{x}$, as follows from the definitions (41). The results can be summarized by

$$rY_{1q}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\,x_q, \tag{53}$$

for $q = 1, 0, -1$, where q appears explicitly as a magnetic quantum number. This equation reveals a relationship between vector operators and the angular momentum value $\ell = 1$, something we will have more to say about presently.

Now the matrix elements (50) become a product of a radial integral times an angular integral,

$$\begin{aligned}\langle n\ell m|x_q|n'\ell'm'\rangle = &\int_0^\infty r^2\,dr\,R^*_{n\ell}(r)rR_{n'\ell'}(r)\\ &\times\sqrt{\frac{4\pi}{3}}\int d\Omega\,Y^*_{\ell m}(\theta,\phi)Y_{1q}(\theta,\phi)Y_{\ell'm'}(\theta,\phi).\end{aligned}\tag{54}$$

We see that all the dependence on the three magnetic quantum numbers (m, q, m') is contained in the angular part of the integral. Moreover, the angular integral can be evaluated by the three-$Y_{\ell m}$ formula, Eq. (18.67), whereupon it becomes proportional to the Clebsch-Gordan coefficient,

$$\langle \ell m|\ell' 1 m' q\rangle.\tag{55}$$

The radial integral is independent of the three magnetic quantum numbers (m, q, m'), and the trick we have just used does not help us to evaluate it. But it is only one integral, and after it has been done, all the other integrals can be evaluated just by computing or looking up Clebsch-Gordan coefficients.

The selection rule $m = q + m'$ in the Clebsch-Gordan coefficient (55) means that many of the integrals vanish, so we have exaggerated the total number of integrals that need to be done. But had we worked with the Cartesian components x_i of $\mathbf{x}$, this selection rule might not have been obvious. In any case, even with the selection rule, there may still be many nonzero integrals to be done (nine, in the case $3d \to 2p$).

The example we have just given of simplifying the calculation of matrix elements for a dipole transition is really an application of the Wigner-Eckart theorem, which we take up later in these notes.

The process we have just described is not just a computational trick, rather it has a physical interpretation. The initial and final states of the atom are eigenstates of L^2 and L_z, and the photon is a particle of spin 1 (see Notes 40). Conservation of angular momentum requires that the angular momentum of the initial state (the atom, with quantum numbers ℓ and m) should be the same as the angular momentum of the final state (the atom, with quantum numbers ℓ' and m', plus the photon with spin 1). Thus, the selection rule $m = m' + q$ means that q is the z-component of the spin of the emitted photon, so that the z-component of angular momentum is conserved in the emission process. As for the selection rule $\ell \in \{\ell' - 1, \ell', \ell' + 1\}$, it means that the amplitude is zero unless the possible total angular momentum quantum number of the final state, obtained by combining $\ell' \otimes 1$, is the total angular momentum quantum number of the initial state. This example shows the effect of symmetries and conservation laws on the selection rules for matrix elements.

This is only an incomplete accounting of the symmetry principles at work in the matrix element (50) or (54); as we will see in Notes 20, parity also plays an important role.

14. Significance of the Spherical Basis

To understand the deeper significance of the spherical basis we examine Table 1. The first row of this table summarizes the principal results obtained in Notes 13, in which we worked out the matrix representations of angular momentum and rotation operators. To review those results, we start with a ket space upon which proper rotations act by means of unitary operators $U(\mathsf{R})$, as indicated in the second column of the table. We refer only to proper rotations $\mathsf{R} \in SO(3)$, and we note that the representation may be double-valued. The rotation operators have generators, defined by Eq. (12.13), that is, that equation can be taken as the definition of $\mathbf{J}$ when the rotation operators $U(\mathsf{R})$ are given. [Equation (12.11) is equivalent.] The components of $\mathbf{J}$ satisfy the usual commutation relations (12.24) since the operators $U(\mathsf{R})$ form a representation of the rotation group. Next, since J^2 and J_z commute, we construct their simultaneous eigenbasis, with an extra index γ to resolve degeneracies. Also, we require states with different m but the same γ and j to be related by raising and lowering operators. This creates the standard angular momentum basis (SAMB), indicated in the fourth column. In the last column, we show how the vectors of the standard angular momentum basis transform under rotations. A basis vector $|\gamma jm\rangle$, when rotated, produces a linear combination of other basis vectors for the same values of γ and j but different values of m. This implies that the space spanned by $|\gamma jm\rangle$ for fixed γ and j, but for $m = -j, \ldots, +j$ is invariant under rotations. This space has dimensionality $2j + 1$. It is, in fact, an irreducible invariant space (more on irreducible subspaces below). One of the results of the analysis of Notes 13 is that the matrices $D^j_{m'm}(U)$ are universal matrices, dependent only on the angular momentum commutation relations and otherwise independent of the nature of the system.

Space	Action	Ang Mom	SAMB	Action on SAMB
Kets	$\|\psi\rangle \mapsto U\|\psi\rangle$	$\mathbf{J}$	$\|\gamma jm\rangle$	$U\|\gamma jm\rangle = \sum_{m'} \|\gamma jm'\rangle D^j_{m'm}$
3D Space	$\mathbf{x} \mapsto \mathsf{R}\mathbf{x}$	$i\mathbf{J}$	$\hat{\mathbf{e}}_q$	$\mathsf{R}\hat{\mathbf{e}}_q = \sum_{q'} \hat{\mathbf{e}}_{q'} D^1_{q'q}$
Operators	$A \mapsto UAU^\dagger$	$\ldots$	T^k_q	$UT^k_qU^\dagger = \sum_{q'} T^k_{q'} D^k_{q'q}$

Table 1. The rows of the table indicate different vector spaces upon which rotations act by means of unitary operators. The first row refers to a ket space (a Hilbert space of a quantum mechanical system), the second to ordinary three-dimensional space (physical space), and the third to the space of operators. The operators in the third row are the usual linear operators of quantum mechanics that act on the ket space, for example, the Hamiltonian. The first column identifies the vector space. The second column shows how rotations $\mathsf{R} \in SO(3)$ act on the given space. The third column shows the generators of the rotations, that is, the 3-vector of Hermitian operators that specify infinitesimal rotations. The fourth column shows the standard angular momentum basis (SAMB), and the last column, the transformation law of vectors of the standard angular momentum basis under rotations.

At the beginning of Notes 13 we remarked that the analysis of those notes applies to other spaces besides ket spaces. All that is required is that we have a vector space upon which rotations

act by means of unitary operators. For other vectors spaces the notation may change (we will not call the vectors kets, for example), but otherwise everything else goes through.

The second row of Table 1 summarizes the case in which the vector space is ordinary three-dimensional (physical) space. Rotations act on this space by means of the matrices R, which, being orthogonal, are also unitary (an orthogonal matrix is a special case of a unitary matrix). The action consists of just rotating vectors in the usual sense, as indicated in the second column.

The generators of rotations in this case must be a vector $\mathbf{J}$ of Hermitian operators, that is, Hermitian matrices, that satisfy

$$U(\hat{\mathbf{n}},\theta) = 1 - \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{J}, \tag{56}$$

when θ is small. Here U really means the same thing as R, since we are speaking of the action on three-dimensional space, and 1 means the same as the identity matrix I. We will modify this definition of $\mathbf{J}$ slightly by writing $\mathbf{J}' = \mathbf{J}/\hbar$, thereby absorbing the $\hbar$ into the definition of $\mathbf{J}$ and making $\mathbf{J}'$ dimensionless. This is appropriate when dealing with ordinary physical space, since it has no necessary relation to quantum mechanics. (The spherical basis is also useful in classical mechanics, for example.) Then we will drop the prime, and just remember that in the case of this space, we will use dimensionless generators. Then we have

$$U(\hat{\mathbf{n}},\theta) = 1 - i\theta\hat{\mathbf{n}}\cdot\mathbf{J}. \tag{57}$$

But this is equivalent to

$$R(\hat{\mathbf{n}},\theta) = \mathsf{I} + \theta\hat{\mathbf{n}}\cdot\mathbf{J}, \tag{58}$$

as in Eq. (11.32), where the vector of matrices $\mathbf{J}$ is defined by Eq. (11.22). These imply

$$\mathbf{J} = i\mathbf{J}, \tag{59}$$

as indicated in the third column of Table 1. Writing out the matrices J_i explicitly, we have

$$J_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad J_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad J_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{60}$$

These matrices are indeed Hermitian, and they satisfy the dimensionless commutation relations,

$$[J_i, J_j] = i\epsilon_{ijk}\, J_k, \tag{61}$$

as follows from Eqs. (11.34) and (59).

We can now construct the standard angular momentum basis on three-dimensional space. In addition to Eq. (60), we need the matrices for J^2 and $J_\pm$. These are

$$J^2 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{62}$$

and

$$J_\pm = \begin{pmatrix} 0 & 0 & \mp 1 \\ 0 & 0 & -i \\ \pm 1 & i & 0 \end{pmatrix}. \tag{63}$$

We see that $J^2 = 2\mathsf{I}$, which means that every vector in ordinary space is an eigenvector of J^2 with eigenvalue $j(j+1) = 2$, that is, with $j = 1$. An irreducible subspace with $j = 1$ in any vector space must be 3-dimensional, but in this case the entire space is 3-dimensional, so the entire space consists of a single irreducible subspace under rotations with $j = 1$.

The fact that physical space carries the angular momentum value $j = 1$ is closely related to the fact that vector operators are irreducible tensor operators of order 1, as explained below. It is also connected with the fact that the photon, which is represented classically by the vector field $\mathbf{A}(\mathbf{x})$ (the vector potential), is a spin-1 particle.

Since every vector in three-dimensional space is an eigenvector of J^2, the standard basis consists of the eigenvectors of J_3, related by raising and lowering operators (this determines the phase conventions of the vectors, relative to that of the stretched vector). But we can easily check that the spherical unit vectors (41) are the eigenvectors of J_3, that is,

$$J_3 \hat{\mathbf{e}}_q = q\, \hat{\mathbf{e}}_q, \qquad q = 0, \pm 1. \tag{64}$$

Furthermore, it is easy to check that these vectors are related by raising and lowering operators, that is,

$$J_\pm \hat{\mathbf{e}}_q = \sqrt{(1 \mp q)(1 \pm q + 1)}\, \hat{\mathbf{e}}_{q\pm 1}, \tag{65}$$

where $J_\pm$ is given by Eq. (63). Only the overall phase of the spherical basis vectors is not determined by these relations. The overall phase chosen in the definitions (41) has the nice feature that $\hat{\mathbf{e}}_0 = \hat{\mathbf{z}}$.

Since the spherical basis is a standard angular momentum basis, its vectors must transform under rotations according to Eq. (13.85), apart from notation. Written in the notation appropriate for three-dimensional space, that transformation law becomes

$$\mathsf{R}\hat{\mathbf{e}}_q = \sum_{q'} \hat{\mathbf{e}}_{q'} D^1_{q'q}(\mathsf{R}). \tag{66}$$

We need not prove this as an independent result; it is just a special case of Eq. (13.85). This transformation law is also shown in the final column of Table 1, in order to emphasize its similarity to related transformation laws on other spaces.

Equation (66) has an interesting consequence, obtained by dotting both sides with $\hat{\mathbf{e}}^*_{q'}$. We use a round bracket notation for the dot product on the left hand side, and we use the orthogonality relation (42) on the right hand side, which picks out one term from the sum. We find

$$\left(\hat{\mathbf{e}}^*_{q'}, \mathsf{R}\hat{\mathbf{e}}_q\right) = D^1_{q'q}(\mathsf{R}), \tag{67}$$

which shows that $D^1_{q'q}$ is just the matrix representing the rotation operator on three-dimensional space with respect to the spherical basis. The usual rotation matrix contains the matrix elements

with respect to the Cartesian basis, that is,

$$\left(\hat{\mathbf{c}}_i, \mathsf{R}\hat{\mathbf{c}}_j\right) = R_{ij}. \tag{68}$$

See Eq. (11.7). For a given rotation, matrices R and D^1 are similar (they differ only by a change of basis).

15. Reducible and Irreducible Spaces of Operators

In the third row of Table 1 we consider the vector space of operators. The operators in question are the operators that act on the ket space of our quantum mechanical system, that is, they are the usual operators of quantum mechanics, for example, the Hamiltonian. Linear operators can be added and multiplied by scalars, so they form a vector space in the mathematical sense, but of course they also act on vectors (that is, kets). So the word "vector" is used in two different senses here. Rotations act on operators according to our definition (6), also shown in the second column of the table. Thus we have another example of a vector space upon which rotation operators act, and we can expect that the entire construction of Notes 13 will go through again, apart from notation.

Rather than filling in the rest of the table, however, let us return to the definition of a vector operator, Eq. (14), and interpret it in a different light. That definition concerns the three components V_1, V_2 and V_3 of a vector operator, each of which is an operator itself, and it says that if we rotate any one of these operators, we obtain a linear combination of the same three operators. Thus, any linear combination of these three operators is mapped into another such linear combination by any rotation, or, equivalently, the space of operators spanned by these three operators is invariant under rotations. Thus we view the three components of $\mathbf{V}$ as a set of "basis operators" spanning this space, which is a 3-dimensional subspace of the space of all operators. (We assume $\mathbf{V} \neq 0$.) A general element of this subspace of operators is an arbitrary linear combination of the three basis operators, that is, it has the form

$$a_1V_1 + a_2V_2 + a_3V_3 = \mathbf{a} \cdot \mathbf{V}, \tag{69}$$

a dot product of a vector of numbers $\mathbf{a}$ and a vector of operators $\mathbf{V}$.

If a subspace of a vector space is invariant under rotations, then we may ask whether it contains any smaller invariant subspaces. If not, we say it is *irreducible*. If so, it can be decomposed into smaller invariant subspaces, and we say it is *reducible*. The invariant subspaces of a reducible space may themselves be reducible or irreducible; if reducible, we decompose them further. We continue until we have only irreducible subspaces. Thus, every invariant subspace can be decomposed into irreducible subspaces, which in effect form the building blocks of any invariant subspace.

In the case of a ket space, the subspaces spanned by $|\gamma jm\rangle$ for fixed γ and j but $m = -j, \ldots, +j$ is, in fact, an irreducible subspace. The proof of this will not be important to us, but it is not hard. What about the three-dimensional space of operators spanned by the components of a vector operator? It turns out that it, too, is irreducible.

A simpler example of an irreducible subspace of operators is afforded by any scalar operator K. If $K \neq 0$, K can be thought of as a basis operator in a one-dimensional space of operators, in which the general element is aK, where a is a number (that is, the space contains all multiples of K). Since K is invariant under rotations [see Eq. (8)], this space is invariant. It is also irreducible, because a one-dimensional space contains no smaller subspace, so if invariant it is automatically irreducible.

We see that both scalar and vector operators are associated with irreducible subspaces of operators. What about second rank tensor operators T_{ij}? Such an "operator" is really a tensor of operators, that is, 9 operators that we can arrange in a 3×3 matrix. Assuming these operators are linearly independent, they span a 9-dimensional subspace of operators that is invariant under rotations, since according to Eq. (24) when we rotate any of these operators we get a linear combination of the same operators. This space, however, is reducible.

To see this, let us take the example (25) of a tensor operator, that is, $T_{ij} = V_i W_j$ where $\mathbf{V}$ and $\mathbf{W}$ are vector operators. This is not the most general form of a tensor operator, but it will illustrate the points we wish to make. A particular operator in the space of operators spanned by the components T_{ij} is the trace of T_{ij}, that is,

$$\operatorname{tr} T = T_{11} + T_{22} + T_{33} = \mathbf{V} \cdot \mathbf{W}. \tag{70}$$

Being a dot product of two vectors, this is a scalar operator, and is invariant under rotations. Therefore by itself it spans a 1-dimensional, irreducible subspace of the 9-dimensional space of operators spanned by the components of T_{ij}. The remaining (orthogonal) 8-dimensional subspace can be reduced further, for it possesses a 3-dimensional invariant subspace spanned by the operators,

$$\begin{aligned} X_3 &= T_{12} - T_{21} = V_1 W_2 - V_2 W_1, \\ X_1 &= T_{23} - T_{32} = V_2 W_3 - V_3 W_2, \\ X_2 &= T_{31} - T_{13} = V_3 W_1 - V_1 W_3, \end{aligned} \tag{71}$$

or, in other words,

$$\mathbf{X} = \mathbf{V} \times \mathbf{W}. \tag{72}$$

The components of $\mathbf{X}$ form a vector operator, so by themselves they span an irreducible invariant subspace under rotations. As we see, the components of $\mathbf{X}$ contain the antisymmetric part of the original tensor T_{ij}.

The remaining 5-dimensional subspace is irreducible. It is spanned by operators containing the symmetric part of the tensor T_{ij}, with the trace removed (or, as we say, the symmetric, traceless part of T_{ij}). The following five operators form a basis in this subspace:

$$\begin{aligned} S_1 &= T_{12} + T_{21}, \\ S_2 &= T_{23} + T_{32}, \\ S_3 &= T_{31} + T_{13}, \\ S_4 &= T_{11} - T_{22}, \\ S_5 &= T_{11} + T_{22} - 2T_{33}. \end{aligned} \tag{73}$$

The original tensor T_{ij} breaks up in three irreducible subspaces, a 1-dimensional scalar (the trace), a 3-dimensional vector (the antisymmetric part), and the 5-dimensional symmetric, traceless part. Notice that these dimensionalities are in accordance with the Clebsch-Gordan decomposition,

$$1 \otimes 1 = 0 \oplus 1 \oplus 2, \tag{74}$$

which corresponds to the count of dimensionalities,

$$3 \times 3 = 1 + 3 + 5 = 9. \tag{75}$$

This Clebsch-Gordan series arises because the vector operators $\mathbf{V}$ and $\mathbf{W}$ form two $\ell = 1$ irreducible subspaces of operators, and when we form T according to $T_{ij} = V_i W_j$, we are effectively combining angular momenta as indicated by Eq. (74). The only difference from our usual practice is that we are forming products of vector spaces of operators, instead of tensor products of ket spaces.

We have examined this decomposition in the special case $T_{ij} = V_i W_j$, but the decomposition itself applies to any second rank tensor T_{ij}. More generally, Cartesian tensors of any rank ≥ 2 are reducible.

It is possible that a given tensor T_{ij} may have one or more of the three irreducible components that vanish. The quadrupole moment tensor (26), for example, is already symmetric and traceless, so its nine components are actually linear combinations of just five independent operators. For another example, an antisymmetric tensor $T_{ij} = -T_{ji}$ contains only the three-dimensional (vector) subspace.

For many purposes it is desirable to organize tensors into their irreducible subspaces. This can be done by going over from the Cartesian to the spherical basis, and then constructing linear combinations using Clebsch-Gordan coefficients to end up with tensors transforming according to an irreducible representation of the rotations. We will say more about this process later.

16. Irreducible Tensor Operators

So far we have said nothing about a standard angular momentum basis of operators. The Cartesian components V_i of a vector operator do form a basis in a 3-dimensional, irreducible subspace of operators, but they do not transform under rotations as a standard angular momentum basis. We see this from the definition (14), which shows that if we rotate the basis operators V_i in this subspace, the coefficients of the linear combinations of the basis operators we obtain are Cartesian components of the rotation matrix R. When we rotate the basis vectors of a standard angular momentum basis, the coefficients are components of the D-matrices, as we see in Eq. (13.85). We now define a class of operators that do transform under rotations as a standard angular momentum basis.

We define an *irreducible tensor operator* of order k as a set of $2k+1$ operators T^k_q, for $q = -k, \ldots, +k$, that satisfy

$$\boxed{U\, T^k_q\, U^\dagger = \sum_{q'} T^k_{q'}\, D^k_{q'q}(U),} \tag{76}$$

for all rotation operators U. We denote the irreducible tensor operator itself by T^k, and its $2k+1$ components by T^k_q. This definition is really a version of Eq. (13.85), applied to the space of operators. It means that the components of an irreducible tensor operator are basis operators in a standard angular momentum basis that spans an irreducible subspace of operators. Thus we place T^k_q in the SAMB column of the third row of Table 1, and the transformation law (76) in the last column. The three transformation laws in the last column (for three different kinds of spaces) should be compared. We see that the order k of an irreducible tensor operator behaves like an angular momentum quantum number j, and q behaves like m.

However, unlike the standard angular momentum basis vectors in ket spaces, irreducible tensor operators are restricted to integer values of angular momentum quantum number k. The physical reason for this is that operators, which represent physically observable quantities, must be invariant under a rotation of 2π; the mathematical reason is that our definition of a rotated operator, given by Eq. (6), is quadratic $U(\mathsf{R})$, so that the representation of rotations on the vector space of operators is always a single-valued representation of $SO(3)$.

Let us examine some examples of irreducible tensor operators. A scalar operator K is an irreducible tensor operator of order 0, that is, it is an example of an irreducible tensor operator T^0_0. This follows easily from the fact that K commutes with any rotation operator U, and from the fact that the $j=0$ rotation matrices are simply given by the 1×1 matrix (1) [see Eq. (13.68)].

Irreducible tensor operators of order 1 are constructed from vector operators by transforming from the Cartesian basis to the spherical basis. If we let $\mathbf{V}$ be a vector operator as defined by Eq. (13), and define its spherical components by

$$V_q = T^1_q = \hat{\mathbf{e}}_q \cdot \mathbf{V}, \tag{77}$$

then we have

$$\begin{aligned} U(\mathsf{R})V_q U(\mathsf{R})^\dagger &= \hat{\mathbf{e}}_q \cdot (\mathsf{R}^{-1}\mathbf{V}) = (\mathsf{R}\hat{\mathbf{e}}_q)\cdot \mathbf{V} \\ &= \sum_{q'} V_{q'} D^1_{q'q}(\mathsf{R}), \end{aligned} \tag{78}$$

where we use Eq. (66).

The electric quadrupole operator is given as a Cartesian tensor in Eq. (26). This Cartesian tensor is symmetric and traceless, so it contains only 5 independent components, which span an irreducible subspace of operators. In fact, this subspace is associated with angular momentum value $k=2$. It is possible to introduce a set of operators T^2_q, $q=-2,\ldots,+2$ that form a standard angular momentum basis in this space, that is, that form an order 2 irreducible tensor operator. These can be regarded as the spherical components of the quadrupole moment tensor. We will explore this subject in more detail later.

17. Commutation Relations of an Irreducible Tensor Operator with J

Above we presented two equivalent definitions of scalar and vector operators, one involving transformation properties under rotations, and the other involving commutation relations with **J**. We will now do the same with irreducible tensor operators. To this end, we substitute the infinitesimal form (15) of the rotation operator U into both sides of the definition (76).

On the right we will need the D-matrix for an infinitesimal rotation. Since the D-matrix contains just the matrix elements of U with respect to a standard angular momentum basis [this is the definition of the D-matrices, see Eq. (13.56)], we require these matrix elements in the case of an infinitesimal rotation. For $\theta \ll 1$, Eq. (13.56) becomes

$$D^j_{m'm}(\hat{\mathbf{n}},\theta) = \langle jm'|\Big(1 - \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{J}\Big)|jm\rangle = \delta_{m'm} - \frac{i}{\hbar}\theta\langle jm'|\hat{\mathbf{n}}\cdot\mathbf{J}|jm\rangle. \tag{79}$$

Changing notation $(jm'm) \to (kq'q)$ and substituting this and Eq. (15) into the definition (76) of an irreducible tensor operator, we obtain

$$\Big(1 - \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{J}\Big)T^k_q\Big(1 + \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\mathbf{J}\Big) = \sum_{q'} T^k_{q'}\Big(\delta_{q'q} - \frac{i}{\hbar}\theta\langle kq'|\hat{\mathbf{n}}\cdot\mathbf{J}|kq\rangle\Big), \tag{80}$$

or, since $\hat{\mathbf{n}}$ arbitrary unit vector,

$$[\mathbf{J}, T^k_q] = \sum_{q'} T^k_{q'}\langle kq'|\mathbf{J}|kq\rangle. \tag{81}$$

The operators **J** on the left- and right-hand sides of Eqs. (80) and (81) are not the same operators. On the left **J** is the angular momentum on the same space upon which the operators T^k_q act; in practice this is usually the state space of a quantum system. The **J** on the right is the angular momentum operator on a model space in which the matrices $D^k_{q'q}$ are defined. See the discussion in Sec. 18.13.

Equation (81) specifies a complete set of commutation relations of the components of **J** with the components of an irreducible tensor operator, but it is usually transformed into a different form. First we take the z-component of both sides and use $J_z|kq\rangle = \hbar q|kq\rangle$, so that

$$\langle kq'|J_z|kq\rangle = q\hbar\,\delta_{q'q}. \tag{82}$$

This is Eq. (13.47) with a change of notation. Then Eq. (81) becomes Eq. (89a) below. Next dot both sides of Eq. (81) with $\hat{\mathbf{x}} \pm i\hat{\mathbf{y}}$, and use

$$J_\pm|kq\rangle = \sqrt{(k \mp q)(k \pm q + 1)}\hbar\,|k, q \pm 1\rangle, \tag{83}$$

or

$$\langle kq'|J_\pm|kq\rangle = \sqrt{(k \mp q)(k \pm q + 1)}\hbar\,\delta_{q',q\pm1}. \tag{84}$$

This is Eq. (13.48b) with a change of notation. Then we obtain Eq. (89b) below. Finally, take the i-th component of Eq. (81),

$$[J_i, T^k_q] = \sum_{q'} T^k_{q'}\langle kq'|J_i|kq\rangle, \tag{85}$$

and form the commutator of both sides with J_i,

$$\begin{aligned}[J_i,[J_i,T^k_q]] &= \sum_{q'}[J_i,T^k_{q'}]\langle kq'|J_i|kq\rangle = \sum_{q'q''} T^k_{q''}\langle kq''|J_i|kq'\rangle\langle kq'|J_i|kq\rangle \\ &= \sum_{q''} T^k_{q''}\langle kq''|J_i^2|kq\rangle,\end{aligned} \tag{86}$$

where we have used Eq. (81) again to create a double sum. Finally summing both sides over i, we obtain,

$$\sum_i [J_i,[J_i,T^k_q]] = \sum_{q''} T^k_{q''}\langle kq''|J^2|kq\rangle. \tag{87}$$

But

$$\langle kq''|J^2|kq\rangle = k(k+1)\hbar^2\,\delta_{q''q}, \tag{88}$$

a version of Eq. (13.46), so we obtain Eq. (89c) below.

In summary, an irreducible tensor operator satisfies the following commutation relations with the components of angular momentum:

$$[J_z,T^k_q] = \hbar q\,T^k_q, \tag{89a}$$

$$[J_\pm,T^k_q] = \hbar\sqrt{(k\mp q)(k\pm q+1)}\,T^k_{q\pm1}, \tag{89b}$$

$$\sum_i [J_i,[J_i,T^k_q]] = \hbar^2 k(k+1)\,T^k_q. \tag{89c}$$

We see that forming the commutator with $J_\pm$ plays the role of a raising or lowering operator for the components of an irreducible tensor operator. As we did with scalar and vector operators, we can show that these angular momentum commutation relations are equivalent to the definition (76) of an irreducible tensor operator. This is done by showing that Eqs. (89) are equivalent to Eq. (76) in the case of infinitesimal rotations, and that if Eq. (76) is true for any two rotations, it is also true for their product. Thus by building up finite rotations as products of infinitesimal ones we show the equivalence of Eqs. (76) and (89). Many books take Eqs. (89) as the definition of an irreducible tensor operator.

18. Statement and Applications of the Wigner-Eckart Theorem

The Wigner-Eckart theorem is not difficult to remember and it is quite easy to use. In this section we discuss the statement of the theorem and ways of thinking about it and its applications, before turning to its proof.

The Wigner-Eckart theorem concerns matrix elements of an irreducible tensor operator with respect to a standard angular momentum basis of kets, something we will write in a general notation as $\langle\gamma' j'm'|T^k_q|\gamma jm\rangle$. As an example of such a matrix element, you may think of the dipole matrix elements $\langle n'\ell'm'|x_q|n\ell m\rangle$ that we examined in Sec. 13. In that case the operator (the position or dipole operator) is an irreducible tensor operator with $k=1$.

The matrix element $\langle \gamma' j' m' | T^k_q | \gamma j m \rangle$ depends on 8 indices, $(\gamma' j' m'; \gamma j m; kq)$, and in addition it depends on the specific operator T in question. The Wigner-Eckart theorem concerns the dependence of this matrix element on the three magnetic quantum numbers $(m'mq)$, and states that that dependence is captured by a Clebsch-Gordan coefficient. More specifically, the Wigner-Eckart theorem states that $\langle \gamma' j' m' | T^k_q | \gamma j m \rangle$ is proportional to the Clebsch-Gordan coefficient $\langle j' m' | jkmq \rangle$, with a proportionality factor that is independent of the magnetic quantum numbers. That proportionality factor depends in general on everything else besides the magnetic quantum numbers, that is, $(\gamma' j'; \gamma j; k)$ and the operator in question. The standard notation for the proportionality factor is $\langle \gamma' j' \| T^k \| \gamma j \rangle$, something that looks like the original matrix element except the magnetic quantum numbers are omitted and a double bar is used. The quantity $\langle \gamma' j' \| T^k \| \gamma j \rangle$ is called the *reduced matrix element*. With this notation, the Wigner-Eckart theorem states

$$\boxed{\langle \gamma' j' m' | T^k_q | \gamma j m \rangle = \langle \gamma' j' \| T^k \| \gamma j \rangle \, \langle j' m' | jkmq \rangle.} \tag{90}$$

The reduced matrix element can be thought of as depending on the irreducible tensor operator T^k and the two irreducible subspaces $(\gamma' j')$ and (γj) that it links. Some authors (for example, Sakurai) include a factor of $1/\sqrt{2j+1}$ on the right hand side of Eq. (90), but here that factor has been absorbed into the definition of the reduced matrix element. The version (90) is easier to remember and closer to the basic idea of the theorem.

To remember the Clebsch-Gordan coefficient it helps to suppress the bra $\langle \gamma' j' m' |$ from the matrix element and think of the ket $T^k_q | \gamma j m \rangle$, or, more precisely, the $(2j+1)(2k+1)$ kets that are produced by letting m and q vary over their respective ranges. This gives an example of an operator with certain angular momentum indices multiplying a ket with certain angular momentum indices. It turns out that such a product of an operator times a ket has much in common with the product (i.e., the tensor product) of two kets, insofar as the transformation properties of the product under rotations are concerned. That is, suppose we were multiplying a ket $|kq\rangle$ with the given angular momentum quantum numbers times another ket $|jm\rangle$ with different angular momentum quantum numbers. Then we could find the eigenstates of total angular momentum by combining the constituent angular momenta according to $k \otimes j$. Actually, in thinking of kets $T^k_q | jm \rangle$, it is customary to think of the product of the angular momenta in the reverse order, that is, $j \otimes k$. This is an irritating convention because it makes the Wigner-Eckart theorem harder to remember, but I suspect it is done this way because in practice k tends to be small and j large.

In any case, thinking of the product of kets, the product

$$|jm\rangle \otimes |kq\rangle = |jkmq\rangle \tag{91}$$

contains various components of total J^2 and J_z, that is, it can be expanded as a linear combination of eigenstates of total J^2 and J^z, with expansion coefficients that are the Clebsch-Gordan coefficients. The coefficient with total angular momentum j' and z-component m' is the Clebsch-Gordan coefficient $\langle j' m' | jkmq \rangle$, precisely what appears in the Wigner-Eckart theorem (90).

Probably the most useful application of the Wigner-Eckart theorem is that it allows us to easily write down selection rules for the given matrix element, based on the selection rules of the Clebsch-Gordan coefficient occurring in Eq. (90). In general, a *selection rule* is a rule that tells us when a matrix element must vanish on account of some symmetry consideration. The Wigner-Eckart theorem provides us with all the selection rules that follow from rotational symmetry; a given matrix element may have other selection rules based on other symmetries (for example, parity). The selection rules that follow from the Wigner-Eckart theorem are that the matrix element $\langle \gamma j' m' | T^k_q | \gamma j m \rangle$ vanishes unless $m' = m + q$ and j' takes on one of the values, $|j - k|, |j - k| + 1, \ldots, j + k$.

Furthermore, suppose we actually have to evaluate the matrix elements $\langle \gamma' j' m' | T^k_q | \gamma j m \rangle$ for all $(2k + 1)(2j + 1)$ possibilities we get by varying q and m. We must do this, for example, in computing atomic transition rates. (We need not vary m' independently, since the selection rules enforce $m' = m+q$.) Then the Wigner-Eckart theorem tells us that we actually only have to do one of these matrix elements (presumably, whichever is the easiest), because if we know the left hand side of Eq. (90) for one set of magnetic quantum numbers, and if we know the Clebsch-Gordan coefficient on the right-hand side, then we can determine the proportionality factor, that is, the reduced matrix element. Then all the other matrix elements for other values of the magnetic quantum numbers follow by computing (or looking up) Clebsch-Gordan coefficients. This procedure requires that the first matrix element we calculate be nonzero.

In some other cases, we have analytic formulas for the reduced matrix element. That was the case of the application in Sec. 13, where the three-$Y_{\ell m}$ formula allowed us to compute the proportionality factor explicitly.

19. The Wigner-Eckart Theorem for Scalar Operators

Let us consider a scalar operator for which $k = q = 0$, such as the Hamiltonian H for an isolated system, that is, with $T^0_0 = H$. In this case the Clebsch-Gordan coefficient is

$$\langle j' m' | j 0 m 0 \rangle = \delta_{j' j}\, \delta_{m' m}, \tag{92}$$

so the Wigner-Eckart theorem can be written

$$\langle \gamma' j' m' | H | \gamma j m \rangle = C^j_{\gamma' \gamma}\, \delta_{j' j}\, \delta_{m' m}, \tag{93}$$

where

$$C^j_{\gamma' \gamma} = \langle \gamma' j \| H \| \gamma j \rangle. \tag{94}$$

We write it this way because $C^j_{\gamma' \gamma}$ can be seen as a set of matrices, labeled by j and indexed by $(\gamma' \gamma)$. The size of the j-th matrix is N_j, the multiplicity of the j value in the system under consideration. In practice the multiplicity is often infinite. The problem of finding the energy eigenvalues of the system amounts to diagonalizing each of the matrices $C^j_{\gamma' \gamma}$.

20. Proof of the Wigner-Eckart Theorem

Consider the product of kets $|jm\rangle \otimes |kq\rangle = |jkmq\rangle$ with the given angular momentum quantum numbers, and consider the $(2j+1)(2k+1)$-dimensional product space spanned by such kets when we allow the magnetic quantum numbers m and q to vary over their respective ranges. The eigenstates $|JM\rangle$ of total J^2 and J_z in this space are given by the Clebsch-Gordan expansion,

$$|JM\rangle = \sum_{mq} |jkmq\rangle\langle jkmq|JM\rangle. \tag{95}$$

Moreover, the states $|JM\rangle$ for fixed J and $M = -J, \ldots, +J$ form a standard angular momentum basis in an invariant, irreducible subspace of dimension $2J+1$ in the product space. This means that the basis states $|JM\rangle$ are not only eigenstates of total J^2 and J_z, but they are also linked by raising and lowering operators. Equivalently, the states $|JM\rangle$ transform as a standard angular momentum basis under rotations,

$$U|JM\rangle = \sum_{M'} |JM'\rangle D^J_{M'M}(U). \tag{96}$$

Now consider the $(2j+1)(2k+1)$ kets $T^k_q|\gamma jm\rangle$ obtained by varying m and q. We construct linear combinations of these with the same Clebsch-Gordan coefficients as in Eq. (95),

$$|X; JM\rangle = \sum_{mq} T^k_q|\gamma jm\rangle\langle jkmq|JM\rangle, \tag{97}$$

and define the result to be the ket $|X; JM\rangle$, as indicated. The indices JM in the ket $|X; JM\rangle$ indicate that the left-hand side depends on these indices, because the right hand side does; initially we assume nothing else about this notation. Similarly, X simply stands for everything else the left-hand side depends on, that is, X is an abbreviation for the indices (γkj).

However, in view of the similarity between Eqs. (95) and (97), we can guess that $|X; JM\rangle$ is actually an eigenstate of J^2 and J_z with quantum numbers J and M, and that the states $|X; JM\rangle$ are related by raising and lowering operators. That is, we guess

$$J_z|X; JM\rangle = M\hbar\,|X; JM\rangle, \tag{98a}$$

$$J_\pm|X; JM\rangle = \sqrt{(J \mp M)(J \pm M + 1)}\hbar\,|X; J, M \pm 1\rangle, \tag{98b}$$

$$J^2|X; JM\rangle = J(J+1)\hbar^2\,|X; JM\rangle. \tag{98c}$$

If true, this is equivalent to the transformation law,

$$U|X; JM\rangle = \sum_{M'} |X; JM'\rangle\, D^J_{M'M}(U), \tag{99}$$

exactly as in Eq. (96). Equations (98) and (99) are equivalent because Eq. (98) can be obtained from Eq. (99) by specializing to infinitesimal rotations, while Eq. (99) can be obtained from Eq. (98) by building up finite rotations out of infinitesimal ones.

In Sec. 21 below we will prove that these guesses are correct. For now we merely explore the consequences. To begin, since $|X;JM\rangle$ is an eigenstate of J^2 and J_z with quantum numbers J and M, it can be expanded as a linear combination of the standard basis kets $|\gamma jm\rangle$ with the same values $j = J$ and $m = M$, but in general all possible values of γ. That is, we have an expansion of the form,

$$|X;JM\rangle = \sum_{\gamma'} |\gamma' JM\rangle\, C^{kJMj}_{\gamma'\gamma}, \tag{100}$$

where the indices on the expansion coefficients $C^{kJMj}_{\gamma'\gamma}$ simply list all the parameters they can depend on. These coefficients, do not, however, depend on M, as we show by applying raising or lowering operators to both sides, and using Eq. (98*b*). This gives

$$\begin{aligned}\sqrt{(J\mp M)(J\pm M+1)}\hbar\,|X;J,M\pm 1\rangle \\ = \sum_{\gamma'} \sqrt{(J\mp M)(J\pm M+1)}\hbar\,|\gamma' J,M\pm 1\rangle\, C^{kJMj}_{\gamma'\gamma},\end{aligned} \tag{101}$$

or, after canceling the square roots,

$$|X;J,M\pm 1\rangle = \sum_{\gamma'} |\gamma' J,M\pm 1\rangle\, C^{kJMj}_{\gamma'\gamma}. \tag{102}$$

Comparing this to Eq. (100), we see that the expansion coefficients are the same for all M values, and thus independent of M. We will henceforth write simply $C^{kJj}_{\gamma'\gamma}$ for them.

Now we return to the definition (97) of the kets $|X;JM\rangle$ and use the orthogonality of the Clebsch-Gordan coefficients (18.50) to solve for the kets $T^k_q|\gamma jm\rangle$. This gives

$$T^k_q|\gamma jm\rangle = \sum_{JM} |X;JM\rangle\langle JM|jkmq\rangle = \sum_{\gamma'' JM} |\gamma'' JM\rangle\, C^{kJj}_{\gamma''\gamma}\,\langle JM|jkmq\rangle, \tag{103}$$

where we use Eq. (100), replacing γ' with γ''. Now multiplying this by $\langle\gamma' j' m'|$ and using the orthonormality of the basis $|\gamma jm\rangle$, we obtain

$$\langle\gamma' j' m'|T^k_q|\gamma jm\rangle = C^{kj'j}_{\gamma'\gamma}\,\langle j'm'|jkmq\rangle, \tag{104}$$

which is the Wigner-Eckart theorem (90) if we identify

$$C^{kj'j}_{\gamma'\gamma} = \langle\gamma' j'\|T^k\|\gamma j\rangle. \tag{105}$$

21. Proof of Eq. (99)

To complete the proof of the Wigner-Eckart theorem we must prove Eq. (99), that is, we must show that the kets $|X;JM\rangle$ transform under rotations like the vectors of a standard angular momentum basis. To do this we call on the definition of $|X;JM\rangle$, Eq. (97), and apply U to both sides,

$$U|X;JM\rangle = \sum_{mq} UT^k_q U^\dagger\, U|\gamma jm\rangle\langle jkmq|JM\rangle. \tag{106}$$

Next we use the definition of an irreducible tensor operator (76) and the transformation law for standard basis vectors under rotations, Eq. (13.85), to obtain

$$U|X;JM\rangle = \sum_{\substack{mq\\m'q'}} T^k_{q'}|\gamma jm'\rangle\, D^j_{m'm}(U)\, D^k_{q'q}(U)\, \langle jkmq|JM\rangle. \tag{107}$$

We now call on Eq. (18.64) with a change of indices,

$$D^j_{m'm}(U)D^k_{q'q}(U) = \sum_{J'M'M''} \langle jkm'q'|J'M'\rangle\, D^{J'}_{M'M''}(U)\, \langle J'M''|jkmq\rangle, \tag{108}$$

which expresses the product of D-matrices in Eq. (107) in terms of single D-matrices. When we substitute Eq. (108) into Eq. (107), the $m'q'$-sum is doable by the definition (97),

$$\sum_{m'q'} T^k_{q'}|\gamma jm'\rangle\langle jkm'q'|J'M'\rangle = |X;J'M'\rangle, \tag{109}$$

and the mq-sum is doable by the orthogonality of the Clebsch-Gordan coefficients,

$$\sum_{mq}\langle J'M''|jkmq\rangle\langle jkmq|JM\rangle = \delta_{J'J}\,\delta_{M''M}. \tag{110}$$

Altogether, Eq. (107) becomes

$$U|X;JM\rangle = \sum_{J'M'M''} |X;J'M'\rangle D^{J'}_{M'M''}(U)\,\delta_{J'J}\,\delta_{M''M} = \sum_{M'} |X;JM'\rangle D^J_{M'M}(U). \tag{111}$$

This proves Eq. (99).

Instead of proving Eq. (99), many authors (for example, Sakurai) prove the equivalent set of statements (98), which involve the actions of the angular momentum operators on the states $|X;JM\rangle$. I think the transformation properties under rotations are little easier. In either case, the rest of the proof is the same.

22. Products of Irreducible Tensor Operators

As we have seen, the idea behind the Wigner-Eckart theorem is that a product of an irreducible tensor operator T^k_q times a ket of the standard basis $|\gamma jm\rangle$ transforms under rotations exactly as the tensor product of two kets of standard bases with the same quantum numbers, $|jm\rangle\otimes|kq\rangle$. Similarly, it turns out that the product of two irreducible tensor operators, say, $X^{k_1}_{q_1}Y^{k_2}_{q_2}$, transforms under rotations exactly like the tensor product of kets with the same quantum numbers, $|k_1q_1\rangle\otimes|k_2q_2\rangle$. In particular, such a product of operators can be represented as a linear combination of irreducible tensor operators with order k lying in the range $|k_1-k_2|,\ldots,k_1+k_2$, with coefficients that are Clebsch-Gordan coefficients. That is, we can write

$$X^{k_1}_{q_1}Y^{k_2}_{q_2} = \sum_{kq} T^k_q\, \langle kq|k_1k_2q_1q_2\rangle, \tag{112}$$

where the T^k_q are new irreducible tensor operators.

To prove this, we first solve for T^k_q,

$$T^k_q = \sum_{q_1 q_2} X^{k_1}_{q_1} Y^{k_2}_{q_2} \langle k_1 k_2 q_1 q_2 | k q \rangle, \tag{113}$$

which we must show is an irreducible tensor operator. To do this, we conjugate both sides of this with a rotation operator U and use the fact that X and Y are irreducible tensor operators,

$$\begin{aligned} U T^k_q U^\dagger &= \sum_{q_1 q_2} U X^{k_1}_{q_1} U^\dagger \, U Y^{k_2}_{q_2} U^\dagger \, \langle k_1 k_2 q_1 q_2 | k q \rangle \\ &= \sum_{\substack{q_1 q_2 \\ q_1' q_2'}} X^{k_1}_{q_1'} Y^{k_2}_{q_2'} \, D^{k_1}_{q_1' q_1}(U) D^{k_2}_{q_2' q_2}(U) \, \langle k_1 k_2 q_1 q_2 | k q \rangle. \end{aligned} \tag{114}$$

Next we use Eq. (18.64) with a change of symbols,

$$D^{k_1}_{q_1' q_1}(U) D^{k_2}_{q_2' q_2}(U) = \sum_{K Q Q'} \langle k_1 k_2 q_1' q_2' | K Q' \rangle D^K_{Q' Q}(U) \langle K Q | k_1 k_2 q_1 q_2 \rangle, \tag{115}$$

which we substitute into Eq. (114). Then the $q_1' q_2'$-sum is doable in terms of the expression (113) for T^k_q,

$$\sum_{q_1' q_2'} X^{k_1}_{q_1'} Y^{k_2}_{q_2'} \langle k_1 k_2 q_1' q_2' | K Q' \rangle = T^K_{Q'}, \tag{116}$$

and the $q_1 q_2$-sum is doable by the orthogonality of the Clebsch-Gordan coefficients,

$$\sum_{q_1 q_2} \langle K Q | k_1 k_2 q_1 q_2 \rangle \langle k_1 k_2 q_1 q_2 | k q \rangle = \delta_{Kk} \, \delta_{Qq}. \tag{117}$$

Then Eq. (114) becomes

$$U T^k_q U^\dagger = \sum_{K Q Q'} T^K_{Q'} D^K_{Q' Q} \, \delta_{Kk} \, \delta_{Qq} = \sum_{q'} T^k_{q'} D^k_{q' q}(U). \tag{118}$$

This shows that T^k_q is an irreducible tensor operator, as claimed.

As an application, two vector operators $\mathbf{V}$ and $\mathbf{W}$, may be converted into $k = 1$ irreducible tensor operators V_q and W_q by going over to the spherical basis. From these we can construct $k = 0, 1, 2$ irreducible tensor operators according to

$$T^k_q = \sum_{q_1 q_2} V_{q_1} W_{q_2} \langle 1 1 q_1 q_2 | k q \rangle. \tag{119}$$

This will yield the same decomposition of a second rank tensor discussed in Sec. 15, where we found a scalar ($k = 0$), a vector ($k = 1$), and a symmetric, traceless tensor ($k = 2$).

Problems

1. This will help you understand irreducible tensor operators better. Let $\mathcal{E}$ be a ket space for some system of interest, and let $\mathcal{A}$ be the space of linear operators that act on $\mathcal{E}$. For example, the ordinary Hamiltonian is contained in $\mathcal{A}$, as are the components of the angular momentum $\mathbf{J}$, the rotation operators $U(\mathsf{R})$, etc. The space $\mathcal{A}$ is a vector space in its own right, just like $\mathcal{E}$; operators can be added, multiplied by complex scalars, etc. Furthermore, we may be interested in certain subspaces of $\mathcal{A}$, such as the 3-dimensional space of operators spanned by the components V_x, V_y, V_z of a vector operator $\mathbf{V}$.

Now let $\mathcal{S}$ be the space of linear operators that act on $\mathcal{A}$. We call an element of $\mathcal{S}$ a "super" operator because it acts on ordinary operators; ordinary operators in $\mathcal{A}$ act on kets in $\mathcal{E}$. We will denote super-operators with a hat, to distinguish them from ordinary operators. (This terminology has nothing to do with supersymmetry.)

Given an ordinary operator $A \in \mathcal{A}$, it is possible to associate it in several different ways with a super-operator. For example, we can define a super operator $\hat{A}_L$, which acts by left multiplication:

$$\hat{A}_L X = AX, \tag{120}$$

where X is an arbitrary ordinary operator. This equation obviously defines a linear super-operator, that is, $\hat{A}_L(X+Y) = \hat{A}_L X + \hat{A}_L Y$, etc. Similarly, we can define a super-operator associated with A by means of right multiplication, or by means of the forming of the commutator, as follows:

$$\begin{aligned} \hat{A}_R X &= XA, \\ \hat{A}_C X &= [A, X]. \end{aligned} \tag{121}$$

There are still other ways of associating an ordinary operator with a super-operator. Let R be a classical rotation, and let $U(\mathsf{R})$ be a representation of the rotations acting on the ket space $\mathcal{E}$. Thus, the operators $U(\mathsf{R})$ belong to the space $\mathcal{A}$. Now associate such a rotation operator $U(\mathsf{R})$ in $\mathcal{A}$ with a super-operator $\hat{U}(\mathsf{R})$ in $\mathcal{S}$, defined by

$$\hat{U}(\mathsf{R})X = U(\mathsf{R})\, X\, U(\mathsf{R})^\dagger. \tag{122}$$

Again, $\hat{U}(\mathsf{R})$ is obviously a linear super-operator.

(a) Show that $\hat{U}(\mathsf{R})$ forms a representation of the rotations, that is, that

$$\hat{U}(\mathsf{R}_1)\hat{U}(\mathsf{R}_2) = \hat{U}(\mathsf{R}_1\mathsf{R}_2). \tag{123}$$

This is easy.

Now let $U(\mathsf{R})$ be infinitesimal as in Eq. (15), and let

$$\hat{U}(\mathsf{R}) = 1 - \frac{i}{\hbar}\theta\hat{\mathbf{n}}\cdot\hat{\mathbf{J}}. \tag{124}$$

(Here the hat on $\hat{\mathbf{n}}$ denotes a unit vector, while that on $\hat{\mathbf{J}}$ denotes a super-operator.) Express the super-operator $\hat{\mathbf{J}}$ in terms of ordinary operators. Write Eqs. (89) in super-operator notation. Work out the commutation relations of the super-operators $\hat{\mathbf{J}}$.

(b) Now write out nine equations, specifying the action of the three super-operators $\hat{J}_i$ on the the basis operators V_j. Write the answers as linear combinations of the V_j's. Then write out six more equations, specifying the action of the super raising and lowering operators, $\hat{J}_\pm$, on the three V_j.

Now find the operator A that is annihilated by $\hat{J}_+$. Do this by writing out the unknown operator as a linear combination of the V_j's, in the form

$$A = a_x V_x + a_y V_y + a_z V_z, \tag{125}$$

and then solving for the coefficients a_i. Show that this operator is an eigenoperator of $\hat{J}_z$ with eigenvalue $+\hbar$. In view of these facts, the operator A must be a "stretched" operator for $k = 1$; henceforth write T^1_1 for it. This operator will have an arbitrary, complex multiplicative constant, call it c. Now apply $\hat{J}_-$, and generate T^1_0 and T^1_{-1}. Choose the constant c to make T^1_0 look as simple as possible. Then write

$$T^1_q = \hat{\mathbf{e}}_q \cdot \mathbf{V}, \tag{126}$$

and thereby "discover" the spherical basis.

2. This problem concerns quadrupole moments and spins. It provides some background for problem 3.

(a) In the case of a nucleus, the spin Hilbert space $\mathcal{E}_{\text{spin}} = \text{span}\{|sm\rangle, m = -s, \ldots, +s\}$ is actually the ground state of the nucleus. It is customary to denote the angular momentum j of the ground state by s. This state is $(2s+1)$-fold degenerate. The nuclear spin operator $\mathbf{S}$ is really the restriction of the total angular momentum of the nucleus $\mathbf{J}$ to this subspace of the (much larger) nuclear Hilbert space.

Let A^k_q and B^k_q be two irreducible tensor operators on $\mathcal{E}_{\text{spin}}$. As explained in these notes, when we say "irreducible tensor operator" we are really talking about the collection of $2k+1$ operators obtained by setting $q = -k, \ldots, +k$. Use the Wigner-Eckart theorem to explain why any two such operators of the same order k are proportional to one another. This need not be a long answer.

Thus, all scalars are proportional to a standard scalar (1 is convenient), and all vector operators (for example, the magnetic moment $\boldsymbol{\mu}$) are proportional to a standard vector ($\mathbf{S}$ is convenient), etc.

For a given s, what is the maximum value of k? What is the maximum order of an irreducible tensor operator that can exist on space $\mathcal{E}_{\text{spin}}$ for a proton (nucleus of ordinary hydrogen)? A deuteron (heavy hydrogen)? An alpha particle (nucleus of helium)? These rules limit the electric and magnetic multipole moments that a nucleus is allowed to have, as is discussed more fully in Notes 26.

(b) Let $\mathbf{A}$ and $\mathbf{B}$ be two vector operators (on any Hilbert space, not necessarily $\mathcal{E}_{\text{spin}}$), with spherical components A_q, B_q, as in Eq. (77). As explained in the notes, A_q and B_q are $k = 1$ irreducible

tensor operators. As explained in Sec. 22, it is possible to construct irreducible tensor operators T^k_q for $k = 0, 1, 2$ out of the nine operators, $\{A_q B_{q'}, q, q' = -1, 0, 1\}$. Write out the three operators T^0_0, T^1_1 and T^2_2 in terms of the Cartesian products $A_i B_j$. Just look up the Clebsch-Gordan coefficients. There are nine operators in T^0_0, T^1_q and T^2_q, but I'm only asking you to compute these three to save you some work.

Show that T^0_0 is proportional to $\mathbf{A} \cdot \mathbf{B}$, that T^1_1 is proportional to a spherical component of $\mathbf{A} \times \mathbf{B}$, and that T^2_2 can be written in terms of the components of the symmetric and traceless part of the Cartesian tensor $A_i B_j$, which is

$$\frac{1}{2}(A_i B_j + A_j B_i) - \frac{1}{3}(\mathbf{A} \cdot \mathbf{B})\delta_{ij}. \tag{127}$$

(c) In classical electrostatics, the quadrupole moment tensor Q_{ij} of a charge distribution $\rho(\mathbf{x})$ is defined by

$$Q_{ij} = \int d^3\mathbf{x}\, \rho(\mathbf{x})[3x_i x_j - r^2\, \delta_{ij}], \tag{128}$$

where $\mathbf{x}$ is measured relative to some origin inside the charge distribution. The quadrupole moment tensor is a symmetric, traceless tensor. The quadrupole energy of interaction of the charge distribution with an external electric field $\mathbf{E} = -\nabla\phi$ is

$$E_{\rm quad} = \frac{1}{6}\sum_{ij} Q_{ij} \frac{\partial^2 \phi(0)}{\partial x_i \partial x_j}. \tag{129}$$

This energy must be added to the monopole and dipole energies, plus the higher multipole energies.

In the case of a nucleus, we choose the origin to be the center of mass, whereupon the dipole moment and dipole energy vanish. The monopole energy is just the usual Coulomb energy $q\phi(0)$, where q is the total charge of the nucleus. Thus, the quadrupole term is the first nonvanishing correction. However, the energy must be understood in the quantum mechanical sense.

Let $\{\mathbf{x}_\alpha, \alpha = 1, \ldots, Z\}$ be the position operators for the protons in a nucleus. The neutrons are neutral, and do not contribute to the electrostatic energy. The electric quadrupole moment operator for the nucleus is defined by

$$Q_{ij} = e\sum_\alpha (3x_{\alpha i} x_{\alpha j} - r^2_\alpha\, \delta_{ij}), \tag{130}$$

where e is the charge of a single proton. In an external electric field, the nuclear Hamiltonian contains a term $H_{\rm quad}$, exactly in the form of Eq. (129), but now interpreted as an operator.

The operator Q_{ij}, being symmetric and traceless, constitutes the Cartesian specification of a $k = 2$ irreducible tensor operator, that you could turn into standard form $T^2_q, q = -2, \ldots, +2$ using the method of part (b) if you wanted to. We'll stay with the Cartesian form here, however. When the operator Q_{ij} is restricted to the ground state (really a manifold of $2s + 1$ degenerate states), it remains a $k = 2$ irreducible tensor operator. According to part (a), it must be proportional to some standard irreducible tensor operator, for which $3S_i S_j - S^2\delta_{ij}$ is convenient. That is, we must be able to write

$$Q_{ij} = a(3S_i S_j - S^2\delta_{ij}), \tag{131}$$

for some constant a.

It is customary in nuclear physics to denote the "quadrupole moment" of the nucleus by the real number Q, defined by

$$Q = \langle ss|Q_{33}|ss\rangle, \tag{132}$$

where $|ss\rangle$ is the stretched state. Don't confuse Q_{ij}, a tensor of operators, with Q, a single number.

The book, *Modern Quantum Mechanics* by J. J. Sakurai gives the interaction energy of a nucleus in an external electric field as

$$H_{\rm int} = \frac{eQ}{2s(s-1)\hbar^2}\Big[\Big(\frac{\partial^2\phi}{\partial x^2}\Big)S_x^2 + \Big(\frac{\partial^2\phi}{\partial y^2}\Big)S_y^2 + \Big(\frac{\partial^2\phi}{\partial z^2}\Big)S_z^2\Big], \tag{133}$$

where ϕ is the electrostatic potential for the external field satisfying the Laplace equation $\nabla^2\phi = 0$ and where the coordinate axes are chosen so that the off-diagonal elements of $\partial^2\phi/\partial x_i\partial x_j$ vanish. Here ϕ and its derivatives are evaluated at the center of mass of the nucleus and ϕ satisfies the Laplace equation rather than the Poisson equation because the sources of the external electric field are outside the nucleus.

Express the quantity a in Eq. (131) in terms of Q, and derive a version of Eq. (133). This equation, copied out of the book, has an error in it; correct it.

3. This is Sakurai, problem 3.29, p. 247; or Sakurai and Napolitano, problem 3.33, p. 261.

A spin-$\frac{3}{2}$ nucleus situated at the origin is subjected to an external inhomogeneous electric field. The basic electric quadrupole interaction is given by Eq. (133) (but corrected), where as above ϕ satisfies the Laplace equation and the off-diagonal components $\partial^2\phi/\partial x_i\partial x_j$ vanish. Show that the interaction energy can be written

$$A(3S_z^2 - S^2) + B(S_+^2 + S_-^2), \tag{134}$$

and express A and B in terms of the nonvanishing second derivatives of ϕ, evaluated at the origin. Determine the energy eigenkets (in terms of $|m\rangle$, where $m = \pm\frac{3}{2}, \pm\frac{1}{2}$) and the corresponding energy eigenvalues. Is there any degeneracy?

4. Some questions on the Mössbauer effect and the Pound-Rebka experiment.

The gravitational red shift is a prediction of general relativity, but the basic physics behind it can be understood in elementary terms. In the Pound-Rebka experiment, photons were launched upward from the ground, just outside a building at Harvard University. These photons were then received by a detector just outside the window of an upper floor of the building, approximately 20 meters above the ground.

Suppose at the very moment a photon is released at the ground, a physicist with a detector in hand jumps out of the upper storey window. As the photon is climbing upward in the earth's gravitational field, suffering a red shift in the process, the physicist is falling, accelerating downward. At a certain point the detector captures the photon and the physicist measures its frequency. This

frequency is blue shifted compared to what it would be if the physicist had just held the detector out the window, instead of jumping, because of the Doppler shift due to the downward motion of the detector.

It turns out that the gravitational red shift and the blue shift due to the falling detector (cum physicist) exactly cancel. Thus, the physicist finds a measured frequency of the photon exactly equal to the frequency it had when emitted at ground level. You can use this fact to calculate the gravitational red shift as seen by a detector that is just held out the window, not falling.

This situation is similar to that illustrated in the "shoot the monkey" demonstration used in elementary physics classes, except that instead of an arrow shot at the monkey particles of light are used. The basic physical reasoning used here is close to that employed by Einstein in his 1911 paper which first predicted the gravitational red shift.

(a) If an atom is free (not a part of a crystal lattice or otherwise bound to anything else), then it suffers some recoil on emitting a photon, which produces a shift $\Delta\omega$ in the frequency of the emitted photon. In the case of the 14.4 KeV photon emitted by the ^{57}Fe nucleus, calculate the fractional shift $\Delta\omega/\omega$ due to this recoil and compare to the natural line width.

(b) If the ^{57}Fe atom is free-floating in a gas at 300 K, calculate the average $\Delta\omega/\omega$ due to the Doppler shift due to the thermal motion of the atom.

(c) Calculate the $\Delta\omega/\omega$ for the gravitational red shift of the same photon climbing (as in the Pound-Rebka experiment) about 20 meters in the earth's gravitational field, and compare to the $\Delta\omega/\omega$ due to the natural line width. You will see that the experiment was a delicate one that required careful measurement and attention to systematic errors.