FIGURE 59.2. The  $B$ -field dependence of the fine-structure levels of a  ${}^2P$  state.

system stays in the upper level of the two levels with  $m_j = +\frac{1}{2}$  for all values of  $\vec{B}$ . The time evolution operator  $U(t, 0)$  will in the adiabatic switching process create a state which at any  $t$  is that linear combination of the states  $|m_l = m_j - \frac{1}{2}, m_s = +\frac{1}{2}\rangle$  and  $|m_l = m_j + \frac{1}{2}, m_s = -\frac{1}{2}\rangle$ , which is the energy eigenstate of the upper of the two levels with this particular  $m_j$  value, if the initial state at  $t = 0$  was the upper of the two levels with this particular  $m_j$  value. Similarly, if the initial state at  $t = 0$  was the lower of the two energy states with a particular  $m_j$  value, the time evolution operator,  $U(t, 0)$ , valid for an adiabatic switching process, will create a state at a later time  $t$ , which is still the lower of the two energy eigenstates with this  $m_j$  value corresponding to the energy valid for the  $B_z$  value for this particular  $t$ .

To find the time evolution operator for the Hamiltonian

$$H = a(t)\mathbf{1} + b(t)\sigma_z + C\sigma_x, \quad (7)$$

we shall try a solution of the form

$$U(t, 0) = e^{-\frac{i}{\hbar} \int_0^t d\tau a(\tau)\mathbf{1}} U'(t, 0) \quad (8)$$

in an attempt to get a simpler equation for  $U'$ . Substituting into

$$-\frac{\hbar}{i} \frac{dU}{dt} = HU, \quad (9)$$

we get

$$\begin{aligned} a(t)\mathbf{1}e^{-\frac{i}{\hbar} \int_0^t d\tau a(\tau)\mathbf{1}} U' - \frac{\hbar}{i} e^{-\frac{i}{\hbar} \int_0^t d\tau a(\tau)\mathbf{1}} \frac{dU'}{dt} \\ = (a(t)\mathbf{1} + b(t)\sigma_z + C\sigma_x)e^{-\frac{i}{\hbar} \int_0^t d\tau a(\tau)\mathbf{1}} U', \end{aligned} \quad (10)$$

leading to the simpler equation

$$-\frac{\hbar}{i} \frac{dU'}{dt} = (b(t)\sigma_z + C\sigma_x)U'. \quad (11)$$

We shall try to put this equation into a more suggestive form by rewriting it as

$$\begin{aligned} -\frac{\hbar}{i} \frac{dU'}{dt} &= \sqrt{(b^2(t) + C^2)} \left( \frac{b(t)}{\sqrt{b^2 + C^2}} \sigma_z + \frac{C}{\sqrt{b^2 + C^2}} \sigma_x \right) U' \\ &= \sqrt{(b^2(t) + C^2)} (\cos \Theta(t) \sigma_z + \sin \Theta(t) \sigma_x) U'. \end{aligned} \quad (12)$$

Because  $\cos \Theta \sigma_z + \sin \Theta \sigma_x$  suggests a  $\sigma_z$ , this form suggests we might try a rotation operator about the  $y$  axis (in the abstract sense) to convert the effective Hamiltonian on the right from one depending on the two noncommuting operators,  $\sigma_z$  and  $\sigma_x$ , to a new effective Hamiltonian depending on a single  $\sigma_z$ . For this reason, we try to find a solution for  $U'$  by trying the substitution

$$U'(t, 0) = e^{-i\frac{\Theta}{2}\sigma_y} U''(t, 0). \quad (13)$$

This substitution leads to

$$\begin{aligned} -\frac{\hbar}{i} \frac{dU'}{dt} &= e^{-i\frac{\Theta}{2}\sigma_y} \left( -\frac{\hbar}{i} \frac{dU''}{dt} \right) + \frac{\hbar}{2} \sigma_y \frac{d\Theta}{dt} e^{-i\frac{\Theta}{2}\sigma_y} U'' \\ &= \sqrt{b^2 + C^2} (\cos \Theta \sigma_z + \sin \Theta \sigma_x) e^{-i\frac{\Theta}{2}\sigma_y} U''. \end{aligned} \quad (14)$$

Left-multiplying by  $e^{i\frac{\Theta}{2}\sigma_y}$ , this equation can be transformed into

$$-\frac{\hbar}{i} \frac{dU''}{dt} = \left[ \sqrt{b^2 + C^2} e^{+i\frac{\Theta}{2}\sigma_y} (\cos \Theta \sigma_z + \sin \Theta \sigma_x) e^{-i\frac{\Theta}{2}\sigma_y} \right] U'' - \frac{\hbar}{2} \sigma_y \frac{d\Theta}{dt} U''. \quad (15)$$

To evaluate the last term, we shall differentiate

$$\sin \Theta(t) = \frac{C}{\sqrt{b^2(t) + C^2}},$$

$$\cos \Theta \frac{d\Theta}{dt} = -\frac{bC}{(b^2 + C^2)^{\frac{3}{2}}} \frac{db}{dt}. \quad (16)$$

Recalling  $b(t) = b_0 + b_1 t$ , with  $b_1 t = -\frac{1}{2}\hbar\omega_L(0)\frac{2t}{T}$ , we can use

$$\frac{db}{dt} = -\frac{1}{T}\hbar\omega_L(0), \quad \text{and } \cos \Theta = \frac{b}{\sqrt{b^2 + C^2}}, \quad (17)$$

to write the last term in eq. (17) as

$$-\frac{\hbar}{2}\sigma_y \frac{d\Theta}{dt} U'' = -\frac{C\hbar\omega_L(0)}{2T(b^2 + C^2)} \hbar\sigma_y U''. \quad (18)$$

In the limit,  $T \rightarrow \infty$ , therefore, this term can be neglected and we can get  $U''$  from the equation

$$-\frac{\hbar}{i} \frac{dU''}{dt} = \left[ \sqrt{b^2 + C^2} e^{i\frac{\Theta}{2}\sigma_y} (\cos \Theta \sigma_z + \sin \Theta \sigma_x) e^{-i\frac{\Theta}{2}\sigma_y} \right] U''. \quad (19)$$

Now, we can use the inverse rotation operation  $e^{i\Theta J_z} J_z e^{-i\Theta J_z} = J_z$  to rewrite

$$e^{i\frac{\Theta}{2}\sigma_y} (\cos \Theta \sigma_z + \sin \Theta \sigma_x) e^{-i\frac{\Theta}{2}\sigma_y} = e^{i\frac{\Theta}{2}\sigma_y} \sigma_z e^{-i\frac{\Theta}{2}\sigma_y} = \sigma_z, \quad (20)$$

leading to the simple differential equation for  $U''$

$$-\frac{\hbar}{i} \frac{dU''}{dt} = \sqrt{b^2(t) + C^2} \sigma_z U'', \quad (21)$$

with solution

$$U''(t, 0) = e^{-\frac{i}{\hbar} \int_0^t d\tau \sqrt{b^2(\tau) + C^2} \sigma_z}. \quad (22)$$

Combining eqs. (8), (13), and (22), we have

$$U(t, 0) = e^{-\frac{i}{\hbar} \int_0^t d\tau a(\tau) \mathbf{1}} e^{-i\frac{\Theta(t)}{2}\sigma_y} e^{-\frac{i}{\hbar} \int_0^t d\tau \sqrt{b^2(\tau) + C^2} \sigma_z}, \quad (23)$$

or

$$U(t, 0) = e^{-i\chi(t) \mathbf{1}} e^{-i\frac{\Theta(t)}{2}\sigma_y} e^{-i\phi(t)\sigma_z}, \quad (24)$$

where we have used

$$\chi(t) \equiv \frac{1}{\hbar} \int_0^t d\tau a(\tau); \quad \phi(t) \equiv \frac{1}{\hbar} \int_0^t d\tau \sqrt{b^2(\tau) + C^2}. \quad (25)$$

Together with

$$e^{-i\frac{\Theta}{2}\sigma_y} = \cos \frac{\Theta}{2} \mathbf{1} - i \sin \frac{\Theta}{2} \sigma_y, \quad (26)$$

these equations lead to

$$\begin{aligned} U(t, 0) &= \begin{pmatrix} e^{-i\chi(t)} & 0 \\ 0 & e^{-i\chi(t)} \end{pmatrix} \begin{pmatrix} \cos \frac{\Theta}{2} & -\sin \frac{\Theta}{2} \\ \sin \frac{\Theta}{2} & \cos \frac{\Theta}{2} \end{pmatrix} \begin{pmatrix} e^{-i\phi(t)} & 0 \\ 0 & e^{+i\phi(t)} \end{pmatrix} \\ &= \begin{pmatrix} \cos \frac{\Theta}{2} e^{-i(\chi+\phi)} & -\sin \frac{\Theta}{2} e^{-i(\chi-\phi)} \\ \sin \frac{\Theta}{2} e^{-i(\chi+\phi)} & \cos \frac{\Theta}{2} e^{-i(\chi-\phi)} \end{pmatrix}. \end{aligned} \quad (27)$$

The remaining job is to express the trigonometric functions of  $\frac{\Theta}{2}$  in terms of  $b$  and  $C$ , from the defining relations

$$\cos \Theta = \frac{b}{\sqrt{b^2 + C^2}}, \quad \sin \Theta = \frac{C}{\sqrt{b^2 + C^2}},$$

via

$$\cos^2 \frac{\Theta}{2} = \frac{1}{2}(1 + \cos \Theta), \quad \sin \frac{\Theta}{2} = \sin \Theta / (2 \cos \frac{\Theta}{2}),$$

leading to

$$\begin{aligned} \cos \frac{\Theta}{2} &= \frac{\sqrt{\sqrt{b^2 + C^2} + b}}{\sqrt{2(b^2 + C^2)^{\frac{1}{4}}}} = \frac{C}{\sqrt{2(b^2 + C^2)^{\frac{1}{4}}}} \frac{1}{\sqrt{\sqrt{b^2 + C^2} - b}} \\ \sin \frac{\Theta}{2} &= \frac{C}{\sqrt{2(b^2 + C^2)^{\frac{1}{4}}}} \frac{1}{\sqrt{\sqrt{b^2 + C^2} + b}} = \frac{\sqrt{\sqrt{b^2 + C^2} - b}}{\sqrt{2(b^2 + C^2)^{\frac{1}{4}}}}, \end{aligned} \quad (28)$$

where the second form of each trigonometric function is obtained from the first by multiplying both the numerator and the denominator with the common factor,  $\sqrt{\sqrt{b^2 + C^2} - b}$ .

Now, if at  $t = 0$ , in the huge positive  $B_0$ -field limit, the one-electron atom is in the upper of the two eigenstates of a particular  $m_j$ ,

$$|\psi(t=0)\rangle = |m_l = m_j - \frac{1}{2}, m_s = +\frac{1}{2}\rangle. \quad (29)$$

At a later time, using the first column of the matrix of eq. (27), we have

$$\begin{aligned} |\psi(t)\rangle &= \cos \frac{\Theta}{2} e^{-i(\chi+\phi)} |m_l = m_j - \frac{1}{2}, m_s = +\frac{1}{2}\rangle \\ &\quad + \sin \frac{\Theta}{2} e^{-i(\chi+\phi)} |m_l = m_j + \frac{1}{2}, m_s = -\frac{1}{2}\rangle \\ &= c_{+\frac{1}{2}} |m_l = m_j - \frac{1}{2}, m_s = +\frac{1}{2}\rangle + c_{-\frac{1}{2}} |m_l = m_j + \frac{1}{2}, m_s = -\frac{1}{2}\rangle, \end{aligned} \quad (30)$$

where the ratio of coefficients is given by the time-dependent function

$$\frac{c_{+\frac{1}{2}}}{c_{-\frac{1}{2}}} = \frac{C}{\sqrt{b^2 + C^2} - b}. \quad (31)$$

Here, we have used the second form for the functions  $\cos \frac{\Theta}{2}$  and  $\sin \frac{\Theta}{2}$  from eq. (28). We shall now show this is precisely the ratio of coefficients for the *upper* of the two eigenstates for this particular  $m_j$  value at this particular time. If we imagine we have stopped the field-switching process at this particular value of  $t$ , we can diagonalize  $H(t)$ , as given by eq. (6), with the matrix  $H(t) - E\mathbf{1}$  given by

$$H - E\mathbf{1} = \begin{pmatrix} (a - E) + b & C \\ C & (a - E) - b \end{pmatrix}. \quad (32)$$

The determinant of this matrix must be set equal to zero to obtain the two eigenvalues for  $E$ , leading to

$$(a - E)^2 - b^2 - C^2 = 0, \quad (33)$$

with

$$(E_{\pm} - a) = \pm\sqrt{b^2 + C^2}, \quad (34)$$

where  $E_+$ , ( $E_-$ ), correspond to  $E_{\text{upper}}$ , ( $E_{\text{lower}}$ ), respectively. The coefficients of the two eigenvectors are given by the linear equations

$$\begin{aligned} [(a - E) + b]c_{+\frac{1}{2}} + Cc_{-\frac{1}{2}} &= 0, \\ Cc_{+\frac{1}{2}} + [(a - E) - b]c_{-\frac{1}{2}} &= 0. \end{aligned} \quad (35)$$

For the upper energy eigenstate,  $E_+ = a + \sqrt{b^2 + C^2}$ , this equation leads to the ratio

$$\frac{c_{+\frac{1}{2}}}{c_{-\frac{1}{2}}} = \frac{C}{\sqrt{b^2 + C^2} - b}. \quad (36)$$

This equation is precisely the ratio of coefficients of eq. (31) given by the time evolution operator  $U(t, 0)$  acting on the initial state  $|\psi(t=0)\rangle$ , which corresponds to the *upper* of the two states with this value of  $m_j$  at the initial time  $t = 0$  when the magnetic field has its maximum positive value. The ratio of eq. (36) leads to the normalized coefficients

$$c_{+\frac{1}{2}} = \frac{C}{\sqrt{2}(b^2 + C^2)^{\frac{1}{4}}} \frac{1}{\sqrt{\sqrt{b^2 + C^2} - b}}, \quad c_{-\frac{1}{2}} = \frac{\sqrt{\sqrt{b^2 + C^2} - b}}{\sqrt{2}(b^2 + C^2)^{\frac{1}{4}}}. \quad (37)$$

The coefficients  $c_{+\frac{1}{2}}$  and  $c_{-\frac{1}{2}}$  of the eigenvalue problem at this fixed  $t$  could each be multiplied by an arbitrary phase factor, such as  $e^{-i(\chi(t)+\phi(t))}$ , because the energy eigenvectors are determined only to within such a phase. By choosing this particular phase factor, we make the state vector identical to that produced by the time evolution operator  $U(t, 0)$  in this adiabatic limit. Also, the process of “stopping” the switching at some fixed value of  $t$  to diagonalize  $H(t)$  can be justified only in this adiabatic limit, where the switching time  $T \rightarrow \infty$ . In this adiabatic limit, however, an initial state that was the *upper* of the two energy eigenstates of a particular  $m_j$  at  $t = 0$  will evolve into the *upper* of the energy eigenstates with this value of  $m_j$  valid for the appropriate magnetic field strength,  $B_z(t)$ . Thus, the state with asymptotic quantum numbers,  $|m_l, m_s\rangle = |0, +\frac{1}{2}\rangle$  at  $t = 0$ , with  $B_z$  positive and huge (see Fig. 59.2), will go through the pure  $p_{\frac{3}{2}}$  state at  $t = \frac{1}{2}T$ , when  $B_z = 0$ , and end in the state with asymptotic quantum numbers,  $|m_l, m_s\rangle = |+1, -\frac{1}{2}\rangle$ , at  $t = T$  in an adiabatic switching process for which  $T \rightarrow \infty$ .

In exactly the same way: If the initial state at  $t = 0$ , with maximum positive (huge-field value) of  $B_z$ , corresponds to the *lower* of the two energy states of a particular  $m_j$ ,  $|\psi(t=0)\rangle = |m_s = -\frac{1}{2}\rangle$ . Now, the state at a later time  $t$  is given by the second column of the  $U(t, 0)$  matrix of eq. (27), leading to the state  $|\psi(t)\rangle$  with coefficients given by the ratio

$$\frac{c_{+\frac{1}{2}}}{c_{-\frac{1}{2}}} = -\frac{\sin \frac{\Theta}{2}}{\cos \frac{\Theta}{2}} = -\frac{C}{\sqrt{b^2 + C^2} + b}, \quad (38)$$

where we have used the first form of the expressions for the trigonometric functions of eq. (28). From eq. (35), this ratio of coefficients is in agreement with the energy eigenvectors corresponding to the *lower* eigenvalue, with  $E_- = a - \sqrt{b^2 + C^2}$ . Thus, a state that was initially the *lower* of the two states with a particular value of  $m_J$  will evolve into the *lower* of these two states at the later time  $t$  in the adiabatic field-switching process. This result is what we set out to prove.

## Problems

**25.** A system of  $J = 1$  particles with magnetic moments,  $\vec{\mu} = (e\hbar/2mc)g_J\vec{J}$ , is in a strong uniform magnetic field,  $\vec{B}_0$ , with a second weak field,  $\vec{B}_1$ , rotating with circular frequency,  $\omega$ , in a plane perpendicular to  $\vec{B}_0$ . Assuming the system is in a state with  $M_J = +1$  at  $t = 0$ , where we use the direction of  $\vec{B}_0$  as quantization direction, calculate an exact expression, valid for all values of  $\omega$ ,  $\omega_0 = (eg_J B_0)/(2mc)$ , and  $\omega_1 = (eg_J B_1)/(2mc)$ , for the probability,  $P_{M_J}(t)$ , the system is in a state with  $M_J = 0$ , or  $M_J = -1$  at a later finite time  $t$ . Compare this with the results given by perturbation theory for  $U(t, 0)$ , valid for  $\omega_1 \ll (\omega_0 + \omega)$  [for  $(\omega_0 + \omega) \neq 0$ ]. Also, calculate the exact values for

$$\frac{dP_{M_J}(t)}{dt} \quad \text{for } M_J = 0 \text{ and } M_J = -1,$$

giving the rate at which transitions,  $M_J = +1 \rightarrow 0$  and  $M_J = +1 \rightarrow -1$ , take place. Compare these with the perturbation theory results for the case of a general perturbing frequency not on resonance. For the resonance case,  $(\omega_0 + \omega) \approx 0$ , show the exact result agrees with the perturbation theory result in the limit  $\omega_1 \rightarrow 0$  for large but finite  $t$ ; i.e., you need to take the limits as follows:

$$\lim_{t \rightarrow \infty} \left[ \lim_{\omega_1 \rightarrow 0} \frac{dP_{M_J}(t)}{dt} \right].$$

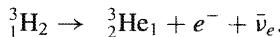
**26.** A sample in a uniform magnetic field,  $\vec{B}_0$ , containing a large number of identical nuclear spins, with  $s = \frac{1}{2}$ , has a magnetization,  $\vec{M}$ , given by the thermal equilibrium value, attained through the so-called spin-lattice relaxation process:

$$M_z = \frac{\left[ e^{i\omega_0/2kT} - e^{-i\omega_0/2kT} \right]}{\left[ e^{i\omega_0/2kT} + e^{-i\omega_0/2kT} \right]}, \quad M_x = M_y = 0,$$

where  $\omega_0 = eg_J B_0/2Mc$ . Write the spin density matrix for this sample. If a  $\vec{B}_1$  field, rotating with circular frequency,  $\omega$ , in a plane normal to  $\vec{B}_0$  is turned on at  $t = 0$ , find the density matrix at a later time,  $t$ . Show the  $\vec{B}_1$  field induces a magnetization,  $\vec{M}(t)$ , including  $x$  and  $y$  components. Note: In a real sample, these perpendicular components of  $\vec{M}$  are destroyed by random collision or spin-spin relaxation processes, not included in our Hamiltonian.

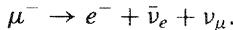
**27.** The endpoint part of the spectrum of the beta decay of tritium,  ${}^3\text{H}_2$ , is being reexamined carefully in an attempt to pin down a possible nonzero rest mass for

the electron neutrino. Because other experimental evidence indicates the neutrino rest mass must be less than 10–30 eV, the exact atomic energy of the recoiling  ${}^3_2\text{He}_1$  one-electron ion must be taken into account carefully. The beta-decay endpoint energy is 18.65 keV. The atomic electron of the tritium atom is initially in its  $1s$  ground state, but finds itself in the field of a  $Z = 2$  nucleus,  ${}^3_2\text{He}_1$ , after the beta decay



Show this beta-decay process constitutes a “sudden” process as far as the perturbation on the atomic electron is concerned, by showing the  $\Delta t$  for this process; i.e., the  $\Delta t$  it takes for the fragments,  $e^-$  and  $\bar{\nu}_e$  to leave the atom is small compared with a hydrogenic period,  $T$ . Therefore, the probability the He ion end in a state  $nlm_l$  can be calculated easily. In particular, calculate the probability of finding the He ion in its  $1s$ ,  $2s$ , and  $3s$  state. Can it be in a state with  $l \neq 0$ ? Show, in principle, a probability the He atom be completely ionized also exists, leaving a bare  ${}^3_2\text{He}_1$  nucleus and an additional  $e^-$  in a continuum state, but make a rough estimate to show this probability is effectively negligible.

- 28.** A  $\mu$ -mesic He atom consisting of a He nucleus, ( $Z = 2$ ), and one  $\mu^-$  and one  $e^-$ , is in its ground state. By taking the overlap of a  $1s$  electron and a  $1s$   $\mu^-$  wave function for  $Z = 2$ , show effectively the electron sees a charge of  $Z = 2$  almost completely shielded by the full negative charge of the  $\mu^-$ , so the electron  $1s$  wave function is to good approximation a hydrogenic  $1s$  wave function for  $Z = 1$ . Conversely, the  $\mu^-$  sees essentially the full  $Z = 2$  of the He nucleus, and its  $1s$  wave function is to good approximation that for a single  $\mu^-$  with a Bohr radius for  $Z = 2$  and the  $\mu^-$ -He reduced mass. The  $\mu^-$  of the  $\mu$ -mesic He atom will decay, via



- Show the  $\Delta t$  for the fragments,  $e^-$ ,  $\bar{\nu}_e$ , and  $\nu_\mu$ , to leave the atom is so short compared with atomic periods this perturbation constitutes a sudden process. For this sudden process, calculate the probability of finding the remaining He ion ( $Z = 2$  nucleus +  $e^-$ ) in the  $1s$ ,  $2s$ , and  $3s$  states of this system. Could it be in a state with  $l \neq 0$ ?

# Atom–Photon Interactions

## Interaction of Electromagnetic Radiation with Atomic Systems

So far, we have considered quantum systems in external oscillating magnetic (or electric) fields, where the perturbing fields were considered as classical oscillating fields. This approach would permit us to study induced absorption or emission processes in an atomic system, particularly if the intensity of the electromagnetic fields is such that the density of photons is very great in the region of interest. To study processes involving a small number of photons interacting with an atomic system, we must first quantize the electromagnetic or radiation field itself. So far, our time-dependent perturbation theory would not permit us to study the spontaneous emission of photons by an atomic system, i.e., a situation in which the initial state consists of an atom in an excited state and no photons, and the final state is the atom in a lower state (perhaps the ground state) and one photon of the appropriate energy. In order to treat this problem rigorously, we need to quantize the radiation field.

(References for this material: Chapter 2 in J. J. Sakurai, *Advanced Quantum Mechanics*, Reading, MA: Addison-Wesley, 1967; and Chapter 1 in Berestetskii, Lifshitz, and Pitaevskii, *Quantum Electrodynamics*, New York: Pergamon Press, 1982; Vol. 4 of the Landau-Lifshitz series. For the general electric and magnetic multipole radiation fields of vital importance in nuclear physics, see also Judah M. Eisenberg and Walter Greiner, *Nuclear Theory. Vol. 2. Excitation Mechanisms of the Nucleus*, Amsterdam: North Holland, 1970.)

Before quantizing the electromagnetic field, let us consider the Hamiltonian for an atom in an electromagnetic field by first considering the electromagnetic field as a classical field. The electric and magnetic field vectors,  $\vec{E}$  and  $\vec{B}$ , will be derived from a vector and a scalar potential,  $\vec{A}$  and  $\Phi$ . For our purposes, it will be convenient to choose these in the so-called radiation or Coulomb gauge. We will

separate the scalar potential,  $\Phi$ , and the so-called longitudinal part of the vector potential,  $\vec{A}_{\parallel}$ , from the transverse part of the vector potential,  $\vec{A}_{\perp}$ . Here,

$$\vec{A} = \vec{A}_{\parallel} + \vec{A}_{\perp}, \quad \text{with} \quad \vec{\nabla} \cdot \vec{A}_{\perp} = 0, \quad [\vec{\nabla} \times \vec{A}_{\parallel}] = 0. \quad (1)$$

The terms arising from  $\Phi$  and  $\vec{A}_{\parallel}$  will be absorbed into  $H_{\text{atom}}$ , i.e., the atomic part of our full Hamiltonian. This absorption will include, e.g., all Coulomb terms, such as the Coulomb repulsion electron-electron potential terms and the Coulomb attraction electron-nucleus terms in an atom. Conversely,  $\vec{A}_{\perp}$  will serve as the source of the radiation field. We will then seek the full Hamiltonian in the form

$$H = H_{\text{atom}} + H_{\text{radiation}} + H_{\text{interaction}}. \quad (2)$$

Guided by our earlier discussion of an atom in an external electromagnetic field, we shall try a Hamiltonian of the form

$$H = \sum_{i=1}^N \frac{1}{2m_i} \left( \vec{p}_i - \frac{e_i}{c} \vec{A}_{\perp}(\vec{r}_i, t) \right) \cdot \left( \vec{p}_i - \frac{e_i}{c} \vec{A}_{\perp}(\vec{r}_i, t) \right) + \sum_{i < k}^N V(\vec{r}_i, \vec{r}_k) \\ - \sum_{i=1}^N \frac{e_i \hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot [\vec{\nabla} \times \vec{A}_{\perp}] + H_{\text{radiation}}, \quad (3)$$

where  $H_{\text{interaction}}$  includes all cross terms, coupling  $\vec{A}_{\perp}$  to atomic operators, such as  $\vec{p}_i$  or  $\vec{s}_i$ .

## A The Electromagnetic Radiation Field

To derive the expression for  $H_{\text{radiation}}$ , let us look at the radiation fields

$$\vec{E}_{\text{rad.}} = -\frac{1}{c} \frac{\partial \vec{A}_{\perp}}{\partial t}, \quad \vec{B}_{\text{rad.}} = [\vec{\nabla} \times \vec{A}_{\perp}], \quad (4)$$

where the Maxwell equations and the condition,  $\vec{\nabla} \cdot \vec{A}_{\perp} = 0$ , lead to

$$\nabla^2 \vec{A}_{\perp} - \frac{1}{c^2} \frac{\partial^2 \vec{A}_{\perp}}{\partial t^2} = 0. \quad (5)$$

We shall solve this vector wave equation in our cubical laboratory of volume  $L^3$  with the usual boundary conditions, leading to a finely discrete spectrum of  $\vec{k}$  values, in terms of basic vector solutions,  $\vec{u}_{\vec{k}\alpha}$ ,

$$\vec{u}_{\vec{k}\alpha} = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \vec{e}_{\alpha}, \quad (6)$$

with

$$\vec{k} \equiv \vec{k}_{n_1 n_2 n_3} = (k_x, k_y, k_z), \quad \text{and} \quad k_x = \frac{2\pi}{L} n_1, \quad k_y = \frac{2\pi}{L} n_2, \quad k_z = \frac{2\pi}{L} n_3, \quad (7)$$

where the  $n_i$  are positive or negative integers and the vectors  $\vec{e}_\alpha$  are unit polarization vectors. When we expand  $\vec{A}_\perp$  in terms of these  $\vec{u}_{\vec{k}\alpha}$ , the condition,  $\nabla \cdot \vec{A}_\perp = 0$ , leads to  $\vec{\nabla} \cdot \vec{u}_{\vec{k}\alpha} = 0$ , with

$$\vec{\nabla} \cdot \vec{u}_{\vec{k}\alpha} = \frac{i}{\sqrt{L^3}} (\vec{k} \cdot \vec{e}_\alpha) e^{i\vec{k} \cdot \vec{r}} = 0, \quad (8)$$

leading to

$$(\vec{k} \cdot \vec{e}_\alpha) = 0, \quad (9)$$

so the unit polarization vectors,  $\vec{e}_\alpha$ , must be orthogonal to  $\vec{k}$ . The index  $\alpha$  can thus be chosen, so the triad of vectors,  $\vec{e}_1$ ,  $\vec{e}_2$ , and  $\vec{k}/k \equiv \vec{e}_3$ , form an orthogonal triad of unit vectors (see Fig. 60.1). For a fixed  $\vec{k}$  specified by the integers,  $n_1, n_2, n_3$ , the index  $\alpha$  can take on the values 1, and 2, corresponding to the two linear polarization vectors. The index  $\alpha$  is thus indirectly dependent on  $\vec{k}$ . The vector potential,  $\vec{A}_\perp$ , can be expanded in terms of the  $\vec{u}_{\vec{k}\alpha}$  through

$$\vec{A}_\perp(\vec{r}, t) = \sum_{\vec{k}} \sum_{\alpha=1,2} (c_{\vec{k}\alpha}(t) \vec{u}_{\vec{k}\alpha}(\vec{r}) + c_{\vec{k}\alpha}^*(t) \vec{u}_{\vec{k}\alpha}^*(\vec{r})), \quad (10)$$

where we have assumed  $\vec{A}_\perp$  is real. The wave equation, eq. (5), then leads to

$$-c^2 k^2 c_{\vec{k}\alpha} - \ddot{c}_{\vec{k}\alpha} = 0, \quad (11)$$

or

$$\ddot{c}_{\vec{k}\alpha} + \omega^2 c_{\vec{k}\alpha} = 0, \quad \text{with } \omega = kc, \quad (12)$$

and

$$c_{\vec{k}\alpha}(t) = c_{\vec{k}\alpha}(0) e^{-i\omega t}, \quad c_{\vec{k}\alpha}^*(t) = c_{\vec{k}\alpha}^*(0) e^{+i\omega t}, \quad (13)$$

so

$$\vec{A}_\perp(\vec{r}, t) = \sum_{\vec{k}} \sum_{\alpha=1,2} \frac{\vec{e}_\alpha}{\sqrt{L^3}} \left( c_{\vec{k}\alpha}(0) e^{i(\vec{k} \cdot \vec{r} - \omega t)} + c_{\vec{k}\alpha}^*(0) e^{-i(\vec{k} \cdot \vec{r} - \omega t)} \right). \quad (14)$$

The classical Hamiltonian for the radiation field can then be obtained from the energy density of the electromagnetic field, via

$$\begin{aligned} H_{\text{radiation}} &= \frac{1}{8\pi} \int_{\text{Vol.}} d\vec{r} \left( (\vec{E}_{\text{rad.}} \cdot \vec{E}_{\text{rad.}}) + (\vec{B}_{\text{rad.}} \cdot \vec{B}_{\text{rad.}}) \right) \\ &= \frac{1}{8\pi} \int_{\text{Vol.}} d\vec{r} \left( \left( -\frac{1}{c} \frac{\partial \vec{A}_\perp}{\partial t} \right)^2 + ([\vec{\nabla} \times \vec{A}_\perp]^2) \right) \\ &= \frac{1}{2\pi} \sum_{\vec{k}, \alpha} \frac{\omega^2}{c^2} c_{\vec{k}\alpha}(t) c_{\vec{k}\alpha}^*(t), \end{aligned} \quad (15)$$

where the volume integral is over the volume of the cubical laboratory, and the last step involves the orthonormality of the spatial functions and the orthonormality of the polarization vectors.

$$\frac{1}{L^3} \int_{\text{Vol.}} d\vec{r} e^{i\vec{k} \cdot \vec{r}} e^{-i\vec{k}' \cdot \vec{r}} = \delta_{\vec{k}, \vec{k}'} = \delta_{\vec{n}, \vec{n}'} = \delta_{n_1 n'_1} \delta_{n_2 n'_2} \delta_{n_3 n'_3}, \quad (16)$$

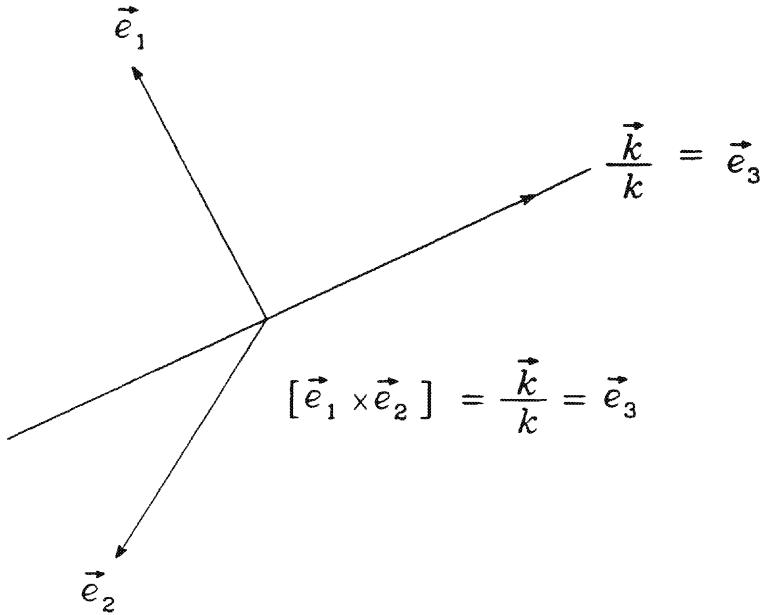


FIGURE 60.1.

so

$$\begin{aligned} \int_{\text{Vol.}} d\vec{r} (\vec{u}_{k\alpha}^* \cdot \vec{u}_{k'\alpha'}) &= \delta_{\vec{k}, \vec{k}'} \delta_{\alpha, \alpha'}, \\ \int_{\text{Vol.}} d\vec{r} (\vec{u}_{\vec{k}\alpha} \cdot \vec{u}_{\vec{k}'\alpha'}) &= \delta_{\vec{k}, -\vec{k}'} \delta_{\alpha, \alpha'}. \end{aligned} \quad (17)$$

To get the last form of eq. (15), we shall also use

$$\begin{aligned} \left( -\frac{\partial \vec{A}_\perp}{c \partial t} \right) \cdot \left( -\frac{\partial \vec{A}_\perp}{c \partial t} \right) &= \frac{1}{c^2} \sum_{\vec{k}, \alpha} \sum_{\vec{k}', \alpha'} (i\omega)(i\omega') \\ &\times \left( c_{\vec{k}\alpha} \vec{u}_{\vec{k}\alpha} - c_{\vec{k}\alpha}^* \vec{u}_{\vec{k}\alpha}^* \right) \cdot \left( c_{\vec{k}'\alpha'} \vec{u}_{\vec{k}'\alpha'} - c_{\vec{k}'\alpha'}^* \vec{u}_{\vec{k}'\alpha'}^* \right), \end{aligned} \quad (18)$$

and

$$\begin{aligned} [\vec{\nabla} \times \vec{A}_\perp] \cdot [\vec{\nabla} \times \vec{A}_\perp] &= \frac{1}{L^3} \sum_{\vec{k}, \alpha} \sum_{\vec{k}', \alpha'} i[\vec{k} \times \vec{e}_\alpha] \cdot i[\vec{k}' \times \vec{e}_{\alpha'}] \\ &\times \left( c_{\vec{k}\alpha} e^{i\vec{k} \cdot \vec{r}} - c_{\vec{k}\alpha}^* e^{-i\vec{k} \cdot \vec{r}} \right) \left( c_{\vec{k}'\alpha'} e^{i\vec{k}' \cdot \vec{r}} - c_{\vec{k}'\alpha'}^* e^{-i\vec{k}' \cdot \vec{r}} \right) \\ &= -\frac{1}{L^3} \sum_{\vec{k}, \alpha} \sum_{\vec{k}', \alpha'} [(\vec{k} \cdot \vec{k}')(\vec{e}_\alpha \cdot \vec{e}_{\alpha'}) - (\vec{k} \cdot \vec{e}_{\alpha'})(\vec{k}' \cdot \vec{e}_\alpha)] \\ &\times \left( c_{\vec{k}\alpha} e^{i\vec{k} \cdot \vec{r}} - c_{\vec{k}\alpha}^* e^{-i\vec{k} \cdot \vec{r}} \right) \left( c_{\vec{k}'\alpha'} e^{i\vec{k}' \cdot \vec{r}} - c_{\vec{k}'\alpha'}^* e^{-i\vec{k}' \cdot \vec{r}} \right). \end{aligned} \quad (19)$$

When integrated over the volume of our cubical laboratory, only terms with  $\vec{k}' = \pm \vec{k}$  survive [see eq. (17)]. For both of these,  $(\vec{k} \cdot \vec{e}_{\alpha'})(\vec{k}' \cdot \vec{e}_{\alpha}) = 0$ . Terms with  $\vec{k}' = \vec{k}$ ,  $\alpha' = \alpha$ , receive a contribution  $2\frac{\omega^2}{c^2} c_{\vec{k}\alpha} c_{\vec{k}\alpha}^*$  from eq. (18) and  $2k^2 c_{\vec{k}\alpha} c_{\vec{k}\alpha}^*$  from eq. (19) when integrated over the volume of the cubical laboratory. Terms with  $\vec{k}' = -\vec{k}$ ,  $\alpha' = \alpha$ , conversely, get a contribution of  $-\frac{\omega^2}{c^2}(c_{\vec{k}\alpha} c_{-\vec{k}\alpha} + c_{\vec{k}\alpha}^* c_{-\vec{k}\alpha}^*)$  from eq. (18) and a contribution  $+k^2(c_{\vec{k}\alpha} c_{-\vec{k}\alpha} + c_{\vec{k}\alpha}^* c_{-\vec{k}\alpha}^*)$  from eq. (19), so these two contributions cancel, whereas the terms with  $\vec{k}' = \vec{k}$  add to give the final result of eq. (15).

$$H_{\text{radiation}} = \frac{1}{2\pi} \sum_{\vec{k}, \alpha} \frac{\omega^2}{c^2} c_{\vec{k}\alpha} c_{\vec{k}\alpha}^*. \quad (20)$$

Now, it will be convenient to rewrite the complex (time-dependent) functions,  $c_{\vec{k}\alpha}$ , in terms of two real time-dependent functions,  $Q_{\vec{k}\alpha}$  and  $P_{\vec{k}\alpha}$ , via

$$\begin{aligned} \frac{1}{c\sqrt{2\pi}} c_{\vec{k}\alpha} &= \sqrt{\frac{1}{2}} \left( Q_{\vec{k}\alpha} + \frac{i}{\omega} P_{\vec{k}\alpha} \right), \\ \frac{1}{c\sqrt{2\pi}} c_{\vec{k}\alpha}^* &= \sqrt{\frac{1}{2}} \left( Q_{\vec{k}\alpha} - \frac{i}{\omega} P_{\vec{k}\alpha} \right), \end{aligned} \quad (21)$$

giving us the *classical* radiation Hamiltonian

$$H_{\text{radiation}} = \frac{1}{2} \sum_{\vec{k}, \alpha} (P_{\vec{k}\alpha}^2 + \omega^2 Q_{\vec{k}\alpha}^2). \quad (22)$$

Comparing this with the simple 1-D harmonic oscillator Hamiltonian

$$H_{\text{harm. osc.}} = \left( \frac{P^2}{2m} + \frac{m\omega^2}{2} Q^2 \right), \quad (23)$$

the classical radiation Hamiltonian involves a superposition of an infinite number of (uncoupled) harmonic oscillator Hamiltonians if we set the parameter  $m = 1$ . (Note, however, this is not a physical mass for our problem).

## B The Quantized Radiation Field

To quantize the above Dirac assumed the classical variables,  $P_{\vec{k}\alpha}$  and  $Q_{\vec{k}\alpha}$ , are replaced by quantum-mechanical operators that satisfy the commutation relations

$$[P_{\vec{k}\alpha}, Q_{\vec{k}'\alpha'}] = \frac{\hbar}{i} \delta_{\vec{k}, \vec{k}'} \delta_{\alpha, \alpha'}, \quad [P_{\vec{k}\alpha}, P_{\vec{k}'\alpha'}] = 0, \quad [Q_{\vec{k}\alpha}, Q_{\vec{k}'\alpha'}] = 0. \quad (24)$$

As for the simple 1-D oscillator, it will now be convenient to introduce dimensionless  $p_{\vec{k}\alpha}$ ,  $q_{\vec{k}\alpha}$  via

$$P_{\vec{k}\alpha} = \sqrt{\hbar\omega} p_{\vec{k}\alpha}, \quad Q_{\vec{k}\alpha} = \sqrt{\frac{\hbar}{\omega}} q_{\vec{k}\alpha}, \quad (25)$$

so the  $p_{\vec{k}\alpha}$  and  $q_{\vec{k}\alpha}$  satisfy the commutation relations

$$[p_{\vec{k}\alpha}, q_{\vec{k}'\alpha'}] = \frac{1}{i} \delta_{\vec{k}, \vec{k}'} \delta_{\alpha, \alpha'}, \quad [p_{\vec{k}\alpha}, p_{\vec{k}'\alpha'}] = 0, \quad [q_{\vec{k}\alpha}, q_{\vec{k}'\alpha'}] = 0. \quad (26)$$

In terms of these operators, the radiation Hamiltonian can be written as

$$H_{\text{radiation}} = \frac{1}{2} \sum_{\vec{k}, \alpha} \hbar \omega (p_{\vec{k}\alpha}^2 + q_{\vec{k}\alpha}^2). \quad (27)$$

As for the 1-D harmonic oscillator, it will be useful to introduce annihilation and creation operators,

$$\begin{aligned} a_{\vec{k}\alpha} &= \sqrt{\frac{1}{2}} (q_{\vec{k}\alpha} + i p_{\vec{k}\alpha}), \\ a_{\vec{k}\alpha}^\dagger &= \sqrt{\frac{1}{2}} (q_{\vec{k}\alpha} - i p_{\vec{k}\alpha}), \end{aligned} \quad (28)$$

with commutation relations

$$\begin{aligned} [a_{\vec{k}\alpha}, a_{\vec{k}'\alpha'}^\dagger] &= \delta_{\vec{k}, \vec{k}'} \delta_{\alpha, \alpha'} \\ [a_{\vec{k}\alpha}, a_{\vec{k}'\alpha'}] &= [a_{\vec{k}\alpha}^\dagger, a_{\vec{k}'\alpha'}^\dagger] = 0. \end{aligned} \quad (29)$$

In terms of these operators,

$$H_{\text{radiation}} = \frac{1}{2} \sum_{\vec{k}, \alpha} \hbar \omega (a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} + a_{\vec{k}\alpha} a_{\vec{k}\alpha}^\dagger) = \sum_{\vec{k}, \alpha} \hbar \omega (a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} + \frac{1}{2}). \quad (30)$$

Now, we can introduce the operator

$$N_{\vec{k}\alpha} = a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha}, \quad (31)$$

which we would have interpreted as the operator which counts the number of oscillator quanta of type  $\vec{k}\alpha$ . We will now interpret this as the operator that counts the number of photons of type  $\vec{k}\alpha$ , where we will substantiate this interpretation. The eigenvectors of  $H_{\text{radiation}}$  are of the form

$$|n_{\vec{k}_1\alpha_1} n_{\vec{k}_2\alpha_2} n_{\vec{k}_3\alpha_3} \cdots n_{\vec{k}\alpha} \cdots \rangle,$$

where

$$a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} | \cdots n_{\vec{k}\alpha} \cdots \rangle = n_{\vec{k}\alpha} | \cdots n_{\vec{k}\alpha} \cdots \rangle, \quad (32)$$

$$a_{\vec{k}\alpha} | \cdots n_{\vec{k}\alpha} \cdots \rangle = \sqrt{n_{\vec{k}\alpha}} | \cdots (n_{\vec{k}\alpha} - 1) \cdots \rangle, \quad (33)$$

$$a_{\vec{k}\alpha}^\dagger | \cdots n_{\vec{k}\alpha} \cdots \rangle = \sqrt{(n_{\vec{k}\alpha} + 1)} | \cdots (n_{\vec{k}\alpha} + 1) \cdots \rangle. \quad (34)$$

The state of no photons, the vacuum state, is of the form

$$|000 \cdots 0 \cdots 0\rangle \equiv |0\rangle$$

and satisfies

$$a_{\vec{k}\alpha} |0\rangle = 0 \quad \text{for all } \vec{k}\alpha. \quad (35)$$

The state of a single photon of type  $\vec{k}\alpha$  is

$$a_{\vec{k}\alpha}^\dagger |0\rangle.$$

The most general many-photon state has the form

$$\prod_{\vec{k}_i \alpha_i} \frac{(a_{\vec{k}_i \alpha_i}^\dagger)^{n_{\vec{k}_i \alpha_i}}}{\sqrt{(n_{\vec{k}_i \alpha_i})!}} |0\rangle.$$

# Photons: The Quantized Radiation Field

In order to interpret the number  $n_{\vec{k}\alpha}$  as the number of photons of type  $\vec{k}\alpha$ , we shall look at the properties of the quantized radiation field in more detail. Combining eqs. (21), (25), and (28) of the last chapter, the expansion of  $\vec{A}_\perp$  can be written as

$$\vec{A}_\perp(\vec{r}, t) = \sum_{\vec{k}, \alpha} c \sqrt{\frac{2\pi\hbar}{\omega}} (a_{\vec{k}\alpha} \vec{u}_{\vec{k}\alpha}(\vec{r}) + a_{\vec{k}\alpha}^\dagger \vec{u}_{\vec{k}\alpha}^*(\vec{r})), \quad (1)$$

where the  $a_{\vec{k}\alpha}$  are time dependent (given in Heisenberg representation), with

$$a_{\vec{k}\alpha} \equiv a_{\vec{k}\alpha}(t) = a_{\vec{k}\alpha}(0)e^{-i\omega t}, \quad a_{\vec{k}\alpha}^\dagger \equiv a_{\vec{k}\alpha}^\dagger(t) = a_{\vec{k}\alpha}^\dagger(0)e^{+i\omega t}. \quad (2)$$

The radiation fields are then given by

$$\vec{E}(\vec{r}, t) = i \sum_{\vec{k}, \alpha} \sqrt{2\pi\hbar\omega} (a_{\vec{k}\alpha} \vec{u}_{\vec{k}\alpha}(\vec{r}) - a_{\vec{k}\alpha}^\dagger \vec{u}_{\vec{k}\alpha}^*(\vec{r})), \quad (3)$$

$$\vec{B}(\vec{r}, t) = i c \sum_{\vec{k}, \alpha} \sqrt{\frac{2\pi\hbar}{\omega}} (a_{\vec{k}\alpha} [\vec{k} \times \vec{u}_{\vec{k}\alpha}(\vec{r})] - a_{\vec{k}\alpha}^\dagger [\vec{k} \times \vec{u}_{\vec{k}\alpha}^*(\vec{r})]). \quad (4)$$

## A Photon Energy

Because the radiation Hamiltonian

$$H_{\text{radiation}} = \sum_{\vec{k}, \alpha} \hbar\omega (a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} + \frac{1}{2}) \quad (5)$$

contains an infinite zero-point energy for the vacuum state through the factor of  $\frac{1}{2}$  associated with each of the infinite number of possible states  $\vec{k}\alpha$ , we must measure the energy *relative* to the energy of the vacuum state,  $E_{\text{rad.}}^0$ .

$$(H_{\text{rad.}} - E_{\text{rad.}}^0)|\cdots n_{\vec{k}\alpha} \cdots\rangle = \sum_{\vec{k},\alpha} \hbar\omega n_{\vec{k}\alpha} |\cdots n_{\vec{k}\alpha} \cdots\rangle. \quad (6)$$

Thus, the single photon state, with  $n_{\vec{k}\alpha} = 1$ , has an energy  $\hbar\omega$ , with  $\omega = kc$ .

## B Photon Linear Momentum

Because the *classical* momentum density of the electromagnetic field is given by  $(1/4\pi c)[\vec{E} \times \vec{B}]$ , we need to integrate the quantized operator form of this quantity over the volume of our cubical laboratory to obtain the linear momentum of the photon field. Because the quantized expressions for  $\vec{E}$  and  $\vec{B}$  of eqs. (3) and (4) contain noncommuting operators, we need to use the symmetrized, hermitian form of the momentum density operator.

$$\begin{aligned} \vec{p} &= \frac{1}{8\pi c} \int_{\text{Vol.}} d\vec{r} ([\vec{E} \times \vec{B}] - [\vec{B} \times \vec{E}]) = \frac{1}{8\pi c} (-c2\pi\hbar) \sum_{\vec{k},\alpha} \sum_{\vec{k}',\alpha'} \sqrt{\frac{\omega}{\omega'}} \frac{1}{L^3} \times \\ &\left( -[\vec{e}_\alpha \times [\vec{k}' \times \vec{e}_{\alpha'}]] \left( a_{\vec{k}\alpha} a_{\vec{k}'\alpha'}^\dagger \int_{\text{Vol.}} d\vec{r} e^{i(\vec{k}-\vec{k}') \cdot \vec{r}} + a_{\vec{k}\alpha}^\dagger a_{\vec{k}'\alpha'} \int_{\text{Vol.}} d\vec{r} e^{i(\vec{k}'-\vec{k}) \cdot \vec{r}} \right) \right. \\ &+ [[\vec{k}' \times \vec{e}_{\alpha'}] \times \vec{e}_\alpha] \left( a_{\vec{k}'\alpha'} a_{\vec{k}\alpha}^\dagger \int_{\text{Vol.}} d\vec{r} e^{i(\vec{k}'-\vec{k}) \cdot \vec{r}} + a_{\vec{k}'\alpha'}^\dagger a_{\vec{k}\alpha} \int_{\text{Vol.}} d\vec{r} e^{i(\vec{k}-\vec{k}') \cdot \vec{r}} \right) \left. + \cdots + \cdots \right). \end{aligned} \quad (7)$$

The orthonormality of the  $e^{i\vec{k}\cdot\vec{r}}/L^{\frac{3}{2}}$  requires  $\vec{k}' = \vec{k}$ , so

$$-[\vec{e}_\alpha \times [\vec{k}' \times \vec{e}_{\alpha'}]] = [[\vec{k}' \times \vec{e}_{\alpha'}] \times \vec{e}_\alpha] = -(\vec{e}_\alpha \cdot \vec{e}_{\alpha'}) \vec{k}' + (\vec{e}_\alpha \cdot \vec{k}') \vec{e}_{\alpha'} = -\delta_{\alpha,\alpha'} \vec{k}, \quad (8)$$

and the above therefore yields

$$\vec{p} = \frac{1}{8\pi c} (-c2\pi\hbar) \sum_{\vec{k},\alpha} 2\vec{k} \left( -a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} - a_{\vec{k}\alpha} a_{\vec{k}\alpha}^\dagger \right) + \cdots + \cdots. \quad (9)$$

The  $\cdots$  terms in these equations indicate similar  $a^\dagger a^\dagger$  and  $aa$  terms exist that contribute for values of  $\vec{k}' = -\vec{k}$ . Contributions from the  $-[\vec{B} \times \vec{E}]$  term, however, cancel those from the  $[\vec{E} \times \vec{B}]$  term for terms of this type. Thus,

$$\vec{p} = \frac{1}{2} \sum_{\vec{k},\alpha} \hbar \vec{k} (a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} + a_{\vec{k}\alpha} a_{\vec{k}\alpha}^\dagger) = \sum_{\vec{k},\alpha} \hbar \vec{k} (a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} + \frac{1}{2}). \quad (10)$$

Now, because for every  $\vec{k}$  with  $n_1, n_2, n_3$  a vector  $-\vec{k}$  with  $-n_1, -n_2, -n_3$  exists, the sum  $\frac{1}{2} \sum_{\vec{k},\alpha} \vec{k} = 0$ , so finally

$$\vec{p} = \sum_{\vec{k},\alpha} a_{\vec{k}\alpha}^\dagger a_{\vec{k}\alpha} \hbar \vec{k}, \quad (11)$$

and a photon of type  $\vec{k}\alpha$  carries a linear momentum,  $\hbar\vec{k}$ . A many-photon state carries the total linear momentum  $\sum_{\vec{k}\alpha}(\hbar\vec{k})n_{\vec{k}\alpha}$ .

## C Photon Rest Mass

From the relativistic relation for the rest mass,  $m_0$ , of a particle,  $(E^2 - c^2 p^2) = m_0^2 c^4$ , we have for the photon

$$(E^2 - c^2 p^2)a_{\vec{k}\alpha}^\dagger |0\rangle = ((\hbar\omega)^2 - c^2(\hbar k)^2)a_{\vec{k}\alpha}^\dagger |0\rangle = 0, \quad (12)$$

so the rest mass of the photon is zero.

## D Angular Momentum: Photon Spin

We begin with the classical expression for the angular momentum density of the electromagnetic field,  $(1/4\pi c)[\vec{r} \times [\vec{E} \times \vec{B}]]$ , leading to the classical expression for the total angular momentum of the radiation field in our cubical laboratory

$$\vec{J} = \frac{1}{4\pi c} \int_{\text{Vol.}} d\vec{r} [\vec{r} \times [\vec{E} \times \vec{B}]]. \quad (13)$$

Before transcribing this to the hermitian quantized form, let us first expand the momentum density, using (in summation convention format for repeated Greek indices)

$$[\vec{E} \times [\vec{\nabla} \times \vec{A}]]_j = \epsilon_{j\alpha\beta} E_\alpha \epsilon_{\beta\mu\nu} \frac{\partial A_\nu}{\partial x_\mu} = E_\alpha \frac{\partial A_\alpha}{\partial x_j} - E_\alpha \frac{\partial A_j}{\partial x_\alpha}, \quad (14)$$

and

$$\begin{aligned} [\vec{r} \times [\vec{E} \times \vec{B}]]_i &= \epsilon_{i\mu\nu} x_\mu \left( E_\alpha \frac{\partial}{\partial x_\nu} A_\alpha - E_\alpha \frac{\partial}{\partial x_\alpha} A_\nu \right) \\ &= E_\alpha \epsilon_{i\mu\nu} x_\mu \frac{\partial}{\partial x_\nu} A_\alpha - \epsilon_{i\mu\nu} x_\mu \frac{\partial}{\partial x_\alpha} (E_\alpha A_\nu) \\ &= E_\alpha \epsilon_{i\mu\nu} x_\mu \frac{\partial}{\partial x_\nu} A_\alpha - \epsilon_{i\mu\nu} \frac{\partial}{\partial x_\alpha} (E_\alpha x_\mu A_\nu) + \epsilon_{i\alpha\nu} E_\alpha A_\nu \\ &= E_\alpha [\vec{r} \times \vec{\nabla}]_i A_\alpha - \frac{\partial}{\partial x_\alpha} (E_\alpha [\vec{r} \times \vec{A}]_i) + [\vec{E} \times \vec{A}]_i, \end{aligned} \quad (15)$$

where we have used  $(\vec{\nabla} \cdot \vec{E}) = 0$  for the radiation field in a source-free region in the second line. Using the final form we can express the total *classical* angular momentum in our cube of volume  $L^3$  by

$$\vec{J}_i = \frac{1}{4\pi c} \left( \int_{\text{Vol.}} d\vec{r} (E_\alpha [\vec{r} \times \vec{\nabla}]_i A_\alpha) - \int_{\text{Vol.}} d\vec{r} (\vec{\nabla} \cdot (\vec{E} [\vec{r} \times \vec{A}]_i)) + \int_{\text{Vol.}} d\vec{r} [\vec{E} \times \vec{A}]_i \right). \quad (16)$$

In the second term, we use Gauss's theorem to convert the volume integral of the divergence to a surface integral

$$\int_{\text{Surf.}} d(\text{Area})(\vec{E} \cdot \vec{n})[\vec{r} \times \vec{A}]_i.$$

Because the radiation  $\vec{A}$  has the value zero on the six faces of our cube, the second term is zero, and the classical expression for the total angular momentum of the radiation field in our cube can be evaluated through the two integrals

$$\begin{aligned} \vec{J} &= \frac{1}{4\pi c} \int_{\text{Vol.}} d\vec{r} (E_\alpha [\vec{r} \times \vec{\nabla}] A_\alpha) + \frac{1}{4\pi c} \int_{\text{Vol.}} d\vec{r} [\vec{E} \times \vec{A}] \\ &= \vec{L} + \vec{S}. \end{aligned} \quad (17)$$

Here, the first integral dependent on the position vector  $\vec{r}$  from some center (such as the position of the atomic system) to a field point in our cube has been identified as the orbital angular momentum of the radiation field, whereas the second term (independent of such an  $\vec{r}$ ) has been identified as the spin angular momentum of the radiation field. Because we are interested in the spin of the photon, we shall look at this second spin term in more detail. To convert this  $\vec{S}$  to the quantized form, we must replace  $[\vec{E} \times \vec{A}]$  by its symmetrized, hermitian form. Thus, for the quantized radiation fields, expressed through eqs. (1) and (3), we have

$$\begin{aligned} \vec{S} &= \frac{1}{8\pi c} \int_{\text{Vol.}} d\vec{r} ([\vec{E} \times \vec{A}] - [\vec{A} \times \vec{E}]) \\ &= \frac{1}{8\pi c} (ic2\pi\hbar) \sum_{\vec{k}} \sum_{\alpha, \alpha'} [\vec{e}_\alpha \times \vec{e}_{\alpha'}] 2(a_{k\alpha}^* a_{k\alpha'}^\dagger - a_{k\alpha}^\dagger a_{k\alpha'}^*) \\ &= -i\hbar \sum_{\vec{k}} \sum_{\alpha, \alpha'} a_{k\alpha}^\dagger a_{k\alpha'}^* [\vec{e}_\alpha \times \vec{e}_{\alpha'}] \\ &= -i\hbar \sum_{\vec{k}} (a_{\vec{k}1}^\dagger a_{\vec{k}2} - a_{\vec{k}2}^\dagger a_{\vec{k}1}) [\vec{e}_1 \times \vec{e}_2] \\ &= -i\hbar \sum_{\vec{k}} (a_{\vec{k}1}^\dagger a_{\vec{k}2} - a_{\vec{k}2}^\dagger a_{\vec{k}1}) \vec{e}_3, \end{aligned} \quad (18)$$

where we have again used the orthonormality of the  $e^{i\vec{k}\cdot\vec{r}}/L^{3/2}$ , as in the calculations for eq. (7), and, again, terms of type  $a^\dagger a^\dagger$  and of type  $aa$  disappear because of cancellations of the contributions from the  $[\vec{E} \times \vec{A}]$  and  $-[\vec{A} \times \vec{E}]$  terms. For our final result, it will be convenient to switch from Cartesian components of vectors along our triad of unit vectors ( $\vec{e}_1, \vec{e}_2, \vec{e}_3 = \vec{k}/k$ ) to spherical vector components, with  $m = +1, 0, -1$ , and define

$$\vec{e}_{+1} = -\sqrt{\frac{1}{2}}(\vec{e}_1 + i\vec{e}_2), \quad \vec{e}_0 = \vec{e}_3, \quad \vec{e}_{-1} = +\sqrt{\frac{1}{2}}(\vec{e}_1 - i\vec{e}_2). \quad (19)$$

Note carefully the difference between  $\vec{e}_{+1}$  and  $\vec{e}_1$ . Also,

$$\vec{e}_m^* = (-1)^m \vec{e}_{-m}. \quad (20)$$

Finally, the  $\vec{e}_{m=\pm 1}$  are the natural base vectors for right and left circular polarizations, just as  $\vec{e}_1$  and  $\vec{e}_2$  were the natural unit vectors for plane polarizations.

Finally, we shall also define the analogous spherical vector components of the photon creation operators

$$a_{\vec{k}m=+1}^{\dagger} = -\sqrt{\frac{1}{2}}(a_{\vec{k}1}^{\dagger} + ia_{\vec{k}2}^{\dagger}), \quad a_{\vec{k}m=-1}^{\dagger} = +\sqrt{\frac{1}{2}}(a_{\vec{k}1}^{\dagger} - ia_{\vec{k}2}^{\dagger}). \quad (21)$$

Note: The photon creation operator has no  $m = 0$  component. From hermitian conjugation, we have

$$a_{\vec{k}m=+1} = -\sqrt{\frac{1}{2}}(a_{\vec{k}1} - ia_{\vec{k}2}), \quad a_{\vec{k}m=-1} = +\sqrt{\frac{1}{2}}(a_{\vec{k}1} + ia_{\vec{k}2}). \quad (22)$$

Also,

$$\sum_{\alpha=1,2} a_{k\alpha}^{\dagger} \vec{e}_{\alpha} = \sum_{m=+1,-1} a_{\vec{k}m}^{\dagger} \vec{e}_m^* = \sum_{m=+1,-1} (-1)^m a_{\vec{k}m}^{\dagger} \vec{e}_{-m}, \quad (23)$$

whereas

$$\sum_{\alpha=1,2} a_{k\alpha} \vec{e}_{\alpha} = \sum_{m=+1,-1} a_{\vec{k}m} \vec{e}_m. \quad (24)$$

Finally, we have

$$(a_{\vec{k}1}^{\dagger} a_{\vec{k}2} - a_{\vec{k}2}^{\dagger} a_{\vec{k}1}) = i(a_{\vec{k}m=+1}^{\dagger} a_{\vec{k}m=+1} - a_{\vec{k}m=-1}^{\dagger} a_{\vec{k}m=-1}), \quad (25)$$

so our expression for the photon spin can be written as

$$\vec{S} = \sum_{\vec{k}} \sum_{m=\pm 1} (\hbar m) a_{\vec{k}m}^{\dagger} a_{\vec{k}m} \left( \frac{\vec{k}}{k} \right) \quad (26)$$

and

$$\vec{S}(a_{\vec{k}m=\pm 1}^{\dagger} |0\rangle) = (\pm \hbar) \left( \frac{\vec{k}}{k} \right) (a_{\vec{k}m=\pm 1}^{\dagger} |0\rangle). \quad (27)$$

Thus, the photon spin vector has projections along the direction of the  $\vec{k}$  vector of  $\pm \hbar$  (right circularly polarized photons) or of  $-\hbar$  (left circularly polarized photons). It thus appears to be a spin-1 particle, *but* the  $m_s = 0$  component is completely missing. The photon has only longitudinal spin projections, either parallel or antiparallel to the direction of its linear momentum vector,  $\vec{k}$ . These are quantized, however, with values  $\pm \hbar$ . The operator  $(\vec{S} \cdot \vec{S})$  does *not* have eigenvalue  $s(s+1)\hbar^2 = 2\hbar^2$ . Instead, this eigenvalue is  $\hbar^2$ .

$$\begin{aligned} (\vec{S} \cdot \vec{S})(a_{\vec{k}m=\pm 1}^{\dagger} |0\rangle) &= \hbar^2 \sum_{\vec{k}'} \sum_{m'=\pm 1} \sum_{\vec{k}''} \sum_{m''=\pm 1} m' m'' \frac{(\vec{k}' \cdot \vec{k}'')}{k' k''} \\ &\times a_{\vec{k}'m'}^{\dagger} a_{\vec{k}'m'}^{\dagger} a_{\vec{k}''m''}^{\dagger} a_{\vec{k}''m''}^{\dagger} (a_{\vec{k}m}^{\dagger} |0\rangle) = \hbar^2 (a_{\vec{k}m}^{\dagger} |0\rangle). \end{aligned} \quad (28)$$

## Vector Spherical Harmonics

To deal with the orbital angular momentum carried by the radiation field, it will be convenient to convert the expansion of the field vector,  $\vec{A}_\perp$ , to an expansion in terms of photon creation and annihilation operators with circular polarizations, with  $m = \pm 1$ , and write

$$\vec{A}_\perp(\vec{r}, t) = \frac{c}{L^{\frac{3}{2}}} \sum_{\vec{k}} \sum_{\lambda=\pm 1} \sqrt{\frac{2\pi\hbar}{\omega}} (a_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{r}} \vec{e}_\lambda + a_{\vec{k}\lambda}^\dagger e^{-i\vec{k}\cdot\vec{r}} \vec{e}_\lambda^*). \quad (1)$$

(Note: We shall reserve later letters in the Greek alphabet, such as  $\lambda, \mu, \nu$  for spherical components, with  $\mu = +1, 0, -1$ , whereas early letters, such as  $\alpha, \beta$ , will be reserved for Cartesian components, with  $\alpha = 1, 2, 3$ .)

We will need to consider the expansion

$$e^{i\vec{k}\cdot\vec{r}} \vec{e}_\lambda = \sum_{l=0}^{\infty} j_l(kr) \sqrt{4\pi(2l+1)} i^l Y_{l0}(\theta, \phi) \vec{e}_\lambda, \quad (2)$$

with  $\lambda = \pm 1$ . Now, it will be useful to couple the spherical components of the vector,  $\vec{e}_\lambda$ , a spherical tensor of rank 1, with the components of the spherical harmonics,  $i^l Y_{lm}$ , which of course are spherical tensors of rank  $l$ , to vector operators of resultant spherical tensor rank  $L$ , with  $L = (l+1), l, (l-1)$ , which are defined by

$$\vec{V}_{[l1]LM} = \sum_{\mu=-1}^{+1} \langle l(M-\mu) 1 \mu | LM \rangle i^l Y_{l(M-\mu)}(\theta, \phi) \vec{e}_\mu, \quad (3)$$

where the  $\vec{V}_{[l1]LM}$  are the so-called vector spherical harmonics. (Note: This vector is similar to our coupled orbital-spin functions,  $\mathcal{Y}_{[ls]jm_j}$ , introduced in Chapter 52.

As there, it will again prove convenient to include the factor  $i^l$  together with the spherical harmonic. Also, the  $\mu$  sum involves all three spherical components of  $\vec{e}_\mu$ .) With this definition, we have

$$e^{i\vec{k}\cdot\vec{r}}\vec{e}_\mu = \sum_l \sum_L j_l(kr) \sqrt{4\pi(2L+1)} \langle l01\mu | L\mu \rangle \vec{V}_{[l1]LM}, \quad (4)$$

with  $\mu = \pm 1$  only and  $L = (l+1), l, (l-1)$ .

## A Properties of Vector Spherical Harmonics

1. Orthonormality. The vector spherical harmonics form an orthonormal set with respect to a scalar product involving both the scalar product of the vectors and an integration over the angular part of our space

$$\begin{aligned} & \int \int d\Omega (\vec{V}_{[l'1]L'M'}^* \cdot \vec{V}_{[l1]LM}) \\ &= \sum_{\mu, \nu} (\vec{e}_\nu^* \cdot \vec{e}_\mu) (-i)^{l'} (i)^l \int \int d\Omega Y_{l'(M'-\nu)}^* Y_{l(M-\mu)} \\ & \times \langle l'(M'-\nu)1\nu | L'M' \rangle \langle l(M-\mu)1\mu | LM \rangle \\ &= \sum_{\mu, \nu} \delta_{\nu\mu} \delta_{l'l} \delta_{(M'-\nu)(M-\mu)} \langle l'(M'-\nu)1\nu | L'M' \rangle \langle l(M-\mu)1\mu | LM \rangle \\ &= \delta_{l'l} \delta_{M'M} \sum_\mu \langle l(M-\mu)1\mu | L'M \rangle \langle l(M-\mu)1\mu | LM \rangle \\ &= \delta_{l'l} \delta_{M'M} \delta_{L'L}, \end{aligned} \quad (5)$$

where this follows from the orthonormality of the unit vectors,  $(\vec{e}_\nu^* \cdot \vec{e}_\mu) = \delta_{\nu\mu}$ , the orthonormality of the spherical harmonics, and the orthonormality of the Clebsch-Gordan coefficients. [Note, in particular: When spherical components are used for the unit vectors,  $\vec{e}$ , we must take the scalar product of a starred with an unstarred spherical component,  $(\vec{e}_\nu^* \cdot \vec{e}_\mu)$  (*not*  $(\vec{e}_\nu \cdot \vec{e}_\mu)$ ), to get a Kronecker delta in the two spherical components.]

2. Parity.

Under space inversion, the spherical harmonics, and the vectors,  $\vec{e}$ , transform as

$$Y_{l(M-\mu)}(\theta, \phi) \rightarrow Y_{l(M-\mu)}(\pi - \theta, \phi + \pi) = (-1)^l Y_{l(M-\mu)}(\theta, \phi)$$

$$\vec{e}_\mu \rightarrow -\vec{e}_\mu.$$

$$\text{Thus, } \vec{V}_{[l1]LM} \rightarrow (-1)^{l+1} \vec{V}_{[l1]LM}. \quad (6)$$

The parity of the vector spherical harmonics is therefore given by  $(-1)^{l+1}$ .

3. Complex Conjugation.

$$\begin{aligned} \vec{V}_{[l1]LM}^* &= \sum_\mu \langle l(M-\mu)1\mu | LM \rangle (-i)^l Y_{l(M-\mu)}^* \vec{e}_\mu^* \\ &= \sum_\mu (-1)^{l+1-L} \langle l(\mu-M)1-\mu | L-M \rangle \\ &\quad \times i^l (-1)^l (-1)^{(M-\mu)} Y_{l(\mu-M)} (-1)^\mu \vec{e}_{-\mu} \end{aligned}$$

$$\begin{aligned}
&= (-1)^{M-L+1} \sum_{\mu} \langle l(\mu - M) 1 - \mu | L - M \rangle i^l Y_{l(\mu-M)} \vec{e}_{-\mu} \\
&= (-1)^{L-M-1} \vec{V}_{[l]L-M}.
\end{aligned} \tag{7}$$

#### 4. Transformation properties under rotations.

Let  $\vec{W}$  be any vector, with an expansion in Cartesian components given by

$$\vec{W} = W_1 \vec{e}_1 + W_2 \vec{e}_2 + W_3 \vec{e}_3 \tag{8}$$

and an expansion in spherical components,  $v = +1, 0, -1$ , given by

$$\vec{W} = \sum_v W_v \vec{e}_v^* = \sum_v W_v (-1)^v \vec{e}_{-v} = \sum_v W_v^* \vec{e}_v = \sum_v (-1)^v W_{-v} \vec{e}_v. \tag{9}$$

Then, we shall show that the scalar product  $(\vec{W} \cdot \vec{V}_{[l]LM})$  transforms under rotations as a spherical tensor of rank  $L$  with spherical components given by  $M$ . Using  $(\vec{e}_\mu \cdot \vec{e}_v^*) = \delta_{\mu,v}$ , we have

$$\begin{aligned}
(\vec{W} \cdot \vec{V}_{[l]LM}) &= \sum_{\mu, v} \langle l(M - \mu) 1 \mu | LM \rangle i^l Y_{l(M-\mu)}(\theta, \phi) (\vec{e}_\mu \cdot \vec{e}_v^*) W_v \\
&= \sum_{\mu} \langle l(M - \mu) 1 \mu | LM \rangle i^l Y_{l(M-\mu)}(\theta, \phi) W_\mu.
\end{aligned} \tag{10}$$

Now, under an arbitrary rotation in 3-D space (specified by the Euler angles,  $\alpha, \beta, \gamma$ ),

$$\begin{aligned}
(\vec{W} \cdot \vec{V}_{[l]LM})_{\text{rot.}} &= R(\alpha, \beta, \gamma) (\vec{W} \cdot \vec{V}_{[l]LM}) R^{-1}(\alpha, \beta, \gamma) \\
&= \sum_{\mu} \langle l(M - \mu) 1 \mu | LM \rangle i^l Y_{l(M-\mu)}(\theta', \phi') W'_\mu,
\end{aligned} \tag{11}$$

where  $\theta', \phi'$  are the angular variables of the rotated system with respect to the original coordinate axes, and  $W'$  are the components of the rotated vector,  $\vec{W}$ . Thus,

$$\begin{aligned}
Y_{l(M-\mu)}(\theta', \phi') &= \sum_m Y_{lm}(\theta, \phi) D_{m(M-\mu)}^l(\alpha, \beta, \gamma)^* \\
W'_\mu &= \sum_v W_v D_{v\mu}^1(\alpha, \beta, \gamma)^*,
\end{aligned} \tag{12}$$

where we have used the conventions of Chapter 29 for the matrix elements of the rotation operators, the so-called Wigner or rotation  $D$  functions. We shall also use (see Chapter 30)

$$\begin{aligned}
D_{m(M-\mu)}^l(\alpha, \beta, \gamma) D_{v\mu}^1(\alpha, \beta, \gamma) &= \\
\sum_{\bar{L}} \langle lm 1 v | \bar{L}(m+v) \rangle \langle l(M-\mu) 1 \mu | \bar{L} M \rangle D_{(m+v)M}^{\bar{L}}(\alpha, \beta, \gamma).
\end{aligned} \tag{13}$$

Combining eqs. (11), (12), and the complex conjugate of eq. (13), we have

$$\begin{aligned}
&(\vec{W} \cdot \vec{V}_{[l]LM})_{\text{rot.}} \\
&= \sum_{m, v} i^l Y_{lm}(\theta, \phi) W_v \sum_{\bar{L}} \langle lm 1 v | \bar{L}(m+v) \rangle D_{(m+v)M}^{\bar{L}}(\alpha, \beta, \gamma)^*
\end{aligned}$$

$$\begin{aligned}
& \times \sum_{\mu} \langle l(M-\mu)1\mu | LM \rangle \langle l(M-\mu)1\mu | \bar{L}M \rangle \\
& = \sum_{m,v} i^l Y_{lm}(\theta, \phi) W_v \sum_{\bar{L}} \langle lm1v | \bar{L}(m+v) \rangle D_{(m+v)M}^{\bar{L}}(\alpha, \beta, \gamma)^* \delta_{\bar{L}L} \\
& = \sum_{m,v} i^l Y_{lm}(\theta, \phi) W_v \langle lm1v | L(m+v) \rangle D_{(m+v)M}^L(\alpha, \beta, \gamma)^*, \tag{14}
\end{aligned}$$

where we have used the orthonormality of the Clebsch–Gordan coefficients. Thus

$$(\vec{W} \cdot \vec{V}_{[l1]LM})_{\text{rot.}} = \sum_{m'} (\vec{W} \cdot \vec{V}_{[l1]Lm'}) D_{m'M}^L(\alpha, \beta, \gamma)^*. \tag{15}$$

The quantity  $(\vec{W} \cdot \vec{V}_{[l1]LM})$  is the  $M^{\text{th}}$  component of a spherical tensor of rank  $L$ .

## B The Vector Spherical Harmonics of the Radiation Field

Now, we shall examine the types of vector spherical harmonics that actually occur in the expansion of the radiation field,  $\vec{A}_\perp(\vec{r}, t)$ . We shall examine the vector spherical harmonics for a fixed  $L$  that occur in the expansion

$$e^{i\vec{k}\cdot\vec{r}} \vec{e}_\mu = \sum_L \sum_{l=L, (L\pm 1)} \langle l01\mu | L\mu \rangle j_l(kr) \sqrt{4\pi(2l+1)} \vec{V}_{[l1]L\mu}. \tag{16}$$

We shall need the Clebsch–Gordan coefficients:

$$\begin{aligned}
\langle L01\pm 1 | L\pm 1 \rangle &= \mp \frac{1}{\sqrt{2}} = \frac{-\mu}{\sqrt{2}}, \\
\langle (L-1)01\pm 1 | L\pm 1 \rangle &= \sqrt{\frac{(L+1)}{2(2L-1)}}, \\
\langle (L+1)01\pm 1 | L\pm 1 \rangle &= \sqrt{\frac{L}{2(2L+3)}}. \tag{17}
\end{aligned}$$

With these coefficients, we have

$$\begin{aligned}
e^{i\vec{k}\cdot\vec{r}} \vec{e}_{\mu=\pm 1} &= \sum_L \sqrt{2\pi(2L+1)} \left[ \left( -\mu j_L(kr) \vec{V}_{[l1]L\mu} \right) + \right. \\
&\quad \left. \left( \sqrt{\frac{(L+1)}{(2L+1)}} j_{L-1}(kr) \vec{V}_{[(L-1)1]L\mu} + \sqrt{\frac{L}{(2L+1)}} j_{L+1}(kr) \vec{V}_{[(L+1)1]L\mu} \right) \right]. \tag{18}
\end{aligned}$$

It will now be convenient to define these two pieces in the vector spherical harmonic expansion of  $\vec{A}_\perp$ , through

$$(1) : \quad j_L(kr) \vec{V}_{[l1]L\mu} \equiv \vec{A}(\vec{r}, \mathcal{M})_{L\mu}, \tag{19}$$

II:

$$\left( \sqrt{\frac{(L+1)}{(2L+1)}} j_{L-1} \vec{V}_{[(L-1)]L\mu} + \sqrt{\frac{L}{(2L+1)}} j_{L+1} \vec{V}_{[(L+1)]L\mu} \right) \equiv \vec{A}(\vec{r}, \mathcal{E})_{L\mu}, \quad (20)$$

where  $\vec{A}(\vec{r}, \mathcal{M})_{L\mu}$  is designated by the letter,  $\mathcal{M}$ , because (as we shall show) it is the term in the  $\vec{A}_\perp$  expansion giving rise to the *magnetic*  $2^L$ -pole radiation field. This term has parity given by  $(-1)^{L+1}$ . Conversely,  $\vec{A}(\vec{r}, \mathcal{E})_{L\mu}$  is designated by the letter,  $\mathcal{E}$ , because it gives rise to the *electric*  $2^L$ -pole radiation field. Its parity is given by  $(-1)^L$ . Finally, one linear combination of the  $\vec{V}_{[l]L\mu}$  exists, which is *missing* in the expansion of  $\vec{A}_\perp$  in vector spherical harmonics. The missing linear combination to be designated by the letter,  $\mathcal{L}$ , is

III:

$$\left( \sqrt{\frac{L}{(2L+1)}} j_{L-1} \vec{V}_{[(L-1)]L\mu} - \sqrt{\frac{(L+1)}{(2L+1)}} j_{L+1} \vec{V}_{[(L+1)]L\mu} \right) \equiv \vec{A}(\vec{r}, \mathcal{L})_{L\mu}. \quad (21)$$

This piece, with parity also given by  $(-1)^L$ , is missing in the expansion of  $\vec{A}_\perp$  because  $(\vec{\nabla} \cdot \vec{A}(\vec{r}, \mathcal{L})) \neq 0$ . This piece therefore occurs in the expansion of  $\vec{A}_\parallel$ , that is, the *longitudinal* part of the vector potential. Hence, the designation by the letter,  $\mathcal{L}$  and its absence in the expansion of the radiation field,  $\vec{A}_\perp$ . Finally, we quote a useful alternate form for the fields,  $\vec{A}(\vec{r}, \mathcal{T})_{L\mu}$ . (The derivation of these formulae is given in an appendix.)

$$\begin{aligned} \text{I : } \vec{A}(\vec{r}, \mathcal{M})_{L\mu} &= \frac{1}{\sqrt{L(L+1)}} \vec{L}(j_L(kr) i^L Y_{L\mu}(\theta, \phi)), \\ \text{II : } \vec{A}(\vec{r}, \mathcal{E})_{L\mu} &= -\frac{1}{k} \frac{1}{\sqrt{L(L+1)}} [\vec{\nabla} \times \vec{L}(j_L(kr) i^L Y_{L\mu}(\theta, \phi))] \\ &= -\frac{1}{k} [\vec{\nabla} \times \vec{A}(\vec{r}, \mathcal{M})_{L\mu}], \\ \text{III : } \vec{A}(\vec{r}, \mathcal{L})_{L\mu} &= \frac{1}{ik} \vec{\nabla}(j_L(kr) i^L Y_{L\mu}(\theta, \phi)), \end{aligned} \quad (22)$$

where the operator,  $\vec{L}$ , is the dimensionless  $-i[\vec{r} \times \vec{\nabla}]$ . All three pieces of the vector potential,  $\vec{A}$ , are derivable from simple operators acting on the scalar function,  $j_L(kr) i^L Y_{L\mu}(\theta, \phi)$ .

Having attained all of these properties of the  $\vec{A}(\vec{r}, \mathcal{T})$ , we can combine eqs. (1), (4), (18), (19), and (20) to give the expansion of the radiation field

$$\begin{aligned} \vec{A}_\perp(\vec{r}, t) = \frac{2\pi c}{\sqrt{\text{Vol.}}} \sum_{\vec{k}} \sum_{\mu=\pm 1} \sum_L \sqrt{\frac{\hbar(2L+1)}{\omega}} &\left[ a_{\vec{k}\mu}^-( -\mu \vec{A}(\vec{r}, \mathcal{M})_{L\mu} + \vec{A}(\vec{r}, \mathcal{E})_{L\mu} \right. \\ &\left. + a_{\vec{k}\mu}^\dagger ( -\mu \vec{A}(\vec{r}, \mathcal{M})_{L\mu}^* + \vec{A}(\vec{r}, \mathcal{E})_{L\mu}^* ) \right]. \end{aligned} \quad (23)$$

(We have written, Vol., explicitly for the volume of our cubical laboratory, to avoid confusion with the angular momentum index,  $L$ .) Also, recall the  $a_{\vec{k}\mu}$  are time de-

pendent,  $a_{\vec{k}\mu}(t) = a_{\vec{k}\mu}(0)e^{-i\omega t}$  and, finally, from eq. (7), note  $\vec{A}(\vec{r}, \mathcal{M}(\text{or } \mathcal{E}))_{L\mu}^* = (-1)^{L+1-\mu} \vec{A}(\vec{r}, \mathcal{M}(\text{or } \mathcal{E}))_{L-\mu}$ .

The  $\vec{A}(\vec{r}, \mathcal{M})_{L\mu}$  and  $\vec{A}(\vec{r}, \mathcal{E})_{L\mu}$  lead to the radiation  $\vec{E}$  and  $\vec{B}$  fields. In particular,

$$\begin{aligned}\vec{E}(\vec{r}, t; \mathcal{M})_{L\mu} &= ik\vec{A}(\vec{r}, \mathcal{M})_{L\mu}e^{-i\omega t}, \\ \vec{B}(\vec{r}, t; \mathcal{M})_{L\mu} &= [\vec{\nabla} \times \vec{A}(\vec{r}, \mathcal{M})_{L\mu}]e^{-i\omega t} = -k\vec{A}(\vec{r}, \mathcal{E})_{L\mu}e^{-i\omega t},\end{aligned}\quad (24)$$

where we have used the second relation of eq. (22) in the last step. Similarly,

$$\begin{aligned}\vec{E}(\vec{r}, t; \mathcal{E})_{L\mu} &= ik\vec{A}(\vec{r}, \mathcal{E})_{L\mu}e^{-i\omega t} = -i\vec{B}(\vec{r}, t; \mathcal{M})_{L\mu}, \\ \vec{B}(\vec{r}, t; \mathcal{E})_{L\mu} &= -k\vec{A}(\vec{r}, \mathcal{M})_{L\mu}e^{-i\omega t} = i\vec{E}(\vec{r}, t; \mathcal{M})_{L\mu},\end{aligned}\quad (25)$$

where we have used

$$[\vec{\nabla} \times [\vec{\nabla} \times \vec{A}]] = -\nabla^2 \vec{A} = k^2 \vec{A}$$

for this divergence-free  $\vec{A}$  together with the second of the relations of eq. (22) in the expression for the  $\vec{B}$  field.

In many atomic and other quantum systems, we shall be interested in the radiation fields in the limit in which the parameter,  $(kr)$ , is a small quantity,  $(r \ll \lambda)$ , i.e., dimension of the radiating quantum system  $\ll$  wavelength of the emitted photon. In this case, we may need only the dominant term in the expansion of the spherical Bessel functions,  $j_L(kr)$ , which gives the radial dependence of the above fields. Recall

$$j_L(kr) \approx \frac{2^L L!}{(2L+1)!} (kr)^L \quad \text{for } kr \ll 1. \quad (26)$$

Thus, in this limit,

$$\vec{A}(\vec{r}, \mathcal{E}) \sim (kr)^{L-1}, \quad \vec{A}(\vec{r}, \mathcal{M}) \sim (kr)^L, \quad (27)$$

and therefore for the  $\mathcal{E}$ -type fields

$$\begin{aligned}\vec{E}(\vec{r}, \mathcal{E}) &\sim ik(kr)^{L-1}, \\ \vec{B}(\vec{r}, \mathcal{E}) &\sim -k(kr)^L.\end{aligned}\quad (28)$$

For the  $\mathcal{E}$ -type fields of a definite  $L$ , the  $\vec{E}$ -field is dominant and has the  $r$  dependence of an electric  $2^L$ -pole field. Conversely, for  $\mathcal{M}$ -type fields,

$$\begin{aligned}\vec{E}(\vec{r}, \mathcal{M}) &\sim ik(kr)^L, \\ \vec{B}(\vec{r}, \mathcal{M}) &\sim -k(kr)^{L-1}.\end{aligned}\quad (29)$$

Now, the  $\vec{B}$ -field dominates for a definite  $L$  and has the  $r$  dependence of a magnetic  $2^L$ -pole field.

Before examining the electric and magnetic multipole radiation fields in detail, we shall (in the next chapter) examine first the dominant electric dipole approximation for quantum systems, such as atoms, for which the approximation  $kr \ll 1$  is a very good one.

## C Mathematical Appendix

In this appendix, we shall derive the alternate form for the  $\vec{A}(\vec{r}, T)$ , given in eq. (22).

### 1. The relation

$$\vec{A}(\vec{r}, \mathcal{M})_{L\mu} \equiv j_L(kr) \vec{V}_{[l1]L\mu} = \frac{1}{\sqrt{L(L+1)}} \vec{L}(j_L(kr) i^L Y_{L\mu}(\theta, \phi)).$$

To derive this relation, we shall write

$$\vec{L} = \sum_{\mu} L_{\mu} \vec{e}_{\mu}^* \quad (30)$$

and use the fact that the operators,  $L_{\mu} = -i[\vec{r} \times \vec{\nabla}]_{\mu}$ , act only on the angles  $\theta, \phi$ , (not on  $r$ ). Thus,

$$\begin{aligned} \vec{L}(i^L Y_{LM}) &= \sum_{\mu} \vec{e}_{\mu}^* i^L (L_{\mu} Y_{LM}) \\ &= \sum_{\mu} (-1)^{\mu} \vec{e}_{-\mu} \langle LM | 1\mu | L(M+\mu) \rangle i^L Y_{L(M+\mu)} \sqrt{L(L+1)} \\ &= \sum_{\mu} \vec{e}_{-\mu} (-1)^{\mu-\mu} \langle L(M+\mu) | 1 - \mu | LM \rangle i^L Y_{L(M+\mu)} \sqrt{L(L+1)} \\ &= \sqrt{L(L+1)} \sum_{\mu} \langle L(M-\mu) | 1\mu | LM \rangle i^L Y_{L(M-\mu)} \vec{e}_{\mu} \\ &= \sqrt{L(L+1)} \vec{V}_{[l1]LM}, \end{aligned} \quad (31)$$

where we have used the Wigner–Eckart theorem for the well-known matrix elements of the spherical components,  $L_{\mu}$ , in the second line, the Clebsch–Gordan coefficient symmetry property involving  $1 \leftrightarrow 3$  interchange in the third line, and finally have renamed the dummy summation index  $\mu \leftrightarrow -\mu$  in the next line; leading to the desired result.

### 2. The gradient formula:

$$\begin{aligned} \frac{1}{i} \vec{\nabla} (f(r) i^l Y_{lm}(\theta, \phi)) &= \sqrt{\frac{l}{(2l+1)}} \left( \frac{df}{dr} + \frac{(l+1)}{r} f(r) \right) \vec{V}_{[(l-1)1]lm} \\ &\quad + \sqrt{\frac{(l+1)}{(2l+1)}} \left( \frac{df}{dr} - \frac{l}{r} f(r) \right) \vec{V}_{[(l+1)1]lm}. \end{aligned} \quad (32)$$

To derive this formula, we shall write

$$\frac{1}{i} \vec{\nabla} (f(r) i^l Y_{lm}(\theta, \phi)) = \frac{1}{i} \sum_{\mu} (-1)^{\mu} \vec{e}_{-\mu} \nabla_{\mu} (f(r) i^l Y_{lm}(\theta, \phi)). \quad (33)$$

We shall again use the Wigner–Eckart theorem to find the matrix elements of  $\nabla_{\mu}$ . It is sufficient to pick one particular spherical component of the operator  $\vec{\nabla}$ . For simplicity, we pick the component with  $\mu = 0$

$$\nabla_0^1 = \frac{\partial}{\partial z} = \cos \theta \frac{\partial}{\partial r} - \frac{1}{r} \sin \theta \frac{\partial}{\partial \theta}. \quad (34)$$

From Chapters 9 and 32, we have [see, in particular, eqs. (33) and (34) of Chapter 9 and eq. (8) of Chapter 32],

$$\cos \theta Y_{lm} = \sum_{l'} \sqrt{\frac{4\pi}{3}} \sqrt{\frac{3(2l+1)}{4\pi(2l'+1)}} \langle l010|l'0 \rangle \langle lm10|l'm \rangle Y_{l'm}, \quad (35)$$

and

$$\begin{aligned} \sin \theta \frac{\partial}{\partial \theta} Y_{lm} &= l \sqrt{\frac{[(l+1)^2 - m^2]}{(2l+1)(2l+3)}} Y_{(l+1)m} - (l+1) \sqrt{\frac{[l^2 - m^2]}{(2l+1)(2l-1)}} Y_{(l-1)m} \\ &= l \sqrt{\frac{(2l+1)}{(2l+3)}} \langle l010|(l+1)0 \rangle \langle lm10|(l+1)m \rangle Y_{(l+1)m} \\ &\quad - (l+1) \sqrt{\frac{(2l+1)}{(2l-1)}} \langle l010|(l-1)0 \rangle \langle lm10|(l-1)m \rangle Y_{(l-1)m}, \end{aligned} \quad (36)$$

where we have used

$$\begin{aligned} \langle lm10|(l+1)m \rangle &= \sqrt{\frac{[(l+1)^2 - m^2]}{(2l+1)(l+1)}}, \\ \langle lm10|(l-1)m \rangle &= -\sqrt{\frac{[l^2 - m^2]}{l(2l+1)}}. \end{aligned} \quad (37)$$

Combining these relations, we get

$$\begin{aligned} &\left( \cos \theta \frac{\partial}{\partial r} - \frac{1}{r} \sin \theta \frac{\partial}{\partial \theta} \right) (f(r) Y_{lm}) = \\ &\sqrt{\frac{(2l+1)(l+1)}{(2l+3)(2l+1)}} \left( \frac{df}{dr} - \frac{l}{r} f(r) \right) Y_{(l+1)m} \langle lm10|(l+1)m \rangle \\ &- \sqrt{\frac{(2l+1)l}{(2l-1)(2l+1)}} \left( \frac{df}{dr} + \frac{(l+1)}{r} f(r) \right) Y_{(l-1)m} \langle lm10|(l-1)m \rangle. \end{aligned} \quad (38)$$

From these, we can read the reduced matrix elements of the operator,  $\vec{\nabla}$ .

$$\begin{aligned} \frac{\langle (l+1) \| \vec{\nabla} \| l \rangle}{\sqrt{(2l+3)}} &= \sqrt{\frac{(2l+1)(l+1)}{(2l+3)(2l+1)}} \left( \frac{df}{dr} - \frac{l}{r} f(r) \right) \\ \frac{\langle (l-1) \| \vec{\nabla} \| l \rangle}{\sqrt{(2l-1)}} &= -\sqrt{\frac{(2l+1)l}{(2l-1)(2l+1)}} \left( \frac{df}{dr} + \frac{(l+1)}{r} f(r) \right). \end{aligned} \quad (39)$$

We can now rewrite

$$\begin{aligned} &\frac{1}{i} \vec{\nabla} (f(r) i^l Y_{lm}) \\ &= i^{l-1} \sum_{\mu} (-1)^{\mu} \vec{e}_{-\mu} \sum_{l'} \langle lm1\mu | l'(m+\mu) \rangle \frac{\langle l' \| \vec{\nabla} \| l \rangle}{\sqrt{(2l'+1)}} Y_{l'(m+\mu)} \end{aligned}$$

$$\begin{aligned}
&= i^{l-1} \sum_{l'=(l\pm 1)} \sum_{\mu} (-1)^{\mu} \vec{e}_{-\mu} \frac{\langle l' \parallel \vec{\nabla} \parallel l \rangle}{\sqrt{(2l+1)}} (-1)^{l-l'+\mu} \langle l'(m+\mu) 1 - \mu | lm \rangle Y_{l'(m+\mu)} \\
&= \sum_{l'=(l\pm 1)} i^{l-1} (-i)^{l'} \frac{\langle l' \parallel \vec{\nabla} \parallel l \rangle}{\sqrt{(2l+1)}} (-1)^{l-l'} \sum_{\mu} \langle l'(m-\mu) 1 \mu | lm \rangle i^{l'} Y_{l'(m-\mu)} \vec{e}_{\mu} \\
&= \sum_{l'=(l\pm 1)} i^{l'-l-1} \sqrt{\frac{(2l'+1)}{(2l+1)}} \vec{V}_{[l']lm} \frac{\langle l' \parallel \vec{\nabla} \parallel l \rangle}{\sqrt{(2l'+1)}}, \tag{40}
\end{aligned}$$

where we have again used a  $1 \leftrightarrow 3$  interchange symmetry property of the Clebsch–Gordan coefficient in line 2, and have again changed the dummy summation index  $\mu \leftrightarrow -\mu$  in line 3 of this relation. Substituting from the two known reduced matrix elements of eq. (39), we get the desired gradient formula of eq. (32). For the special case, when  $f(r) = j_l(kr)$ , we have from the results of Chapter 41 and the mathematical appendix to Chapter 41:

$$\left( \frac{d}{dr} - \frac{l}{r} \right) j_l(kr) = -k j_{l+1}(kr), \tag{41}$$

$$\left( \frac{d}{dr} + \frac{(l+1)}{r} \right) j_l(kr) = +k j_{l-1}(kr). \tag{42}$$

This leads to the relation (III) of eq. (22).

### 3. Derivation of

$$\vec{A}(\vec{r}, \mathcal{E})_{LM} = -\frac{1}{k} [\vec{\nabla} \times \vec{A}(\vec{r}, \mathcal{M})_{LM}].$$

We shall use  $\vec{A}(\vec{r}, \mathcal{M})_{LM} = j_L(kr) \vec{V}_{[L]LM}$  and take the curl of this vector

$$\begin{aligned}
&[\vec{\nabla} \times (j_L(kr) \vec{V}_{[L]LM})] \\
&= [\vec{\nabla} \times (j_L(kr) \sum_{\mu} \langle L(M-\mu) 1 \mu | LM \rangle i^L Y_{L(M-\mu)} \vec{e}_{\mu})] \\
&= \sum_{\mu} \langle L(M-\mu) 1 \mu | LM \rangle [\vec{\nabla} (j_L(kr) i^L Y_{L(M-\mu)}) \times \vec{e}_{\mu}] \\
&= i \sum_{\mu} \langle L(M-\mu) 1 \mu | LM \rangle \left( \sqrt{\frac{L}{(2L+1)}} k j_{L-1}(kr) [\vec{V}_{[(L-1)]L(M-\mu)} \times \vec{e}_{\mu}] \right. \\
&\quad \left. - \sqrt{\frac{(L+1)}{(2L+1)}} k j_{L+1}(kr) [\vec{V}_{[(L+1)]LM} \times \vec{e}_{\mu}] \right), \tag{43}
\end{aligned}$$

where we have used  $[\vec{\nabla} \times (\chi \vec{e})] = [(\vec{\nabla} \chi) \times \vec{e}]$  for the special case in which  $\vec{e}$  is a constant vector and  $\chi$  is a scalar, and where we have used the gradient formula in the last step. Now, we shall use

$$\begin{aligned}
&[\vec{V}_{[l']L(M-\mu)} \times \vec{e}_{\mu}] = \\
&\sum_{\nu} \langle l'((M-\mu-\nu) 1 \nu | L(M-\mu)) i^{l'} Y_{l'(M-\mu-\nu)} [\vec{e}_{\nu} \times \vec{e}_{\mu}] \tag{44}
\end{aligned}$$

In terms of spherical components, the vector product of the unit vectors can be seen to be expressible in terms of a Clebsch–Gordan coefficient

$$[\vec{e}_v \times \vec{e}_\mu] = i\sqrt{2}\langle l v 1 \mu | l(\mu + v) \rangle \vec{e}_{(\mu+v)}, \quad (45)$$

so

$$\begin{aligned} & \sum_\mu \langle L(M - \mu) 1 \mu | LM \rangle [\vec{V}_{[l'1]L(M-\mu)} \times \vec{e}_\mu] \\ &= i\sqrt{2} \sum_{\mu, v} \langle l'(M - \mu - v) 1 v | L(M - \mu) \rangle \langle L(M - \mu) 1 \mu | LM \rangle \\ & \quad \times \langle 1 v 1 \mu | l(\mu + v) \rangle i^{l'} Y_{l'(M-\mu-v)} \vec{e}_{\mu+v} \\ &= i\sqrt{2} \sum_\lambda \left( \sum_\mu \langle l'(M - \lambda) 1 (\lambda - \mu) | L(M - \mu) \rangle \langle L(M - \mu) 1 \mu | LM \rangle \right. \\ & \quad \times \left. \langle 1 (\lambda - \mu) 1 \mu | 1 \lambda \rangle \right) i^{l'} Y_{l'(M-\lambda)} \vec{e}_\lambda, \end{aligned} \quad (46)$$

where, for convenience, we have changed the summation indices by renaming  $(\mu + v) = \lambda$  in the last line. Now, we can do the  $\mu$  sum in the last step. In particular, it can be shown that this sum over  $\mu$  of a product of three  $\mu$ -dependent Clebsch–Gordan coefficients is, for *fixed M* and *fixed λ*, equal to a single Clebsch–Gordan coefficient times an  $l'$  dependent, but (magnetic quantum number)-independent coefficient:

$$\begin{aligned} & \sum_\mu \langle l'(M - \lambda) 1 (\lambda - \mu) | L(M - \mu) \rangle \langle L(M - \mu) 1 \mu | Lm \rangle \langle 1 (\lambda - \mu) 1 \mu | 1 \lambda \rangle \\ &= c_{l'} \langle l'(M - \lambda) 1 \lambda | LM \rangle, \end{aligned} \quad (47)$$

with

$$c_{(L-1)} = \sqrt{\frac{(L+1)}{2L}}, \quad c_{(L+1)} = -\sqrt{\frac{L}{2(L+1)}}. \quad (48)$$

This equation can be shown by direct verification. It also follows more elegantly from angular-momentum recoupling theory (see Chapter 34). The coefficients  $c_{l'}$  introduced here are given by the unitary form of the Racah coefficient,  $c_{l'} = U(l'1L1; L1)$  [see eq. (12) of Chapter 34]. Using eqs. (46) and (47), we have

$$\begin{aligned} & \sum_\mu \langle L(M - \mu) 1 \mu | LM \rangle [\vec{V}_{[l'1]L(M-\mu)} \times \vec{e}_\mu] \\ &= i\sqrt{2} c_{l'} \sum_\lambda \langle l'(M - \lambda) 1 \lambda | LM \rangle i^{l'} Y_{l'(M-\lambda)} \vec{e}_\lambda \\ &= i\sqrt{2} c_{l'} \vec{V}_{[l'1]LM}. \end{aligned} \quad (49)$$

Using this result, together with the  $c_{l'}$  of eq. (48) and eq.(43), we get

$$\begin{aligned} & [\vec{\nabla} \times (j_L(kr) \vec{V}_{[L1]LM})] = \\ & -k \left( \sqrt{\frac{(L+1)}{(2L+1)}} j_{(L-1)}(kr) \vec{V}_{[(L-1)1]LM} + \sqrt{\frac{L}{(2L+1)}} j_{(L+1)}(kr) \vec{V}_{[(L+1)1]LM} \right) \\ &= -k \vec{A}(\vec{r}, \mathcal{E})_{LM}, \end{aligned} \quad (50)$$

leading to the desired result

$$\vec{A}(\vec{r}, \mathcal{E})_{LM} = -\frac{1}{k} [\vec{\nabla} \times \vec{A}(\vec{r}, \mathcal{M})_{LM}]. \quad (51)$$

# The Emission of Photons by Atoms: Electric Dipole Approximation

We shall now look at the interaction of an atomic system with the radiation field in detail. We have

$$H = H_{\text{atom}} + H_{\text{radiation}} + H_{\text{interaction}}, \quad (1)$$

where  $H_{\text{radiation}}$  will be written in terms of the photon creation and annihilation operators as in Chapters 60 and 61,  $H_{\text{atom}}$  has the usual kinetic and potential energy terms, and  $H_{\text{interaction}}$  is given by

$$\begin{aligned} H_{\text{interaction}} &= \\ &\sum_{i=1}^n \left( \frac{-e_i}{2m_i c} (\vec{p}_i \cdot \vec{A}_\perp(\vec{r}_i, t) + \vec{A}_\perp(\vec{r}_i, t) \cdot \vec{p}_i) + \frac{e_i^2}{2m_i c^2} (\vec{A}_\perp(\vec{r}_i, t) \cdot \vec{A}_\perp(\vec{r}_i, t)) \right) \\ &- \sum_{i=1}^n \frac{e_i \hbar}{2m_i c} g_{s_i} (\vec{s}_i \cdot [\vec{\nabla}_i \times \vec{A}_\perp(\vec{r}_i, t)]). \end{aligned} \quad (2)$$

We can combine the two terms,  $\vec{p}_i \cdot \vec{A}_\perp(\vec{r}_i, t)$  and  $\vec{A}_\perp(\vec{r}_i, t) \cdot \vec{p}_i$ , because  $\vec{A}_\perp$  is divergence-free.

$$\vec{p}_i \cdot \vec{A}_\perp(\vec{r}_i, t) = \vec{A}_\perp(\vec{r}_i, t) \cdot \vec{p}_i + \frac{\hbar}{i} \sum_{\alpha} \frac{\partial}{\partial x_{i,\alpha}} (A_\perp(\vec{r}_i, t))_{\alpha} = \vec{A}_\perp(\vec{r}_i, t) \cdot \vec{p}_i, \quad (3)$$

because  $\partial(A_\perp)_{\alpha}/\partial x_{\alpha} = 0$ . In the above,

$$\vec{A}(\vec{r}, t) = \frac{c}{\sqrt{L^3}} \sum_{\vec{k}} \sum_{\lambda} \sqrt{\frac{2\pi\hbar}{\omega}} (a_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{r}} \vec{e}_{\lambda} + a_{\vec{k}\lambda}^* e^{-i\vec{k}\cdot\vec{r}} \vec{e}_{\lambda}^*). \quad (4)$$

For an atomic system, we can expect the quantity,  $\vec{k} \cdot \vec{r}_i$ , to be very small:

$$kr_i = \frac{2\pi}{\lambda} a_0 \approx \frac{2\pi(10)^{-8}\text{cm}}{6,000 \times (10)^{-8}\text{cm}} \approx (10)^{-3},$$

assuming the photon is in the visible part of the spectrum. For such a system, we can use  $e^{i\vec{k} \cdot \vec{r}_i} \approx 1$  to very good approximation. As a second example, think of a nuclear system. For a nucleus,

$$kr_i = \frac{\hbar\omega r_i}{\hbar c} = \frac{(\hbar\omega)_\gamma R_{\text{nucleus}}}{\hbar c} = \frac{(\hbar\omega)_\gamma R_{\text{nucleus}}}{200\text{MeVfermi}},$$

so, for a heavy nucleus, with  $R_{\text{nucleus}} \approx 10$  fermi and emitted  $\gamma$  photon of energy 2 MeV, we would have  $kr_i \approx (10)^{-1}$ , still small, but now large enough so higher order terms in the expansion in powers of  $kr_i$  become important. This will be particularly true for transitions between low-lying states in a nucleus that often have the same parity so the zeroth-order term will lead to electric dipole matrix elements that are rigorously zero because of parity selection rules. In such a system then, we will find it advantageous to make full use of the expansion of  $\vec{A}_\perp$  in vector spherical harmonics. With the full expansion, we will get higher order electric and magnetic multipole moment matrix elements. For the atomic case, however, where the zeroth-order term dominates, we can dispense with the vector spherical harmonic formalism. In this case (as we shall see), the atomic transition probability matrix elements will involve only matrix elements of the atomic electric dipole moment operator.

For the atomic system, we can take

$$H_{\text{interaction}} = H_{\text{perturbation}}^{(1)} = -\sum_i \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}(\vec{r}_i, t), \quad (5)$$

where we take only the zeroth-order term in the  $kr_i$  expansion of  $\vec{A}$ , so

$$\vec{A} = \frac{c}{\sqrt{L^{\frac{3}{2}}}} \sum_{\vec{k}} \sum_{\lambda} \sqrt{\frac{2\pi\hbar}{\omega}} (a_{\vec{k}\lambda} \vec{e}_{\lambda} + a_{\vec{k}\lambda}^{\dagger} \vec{e}_{\lambda}^*). \quad (6)$$

The term quadratic in  $\vec{A}(\vec{r}_i, t)$  is a second-order perturbation term, and the magnetic dipole moment term

$$\sum_{i=1}^n \frac{e_i \hbar}{2m_i c} g_{s_i} (\vec{s}_i \cdot [\vec{\nabla}_i \times \vec{A}_\perp(\vec{r}_i, t)])$$

is of order

$$(\hbar k)/p_i = kr_i$$

times the

$$\sum_i \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}(\vec{r}_i, t)$$

term, and can therefore be neglected in the  $kr_i \ll 1$  or electric dipole approximation.

In doing the perturbation calculation, the state vectors must now carry the information about both the atomic system ( $H_{\text{atom}}^{(0)}$ ) and the photons ( $H_{\text{radiation}}^{(0)}$ ). The initial and final states,  $|i\rangle$  and  $|f\rangle$ , must carry both the quantum numbers for the atomic system, such as  $n_i l_i m_l m_s$  to be denoted by the shorthand symbol  $A_i$ , and the quantum numbers for the radiation field, i.e., the photon numbers,  $n_{\vec{k}\mu}$ , for all  $\vec{k}, \mu$  of the initial state, similarly for the final state. For the spontaneous emission of a photon from an atom in an initial state,  $A_i$ , to a lower final state,  $A_f$ , we shall need

$$|i\rangle = |A_i \ 0\rangle, \quad |f\rangle = |A_f \ n_{\vec{k}\mu} = 1\rangle,$$

where  $A_i$  designates the atomic quantum numbers of the initial excited atomic state, 0 designates all  $n_{\vec{k}\mu} = 0$ , the photon vacuum state, and  $A_f$  designates the atomic quantum numbers of the final state. Our first-order perturbation theory result can be read from the generalized diagram of Fig. 63.1(a), where we generalize the state vector lines by a straight line for the atomic system and a wiggly line for the photon.

$$\langle A_f \ n_{\vec{k}\mu} = 1 | U^{(1)}(t, t_0) | A_i \ 0 \rangle =$$

$$-\frac{i}{\hbar} \int_{t_0}^t d\tau e^{-\frac{i}{\hbar}(E_f^{(0)} + \hbar\omega)(t-\tau)} \langle A_f \ n_{\vec{k}\mu} = 1 | H_{\text{interaction}} | A_i \ 0 \rangle e^{-\frac{i}{\hbar}E_i^{(0)}(\tau-t_0)}. \quad (7)$$

(Note: For our time-dependent perturbation theory formalism, it is best to convert to the Schrödinger picture, where we consider the state vectors to be time-dependent and the operators to be time-independent.) The energies  $E_i^{(0)}$  and  $E_f^{(0)}$  are the eigenvalues of  $H_{\text{atom}}^{(0)}$ . The final energy includes the energy of the photon. The energy for any time interval of the diagram includes the energies of all atom and photon lines. We then get

$$\begin{aligned} \lim_{(t-t_0) \rightarrow \infty} \frac{\left| \langle A_f \ n_{\vec{k}\mu} = 1 | U(t, t_0) | A_i \ 0 \rangle \right|^2}{(t - t_0)} &= \frac{2\pi}{\hbar} \delta(E_f^{(0)} + \hbar\omega - E_i^{(0)}) \\ &\times \left| \langle A_f \ n_{\vec{k}\mu} = 1 | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_\mu^*) a_{\vec{k}\mu}^\dagger \frac{1}{L^{\frac{3}{2}}} c \sqrt{\frac{2\pi\hbar}{\omega}} | A_i \ 0 \rangle \right|^2 \\ &= \frac{2\pi}{\hbar} \delta(E_f^{(0)} + \hbar\omega - E_i^{(0)}) \frac{c^2}{L^3} \frac{2\pi\hbar}{\omega} \left| \langle A_f | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_\mu^*) | A_i \rangle \right|^2, \end{aligned} \quad (8)$$

where we have carried out the photon part of the matrix element,

$$\langle n_{\vec{k}\mu} = 1 | a_{\vec{k}\mu}^\dagger | 0 \rangle = 1,$$

so the last matrix element is a matrix element of a purely atomic operator between purely atomic states. It will now be convenient to convert this atomic matrix element to a different form in which we will recognize the electric dipole moment operator of the atomic system. Using

$$H_{\text{atom}}^{(0)} = \sum_i \frac{\vec{p}_i^2}{2m_i} + \sum_{i < k} V(\vec{r}_i, \vec{r}_k), \quad (9)$$

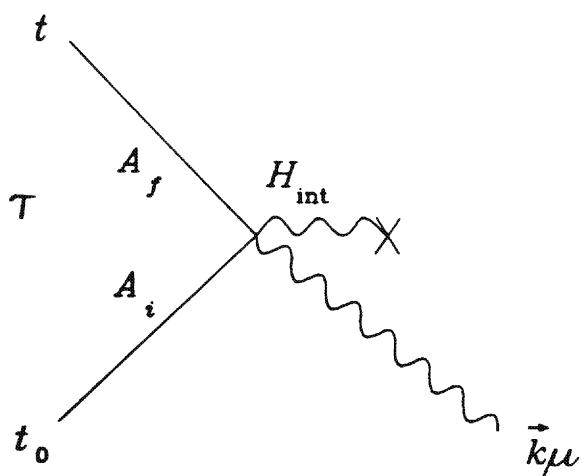
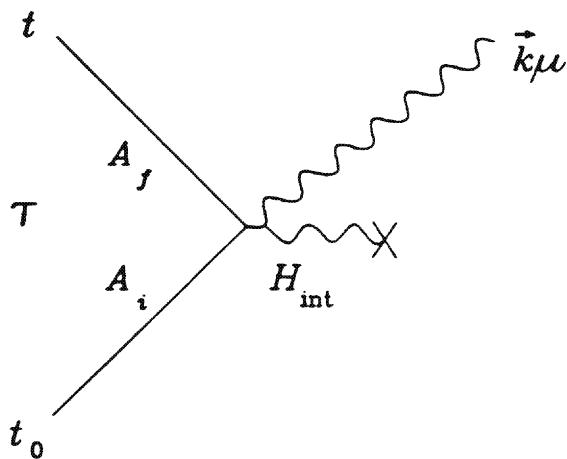


FIGURE 63.1. First-order diagrams for (a) photon emission and (b) photon absorption.

we have the simple commutator relation

$$[H_{\text{atom}}^{(0)}, \vec{r}_i] = \frac{\hbar}{i} \frac{\vec{p}_i}{m_i}, \quad (10)$$

so

$$\begin{aligned} & \langle A_f | \sum_i \frac{e_i}{c} \left( \frac{\vec{p}_i}{m_i} \cdot \vec{e}_\mu^* \right) | A_i \rangle \\ &= \frac{i}{\hbar c} \langle A_f | H_{\text{atom}}^{(0)} \left( \left( \sum_i e_i \vec{r}_i \right) \cdot \vec{e}_\mu^* \right) - \left( \left( \sum_i e_i \vec{r}_i \right) \cdot \vec{e}_\mu^* \right) H_{\text{atom}}^{(0)} | A_i \rangle \\ &= \frac{i}{\hbar c} (E_f^{(0)} - E_i^{(0)}) \langle A_f | \left( \left( \sum_i e_i \vec{r}_i \right) \cdot \vec{e}_\mu^* \right) | A_i \rangle \\ &= -\frac{i\omega}{c} \langle A_f | \left( \left( \sum_i e_i \vec{r}_i \right) \cdot \vec{e}_\mu^* \right) | A_i \rangle. \end{aligned} \quad (11)$$

The atomic operator in this matrix element is the electric dipole moment vector of the atomic system

$$\sum_i e_i \vec{r}_i = \vec{\mu}^{(\text{electric})}. \quad (12)$$

Now, to get the final transition probability, we also need the density of states,  $\rho(E)$ , for the photons with energy between  $E$  and  $E + dE$  in the photon continuum, or the finely discrete spectrum of the photon waves in our cubical laboratory of volume  $L^3$ . In Chapter 57, we calculated this quantity and found

$$\rho(E)dE = \frac{L^3}{(2\pi)^3} k^2 dk d\Omega, \quad (13)$$

where  $d\Omega$  is the element of solid angle about the direction of  $\vec{k}$ . In Chapter 57, we dealt with matter waves. Now, the waves in our cube are electromagnetic. Therefore, now,

$$k = \frac{\omega}{c}, \quad E = \hbar\omega, \quad \text{and } dk = \frac{1}{\hbar c} dE. \quad (14)$$

Thus,

$$\rho(E) = \frac{L^3}{(2\pi)^3 \hbar c^3} \frac{\omega^2}{d\Omega}. \quad (15)$$

With this  $\rho(E)$  and the above matrix element, we then get our expression for the transition probability per second that the atom makes a transition from the excited state,  $A_i$ , to a lower state,  $A_f$ , with the emission of a photon with energy between  $E$  and  $E + dE$ , where  $E = \hbar\omega = (E_i^{(0)} - E_f^{(0)})$ , the photon being emitted into an element of solid angle  $d\Omega$  about the direction of  $\vec{k}$ , with circular polarization given by  $\mu = \pm 1$ ,

$$\left[ \frac{\text{Transition Probability}}{\text{second}} \right]_{\text{atom } A_i \rightarrow A_f + \text{photon of type } \vec{k}, \mu \text{ into } d\Omega}$$

$$\begin{aligned}
&= \frac{2\pi}{\hbar} \rho(E) \frac{c^2}{L^3} \frac{2\pi\hbar}{\omega} \frac{\omega^2}{c^2} \left| \langle A_f | \left( \sum_i e_i \vec{r}_i \right) \cdot \vec{e}_\mu^* | A_i \rangle \right|^2 \\
&= \frac{\omega^3 d\Omega}{2\pi\hbar c^3} \left| \langle A_f | (\vec{\mu}^{(\text{el.})} \cdot \vec{e}_\mu^*) | A_i \rangle \right|^2.
\end{aligned} \quad (16)$$

If we want the total transition probability per second that the photon with energy  $\hbar\omega = (E_i^{(0)} - E_f^{(0)})$  be emitted into any direction with either polarization, we must still integrate over all possible photon directions and sum over the two possible photon polarizations for each direction.

$$\left[ \frac{\text{Transition Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} = \frac{\omega^3}{2\pi\hbar c^3} \sum_{\mu=\pm 1} \int \int d\Omega \left| \langle A_f | (\vec{\mu}^{(\text{el.})} \cdot \vec{e}_\mu^*) | A_i \rangle \right|^2. \quad (17)$$

To carry out the polarization sum, it will be convenient to expand the electric dipole moment vector in spherical components

$$\vec{\mu}^{(\text{el.})} = \sum_v (\vec{\mu}^{(\text{el.})})_v' \vec{e}_v = \sum_v (-1)^v (\vec{\mu}^{(\text{el.})})_{-v}' \vec{e}_v, \quad (18)$$

and use the orthogonality relation in spherical component form,  $(\vec{e}_v \cdot \vec{e}_\mu^*) = \delta_{v,\mu}$ , and subsequently change the dummy summation index  $v \rightarrow -v$ , after the  $\mu$  sums have been performed in eq. (17). This method gives us

$$\left[ \frac{\text{Transition Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} = \frac{\omega^3}{2\pi\hbar c^3} \sum_{v=\pm 1} \int \int d\Omega \left| \langle A_f | (\vec{\mu}^{(\text{el.})})_v' | A_i \rangle \right|^2. \quad (19)$$

Also, the circular polarization index,  $v$  or  $\mu$ , is defined relative to the photon direction,  $\vec{k}$ . If we name the direction of  $\vec{k}$  a  $z'$  direction, where the  $z'$  axis makes polar and azimuth angles,  $\theta$  and  $\phi$ , with respect to a laboratory reference frame,  $x$ ,  $y$ ,  $z$  (see Fig. 63.2), then the electric dipole moment vector in eqs. (18) and (19) has spherical components relative to this primed coordinate system. Hence, these components are designated by  $\mu'_v$ , with  $v = \pm 1$ . Using the transformation from primed to unprimed spherical components, we have

$$\langle A_f | (\mu^{(\text{el.})})_v' | A_i \rangle = \sum_{m=\pm 1,0} \langle A_f | (\mu^{(\text{el.})})_m | A_i \rangle D_{mv}^1(\phi, \theta, 0)^*, \quad (20)$$

so

$$\begin{aligned}
\int \int d\Omega \left| \langle A_f | (\mu^{(\text{el.})})_v' | A_i \rangle \right|^2 &= \sum_m \sum_{m'} \langle A_f | (\mu^{(\text{el.})})_m | A_i \rangle \langle A_f | (\mu^{(\text{el.})})_{m'} | A_i \rangle^* \\
&\times \int \int d\Omega D_{mv}^1(\phi, \theta, 0)^* D_{m'v}^1(\phi, \theta, 0).
\end{aligned} \quad (21)$$

Now, using a special case of the  $D$  function orthonormality integral [see eq. (30) of Chapter 30],

$$\int \int d\Omega D_{mv}^1(\phi, \theta, 0)^* D_{m'v}^1(\phi, \theta, 0) = \frac{4\pi}{3} \delta_{m,m'}, \quad (22)$$

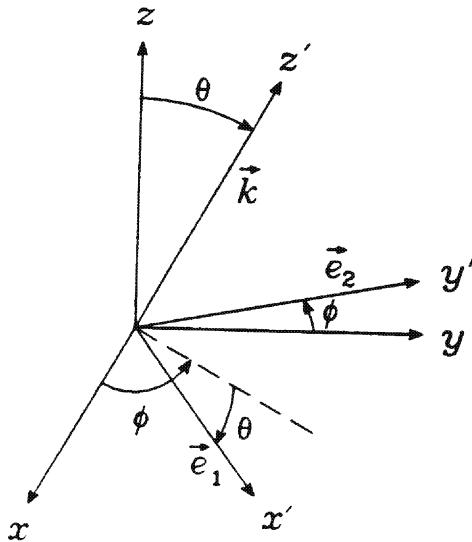


FIGURE 63.2.

and summing over the two possible polarizations,  $\nu = \pm 1$ , we get

$$\sum_{\nu=\pm 1} \int \int d\Omega | \langle A_f | (\mu^{(\text{el.})})'_{\nu} | A_i \rangle |^2 = \frac{8\pi}{3} \sum_{m=\pm 1,0} | \langle A_f | (\mu^{(\text{el.})})_m | A_i \rangle |^2. \quad (23)$$

Substituting this into eq. (19),

$$\left[ \frac{\text{Transition Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} = \frac{4\omega^3}{3\hbar c^3} \sum_{m=\pm 1,0} | \langle A_f | (\mu^{(\text{el.})})_m | A_i \rangle |^2. \quad (24)$$

Finally, if the atomic quantum numbers in the state vectors are given by

$$| A_i \rangle = | a_i J_i M_i \rangle, \quad | A_f \rangle = | a_f J_f M_f \rangle,$$

where  $a_i$  and  $a_f$  are all quantum numbers other than the total angular momentum quantum numbers  $J_i$ ,  $M_i$  and  $J_f$ ,  $M_f$ , and if the initial and final states have degeneracies  $(2J_i + 1)$  and  $(2J_f + 1)$ , we can use the Wigner-Eckart theorem and do the  $M$  sums. If we average over the initial  $M_i$  substates, assuming each is occupied with an equal probability of  $[1/(2J_i + 1)]$ , we have

$$\begin{aligned} & \left[ \frac{\text{Transition Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} \\ &= \frac{1}{(2J_i + 1)} \frac{64\pi^4 \nu^3}{3\hbar c^3} \sum_{M_i} \sum_m \sum_{M_f} \langle J_i M_i | J_f M_f \rangle^2 \frac{| \langle a_f J_f | \vec{\mu}^{(\text{el.})} | a_i J_i \rangle |^2}{(2J_f + 1)} \\ &= \frac{1}{(2J_i + 1)} \frac{64\pi^4 \nu^3}{3\hbar c^3} | \langle a_f J_f | \vec{\mu}^{(\text{el.})} | a_i J_i \rangle |^2. \end{aligned} \quad (25)$$

This result agrees with our earlier result, obtained via the “correspondence principle arguments” or “guess.”

Final note: We might have been interested in the transition probability per second that the atom makes a transition from the atomic state  $A_i$  to  $A_f$  and that the photon be emitted into a  $d\Omega$  about the direction of  $\vec{k}$ , but now with a linear polarization vector  $\vec{e}_\alpha$ , with  $\alpha = 1$ , or 2. In that case,

$$\left[ \frac{\text{Transition Prob.}}{\text{second}} \right]_{i \rightarrow f} = \frac{\omega^3 d\Omega}{2\pi\hbar c^3} \left| \langle A_f | (\vec{\mu}^{(\text{el.})} \cdot \vec{e}_\alpha) | A_i \rangle \right|^2, \quad (26)$$

where, now,

$$\begin{aligned} \vec{e}_1 &= \vec{e}_{x'} = \cos \theta \cos \phi \vec{e}_x + \cos \theta \sin \phi \vec{e}_y - \sin \theta \vec{e}_z \\ \vec{e}_2 &= \vec{e}_{y'} = -\sin \phi \vec{e}_x + \cos \phi \vec{e}_y. \end{aligned} \quad (27)$$

Now, summing over the two polarizations, and integrating over all possible photon directions, we have

$$\begin{aligned} \left[ \frac{\text{Transition Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} &= \\ \frac{\omega^3}{2\pi\hbar c^3} \int \int d\Omega &\left[ (\cos^2 \theta \cos^2 \phi + \sin^2 \phi) |\langle A_f | \mu_x^{(\text{el.})} | A_i \rangle|^2 \right. \\ &+ (\cos^2 \theta \sin^2 \phi + \cos^2 \phi) |\langle A_f | \mu_y^{(\text{el.})} | A_i \rangle|^2 \\ &\left. + \sin^2 \theta |\langle A_f | \mu_z^{(\text{el.})} | A_i \rangle|^2 + \dots + \dots \right] \\ &= \frac{4\omega^3}{3\hbar c^3} (|\langle A_f | \mu_x^{(\text{el.})} | A_i \rangle|^2 + |\langle A_f | \mu_y^{(\text{el.})} | A_i \rangle|^2 + |\langle A_f | \mu_z^{(\text{el.})} | A_i \rangle|^2), \end{aligned} \quad (28)$$

where the six angular integrals for the cross terms, indicated by  $+\dots+\dots$  above, are zero.

# 64

## The Photoelectric Effect: Hydrogen Atom

As our second example, let us calculate the cross section for the photoelectric effect for an atom. For simplicity, we will choose the simplest atom, hydrogen. We assume we have an incoming beam of photons of definite  $\vec{k}$ , hence definite energy,  $\hbar\omega$ , and definite polarization. We also assume the incident photon beam is linearly polarized, with polarization in the direction of  $\vec{e}_\alpha$ , and  $\hbar\omega$  is greater than the ionization energy of hydrogen,  $((\mu e^4)/(2\hbar^2))$ . Therefore, when a photon of energy  $\hbar\omega$  is absorbed, the hydrogen atom makes a transition from the  $1s$  ground state into the continuum, (see Fig. 64.1). For simplicity, let us further assume  $\hbar\omega \gg (\mu e^4)/(2\hbar^2)$  so the final electron kinetic energy  $p_f^2/2\mu$  is large enough the final electron continuum wave function can be approximated by a plane wave. For the moment, therefore, we shall avoid the more complicated exact Coulomb relative motion function discussed in the appendix to Chapter 42. To calculate the differential cross section for the photoelectric process, we need to know the flux in the incoming photon beam, and the transition probability per second that the hydrogen atom makes a transition from the  $1s$  ground state to a continuum state with the absorption of a photon.

To get the incident flux for an initial photon state,  $|\cdots n_{\vec{k}\alpha} \cdots\rangle$ , the photon number density is given by

$$\text{photon number density} = \frac{n_{\vec{k}\alpha}}{L^3}.$$

(Our photon plane waves are assumed to fill the whole volume  $L^3$  of our cube. Even if the real photon beam has a finite extent, it will fill a macroscopic volume. Because all final physically relevant results will have to be independent of  $L^3$ , the exact value of the macroscopic volume cannot play a role). To get the incident

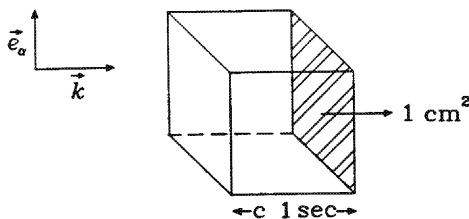
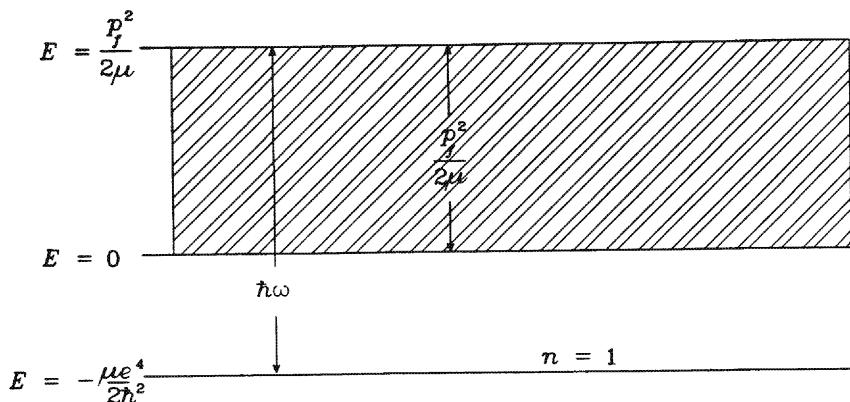


FIGURE 64.1. Photoelectric effect in hydrogen.

photon flux, all photons in a volume element of cross-sectional area  $1 \text{ cm}^2$  normal to  $\vec{k}$  and of length  $c \times 1 \text{ sec}$ . parallel to  $\vec{k}$  will traverse the cross-sectional area in 1 sec. Thus, the number of photons streaming across unit area normal to  $\vec{k}$  per second is given by

$$\text{Incident photon flux} = \left( \frac{n_{\vec{k}\alpha} c}{L^3} \right). \quad (1)$$

Our initial and final states are

$$\begin{aligned} |i\rangle &= |A_i = (n = 1, l = 0, m_l = 0); n_{\vec{k}\alpha}\rangle, \\ |f\rangle &= |A_f = \vec{p}_f; (n_{\vec{k}\alpha} - 1)\rangle. \end{aligned} \quad (2)$$

We will approximate the final-state continuum atomic wave function by

$$\langle \vec{r} | \vec{p}_f \rangle = \frac{e^{i(\vec{k}_f \cdot \vec{r})}}{L^{\frac{3}{2}}}, \quad (3)$$

with  $\vec{p}_f = \hbar \vec{k}_f$ . Here, we have neglected the effect of the (far-reaching) Coulomb potential on this relative motion wave function. Energy conservation gives

$$\hbar\omega = \hbar k c = \frac{\hbar^2 k_f^2}{2\mu} + \frac{\mu e^4}{2\hbar^2} = \frac{\mu e^4}{2\hbar^2} ((k_f a_0)^2 + 1). \quad (4)$$

The differential cross section for the emission of the atomic electron into an element of solid angle,  $d\Omega_f$ , about the direction of  $\vec{p}_f$  is then given by the ratio of (1) the transition probability per second that the atomic electron makes a transition from the  $1s$  ground state to the continuum state with energy between  $E_f$  and  $E_f + dE_f$  and momenta with directions within an element of solid angle  $d\Omega_f$  about the direction of  $\vec{p}_f$ , and (2) the incident photon flux.

$$d\sigma = \frac{2\pi}{\hbar} \rho(E_f) \frac{1}{\text{inc. photon flux}} \times \left| \langle \vec{p}_f, (n_{\vec{k}\alpha} - 1) | \sum_{j=1}^2 \frac{e_j}{m_j c} (\vec{p}_j \cdot \vec{e}_\alpha) \frac{c}{L^{\frac{3}{2}}} \sqrt{\frac{2\pi\hbar}{\omega}} a_{\vec{k}\alpha} | 100, n_{\vec{k}\alpha} \rangle \right|^2, \quad (5)$$

where only the photon annihilation operator piece of

$$A_\perp = \frac{c}{L^{\frac{3}{2}}} \sum_{\vec{k},\alpha} \sqrt{\frac{2\pi\hbar}{\omega}} (a_{\vec{k}\alpha} \vec{e}_\alpha e^{i\vec{k}\cdot\vec{r}_j} + a_{\vec{k}\alpha}^\dagger \vec{e}_\alpha e^{-i\vec{k}\cdot\vec{r}_j}) \quad (6)$$

can contribute to the matrix element, and we have made the electric dipole approximation

$$e^{i\vec{k}\cdot\vec{r}_j} \approx 1.$$

Our plane wave approximation requires  $k_f a_0 \gg 1$ . In this limit energy conservation, eq. (4) gives  $\hbar k c \approx (\hbar^2 k_f^2)/2\mu$ , so

$$\frac{k^2}{k_f^2} \approx \frac{(\hbar^2 k_f^2)/2\mu}{2\mu c^2}, \quad (7)$$

and therefore  $k/k_f \ll 1$ , provided the kinetic energy of the photoelectron is much less than  $2(\text{electron rest energy}) \approx 1\text{MeV}$ . Therefore, both the plane wave approximation,  $k_f a_0 \gg 1$ , and the electric dipole approximation,  $ka_0 \ll 1$ , can be satisfied simultaneously.

The density of states  $\rho(E_f)$  is given by the number of free electron states between energies  $E_f$  and  $E_f + dE_f$  in our cube of volume  $L^3$ . We counted this in Chapter 57.

$$\rho(E_f) = \frac{L^3}{(2\pi)^3} \frac{\mu p_f}{\hbar^3} d\Omega_f. \quad (8)$$

The photon part of the matrix element is simply

$$\langle (n_{\vec{k}\alpha} - 1) | a_{\vec{k}\alpha} | n_{\vec{k}\alpha} \rangle = \sqrt{n_{\vec{k}\alpha}}, \quad (9)$$

so

$$\begin{aligned}
 d\sigma &= \frac{2\pi}{\hbar} \left( \frac{L^3}{(2\pi)^3} \frac{\mu p_f}{\hbar^3} d\Omega_f \right) \left( \frac{L^3}{n_{k_\alpha} c} \right) \frac{c^2 2\pi\hbar}{L^3 \omega} n_{k_\alpha} \\
 &\times \left| \langle \vec{p}_f | \sum_{j=1}^2 \frac{e_j}{m_j c} (\vec{p}_j \cdot \vec{e}_\alpha) | 100 \rangle \right|^2 \\
 &= \frac{L^3}{2\pi} \frac{\mu p_f c}{\hbar^3 \omega} d\Omega_f \left| \langle \vec{p}_f | \sum_{j=1}^2 \frac{e_j}{m_j c} (\vec{p}_j \cdot \vec{e}_\alpha) | 100 \rangle \right|^2. \quad (10)
 \end{aligned}$$

In the atomic matrix element, we shall write the momentum operator

$$\sum_{j=1}^2 \frac{e_j \vec{p}_j}{m_j} = \frac{\hbar}{i} \left( -\frac{e}{m_e} \vec{\nabla}_1 + \frac{e}{m_{\text{proton}}} \vec{\nabla}_2 \right) = -\frac{\hbar}{i} \frac{e}{\mu} \vec{\nabla}, \quad (11)$$

where we have expressed the  $\vec{\nabla}_1$  and  $\vec{\nabla}_2$  operators in terms of the relative motion  $\vec{\nabla}$  operator, with relative motion vector,  $\vec{r} = \vec{r}_1 - \vec{r}_2$ . In addition, it will be convenient to calculate the atomic matrix element in the right-handed form by using

$$\left| \langle \vec{p}_f | \frac{e}{\mu c} (\vec{e}_\alpha \cdot \vec{p}) | 100 \rangle \right| = \left| \langle 100 | \frac{e}{\mu c} (\vec{e}_\alpha \cdot \vec{p}) | \vec{p}_f \rangle \right|,$$

where

$$\begin{aligned}
 \langle 100 | \frac{e}{\mu c} (\vec{e}_\alpha \cdot \vec{p}) | \vec{p}_f \rangle &= \frac{e}{\mu c} \int d\vec{r} \psi_{100}(\vec{r}) (\vec{e}_\alpha \cdot \frac{\hbar}{i} \vec{\nabla}) \frac{e^{i\frac{\hbar}{\mu}(\vec{p}_f \cdot \vec{r})}}{L^{\frac{3}{2}}} \\
 &= \frac{e}{\mu c} \frac{(\vec{e}_\alpha \cdot \vec{p}_f)}{L^{\frac{3}{2}}} \int d\vec{r} \left( 2 \left( \frac{1}{a_0} \right)^{\frac{3}{2}} e^{-\frac{r}{a_0}} \frac{1}{\sqrt{4\pi}} e^{i\vec{k}_f \cdot \vec{r}} \right) \\
 &= \frac{e}{\mu c} \frac{(\vec{e}_\alpha \cdot \vec{p}_f)}{L^{\frac{3}{2}}} 2 \left( \frac{1}{a_0} \right)^{\frac{3}{2}} \sqrt{4\pi} \int_0^\infty dr r^2 j_0(k_f r) e^{-\frac{r}{a_0}}. \quad (12)
 \end{aligned}$$

The radial integral is given by

$$\frac{1}{2ik_f} \int_0^\infty dr r \left( e^{-(\frac{1}{a_0} - ik_f)r} - e^{-(\frac{1}{a_0} + ik_f)r} \right) = \frac{2}{a_0} \frac{1}{\left[ \left( \frac{1}{a_0} \right)^2 + k_f^2 \right]^2}, \quad (13)$$

so

$$\begin{aligned}
 \langle 100 | \frac{e}{\mu c} (\vec{e}_\alpha \cdot \vec{p}) | \vec{p}_f \rangle &= \frac{e}{\mu c} \frac{p_f \cos \theta}{L^{\frac{3}{2}}} \frac{8\sqrt{\pi} \left( \frac{1}{a_0} \right)^{\frac{5}{2}}}{\left[ \left( \frac{1}{a_0} \right)^2 + k_f^2 \right]^2} \\
 &= \frac{e\hbar^3}{\mu^3 c \omega^2} \frac{k_f \cos \theta}{L^{\frac{3}{2}}} 2\sqrt{\pi} \left( \frac{1}{a_0} \right)^{\frac{5}{2}}, \quad (14)
 \end{aligned}$$

where we have used the energy conservation eq. (4) in the last step to make the replacement

$$\left[ \left( \frac{1}{a_0} \right)^2 + k_f^2 \right] = \frac{2\mu\omega}{\hbar},$$

and the angle between  $\vec{p}_f = \hbar\vec{k}_f$  and  $\vec{e}_1$  has been named  $\theta$  (see Fig. 64.2). With this matrix element, eq. (10) yields

$$d\sigma = \frac{2\hbar^4 e^2 k_f^3}{\mu^5 \omega^5 c a_0^5} \cos^2 \theta d\Omega, \quad (15)$$

or, in atomic units,

$$d\sigma = 2 \frac{e^2}{\hbar c} (k_f a_0)^3 \left( \frac{\mu e^4}{\hbar^2} \right)^5 a_0^2 \cos^2 \theta d\Omega. \quad (16)$$

For an unpolarized incident photon beam, with equal probability of photon polarization in the  $\vec{e}_1$  and  $\vec{e}_2$  direction (see Fig. 64.2), the differential cross section for the photoelectron to be emitted in the direction shown is

$$d\sigma = 2 \frac{e^2}{\hbar c} (k_f a_0)^3 \left( \frac{\mu e^4}{\hbar^2} \right)^5 a_0^2 \frac{(\cos^2 \theta + \sin^2 \theta \cos^2 \phi)}{2} d\Omega. \quad (17)$$

Integrating over all directions, this equation gives the total cross section for the photoionization effect,

$$\sigma = \frac{8\pi}{3} \frac{e^2}{\hbar c} (k_f a_0)^3 \left( \frac{\mu e^4}{\hbar^2} \right)^5 a_0^2, \quad (18)$$

or, finally, in terms of the fine structure constant,  $\alpha$ , and the 1s atomic binding energy,  $|E_{n=1}|$ , and with the approximation,  $\hbar k_f \approx \sqrt{2\mu\hbar\omega}$ , valid for the case  $\hbar\omega \gg \mu e^4/\hbar^2$ , which we have considered, we have

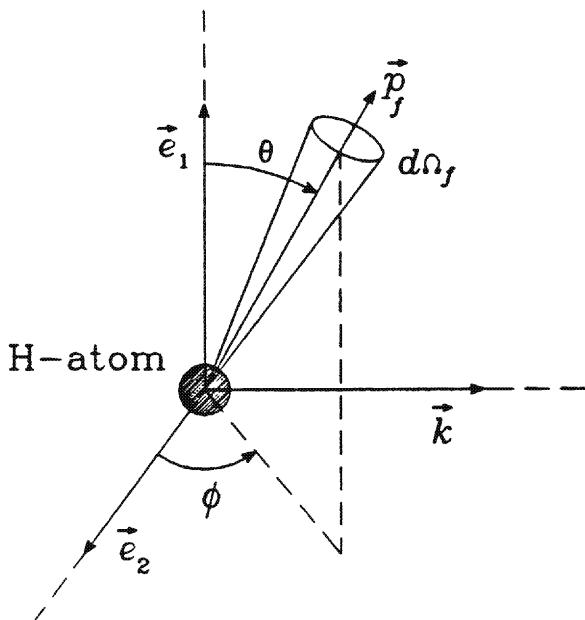
$$\sigma \approx \frac{256\pi}{3} \alpha \left( \frac{|E_{n=1}|}{\hbar\omega} \right)^{\frac{7}{2}} a_0^2. \quad (19)$$

In this expression, valid for  $k_f a_0 \gg 1$ , we have for simplicity used the plane wave approximation for the Coulomb continuum wave function. Using the results of the mathematical appendix to Chapter 42, we could just as easily have used the exact Coulomb wave function for the final continuum wave function. For this purpose, it will be useful to convert the atomic matrix element of eq. (10) to a matrix element of the atomic electric dipole moment matrix element. This result can be accomplished by the same trick used in eq. (10) of Chapter 63, using the commutator relation

$$[H^{(0)}, \vec{p}_j] = \frac{\hbar}{i} \frac{\vec{p}_j}{m_j}, \quad (20)$$

which converts the atomic operator to

$$\sum_{j=1}^2 \frac{e_j}{m_j c} (\vec{p}_j \cdot \vec{e}_\alpha) = \sum_{j=1}^2 \frac{ie_j}{\hbar c} [H^{(0)}, (\vec{r}_j \cdot \vec{e}_\alpha)] = \frac{-ie}{\hbar c} [H^{(0)}, (\vec{r} \cdot \vec{e}_\alpha)], \quad (21)$$

FIGURE 64.2. The incident photon  $\vec{k}$  and photoelectron  $\vec{p}_f$  vectors.

where  $\vec{r}$  is the relative motion vector,  $\vec{r} = \vec{r}_1 - \vec{r}_2$ . Using the zeroth-order energy eigenvalues of the ground state and the continuum state and the result for the matrix element of  $\vec{r} \cdot \vec{e}_\alpha$ , as derived through eq. (44) of the mathematical appendix to Chapter 42, this yields

$$\begin{aligned} \langle \vec{p}_f | \sum_{j=1}^2 \frac{e_j}{m_j c} (\vec{p}_j \cdot \vec{e}_\alpha) | 100 \rangle &= -\frac{ie\omega}{c} \langle \vec{p}_f | \vec{r} \cdot \vec{e}_\alpha | 100 \rangle \\ &= -\frac{ie\omega}{c} a_0^{\frac{5}{2}} \frac{\sqrt{4\pi}}{L^{\frac{3}{2}}} \cos \theta \frac{8i\gamma^5}{(\gamma^2 + 1)^3} \left[ \frac{(1 + \gamma^2)\pi\gamma}{\sinh \pi\gamma} \right]^{\frac{1}{2}} e^{(\gamma\pi)/2} e^{-2\gamma \tan^{-1}(1/\gamma)}, \quad (22) \end{aligned}$$

where  $\theta$  is the angle between the polarization vector of the incident photon and the vector  $\vec{p}_f$  (see Fig. 64.2) and  $\gamma$  is the Coulomb parameter

$$\gamma = \frac{\mu e^2}{\hbar^2 k} = \frac{1}{ka_0}. \quad (23)$$

Using the expression for the differential cross section, given by eq. (10), and the energy conservation relation, eq. (4), to yield

$$\frac{\mu k_f \hbar \omega}{\hbar^2} = \frac{k_f}{2} \left( k_f^2 + \frac{\mu^2 e^4}{\hbar^4} \right) = \frac{1}{2a_0^3} \frac{(\gamma^2 + 1)}{\gamma^3}, \quad (24)$$

we have the exact result

$$d\sigma = \frac{e^2}{\hbar c} 128\pi a_0^2 \frac{\gamma^8}{(\gamma^2 + 1)^4} \frac{e^{-4\gamma \tan^{-1}(1/\gamma)}}{(1 - e^{-2\gamma\pi})} \cos^2 \theta d\Omega \quad (25)$$

for a polarized incident beam with angle  $\theta$  between  $\vec{p}_f$  and the incident beam polarization vector  $\vec{e}$ , with a similar result for an unpolarized incident beam, cf., eqs. (16) and (17). This method leads to a total cross section

$$\sigma = \frac{e^2}{\hbar c} \frac{512\pi^2}{3} a_0^2 \frac{\gamma^8}{(\gamma^2 + 1)^4} \frac{e^{-4\gamma \tan^{-1}(1/\gamma)}}{(1 - e^{-2\gamma\pi})}, \quad (26)$$

where  $\gamma^2/(\gamma^2 + 1) = (|E_{n=1}|/\hbar\omega)$ . Also, this expression is valid for all (non-relativistic) values of  $(k_f a_0) = \gamma^{-1}$ . We have now made only the electric dipole approximation,  $(ka_0) \ll 1$ , where  $\hbar c$  is the photon energy. In the high energy limit, with  $\gamma \ll 1$ , the above yields

$$\sigma \approx \frac{e^2}{\hbar c} \frac{256\pi}{3} a_0^2 \gamma^7 \approx \frac{e^2}{\hbar c} \frac{256\pi}{3} a_0^2 \left( \frac{|E_{n=1}|}{\hbar\omega} \right)^{\frac{7}{2}} \quad (27)$$

in agreement with our earlier plane wave approximation.

## Problems

**29.** Show the intensity loss of a parallel beam of light per thickness,  $dx$ , of atomic absorber caused by stimulated absorption and emission processes is given (in electric dipole approximation) by

$$\begin{aligned} \text{Energy Loss} &= \frac{4\pi^2}{3\hbar} \rho(v_{ul}) v_{ul} N_0 |\langle a_u J_u \| \sum_i e_i \vec{r}_i \| a_l J_l \rangle|^2 \\ &\times \frac{e^{-(E_l/kT)}}{\left[ \sum_n g_n e^{-(E_n/kT)} \right]} \left( 1 - e^{-(hv_{ul}/kT)} \right), \end{aligned}$$

where we assume:

- (a) the number of photons of type,  $\vec{k}\alpha$ , is large,  $n_{\vec{k}\alpha} \gg 1$ , so  $(n_{\vec{k}\alpha} + 1) \approx n_{\vec{k}\alpha}$ ;
- (b) the atoms are in a gas sample in thermal equilibrium, so the number of atoms in the lower (similarly upper) state are given by  $N_0 f_l$ , where

$$f_l = \frac{g_l e^{-(E_l/kT)}}{\left[ \sum_n g_n e^{-(E_n/kT)} \right]};$$

$N_0$  = total number of atoms per unit volume, and degeneracy factors such as  $g_l$ ,  $g_u$ , or  $g_n$  are given by  $g_l = (2J_l + 1), \dots$ , assuming all other degeneracies are removed by some interaction;

(c) the intensity of the incoming beam is given by  $c\rho(v)dv$ , where  $\rho(v)dv$  is the energy density between frequencies  $v$  and  $v + dv$  in the incoming beam,

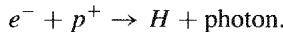
$$\int_0^\infty d\omega \rho(\omega) = \int_0^\infty dv \rho(v), \quad \text{so } \rho(\omega) = \rho(v)/(2\pi);$$

(d) the atoms in the gas sample have arbitrary orientations, so we have to average over all atomic orientations; for this reason, the above result is valid for both incident light with definite polarization,  $\alpha$ , and for unpolarized light; recall

$$\int d\Omega D_{M_1 M}^1 D_{M_2 M}^{1*} = \frac{4\pi}{3} \delta_{M_1 M_2}.$$

In the above, the double-barred matrix element is the standard reduced matrix element;  $a_l$  is shorthand for all quantum numbers other than  $J_l$  and  $M_{J_l}$ , similarly for  $a_u$ , and  $\hbar\nu_{ul} = (E_u - E_l)$ .

**30.** In a hot, completely ionized hydrogen gas both electron-electron and electron-proton scattering must be considered. In the electron-proton scattering with an initial  $\vec{p}_0$ , the most probable process is elastic scattering. There is, however, the possibility of a radiative capture process in which the proton captures an electron to make a hydrogen atom in a bound state, with the emission of a photon of energy,  $\hbar\omega$ ,



For a center of mass energy in the incident beam of  $p_0^2/(2\mu) \geq 100$  eV ( $\gg 13.6$  eV), assume the electron-proton relative motion function can be approximated by a plane wave.

(a) With  $p_0^2/(2\mu) = 100$  eV, show this radiative capture cross section can be calculated in electric dipole approximation. In this case, calculate the differential cross section for the emission of a photon with momentum,  $\hbar\vec{k}$ , making an angle  $\theta$  with the beam direction,  $\vec{p}_0 = \hbar\vec{k}_0$ , leaving the hydrogen atom in its ground state. What is the total cross section for this capture process into the hydrogen ground state?

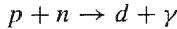
(b) With  $p_0^2/(2\mu) = 10^4$  eV, the problem can still be treated nonrelativistically, with considerable accuracy. (For this energy,  $\beta^2 \approx .04$ .) Show, however, at this energy, the multipole expansion is not valid. The electric dipole approximation would be bad. Repeat the calculation for the differential cross section for the radiative capture process into the hydrogen atom ground state, valid for this incident energy. Now,  $ka_0 \approx 2.7$ , and we cannot make approximations in the expansion of  $e^{i(\vec{k} \cdot \vec{r}_e)}$ . Also, the ratio  $k/k_0 \approx 0.1$ , so we must now consider both the

$$\sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{A}_\perp) \quad \text{and} \quad - \sum_i \frac{e_i \hbar}{2m_i c} g_{s_i} (\vec{s}_i \cdot [\vec{\nabla}_i \times \vec{A}_\perp])$$

terms in the interaction Hamiltonian, by showing the contributions of the second (magnetic moment) term are of order  $(k/k_0)$  compared with the contributions of the first  $(\vec{p}_i \cdot \vec{A}_\perp)$  term. Show, however, no cross terms exist in the nonzero matrix elements for the radiative capture process, so the contributions of the magnetic

moment term to the cross section are smaller by a factor  $(k/k_0)^2 \approx .01$  and to within this accuracy could be neglected for our case.

**31.** Compared with the elastic proton neutron scattering process, the radiative capture process



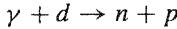
leading to the formation of a deuteron with the emission of a  $\gamma$  photon of energy  $\hbar\omega$  is quite improbable. Convince yourself that in the 2–20-MeV incident center of mass energy range this radiative capture process is dominated by the electric dipole term and can be calculated in electric dipole approximation. (The spins and magnetic moments of the particles therefore play no role in the dynamics.) In this approximation, calculate the total cross section for radiative capture as a function of incident energy,  $E_0$ , or rather as a function of  $k_0$  [with  $E_0 = \hbar^2 k_0^2 / (2\mu) = \hbar^2 k_0^2 / M$ ]. Assume the deuteron bound-state wave function can be approximated by the Hulthen wave function

$$\sqrt{\frac{2\eta(1+\eta)}{r_0(\eta-1)^2}} \left( \frac{e^{-(r/r_0)} - e^{-\eta(r/r_0)}}{r} \right) Y_{00} \chi_{S=1, M_S} \chi_{I=0, M_I=0},$$

with  $\eta = 6.2$ ;  $r_0 = 4.26$  fm. Recall the deuteron bound state has  $S = 1$ ,  $I = 0$ . The deuteron binding energy is 2.226 MeV.

Assume the incident proton beam and neutron target are both unpolarized. Also convince yourself an incident plane wave approximation can be used for the neutron–proton relative motion function for the whole range of  $r$  values from  $\infty \rightarrow 0$ .

**32.** Calculate the differential and total cross sections for the photo-dissociation of the deuteron into a free neutron and proton



in the energy range for which the incident  $\gamma$  photon has an energy  $\hbar\omega$  in the 4–20-MeV range, where the photodissociation process is dominated by the electric dipole matrix element. (See problem 31.)

# Spontaneous Photon Emission: General Case: Electric and Magnetic Multipole Radiation

For the general case, for a quantum system with  $kr_i$  *not* necessarily very small, we need to use the full first-order piece of the interaction Hamiltonian

$$\begin{aligned}
 H_{\text{int.}} &= -\sum_{i=1}^n \left( \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{A}_{\perp}) + \frac{e\hbar g_{s,i}}{2m_i c} (\vec{s}_i \cdot [\vec{\nabla} \times \vec{A}_{\perp}]) \right) \\
 &= -\sum_{\vec{k}} \sum_{\mu=\pm 1} \sum_L \frac{c2\pi}{\sqrt{\text{Vol.}}} \sqrt{\frac{\hbar(2L+1)}{\omega}} \\
 &\quad \times \left[ \sum_i \frac{e_i}{m_i c} \vec{p}_i \cdot \left( a_{\vec{k}\mu} (\vec{A}(\vec{r}_i, \mathcal{E})_{L\mu} - \mu \vec{A}(\vec{r}_i, \mathcal{M})) \right. \right. \\
 &\quad \quad \left. \left. + a_{\vec{k}\mu}^\dagger (\vec{A}(\vec{r}_i, \mathcal{E})_{L\mu}^* - \mu \vec{A}(\vec{r}_i, \mathcal{M})_{L\mu}^*) \right) \right] \\
 &\quad + i \sum_i \frac{e\hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot \left( a_{\vec{k}\mu} [\vec{k} \times (\vec{A}(\vec{r}_i, \mathcal{E})_{L\mu} - \mu \vec{A}(\vec{r}_i, \mathcal{M}))] \right. \\
 &\quad \quad \left. \left. - a_{\vec{k}\mu}^\dagger [\vec{k} \times (\vec{A}(\vec{r}_i, \mathcal{E})_{L\mu}^* - \mu \vec{A}(\vec{r}_i, \mathcal{M})_{L\mu}^*)] \right) \right]. \quad (1)
 \end{aligned}$$

To calculate the spontaneous emission probability, we need matrix elements of the type

$$|\langle A_f; n_{\vec{k}\mu} = 1 | H_{\text{int.}} | A_i; 0 \rangle| = |\langle A_i 0 | H_{\text{int.}} | A_f; n_{\vec{k}\mu} = 1 \rangle|.$$

We prefer to work with the latter form (to avoid the complex conjugate fields) and will calculate

$$\langle A_i; 0 | H_{\text{int.}} | A_f; n_{\vec{k}\mu} = 1 \rangle = -\frac{2\pi c}{\sqrt{\text{Vol.}}} \sum_L \sqrt{\frac{\hbar(2L+1)}{\omega}}$$

$$\times \langle A_i | \sum_i \frac{e_i}{m_i c} (\vec{p}_i + \frac{i}{2} g_{s,i} \hbar [\vec{s}_i \times \vec{k}]) \cdot (\vec{A}(\vec{r}_i, \mathcal{E})_{L\mu} - \mu \vec{A}(\vec{r}_i, \mathcal{M})_{L\mu}) | A_f \rangle. \quad (2)$$

The perturbing terms are of the form

$$(\vec{W} \cdot \vec{A}(\vec{r}_i; \mathcal{E} \text{ or } \mathcal{M})_{L\mu})$$

and hence of the form  $(\vec{W} \cdot \vec{V}_{[L]LM})$ , where

$$\vec{W} = \sum_i \frac{e_i}{m_i c} (\vec{p}_i + \frac{i}{2} g_{s,i} \hbar [\vec{s}_i \times \vec{k}]), \quad (3)$$

and where we must remember  $\mu$  is a circular polarization index with respect to a photon vector,  $\vec{k}$ , whose direction is identified as that of a  $z'$  axis rotated relative to the laboratory axes,  $x$ ,  $y$ ,  $z$ , via the arbitrary angles  $\phi$ ,  $\theta$ . Thus,

$$(\vec{W} \cdot \vec{V}_{[L]LM}) = \sum_M (\vec{W} \cdot \vec{V}_{[L]LM}) D_{M\mu}^L(\phi, \theta, 0)^*, \quad (4)$$

where the  $M$  quantum number now refers to the projection of  $L$  onto the laboratory  $z$  axis. The transition probability can then be expressed by

$$\begin{aligned} & \left[ \frac{\text{Transition Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f + \text{photon } \vec{k}\mu \text{ into } d\Omega} = \\ & \frac{2\pi}{\hbar} \frac{\text{Vol. } \omega^2 d\Omega}{(2\pi)^3} \frac{(2\pi c)^2 \hbar}{\text{Vol. } \omega_{L,M}} \sum_{L,M} \sqrt{(2L+1)} \sum_{L'M'} \sqrt{(2L'+1)} \\ & \times \langle A_i | \sum_i \frac{e_i}{m_i c} (\vec{p}_i + \frac{i}{2} g_{s,i} \hbar [\vec{s}_i \times \vec{k}]) \cdot (\vec{A}(\vec{r}_i, \mathcal{E})_{LM} - \mu \vec{A}(\vec{r}_i, \mathcal{M})_{LM}) | A_f \rangle^* \\ & \times \langle A_i | \sum_i \frac{e_i}{m_i c} (\vec{p}_i + \frac{i}{2} g_{s,i} \hbar [\vec{s}_i \times \vec{k}]) \cdot (\vec{A}(\vec{r}_i, \mathcal{E})_{L'M'} - \mu \vec{A}(\vec{r}_i, \mathcal{M})_{L'M'}) | A_f \rangle \\ & \times D_{M\mu}^L(\phi, \theta, 0) D_{M'\mu}^{L'}(\phi, \theta, 0)^*. \end{aligned} \quad (5)$$

To get the transition probability that the quantum system makes a transition from state  $A_i$  to  $A_f$  with the emission of a photon, we need to sum over both polarizations and integrate over all photon directions. For this purpose, we use the orthonormality integral

$$\int \int d\Omega D_{M'\mu}^{L'}(\phi, \theta, 0)^* D_{M\mu}^L(\phi, \theta, 0) = \delta_{L'L} \delta_{M'M} \frac{4\pi}{(2L+1)} \quad (6)$$

to get

$$\begin{aligned} & \left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} = \sum_{\mu=\pm 1} \int \int d\Omega \left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f + \text{photon } \vec{k}\mu} \\ & = \frac{4\pi \omega}{\hbar c} \sum_{\mu=\pm 1} \sum_{LM} \left( \langle A_i | \vec{W} \cdot (\vec{A}(\vec{r}, \mathcal{E})_{LM} - \mu \vec{A}(\vec{r}, \mathcal{M})_{LM}) | A_f \rangle^* \right. \\ & \times \langle A_i | \vec{W} \cdot (\vec{A}(\vec{r}, \mathcal{E})_{LM} - \mu \vec{A}(\vec{r}, \mathcal{M})_{LM}) | A_f \rangle \Big) \\ & = \frac{4\pi \omega}{\hbar c} \left( 2 \sum_{LM} |\langle A_i | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{E})_{LM} | A_f \rangle|^2 \right) \end{aligned}$$

$$\begin{aligned}
& + 2 \sum_{LM} |\langle A_i | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{M})_{LM} | A_f \rangle|^2 \\
& - \left( \sum_{\mu} \mu \right) \sum_{LM} \langle A_i | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{E})_{LM} | A_f \rangle^* \langle A_i | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{M})_{LM} | A_f \rangle \\
& - \left( \sum_{\mu} \mu \right) \sum_{LM} \langle A_i | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{M})_{LM} | A_f \rangle^* \langle A_i | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{E})_{LM} | A_f \rangle \Big). \quad (7)
\end{aligned}$$

Now, in the last two terms, the cross terms between type  $\mathcal{E}$  and  $\mathcal{M}$  matrix elements, the matrix elements are now independent of  $\mu$ , so the sum,  $\sum_{\mu} \mu = (-1 + 1) = 0$ . The cross terms therefore do not contribute to the total transition probability (no interference between  $\mathcal{E}$  and  $\mathcal{M}$ ), and the total transition probability is given by

$$\left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} = \frac{8\pi\omega}{\hbar c} \sum_{LM} \left( \left| \langle A_i | \sum_{i=1}^n \vec{W}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM} | A_f \rangle \right|^2 \right. \\
\left. + \left| \langle A_i | \sum_{i=1}^n \vec{W}_i \cdot \vec{A}(\vec{r}_i, \mathcal{M})_{LM} | A_f \rangle \right|^2 \right). \quad (8)$$

Usually, because of parity or angular momentum selection rules either the  $\mathcal{E}$  or the  $\mathcal{M}$  term is dominant, and the  $L$  in the sum will also be determined by selection rules. For example, in a  $2^+ \rightarrow 0^+$  transition in even-even nuclei (even proton and neutron number), where the first excited state is often a  $2^+$  state and the ground state is almost always a  $0^+$  state, the dominant term is an  $\mathcal{E}$  type with  $L = 2$  only. The transition probability is then determined by an electric quadrupole radiation matrix element. Usually, also, the first term with a nonzero matrix element in the  $L$  expansion will make the dominant contribution. The higher-order terms, with  $L = L_{\text{dominant}} + \Delta L$ , usually with a  $\Delta L$  of 2, will be negligible compared with this dominant term.

## A Electric Multipole Radiation

To calculate the transition probability for the  $L^{\text{th}}$  electric multipole term, we need to evaluate the matrix element,  $\langle A_i | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{E})_{LM} | A_f \rangle$ , or (going back to the photon emission form),  $\langle A_f | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{E})_{LM}^* | A_i \rangle$ . Recall

$$\vec{A}(\vec{r}, \mathcal{E})_{LM} = \sqrt{\frac{(L+1)}{(2L+1)}} j_{L-1} \vec{V}_{[(L-1)]LM} + \sqrt{\frac{L}{(2L+1)}} j_{L+1} \vec{V}_{[(L+1)]LM}. \quad (9)$$

For small values of  $kr$ , the spherical Bessel function  $j_L(kr)$  is of order

$$j_L(kr) \approx \frac{2^L L!}{(2L+1)!} (kr)^L = \frac{1}{(2L+1)!!} (kr)^L, \quad (10)$$

where  $(2L+1)!! \equiv (2L+1)(2L-1)\cdots 5 \cdot 3 \cdot 1$ , so the second  $l = (L+1)$  term in the expression for  $\vec{A}(\vec{r}, \mathcal{E})_{LM}$  is of order

$$\frac{(kr)^2}{(2L+3)(2L+1)} \sqrt{\frac{L}{(L+1)}}$$

times the first  $l = (L-1)$  term. Even for  $kr \approx 0.5$ , the second term is at most of order .01 of the first term. For all quantum systems, therefore, the second term is negligible compared with the first. We also recall the longitudinal vector field,  $\vec{A}(\vec{r}, \mathcal{L})_{LM}$ , which is *not* part of the radiation field, but mathematically somewhat simpler than  $\vec{A}(\vec{r}, \mathcal{E})_{LM}$ , is

$$\vec{A}(\vec{r}, \mathcal{L})_{LM} = \sqrt{\frac{L}{(2L+1)}} j_{L-1} \vec{V}_{[(L-1)1]LM} - \sqrt{\frac{(L+1)}{(2L+1)}} j_{L+1} \vec{V}_{[(L+1)1]LM}. \quad (11)$$

Again, for small values of  $kr$ , the second term of this longitudinal field is negligible compared with the first term. Thus, for reasonably small values of  $kr$ , we have

$$\vec{A}(\vec{r}, \mathcal{E})_{LM} \approx \sqrt{\frac{(L+1)}{L}} \vec{A}(\vec{r}, \mathcal{L})_{LM} = \frac{1}{ik} \sqrt{\frac{(L+1)}{L}} \vec{\nabla}(\Phi_{LM}), \quad (12)$$

where the scalar function  $\Phi_{LM}$  is

$$\Phi_{LM}(\vec{r}) = j_L(kr) i^L Y_{LM}(\theta, \phi), \quad (13)$$

so the vector field is derivable through the gradient of a simple scalar function. It is this mathematical simplicity that leads us to use the above approximation. In addition, the source vector

$$\vec{W} = \sum_{i=1}^n \vec{W}_i = \sum_i \frac{e_i}{m_i c} (\vec{p}_i + \frac{i\hbar}{2} g_{s,i} [\vec{s}_i \times \vec{k}]) \quad (14)$$

can also be simplified for the electric multipole case. The second term is of order  $kr_i$  compared with the first term and can therefore usually be neglected. We therefore make the approximation

$$\langle A_i | \sum_i \vec{W}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM} | A_f \rangle \approx \frac{1}{ik} \sqrt{\frac{L+1}{L}} \langle A_i | \sum_i \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{\nabla}_i \Phi_{LM}(\vec{r}_i) | A_f \rangle, \quad (15)$$

with a similar approximation for the matrix element

$$\langle A_f | \sum_i \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^* | A_i \rangle$$

actually needed for the spontaneous emission process taking the quantum system from state  $A_i \rightarrow A_f$ . We shall also find it convenient to write the operator in symmetrized form to get

$$\langle A_f | \sum_{i=1}^n \frac{e_i}{2m_i c} (\vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^* + \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^* \cdot \vec{p}_i) | A_i \rangle$$

$$\begin{aligned}
&= \langle A_f | \sum_{i=1}^n \frac{e_i}{2m_i c} \left( \frac{\hbar}{i} \vec{\nabla}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^* + \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^* \cdot \frac{\hbar}{i} \vec{\nabla}_i \right) | A_i \rangle \\
&= \int d\vec{r}_1 \cdots d\vec{r}_n \sum_{i=1}^n \frac{e_i}{c} \frac{\hbar}{2im_i} \left( \psi_{A_f}^*(\vec{\nabla}_i \psi_{A_i}) - \psi_{A_i}(\vec{\nabla}_i \psi_{A_f}^*) \right) \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^* \\
&= \frac{1}{c} \int d\vec{r}_1 \cdots d\vec{r}_n \sum_{i=1}^n e_i \vec{S}_{A_f A_i}(\vec{\nabla}_i) \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^*, \tag{16}
\end{aligned}$$

where we have used the coordinate representation for the  $n$  particle system and have let the operator  $\vec{\nabla}_i$  act to the right in the first term and to the left in the second term of the  $n$  particle matrix element. We have named the resultant operator,  $\vec{S}_{A_f A_i}$ , the transition probability density current,

$$\vec{S}_{A_f A_i} = \frac{\hbar}{2im} \left( \psi_{A_f}^* \vec{\nabla} \psi_{A_i} - \psi_{A_i} \vec{\nabla} \psi_{A_f}^* \right), \tag{17}$$

dependent *not* on a single function  $\psi$  and its complex conjugate  $\psi^*$ , but on the function  $\psi_{A_i}$  and on  $\psi_{A_f}^*$ . The full vector,  $\vec{S}_{A_f A_i}$ , is a sum over the  $n$  single-particle terms, each dependent on its own  $\vec{r}_i$ . To convert this probability density current operator to a charge current density operator, it will be useful to multiply this  $\vec{S}$  vector by the charge density of our  $n$  particle system. Our system was imagined to be a system of  $n$  point particles with charges  $e_i$  at position vectors,  $\vec{r}_i$ . For such a system, the charge density could be expressed by

$$\rho(\vec{r}) = \sum_{i=1}^n e_i \delta(\vec{r} - \vec{r}_i), \tag{18}$$

with

$$\sum_{i=1}^n e_i \delta(\vec{r} - \vec{r}_i) \vec{S}_{A_f A_i} = \vec{j}_{A_f A_i}(\vec{r}), \tag{19}$$

where  $\vec{j}$  is now the charge current density vector. The matrix element of eq. (8) can thus be written in the form

$$\begin{aligned}
&\langle A_f | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^*) | A_i \rangle \\
&= \frac{1}{c} \int d\vec{r} \int d\vec{r}_1 \cdots d\vec{r}_n \sum_{i=1}^n e_i \delta(\vec{r} - \vec{r}_i) \vec{S}_{A_f A_i}(\vec{\nabla}) \cdot \vec{A}(\vec{r}, \mathcal{E})_{LM}^* \\
&= \frac{1}{c} \int d\vec{r} \int d\vec{r}_1 \cdots d\vec{r}_n \vec{j}_{A_f A_i}(\vec{r}) \cdot \vec{A}(\vec{r}, \mathcal{E})_{LM}^* \\
&\approx -\frac{1}{ick} \sqrt{\frac{(L+1)}{L}} \int d\vec{r} \int d\vec{r}_1 \cdots d\vec{r}_n \vec{j}_{A_f A_i}(\vec{r}) \cdot \vec{\nabla} \Phi_{LM}^*(\vec{r}) \\
&= -\frac{1}{ick} \sqrt{\frac{(L+1)}{L}} \int d\vec{r} \langle A_f | \vec{j}(\vec{r}) \cdot \vec{\nabla} \Phi_{LM}^*(\vec{r}) | A_i \rangle. \tag{20}
\end{aligned}$$

We have added an *extra* integral,  $\int d\vec{r}$ , to the  $3n$  integrals of our  $n$  particle coordinate representation expression to accomodate the delta function. We have also

used the approximate expression of eq. (12) for  $\vec{A}(\vec{r}, \mathcal{E})_{LM}$ . Now, we shall rewrite the volume integral as

$$\begin{aligned} & \int_{\text{Vol.}} d\vec{r} \langle A_f | \vec{j}(\vec{r}) \cdot \vec{\nabla} \Phi_{LM}^* | A_i \rangle \\ &= \int_{\text{Vol.}} d\vec{r} \langle A_f | (\vec{\nabla} \cdot (\Phi_{LM}^* \vec{j})) | A_i \rangle - \int_{\text{Vol.}} d\vec{r} \langle A_f | \Phi_{LM}^* (\vec{\nabla} \cdot \vec{j}) | A_i \rangle \\ &= \int_{\text{Surface}} d\text{Area} \langle A_f | \Phi_{LM}^* (\vec{j} \cdot \vec{n}) | A_i \rangle - \int_{\text{Vol.}} d\vec{r} \langle A_f | \Phi_{LM}^* (\vec{\nabla} \cdot \vec{j}) | A_i \rangle \\ &= - \int_{\text{Vol.}} d\vec{r} \langle A_f | \Phi_{LM}^* (\vec{\nabla} \cdot \vec{j}) | A_i \rangle, \end{aligned} \quad (21)$$

where we have used Gauss's theorem to convert the volume integral, over the volume of our cube of side  $L$ , of the divergence of  $\Phi_{LM}^* \vec{j}$  to a surface integral, over the surface of our cube of the outward normal component of this vector. This surface integral is zero, because our radiation field has the value zero on the surface of our cube. Now, we shall use charge conservation in the form of the continuity equation,

$$(\vec{\nabla} \cdot \vec{j}) + \frac{\partial \rho}{\partial t} = 0, \quad (22)$$

or, more precisely,

$$(\vec{\nabla} \cdot \vec{j}_{A_f A_i}) + \frac{\partial \rho_{A_f A_i}}{\partial t} = 0, \quad (23)$$

to transform the needed matrix element into

$$\begin{aligned} & \langle A_f | \sum_{i=1}^n \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^*) | A_i \rangle \\ &= - \frac{1}{ick} \sqrt{\frac{(L+1)}{L}} \int d\vec{r}_1 \cdots d\vec{r}_n \int d\vec{r} \Phi_{LM}^* \left( \frac{\partial \rho_{A_f A_i}}{\partial t} \right) \\ &= - \frac{1}{ick} \sqrt{\frac{(L+1)}{L}} \int d\vec{r}_1 \cdots d\vec{r}_n \int d\vec{r} \Phi_{LM}^* \frac{\partial}{\partial t} (\psi_{A_f}^* \rho \psi_{A_i}) \\ &= - \frac{1}{ick} \sqrt{\frac{(L+1)}{L}} \int d\vec{r}_1 \cdots d\vec{r}_n \int d\vec{r} \Phi_{LM}^* \left( \frac{i}{\hbar} (H \psi_{A_f}^*) \rho \psi_{A_i} \right. \\ & \quad \left. - \frac{i}{\hbar} \psi_{A_f}^* \rho (H \psi_{A_i}) \right) \\ &= - \frac{1}{\hbar ck} \sqrt{\frac{(L+1)}{L}} (E_{A_f}^{(0)} - E_{A_i}^{(0)}) \int d\vec{r}_1 \cdots d\vec{r}_n \int d\vec{r} \Phi_{LM}^*(\vec{r}) \psi_{A_f}^* \rho \psi_{A_i} \\ &= - \frac{1}{\hbar ck} (-\hbar \omega) \sqrt{\frac{(L+1)}{L}} \int d\vec{r} \Phi_{LM}^*(\vec{r}) \langle A_f | \rho(\vec{r}) | A_i \rangle \\ &= \sqrt{\frac{(L+1)}{L}} \langle A_f | \int d\vec{r} \sum_{i=1}^n e_i \delta(\vec{r} - \vec{r}_i) \Phi_{LM}^*(\vec{r}) | A_i \rangle \\ &= \sqrt{\frac{(L+1)}{L}} \langle A_f | \sum_{i=1}^n e_i \Phi_{LM}^*(\vec{r}_i) | A_i \rangle \end{aligned}$$

$$= \sqrt{\frac{(L+1)}{L}} \langle A_f | \sum_{i=1}^n e_i j_L(kr_i) (-i)^L Y_{LM}^*(\theta_i, \phi_i) | A_i \rangle. \quad (24)$$

Now, we make the approximation,  $j_L(kr_i) \approx (kr_i)^L / (2L+1)!!$ , valid for  $kr_i \ll 1$ , and set  $k = \omega/c$  to get our final result

$$\begin{aligned} & \langle A_f | \sum_{i=1}^n \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^*) | A_i \rangle \\ &= \left(\frac{\omega}{c}\right)^L \sqrt{\frac{(L+1)}{L}} \frac{(-i)^L}{(2L+1)!!} \langle A_f | \sum_{i=1}^n e_i r_i^L Y_{LM}^*(\theta_i, \phi_i) | A_i \rangle. \end{aligned} \quad (25)$$

Now, with

$$\left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{A_i \rightarrow A_f} = \frac{8\pi\omega}{\hbar c} \sum_M \left| \langle A_f | \sum_{i=1}^n \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM} | A_i \rangle \right|^2, \quad (26)$$

this transition probability per second is given by

$$\frac{1}{\tau_{\mathcal{E}L}} = \frac{8\pi}{\hbar} \left(\frac{\omega}{c}\right)^{2L+1} \frac{(L+1)}{L[(2L+1)!!]^2} \sum_M \left| \langle A_f | \sum_{i=1}^n e_i r_i^L Y_{LM}(\theta_i, \phi_i) | A_i \rangle \right|^2, \quad (27)$$

where we have expressed this transition probability per unit time in terms of the inverse of the mean lifetime,  $\tau_{\mathcal{E}L}$ , for the photon emission process via the electric  $2^L$ -pole moment radiation matrix element. The matrix element involves a sum over the  $(2L+1)$  spherical components of the electric  $2^L$ -pole moment operator.

In particular, with  $L = 1$ , and

$$\begin{pmatrix} rY_{1+1} \\ rY_{10} \\ rY_{1-1} \end{pmatrix} = \sqrt{\frac{3}{4\pi}} \begin{pmatrix} \vec{r}_{+1} = -\sqrt{\frac{1}{2}}(x+iy) \\ \vec{r}_0 = z \\ \vec{r}_{-1} = +\sqrt{\frac{1}{2}}(x-iy) \end{pmatrix}, \quad (28)$$

so, we regain our earlier electric dipole result

$$\frac{1}{\tau_{\mathcal{E}1}} = \frac{4\omega^3}{3\hbar c^3} \sum_M \left| \langle A_f | \sum_{i=1}^n (e_i \vec{r}_i)_M | A_i \rangle \right|^2. \quad (29)$$

For the case of general  $L$ , with initial and final states specified by

$$|A_i\rangle = |a_i J_i M_i\rangle, \quad |A_f\rangle = |a_f J_f M_f\rangle, \quad (30)$$

we assume all other degeneracies have been removed so the initial and final states are  $(2J_i+1)$ -fold and  $(2J_f+1)$ -fold degenerate, with  $J_i$ ,  $M_i$  and  $J_f$ ,  $M_f$ , the total angular momentum quantum numbers for the quantum system. Again,  $a_i$  and  $a_f$  are shorthand for all other quantum numbers. Then, averaging over the initial  $M_i$  states, summing over the final  $M_f$ , and using the Wigner-Eckart theorem to express the  $M_i$ ,  $M_f$ -dependent matrix elements in terms of the reduced or double-barred matrix element, we have

$$\frac{1}{\tau_{\mathcal{E}L}} = \frac{8\pi}{\hbar} \left(\frac{\omega}{c}\right)^{2L+1} \frac{(L+1)}{L[(2L+1)!!]^2} \frac{1}{(2J_i+1)}$$

$$\times \left| \langle a_f J_f | \sum_i e_i r_i^L Y_L(\theta_i, \phi_i) | a_i J_i \rangle \right|^2. \quad (31)$$

The electric  $2^L$ -pole operator has parity  $(-1)^L$ . We are thus led to the parity selection rule:

$$\text{final state parity} = \text{initial state parity}, \quad \text{for } L = \text{even},$$

$$\text{final state parity} \neq \text{initial state parity}, \quad \text{for } L = \text{odd}.$$

In addition, we have the angular momentum selection rule given by the angular momentum addition rule,  $\vec{J}_i + \vec{L} = \vec{J}_f$ , so  $|J_f - J_i| \leq L \leq (J_f + J_i)$ . Also, the transition probability is proportional to  $\omega^{2L+1}$  and is thus a sensitive function of the photon energy, especially for the higher  $2^L$ -pole cases.

## B Magnetic Multipole Radiation

For the  $L^{th}$  magnetic multipole term, we need to evaluate the matrix element  $\langle A_f | \vec{W} \cdot \vec{A}(\vec{r}, \mathcal{M})_{LM}^* | A_i \rangle$ . Now, as we shall see, both pieces of the  $\vec{W}$  vector will be equally important, and we shall need both

$$-\langle A_f | \sum_{i=1}^n \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^* | A_i \rangle$$

and

$$-\langle A_f | \sum_{i=1}^n \frac{e_i \hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot [\vec{\nabla}_i \times \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^*] | A_i \rangle.$$

Let us first evaluate the first term:

$$\begin{aligned} & -\langle A_f | \sum_{i=1}^n \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^* | A_i \rangle \\ &= -\int d\vec{r}_1 \cdots d\vec{r}_n \psi_{A_f}^* \sum_{i=1}^n \frac{\hbar}{i} \vec{\nabla}_i \cdot (\vec{A}(\vec{r}_i, \mathcal{M})_{LM}^* \psi_{A_i}) \\ &= -\int d\vec{r}_1 \cdots d\vec{r}_n \psi_{A_f}^* \sum_{i=1}^n \frac{e_i}{m_i c} \frac{\hbar}{i} \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^* \cdot (\vec{\nabla}_i \psi_{A_i}) \\ &= -\int d\vec{r}_1 \cdots d\vec{r}_n \psi_{A_f}^* \sum_{i=1}^n \frac{e_i}{m_i c} \frac{\hbar}{i} \left( \frac{\vec{L} \Phi_{LM}(\vec{r}_i)}{\sqrt{L(L+1)}} \right)^* \cdot (\vec{\nabla}_i \psi_{A_i}), \end{aligned} \quad (32)$$

where we have used  $(\vec{\nabla}_i \cdot \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^*) = 0$  and have expressed  $\vec{A}(\vec{r}_i, \mathcal{M})_{LM}$  in terms of the scalar function  $\Phi_{LM}(\vec{r}_i)$  through eq. (22) of Chapter 62. Now we use

$$\begin{aligned} \left( \frac{\vec{L} \Phi_{LM}(\vec{r}_i)}{\sqrt{L(L+1)}} \right)^* \cdot (\vec{\nabla}_i \psi_{A_i}) &= -\frac{1}{i} [\vec{r}_i \times (\vec{\nabla}_i \Phi_{LM}^*(\vec{r}_i))] \cdot (\vec{\nabla}_i \psi_{A_i}) \\ &= +\frac{1}{i} (\vec{\nabla}_i \Phi_{LM}^*(\vec{r}_i)) \cdot [\vec{r}_i \times (\vec{\nabla}_i \psi_{A_i})] \end{aligned} \quad (33)$$

to obtain

$$\begin{aligned}
& - \langle A_f | \sum_{i=1}^n \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^* | A_i \rangle \\
& = - \frac{1}{i \sqrt{L(L+1)}} \langle A_f | \sum_{i=1}^n \frac{e_i \hbar}{m_i c} (\vec{\nabla}_i \Phi_{LM}^*(\vec{r}_i)) \cdot \frac{1}{i} [\vec{r}_i \times \vec{\nabla}_i] | A_i \rangle \\
& = \frac{i}{\sqrt{L(L+1)}} \langle A_f | \sum_{i=1}^n \frac{e_i \hbar}{m_i c} (\vec{\nabla}_i \Phi_{LM}^*(\vec{r}_i)) \cdot \vec{l}_i | A_i \rangle,
\end{aligned} \tag{34}$$

where  $\vec{l}_i$  is the (dimensionless) single-particle, orbital angular momentum operator acting on particle with index,  $i$ .

In similar manner, we can transcribe the second term into the same type of form

$$\begin{aligned}
& - \langle A_f | \sum_{i=1}^n \frac{e_i \hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot [\vec{\nabla}_i \times \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^* | A_i \rangle \\
& = +k \langle A_f | \sum_{i=1}^n \frac{e_i \hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot \vec{A}(\vec{r}_i, \mathcal{E})_{LM}^* | A_i \rangle \\
& \approx k \sqrt{\frac{(L+1)}{L}} \langle A_f | \sum_{i=1}^n \frac{e_i \hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot \vec{A}(\vec{r}_i, \mathcal{L})_{LM}^* | A_i \rangle \\
& = \frac{k}{-ik} \sqrt{\frac{(L+1)}{L}} \langle A_f | \sum_{i=1}^n \frac{e_i \hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot (\vec{\nabla}_i \Phi_{LM}^*(\vec{r}_i)) | A_i \rangle,
\end{aligned} \tag{35}$$

where we have used  $[\vec{\nabla}_i \times \vec{A}(\vec{r}_i, \mathcal{M})_{LM}] = -k \vec{A}(\vec{r}_i, \mathcal{E})_{LM}$  and have approximated  $\vec{A}(\vec{r}_i, \mathcal{E})_{LM}$ , as we did for the electric multipole case to express this vector in terms of a gradient of the scalar function,  $\Phi_{LM}(\vec{r}_i) = j_L(kr_i) i^L Y_{LM}(\theta_i, \phi_i)$ . Combining eqs. (34) and (35), we get

$$\begin{aligned}
& - \langle A_f | \sum_{i=1}^n \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^* + \sum_{i=1}^n \frac{e_i \hbar g_{s,i}}{2m_i c} \vec{s}_i \cdot [\vec{\nabla}_i \times \vec{A}(\vec{r}_i, \mathcal{M})_{LM}^*] | A_i \rangle \\
& = i \sqrt{\frac{(L+1)}{L}} \langle A_f | \sum_{i=1}^n \frac{e_i \hbar}{2m_i c} (\vec{\nabla}_i \Phi_{LM}^*(\vec{r}_i)) \cdot \left( \frac{2}{(L+1)} \vec{l}_i + g_{s,i} \vec{s}_i \right) | A_i \rangle \\
& \approx i^{L+1} (-1)^{L+M} \sqrt{\frac{(L+1)}{L}} \frac{1}{(2L+1)!!} \\
& \times \langle A_f | \sum_{i=1}^n \frac{e_i \hbar}{2m_i c} \vec{\nabla}_i \left( (kr_i)^L Y_{L,-M}(\theta_i, \phi_i) \right) \cdot \left( \frac{2}{(L+1)} \vec{l}_i + g_{s,i} \vec{s}_i \right) | A_i \rangle,
\end{aligned} \tag{36}$$

where we have again used the approximation,

$$j_L(kr_i) \approx \frac{(kr_i)^L}{(2L+1)!!}. \tag{37}$$

From this result, we get the final expression for the transition probability per second that the quantum system make a transition  $A_i \rightarrow A_f$  via a magnetic  $2^L$ -pole photon

emission,

$$\frac{1}{\tau_{ML}} = \frac{8\pi}{\hbar} \left(\frac{\omega}{c}\right)^{2L+1} \frac{(L+1)}{L} \frac{1}{[(2L+1)!!]^2} \sum_M \times \left| \langle A_f | \sum_{i=1}^n \frac{e_i \hbar}{2m_i c} \vec{\nabla}_i \left( r_i^L Y_{L,M}(\theta_i, \phi_i) \right) \cdot \left( \frac{2}{(L+1)} \vec{l}_i + g_{s,i} \vec{s}_i \right) | A_i \rangle \right|^2, \quad (38)$$

where we have renamed  $M \rightarrow -M$  in the dummy summation index. Now, we can use the gradient formula (see the mathematical appendix to Chapter 62),

$$\begin{aligned} \frac{1}{i} \vec{\nabla} \left( i^L f(r) Y_{LM} \right) &= \left( \frac{df}{dr} + \frac{(L+1)}{r} f \right) \sqrt{\frac{L}{(2L+1)}} \vec{V}_{[(L-1)1]LM} \\ &\quad + \left( \frac{df}{dr} - \frac{L}{r} f \right) \sqrt{\frac{(L+1)}{(2L+1)}} \vec{V}_{[(L+1)1]LM}. \end{aligned} \quad (39)$$

In particular, the second term disappears for  $f(r) = r^L$ , so

$$\begin{aligned} \frac{1}{i} \vec{\nabla} \left( i^L r^L Y_{LM} \right) &= \sqrt{L(2L+1)} r^{L-1} \vec{V}_{[(L-1)1]LM} \\ &= \sqrt{L(2L+1)} \sum_{\mu} \langle (L-1)(M-\mu)1\mu | LM \rangle i^{L-1} r^{L-1} Y_{(L-1)(M-\mu)} \vec{e}_{\mu}. \end{aligned} \quad (40)$$

We therefore have

$$\begin{aligned} &\vec{V}_i \left( r_i^L Y_{LM}(\theta_i, \phi_i) \right) \cdot \left( \frac{2}{(L+1)} \vec{l}_i + g_{s,i} \vec{s}_i \right) = \sqrt{L(2L+1)} \\ &\times \sum_{\mu} \langle (L-1)(M-\mu)1\mu | LM \rangle r_i^{L-1} Y_{(L-1)(M-\mu)}(\theta_i, \phi_i) \\ &\times \left( \frac{2}{(L+1)} (\vec{l}_i)_{\mu} + g_{s,i} (\vec{s}_i)_{\mu} \right) \\ &= \sqrt{L(2L+1)} \left[ r_i^{L-1} Y_{(L-1)}(\theta_i, \phi_i) \times \left( \frac{2}{(L+1)} \vec{l}_i^1 + g_{s,i} \vec{s}_i^1 \right) \right]_M^L, \end{aligned} \quad (41)$$

where the square bracket denotes the angular momentum coupling of the spherical harmonic of rank  $(L-1)$  with the vectors of spherical rank 1 to resultant angular momentum  $L$ . With this result, we can transcribe

$$\begin{aligned} \frac{1}{\tau_{ML}} &= \frac{8\pi}{\hbar} \left(\frac{\omega}{c}\right)^{2L+1} \frac{(L+1)}{[(2L+1)!!(2L-1)!!]} \sum_M \\ &\left| \langle A_f | \sum_{i=1}^n \frac{e_i \hbar}{2m_i c} \left[ r_i^{L-1} Y_{(L-1)}(\theta_i, \phi_i) \times \left( \frac{2}{(L+1)} \vec{l}_i^1 + g_{s,i} \vec{s}_i^1 \right) \right]_M^L | A_i \rangle \right|^2. \end{aligned} \quad (42)$$

We note, in particular, with  $L = 1$ , for which

$$\sqrt{L(2L+1)} \left[ r_i^{L-1} Y_{(L-1)} \times \left( \frac{2}{(L+1)} \vec{l}_i^1 + g_{s,i} \vec{s}_i^1 \right) \right]_M^L = \sqrt{\frac{3}{4\pi}} \left( \vec{l}_i + g_{s,i} \vec{s}_i \right)_M, \quad (43)$$

we have

$$\frac{1}{\tau_{M1}} = \frac{4\omega^3}{3\hbar c^3} \sum_M \left| \langle A_f | \sum_{i=1}^n (\vec{\mu}_i^{(\text{magnetic})})_M | A_i \rangle \right|^2, \quad (44)$$

where

$$\vec{\mu}_i^{(\text{magnetic})} = \frac{e\hbar}{2m_i c} (\vec{l}_i + g_{s,i} \vec{s}_i) \quad (45)$$

is the magnetic moment for the  $i^{\text{th}}$  particle. Just as we had the generalized electric  $2^L$ -pole operator given (in spherical form) by

$$\sum_i e_i r_i^L Y_{LM}(\theta_i, \phi_i),$$

we now have the magnetic  $2^L$ -pole operator given by

$$\sum_i \sqrt{L(2L+1)} \left[ r_i^{L-1} Y_{(L-1)}(\theta_i, \phi_i) \times \frac{e\hbar}{2m_i c} \left( \frac{2}{(L+1)} \vec{l}_i^1 + g_{s,i} \vec{s}_i^1 \right) \right]_M^L.$$

Finally, if we use the Wigner–Eckart theorem, we get

$$\begin{aligned} \frac{1}{\tau_{ML}} &= \frac{8\pi}{\hbar} \left( \frac{\omega}{c} \right)^{2L+1} \frac{(L+1)}{(2L+1)!!(2L-1)!!} \frac{1}{(2J_i+1)} \times \\ &\left| \langle a_f J_f | \sum_{i=1}^n \frac{e\hbar}{2m_i c} \left[ r_i^{L-1} Y_{(L-1)}(\theta_i, \phi_i) \times \left( \frac{2}{(L+1)} \vec{l}_i^1 + g_{s,i} \vec{s}_i^1 \right) \right]_M^L | a_i J_i \rangle \right|^2. \end{aligned} \quad (46)$$

Let us end by comparing the orders of magnitude of a typical  $\mathcal{M}1$  and a typical  $\mathcal{E}1$  matrix element.

$$\frac{\mathcal{M}1 \text{ matrix element}}{\mathcal{E}1 \text{ matrix element}} \approx \frac{\mathcal{M}L \text{ matrix element}}{\mathcal{E}L \text{ matrix element}} \approx \frac{e\hbar}{mc} \frac{1}{er}. \quad (47)$$

For an atom, with  $r \approx a_0$ , this ratio is  $\approx \frac{e^2}{\hbar c} \approx 10^{-2}$ . The other useful ratio of matrix elements is

$$\frac{\mathcal{E}2 \text{ matrix element}}{\mathcal{E}1 \text{ matrix element}} \approx \frac{\mathcal{E}(L+1) \text{ matrix element}}{\mathcal{E}L \text{ matrix element}} \approx \frac{\omega}{c} r. \quad (48)$$

For an atom, this ratio is of order  $(\hbar\omega)a_0/(\hbar c)$ . If we were to take  $\hbar\omega = e^2/a_0$ , i.e., an  $\hbar\omega$  equal to one atomic unit of energy, again, this ratio would be  $\frac{e^2}{\hbar c} \approx (10)^{-2}$ . Note, however, this  $\hbar\omega = (8/3)\hbar\omega_{(\text{Lyman } \alpha)}$  and would correspond to a wavelength of  $456 \times (10)^{-8}$  cm. For a wavelength in the visible part of the spectrum, therefore, the ratio would be of order  $(10)^{-3}$ . Thus, the  $\mathcal{M}1$  and  $\mathcal{E}2$  matrix elements are very roughly of the same order, with the  $\mathcal{E}2$  matrix element possibly smaller by a factor of 10, but with both  $\sim (10)^{-2} - (10)^{-3}$  times the order of magnitude of a typical  $\mathcal{E}1$  matrix element.

For nuclei with

$$\frac{\hbar}{mcr} = \frac{\hbar c}{mc^2} \frac{1}{r} \approx \frac{0.2 \text{ fm}}{r_{\text{nucleus}}},$$

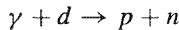
this number varies from  $(10)^{-1}$  to  $(10)^{-2}$  for light to heavy nuclei. The ratio  $(\hbar\omega)r/(\hbar c)$  is strongly frequency dependent and again varies by nearly a factor of 10 with the mass of the nucleus but is again of the order of  $(10)^{-1}$  to  $(10)^{-2}$ . Thus, roughly,  $\mathcal{M}1$  and  $\mathcal{E}2$  matrix elements are of the same order of magnitude, similarly for  $\mathcal{M}2$  and  $\mathcal{E}3$  matrix elements.

Finally, the  $\mathcal{M}1$  and  $\mathcal{E}2$  operators both have positive parity, thus they cannot change the parity of the state  $A_i$ , whereas the  $\mathcal{E}1$  operator, as well as  $\mathcal{M}2$  and  $\mathcal{E}3$ ,  $\mathcal{M}4$  and  $\mathcal{E}5$  operators, . . . , have negative parity and have nonzero matrix elements only between states of opposite parity.

## Problems

**33.** The 21-cm line in the hydrogen atom, famous through radio astronomy and the hydrogen maser, involves the transition,  $F = 1 \rightarrow F = 0$ , from the  $F = 1$  hyperfine level to the  $F = 0$  hyperfine level of the  $1s$  ground state of the hydrogen atom, where  $\vec{F} = \vec{s}_e + \vec{s}_p$ . Calculate the mean life for the spontaneous emission of the 21-cm photon. Show the transition must proceed via the intrinsic spin part of the magnetic dipole term. (The long mean life results from the  $\mathcal{M}1$  character of the transition, but also from the extremely low value of the transition frequency of  $1.420,405,752 \times 10^9 \text{ sec}^{-1}$ . In the observation of this line from interstellar hydrogen, induced emission and absorption processes may also have to be considered.)

**34.** At low  $\gamma$  photon energies, with  $\hbar\omega$  somewhat greater than the deuteron binding energy of 2.226 MeV, the photo dissociation of the deuteron



cannot proceed via the electric dipole term (cf., problems 32. and 31.), because the relative motion function for the  $p-n$  relative motion will be predominantly  $s$  wave,  $l = 0$ , just above threshold, and the bound-state wave function of the deuteron is an almost pure  $l = 0$  wave function. At low  $\gamma$  photon energies,  $2.226 \text{ MeV} < \hbar\omega \leq 4 \text{ MeV}$ , just above threshold, the photo-dissociation must therefore proceed via the magnetic dipole term.

Show that only the spin terms of the magnetic dipole operator can contribute to the matrix element. Because the bound state of the deuteron has  $S = 1$ , and because the orbital wave functions for two  $S = 1$  states at *different* energies (one the bound state, the second the relative motion function in the continuum) must be orthogonal to each other\*, show that the magnetic dipole operator has zero matrix element between the  $S = 1$  bound state and an  $S = 1$  continuum state. The photodissociation process near threshold thus proceeds only into  $S = 0$  continuum states. For these, we can approximate the radial  $s$  wave continuum function by a phase-shifted  $l = 0$  radial function,

$$r R_{l=0}(r) = A_0 \sin(k_0 r + \delta_0), \quad r \rightarrow \text{large},$$

where  $\hbar^2 k_0^2/M = \hbar\omega - 2.226$  MeV, and  $\delta_0$  is the singlet phase shift given approximately in terms of the singlet scattering length

$$a_{\text{sc.l.}}^{S=0} = -23.68 \text{ fm}, \quad \text{by} \quad \tan \delta_0 \approx -k_0 a_{\text{sc.l.}}^{S=0}.$$

For the bound-state wave function of the deuteron, use the Hulthen wave function (see problem 31). For purposes of estimating the radial overlap, assume the continuum wave function,  $A_0 \sin(k_0 r + \delta_0)$ , is valid all the way to  $r = 0$ . Also, recall the  $S = 0, l = 0$  two-nucleon wave function must have isospin,  $I = 1$ . With the above approximations, calculate the differential and total cross sections for the photodissociation process and compare with the electric dipole result of problem 32. Also, recall  $g_s = 2 \times 2.793$  for the proton and  $g_s = 2 \times (-1.913)$  for the neutron.

\*Footnote: For the highly approximate radial wave functions that we use here, this orthogonality would not be satisfied exactly, but this is a fault of our approximations. Also, note: We no longer use the plane wave approximations of problems 31 and 32, valid at higher energies.

35. The ground state of the nucleus,  $^{111}\text{In}_{62}$ , with 49 protons and 62 neutrons, has spin and parity,  $\frac{9}{2}^+$ . The first excited state of this nucleus is an isomeric (metastable) state with spin and parity,  $\frac{1}{2}^-$ , at an excitation energy of 0.5363 MeV. Show the transition from the  $\frac{1}{2}^-$  state to the  $\frac{9}{2}^+$  state can proceed only via the emission of a magnetic  $2^4$ -pole or an electric  $2^5$ -pole photon, i.e.,  $\mathcal{M}$ -type with  $L = 4$ , or  $\mathcal{E}$ -type with  $L = 5$ . Prove, by calculating both rates, the  $\mathcal{M}4$  rate predominates and make a prediction of the mean life of the excited  $\frac{1}{2}^-$  state. The nuclear shell model would lead us to believe the transition matrix element results from the last odd proton making a transition from a  $2p_{\frac{1}{2}}$  shell model orbit, with  $l = 1, j = \frac{1}{2}$ , to a  $1g_{\frac{9}{2}}$  shell model orbit, with  $l = 4, j = \frac{9}{2}$ . The radial wave functions can be approximated by the 3-D harmonic oscillator wave functions

$$\text{For } 2p : \quad R_{2p}(\rho) = \left[ \frac{m\omega_0}{\hbar} \right]^{\frac{3}{4}} \frac{1}{\sqrt{2\Gamma(\frac{7}{2})}} (5\rho - 2\rho^3) e^{-\frac{1}{2}\rho^2},$$

$$\text{For } 1g : \quad R_{1g}(\rho) = \left[ \frac{m\omega_0}{\hbar} \right]^{\frac{3}{4}} \frac{2}{\sqrt{\Gamma(\frac{11}{2})}} \rho^4 e^{-\frac{1}{2}\rho^2},$$

where the oscillator length,  $\sqrt{\hbar/m\omega_0}$ , is determined by the nucleon mass,  $m$ , and the shell model  $\hbar\omega_0$ , which for a nucleus with a mass of 111 is approximately,  $\hbar\omega_0 = 8.5$  MeV. In the above,  $\rho = r\sqrt{m\omega_0/\hbar}$ . The proton  $g_s$  factor is  $2 \times 2.793$ . First, calculate the needed matrix elements, as if a single proton were making a transition from  $p_{\frac{1}{2}} \rightarrow g_{\frac{9}{2}}$ . The actual transition in  $^{111}\text{In}_{62}$  actually involves a transition from the proton configuration

$$(\text{closed } j \text{ shells})(g_{\frac{9}{2}})^8(p_{\frac{1}{2}})^1 \rightarrow (\text{closed } j \text{ shells})(g_{\frac{9}{2}})^9.$$

As the  $p_{\frac{1}{2}}$  proton is converted to a  $g_{\frac{5}{2}}$  proton, it finds only two of the 10 possible  $g_{\frac{5}{2}}$  orbits still vacant. This gives an additional factor of  $\sqrt{2/10}$  relative to the simple single-particle matrix element. Take this factor of  $\sqrt{2/10}$  into account in calculating the actual mean life of the  $\frac{1}{2}^-$  excited state. The observed lifetime is 7.7 minutes. (In comparing your actual result with this experimental value, remember our model for the transition is based on many approximations.)

**36.** The ground state of an odd  $Z$  nucleus has angular momentum and parity  $\frac{7}{2}^+$ . The first excited state of this nucleus at 0.32-MeV excitation energy has angular momentum and parity  $\frac{11}{2}^-$ . Show the transition from the  $\frac{11}{2}^-$  state to the  $\frac{7}{2}^+$  state will proceed predominantly via the emission of a magnetic  $2^2$ -pole or an electric  $2^3$ -pole photon (i.e., an  $M$ -type with  $L = 2$  or a  $E$ -type with  $L = 3$ ), or even higher multipoles. Show, by calculating both the  $ML = 2$  and  $EL = 3$  matrix elements which of the two rates predominates. Make a prediction of the mean life of the excited state under the assumption the transition matrix element results from a single odd proton making a transition from an  $1h_{\frac{11}{2}}$  orbit, with  $l = 5$ ,  $j = \frac{11}{2}$ , to a  $1g_{\frac{5}{2}}$  orbit, with  $l = 4$ ,  $j = \frac{7}{2}$ . The radial wave functions can be approximated by 3-D harmonic oscillator wave functions:

$$\text{For } 1h : \quad R_{1h}(\rho) = \frac{1}{a^{\frac{3}{2}}} \sqrt{\frac{2}{\Gamma(\frac{13}{2})}} \rho^5 e^{-\frac{1}{2}\rho^2},$$

$$\text{For } 1g : \quad R_{1g}(\rho) = \frac{1}{a^{\frac{3}{2}}} \sqrt{\frac{2}{\Gamma(\frac{11}{2})}} \rho^4 e^{-\frac{1}{2}\rho^2},$$

with  $\rho = r/a$ , and  $a = 2.3$  fm. The proton  $g_s$  factor is  $2 \times 2.793$ .

**37.** A nucleus may make a transition from an excited state to a lower state by the emission of a  $\gamma$  photon or by the competing so-called internal conversion process in which the nuclear energy loss is transferred to an atomic  $K$  shell electron, with  $n = 1, l = 0$ , which is kicked out of the atomic  $K$  shell into the electron continuum. Assume the nuclear energy difference is such that the outgoing electron can be treated nonrelativistically, but is big enough, so the nuclear energy difference

$$E_i^{\text{nuc.}} - E_f^{\text{nuc.}} = \hbar\omega = \frac{p_f^2}{2m} - \left(-\frac{Z^2 e^2}{2a_0}\right)$$

leads to

$$\frac{p_f^2}{2m} \gg \frac{Z^2 e^2}{2a_0},$$

so the final free electron wave function can be approximated by a plane wave, with  $\vec{p}_f = \hbar\vec{k}_f$ . The interaction responsible for this process is the Coulomb interaction between the  $Z$  protons in the nucleus and the two  $K$  shell electrons in the atom

$$H_{\text{int.}} = -e^2 \sum_{j=1}^Z \sum_{k=1}^2 \frac{1}{|\vec{r}_j - \vec{r}_k|}$$

$$= -e^2 \sum_{j=1}^Z \sum_{k=1}^2 \sum_L \frac{r_j^L}{\bar{r}_k^{L+1}} \frac{4\pi}{(2L+1)} \sum_M Y_{LM}(\theta_j, \phi_j) Y_{LM}^*(\bar{\theta}_k, \bar{\phi}_k),$$

where we have assumed the probability of finding the atomic electron inside the nucleus is negligible, so  $r_j < \bar{r}_k$ , where  $\vec{r}_j$  gives the position of a proton within the nucleus, and  $\vec{r}_k$  gives the position of the atomic electron. Assume the atomic  $K$  shell electron wave function can be approximated by the hydrogenic  $1s$  wave functions

$$2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Z\bar{r}/a_0} Y_{00}(\bar{\theta}, \bar{\phi}).$$

Assume the angular momenta and parities of the initial and final nuclear states are such that the competing photon emission process would proceed via the emission of an electric  $2^L$ -pole photon. Calculate the so-called internal conversion coefficient, which is the ratio

$$R = \frac{\text{Prob./sec. for nuclear transition } i \rightarrow f \text{ via K-shell conversion}}{\text{Prob./sec. for nuclear transition } i \rightarrow f \text{ via photon emission}}$$

and show under the above assumptions this ratio is

$$R = \left(\frac{e^2}{\hbar c}\right)^4 Z^3 \frac{L}{L+1} \left(\frac{2mc^2}{\hbar\omega}\right)^{L+\frac{5}{2}}.$$

In arriving at this result, we have used

$$\int_0^\infty dr r^2 \frac{j_L(k_f r)}{r^{L+1}} e^{-Zr/a_0} \approx \int_0^\infty dr \frac{j_L(k_f r)}{r^{L-1}} \quad \text{for } \frac{k_f a_0}{Z} \gg 1,$$

and

$$\int_0^\infty d\rho \frac{j_L(\rho)}{\rho^{L-1}} = - \left[ \frac{j_{L-1}(\rho)}{\rho^{L-1}} \right]_0^\infty = \frac{1}{(2L-1)!!},$$

which follows via eq. (5) of the appendix to Chapter 41, with replacement  $l \rightarrow l-1$ .

**38. Auger Effect.** In the two-electron He atom, states in which both electrons are excited have an energy higher than the energy of a  $\text{He}^+$  ion in its  $n = 1$   $1s$  ground state and a free electron, with energy  $\hbar^2 k_f^2 / 2m$ . Such doubly excited states dissociate into a  $\text{He}^+$  ion plus the free electron (the Auger effect).

Calculate the probability per second that the  $(2s)^2 {}^1S_0$  state of the He atom dissociate into a  $\text{He}^+$  ion in its  $1s$  state and a free electron with energy  $\hbar^2 k_f^2 / 2m$ . The interaction is the Coulomb potential between the two electrons,

$$\frac{e^2}{|\vec{r}_1 - \vec{r}_2|}.$$

Show, in particular, this Auger process is much more probable than a characteristic radiative decay process in an atom, by making the rough approximation that the free electron wave function can be replaced by a plane wave and the He bound

wave functions can be approximated by hydrogenic wave functions, with

$$R_{1s} = 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}}, \quad R_{2s} = \frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \left(2 - \frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}}.$$

**39.** The directional correlation between successively emitted  $\gamma$  photons is used to give information about the angular momenta of excited states in nuclei. Assuming the  $\gamma$  cascade is a  $1^+ \rightarrow 1^- \rightarrow 0^+$  cascade and the emission probability for each photon is given in electric dipole approximation, calculate the directional correlation function,  $W(\theta_{12})d\Omega_1 d\Omega_2$ . The function  $W(\theta_{12})d\Omega_1 d\Omega_2$  is the probability the second photon ( $\hbar\omega_2$ , emitted in the transition  $1^- \rightarrow 0^+$ ) is emitted within a solid angle element  $d\Omega_2$  about an angle,  $\theta_{12}$ , relative to the direction of the first photon, ( $\hbar\omega_1$ , emitted in the transition  $1^+ \rightarrow 1^-$ ). Use first-order time-dependent perturbation theory for the probability/second for the emission of each photon, so energy is conserved for each step of the cascade. Take the direction of emission of the first photon to be the  $z$  direction and assume the first photon is emitted into an element of solid angle  $d\Omega_1$  about the  $z$  direction. Assume all  $M$  sublevels of the initial  $1^+$  state are populated with equal probability, and calculate first the probability for the population of each  $M$  sublevel of the intermediate  $1^-$  level. Show  $W(\theta_{12})d\Omega_1 d\Omega_2$  has the general form

$$W(\theta_{12})d\Omega_1 d\Omega_2 = (a + b \cos \theta_{12} + c \cos^2 \theta_{12})d\Omega_1 d\Omega_2.$$

Find the relative magnitudes of  $c$ ,  $b$ , and  $a$ , and show how these constants are related to the two reduced electric dipole moment matrix elements for the two transitions. You will have to relate the two circular components of the photon polarization vector relative to the  $z'$  axis, making azimuth and polar angles,  $\phi_{12}, \theta_{12}$ , with respect to the  $x, y, z$  coordinate system to the spherical components of the unit vectors  $\vec{e}$  defined relative to the  $x, y, z$  coordinate system, by

$$\vec{e}_{\pm 1}' = \sum_m \vec{e}_m D_{m,\pm 1}^1(\phi_{12}, \theta_{12}, 0)^*.$$

# 66

## Scattering of Photons by Atomic Systems

We shall next use our interaction between the atomic system and the radiation field to study the scattering of photons from atoms or molecules. We shall study both elastic scattering processes and inelastic scattering processes. In the low frequency limit, the elastic scattering is known as Rayleigh scattering; at high frequency, it is known as Thomson scattering. The inelastic scattering process goes by the name of Raman scattering.

Because we start with a photon of type  $\vec{k}\mu$  and end with a photon of type  $\vec{k}'\mu'$ , with  $\vec{k}' \neq \vec{k}$ , the process will involve both a photon annihilation operator and a photon creation operator. We will thus have to deal with a second-order perturbation process, and we will need both first- and second-order perturbation terms

$$\begin{aligned} H_{\text{perturbation}} &= H_{\text{int.}}^{(1)} + H_{\text{int.}}^{(2)} \\ &= -\sum_{i=1}^n \frac{e_i}{m_i c} \vec{p}_i \cdot \vec{A}_\perp(\vec{r}_i) + \sum_{i=1}^n \frac{e_i^2}{2m_i c^2} \vec{A}_\perp(\vec{r}_i) \cdot \vec{A}_\perp(\vec{r}_i). \end{aligned} \quad (1)$$

Because we are dealing with atoms or molecules, it will be sufficient to use the electric dipole approximation, and approximate  $\vec{A}_\perp$  by

$$\vec{A}_\perp(\vec{r}_i) = \frac{c}{\sqrt{\text{Vol.}}} \sum_{\vec{k}} \sum_{\mu=\pm 1} \sqrt{\frac{2\pi\hbar}{\omega}} (a_{\vec{k}\mu} \vec{e}_\mu + a_{\vec{k}\mu}^\dagger \vec{e}_\mu^*). \quad (2)$$

We use the second-order perturbation theory formula, eq. (58) of Chapter 57, to get the transition probability that a photon of type  $\vec{k}\mu$  is converted to one of type  $\vec{k}'\mu'$  through a scattering process, with the atomic system starting in the initial state,  $A_i$ , and ending in the final state,  $A_f$ , with  $A_f = A_i$  for the elastic scattering

process, and  $A_f \neq A_i$  for the inelastic scattering process. Thus,

$$\left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{\vec{k}\mu \rightarrow \vec{k}'\mu'} = \frac{2\pi}{\hbar} \rho(E_f) \times \left| \langle A_f \vec{k}'\mu' | H_{\text{int.}}^{(2)} | A_i \vec{k}\mu \rangle + \sum_a \frac{\langle A_f \vec{k}'\mu' | H_{\text{int.}}^{(1)} | a \rangle \langle a | H_{\text{int.}}^{(1)} | A_i \vec{k}\mu \rangle}{(E_i^{(0)} - E_a^{(0)})} \right|^2, \quad (3)$$

where we have used the shorthand notation,  $\vec{k}\mu$ , for the state with photon number  $n_{\vec{k}\mu} = 1$ , where  $E_i^{(0)}$  and  $E_a^{(0)}$  include the eigenvalues of both  $H_{\text{atom}}^{(0)}$  and  $H_{\text{radiation}}^{(0)}$  and the intermediate states  $|a\rangle$  include states of two types: either states with all photon numbers equal to zero,  $|A_{\text{Intermediate}}\rangle \equiv |A_I\rangle$ , or states with both a photon of type  $\vec{k}\mu$  and of type  $\vec{k}'\mu'$ ,  $|A_I \vec{k}\mu, \vec{k}'\mu'\rangle$ . The three types of needed perturbation terms are illustrated by the diagrams of Fig. 66.1. In the term of type (2), the photon  $\vec{k}\mu$  is annihilated at time  $\tau_1$  and the photon  $\vec{k}'\mu'$  is created at later time  $\tau_2$ , whereas in the term of type (3) the photon  $\vec{k}'\mu'$  is created at the earlier time  $\tau_1$  and the photon  $\vec{k}\mu$  is annihilated at the later time  $\tau_2$ . Therefore,

$$\left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{\vec{k}\mu \rightarrow \vec{k}'\mu'} = \frac{2\pi}{\hbar} \rho(E_f) \times \left| \langle A_f \vec{k}'\mu' | H_{\text{int.}}^{(2)} | A_i \vec{k}\mu \rangle + \sum_{A_I} \frac{\langle A_f \vec{k}'\mu' | H_{\text{int.}}^{(1)} | A_I \rangle \langle A_I | H_{\text{int.}}^{(1)} | A_i \vec{k}\mu \rangle}{(E_{A_I}^{(0)} + \hbar\omega - E_{A_I}^{(0)})} + \sum_{A_I} \frac{\langle A_f \vec{k}'\mu' | H_{\text{int.}}^{(1)} | A_I \vec{k}'\mu', \vec{k}\mu \rangle \langle A_I \vec{k}'\mu', \vec{k}\mu | H_{\text{int.}}^{(1)} | A_i \vec{k}\mu \rangle}{(E_{A_I}^{(0)} - E_{A_I}^{(0)} - \hbar\omega')} \right|^2. \quad (4)$$

The energy conservation delta function that led to this relation requires only that  $E_{A_f}^{(0)} + \hbar\omega' = E_{A_I}^{(0)} + \hbar\omega$ . The intermediate energies,  $E_{A_I}^{(0)}$ , can therefore go to arbitrarily high values, and the sum,  $\sum_{A_I}$ , will in general include an integral over atomic continuum states. The three contributions to the needed matrix element are

$$(1) : \langle A_f \vec{k}'\mu' | H_{\text{int.}}^{(2)} | A_i \vec{k}\mu \rangle = \frac{c^2}{\text{Vol. } \sqrt{\omega\omega'}} (\vec{e}_\mu \cdot \vec{e}_{\mu'}^*) \sum_{i=1}^n \frac{e_i^2}{2m_i c^2} \langle A_f \vec{k}'\mu' | (a_{\vec{k}'\mu'}^\dagger a_{\vec{k}\mu} + a_{\vec{k}\mu} a_{\vec{k}'\mu'}^\dagger) | A_i \vec{k}\mu \rangle = \frac{c^2}{\text{Vol. } \sqrt{\omega\omega'}} (\vec{e}_\mu \cdot \vec{e}_{\mu'}^*) \sum_{i=1}^n \frac{e_i^2}{2m_i c^2} 2\delta_{A_f A_i} \delta_{\omega' \omega}. \quad (5)$$

(Note:  $a_{\vec{k}\mu}$  commutes with  $a_{\vec{k}'\mu'}^\dagger$  because we must have  $\vec{k}' \neq \vec{k}$  to have a scattering process. However,  $\omega' = \omega$  follows from energy conservation through the energy delta function of the Golden Rule. Note, finally, we have put a prime on the unit vector associated with  $\vec{k}'\mu'$  to indicate it is associated with a different  $z'$  axis than that associated with  $\vec{k}\mu$ .)

$$(2) : \langle A_f \vec{k}'\mu' | H_{\text{int.}}^{(1)} | A_I \rangle \langle A_I | H_{\text{int.}}^{(1)} | A_i \vec{k}\mu \rangle = \frac{c^2}{\text{Vol. } \sqrt{\omega\omega'}} \langle A_f | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_{\mu'}^*) | A_I \rangle \langle A_I | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_\mu) | A_i \vec{k}\mu \rangle, \quad (6)$$

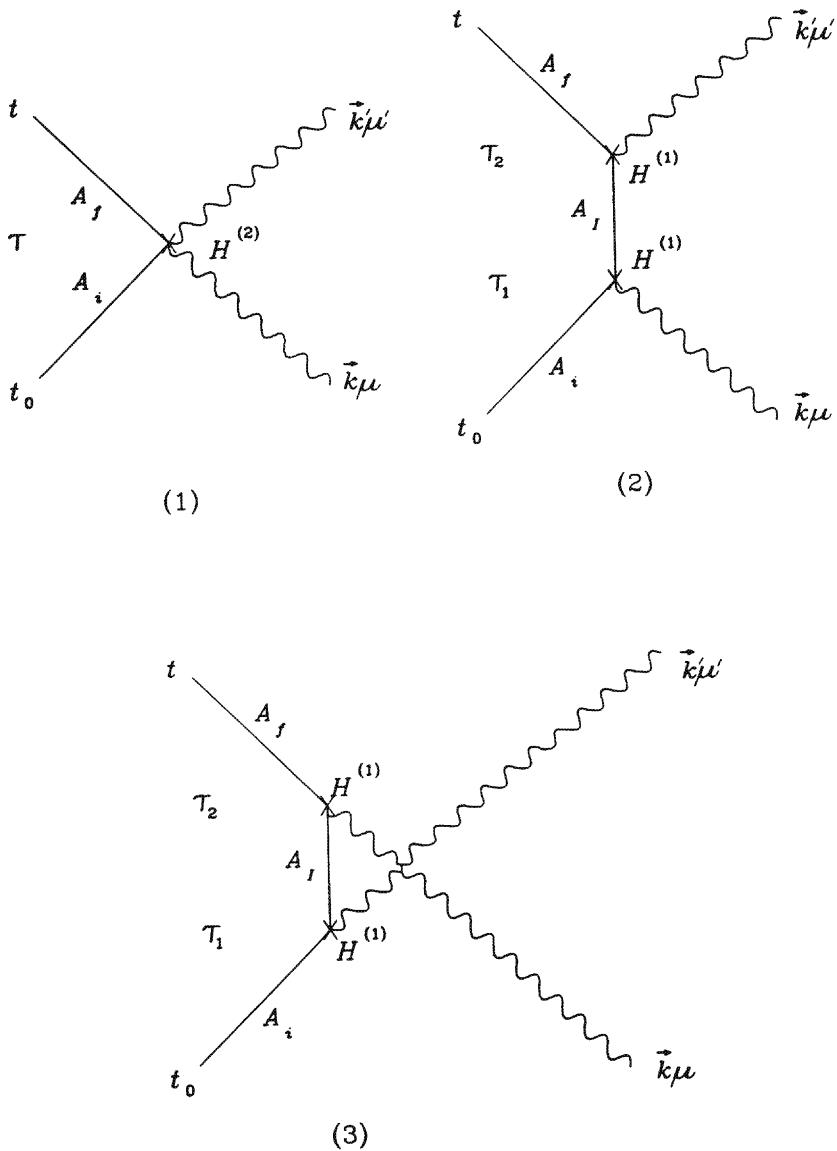


FIGURE 66.1. The three types of second-order perturbation terms for photon-atom scattering.

$$(3) : \langle A_f \vec{k}' \mu' | H_{\text{int}}^{(1)} | A_I \vec{k}' \mu', \vec{k} \mu \rangle \langle A_I \vec{k}' \mu', \vec{k} \mu | H_{\text{int}}^{(1)} | A_i \vec{k} \mu \rangle \\ = \frac{c^2}{\text{Vol. } \sqrt{\omega \omega'}} \langle A_f | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_\mu) | A_I \rangle \langle A_I | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_{\mu'}^*) | A_i \rangle. \quad (7)$$

## A Thomson Scattering

Let us first look at a very special case, the case of elastic scattering of high-energy photons. This is the case of so-called Thomson scattering. We assume  $\hbar\omega$  is much greater than a typical atomic energy, or a typical atomic energy difference, such as  $E_{A_1}^{(0)} - E_{A_i}^{(0)}$ , found in the energy denominators of terms (2) and (3). The atomic matrix elements of terms (2) and (3) thus make a contribution of order

$$\frac{e^2}{mc^2} \frac{p^2}{m} \times \frac{1}{\hbar\omega},$$

where the  $(1/\hbar\omega)$  gives the order of magnitude of the energy denominator factor in this case. Conversely, term (1) makes a contribution of order

$$\frac{e^2}{mc^2}.$$

Thus, terms (2) and (3) are smaller by a factor that is the ratio of (an atomic kinetic energy matrix element)/( $\hbar\omega$ ), and in this case terms (2) and (3) can be neglected compared with term (1). In this case, therefore, with  $\hbar\omega' = \hbar\omega \gg$  typical atomic energy, we have

$$\left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{\vec{k}\mu \rightarrow \vec{k}'\mu'} = \frac{2\pi}{\hbar} \rho(E_f) \left[ \frac{c^2}{\text{Vol.}} \frac{2\pi\hbar}{\omega} (\vec{e}_\mu \cdot \vec{e}'_\mu)^* \frac{Ze^2}{mc^2} \right]^2, \quad (8)$$

where  $m$  is the electron mass and we have neglected the term of order  $1/m_{\text{nucleus}}$  compared with  $1/m$ . We also need

$$\rho(E_f) = \frac{\text{Vol.}}{(2\pi)^3 \hbar c^3} \frac{\omega^2}{d\Omega'}. \quad (9)$$

To obtain the differential scattering cross section,  $d\sigma$ , we need (a) the above transition probability per second that the photon with incident  $\vec{k}$  and polarization  $\vec{e}_\mu$  be scattered into a  $d\Omega'$  about  $\vec{k}'$  with polarization  $\vec{e}'_\mu$ , and (b) we must divide this by the incident photon flux. For us,

$$\text{Incident photon flux} = \frac{(n_{\vec{k}\mu} = 1)c}{\text{Vol.}}. \quad (10)$$

Putting all the factors together, we have in this approximation

$$\left( \frac{d\sigma}{d\Omega'} \right)_{\text{Thomson}} = \frac{Z^2 e^4}{m^2 c^4} (\vec{e}_\mu \cdot \vec{e}'_\mu)^2. \quad (11)$$

We note

$$\frac{e^2}{mc^2} = r_0 = \text{"classical electron radius"} = 2.8 \times (10)^{-13} \text{cm.} \quad (12)$$

Above, we have written this cross section in terms of the circular polarization vectors,  $\vec{e}_\mu$  and  $\vec{e}'_\mu$ . We could just as well have taken linear polarization vectors,

$\vec{e}_\alpha$  and  $\vec{e}'_{\alpha'}$ , to get

$$\left( \frac{d\sigma}{d\Omega'} \right)_{\text{Thomson}} = Z^2 r_0^2 (\vec{e}_\alpha \cdot \vec{e}'_{\alpha'})^2. \quad (13)$$

If we choose the original photon direction,  $\vec{k}$ , along the  $z$  axis, and the scattered photon,  $\vec{k}'$ , along the  $z'$  axis, as shown in Fig. 66.2,

$$\begin{aligned} (\vec{e}_{x'} \cdot \vec{e}_x) &= \cos \theta \cos \phi, & (\vec{e}_{x'} \cdot \vec{e}_y) &= \cos \theta \sin \phi, \\ (\vec{e}_{y'} \cdot \vec{e}_x) &= -\sin \phi, & (\vec{e}_{y'} \cdot \vec{e}_y) &= \cos \phi. \end{aligned} \quad (14)$$

For unpolarized incident photons and for detectors insensitive to the polarization of the scattered photons, we then have

$$\left( \frac{d\sigma}{d\Omega'} \right)_{\text{Thomson}} = \frac{1}{2} Z^2 r_0^2 \sum_{\alpha=x,y} \sum_{\alpha'=x',y'} (\vec{e}_\alpha \cdot \vec{e}'_{\alpha'})^2 = \frac{1}{2} Z^2 r_0^2 (\cos^2 \theta + 1), \quad (15)$$

with total cross section

$$\sigma_{\text{Thomson}} = \frac{8\pi}{3} Z^2 r_0^2. \quad (16)$$

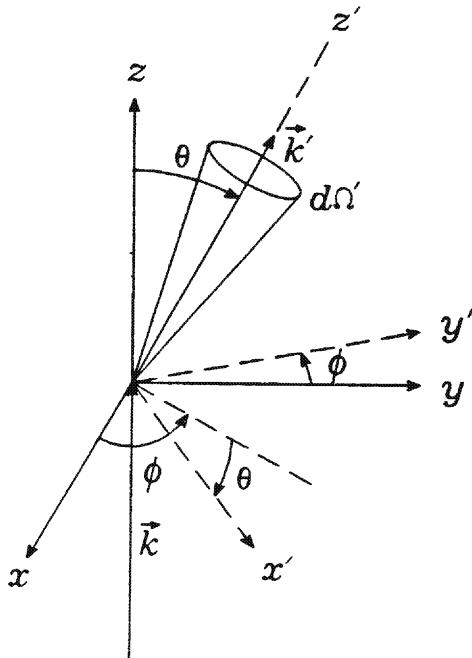


FIGURE 66.2. The incident photon  $\vec{k}$  and scattered photon  $\vec{k}'$  vectors.

## B Rayleigh and Raman Scattering

For the general case of photons of arbitrary  $\hbar\omega$ , or for photons of low frequency, it will be necessary to go back to eqs. (4)–(7). Now, terms of type (1), (2), and (3) all contribute. In the general case, it will be possible to combine terms (1), (2), and (3) most neatly by the following substitutions.

In term (1), use the identity

$$(\vec{e}_{\mu'}^* \cdot \vec{e}_\mu) = \frac{i}{\hbar} \left( (\vec{p}_i \cdot \vec{e}_{\mu'}^*)(\vec{r}_i \cdot \vec{e}_\mu) - (\vec{r}_i \cdot \vec{e}_\mu)(\vec{p}_i \cdot \vec{e}_{\mu'}^*) \right) = \frac{i}{\hbar} [(\vec{p}_i)_{\mu'}^*, (\vec{r}_i)_\mu], \quad (17)$$

where the Heisenberg commutation relation between  $\vec{p}$  and  $\vec{r}$  in *spherical* components can be written as

$$[(\vec{p})_\mu^*, (\vec{r})_v] = \frac{\hbar}{i} \delta_{\mu v}. \quad (18)$$

[Eq. (17), however, also involves direction cosines between the unit vectors in the primed and unprimed coordinates.]

In term (2), we will use the identity

$$\begin{aligned} \langle A_I | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_\mu) | A_I \rangle &= \frac{i}{\hbar} \langle A_I | \sum_i \frac{e_i}{c} [H_{\text{atom}}^{(0)}, \vec{r}_i] \cdot \vec{e}_\mu | A_I \rangle \\ &= \frac{i}{\hbar c} (E_{A_I}^{(0)} - E_{A_i}^{(0)}) \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_\mu | A_I \rangle. \end{aligned} \quad (19)$$

In term (3), we will use the identity

$$\begin{aligned} \langle A_f | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}_\mu) | A_I \rangle &= \frac{i}{\hbar} \langle A_f | \sum_i \frac{e_i}{c} [H_{\text{atom}}^{(0)}, \vec{r}_i] \cdot \vec{e}_\mu | A_I \rangle \\ &= \frac{i}{\hbar c} (E_{A_f}^{(0)} - E_{A_I}^{(0)}) \langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_\mu | A_I \rangle. \end{aligned} \quad (20)$$

Combining these three terms, we get

$$\begin{aligned} \left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{\vec{k}_\mu \rightarrow \vec{k}'_{\mu'}} &= \frac{2\pi}{\hbar} \rho(E_f) \left[ \frac{c^2}{\text{Vol.}} \frac{2\pi\hbar}{\sqrt{\omega\omega'}} \right]^2 \frac{1}{\hbar^2 c^4} \\ &\times \left| \sum_{A_I} \left[ \langle A_f | \sum_i \frac{e_i}{m_i} (\vec{p}_i \cdot \vec{e}_{\mu'}^*) | A_I \rangle \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_\mu | A_I \rangle \left( 1 + \frac{E_{A_I}^{(0)} - E_{A_i}^{(0)}}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} \right) \right. \right. \\ &\quad \left. \left. + \langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_\mu | A_I \rangle \langle A_I | \sum_i \frac{e_i}{m_i} (\vec{p}_i \cdot \vec{e}_{\mu'}^*) | A_I \rangle \left( -1 + \frac{E_{A_f}^{(0)} - E_{A_I}^{(0)}}{E_{A_I}^{(0)} - E_{A_f}^{(0)} - \hbar\omega'} \right) \right] \right|^2, \end{aligned} \quad (21)$$

where we have inserted a unit operator in the form of,  $\sum_{A_I} |A_I\rangle\langle A_I| = 1$ , between the two operators of term (1), and have used the commutator relation,  $[(\vec{p}_i)_{\mu'}^*, (\vec{r}_j)_\mu] = 0$  for  $j \neq i$ . We will further make use of the two identities

$$\left( 1 + \frac{E_{A_I}^{(0)} - E_{A_i}^{(0)}}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} \right) = \frac{\hbar\omega}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}},$$

$$\left( -1 + \frac{E_{A_f}^{(0)} - E_{A_I}^{(0)}}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'} \right) = \frac{\hbar\omega}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'}, \quad (22)$$

and use the commutator relation

$$\frac{\vec{p}_i}{m_i} = \frac{i}{\hbar} [H_{\text{atom}}^{(0)}, \vec{r}_i] \quad (23)$$

once more to convert the remaining atomic matrix elements in eq. (21) to electric dipole form, and obtain

$$\begin{aligned} \left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{\vec{k}\mu \rightarrow \vec{k}'\mu'} &= \frac{2\pi}{\hbar} \rho(E_f) \frac{(2\pi)^2}{\omega\omega' \text{Vol.}^2} \omega^2 \\ &\times \left| \sum_{A_I} \frac{(E_{A_f}^{(0)} - E_{A_I}^{(0)}) \langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu'}^* | A_I \rangle \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu} | A_I \rangle}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} \right. \\ &\quad \left. + \sum_{A_I} \frac{(E_{A_I}^{(0)} - E_{A_f}^{(0)}) \langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu} | A_I \rangle \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu'}^* | A_I \rangle}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'} \right|^2. \end{aligned} \quad (24)$$

Now, we shall further make use of the identities

$$\begin{aligned} \frac{E_{A_f}^{(0)} - E_{A_I}^{(0)}}{E_{A_i}^{(0)} - E_{A_I}^{(0)} + \hbar\omega} &= 1 - \frac{\hbar\omega'}{E_{A_i}^{(0)} - E_{A_I}^{(0)} + \hbar\omega}, \\ \frac{E_{A_I}^{(0)} - E_{A_f}^{(0)}}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'} &= -1 - \frac{\hbar\omega'}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'}, \end{aligned} \quad (25)$$

and use the completeness of the atomic states  $|A_I\rangle$  to note

$$\begin{aligned} \sum_{A_I} &\left( \langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu'}^* | A_I \rangle \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu} | A_I \rangle \right. \\ &\quad \left. - \langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu} | A_I \rangle \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu'}^* | A_I \rangle \right) \\ &= 0. \end{aligned} \quad (26)$$

With these relations, we can convert the transition probability for the scattering process into

$$\begin{aligned} \left[ \frac{\text{Trans. Prob.}}{\text{second}} \right]_{\vec{k}\mu \rightarrow \vec{k}'\mu'} &= \frac{2\pi}{\hbar} \rho(E_f) \frac{(2\pi)^2}{\omega\omega' \text{Vol.}^2} \hbar^2 \omega^2 \omega'^2 \\ &\times \left| \sum_{A_I} \frac{\langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu'}^* | A_I \rangle \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu} | A_I \rangle}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} \right. \\ &\quad \left. + \sum_{A_I} \frac{\langle A_f | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu} | A_I \rangle \langle A_I | \sum_i e_i \vec{r}_i \cdot \vec{e}_{\mu'}^* | A_I \rangle}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'} \right|^2. \end{aligned} \quad (27)$$

In this expression, our polarization vectors,  $\vec{e}_{\mu}$ , for the incident photon of type  $\vec{k}\mu$  are defined with respect to the laboratory axes, but the circular polarization vectors,  $\vec{e}_{\mu'}^*$ , are again defined with respect to the direction of the vector  $\vec{k}'$ , which

can be used to define the  $z'$  direction, where the  $x'$ ,  $y'$ ,  $z'$  axes are rotated through the Euler angles  $\phi$ ,  $\theta$ , 0, relative to the laboratory axes (see Fig. 66.2), so

$$\vec{e}'_{\mu'} = \sum_{m=\pm 1,0} \vec{e}_m D_{m\mu'}^1(\phi, \theta, 0)^*. \quad (28)$$

To obtain the differential scattering cross section,  $d\sigma$ , we must again divide the transition probability per second that the photon with incident  $\vec{k}$  and polarization  $\vec{e}_\mu$  be scattered into a  $d\Omega'$  about  $\vec{k}'$  with polarization  $\vec{e}'_{\mu'}$  by the incident photon flux. For us,

$$\text{Incident photon flux} = \frac{(n_{k\mu} = 1)c}{\text{Vol.}}. \quad (29)$$

We also need  $\rho(E_f)$ , which is now

$$\rho(E_f) = \frac{\text{Vol.}}{(2\pi)^3 \hbar c^3} \frac{\omega'^2}{d\Omega'}. \quad (30)$$

Thus,

$$\begin{aligned} d\sigma &= \frac{2\pi}{\hbar} \frac{\text{Vol.}}{(2\pi)^3 \hbar c^3} \frac{\omega'^2}{d\Omega'} \frac{(2\pi)^2}{\omega \omega' \text{Vol.}^2} \frac{\hbar^2 \omega^2 \omega'^2}{c} \frac{\text{Vol.}}{c} \\ &\times \sum_{m,\bar{m}} D_{m\mu'}^1(\phi, \theta, 0) D_{\bar{m}\mu}^1(\phi, \theta, 0)^* g_{m\mu} g_{\bar{m}\mu}^* \\ &= \frac{\omega \omega'^3}{c^4} d\Omega' \sum_{m,\bar{m}} D_{m\mu'}^1(\phi, \theta, 0) D_{\bar{m}\mu}^1(\phi, \theta, 0)^* g_{m\mu} g_{\bar{m}\mu}^*, \end{aligned} \quad (31)$$

where

$$\begin{aligned} g_{m\mu} &= \sum_{A_i} \left[ \frac{\langle A_f | (\vec{\mu}^{(\text{el.})})_m^* | A_i \rangle \langle A_i | (\vec{\mu}^{(\text{el.})})_\mu | A_i \rangle}{E_{A_i}^{(0)} - E_{A_f}^{(0)} + \hbar\omega} \right. \\ &\quad \left. + \frac{\langle A_f | (\vec{\mu}^{(\text{el.})})_\mu^* | A_i \rangle \langle A_i | (\vec{\mu}^{(\text{el.})})_m | A_i \rangle}{E_{A_i}^{(0)} - E_{A_f}^{(0)} - \hbar\omega} \right]. \end{aligned} \quad (32)$$

Note: We sum over all three values  $m = +1, 0, -1$ , similarly for  $\bar{m}$ , where these are defined with respect to the laboratory  $z$  axis of Fig. 66.2, which is chosen along the direction of  $\vec{k}$ , whereas  $\mu = +1$ , or  $-1$ , is fixed by the polarization of the incident photon. Also, in general, it will be very challenging to evaluate the matrix element sums over intermediate states in  $g_{m\mu}$ . These sums will in general involve an infinite number of discrete states and an integral over continuum states. In the extreme low frequency limit, however, in which  $\hbar\omega$  and  $\hbar\omega'$  in the energy denominators can be neglected, the  $g_{m\mu}$  are essentially pure atomic properties, dependent only on the nature of the states,  $|A_i\rangle$  and  $|A_f\rangle$ . For elastic scattering, with an unpolarized incident beam and a detector insensitive to the polarization of the scattered photons, we then have

$$\left( \frac{d\sigma}{d\Omega'} \right)_{\text{Rayleigh}} = \frac{1}{2} \frac{\omega^4}{c^4} \sum_{\mu=\pm 1} \sum_{\mu'=\pm 1} \sum_{m,\bar{m}} D_{m\mu'}^1(\phi, \theta, 0) D_{\bar{m}\mu}^1(\phi, \theta, 0)^* g_{m\mu} g_{\bar{m}\mu}^*, \quad (33)$$

leading to the total cross section

$$\sigma_{\text{Rayleigh}} = \frac{4\pi}{3} \frac{\omega^4}{c^4} \sum_{\mu=\pm 1} \sum_{m=\pm 1,0} |g_{m\mu}|^2. \quad (34)$$

This cross section is of order of magnitude

$$\left(\frac{2\pi}{\lambda}\right)^4 \left(\frac{(ea_0)^2}{\frac{e^2}{a_0}}\right)^2 \approx \left(\frac{2\pi}{\lambda}\right)^4 a_0^6.$$

For  $\lambda = 6,000 \times (10)^{-8}$  cm, we have  $\sigma \approx (10)^{-12} a_0^2$ . Note, finally, the  $\omega^4$  dependence of the formula.

# Resonance Fluorescence Cross Section

In the last chapter, we saw both the elastic and inelastic photon scattering cross sections were given in terms of the amplitudes,  $g_{m\mu}$ , where

$$\sigma_{\text{elastic}} = \frac{8\pi}{3} \frac{\omega^4}{c^4} \sum_{m=\pm 1,0} |g_{m\mu}|^2, \quad \sigma_{\text{inelastic}} = \frac{8\pi}{3} \frac{\omega\omega'^3}{c^4} \sum_{m=\pm 1,0} |g_{m\mu}|^2, \quad (1)$$

where  $\mu = \pm 1$  indicates the circular polarization of the incident photon, and where

$$g_{m\mu} = \sum_{A_I} \left[ \frac{\langle A_f | (\mu^{(\text{el.})})_m^* | A_I \rangle \langle A_I | \mu_\mu^{(\text{el.})} | A_i \rangle}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} + \frac{\langle A_f | (\mu_\mu^{(\text{el.})})^* | A_I \rangle \langle A_I | (\mu^{(\text{el.})})_m^* | A_i \rangle}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'} \right]. \quad (2)$$

In the second term of this sum, the energy denominator can never be zero because we assume  $E_{A_i}^{(0)}$  is the ground-state energy of the atom, so  $E_{A_i}^{(0)} > E_{A_I}^{(0)}$  for all  $A_I$ . In the first term of the sum, however, it may be possible that the incident photon energy is such that  $\hbar\omega = E_{A_I}^{(0)} - E_{A_i}^{(0)}$  for some specific excited state,  $E_{A_I}^{(0)}$ . In that case, we would have a zero energy denominator for one specific term in the sum over the states  $A_I$ . This is very similar to the zero denominators which had to be avoided in the scattering Green's function formulation of the scattering problem, where we avoided this difficulty by replacing the energy  $E$  in the operator form of the Green's function formulation by an  $E + i\epsilon$ . Let us attempt the same type of change here, and make the replacement

$$\begin{aligned} & \sum_{A_I} \frac{\langle A_f | (\mu^{(\text{el.})})_m^* | A_I \rangle \langle A_I | \mu_\mu^{(\text{el.})} | A_i \rangle}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} \\ & \rightarrow \langle A_f | (\mu^{(\text{el.})})_m^* | A_I \rangle \frac{1}{E - H_0 + i\epsilon} \langle A_I | \mu_\mu^{(\text{el.})} | A_i \rangle \end{aligned}$$

$$\begin{aligned}
&= \int d\vec{r}_1 \cdots d\vec{r}_n \int d\vec{r}'_1 \cdots d\vec{r}'_n \psi_{A_f}^*(\vec{r}_1, \dots, \vec{r}_n) \sum_i \mu_m^{(\text{el.})*}(\vec{r}_i) \\
&\times \left[ \sum_{A_I} \frac{\psi_{A_I}(\vec{r}_1, \dots, \vec{r}_n) \psi_{A_I}^*(\vec{r}'_1, \dots, \vec{r}'_n)}{E - E_{A_I}^{(0)} + i\epsilon} \right] \sum_i \mu_\mu^{(\text{el.})}(\vec{r}'_i) \psi_{A_I}(\vec{r}'_1, \dots, \vec{r}'_n) \\
&= \int d\vec{r} \int d\vec{r}' \psi_{A_f}^*(\vec{r}) \mu_m^{(\text{el.})*}(\vec{r}) G(\vec{r}, \vec{r}'; E) \mu_\mu^{(\text{el.})}(\vec{r}') \psi_{A_I}(\vec{r}'), \tag{3}
\end{aligned}$$

where  $E$  is the incident energy,  $E = E_{A_i}^{(0)} + \hbar\omega$ , and we have used the shorthand notation,  $\vec{r} \equiv \vec{r}_1 \cdots \vec{r}_n$ , similarly for  $\vec{r}'$ , in the last line, in which the Green's function is expressed in coordinate representation. With this Green's function representation of the energy denominator, the energy of any excited state must be replaced by

$$E_{A_I}^{(0)} \rightarrow E_{A_I}^{(0)} - i\epsilon \equiv E_{A_I}^{(0)} - i\frac{\Gamma_I}{2}. \tag{4}$$

This relation makes sense, because any excited atomic state may decay to lower atomic states if the interaction of the atom with the radiation field is taken into account. This decay can be interpreted in terms of the level width (as we shall prove in the next chapter). With the imaginary part of the energy for the state,  $A_I$ , we have

$$\Psi_{A_I}(\vec{r}, t) = e^{-\frac{i}{\hbar} E_{A_I}^{(0)} t} e^{-\frac{\Gamma_I}{2} t}, \tag{5}$$

so  $(\Gamma_I/\hbar)$  gives  $(1/\tau_I)$ , where  $\tau_I$  is the mean lifetime of the excited state  $A_I$ . Because  $\tau_I$  is of order of  $(10)^{-8}$  sec. in atoms,  $\Gamma_I$  is of order  $\hbar/\tau_I \approx (10)^{-7}$  eV in atoms.

If there is an atomic excited state with energy such that

$$E_{A_R}^{(0)} \approx E_{A_i}^{(0)} + \hbar\omega, \tag{6}$$

the single term, with  $I = R$  (resonant state) predominates and all other terms in the sum,  $\sum_{A_I}$ , can be neglected for incident photons in this energy range. Therefore, with  $A_f = A_i$  (elastic scattering process),

$$g_{m\mu} \approx \frac{\langle A_i | \mu_m^{(\text{el.})*} | A_R \rangle \langle A_R | \mu_\mu^{(\text{el.})} | A_i \rangle}{(\hbar\omega + E_{A_i}^{(0)} - E_{A_R}^{(0)}) + \frac{i}{2}\Gamma_R}. \tag{7}$$

In this case, a strong enhancement of the scattering cross section exists at this resonant frequency,  $\hbar\omega = (E_{A_R}^{(0)} - E_{A_i}^{(0)})$ . A resonance fluorescence exists, and near  $\hbar\omega = \hbar\omega_{\text{resonance}}$ , assuming unpolarized incident photons, the resonance fluorescence cross section is

$$\sigma_{\text{resonance}} = \frac{4\pi}{3} \frac{\omega^4}{c^4} \sum_{\mu=\pm 1} \sum_{m=\pm 1,0} \frac{|\langle A_i | \mu_m^{(\text{el.})*} | A_R \rangle|^2 |\langle A_R | \mu_\mu^{(\text{el.})} | A_i \rangle|^2}{(E_{A_i}^{(0)} + \hbar\omega - E_{A_R}^{(0)})^2 + \frac{1}{4}\Gamma_R^2}. \tag{8}$$

At exact resonance, the energy denominator is given by  $\frac{1}{4}\Gamma_R^2$ , a quantity of order  $(10)^{-14}$  eV<sup>2</sup>, whereas the denominator for an average term far off resonance can be expected to be of order 1 eV<sup>2</sup>, where we have taken a characteristic atomic energy difference to be 1 eV. Thus, we can expect an enhancement at exact resonance by

a factor of the order of  $10^{14}$  compared with the ordinary photon scattering cross section.

## A The Photon Scattering Cross Section and the Polarizability Tensor

Because of the difficulty of performing the intermediate state sum in the factors,  $g_{m\mu}$ , needed to evaluate the scattering cross sections from the underlying atomic structure, it may be useful to see how these  $g_{m\mu}$  are related to other physically measurable quantities. We want to investigate the possibility these sums can be estimated from other physically measurable quantities.

So far, we have found it convenient to express the differential and total cross sections in terms of the circular polarizations of the incident and scattered photons. In terms of these, we had

$$\left( \frac{d\sigma}{d\Omega'} \right)_{\vec{k}\mu \rightarrow \vec{k}'\mu'} = \frac{\omega\omega'^3}{c^4} \sum_{m=\pm 1,0} \sum_{\tilde{m}=\pm 1,0} D_{m\mu}^1(\phi, \theta, 0) D_{\tilde{m}\mu'}^1(\phi, \theta, 0)^* g_{m\mu} g_{\tilde{m}\mu}^*, \quad (9)$$

where the  $g_{m\mu}$  are given in terms of spherical components of the electric dipole moment vector in eq. (32) of Chapter 66. Note,  $\mu = \pm 1$ . The total cross section for unpolarized incident photons with detectors insensitive to the polarizations of the scattered photons was then given by

$$\sigma = \frac{4\pi}{3} \frac{\omega\omega'^3}{c^4} \sum_{\mu=\pm 1} \sum_{m=\pm 1,0} |g_{m\mu}|^2. \quad (10)$$

With  $\omega' = \omega$ , these expressions are valid for the elastic processes. Also, for  $\omega$  and  $\omega'$  not necessarily very small, the  $g_{m\mu}$  are  $\omega$ -dependent quantities. Because atoms (unlike molecules) are spherically symmetric systems, which in general have all possible orientations with respect to the incident photon beam coordinate system, we could have averaged over all possible orientations of the atom, leading to

$$\overline{|g_{m\mu}|^2} = \frac{1}{3} \sum_{v=\pm 1,0} |g_{mv}|^2, \quad (11)$$

where the bar denotes the averaging over all possible orientations of the atom. With this averaging, the total cross section, for unpolarized incident photons and detectors insensitive to polarization direction, becomes

$$\sigma = \frac{8\pi}{9} \frac{\omega\omega'^3}{c^4} \sum_{m=\pm 1,0} \sum_{v=\pm 1,0} |g_{mv}|^2. \quad (12)$$

All these formulae could have been transcribed to the case of linearly polarized incident photons and linearly polarized scattered photons, with

$$\left( \frac{d\sigma}{d\Omega'} \right)_{\vec{k}\alpha \rightarrow \vec{k}'\alpha'} = \frac{\omega\omega'^3}{c^4} \left| \sum_{A_f} \frac{\langle A_f | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_{\alpha'} | A_f \rangle \langle A_f | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_{\alpha} | A_i \rangle}{E_{A_f}^{(0)} + \hbar\omega - E_{A_i}^{(0)}} \right|$$

$$\begin{aligned}
& + \sum_{A_I} \frac{\langle A_f | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_\alpha | A_I \rangle \langle A_I | \sum_i (e_i \vec{r}_i) \cdot \vec{e}'_\alpha | A_I \rangle}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'} \Big|^2 \\
& = \frac{\omega\omega'^3}{c^4} \sum_{j=x,y,z} \sum_{\bar{j}=x,y,z} (\vec{e}_j \cdot \vec{e}'_\alpha)(\vec{e}_{\bar{j}} \cdot \vec{e}'_{\alpha'}) g_{j\alpha} g_{\bar{j}\alpha}^*, \tag{13}
\end{aligned}$$

where we have used

$$g_{\alpha'\alpha} = \sum_{j=x,y,z} (\vec{e}_j \cdot \vec{e}'_\alpha) g_{j\alpha},$$

and the direction cosines,  $(\vec{e}_j \cdot \vec{e}'_\alpha)$ , can be read from eq. (27) of Chapter 63. These have the property

$$\sum_{\alpha'=x',y'} \int \int d\Omega' (\vec{e}_j \cdot \vec{e}'_{\alpha'})(\vec{e}_{\bar{j}} \cdot \vec{e}'_{\alpha'}) = \frac{8\pi}{3} \delta_{j,\bar{j}}, \tag{14}$$

[cf., eq. (28) of Chapter 63]. This leads to a total cross section, for an unpolarized incident photon and detectors insensitive to the polarization of the scattered photon,

$$\sigma = \frac{8\pi}{3} \frac{\omega\omega'^3}{c^4} \frac{1}{2} \sum_{\alpha=x,y} \sum_{j=x,y,z} |g_{j\alpha}|^2. \tag{15}$$

The  $g_{j\alpha}$ , with  $\alpha = x, y$  only, now have the form

$$\begin{aligned}
g_{j\alpha} &= \sum_{A_I} \left[ \frac{\langle A_f | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_j | A_I \rangle \langle A_I | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_\alpha | A_I \rangle}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} \right. \\
&\quad \left. + \frac{\langle A_f | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_\alpha | A_I \rangle \langle A_I | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_j | A_I \rangle}{E_{A_i}^{(0)} - E_{A_I}^{(0)} - \hbar\omega'} \right] \\
&= \langle A_f | \mathcal{O}_{j\alpha} | A_I \rangle, \tag{16}
\end{aligned}$$

where the operator,  $\mathcal{O}_{jk}$ , is

$$\begin{aligned}
\mathcal{O}_{jk} &= \sum_{A_I} \left[ \sum_i (e_i \vec{r}_i) \cdot \vec{e}_j | A_I \rangle \frac{1}{E - H_0 + i\epsilon} \langle A_I | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_k \right. \\
&\quad \left. + \sum_i (e_i \vec{r}_i) \cdot \vec{e}_k | A_I \rangle \frac{1}{E - H_0 - \hbar\omega - \hbar\omega'} \langle A_I | \sum_i (e_i \vec{r}_i) \cdot \vec{e}_j \right], \tag{17}
\end{aligned}$$

where  $E = E_{A_i}^{(0)} + \hbar\omega$  and the unit vectors  $\vec{e}_j$  and  $\vec{e}_k$  both refer to the laboratory frame. In the low frequency limit, in which  $\hbar\omega(\hbar\omega') \ll E_{A_i}^{(0)} - E_{A_I}^{(0)}$ , so we can let  $\hbar\omega \rightarrow 0, \hbar\omega' \rightarrow 0$ , only the symmetric part of the second rank Cartesian tensor,  $\mathcal{O}_{jk}$ , survives, and we can identify it with the polarizability tensor of the atom. The diagonal matrix elements of  $\mathcal{O}_{jk}$  in the atomic ground state,  $A_i$ , can be identified with the atomic polarizability tensor,  $\alpha_{jk}$ . To see this, consider the atom to be perturbed by a static external electric field,  $\vec{\mathcal{E}}^{\text{ext.}}$ , with

$$H_{\text{perturbation}} = - \sum_i (e_i \vec{r}_i) \cdot \vec{\mathcal{E}}^{\text{ext.}}. \tag{18}$$

Stationary-state perturbation theory gives

$$\begin{aligned}\Delta E &= \sum_{A_I} \frac{\langle A_i | \sum_i (e_i \vec{r}_i) \cdot \vec{\mathcal{E}}^{\text{ext.}} | A_I \rangle \langle A_I | \sum_i (e_i \vec{r}_i) \cdot \vec{\mathcal{E}}^{\text{ext.}} | A_i \rangle}{E_{A_I}^{(0)} - E_{A_I}^{(0)}} \\ &= \frac{1}{2} \sum_{jk} \langle A_i | \mathcal{O}_{jk} (\omega = \omega' = 0) | A_i \rangle \mathcal{E}_j^{\text{ext.}} \mathcal{E}_k^{\text{ext.}} \\ &= \frac{1}{2} \sum_{jk} \alpha_{jk} \mathcal{E}_j^{\text{ext.}} \mathcal{E}_k^{\text{ext.}},\end{aligned}\quad (19)$$

where  $\alpha_{jk}$  is the polarizability tensor, which gives the strength of an *induced* electric dipole moment in the external field,  $\vec{\mathcal{E}}$ ,

$$\vec{\mu}_j^{\text{induced}} = \sum_k \alpha_{jk} \mathcal{E}_k^{\text{ext.}}. \quad (20)$$

The total cross section for low  $\omega$  elastic scattering, for an unpolarized incident photon beam and detectors insensitive to the polarization of the scattered photons, then follows from eq. (15),

$$\sigma_{\text{Rayleigh}} = \frac{8\pi}{3} \frac{\omega^4}{c^4} \frac{1}{2} \sum_{\beta=x,y} \sum_{j=x,y,z} |\langle A_i | \mathcal{O}_{j\beta} | A_i \rangle|^2 = \frac{8\pi}{3} \frac{\omega^4}{c^4} \frac{1}{2} \sum_{\beta=x,y} \sum_{j=x,y,z} \alpha_{j\beta}^2. \quad (21)$$

If the scattering system is spherically symmetric, e.g., an atom, which will have all possible orientations with respect to the incident photon coordinate system, averaging over all possible orientations of the atoms will lead to

$$\sigma_{\text{Rayleigh}} = \frac{8\pi}{9} \frac{\omega^4}{c^4} \sum_{j=x,y,z} \sum_{k=x,y,z} \alpha_{jk}^2. \quad (22)$$

For finite values of  $\hbar\omega$ , the polarizability tensor will be  $\omega$  dependent. We define

$$\alpha_{jk}(\omega) = |\langle A_i | \mathcal{O}_{jk}(\omega) | A_i \rangle|. \quad (23)$$

If the scattering system is not spherically symmetric, a diatomic molecule, e.g., we must transform from the polarizability tensor components in the laboratory frame, defined by  $\vec{k}$  and  $\vec{e}_\beta$ , to components in the molecular principal axis frame before averaging over all possible orientations of the molecules (see problems 40 and 41).

# 68

## Natural Line Width: Wigner–Weisskopf Treatment

Because we consider a world made of atomic systems and electromagnetic fields, i.e., atomic systems coupled to the photon fields, we must consider not only the atomic bound states with zero photons present, i.e., states such as  $|A_n 0\rangle$ , but also atomic bound states with one photon present, states such as  $|A_{n'}, \vec{k}\mu\rangle$ . Because the coupling between atoms and photons is weak, states with two photons, such as  $|A_{n''}, \vec{k}\mu, \vec{k}'\mu'\rangle$ , may be negligible in dominant order of perturbation theory, although they may also play a role, particularly for systems for which selection rules eliminate the one photon states. Fig. 68.1 shows the discrete spectrum of an atomic system with no photons present, with ground state,  $A_0$ , and excited states,  $A_n$ , with  $n = 1, 2, \dots$ . The figure also shows the continuous spectra of states with one photon present. The atomic eigenstate,  $A_3$ , e.g., is seen to be degenerate with the system where the atom is in the ground state and the photon has energy,  $\hbar\omega = E_{A_3}^{(0)} - E_{A_0}^{(0)}$ . It is also degenerate with the system where the atom is in the first excited state and the photon has energy  $\hbar\omega' = E_{A_3}^{(0)} - E_{A_1}^{(0)}$  and with the system composed of the atom in the second excited state and with photon energy,  $\hbar\omega'' = E_{A_3}^{(0)} - E_{A_2}^{(0)}$ . More precisely, the discrete excited state  $|A_n\rangle$  of the bare atom is coupled to states,  $|A_{n'}, \vec{k}\mu\rangle$ , in the continuum, where the photon energy lies between the above  $\hbar\omega$  and  $\hbar\omega + dE_{\text{photon}}$ , with  $\hbar\omega = E_n^{(0)} - E_{n'}^{(0)}$ , where  $n' < n$ . In other words, the discrete state is coupled to the photon continuum with the weighting factor

$$\rho(E_{\text{photon}})dE_{\text{photon}} = \frac{\text{Vol. } \omega^2 d\Omega}{(2\pi)^3 \hbar c^3} dE_{\text{photon}}.$$

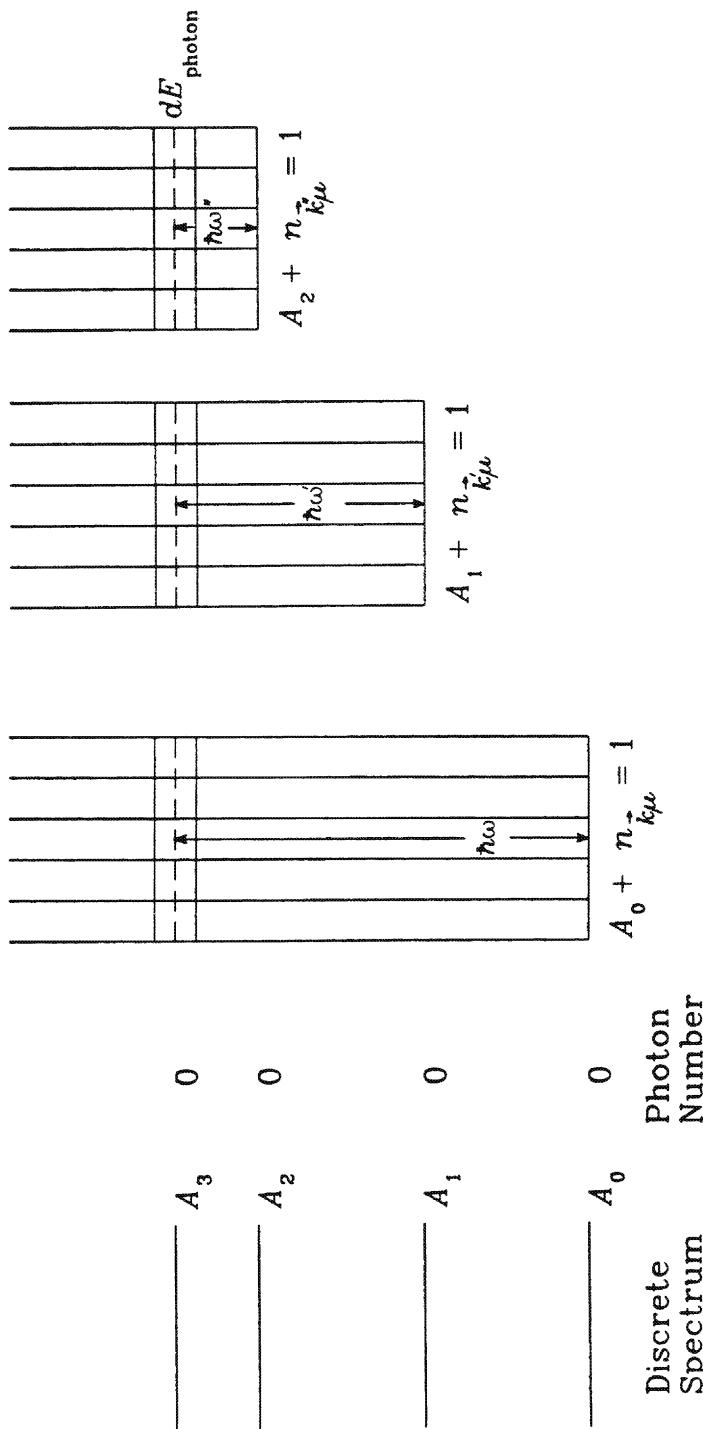


FIGURE 68.1. The degeneracy of excited atomic states and lower atomic states with photon number  $n_{\vec{k}\mu} = 1$ .

If at  $t = 0$  the system is in the state,  $|A_n 0\rangle$ , first-order time-dependent perturbation theory will give us

$$|\psi(t)\rangle = |A_n 0\rangle e^{-\frac{i}{\hbar} E_{A_n}^{(0)} t} + \sum_{n', \vec{k}\mu} |A_{n'}, \vec{k}\mu\rangle c_{n', \vec{k}\mu}(t) e^{-\frac{i}{\hbar} (E_{A_{n'}}^{(0)} + \hbar\omega)t}, \quad (1)$$

where the coefficients,  $c_{n', \vec{k}\mu}(t)$ , can be calculated by time-dependent perturbation theory with the aid of the perturbation diagram of Fig. 68.2(a). Note, however, to first order in perturbation theory, the overlap of this  $|\psi(t)\rangle$  with the  $t = 0$  state  $|A_n 0\rangle$  is still unity

$$\langle A_n 0 | \psi(t) \rangle = 1 \quad (2)$$

because of the orthogonality of the states,  $|A_n 0\rangle$  and  $|A_{n'}, \vec{k}\mu\rangle$ . To get the time evolution of the state  $|A_n 0\rangle$ , i.e., to see how  $c_{n,0}(t)$  evolves with time, we need to go to second-order perturbation theory. With the aid of Fig. 68.2(b) and the diagram rules, we get

$$\begin{aligned} \langle A_n 0 | U(t, 0) | A_n 0 \rangle &= \langle A_n 0 | [1 + U^{(2)}(t, 0)] | A_n 0 \rangle \\ &= e^{-\frac{i}{\hbar} E_{A_n}^{(0)} t} \times 1 + \left( \frac{-i}{\hbar} \right)^2 \sum_{A_I} \sum_{\vec{k}\mu} \int_0^t d\tau_2 e^{-\frac{i}{\hbar} E_{A_n}^{(0)} (t - \tau_2)} \langle A_n 0 | H_{\text{int.}} | A_I, \vec{k}\mu \rangle \\ &\quad \times \int_0^{\tau_2} d\tau_1 e^{-\frac{i}{\hbar} (E_{A_I}^{(0)} + \hbar\omega)(\tau_2 - \tau_1)} \langle A_I, \vec{k}\mu | H_{\text{int.}} | A_n 0 \rangle e^{-\frac{i}{\hbar} (\tau_1 - 0)} \\ &= e^{-\frac{i}{\hbar} E_{A_n}^{(0)} t} \left[ 1 - \frac{1}{\hbar^2} \sum_{A_I} \sum_{\vec{k}\mu} \left| \langle A_n 0 | H_{\text{int.}} | A_I, \vec{k}\mu \rangle \right|^2 \right. \\ &\quad \left. \times \int_0^t d\tau_2 e^{+i(\omega_{nI} - \omega)\tau_2} \int_0^{\tau_2} d\tau_1 e^{-i(\omega_{nI} - \omega)\tau_1} \right], \end{aligned} \quad (3)$$

where we have used the shorthand notation,  $\omega_{nI} = (E_{A_n}^{(0)} - E_{A_I}^{(0)})/\hbar$  and the Schrödinger picture with time-independent  $H_{\text{int.}}$ . The time-dependent integral gives

$$\begin{aligned} F(t) &= \int_0^t d\tau_2 e^{i(\omega_{nI} - \omega)\tau_2} \int_0^{\tau_2} d\tau_1 e^{-i(\omega_{nI} - \omega)\tau_1} \\ &= \frac{i}{(\omega_{nI} - \omega)} \left[ t - \frac{(e^{i(\omega_{nI} - \omega)t} - 1)}{i(\omega_{nI} - \omega)} \right] \\ &= -\frac{[\cos(\omega_{nI} - \omega)t - 1]}{(\omega_{nI} - \omega)^2} + \frac{i}{(\omega_{nI} - \omega)} \left[ t - \frac{\sin(\omega_{nI} - \omega)t}{(\omega_{nI} - \omega)} \right] \\ &= \left[ \frac{\sin^2[\frac{1}{2}(\omega_{nI} - \omega)t]}{2[\frac{1}{2}(\omega_{nI} - \omega)]^2} \right] + \frac{i}{(\omega_{nI} - \omega)} \left[ t - \frac{\sin(\omega_{nI} - \omega)t}{(\omega_{nI} - \omega)} \right] \\ &= \Re[F(t)] + i\Im[F(t)]. \end{aligned} \quad (4)$$

We shall be interested in these time-dependent functions in the limit in which (1)  $t \gg T_{\text{atomic}}$ , where the atomic periods,  $T_{\text{atomic}}$ , are of order  $(10)^{-15}$  sec., (2)  $t \ll t_{\text{laboratory}}$ . For atoms, this means  $t \ll (10)^{-8}$  sec., that is,  $t \ll$  a lifetime of a typical atomic excited state. Because quantities such as  $\omega_{nI}$  and  $\omega$  in the above

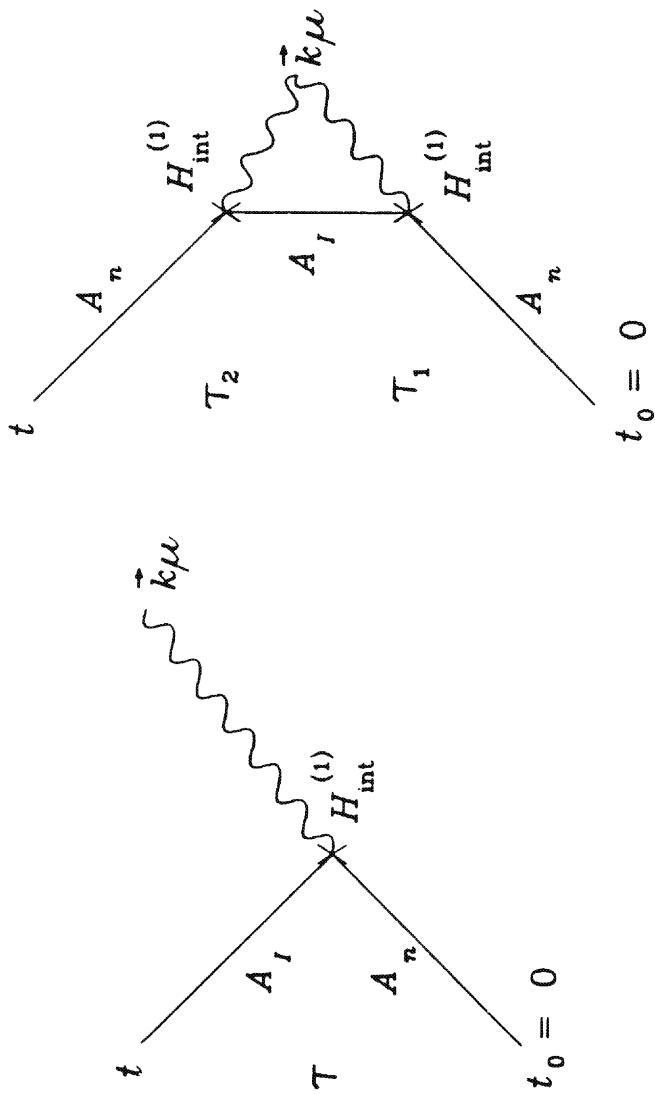


FIGURE 68.2. Perturbation diagrams for eq. (1)–(3).

formulae are of order  $1/T_{\text{atomic}}$ , we shall look at  $F(t)$  in the first limit. For  $t \gg T_{\text{atomic}}$ , we can effectively take  $t \rightarrow \infty$  in  $\Re[F(t)]$  and  $\Im[F(t)]$ . Now, using

$$\begin{aligned} \lim_{t \rightarrow \infty} \left[ t - \frac{\sin(\omega_{nI} - \omega)t}{(\omega_{nI} - \omega)} \right] &\approx t && \text{for } (\omega_{nI} - \omega) \neq 0 \\ &= 0 && \text{for } (\omega_{nI} - \omega) = 0, \end{aligned} \quad (5)$$

we get

$$\begin{aligned} \Re[F(t)] &\approx \frac{1}{(\omega_{nI} - \omega)} t && \text{for } (\omega_{nI} - \omega) \neq 0 \\ \Im[F(t)] &= 0 && \text{for } (\omega_{nI} - \omega) = 0. \end{aligned} \quad (6)$$

$$\begin{aligned} \Re[F(t)] &= \lim_{t \rightarrow \infty} \left[ \frac{\sin^2[\frac{1}{2}(\omega_{nI} - \omega)t]}{2[\frac{1}{2}(\omega_{nI} - \omega)]^2} \right] = \pi t \delta(\omega_{nI} - \omega) \\ &= \pi t \hbar \delta(E_n^{(0)} - E_I^{(0)} - \hbar\omega). \end{aligned} \quad (7)$$

With these results, we get (through second order in perturbation theory)

$$\begin{aligned} \langle A_n 0 | U(t, 0) | A_n 0 \rangle &= \\ e^{-\frac{i}{\hbar} E_{A_n}^{(0)} t} \left[ 1 - \frac{1}{\hbar^2} \pi t \hbar \sum_{A_I, \vec{k}\mu} \delta(E_{A_n}^{(0)} - E_{A_I}^{(0)} - \hbar\omega) \left| \langle A_n 0 | H_{\text{int.}} | A_I, \vec{k}\mu \rangle \right|^2 \right. \\ \left. - \frac{it}{\hbar^2} \sum_{A_I, \vec{k}\mu} \left( \frac{\hbar}{E_{A_n}^{(0)} - E_{A_I}^{(0)} - \hbar\omega} \right) \left| \langle A_n 0 | H_{\text{int.}} | A_I, \vec{k}\mu \rangle \right|^2 \right], \end{aligned} \quad (8)$$

where the prime superscript on the sum of the imaginary part means:  $\hbar\omega \neq (E_{A_n}^{(0)} - E_{A_I}^{(0)})$ . Recall  $\Im[F(t)] = 0$ , when  $(\omega_{nI} - \omega) = 0$  [see eq. (6)]. Now, we will also use

$$\begin{aligned} U(t, 0) | A_n 0 \rangle &= e^{-\frac{i}{\hbar} E_{A_n}^{(0)} t} e^{-\frac{i}{\hbar} \Delta E_{A\mu} t} e^{-\frac{\Gamma_{A_n}}{2\hbar} t} | A_n 0 \rangle + \dots \\ &\approx e^{-\frac{i}{\hbar} E_{A_n}^{(0)} t} \left( 1 - i \frac{\Delta E_{A_n}}{\hbar} t - \frac{\Gamma_{A_n}}{2\hbar} t + \dots \right) | A_n 0 \rangle + \dots, \end{aligned} \quad (9)$$

where the final  $+ \dots$  in this relation stands for the presence of atomic terms other than  $A_n$ . In this equation, we have used requirement (2) above,  $t \ll t_{\text{lab.}}$ . Comparing with eq. (8), we get the level shift

$$\Delta E_{A_n} = \sum_{A_I, \vec{k}\mu} \left( \frac{1}{(E_{A_n}^{(0)} - E_{A_I}^{(0)} - \hbar\omega)} \right) \left| \langle A_n 0 | H_{\text{int.}} | A_I, \vec{k}\mu \rangle \right|^2, \quad (10)$$

and the width

$$\Gamma_{A_n} = 2\pi \sum_{A_I, \vec{k}\mu} \left( \frac{1}{(E_{A_n}^{(0)} - E_{A_I}^{(0)} - \hbar\omega)} \right) \left| \langle A_n 0 | H_{\text{int.}} | A_I, \vec{k}\mu \rangle \right|^2. \quad (11)$$

In these formulae, the sum,  $\sum_{\vec{k}}$ , must be replaced by integrals over the continuous photon spectrum and over the possible angular directions of the photons of a

particular energy,

$$\begin{aligned} \sum_{\vec{k}\mu} &\rightarrow \sum_{\mu=\pm 1} \int \int d\Omega \int dE_{\text{photon}} \rho(E_{\text{photon}}) \\ &= \sum_{\mu=\pm 1} \int \int d\Omega \int dE_{\text{photon}} \frac{\text{Vol.}}{(2\pi)^3} \frac{\omega^2}{\hbar c^3}. \end{aligned}$$

For the width,  $\Gamma_{A_n}$ , the energy Dirac delta function will limit the photon energies to values  $\hbar\omega = (E_{A_n}^{(0)} - E_{A_{n'}}^{(0)})$ , with  $n' < n$ . Thus, only a finite number of terms are involved. For the level shift, however, even though no zero denominator difficulties exist, the integral over photon energies and sum over atomic states,  $A_l$ , should go to  $\infty$  energies and should therefore be treated by relativistic quantum theory. Nevertheless, H. A. Bethe in 1947 used the above formula with an arbitrary cutoff of  $\hbar\omega \approx mc^2$  and obtained remarkable agreement with the then recently observed upward “Lamb shift” of the  $2s_{\frac{1}{2}}$  level relative to the  $2p_{\frac{1}{2}}$  level in hydrogen ( $\Delta E_{A_n} \neq 0$  essentially only for the  $l = 0$  states). The level shift formula also involves a mass renormalization. Even a free electron has an energy  $p^2/2m_{\text{obs}}$ , where the bare mass has to be renormalized because of the presence of the virtual photons of type  $\vec{k}\mu$  to yield the observed mass,  $m_{\text{obs}}$ . [Because both the correct relativistic treatment and the renormalization are best treated in quantum field theory, we defer this subject to the quantum field theory course. For a good account of Bethe’s treatment, however, see Section 2.8 in J. J. Sakurai, *Advanced Quantum Mechanics*, (1967).]

The width,  $\Gamma_{A_n}$ , is given by

$$\frac{\Gamma_{A_n}}{\hbar} = \frac{2\pi}{\hbar} \sum_{n' < n} \sum_{\mu=\pm 1} \int \int d\Omega \frac{\text{Vol.}}{(2\pi)^3} \frac{\omega_{nn'}^2}{\hbar c^3} \frac{c^2}{\text{Vol.} \omega_{nn'}} \left| \langle A_n | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}'_\mu) | A_{n'} \rangle \right|^2. \quad (12)$$

Again, using

$$\frac{\vec{p}_i}{m_i c} = \frac{i}{\hbar c} [H_{\text{atom}}^{(0)}, \vec{r}_i], \quad (13)$$

we convert

$$\begin{aligned} \left| \langle A_n | \sum_i \frac{e_i}{m_i c} (\vec{p}_i \cdot \vec{e}'_\mu) | A_{n'} \rangle \right|^2 &= \left( \frac{\omega_{nn'}}{c} \right)^2 \left| \langle A_n | \sum_i e_i \vec{r}_i \cdot \vec{e}'_\mu | A_{n'} \rangle \right|^2 = \\ \left( \frac{\omega_{nn'}}{c} \right)^2 \sum_{m,m'} D_{m\mu}^{1*} D_{m'\mu}^1 \langle A_n | \sum_i e_i \vec{r}_i \cdot \vec{e}_m | A_{n'} \rangle \langle A_n | \sum_i e_i \vec{r}_i \cdot \vec{e}_{m'} | A_{n'} \rangle^*, \end{aligned} \quad (14)$$

and, again, with the use of

$$\sum_{\mu=\pm 1} \int \int d\Omega D_{m\mu}^{1*} D_{m'\mu}^1 = \frac{8\pi}{3} \delta_{mm'}, \quad (15)$$

we have

$$\frac{\Gamma_{A_n}}{\hbar} = \frac{4}{3} \sum_{n' < n} \frac{\omega_{nn'}^3}{\hbar c^3} \sum_{m=\pm 1,0} \left| \langle A_n | \vec{\mu}_m^{(\text{el.})} | A_{n'} \rangle \right|^2$$

$$= \sum_{n' < n} \left[ \frac{1}{(\tau_{\text{E1}})_{A_n \rightarrow A_{n'}}} \right]. \quad (16)$$

Here,  $(1/\tau_{A_n \rightarrow A_{n'}})$  gives the probability per second that the atom in state  $n$  make a transition to a lower state  $n'$  via the spontaneous emission of a photon, see eq. (24) of Chapter 63. Also,

$$|\psi(t)\rangle = c_{A_n}(t)|A_n\rangle = e^{-\frac{i}{\hbar}(E_{A_n}^{(0)} + \Delta E_{A_n})t} e^{-\frac{\Gamma_{A_n}}{2\hbar}t}|A_n\rangle. \quad (17)$$

Further, a Fourier analysis of this time-dependent function gives a level centered at position,  $E_{A_n}^{(0)} + \Delta E_{A_n}$ , with width,  $\Gamma_{A_n}$ . The decay of the  $n^{\text{th}}$  level is given by

$$|c_{A_n}(t)|^2 = e^{-\frac{\Gamma_{A_n}}{\hbar}t} = e^{-\frac{t}{\tau_n}}, \quad (18)$$

with

$$\frac{1}{\tau_n} = \sum_{n' < n} \left[ \frac{1}{\tau_{A_n \rightarrow A_{n'}}} \right]. \quad (19)$$

## Problems

- 40.** In a diatomic molecule, the scattering matrix sums (for elastic scattering)

$$g_{\beta'\gamma} = \sum_{A_I} \left[ \frac{\langle A_i | (\vec{\mu}^{(\text{el.})} \cdot \vec{e}_{\beta'}) | A_I \rangle \langle A_I | (\vec{\mu}^{(\text{el.})} \cdot \vec{e}_\gamma) | A_i \rangle}{E_{A_i}^{(0)} + \hbar\omega - E_{A_I}^{(0)}} \right. \\ \left. + \frac{\langle A_i | (\vec{\mu}^{(\text{el.})} \cdot \vec{e}_\gamma) | A_I \rangle \langle A_I | (\vec{\mu}^{(\text{el.})} \cdot \vec{e}_{\beta'}) | A_i \rangle}{E_{A_i}^{(0)} - \hbar\omega - E_{A_I}^{(0)}} \right]$$

can be replaced by the approximately frequency-independent polarizability components,  $\alpha_{\beta'\gamma}$ , i.e.,  $g_{\beta'\gamma} \rightarrow \alpha_{\beta'\gamma}$ . (Note, the mixed components used here:  $\beta'$  refers to the primed axes of the scattered photon,  $\gamma$  to the unprimed incident photon coordinate system, where the  $\vec{k}$  of the incident photon is in the  $z$  direction, and the  $\vec{k}'$  of the scattered photon is in the  $z'$  direction.) In the molecular symmetry coordinate system, with  $z''$  parallel to the diatomic molecule axis, with

$$\vec{e}_{z''} = \vec{e}_x \sin \theta \cos \phi + \vec{e}_y \sin \theta \sin \phi + \vec{e}_z \cos \theta,$$

$$\vec{e}_{x''} = \vec{e}_x \cos \theta \cos \phi + \vec{e}_y \cos \theta \sin \phi - \vec{e}_z \sin \theta,$$

$$\vec{e}_{y''} = -\vec{e}_x \sin \phi + \vec{e}_y \cos \phi,$$

the polarizability tensor has the simple diagonal form:  $\alpha_{x''x''} = \alpha_{y''y''} = \alpha_\perp$ ;  $\alpha_{z''z''} = \alpha_\parallel$ ,

$$\alpha_{\beta''\gamma''} = \begin{pmatrix} \alpha_\perp & 0 & 0 \\ 0 & \alpha_\perp & 0 \\ 0 & 0 & \alpha_\parallel \end{pmatrix}.$$

To gain information about the molecular polarizabilities,  $\alpha_{\perp}$  and  $\alpha_{\parallel}$ , the polarizations of the scattered photons are measured, usually in an arrangement with  $\theta' = \frac{\pi}{2}$ ,  $\phi' = 0$ , i.e., scattered photon in the  $x$  direction, incident photon in the  $z$  direction. For this arrangement, show the “degree of polarization” ( $d\sigma_{\parallel}/d\sigma_{\perp}$ ) has the value

$$\frac{d\sigma_{\parallel}}{d\sigma_{\perp}} = \frac{(\alpha_{\parallel} - \alpha_{\perp})^2}{3\alpha_{\parallel}^2 + 8\alpha_{\perp}^2 + 4\alpha_{\parallel}\alpha_{\perp}},$$

for the case when the incident light is polarized in the  $y$  direction and

$$\frac{d\sigma_{\parallel}}{d\sigma_{\perp}} = \frac{2(\alpha_{\parallel} - \alpha_{\perp})^2}{4\alpha_{\parallel}^2 + 9\alpha_{\perp}^2 + 2\alpha_{\parallel}\alpha_{\perp}},$$

for the case of unpolarized incident light.

Note that you have to average over all possible molecular orientations.

In the above,  $d\sigma_{\parallel}$  gives the scattering cross section for the scattered photons polarized parallel to the scattering plane, defined by the vectors  $\vec{k}$  of the incident beam and  $\vec{k}'$  of the scattered beam; i.e., in our arrangement,  $d\sigma_{\parallel}$  is for the scattered photon polarized in the  $z$  direction.  $d\sigma_{\perp}$  gives the scattering cross section for the scattered photon polarized perpendicular to the scattering plane; therefore, in our arrangement,  $d\sigma_{\perp}$  is for the scattered photon polarized in the  $y$  direction.

**41.** For the Raman scattering from diatomic molecules involving rotational excitations, the  $g_{\beta'\gamma}$  of problem 40. can be replaced by the rotational matrix elements of the polarizability tensor components:

$$g_{\beta'\gamma} \rightarrow \langle J_f M_f | \alpha_{\beta'\gamma} | J_i M_i \rangle.$$

Recall, for the diatomic molecule rigid rotator,

$$E_J = \frac{\hbar^2}{2I_e} J(J+1), \quad \text{and} \quad \psi_{JM}(\theta, \phi) = Y_{JM}(\theta, \phi),$$

where  $\theta$  and  $\phi$  are the polar and azimuth angles giving the orientation of the molecular symmetry axis relative to the laboratory frame and  $I_e$  is the moment of inertia of the diatomic molecule in its equilibrium configuration,  $I_e = \mu r_e^2$ .

Calculate the cross sections,  $d\sigma_{\parallel}$  and  $d\sigma_{\perp}$ , as functions of  $\alpha_{\perp}$  and  $\alpha_{\parallel}$ , again, for the special case,  $\theta' = \frac{\pi}{2}$ ,  $\phi' = 0$ , as in problem 40, i.e., scattered photon in the  $x$  direction, incident photon in the  $z$  direction. Assume unpolarized incident light. Calculate these cross sections for both the so-called Stokes process, where the molecule absorbs energy (transition  $J \rightarrow J+2$ ), so  $\hbar\omega' < \hbar\omega$ , and the anti-Stokes process (transition  $J \rightarrow J-2$ ), so  $\hbar\omega' > \hbar\omega$ . Prove only Raman transitions with  $\Delta J = \pm 2$  can occur; keeping in mind transitions with  $\Delta J = 0$  lead to elastic scattering processes.

Raman scattering is particularly important in homonuclear diatomic molecules, such as  $H_2$  and  $N_2$ , which have no permanent electric dipole moments and hence no rotational absorption spectra. Also, the differential cross section for each Raman transition,  $J \rightarrow J'$ , depends on the number of molecules in the initial rotational

state,  $J$ .

$$N_J = N_0 \frac{(2J+1)g_{\text{nuclear}} e^{-E_J/kT}}{\sum_J (2J+1)g_{\text{nuclear}} e^{-E_J/kT}}$$

for a gas sample in thermal equilibrium, where  $N_0$  is the total number of molecules per unit volume. Taking account of the identity of the two spin  $\frac{1}{2}$  protons in the  $H_2$  diatomic molecule, and the identity of the two spin 1 nuclei,  $^{14}N$ , in the diatomic molecule  $N_2$ , show the nuclear spin weights,  $g_{\text{nuclear}}$ , are  $J$ -dependent as follows:

$$g_{\text{nuclear}} = 1 \text{ for even } J, \quad g_{\text{nuclear}} = 3 \text{ for odd } J, \quad \text{in } H_2,$$

$$g_{\text{nuclear}} = 6 \text{ for even } J, \quad g_{\text{nuclear}} = 3 \text{ for odd } J, \quad \text{in } N_2.$$

**42.** For the elastic scattering of an unpolarized incident beam of high-frequency photons from an atom (Thomson limit), calculate the degree of polarization ( $d\sigma_{||}/d\sigma_{\perp}$ ) as a function of scattering angle  $\theta$ .  $d\sigma_{||}$  gives the differential cross section for photons with their linear polarization vector lying in the scattering plane defined by  $\vec{k}$  and  $\vec{k}'$ , and  $d\sigma_{\perp}$  gives the differential cross sections for photons linearly polarized with their polarization vector perpendicular to the scattering plane.

**43.** Calculate the resonance fluorescence cross section for the scattering of unpolarized Lyman  $\alpha$  radiation from cold hydrogen (in its ground state). Show, in particular, at exact resonance,

$$\hbar\omega = (E_{n=2} - E_{n=1}) = \frac{3e^2}{8a_0},$$

the reduced electric dipole moment matrix element drops out of the expression for the cross section, and give an expression for the cross section in terms of the wave length  $\lambda$  of Lyman  $\alpha$ .

**44.** The most-probable decay mode for the  $2S_{\frac{1}{2}}$  state of hydrogen involves the simultaneous emission of two photons, with  $\hbar\omega + \hbar\omega' = E_{2S_{\frac{1}{2}}} - E_{1S_{\frac{1}{2}}}$ .

Convince yourself first the magnetic dipole single-photon emission probability for this transition is equal to zero, and the sequential decay via the emission of an electric dipole photon from the  $2S_{\frac{1}{2}}$  into the  $2P_{\frac{1}{2}}$  level with subsequent fast emission of the electric dipole photon for the transition  $2P_{\frac{1}{2}} \rightarrow 1S_{\frac{1}{2}}$  is very improbable because of the low frequency of 1057 Mc/sec. corresponding to the Lamb shift that has raised the  $2S_{\frac{1}{2}}$  level above the  $2P_{\frac{1}{2}}$  level.

Derive a formula for the probability of double photon emission with one photon in the frequency range  $d\omega = 2\pi d\nu$  about  $\omega = 2\pi\nu$ . Show, in particular,

$$\left[ \frac{\text{Transition Probability}}{\text{second}} \right]_{2s \rightarrow 1s + \hbar\omega' + \hbar\omega} = \frac{2^{10} e^4 \pi^6 v^3 v'^3 d\nu}{3^3 c^6} \times$$

$$\left| \sum_{n=2}^{\infty} I_{1sn} I_{np2s} \left( \frac{1}{E_n - E_2 + \hbar\omega} + \frac{1}{E_n - E_2 + \hbar\omega'} \right) \right|$$

$$+ \text{similar } \int \text{ over continuum p-states} \Bigg|^2,$$

where  $I_{1snp}$  and  $I_{np2s}$  are the radial integrals

$$I_{1snp} = \int_0^\infty dr r^2 R_{1s}(r) r R_{np}(r), \quad I_{np2s} = \int_0^\infty dr r^2 R_{np}(r) r R_{2s}(r),$$

involving discrete excited states. See Chapter 35 for the needed integrals. For the similar contribution from the continuum states with  $l = 1$ , for which the discrete sum has to be replaced by the continuous integral involving positive energies from  $0 \rightarrow \infty$ , see the mathematical appendix to Chapter 42. The total transition probability for the atom to make the transition,  $2s \rightarrow 1s$ , will involve an integration over all frequencies,  $\nu$ , with the restriction,

$$\nu + \nu' = \frac{3}{8} \frac{1}{\hbar} \frac{e^2}{a_0},$$

with  $\nu$  ranging from zero to

$$\nu_{\max.} = \frac{3}{8} \frac{1}{\hbar} \frac{e^2}{a_0}.$$

In making this integral over all allowed frequencies,  $\nu$ , we have to remember a particular photon frequency,  $\nu_0$ , can occur in two ways: either  $\nu = \nu_0$  or  $\nu' = \nu_0$ . Thus, to avoid double counting, we have

$$\left[ \frac{\text{Transition Probability}}{\text{second}} \right]_{2s \rightarrow 1s} = \frac{1}{(\tau = \text{meanlife})} = \frac{1}{2} \int_0^{\nu_{\max.}} d\nu A(\nu).$$

Finally, introducing dimensionless quantities

$$y = \frac{\hbar\omega}{\left(\frac{3e^2}{8a_0}\right)}, \quad (1 - y) = \frac{\hbar\omega'}{\left(\frac{3e^2}{8a_0}\right)},$$

and dimensionless integrals, such as  $\mathcal{I}_{1snp} \equiv I_{1snp}/a_0$ , show

$$\begin{aligned} \frac{1}{\tau} &= \frac{1}{2} \int_0^1 dy A(y) = \frac{3^2}{2^{13}} \frac{c}{\pi a_0} \left( \frac{e^2}{\hbar c} \right)^7 \int_0^1 dy y^3 (1 - y)^3 \\ &\times \left| \sum_{n=2}^{\infty} \mathcal{I}_{1snp} \mathcal{I}_{np2s} \left( \frac{1}{\left[ \frac{1}{3} - \frac{4}{3n^2} + y \right]} + \frac{1}{\left[ \frac{4}{3} - \frac{4}{3n^2} - y \right]} \right) + \text{continuum contribution} \right|^2. \end{aligned}$$

Make a “guesstimate” for the lifetime,  $\tau$ , by evaluating the most important terms of the discrete sum, and show this  $\tau$  is much smaller, by a factor of order  $\sim 10^9$ , than the lifetime for the cascade  $2s_{\frac{1}{2}} \rightarrow 2p_{\frac{1}{2}} \rightarrow 1s_{\frac{1}{2}}$ .

# Introduction to Relativistic Quantum Mechanics

# Dirac Theory: Relativistic Quantum Theory of Spin- $\frac{1}{2}$ Particles

## A Four-Vector Conventions

In relativistic theories, it will be useful to use a four-vector space-time formulation. We shall use the conventions of J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics*, New York: McGraw-Hill, 1964. (These are also the conventions used by J. D. Jackson, *Classical Electrodynamics*, New York: John Wiley, 1967.) We shall therefore use covariant and contravariant vector notation, using Greek letters for 4-D quantities and Latin letters for 3-D quantities, with a metric tensor

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

The time-space four-vector is given by

$$x^\mu = (x^0, x^i) = (ct, x^1, x^2, x^3) = (ct, \vec{r}),$$

whereas

$$x_\mu = g_{\mu\nu} x^\nu = (x_0, x_i) = (x_0, -x^i) = (ct, -\vec{r}),$$

where we use summation convention for repeated indices. The scalar invariant length in four-space is

$$x^\mu x_\mu = g_{\mu\nu} x^\mu x^\nu = g^{\mu\nu} x_\mu x_\nu = (ct)^2 - (\vec{r} \cdot \vec{r}). \quad (1)$$

The four-momentum vector has covariant and contravariant components

$$P_\mu = -\frac{\hbar}{i} \frac{\partial}{\partial x^\mu} = \left( -\frac{\hbar}{ic} \frac{\partial}{\partial t}, -\frac{\hbar}{i} \frac{\partial}{\partial x^i} \right) = \left( -\frac{\hbar}{ic} \frac{\partial}{\partial t}, -\frac{\hbar}{i} \vec{\nabla} \right),$$

and

$$P^\mu = -\frac{\hbar}{i} \frac{\partial}{\partial x_\mu} = \left( -\frac{\hbar}{ic} \frac{\partial}{\partial t}, +\frac{\hbar}{i} \vec{\nabla} \right),$$

where

$$P^\mu P_\mu = \left( \frac{E}{c} \right)^2 - (\vec{p} \cdot \vec{p}). \quad (2)$$

## B The Klein–Gordon Equation

In the early chapters, we saw that the relation between energy and momentum for a free particle

$$\frac{E^2}{c^2} - (\vec{p} \cdot \vec{p}) = m^2 c^2, \quad (3)$$

which becomes the dispersion relation in wave theory, leads via

$$E \rightarrow -\frac{\hbar}{i} \frac{\partial}{\partial t}; \quad \vec{p} \rightarrow \frac{\hbar}{i} \vec{\nabla}$$

to the Klein–Gordon equation

$$\nabla^2 \Psi - \frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2} - \frac{m^2 c^2}{\hbar^2} \Psi = 0 \quad (4)$$

and would lead to a conserved probability density,  $W$ , and probability density current,  $\vec{S}$ , with

$$\frac{\partial W}{\partial t} + (\vec{\nabla} \cdot \vec{S}) = 0, \quad (5)$$

with

$$\vec{S} = \frac{\hbar}{2mi} (\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^*), \quad \text{and} \quad W = -\frac{\hbar}{2mc^2} (\Psi^* \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \Psi^*}{\partial t}), \quad (6)$$

with a real but not positive-definite probability density,  $W$ . It was this seeming difficulty that led Dirac to an alternative approach. (Today, we know the Klein–Gordon equation is a correct relativistic wave equation for spin-0 particles.)

## C Dirac's Reasoning: Historical Approach

Because of the seeming difficulty with the Klein–Gordon equation, Dirac looked for an alternative. He assumed the basic equations might be first order in both space

and time derivatives, so  $ct$  and  $x, y, z$ , appear on an equal footing. He was guided by Maxwell's equations, which are Lorentz-covariant and first order in time and space derivatives, but involve not one scalar field,  $\Psi$ , but six fields,  $E_1, E_2, E_3, B_1, B_2, B_3$ , connected by six of the equations. He, therefore, postulated the relativistic equations have  $N$  fields,  $\psi_\rho$ , with  $\rho = 1, \dots, N$ , such that

$$1. \quad W = \sum_{\rho=1}^N |\psi_\rho|^2, \quad (7)$$

leading to a positive-definite probability density. In addition, he assumed the basic equations are first-order equations, and the Klein-Gordon equation is then a consequence of these first-order equations, where, with  $\rho = 1, \dots, N$ ,

$$2. \quad -\frac{\hbar}{i} \frac{1}{c} \frac{\partial \psi_\rho}{\partial t} - \frac{\hbar}{i} (\alpha_x)_{\rho\sigma} \frac{\partial \psi_\sigma}{\partial x} - \frac{\hbar}{i} (\alpha_y)_{\rho\sigma} \frac{\partial \psi_\sigma}{\partial y} - \frac{\hbar}{i} (\alpha_z)_{\rho\sigma} \frac{\partial \psi_\sigma}{\partial z} - mc\beta_{\rho\sigma} \psi_\sigma = 0, \quad (8)$$

or

$$-\frac{\hbar}{i} \frac{\partial \psi_\rho}{\partial t} = (H)_{\rho\sigma} \psi_\sigma, \quad \text{with } (H)_{\rho\sigma} = c\vec{\alpha}_{\rho\sigma} \cdot \frac{\hbar}{i} \vec{\nabla} + mc^2 \beta_{\rho\sigma}, \quad (9)$$

where summation convention is assumed for repeated Greek indices, the sum running from 1 to  $N$ , and  $(\alpha_x)_{\rho\sigma}, (\alpha_y)_{\rho\sigma}, (\alpha_z)_{\rho\sigma}, \beta_{\rho\sigma}$ , are  $N \times N$  matrices, independent of space-time variables. These are to be chosen so the Klein-Gordon equation follows and the probability interpretation is a valid one.

3. Theorem I. If the the  $\vec{\alpha}$ , and  $\beta$  are hermitian matrices, and if  $W$  is given by eq. (7), probability is conserved: If  $\alpha_x = \alpha_x^\dagger, \alpha_y = \alpha_y^\dagger, \alpha_z = \alpha_z^\dagger, \beta = \beta^\dagger$ ,

$$\frac{d}{dt} \int_{\text{all space}} d\vec{r} \ W = 0. \quad (10)$$

Multiplying the  $\rho^{th}$  Dirac equation by  $\psi_\rho^*$ , the complex conjugate of the  $\rho^{th}$  equation by  $\psi_\rho$ , and summing over the index  $\rho$ :

$$\begin{aligned} & \psi_\rho^* \left[ \frac{1}{c} \frac{\partial \psi_\rho}{\partial t} + \vec{\alpha}_{\rho\sigma} \cdot \vec{\nabla} \psi_\sigma + \frac{imc}{\hbar} \beta_{\rho\sigma} \psi_\sigma \right] \\ & + \psi_\rho \left[ \frac{1}{c} \frac{\partial \psi_\rho^*}{\partial t} + \vec{\alpha}_{\rho\sigma}^* \cdot \vec{\nabla} \psi_\sigma^* - \frac{imc}{\hbar} \beta_{\rho\sigma}^* \psi_\sigma^* \right] = 0. \end{aligned} \quad (11)$$

Now, using the hermiticity of the matrices in the second term,

$$\vec{\alpha}_{\rho\sigma}^* = \vec{\alpha}_{\sigma\rho}, \quad \beta_{\rho\sigma}^* = \beta_{\sigma\rho},$$

and renaming dummy indices  $\rho \leftrightarrow \sigma$  in double sums, such as  $\psi_\rho \beta_{\rho\sigma}^* \psi_\sigma^* = \psi_\rho \beta_{\sigma\rho} \psi_\sigma^* = \psi_\rho^* \beta_{\rho\sigma} \psi_\sigma$ , we are led to a continuity equation

$$\begin{aligned} & \frac{1}{c} \frac{\partial (\psi_\rho^* \psi_\rho)}{\partial t} + \vec{\nabla} \cdot (\psi_\rho^* \vec{\alpha}_{\rho\sigma} \psi_\sigma) = 0 \\ \text{or} \quad & \frac{\partial W}{\partial t} + \vec{\nabla} \cdot \vec{S} = 0, \end{aligned} \quad (12)$$

with

$$W = \psi_\rho^* \psi_\rho \quad \left( \equiv \sum_\rho |\psi_\rho|^2 \right), \quad \vec{S} = c(\psi_\rho^* \vec{\alpha}_{\rho\sigma} \psi_\sigma). \quad (13)$$

If we assume the  $\psi_\rho$  go to zero sufficiently fast as  $r \rightarrow \infty$ ,  $(\vec{S} \cdot \vec{n}) \rightarrow 0$  on the surface at  $\infty$ , so Gauss's theorem applied to the divergence term gives us the desired result.

4. Theorem II. If the matrices,  $\vec{\alpha}$ ,  $\beta$ , satisfy the Dirac conditions

$$\begin{aligned} \alpha_l \alpha_k + \alpha_k \alpha_l &= 2\delta_{lk} \mathbf{1}, \\ \alpha_l \alpha_k + \alpha_k \alpha_l &= 0 \text{ for } l \neq k, \quad (\alpha_l)^2 = \mathbf{1} \text{ for } l = x, y, z, \\ \alpha_l \beta + \beta \alpha_l &= 0, \quad \text{and } \beta^2 = \mathbf{1}, \end{aligned} \quad (14)$$

each of the  $\psi_\rho$  satisfies the Klein-Gordon equation. (In these relations,  $\mathbf{1}$  is the  $N \times N$  unit matrix.) To prove this theorem, let us change to full matrix notation, and let  $\psi$  be an  $N \times 1$ -matrix with  $N$  rows and a single column, whereas  $\beta$  and the  $\alpha_l$  are  $N \times N$  matrices. As a specific example,

$$\beta \psi = \begin{pmatrix} \beta_{11} & \beta_{12} & \cdots & \beta_{1N} \\ \beta_{21} & \beta_{22} & \cdots & \beta_{2N} \\ \vdots & \vdots & \cdots & \vdots \\ \beta_{N1} & \beta_{N2} & \cdots & \beta_{NN} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}. \quad (15)$$

Let us then act with the operator

$$\left( -\frac{1}{c} \frac{\partial}{\partial t} + \vec{\alpha} \cdot \vec{\nabla} + \frac{imc}{\hbar} \beta \right)$$

on the Dirac equation

$$+\frac{1}{c} \frac{\partial \psi}{\partial t} + \vec{\alpha} \cdot \vec{\nabla} \psi + \frac{imc}{\hbar} \beta \psi = 0$$

to obtain

$$\begin{aligned} &-\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + (\vec{\alpha} \cdot \vec{\nabla})(\vec{\alpha} \cdot \vec{\nabla} \psi) - \frac{m^2 c^2}{\hbar^2} \beta^2 \psi + \frac{imc}{\hbar} (\alpha_l \beta + \beta \alpha_l) \frac{\partial \psi}{\partial x^l} \\ &+ \frac{1}{c} \left( \vec{\alpha} \cdot \vec{\nabla} \frac{\partial \psi}{\partial t} - \frac{\partial}{\partial t} \vec{\alpha} \cdot \vec{\nabla} \psi \right) + \frac{imc}{\hbar} \left( \beta \frac{\partial \psi}{\partial t} - \frac{\partial \beta \psi}{\partial t} \right) \\ &= -\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + \left( \alpha_x^2 \frac{\partial^2 \psi}{\partial x^2} + \alpha_y^2 \frac{\partial^2 \psi}{\partial y^2} + \alpha_z^2 \frac{\partial^2 \psi}{\partial z^2} \right) - \frac{m^2 c^2}{\hbar^2} \beta^2 \psi \\ &+ (\alpha_x \alpha_y + \alpha_y \alpha_x) \frac{\partial^2 \psi}{\partial x \partial y} + (\alpha_x \alpha_z + \alpha_z \alpha_x) \frac{\partial^2 \psi}{\partial x \partial z} + (\alpha_y \alpha_z + \alpha_z \alpha_y) \frac{\partial^2 \psi}{\partial y \partial z} \\ &= -\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + \nabla^2 \psi - \frac{m^2 c^2}{\hbar^2} \psi = 0, \end{aligned} \quad (16)$$

where we have used the Dirac relations of eq. (14) in the last step.

5. Theorem III. There is "essentially" only one set of matrices,  $\vec{\alpha}$ ,  $\beta$ , which satisfy the Dirac relations.

(a). The matrices must be at least  $4 \times 4$  matrices. A specific solution to the Dirac relations is:

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (17)$$

where  $\mathbf{1}$  is the  $2 \times 2$  unit matrix, and  $0$  are  $2 \times 2$  zero matrices, and where the  $\vec{\sigma}$  are the  $2 \times 2$  Pauli spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (18)$$

For example,

$$\begin{aligned} \alpha_i \alpha_j + \alpha_j \alpha_i &= \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \\ &= \begin{pmatrix} (\sigma_i \sigma_j + \sigma_j \sigma_i) & 0 \\ 0 & (\sigma_i \sigma_j + \sigma_j \sigma_i) \end{pmatrix} = 2\delta_{ij}\mathbf{1}, \end{aligned} \quad (19)$$

where we have used

$$\sigma_i \sigma_j = \delta_{ij}\mathbf{1} + i\epsilon_{ijk}\sigma_k. \quad (20)$$

(b) The matrices are the specific ones shown through eq. (17) or are related to these by a similarity transformation, with  $4 \times 4$  matrices  $S$ . Thus, with

$$\vec{\alpha}' = S\vec{\alpha}S^{-1}, \quad \beta' = S\beta S^{-1},$$

we would have the Dirac equations

$$\begin{aligned} \frac{1}{c} \frac{\partial \psi}{\partial t} + \vec{\alpha}' \cdot \vec{\nabla} \psi + \frac{imc}{\hbar} \beta' \psi &= 0 \\ = S \left[ \frac{1}{c} \frac{\partial (S^{-1} \psi)}{\partial t} + \vec{\alpha} \cdot \vec{\nabla} (S^{-1} \psi) + \frac{imc}{\hbar} \beta (S^{-1} \psi) \right] &= 0. \end{aligned} \quad (21)$$

These equations would be a linear combination of the old equations, applied to a linear combinations of the old  $\psi_\rho$ .

(c) Higher dimensional realizations, such as  $8 \times 8$  or  $12 \times 12$ , could have been obtained via a blowup process. This, however, would again not have led to anything new. It would merely be a rewriting of the original equations, two or three times over.

## D The Dirac Equation in Four-Dimensional Notation

So far, we have treated the space and time derivative terms of the Dirac equation on a separate footing. We can achieve a more uniform 4-D notation, if we left-multiply the equation by  $\beta$  to get

$$\frac{\beta}{c} \frac{\partial \psi}{\partial t} + (\beta \vec{\alpha}) \cdot \vec{\nabla} \psi + \frac{imc}{\hbar} \psi = 0, \quad (22)$$

and if we define

$$\gamma^0 = \beta, \quad \gamma^i = \beta \vec{\alpha}, \quad \text{with } i = 1, 2, 3; \text{ for } \alpha_x, \alpha_y, \alpha_z, \quad (23)$$

the Dirac equation then has the form

$$\gamma^\mu \frac{\partial \psi}{\partial x^\mu} + \frac{imc}{\hbar} \psi = 0. \quad (24)$$

In terms of the  $\gamma^\mu$ , with  $\mu = 0, 1, 2, 3$ , the Dirac relations can be written in terms of one equation

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu} \mathbf{1}. \quad (25)$$

Note:  $(\gamma^\mu)^2 = g^{\mu\mu} \mathbf{1}$  for the special case  $\mu = \nu$ , so

$$(\gamma^0)^2 = \mathbf{1}, \quad (\gamma^i)^2 = -\mathbf{1}. \quad (26)$$

If we want to diagonalize a particular  $\gamma^\mu$  via a similarity transformation with a matrix  $S$ , the eigenvalues must be either +1 or -1 (for  $\mu = 0$ ), or +i or -i (for  $\mu = 1, 2, 3$ ). Also, from the Dirac relation with  $\mu \neq \nu$ , we get by left-multiplication with a particular  $\gamma^\mu$

$$\gamma^\nu = -(\gamma^\mu \gamma^\nu \gamma^\mu) g^{\mu\mu}, \quad \text{for } \mu \neq \nu. \quad (27)$$

(For the moment, there is *no* summation convention for repeated indices.) Taking the trace of this relation, we have

$$\begin{aligned} \text{Trace}(\gamma^\nu) &= -[\text{Trace}(\gamma^\mu \gamma^\nu \gamma^\mu)] g^{\mu\mu} = -[\text{Trace}(\gamma^\nu (\gamma^\mu)^2)] g^{\mu\mu} \\ &= -[\text{Trace}(\gamma^\nu)] (g^{\mu\mu})^2 = -\text{Trace}(\gamma^\nu). \end{aligned} \quad (28)$$

Thus,

$$\text{Trace}(\gamma^\nu) = 0. \quad (29)$$

Because the eigenvalues of a particular  $\gamma^\nu$  are either +1 or -1, or +i or -i, and the matrix has zero trace, the dimension of the matrix,  $N$ , must be even. The solution  $N = 2$  is ruled out because  $N = 2$  cannot accommodate four independent hermitian matrices. Thus, we have the proof:  $N = 4$ . If we take Dirac's earlier very specific realization, we have

$$\gamma^0 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \quad (30)$$

where  $\sigma^i = \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  are the standard  $2 \times 2$  Pauli  $\sigma$ -matrices, and  $\mathbf{1}$  and  $0$  are  $2 \times 2$  unit and zero matrices. Note,

$$\gamma^{0\ddagger} = \gamma^0, \quad \gamma^{i\ddagger} = -\gamma^i. \quad (31)$$

## E Hermitian Conjugate Equation

As for the nonrelativistic Schrödinger equation, we need both the Dirac equation and its hermitian conjugate equation

$$\frac{\partial \psi^\dagger}{\partial x^\mu} \gamma^{\mu\dagger} - \frac{imc}{\hbar} \psi^\dagger = 0. \quad (32)$$

Now right-multiplying by  $\gamma^0$ , and using  $\gamma^{0\dagger} = \gamma^0$ , as well as  $\gamma^{i\dagger} \gamma^0 = -\gamma^i \gamma^0 = +\gamma^0 \gamma^i$ , we get

$$\frac{\partial}{\partial x^\mu} \psi^\dagger \gamma^0 \gamma^\mu - \frac{imc}{\hbar} \psi^\dagger \gamma^0 = 0. \quad (33)$$

Now, it proves convenient to define

$$\begin{aligned} \bar{\psi} &= \psi^\dagger \gamma^0 = (\psi_1^* \quad \psi_2^* \quad \psi_3^* \quad \psi_4^*) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \\ &= (\psi_1^* \quad \psi_2^* \quad -\psi_3^* \quad -\psi_4^*), \end{aligned} \quad (34)$$

so the Dirac equation

$$\text{I.} \quad \gamma^\mu \frac{\partial \psi}{\partial x^\mu} + \frac{imc}{\hbar} \psi = 0 \quad (35)$$

goes over into the conjugate equation

$$\text{II.} \quad \frac{\partial \bar{\psi}}{\partial x^\mu} \gamma^\mu - \frac{imc}{\hbar} \bar{\psi} = 0. \quad (36)$$

Now, taking  $\bar{\psi} \times (\text{eq. I}) + (\text{eq. II}) \times \psi$  yields

$$\frac{\partial}{\partial x^\mu} (\bar{\psi} \gamma^\mu \psi) = 0. \quad (37)$$

This is the continuity equation in 4-D notation

$$\frac{\partial J^\mu}{\partial x^\mu} = 0, \quad \frac{1}{c} \frac{\partial J^0}{\partial t} + \vec{J} \cdot \vec{J} = 0, \quad (38)$$

with

$$J^0 = \bar{\psi} \gamma^0 \psi = \psi^\dagger \psi = \sum_{\rho=1}^4 |\psi_\rho|^2, \quad J^i = \bar{\psi} \gamma^i \psi = \psi^\dagger \alpha^i \psi = \sum_{\rho,\sigma=1}^4 \psi_\rho^* (\vec{\alpha})_{\rho\sigma} \psi_\sigma. \quad (39)$$

Note:  $\bar{\psi} \gamma^\mu \psi$  appears to be a four-vector, because we expect that all observers, in all Lorentz frames, would expect to obtain a continuity equation of the same form.

## Lorentz Covariance of the Dirac Equation

From the 4-D form of the Dirac equation,

$$\gamma^\mu \frac{\partial}{\partial x^\mu} \psi + \frac{imc}{\hbar} \psi = 0, \quad (1)$$

it might seem tempting to conclude the  $\gamma^\mu$  are the four components of a four-vector contracted with  $\partial/\partial x^\mu$  to make a Lorentz scalar, but this is nonsense. The  $\gamma^\mu$  are merely matrices, introduced to keep track of how the various components,  $\psi_\rho$ , are coupled to each other in the four equations. If an observer,  $O'$ , in another Lorentz frame,  $x'^\mu$ , constructs his Dirac equations, his  $\gamma^\mu$  will have to satisfy all of the same criteria as the  $\gamma^\mu$  for an observer,  $O$ , in the Lorentz frame,  $x^\mu$ . Observer,  $O'$ , might come up with a different solution to the Dirac relations and the hermiticity conditions (as might another observer in  $x^\mu$ ), but his different solution would be related to Dirac's solution by means of a similarity transformation, corresponding again merely to a different linear combination of the  $\psi_\rho$  and the four equations. (Unlike  $\gamma^\mu$ , however, the product  $\bar{\psi} \gamma^\mu \psi = J^\mu$ , is a four-vector, as was surmised in the last chapter.)

An observer,  $O'$ , in a Lorentz frame,  $x'^\mu$ , should therefore obtain Dirac equations, with the standard  $\gamma^\mu$ , of the form

$$\gamma^\mu \frac{\partial}{\partial x'^\mu} \psi'(x') + \frac{imc}{\hbar} \psi'(x') = 0, \quad (2)$$

where the  $x'^\mu$  are related to the  $x^\nu$  via the Lorentz transformation

$$x'^\mu = a^\mu_\nu x^\nu, \quad (3)$$

with inverse relations

$$x^\nu = (a^{-1})^\nu_\mu x'^\mu, \quad (4)$$

with

$$a^\mu_\nu = \frac{\partial x'^\mu}{\partial x^\nu}, \quad (a^{-1})^\nu_\mu = \frac{\partial x^\nu}{\partial x'^\mu}, \quad (5)$$

and

$$a^\mu_\nu (a^{-1})^\nu_\lambda = \delta^\mu_\lambda. \quad (6)$$

The Lorentz invariance of the 4-D length element

$$x'^\mu x'_\mu = x^\nu x_\nu, \quad c^2 t'^2 - \vec{r}' \cdot \vec{r}' = c^2 t^2 - \vec{r} \cdot \vec{r}, \quad (7)$$

leads to the 4-D orthogonality relations

$$a^\mu_\nu a^\nu_\lambda = \delta^\mu_\lambda. \quad (8)$$

The most general Lorentz transformation can be built from a combination of special Lorentz transformations, Lorentz boosts in the direction of some specific space direction, and ordinary rotations in the 3-D subspace,  $x^1, x^2, x^3$ . For example, the special Lorentz transformation

$$\begin{aligned} x'^0 &= \frac{1}{\sqrt{1-\beta^2}}(x^0 - \beta x^1), & ct' &= \frac{1}{\sqrt{1-\beta^2}}(ct - \beta x), \\ x'^1 &= \frac{1}{\sqrt{1-\beta^2}}(-\beta x^0 + x^1), & x' &= \frac{1}{\sqrt{1-\beta^2}}(-vt + x), \end{aligned} \quad (9)$$

or the special rotation

$$\begin{aligned} x'^1 &= x^1 \cos \theta + x^2 \sin \theta, \\ x'^2 &= -x^1 \sin \theta + x^2 \cos \theta. \end{aligned} \quad (10)$$

The special Lorentz transformation could have been written in analogous form

$$\begin{aligned} x'^0 &= x^0 \cosh \chi - x^1 \sinh \chi, \\ x'^1 &= -x^0 \sinh \chi + x^1 \cosh \chi, \end{aligned} \quad (11)$$

with

$$\cosh \chi = \frac{1}{\sqrt{1-\beta^2}}, \quad \sinh \chi = \frac{\beta}{\sqrt{1-\beta^2}}. \quad (12)$$

Also, for the proper Lorentz transformations:  $\det|a^\mu_\nu| = +1$ . For the improper Lorentz transformations:  $\det|a^\mu_\nu| = -1$ . The latter transformations include the space inversions,  $x^i \rightarrow -x^i$ , for  $i = 1, 2, 3$ , and the time reflections,  $x^0 \rightarrow -x^0$ .

Dirac assumed, in the new Lorentz frame, the  $\psi'(x')$  are a linear combination of the  $\psi(x)$ :

$$\psi'(x') = S_L \psi(x), \quad \text{with } S_L \equiv S = S(a^\mu_\nu), \quad (13)$$

that is, the  $4 \times 4$  Lorentz  $S$  matrices are functions of the Lorentz parameters,  $\theta_{ij}$ ,  $\chi_i$ . Then, with

$$\frac{\partial}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu} \frac{\partial}{\partial x^\nu} = (a^{-1})^\nu_\mu \frac{\partial}{\partial x^\nu}, \quad (14)$$

the Dirac equation in the primed frame transforms into

$$\gamma^\mu \frac{\partial}{\partial x'^\mu} \psi'(x') + \frac{imc}{\hbar} \psi'(x') = \gamma^\mu (a^{-1})^\nu_\mu \frac{\partial}{\partial x^\nu} (S\psi(x)) + \frac{imc}{\hbar} (S\psi(x)) = 0. \quad (15)$$

Left-multiplying this equation by  $S^{-1}$  leads to

$$(S^{-1} \gamma^\mu S) (a^{-1})^\nu_\mu \frac{\partial}{\partial x^\nu} \psi(x) + \frac{imc}{\hbar} \psi(x) = 0, \quad (16)$$

which would leave the form of the Dirac equations Lorentz invariant if

$$(S^{-1} \gamma^\mu S) (a^{-1})^\nu_\mu = \gamma^\nu, \quad (17)$$

or, using  $a^\lambda_\nu (a^{-1})^\nu_\mu = \delta^\lambda_\mu$ ,

$$I(a) : \quad (S^{-1} \gamma^\lambda S) = a^\lambda_\nu \gamma^\nu, \quad (18)$$

or

$$I(b) : \quad \gamma^\lambda = a^\lambda_\nu (S \gamma^\nu S^{-1}). \quad (19)$$

Also, the conjugate of the Dirac equations will be Lorentz covariant if

$$\bar{\psi}'(x') = \bar{\psi}(x) S^{-1}, \quad (20)$$

because

$$\begin{aligned} \frac{\partial \bar{\psi}'(x')}{\partial x'^\mu} \gamma^\mu - \frac{imc}{\hbar} \bar{\psi}'(x') &= 0 \rightarrow \frac{\partial x^\nu}{\partial x'^\mu} \frac{\partial}{\partial x^\nu} \bar{\psi}(x) S^{-1} \gamma^\mu - \frac{imc}{\hbar} \bar{\psi}(x) S^{-1} = 0 \\ &\rightarrow (a^{-1})^\nu_\mu \frac{\partial \bar{\psi}(x)}{\partial x^\nu} (S^{-1} \gamma^\mu S) - \frac{imc}{\hbar} \bar{\psi}(x) \\ &\rightarrow \frac{\partial \bar{\psi}(x)}{\partial x^\nu} \gamma^\nu - \frac{imc}{\hbar} \bar{\psi}(x) = 0, \end{aligned} \quad (21)$$

where we have first right-multiplied by  $S$  in the second line and have then used eq. (18) in the last step. Now, combining eq. (20) with

$$\bar{\psi}'(x') = \psi'(x')^\dagger \gamma^0 = \psi(x)^\dagger S^\dagger \gamma^0, \quad (22)$$

we have as a second requirement on the matrix,  $S$ ,

$$II : \quad S^\dagger \gamma^0 = \gamma^0 S^{-1}. \quad (23)$$

## A Construction of the Lorentz Matrix, $S$

As in our study of ordinary rotations, we shall exploit the fact that it is sufficient to know the  $S$  matrix for an infinitesimal transformation (either an ordinary rotation

in three-space or a Lorentz boost along some specific space direction), and obtain the finite transformations by compounding the infinitesimal ones. We take as our simplest first example an ordinary rotation in the 1–2 plane, i.e., a rotation about the  $z$  axis through an infinitesimal angle,  $\delta\theta_{12}$ , for which

$$\begin{aligned} S\psi(x) &= \psi'(x') = \psi'(ct, x', y', z) \\ &= \psi'(ct, x \cos \theta_{12} + y \sin \theta_{12}, -x \sin \theta_{12} + y \cos \theta_{12}, z) \\ &\quad (1 - i\delta\theta_{12}G_{12})\psi(x) = \psi'(ct, x + y\delta\theta_{12}, y - x\delta\theta_{12}, z) \\ &= \psi'(ct, x, y, z) + \delta\theta_{12}\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)\psi(ct, x, y, z) \\ &= \psi'(ct, x, y, z) - i\delta\theta_{12}\frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi(ct, x, y, z), \end{aligned} \quad (24)$$

where we have replaced  $\psi'(ct, x, y, z)$  by  $\psi(ct, x, y, z)$  in the second term of the last line because this term is already proportional to  $\delta\theta_{12}$  and  $\psi'(ct, x, y, z)$  would differ from  $\psi(ct, x, y, z)$  by an infinitesimal of first order. In the above equation,  $G_{12}$  is the generator of this infinitesimal rotation through the angle  $\delta\theta_{12}$ . Thus, we note

$$(1 - i\delta\theta_{12}G_{12})\psi(x) = \psi'(x) - i\delta\theta_{12}L_z\psi(ct, x, y, z), \quad (25)$$

where the orbital part of  $G_{12}$  turns out to be the orbital angular-momentum operator,  $L_z$ . From our experience with nonrelativistic quantum theory, we would expect  $G_{12} = G_{12}^{\text{intrinsic}} + G_{12}^{\text{orbital}}$ , so

$$(1 - i\delta\theta_{12}G_{12})\psi(x) = \left[1 - i\delta\theta_{12}(G_{12}^{\text{intr.}} + L_z)\right]\psi(ct, x, y, z). \quad (26)$$

Therefore, we would expect

$$\psi'(x) = S\psi(x) = (1 - i\delta\theta_{12}G_{12}^{\text{intr.}})\psi(x) \quad (27)$$

for the infinitesimal transformation. Moreover, we would expect  $G_{12}^{\text{intr.}}$  to be related to  $\frac{1}{2}\sigma_z$  in the nonrelativistic limit. Now, note

$$\gamma^1\gamma^2 =$$

$$\begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix} = \begin{pmatrix} -\sigma_x\sigma_y & 0 \\ 0 & -\sigma_x\sigma_y \end{pmatrix} = \begin{pmatrix} -i\sigma_z & 0 \\ 0 & -i\sigma_z \end{pmatrix}. \quad (28)$$

Recall, finally, the iteration of the infinitesimal transformation  $(1 - i\delta\theta_{12}G_{12})$  leads to the finite transformation matrix

$$S = e^{-i\theta_{12}G_{12}}. \quad (29)$$

From the infinitesimal transformation above, we are therefore led to try, for a rotation in the 1–2 plane through a finite angle,  $\theta_{12}$ ,

$$S = e^{-\frac{1}{2}\theta_{12}\gamma^1\gamma^2}. \quad (30)$$

Now, let us test whether this  $S$  satisfies the relations I of eqs. (18) and (19), and II of eqs. (23). From

$$(\gamma^1\gamma^2)(\gamma^1\gamma^2) = -(\gamma^1)^2(\gamma^2)^2 = -\mathbf{1}, \quad (31)$$

we have

$$e^{-\frac{1}{2}\theta\gamma^1\gamma^2} = \cos \frac{\theta}{2} \mathbf{1} - \sin \frac{\theta}{2} \gamma^1 \gamma^2, \quad (32)$$

so

$$(S^{-1}\gamma^\lambda S) = (\cos \frac{\theta}{2} \mathbf{1} + \sin \frac{\theta}{2} \gamma^1 \gamma^2) \gamma^\lambda (\cos \frac{\theta}{2} \mathbf{1} - \sin \frac{\theta}{2} \gamma^1 \gamma^2) \quad (33)$$

leads, with repeated use of the Dirac relation for the  $\gamma^\mu$  to:

$$\begin{aligned} \text{For } \lambda = 1 : \quad S^{-1}\gamma^1 S &= \left( \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} \right) \gamma^1 + 2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} \gamma^2 \\ &= \cos \theta \gamma^1 + \sin \theta \gamma^2 = a_v^1 \gamma^v, \\ \text{For } \lambda = 2 : \quad S^{-1}\gamma^2 S &= -\sin \theta \gamma^1 + \cos \theta \gamma^2 = a_v^2 \gamma^v, \\ \text{For } \lambda = 3 : \quad S^{-1}\gamma^3 S &= \gamma^3 = a_v^3 \gamma^v, \\ \text{For } \lambda = 0 : \quad S^{-1}\gamma^0 S &= \gamma^0 = a_v^0 \gamma^v. \end{aligned} \quad (34)$$

Also, using,  $(\gamma^1 \gamma^2)^\dagger = \gamma^{2\dagger} \gamma^{1\dagger} = (-\gamma^2)(-\gamma^1) = -\gamma^1 \gamma^2$ ,

$$S^\dagger \gamma^0 = \gamma^0 \left( \cos \frac{\theta}{2} \mathbf{1} + \sin \frac{\theta}{2} \gamma^1 \gamma^2 \right) = \gamma^0 S^{-1}, \quad (35)$$

so relations I, II are satisfied by this  $S = S_{12}$ . Similarly, we can show rotations in the 2–3 plane, i.e., about the  $x$  axis, require

$$S_{23} = e^{-\frac{1}{2}\theta_{23}\gamma^2\gamma^3} = \cos \frac{\theta_{23}}{2} \mathbf{1} - \sin \frac{\theta_{23}}{2} \gamma^2 \gamma^3, \quad (36)$$

and rotations about the  $y$  axis, i.e., rotations in the 3–1 plane, require

$$S_{31} = e^{-\frac{1}{2}\theta_{31}\gamma^3\gamma^1} = \cos \frac{\theta_{31}}{2} \mathbf{1} - \sin \frac{\theta_{31}}{2} \gamma^3 \gamma^1. \quad (37)$$

For a special Lorentz transformation in the  $x$  direction; or a special Lorentz transformation in the 0–1 subspace, we are led to try

$$S_{01} = e^{-\frac{1}{2}\chi\gamma^0\gamma^1} = \cosh \frac{\chi}{2} \mathbf{1} - \sinh \frac{\chi}{2} \gamma^0 \gamma^1, \quad (38)$$

where now:  $(\gamma^0 \gamma^1)(\gamma^0 \gamma^1) = +\mathbf{1}$ . Now, let us test this  $S_{01}$  to see whether it satisfies relations I and II. With

$$(S^{-1}\gamma^\lambda S) = \left( \cosh \frac{\chi}{2} \mathbf{1} + \sinh \frac{\chi}{2} \gamma^0 \gamma^1 \right) \gamma^\lambda \left( \cosh \frac{\chi}{2} \mathbf{1} - \sinh \frac{\chi}{2} \gamma^0 \gamma^1 \right), \quad (39)$$

we have:

$$\begin{aligned} \text{For } \lambda = 0 : \quad (S^{-1}\gamma^0 S) &= \left( \cosh^2 \frac{\chi}{2} + \sinh^2 \frac{\chi}{2} \right) \gamma^0 - 2 \cosh \frac{\chi}{2} \sinh \frac{\chi}{2} \gamma^1 \\ &= \cosh \chi \gamma^0 - \sinh \chi \gamma^1 = a_v^0 \gamma^v, \\ \text{For } \lambda = 1 : \quad (S^{-1}\gamma^1 S) &= -\sinh \chi \gamma^0 + \cosh \chi \gamma^1 = a_v^1 \gamma^v, \\ \text{For } \lambda = 2 : \quad (S^{-1}\gamma^2 S) &= \gamma^2 = a_v^2 \gamma^v, \\ \text{For } \lambda = 3 : \quad (S^{-1}\gamma^3 S) &= \gamma^3 = a_v^3 \gamma^v. \end{aligned} \quad (40)$$

Finally,

$$S^\dagger \gamma^0 = \left( \cosh \frac{\chi}{2} \mathbf{1} + \sinh \frac{\chi}{2} \gamma^1 \gamma^0 \right) \gamma^0 = \gamma^0 \left( \cosh \frac{\chi}{2} \mathbf{1} + \sinh \frac{\chi}{2} \gamma^0 \gamma^1 \right) = \gamma^0 S^{-1}, \quad (41)$$

so both relations I and II are satisfied. We therefore expect

$$S_{0i} = e^{-\frac{1}{2}\chi_i \gamma^0 \gamma^i} \quad \text{with } i = 1, 2, 3. \quad (42)$$

Finally, the  $S_{ij}$  and  $S_{0i}$  can be expressed through

$$\begin{aligned} S_{ij} &= \cos \frac{\theta_{ij}}{2} \mathbf{1} - \sin \frac{\theta_{ij}}{2} \gamma^i \gamma^j \\ &= \cos \frac{\theta_{ij}}{2} \begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix} + i \sin \frac{\theta_{ij}}{2} \epsilon_{ijk} \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix} \quad \text{with } i \neq j = 1, 2, 3, \end{aligned} \quad (43)$$

and

$$\begin{aligned} S_{0i} &= \cosh \frac{\chi_i}{2} \mathbf{1} - \sinh \frac{\chi_i}{2} \gamma^0 \gamma^i \\ &= \cosh \frac{\chi_i}{2} \begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix} - \sinh \frac{\chi_i}{2} \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad \text{with } i = 1, 2, 3. \end{aligned} \quad (44)$$

Thus, we can summarize: For any  $\mu-\nu$  plane Lorentz transformation

$$S_{\mu\nu} = e^{-\frac{1}{2}\theta_{\mu\nu} \gamma^\mu \gamma^\nu} = e^{\frac{i}{2}\theta_{\mu\nu} \sigma^{\mu\nu}}, \quad \text{with } \sigma^{\mu\nu} \equiv \frac{i}{2} [\gamma^\mu, \gamma^\nu] = i \gamma^\mu \gamma^\nu. \quad (45)$$

From eqs. (42) and (43), we also have, explicitly,

For 12 – rotations :

$$\begin{aligned} \psi'_1 &= e^{i \frac{\theta_{12}}{2}} \psi_1 \\ \psi'_2 &= e^{-i \frac{\theta_{12}}{2}} \psi_2 \\ \psi'_3 &= e^{i \frac{\theta_{12}}{2}} \psi_3 \\ \psi'_4 &= e^{-i \frac{\theta_{12}}{2}} \psi_4; \end{aligned} \quad (46)$$

or for 23 – rotations :

$$\begin{aligned} \psi'_1 &= \cos \frac{\theta_{23}}{2} \psi_1 + i \sin \frac{\theta_{23}}{2} \psi_2 \\ \psi'_2 &= i \sin \frac{\theta_{23}}{2} \psi_1 + \cos \frac{\theta_{23}}{2} \psi_2 \\ \psi'_3 &= \cos \frac{\theta_{23}}{2} \psi_3 + i \sin \frac{\theta_{23}}{2} \psi_4 \\ \psi'_4 &= i \sin \frac{\theta_{23}}{2} \psi_3 + \cos \frac{\theta_{23}}{2} \psi_4; \end{aligned} \quad (47)$$

or for 01 – boosts :

$$\begin{aligned} \psi'_1 &= \cosh \frac{\chi_{01}}{2} \psi_1 - \sinh \frac{\chi_{01}}{2} \psi_4 \\ \psi'_2 &= \cosh \frac{\chi_{01}}{2} \psi_2 - \sinh \frac{\chi_{01}}{2} \psi_3 \\ \psi'_3 &= - \sinh \frac{\chi_{01}}{2} \psi_2 + \cosh \frac{\chi_{01}}{2} \psi_3 \end{aligned}$$

$$\psi'_4 = -\sinh \frac{\chi_{01}}{2} \psi_1 + \cosh \frac{\chi_{01}}{2} \psi_4. \quad (48)$$

These equations give just the intrinsic transformations. Each  $\psi_i$  must still be acted upon by the appropriate  $e^{-i\theta_{\mu\nu} C_{\mu\nu}^{\text{orbital}}}$ , where these operators act on the space-time coordinates in the  $\psi_i$ . Recalling, from eqs. (24)–(27),  $\psi'(x^\mu) = S_{\text{intr.}} \psi(x^\mu) = S_{\text{intr.}} \psi((a^{-1})^\mu{}_\nu x'^\nu)$ , we have in the specific example of a 12 rotation, [see the first line of eq. (46)],

$$\psi'_1(x'^\mu) = e^{i\frac{\theta_{12}}{2}} \psi_1(x'^0, x'^1 \cos \theta_{12} - x'^2 \sin \theta_{12}, x'^1 \sin \theta_{12} + x'^2 \cos \theta_{12}, x'^3).$$

## B Space Inversions

As a final example, consider the space-inversion operation, with

$$x'^\mu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} x^\nu = g^{\mu\nu} x^\nu. \quad (49)$$

Our basic relations I and II are simply

$$\begin{aligned} S^{-1} \gamma^\lambda S &= g^{\lambda\nu} \gamma^\nu \\ S^\dagger \gamma^0 &= \gamma^0 S^{-1}. \end{aligned} \quad (50)$$

These equations are satisfied by

$$S = e^{i\alpha} \gamma^0, \quad \text{where } \alpha = \text{any real number.} \quad (51)$$

It will prove convenient to choose  $\alpha = 0$  when the limiting nonrelativistic  $\psi$  has positive parity, and  $\alpha = \pi$  when the limiting nonrelativistic  $\psi$  has negative parity.

# Bilinear Covariants

Consider the 16 combinations of  $\gamma$  matrices,  $\Gamma^A$ ,  $A = 1, \dots, 16$ , where

$$\begin{aligned} (S) : \quad & \Gamma^S = \mathbf{1}, \\ (V) : \quad & (\Gamma^V)^\mu = \gamma^\mu = (\gamma^0, \gamma^1, \gamma^2, \gamma^3), \\ (T) : \quad & (\Gamma^T)^{\mu\nu} = \sigma^{\mu\nu} = i\gamma^\mu\gamma^\nu = (i\gamma^0\gamma^1, i\gamma^0\gamma^2, i\gamma^0\gamma^3, i\gamma^1\gamma^2, i\gamma^2\gamma^3, i\gamma^3\gamma^1), \\ (A) : \quad & (\Gamma^A)^\mu = \gamma^5\gamma^\mu = (-i\gamma^1\gamma^2\gamma^3, -i\gamma^0\gamma^2\gamma^3, -i\gamma^0\gamma^3\gamma^1, -i\gamma^0\gamma^1\gamma^2), \\ (P) : \quad & \Gamma^P = \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3, \end{aligned} \quad (1)$$

where we have defined a new  $\gamma$  matrix

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \quad (2)$$

where  $\mathbf{1}$  is a  $2 \times 2$  unit matrix and  $\mathbf{0}$  is a  $2 \times 2$  zero matrix. Note:  $\gamma^5$  also has the following properties:

$$(\gamma^5)^2 = \mathbf{1}, \quad \gamma^5\gamma^\mu = -\gamma^\mu\gamma^5. \quad (3)$$

The 16  $\Gamma^A$  satisfy the following properties:

$$1. \quad (\Gamma^A)^2 = \pm 1, \quad (4)$$

as can be shown by direct verification. Thus, each  $\Gamma^A$  has an inverse and  $(\Gamma^A)^{-1} = \pm\Gamma^A$ .

$$2. \quad \Gamma^A\Gamma^B = \epsilon^{AB}\Gamma^C, \quad \text{where } \epsilon^{AB} = \pm 1, \pm i \text{ only.} \quad (5)$$

This can again be shown by direct verification. In addition:

If, for fixed  $\Gamma^A$ ,  $\Gamma^B$  is allowed to run through all 16 possibilities,  $\Gamma^C$  runs through all 16 possibilities also, and  $\Gamma^C = \mathbf{1}$  only for  $\Gamma^B = \Gamma^A$ . To prove this: Suppose

some  $\Gamma^{B'} \neq \Gamma^B$  existed for which  $\Gamma^A \Gamma^B = \Gamma^A \Gamma^{B'}$ . Because the inverse of  $\Gamma^A$  exists, if we left-multiply with  $(\Gamma^A)^{-1}$ , we would have  $\Gamma^B = \Gamma^{B'}$ , contrary to the initial assumption.

$$3. \quad \text{Trace}(\Gamma^A) = 0, \quad \text{for all } \Gamma^A \text{ except } \Gamma^A = \Gamma^S = \mathbf{1}. \quad (6)$$

For each such  $\Gamma^A$  (other than  $\Gamma^S$ ), a  $\Gamma^N$  exists such that

$$\Gamma^A \Gamma^N = -\Gamma^N \Gamma^A, \quad (7)$$

so

$$\begin{aligned} \text{Trace}(\Gamma^A \Gamma^N) &= -\text{Trace}(\Gamma^N \Gamma^A) \\ &= -\text{Trace}(\Gamma^A \Gamma^N) = 0. \end{aligned} \quad (8)$$

The first step can be shown by verification.

$$\begin{aligned} \text{For } \Gamma^A &= \gamma^\mu, \quad \Gamma^N = \gamma^\nu; \quad (\nu \neq \mu). \\ \text{For } \Gamma^A &= i\gamma^\mu \gamma^\nu, \quad \Gamma^N = \gamma^\nu; \quad (\nu \neq \mu). \\ \text{For } \Gamma^A &= \gamma^5 \gamma^\mu, \quad \Gamma^N = \gamma^\mu. \\ \text{For } \Gamma^A &= \gamma^5, \quad \Gamma^N = \gamma^\mu. \end{aligned} \quad (9)$$

The  $\Gamma^A \Gamma^N$  from this list cover all 15 possibilities, which are therefore traceless.

4. The 16  $\Gamma^A$  are linearly independent. No relation of the form  $\sum_{B=1}^{16} c_B \Gamma^B = 0$  exists.

Proof: For any specific  $\Gamma^A$ ,

$$\text{Trace}\left(\sum_{B=1}^{16} c_B \Gamma^B \Gamma^A\right) = \pm \text{Trace}(\mathbf{1}) c_A = \pm 4c_A. \quad (10)$$

Thus, if  $\sum_{B=1}^{16} c_B \Gamma^B = 0$ ,  $c_A = 0$  for all  $A = 1, \dots, 16$ .

5. If  $F$  is a  $4 \times 4$  matrix that commutes with all four  $\gamma^\mu$ ,  $F$  is a multiple of the unit matrix  $\mathbf{1}$ .

Proof: Let  $F = \sum_B c_B \Gamma^B$ . Then,

$$F \gamma^\mu = \gamma^\mu F \rightarrow \sum_B c_B \Gamma^B \gamma^\mu = \sum_B c_B \gamma^\mu \Gamma^B; \quad \mu = 0, 1, 2, 3, \quad (11)$$

or

$$\sum_{B \neq S} c_B (\Gamma^B \gamma^\mu - \gamma^\mu \Gamma^B) + c_1 \gamma^\mu - c_1 \gamma^\mu = 0. \quad (12)$$

For each  $\Gamma^B$ , at least one  $\gamma^\mu$  exists such that  $\gamma^\mu \Gamma^B = -\Gamma^B \gamma^\mu$ , see eq. (9). Therefore, the sum above can be zero only if each  $c_B$  with  $B \neq 1$  is zero.

## A Transformation Properties of the $\bar{\psi} \Gamma^A \psi$

Substituting for  $\bar{\psi}'(x')$  and  $\psi'(x')$ ,

$$\bar{\psi}'(x') \mathbf{1} \psi'(x') = \bar{\psi}(x) S^{-1} S \psi(x) = \bar{\psi}(x) \mathbf{1} \psi(x). \quad (13)$$

This equation establishes the Lorentz invariance of  $\bar{\psi}\psi$ .

$$\bar{\psi}'(x')\gamma^\mu\psi'(x') = \bar{\psi}(x)S^{-1}\gamma^\mu S\psi(x) = a_v^\mu\bar{\psi}(x)\gamma^v\psi(x), \quad (14)$$

which shows  $\bar{\psi}\gamma^\mu\psi$  is a Lorentz four-vector.

$$\bar{\psi}'(x')i\gamma^\mu\gamma^v\psi'(x') = \bar{\psi}(x)i(S^{-1}\gamma^\mu S)(S^{-1}\gamma^v S)\psi(x) = a_\rho^\mu a_\lambda^v (\bar{\psi}(x)i\gamma^\rho\gamma^\lambda\psi(x)). \quad (15)$$

To see how the (A) and (P) transform, we use

$$\gamma^5\gamma^\mu\gamma^v = \gamma^\mu\gamma^v\gamma^5, \quad \gamma^5\gamma^\mu = -\gamma^\mu\gamma^5. \quad (16)$$

Because the  $S$  for proper Lorentz transformations are built from exponentials of type  $e^{-\frac{\theta}{2}\gamma^\mu\gamma^v}$ ,  $[\gamma^5, S] = 0$  for proper Lorentz transformations. Thus, for proper Lorentz transformations, we have

$$\begin{aligned} \bar{\psi}'(x')\gamma^5\gamma^\mu\psi'(x') &= \bar{\psi}(x)S^{-1}\gamma^5\gamma^\mu S\psi(x) = \bar{\psi}(x)\gamma^5S^{-1}\gamma^\mu S\psi(x) \\ &= a_v^\mu\bar{\psi}(x)\gamma^5\gamma^v\psi(x), \end{aligned} \quad (17)$$

and, again for proper Lorentz transformations,

$$\bar{\psi}'(x')\gamma^5\psi'(x') = \bar{\psi}(x)S^{-1}\gamma^5S\psi(x) = \bar{\psi}(x)\gamma^5S^{-1}S\psi(x) = \bar{\psi}(x)\gamma^5\psi(x). \quad (18)$$

Now, for pure space inversions, we found  $S = e^{i\alpha}\gamma^0$ . Therefore, for this space inversion  $S$ , we have

$$S^{-1}\gamma^5S = -\gamma^5 \quad (19)$$

This relation shows the pseudoscalar character, (P), of  $\bar{\psi}\gamma^5\psi$ . Finally, for the space-inversion,  $S = e^{i\alpha}\gamma^0$ , we also have

$$\begin{aligned} S^{-1}\gamma^\mu S &= (\gamma^0, -\gamma^i), \\ S^{-1}\gamma^5\gamma^\mu S &= (-\gamma^5\gamma^0, \gamma^5\gamma^i), \\ S^{-1}i\gamma^\mu\gamma^v S &= (-i\gamma^0\gamma^i, i\gamma^i\gamma^j). \end{aligned} \quad (20)$$

These relations establish the true four-vector character, (V), of  $\bar{\psi}\gamma^\mu\psi$ , the pseudo or axial vector character, (A), of  $\bar{\psi}\gamma^5\gamma^\mu\psi$ , and finally the true tensor character, (T), of  $\bar{\psi}i\gamma^\mu\gamma^v\psi$ .

## B Lower Index $\gamma$ Matrices

So far, we have defined all of the  $\Gamma^A$  in terms of upper index  $\gamma$  matrices,  $\gamma^\mu$ . In view of the transformation properties of the  $\bar{\psi}\Gamma^A\psi$ , it is useful to define lower index  $\gamma$ -matrices,  $\gamma_\mu$ , through

$$\gamma_0 = \gamma^0, \quad \gamma_i = -\gamma^i, \quad \text{for } i = 1, 2, 3, \quad (21)$$

but with  $\gamma_5$  defined by

$$\gamma_5 = \gamma^5. \quad (22)$$

## Simple Solutions: Free Particle Motion: Plane Wave Solutions

Let us first seek solutions to the equation

$$\gamma^\mu \frac{\partial \psi}{\partial x^\mu} + \frac{imc}{\hbar} \psi = 0, \quad (1)$$

which have the plane wave form

$$\psi = u(\vec{p}) e^{\frac{i}{\hbar} (\vec{p} \cdot \vec{r} - Et)} = u(\vec{p}) e^{-\frac{i}{\hbar} P_\mu x^\mu}, \quad (2)$$

where  $u(\vec{p})$  is a four-component quantity, i.e., a  $4 \times 1$  matrix, and

$$E = \pm \sqrt{(m^2 c^4 + c^2 p^2)}, \quad (3)$$

which follows from the energy-momentum relation leading to the Klein–Gordon equation for the free particle of rest mass  $m$ . Both a positive and negative root exist. To get the simplest of all solutions, let us investigate the case,  $\vec{p} = 0$ , i.e., a particle at rest in our Lorentz frame. In this case,

$$\begin{aligned} \gamma^0 \frac{1}{c} \frac{\partial \psi}{\partial t} &= -\frac{imc}{\hbar} \psi, \\ \text{or } -\frac{i}{\hbar c} E \gamma^0 u(0) &= -\frac{imc}{\hbar} u(0). \end{aligned} \quad (4)$$

If we decompose the  $4 \times 1$  matrix into two  $2 \times 1$  matrices,  $u_A(0)$  and  $u_B(0)$ , this becomes

$$E \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & -1 \end{pmatrix} \begin{pmatrix} u_A(0) \\ u_B(0) \end{pmatrix} = mc^2 \begin{pmatrix} u_A(0) \\ u_B(0) \end{pmatrix}. \quad (5)$$

1. With  $E = +mc^2$ , this equation has two independent solutions, both with  $u_B(0) = 0$ :

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \frac{e^{-\frac{i}{\hbar} mc^2 t}}{\sqrt{\text{Vol.}}}, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \frac{e^{-\frac{i}{\hbar} mc^2 t}}{\sqrt{\text{Vol.}}},$$

where we have used a box normalization with a box of volume,  $\text{Vol.} = L^3$ .

2. With  $E = -mc^2$ , two independent solutions again exist, now both with  $u_A(0) = 0$ :

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \frac{e^{+\frac{i}{\hbar} mc^2 t}}{\sqrt{\text{Vol.}}}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \frac{e^{+\frac{i}{\hbar} mc^2 t}}{\sqrt{\text{Vol.}}}.$$

Similarly, we get the plane wave solutions for  $\vec{p} \neq 0$  from

$$(E\gamma^0 + c\gamma^i p_i - mc^2 \mathbf{1})u(\vec{p}) = 0, \quad (6)$$

or

$$\left[ E \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & -1 \end{pmatrix} - c \begin{pmatrix} \mathbf{0} & \vec{\sigma} \\ -\vec{\sigma} & \mathbf{0} \end{pmatrix} \cdot \vec{p} - mc^2 \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & 1 \end{pmatrix} \right] \begin{pmatrix} u_A(\vec{p}) \\ u_B(\vec{p}) \end{pmatrix} = 0, \quad (7)$$

leading to the two equations

$$\begin{aligned} (E - mc^2)u_A(\vec{p}) - c(\vec{\sigma} \cdot \vec{p})u_B(\vec{p}) &= 0, \\ (E + mc^2)u_B(\vec{p}) - c(\vec{\sigma} \cdot \vec{p})u_A(\vec{p}) &= 0, \end{aligned} \quad (8)$$

with

$$u_A(\vec{p}) = \frac{c(\vec{\sigma} \cdot \vec{p})}{(E - mc^2)}u_B(\vec{p}), \quad u_B(\vec{p}) = \frac{c(\vec{\sigma} \cdot \vec{p})}{(E + mc^2)}u_A(\vec{p}). \quad (9)$$

These equations lead to the same equation for both  $u_A(\vec{p})$  and  $u_B(\vec{p})$ ; e.g.,

$$\left[ (E^2 - m^2 c^4) - c^2 (\vec{\sigma} \cdot \vec{p}) \cdot (\vec{\sigma} \cdot \vec{p}) \right] u_A(\vec{p}) = 0. \quad (10)$$

If we use the general identity for two arbitrary vector operators,  $\vec{A}$ , and  $\vec{B}$ ,

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = (\vec{A} \cdot \vec{B}) + i\vec{\sigma} \cdot [\vec{A} \times \vec{B}], \quad (11)$$

we have, with  $\vec{A} = \vec{B} = \vec{p}$ ,

$$(E^2 - m^2 c^4 - c^2 p^2)u_A(\vec{p}) = 0. \quad (12)$$

This equation just verifies the energy-momentum relation for our relativistic particle. To get solutions, we use eq. (9) to determine  $u_B$  from the two independent possible solutions for  $u_A$  and vice versa. With the  $2 \times 2$  matrix for  $(\vec{\sigma} \cdot \vec{p})$ ,

$$(\vec{\sigma} \cdot \vec{p}) = \begin{pmatrix} p_z & (p_x - ip_y) \\ (p_x + ip_y) & -p_z \end{pmatrix} = \begin{pmatrix} p_z & p_- \\ p_+ & -p_z \end{pmatrix}, \quad (13)$$

this equation leads to

$$\begin{aligned} u^{(1)}(\vec{p}) &= N \begin{pmatrix} 1 \\ \frac{cp_z}{E+mc^2} \\ \frac{cp_+}{E+mc^2} \\ \frac{cp_-}{E+mc^2} \end{pmatrix}, & u^{(2)}(\vec{p}) &= N \begin{pmatrix} 0 \\ \frac{cp_-}{E+mc^2} \\ \frac{cp_+}{E+mc^2} \\ \frac{cp_z}{E+mc^2} \end{pmatrix}, \\ u^{(3)}(\vec{p}) &= N \begin{pmatrix} \frac{cp_z}{E-mc^2} \\ \frac{cp_+}{E-mc^2} \\ 1 \\ 0 \end{pmatrix}, & u^{(4)}(\vec{p}) &= N \begin{pmatrix} 0 \\ \frac{-cp_z}{E-mc^2} \\ \frac{-cp_+}{E-mc^2} \\ 0 \\ 1 \end{pmatrix}, \end{aligned} \quad (14)$$

where the solutions,  $r = 1, 2$ , are associated with the positive energy branch, whereas those with  $r = 3, 4$ , are associated with negative energies, and the normalization factor can be obtained from

$$\int_{\text{Vol.}} d\vec{r} u^{(r)}(\vec{p})^\dagger u^{(r)}(\vec{p}) = 1, \quad (15)$$

where we take box normalization with a cube of Vol.  $L^3$ . For  $(r) = (1)$ , or  $(2)$ , we then have

$$|N|^2 \text{Vol.} \frac{(E + mc^2)^2 + c^2 p^2}{(E + mc^2)^2} = |N|^2 \text{Vol.} \frac{2E}{(E + mc^2)} = 1, \quad (16)$$

where we have used  $c^2 p^2 = E^2 - m^2 c^4$ . Choosing  $N$  real, we have

$$N = \sqrt{\frac{(E + mc^2)}{2E}} \frac{1}{\sqrt{\text{Vol.}}}. \quad (17)$$

For  $(r) = (3)$ , or  $(4)$ , we have

$$|N|^2 \text{Vol.} \frac{(E - mc^2)^2 + c^2 p^2}{(E - mc^2)^2} = |N|^2 \text{Vol.} \frac{2E}{(E - mc^2)} = 1, \quad (18)$$

but now  $E$  is a negative quantity, so, again

$$N = \sqrt{\frac{(|E| + mc^2)}{2|E|}} \frac{1}{\sqrt{\text{Vol.}}}, \quad (19)$$

which is therefore the same as that for the positive energy solutions. We shall discuss these negative-energy solutions in more detail later, when, with Dirac, we “discover” the positron; see Chapter 75. We shall, however, anticipate the positron, and in the solutions with  $(r = 3, 4)$ , put  $E = -|E| = -E_{e^+}$ , and  $\vec{p} = -\vec{p}_{e^+}$ . With this change in notation, we shall rename the plane wave solutions with  $(r = 3, 4)$ ,  $v^{(r)}(\vec{p})$

$$v^{(3)}(\vec{p}) = N \begin{pmatrix} \frac{cp_z}{E+mc^2} \\ \frac{cp_+}{E+mc^2} \\ 1 \\ 0 \end{pmatrix}, \quad v^{(4)}(\vec{p}) = N \begin{pmatrix} \frac{cp_-}{E+mc^2} \\ \frac{-cp_z}{E+mc^2} \\ 0 \\ 1 \end{pmatrix}, \quad (20)$$

where now  $E$  is the positive energy of the positron and  $\vec{p}$  is the momentum vector of the positron, although we leave off the subscripts,  $e^+$ . The normalization constant

is given by eq. (19). Let us show the solutions with  $r = 1, 2$  could also have been obtained from the rest frame solutions with  $u_1(0) = 1$  and  $u_2(0) = 1$ , respectively, by applying a Lorentz boost in the appropriate direction to these rest frame solutions. Let us choose the rest frame of the particle as the primed frame, and the laboratory frame as the unprimed frame. Recall  $\psi'(x') = S\psi(x)$ , so we need  $\psi(x) = S^{-1}\psi'(x')$ . Therefore,

$$\psi(x) = S^{-1}u(0) \frac{1}{\sqrt{L'^3}} e^{-\frac{i}{\hbar}(P'_\mu x'^\mu)}, \quad (21)$$

where we must use the Lorentz contraction to transform the rest frame volume,  $L'^3$ , to the laboratory volume,  $L^3$ . If for this purpose we choose, for the moment, the  $x$  axis along the direction of the electron's  $\vec{p}$ ,

$$L_x = \sqrt{(1 - \beta^2)} L'_x, \quad L_y = L'_y, \quad L_z = L'_z, \quad (22)$$

so

$$L'^3 = \frac{1}{\sqrt{(1 - \beta^2)}} L^3 = \frac{mc^2}{\sqrt{(1 - \beta^2)}} \frac{1}{mc^2} L^3 = \frac{E}{mc^2} L^3. \quad (23)$$

We also need to transform  $P'_\mu x'^\mu$  into the laboratory frame via  $P'_\mu x'^\mu = P_\mu x^\mu$ . With  $x^\mu = (ct, \vec{r})$ , and  $P_\mu = (\frac{E}{c}, -\vec{p})$ , this gives

$$P'_\mu x'^\mu = Et - \vec{p} \cdot \vec{r}. \quad (24)$$

Finally, recall

$$\begin{aligned} S^{-1} &= \left[ \cosh \frac{\chi}{2} \mathbf{1} + \sinh \frac{\chi}{2} \gamma^0 \gamma^i \right] \\ &= \cosh \frac{\chi}{2} \left[ \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} + \tanh \frac{\chi}{2} \begin{pmatrix} \mathbf{0} & (\vec{\sigma} \cdot \vec{e}_i) \\ (\vec{\sigma} \cdot \vec{e}_i) & \mathbf{0} \end{pmatrix} \right], \end{aligned} \quad (25)$$

where we have now chosen  $\vec{p}$  in an arbitrary direction in three-space parallel to a unit vector,  $\vec{e}_i$ , and where

$$\cosh \chi = 2 \cosh^2 \frac{\chi}{2} - 1 = \frac{1}{\sqrt{(1 - \beta^2)}} = \frac{mc^2}{\sqrt{(1 - \beta^2)}} \frac{1}{mc^2} = \frac{E}{mc^2}, \quad (26)$$

and

$$\sinh \chi = \frac{\beta}{\sqrt{(1 - \beta^2)}} = \frac{mv}{\sqrt{(1 - \beta^2)}} \frac{c}{mc^2} = \frac{pc}{mc^2}, \quad (27)$$

so

$$\cosh \frac{\chi}{2} = \sqrt{\frac{(E + mc^2)}{2mc^2}}; \quad \tanh \frac{\chi}{2} = \frac{\sinh \chi}{2 \cosh^2 \frac{\chi}{2}} = \frac{pc}{(E + mc^2)}. \quad (28)$$

We therefore have

$$S^{-1}u(0) = \sqrt{\frac{(E + mc^2)}{2mc^2}} \left[ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \right]$$

$$+ \frac{c}{(E + mc^2)} \begin{pmatrix} 0 & 0 & p_z & p_- \\ 0 & 0 & p_+ & -p_z \\ p_z & p_- & 0 & 0 \\ p_+ & -p_z & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}. \quad (29)$$

Combining eqs. (21), (23), (24), and (29), we have

$$\psi^{(1)}(\vec{p}, \vec{r}) = \sqrt{\frac{(E + mc^2)}{2mc^2}} \begin{pmatrix} 1 \\ 0 \\ \frac{cp_z}{(E + mc^2)} \\ \frac{cp_+}{(E + mc^2)} \end{pmatrix} \sqrt{\frac{mc^2}{E}} \frac{1}{\sqrt{L^3}} e^{-\frac{i}{\hbar}(Et - \vec{p} \cdot \vec{r})},$$

$$\psi^{(2)}(\vec{p}, \vec{r}) = \sqrt{\frac{(E + mc^2)}{2mc^2}} \begin{pmatrix} 1 \\ \frac{cp_-}{(E + mc^2)} \\ -\frac{cp_z}{(E + mc^2)} \\ 0 \end{pmatrix} \sqrt{\frac{mc^2}{E}} \frac{1}{\sqrt{L^3}} e^{-\frac{i}{\hbar}(Et - \vec{p} \cdot \vec{r})}, \quad (30)$$

which agrees with our earlier results, using eqs. (14) and (17).

## A An Application: Coulomb Scattering of Relativistic Electrons in Born Approximation: The Mott Formula

Before a further investigation of the physical significance of the solutions with  $r = 1, 2$  (to find their relationship to electron spin), let us first use these plane wave solutions in our first application. Let us calculate the differential scattering cross section of a relativistic electron from a nucleus of charge  $Ze$ . The interaction will be the Coulomb potential, but, as in our corresponding nonrelativistic calculation, we will have to use a screened Coulomb potential and let the screening parameter  $\rightarrow 0$ . (Compare with Chapter 46.) This is quite realistic because the real target will undoubtedly be made of atoms, where the nucleus of charge,  $Ze$ , is imbedded in the atomic electron cloud. Also, for relativistic electrons, we would expect the plane wave Born approximation to be good because now  $E \gg Ze^2/r_{\text{nucleus}}$ .

The differential cross section is given by

$$d\sigma = \frac{1}{\text{inc. flux}} \frac{2\pi}{\hbar} \rho(E_f) \left| \langle \vec{p}_f | -\frac{Ze^2}{r} |\vec{p}_i \rangle \right|^2. \quad (31)$$

We shall assume the incident beam is in the  $z$  direction, with momentum  $\vec{p}_i = p\vec{e}_z$ . Thus,

$$\vec{S}_{\text{inc.}} = c\bar{\psi}\vec{\gamma}\psi = cu^{(r)\dagger}(\vec{p}_i)\alpha_z u^{(r)}(\vec{p}_i) = cu^{(r)\dagger} \begin{pmatrix} \mathbf{0} & \sigma_z \\ \sigma_z & \mathbf{0} \end{pmatrix} u^{(r)}. \quad (32)$$

With  $(r) = 1$ ,

$$S_z = c \frac{E + mc^2}{2E} \frac{1}{\text{Vol.}} \begin{pmatrix} 1 & 0 & \frac{cp}{E + mc^2} & 0 \end{pmatrix} \begin{pmatrix} \frac{cp}{E + mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{c^2 p}{E} \frac{1}{\text{Vol.}}.$$

Similarly, with  $(r) = 2$ ,

$$S_z = c \frac{E + mc^2}{2E} \frac{1}{\text{Vol.}} \begin{pmatrix} 0 & 1 & 0 & -\frac{cp}{E+mc^2} \end{pmatrix} \begin{pmatrix} 0 \\ \frac{cp}{E+mc^2} \\ 0 \\ -1 \end{pmatrix} = \frac{c^2 p}{E} \frac{1}{\text{Vol.}},$$

so

$$\text{Inc. Flux} = \frac{c^2 p}{E \text{Vol.}} = \frac{v}{\text{Vol.}}. \quad (33)$$

In general,

$$\rho(E_f) dE_f = \frac{\text{Vol.}}{(2\pi)^3} \frac{p_f^2 dp_f d\Omega_f}{\hbar^3}, \quad (34)$$

where now  $c^2 p_f^2 = c^2 p^2 = E^2 - m^2 c^4$ , so  $2c^2 p_f dp_f = 2EdE$  and

$$\rho(E_f) = \frac{\text{Vol.}}{(2\pi)^3} \frac{p E d\Omega_f}{c^2 \hbar^3}. \quad (35)$$

Finally, the matrix element will involve the four-component, relativistic plane-wave states, so

$$\langle \vec{p}_f, (s) | -\frac{Ze^2}{r} |\vec{p}_i, (r) \rangle = - \int d\vec{r} e^{-i\vec{p}_f \cdot \vec{r}} \frac{Ze^2}{r} e^{+i\vec{p}_i \cdot \vec{r}} u^{(s)\dagger}(\vec{p}_f) u^{(r)}(\vec{p}_i), \quad (36)$$

where, for the moment, we have assumed the relativistic electrons in the incident beam are in the intrinsic state,  $(r)$ , and the electrons in the final scattered beam are in the intrinsic state,  $(s)$ . With  $(\vec{p}_f - \vec{p}_i)/\hbar = \vec{q}$ , the needed spatial integral is

$$\int d\vec{r} e^{-i\vec{q} \cdot \vec{r}} \frac{Ze^2}{r} = 4\pi Ze^2 \int_0^\infty dr r j_0(qr) = 4\pi \frac{Ze^2}{q} \int_0^\infty dr \sin qr \rightarrow \lim_{b \rightarrow 0} 4\pi \frac{Ze^2}{q} \int_0^\infty dr \sin qr e^{-br} = 4\pi \frac{Ze^2}{q^2}, \quad (37)$$

where we have used a screened Coulomb potential to regularize the Coulomb radial integral. In addition, we shall assume the incident electron beam is unpolarized, i.e., an equal mixture of both positive energy intrinsic states, with  $(r) = 1$ , or 2, and the detector is insensitive to the electron's intrinsic state. Thus,

$$\frac{d\sigma}{d\Omega} = \frac{E \text{Vol.}}{c^2 p} \frac{2\pi}{\hbar} \frac{\text{Vol.}}{(2\pi)^3} \frac{p E}{c^2 \hbar^3} \left( \frac{4\pi Ze^2}{q^2} \right)^2 \sum_{s=1,2} \frac{1}{2} \sum_{r=1,2} |u^{(s)\dagger}(\vec{p}_f) u^{(r)}(\vec{p}_i)|^2. \quad (38)$$

We have assumed  $\vec{p}_i = p\vec{e}_z$ . We could take the most general direction for  $\vec{p}_f$ , and choose  $\vec{p}_f = p \sin \theta \cos \phi \vec{e}_x + p \sin \theta \sin \phi \vec{e}_y + p \cos \theta \vec{e}_z$ . Because our problem has axial symmetry about the direction of the incident beam, however, we can choose  $\phi = 0$  without loss of generality. Thus,

$$u^{(1)\dagger}(\vec{p}_f) = \sqrt{\frac{E + mc^2}{2E}} \frac{\text{Vol.}}{\text{Vol.}} (1 \quad 0 \quad \frac{cp \cos \theta}{E+mc^2} \quad \frac{cp \sin \theta}{E+mc^2}),$$

$$u^{(1)}(\vec{p}_i) = \sqrt{\frac{E+mc^2}{2E \text{ Vol.}}} \begin{pmatrix} 1 \\ 0 \\ \frac{cp}{(E+mc^2)} \\ 0 \end{pmatrix},$$

$$u^{(2)\dagger}(\vec{p}_f) = \sqrt{\frac{E+mc^2}{2E \text{ Vol.}}} (0 \quad 1 \quad \frac{cp \sin \theta}{E+mc^2} \quad \frac{-cp \cos \theta}{E+mc^2}),$$

$$u^{(2)}(\vec{p}_i) = \sqrt{\frac{E+mc^2}{2E \text{ Vol.}}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{-cp}{(E+mc^2)} \end{pmatrix}.$$

With these equations, we get

$$\begin{aligned} & \frac{1}{2} \sum_{s=1,2} \sum_{r=1,2} |u^{(s)\dagger}(\vec{p}_f) u^{(r)}(\vec{p}_i)|^2 \\ &= \frac{1}{2} \left( \frac{E+mc^2}{2E \text{ Vol.}} \right)^2 \left[ 2 \left( 1 + \frac{c^2 p^2 \cos \theta}{(E+mc^2)^2} \right)^2 + 2 \left( \frac{-c^2 p^2 \sin \theta}{(E+mc^2)^2} \right)^2 \right] \\ &= \left( \frac{E+mc^2}{2E \text{ Vol.}} \right)^2 \left[ 1 + \frac{c^4 p^4}{(E+mc^2)^4} + 2 \frac{\cos \theta c^2 p^2}{(E+mc^2)^2} \right] \\ &= \frac{1}{(2E \text{ Vol.})^2} \left[ (E+mc^2)^2 + (E-mc^2)^2 + 2 \cos \theta (E^2 - m^2 c^4) \right] \\ &= \frac{1}{(2E \text{ Vol.})^2} 2 \left[ E^2 + m^2 c^4 + \cos \theta (E^2 - m^2 c^4) \right] \\ &= \frac{1}{(2E \text{ Vol.})^2} 2 \left[ E^2 + m^2 c^4 + (1 - 2 \sin^2 \frac{\theta}{2}) (E^2 - m^2 c^4) \right] \\ &= \frac{1}{E^2} \frac{1}{\text{Vol.}^2} \left[ E^2 - c^2 p^2 \sin^2 \frac{\theta}{2} \right] = \frac{1}{\text{Vol.}^2} \left[ 1 - \beta^2 \sin^2 \frac{\theta}{2} \right]. \end{aligned} \quad (39)$$

Combining eqs. (38) and (39), we have

$$\frac{d\sigma}{d\Omega} = \frac{4Z^2 e^4 E^2}{c^4 \hbar^4 q^4} \left( 1 - \beta^2 \sin^2 \frac{\theta}{2} \right). \quad (40)$$

Finally, noting  $q = 2k \sin \frac{\theta}{2}$ , as seen in Chapter 46, we get the Mott formula

$$\frac{d\sigma}{d\Omega} = \left( \frac{Z^2 m^2 e^4}{4k^4 \hbar^4 \sin^4 \frac{\theta}{2}} \right) \frac{E^2}{m^2 c^4} \left( 1 - \beta^2 \sin^2 \frac{\theta}{2} \right), \quad (41)$$

or

$$\frac{d\sigma}{d\Omega} = \left( \frac{d\sigma}{d\Omega} \right)_{\text{Rutherford}} \frac{\left( 1 - \beta^2 \sin^2 \frac{\theta}{2} \right)}{(1 - \beta^2)}, \quad (42)$$

where the modification of the nonrelativistic result is shown very explicitly. (We have put  $Z_1 = Z$ ,  $Z_2 = -1$ ,  $\mu \approx m$ , in the Rutherford formula, as derived in eq. (16) of Chapter 46.)

## Dirac Equation for a Particle in an Electromagnetic Field

The electromagnetic scalar and vector potentials,  $\Phi$  and  $\vec{A}$ , combine to form a Lorentz four-vector. (See J. D. Jackson, *Classical Electrodynamics*, New York: John Wiley, 1975.)

$$A^\mu = (A^0, A^i) = (\Phi, \vec{A}), \quad A_\mu = (A_0, A_i) = (\Phi, -\vec{A}). \quad (1)$$

Therefore, if we modify the four-momentum operator,

$$P_\mu = \frac{\hbar}{i} \frac{\partial}{\partial x^\mu} \longrightarrow P_\mu + \frac{e}{c} A_\mu, \quad (2)$$

the Dirac equation for a relativistic particle of charge,  $e$ , and rest mass,  $m$ , in an external field derivable from the potential,  $A_\mu$ , would be

$$\gamma^\mu \left( \frac{\partial}{\partial x^\mu} + \frac{i}{\hbar c} e A_\mu \right) \psi + \frac{imc}{\hbar} \psi = 0, \quad (3)$$

or

$$\left( \frac{\gamma^0}{c} \frac{\partial}{\partial t} + \frac{i}{\hbar} \gamma^0 \frac{e}{c} \Phi + \vec{\gamma} \cdot \left( \vec{\nabla} - \frac{i}{\hbar c} \vec{A} \right) + \frac{imc}{\hbar} \right) \psi = 0. \quad (4)$$

Left-multiplying by  $\gamma^0 = \beta$ , this equation can be rewritten in the Hamiltonian form

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = \left( V + c \vec{\alpha} \cdot \left( \frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A} \right) + \beta m c^2 \right) \psi, \quad (5)$$

with  $e\Phi = V$ , where the momentum operator has been augmented by the vector potential term

$$\vec{p} \rightarrow \vec{\Pi} = \left( \frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A} \right). \quad (6)$$

## A Nonrelativistic Limit of the Dirac Equation

Let us decompose the above  $4 \times 1$  matrix  $\psi$  into two  $2 \times 1$  matrices and factor out the time-dependence, which arises from the rest energy  $E_{\text{rest}} = mc^2$ , by setting

$$\psi = \begin{pmatrix} \psi_A e^{-\frac{i}{\hbar} mc^2 t} \\ \psi_B e^{-\frac{i}{\hbar} mc^2 t} \end{pmatrix} \quad (7)$$

to decompose eq. (5) into the two equations

$$\begin{aligned} -\frac{\hbar}{i} \frac{\partial \psi_A}{\partial t} &= V \psi_A + c(\vec{\sigma} \cdot \vec{\Pi}) \psi_B + (mc^2 - mc^2) \psi_A, \\ -\frac{\hbar}{i} \frac{\partial \psi_B}{\partial t} &= V \psi_B + c(\vec{\sigma} \cdot \vec{\Pi}) \psi_A - 2mc^2 \psi_B. \end{aligned} \quad (8)$$

Now, let us look at the extreme nonrelativistic limit for which

$$-\frac{\hbar}{i} \frac{\partial \psi_B}{\partial t} \quad \text{and} \quad V \psi_B$$

are both negligible compared with  $2mc^2 \psi_B$ . Note,

$$-\frac{\hbar}{i} \frac{\partial \psi_B}{\partial t} \text{ is of order } (E - mc^2) \psi_B,$$

that is, of order of a nonrelativistic energy negligible compared with  $2mc^2$  in the extreme nonrelativistic limit. In this limit, therefore, the second of the two equations above can be solved for  $\psi_B$  to give

$$\psi_B = \frac{1}{2mc} (\vec{\sigma} \cdot \vec{\Pi}) \psi_A + \dots, \quad (9)$$

to give the Schrödinger limit

$$-\frac{\hbar}{i} \frac{\partial \psi_A}{\partial t} = \left( V + \frac{1}{2m} (\vec{\sigma} \cdot \vec{\Pi})(\vec{\sigma} \cdot \vec{\Pi}) \right) \psi_A. \quad (10)$$

With  $\vec{A} = 0$ , so  $(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p}) = (\vec{p} \cdot \vec{p})$  [see eq. (11) of Chapter 72], the above is the Schrödinger equation, so in this limit  $\psi_A \rightarrow \psi_{\text{Schrodinger}}$ . (Remember, however,  $\psi_A$  has two components!)

In the presence of an external magnetic field derivable from  $\vec{A}$ , we get additional terms, now

$$\begin{aligned} (\vec{\sigma} \cdot \vec{\Pi})(\vec{\sigma} \cdot \vec{\Pi}) &= \sum_{j=1}^3 \sigma_j^2 \Pi_j^2 + \sum_{j < k} \sigma_j \sigma_k \Pi_j \Pi_k + \sigma_k \sigma_j \Pi_k \Pi_j \\ &= \vec{\Pi} \cdot \vec{\Pi} + i \epsilon_{jkl} \sigma_l [\Pi_j, \Pi_k], \end{aligned} \quad (11)$$

using for the moment ordinary 3-D vector index notation. With  $\Pi_j = p_j - \frac{e}{c} A_j$ , we now get

$$[\Pi_j, \Pi_k] = -\frac{e\hbar}{ci} \left( \frac{\partial A_k}{\partial x_j} - \frac{\partial A_j}{\partial x_k} \right), \quad (12)$$

and

$$i\epsilon_{jkl}\sigma_l [\Pi_j, \Pi_k] = -\frac{e\hbar\vec{\sigma}}{c} \cdot [\vec{\nabla} \times \vec{A}] = -\frac{e\hbar\vec{\sigma}}{c} \cdot \vec{B}, \quad (13)$$

so

$$-\frac{\hbar}{i} \frac{\partial \psi_A}{\partial t} = \left( V + \frac{1}{2m} (\vec{p} - \frac{e}{c} \vec{A}) \cdot (\vec{p} - \frac{e}{c} \vec{A}) - \frac{e\hbar}{2mc} \vec{\sigma} \cdot \vec{B} \right) \psi_A + \dots \quad (14)$$

The spin-magnetic moment interaction with an external field  $\vec{B}$  comes out of the nonrelativistic limit of the Dirac equation *automatically*. Moreover, it gives the correct  $g_s$ -factor, because

$$-\frac{e\hbar}{2mc} \vec{\sigma} \cdot \vec{B} = -\frac{e\hbar}{2mc} g_s \vec{s} \cdot \vec{B}, \quad \text{with } g_s = 2, \quad (15)$$

because  $\vec{s} = \frac{1}{2}\vec{\sigma}$ . Note: Before Dirac, the spin-magnetic moment term was put into the theory by hand by Uhlenbeck and Goudsmit and the  $g_s$  value was set equal to  $g_s = 2$  empirically to fit the observed spectroscopic data! Finally, in a uniform magnetic field,  $\vec{B}_0$ , with  $\vec{A} = -\frac{1}{2}[\vec{r} \times \vec{B}_0]$ , we get the extreme nonrelativistic limit

$$-\frac{\hbar}{i} \frac{\partial \psi_A}{\partial t} = \left( V + \frac{1}{2m} (\vec{p} \cdot \vec{p}) - \frac{e\hbar}{2mc} (\vec{l} + \vec{\sigma}) \cdot \vec{B}_0 + \frac{e^2}{8mc^2} (r^2 B_0^2 - (\vec{r} \cdot \vec{B}_0)^2) \right) \psi_A + \dots \quad (16)$$

Both the orbital and spin-magnetic moment terms are present, and with their correct  $g$  factors.

## B Angular Momentum

Consider next a Hamiltonian with no external magnetic fields, i.e., with  $\vec{A} = 0$ , and with a spherically symmetric scalar potential,  $\Phi = \Phi(r)$ , and possibly an additional spherically symmetric potential,  $\bar{V}(r)$ , i.e., with a total potential,  $V(r) = \bar{V}(r) + e\Phi(r)$ . Now,

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = H\psi = \left( V(r) + c\gamma^0 \vec{\gamma} \cdot \frac{\hbar}{i} \vec{\nabla} + \gamma^0 mc^2 \right) \psi, \quad (17)$$

where we have gone back to the full relativistic equation and  $\psi$  is the full four-component  $\psi$ . The orbital angular momentum operator,  $[\vec{r} \times \vec{p}]$ , does not commute with this  $H$  because of the presence of the  $c\gamma^0 \vec{\gamma} \cdot \frac{\hbar}{i} \vec{\nabla}$  term. Of course, we still have  $[\vec{L}, V(r)] = 0$ , as in the nonrelativistic theory, but now  $[H, L_j] \neq 0$  because of the  $c\gamma^0 \vec{\gamma} \cdot \vec{p}$  part of  $H$ . Let us express the  $j^{th}$  component of  $\vec{L}$  by

$$L_j = \epsilon_{jmk} x^m p^k,$$

with summation convention for repeated Latin indices, so  $m$  and  $k$  run from  $1 \rightarrow 3$ . Then,

$$[H, L_j] = [c\gamma^0\gamma^l \frac{\hbar}{i} \frac{\partial}{\partial x^l}, \epsilon_{jmk}x^m p^k] = \frac{\hbar c}{i} \epsilon_{jlk}\gamma^0\gamma^l p^k. \quad (18)$$

Now, let us define

$$\Sigma_j = \epsilon_{jmk} \frac{i}{2} \gamma^m \gamma^k, \quad (\Sigma_1 = i\gamma^2\gamma^3, \Sigma_2 = i\gamma^3\gamma^1, \Sigma_3 = i\gamma^1\gamma^2). \quad (19)$$

(Recall the generators of the pure rotation operators from Chapter 70.) We consider the commutator

$$[H, \frac{\hbar}{2}\Sigma_j] = \frac{ci\hbar}{4} [\gamma^0\gamma^l p_l, \epsilon_{jmk}\gamma^m\gamma^k] = \frac{ci\hbar}{4} \gamma^0 \epsilon_{jmk} [\gamma^l, \gamma^m\gamma^k] p_l. \quad (20)$$

From the Dirac relations, we have

$$[\gamma^l, \gamma^m\gamma^k] = 2g^{lm}\gamma^k - 2g^{lk}\gamma^m, \quad \text{with } g^{ll} = -1, \quad g^{lm} = 0 \text{ for } l \neq m, \quad (21)$$

so

$$\begin{aligned} [H, \frac{\hbar}{2}\Sigma_j] &= \frac{ci\hbar}{4} \epsilon_{jmk} \gamma^0 (-2\gamma^k p^m + 2\gamma^m p^k) \\ &= \frac{ci\hbar}{2} \gamma^0 (-\epsilon_{jmk} \gamma^k p^m + \epsilon_{jmk} \gamma^m p^k) \\ &= i\hbar c \gamma^0 \epsilon_{jlk} \gamma^l p^k. \end{aligned} \quad (22)$$

Combining eqs. (18) and (22),

$$[H, L_j + \frac{\hbar}{2}\Sigma_j] = 0. \quad (23)$$

Also,

$$\Sigma_1 = \begin{pmatrix} \sigma_x & \mathbf{0} \\ \mathbf{0} & \sigma_x \end{pmatrix}, \quad \Sigma_2 = \begin{pmatrix} \sigma_y & \mathbf{0} \\ \mathbf{0} & \sigma_y \end{pmatrix}, \quad \Sigma_3 = \begin{pmatrix} \sigma_z & \mathbf{0} \\ \mathbf{0} & \sigma_z \end{pmatrix}. \quad (24)$$

It is thus natural to define the total angular momentum operator

$$J_j = L_j + \frac{\hbar}{2}\Sigma_j = \hbar(\bar{L}_j \mathbf{1} + \frac{1}{2}\Sigma_j), \quad (25)$$

where now  $\bar{L}$  and  $\frac{1}{2}\bar{\Sigma}$  are the dimensionless orbital and spin angular momentum operators. Note: It is the total angular momentum operator which commutes with the Hamiltonian with a spherically symmetric  $V(r)$ .

Also, the plane wave solutions of Chapter 72 have been chosen such that they are eigenstates of  $\Sigma_3$ , if the  $z$  direction is chosen parallel to  $\vec{p}$ . The eigenvalues of  $\Sigma_3$  are +1 for states  $u^{(1)}$  and  $u^{(3)}$ , and -1 for states  $u^{(2)}$  and  $u^{(4)}$ , because

$$\Sigma_3 \begin{pmatrix} 1 \\ \mathbf{0} \\ \frac{cp}{E+mc^2} \\ \mathbf{0} \end{pmatrix} = +1 \begin{pmatrix} 1 \\ \mathbf{0} \\ \frac{cp}{E+mc^2} \\ \mathbf{0} \end{pmatrix}, \quad \Sigma_3 \begin{pmatrix} \frac{cp}{E-mc^2} \\ 0 \\ 1 \\ \mathbf{0} \end{pmatrix} = +1 \begin{pmatrix} \frac{cp}{E-mc^2} \\ 0 \\ 1 \\ \mathbf{0} \end{pmatrix}, \quad (26)$$

and

$$\Sigma_3 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{-cp}{E+mc^2} \end{pmatrix} = -1 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{-cp}{E+mc^2} \end{pmatrix}, \quad \Sigma_3 \begin{pmatrix} 0 \\ \frac{-cp}{E-mc^2} \\ 0 \\ 1 \end{pmatrix} = -1 \begin{pmatrix} 0 \\ \frac{-cp}{E-mc^2} \\ 0 \\ 1 \end{pmatrix}. \quad (27)$$

Final Note: In Chapter 70 you should perhaps have been worried we seemingly obtained the “wrong” sign of the generator,  $G_{12}^{\text{intr.}}$ , relative to that of  $G_{12}^{\text{orb.}}$ . Recall we concluded

$$e^{-i\theta_{12}G_{12}^{\text{intr.}}} = e^{+i\frac{\theta_{12}}{2}\Sigma_3},$$

whereas

$$e^{-i\theta_{12}G_{12}^{\text{orb.}}} = e^{-i\theta_{12}L_z},$$

the latter in agreement with our earlier nonrelativistic rotation theory. But note that  $L_z$  was defined, however, by

$$L_z = \frac{1}{i} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = \frac{1}{i} \left( x^1 \frac{\partial}{\partial x^2} - x^2 \frac{\partial}{\partial x^1} \right) = (x^1 p_2 - x^2 p_1),$$

and, therefore,

$$L_z = -L_3 = -(x^1 p^2 - x^2 p^1).$$

## Pauli Approximation to the Dirac Equation

In the last chapter, we examined the extreme nonrelativistic limit of the Dirac equation and saw that the first two components of  $\psi$  lead to Schrödinger theory,  $\psi_A \rightarrow \psi_{\text{Schroedinger}}$ , the two components of  $\psi_A$  being related to the two spin components of the electron, whereas the third and fourth components, in the form of  $\psi_B$ , were smaller by a factor of order  $p/mc$ . We now want to carry this one step further following an approach first carried through by Pauli. Again, let

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} e^{-\frac{i}{\hbar}mc^2 t}, \quad (1)$$

so, again,

$$\begin{aligned} -\frac{\hbar}{i} \frac{\partial \psi_A}{\partial t} &= V\psi_A + c(\vec{\sigma} \cdot \vec{\Pi})\psi_B, \\ -\frac{\hbar}{i} \frac{\partial \psi_B}{\partial t} &= V\psi_B + c(\vec{\sigma} \cdot \vec{\Pi})\psi_A - 2mc^2\psi_B, \end{aligned} \quad (2)$$

with  $V = e\Phi$ , and  $\vec{\Pi} = \vec{p} - \frac{e}{c}\vec{A}$ . Rewriting the second of these two equations, we have

$$\psi_B = \frac{1}{2mc^2} \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right) \psi_B + \frac{c(\vec{\sigma} \cdot \vec{\Pi})}{2mc^2} \psi_A. \quad (3)$$

Now, in the first term on the right-hand side, we can substitute the zeroth-order approximation for  $\psi_B$  because the operators  $\frac{\hbar}{i} \frac{\partial}{\partial t}$  and  $V$  lead to quantities of order  $E_{\text{nonrelativistic}} \ll 2mc^2$ . In zeroth order, we had

$$\psi_B = \frac{(\vec{\sigma} \cdot \vec{\Pi})}{2mc} \psi_A + \dots, \quad (4)$$

so eq. (3) leads to

$$\psi_B = \frac{1}{4m^2c^3} \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right) (\vec{\sigma} \cdot \vec{\Pi}) \psi_A + \frac{(\vec{\sigma} \cdot \vec{\Pi})}{2mc} \psi_A + \dots . \quad (5)$$

Now, substituting this back into the equation for  $\psi_A$ , we get an equation for  $\psi_A$  in the form,

$$-\frac{\hbar}{i} \frac{\partial \psi_A}{\partial t} = H \psi_A,$$

with

$$\begin{aligned} H \psi_A &= V \psi_A \\ &+ \frac{1}{2m} (\vec{\sigma} \cdot \vec{\Pi}) (\vec{\sigma} \cdot \vec{\Pi}) \psi_A + \frac{(\vec{\sigma} \cdot \vec{\Pi})}{4m^2c^2} \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right) (\vec{\sigma} \cdot \vec{\Pi}) \psi_A + \dots \\ &= \left( \frac{1}{2m} (\vec{\Pi} \cdot \vec{\Pi}) + V - \frac{e\hbar}{2mc} (\vec{\sigma} \cdot \vec{B}) \right) \psi_A + \frac{(\vec{\sigma} \cdot \vec{\Pi})}{4m^2c^2} \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right) (\vec{\sigma} \cdot \vec{\Pi}) \psi_A \\ &+ \dots . \end{aligned} \quad (6)$$

The normalization for a single-particle relativistic theory would be, however,

$$\int d\vec{r} (\psi_A^\dagger \psi_A + \psi_B^\dagger \psi_B) = 1, \quad (7)$$

and, with  $\psi_B \approx (\vec{\sigma} \cdot \vec{\Pi}) \psi_A / 2mc$ , this would be

$$\int d\vec{r} \psi_A^\dagger \left( 1 + \frac{1}{4m^2c^2} (\vec{\sigma} \cdot \vec{\Pi}) (\vec{\sigma} \cdot \vec{\Pi}) + \dots \right) \psi_A = 1, \quad (8)$$

whereas, for the nonrelativistic approximation, we should have had

$$\int d\vec{r} \psi^\dagger \psi = 1. \quad (9)$$

To order  $p^2/m^2c^2$ , if we renormalize  $\psi$  with an operator  $\Omega$

$$\begin{aligned} \psi &= \Omega \psi_A = \left( 1 + \frac{1}{8m^2c^2} (\vec{\sigma} \cdot \vec{\Pi}) (\vec{\sigma} \cdot \vec{\Pi}) + \dots \right) \psi_A, \\ \psi^\dagger &= \psi_A^\dagger \left( 1 + \frac{1}{8m^2c^2} (\vec{\sigma} \cdot \vec{\Pi}) (\vec{\sigma} \cdot \vec{\Pi}) + \dots \right), \end{aligned} \quad (10)$$

or

$$\psi_A = \Omega^{-1} \psi = \left( 1 - \frac{1}{8m^2c^2} (\vec{\sigma} \cdot \vec{\Pi}) (\vec{\sigma} \cdot \vec{\Pi}) + \dots \right) \psi. \quad (11)$$

With this transformation, eq. (6) can be rewritten

$$-\frac{\hbar}{i} \frac{\partial \psi_A}{\partial t} = H \psi_A \quad \rightarrow \quad -\frac{\hbar}{i} \frac{\partial (\Omega^{-1} \psi)}{\partial t} = H (\Omega^{-1} \psi), \quad (12)$$

or, left-multiplying with the operator  $\Omega^{-1}$ ,

$$-\frac{\hbar}{i} \left( \Omega^{-1} \frac{\partial}{\partial t} \Omega^{-1} \right) \psi = (\Omega^{-1} H \Omega^{-1}) \psi, \quad (13)$$

leading to

$$\begin{aligned} & -\frac{\hbar}{i} \frac{\partial \psi}{\partial t} + \frac{1}{8m^2c^2} \left( (\vec{\sigma} \cdot \vec{\Pi})^2 \frac{\hbar}{i} \frac{\partial}{\partial t} + \frac{\hbar}{i} \frac{\partial}{\partial t} (\vec{\sigma} \cdot \vec{\Pi})^2 \right) \psi + \dots \\ & = \left( H - \frac{1}{8m^2c^2} (H(\vec{\sigma} \cdot \vec{\Pi})^2 + (\vec{\sigma} \cdot \vec{\Pi})^2 H) + \dots \right) \psi, \end{aligned} \quad (14)$$

or

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = H' \psi, \quad (15)$$

with

$$\begin{aligned} H' &= H - \frac{1}{8m^2c^2} \left[ \left( (\vec{\sigma} \cdot \vec{\Pi})^2 \frac{\hbar}{i} \frac{\partial}{\partial t} + \frac{\hbar}{i} \frac{\partial}{\partial t} (\vec{\sigma} \cdot \vec{\Pi})^2 \right) \right. \\ &\quad \left. + \left( \left( \frac{(\vec{\sigma} \cdot \vec{\Pi})^2}{2m} + V \right) (\vec{\sigma} \cdot \vec{\Pi})^2 + (\vec{\sigma} \cdot \vec{\Pi})^2 \left( \frac{(\vec{\sigma} \cdot \vec{\Pi})^2}{2m} + V \right) \right) \right] + \dots \\ &= \frac{(\vec{\sigma} \cdot \vec{\Pi})^2}{2m} + V + \frac{1}{4m^2c^2} (\vec{\sigma} \cdot \vec{\Pi}) \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right) (\vec{\sigma} \cdot \vec{\Pi}) \\ &\quad - \frac{1}{8m^2c^2} \left[ (\vec{\sigma} \cdot \vec{\Pi})^2 \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right) + \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right) (\vec{\sigma} \cdot \vec{\Pi})^2 + \frac{1}{m} (\vec{\sigma} \cdot \vec{\Pi})^4 \right] \\ &\quad + \dots, \end{aligned} \quad (16)$$

so  $H'$  can be written with the help of a double commutator as

$$H' = \frac{(\vec{\sigma} \cdot \vec{\Pi})^2}{2m} + V - \frac{1}{8m^2c^2} [(\vec{\sigma} \cdot \vec{\Pi}), [(\vec{\sigma} \cdot \vec{\Pi}), \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right)]] - \frac{1}{8m^3c^2} (\vec{\sigma} \cdot \vec{\Pi})^4. \quad (17)$$

The first commutator gives

$$\begin{aligned} [(\vec{\sigma} \cdot \vec{\Pi}), \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + V \right)] &= \vec{\sigma} \cdot [(\vec{p} - \frac{e}{c} \vec{A}), \left( \frac{\hbar}{i} \frac{\partial}{\partial t} + e\Phi \right)] \\ &= -\frac{e\hbar}{i} \vec{\sigma} \cdot \left( -\vec{\nabla}\Phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \right) = -\frac{e\hbar}{i} (\vec{\sigma} \cdot \vec{\mathcal{E}}). \end{aligned} \quad (18)$$

This leads to the second commutator (using for the moment ordinary 3-D vector index notation),

$$\begin{aligned} [(\vec{\sigma} \cdot \vec{\Pi}), (\vec{\sigma} \cdot \vec{\mathcal{E}})] &= \sigma_k \sigma_j [\Pi_k, \mathcal{E}_j] + [\sigma_k, \sigma_j] \mathcal{E}_j \Pi_k \\ &= (\delta_{kj} + i \epsilon_{kjl} \sigma_l) \frac{\hbar}{i} \frac{\partial \mathcal{E}_j}{\partial x_k} - 2i \epsilon_{jkl} \sigma_l \mathcal{E}_j \Pi_k \\ &= \frac{\hbar}{i} (\vec{\nabla} \cdot \vec{\mathcal{E}}) + \hbar \vec{\sigma} \cdot [\vec{\nabla} \times \vec{\mathcal{E}}] - 2i \vec{\sigma} \cdot [\vec{\mathcal{E}} \times \vec{\Pi}]. \end{aligned} \quad (19)$$

With this result, we then have

$$\begin{aligned} H' &= \frac{(\vec{\sigma} \cdot \vec{\Pi})^2}{2m} + e\Phi - \frac{e\hbar}{4m^2c^2} (\vec{\sigma} \cdot [\vec{\mathcal{E}} \times \vec{\Pi}]) \\ &\quad - \frac{e\hbar^2}{8m^2c^2} (\vec{\nabla} \cdot \vec{\mathcal{E}}) - \frac{e\hbar^2}{8m^2c^2} i \vec{\sigma} \cdot [\vec{\nabla} \times \vec{\mathcal{E}}] - \frac{1}{8m^3c^2} (\vec{\sigma} \cdot \vec{\Pi})^4, \end{aligned} \quad (20)$$

where this  $H'$  includes relativistic corrections to the zeroth-order problem through terms of order  $\beta^2 \times$  (zeroth order terms). In the special case, when no external magnetic fields exist, so  $\vec{A} = 0$  and

$$[\vec{\nabla} \times \vec{\mathcal{E}}] = -\frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0,$$

we have

$$H' = \frac{\vec{p}^2}{2m} + V - \frac{e\hbar}{4m^2c^2} (\vec{\sigma} \cdot [\vec{\mathcal{E}} \times \vec{p}]) - \frac{e\hbar^2}{8m^2c^2} (\vec{\nabla} \cdot \vec{\mathcal{E}}) - \frac{(\vec{p}^2)^2}{8m^3c^2}. \quad (21)$$

The very last term is easily recognized as the relativistic mass correction to the kinetic energy term, because

$$E - mc^2 = \sqrt{(m^2c^4 + c^2 p^2)} - mc^2 = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \dots . \quad (22)$$

If the electric fields,  $\vec{\mathcal{E}}$ , are those of a spherically symmetric potential, e.g., the Coulomb potential in a one-electron atom,  $\vec{\mathcal{E}} = -\vec{\nabla}\Phi = -\frac{1}{r}\vec{\nabla}V$  and the first correction term to the zeroth-order nonrelativistic energy becomes

$$-\frac{e\hbar}{4m^2c^2} (\vec{\sigma} \cdot [\vec{\mathcal{E}} \times \vec{p}]) = \frac{\hbar}{4m^2c^2} \vec{\sigma} \cdot \left( \frac{1}{r} \frac{dV}{dr} [\vec{r} \times \vec{p}] \right) = \frac{\hbar^2}{2m^2c^2} (\vec{s} \cdot \vec{l}) \frac{1}{r} \frac{dV}{dr}. \quad (23)$$

This term gives the combined internal magnetic field spin-orbit coupling term and the Thomas precession term. We see again that it was not put into the theory "by hand" but falls automatically out of the Dirac theory. Finally, the  $\vec{\nabla} \cdot \vec{\mathcal{E}}$  term, which is known as the Darwin term, can be written via Maxwell's equations as

$$\vec{\nabla} \cdot \vec{\mathcal{E}} = 4\pi\rho_{\text{charge}} = 4\pi Ze\delta(\vec{r} = 0) \quad (24)$$

for a one-electron atom. The Darwin term, therefore, can in this case be rewritten as (remembering the electron  $e$  is negative, whereas the nuclear charge  $Ze$  is positive)

$$-\frac{e\hbar^2}{8m^2c^2} \vec{\nabla} \cdot \vec{\mathcal{E}} = \frac{4\pi Ze^2\hbar^2}{8m^2c^2} \delta(\vec{r} = 0), \quad (25)$$

leading to an energy correction in a hydrogenic atom of

$$\Delta E_{nlm} = \frac{4\pi Ze^2\hbar^2}{8m^2c^2} |\psi_{nlm}(\vec{r} = 0)|^2 = \frac{4\pi Ze^2\hbar^2}{8m^2c^2} \delta_{l0} \frac{1}{4\pi} \left( \frac{4Z^3}{n^3 a_0^3} \right) = \frac{me^4 \alpha^2 Z^4}{\hbar^2} \frac{1}{2} \frac{n^4}{n^3} \delta_{l0}. \quad (26)$$

The spin orbit term in a hydrogenic atom, with  $V(r) = -Ze^2/r$ , is

$$\frac{me^4 \alpha^2}{\hbar^2} \frac{Z}{2} \frac{1}{(r/a_0)^3} (\vec{s} \cdot \vec{l}), \quad (27)$$

leading to an energy correction [see eq. (13) of Chapter 26].

$$\Delta E_{nlj} = \frac{me^4 \alpha^2}{\hbar^2} \frac{Z^4}{2} \frac{1}{n^3 l(l + \frac{1}{2})(l + 1)} \times \begin{cases} +\frac{l}{2} & \text{for } j = (l + \frac{1}{2}) \\ -\frac{(l+1)}{2} & \text{for } j = (l - \frac{1}{2}) \end{cases}. \quad (28)$$

For  $l = 0$ ,  $j = \frac{1}{2}$ , the matrix element of  $(\vec{l} \cdot \vec{s})$  is equal to zero. If we take the above formula of eq. (28) and cancel the factor  $l$  in numerator and denominator and then set  $l = 0$ , we get the  $l = 0$ ,  $j = \frac{1}{2}$  result of the Darwin term. Rigorously, this result comes out of the Darwin term and not the  $(\vec{l} \cdot \vec{s})$  term. (In Chapter 26, we “cheated”!!) The rigorous derivation from the Pauli approximation to the Dirac equation gives the  $l = 0$  result via the Darwin term.

## A The Foldy–Wouthuysen Transformation

The uncoupling of the first two components of the Dirac equation from the third and fourth components via the Pauli approximation in a perturbation expansion naturally leads to the question: Is it possible to transform the Dirac Hamiltonian to a new form in which the third and fourth components are completely uncoupled from the first two components? The answer is yes, at least for the free particle with Hamiltonian,  $H = c(\vec{\alpha} \cdot \vec{p}) + \beta mc^2$ . In this case, the transformation was achieved by Foldy and Wouthuysen.

Foldy and Wouthuysen sought a transformation

$$\psi \rightarrow \psi' = U\psi, \quad H \rightarrow H' = UHU^\dagger, \quad (29)$$

via a unitary operator  $U = e^{iG}$  such that the  $4 \times 4$  matrices within  $H'$  factor into a direct sum of  $2 \times 2$  matrices. From our knowledge of Lorentz transformations, one might seek unitary operators of the form

$$U = e^{i(-i\theta\beta\vec{\alpha} \cdot \vec{p})} = \cos(p\theta)\mathbf{1} + \beta(\vec{\alpha} \cdot \frac{\vec{p}}{p})\sin(p\theta), \quad (30)$$

where  $\theta$  is a function of  $p$  and we have used

$$(\beta\vec{\alpha} \cdot \vec{p})(\beta\vec{\alpha} \cdot \vec{p}) = -(\vec{\alpha} \cdot \vec{p})(\vec{\alpha} \cdot \vec{p}) = -p^2\mathbf{1}. \quad (31)$$

The actual solution gives

$$U = \left( \sqrt{\frac{mc^2 + |E|}{2|E|}}\mathbf{1} + \frac{c\beta\vec{\alpha} \cdot \vec{p}}{\sqrt{2|E|(mc^2 + |E|)}} \right). \quad (32)$$

This equation leads to

$$\begin{aligned} H'_{\text{F.W.}} &= UHU^\dagger \\ &= \left( \sqrt{\frac{mc^2 + |E|}{2|E|}}\mathbf{1} + \frac{c\beta\vec{\alpha} \cdot \vec{p}}{\sqrt{2|E|(mc^2 + |E|)}} \right)(c\vec{\alpha} \cdot \vec{p} + \beta mc^2)U^\dagger \\ &= \left( \frac{\beta}{2}\sqrt{2|E|(mc^2 + |E|)} + \frac{c(\vec{\alpha} \cdot \vec{p})\sqrt{2|E|}}{2\sqrt{(mc^2 + |E|)}} \right) \\ &\quad \times \left( \sqrt{\frac{mc^2 + |E|}{2|E|}}\mathbf{1} + \frac{c(\vec{\alpha} \cdot \vec{p})\beta}{\sqrt{2|E|(mc^2 + |E|)}} \right) \end{aligned}$$

$$\begin{aligned}
&= \left( \frac{c}{2} [(\vec{\alpha} \cdot \vec{p}) + \beta(\vec{\alpha} \cdot \vec{p})\beta] \right) + \frac{\beta}{2} \left( (mc^2 + |E|) + \frac{c^2 p^2}{(mc^2 + |E|)} \right) \\
&= \begin{pmatrix} 0 \\ +\beta|E| \end{pmatrix} \\
&= +\beta \sqrt{m^2 c^4 + c^2 p^2}.
\end{aligned} \tag{33}$$

The Dirac equation in  $\psi'$  thus separates into the two equations

$$\begin{aligned}
H'_{\text{F.W.}} \psi'_A &= +\sqrt{m^2 c^4 + c^2 p^2} \psi'_A, \\
H'_{\text{F.W.}} \psi'_B &= -\sqrt{m^2 c^4 + c^2 p^2} \psi'_B.
\end{aligned} \tag{34}$$

For a particle in an arbitrary electromagnetic field, a successful analogue of the Foldy–Wouthuysen transformation has not been found. An expansion in powers of  $p/mc$ , however, can be carried out systematically with the unitary operator

$$U = e^{i\lambda G}, \quad \text{with } i\lambda G = \frac{\beta(\vec{\alpha} \cdot \vec{\Pi})}{2mc}. \tag{35}$$

# The Klein Paradox: An Example from the History of Negative Energy State Difficulties: The Positron Interpretation

One of the simplest problems, first solved in the earliest days of the Dirac theory, is the 1-D motion of a free particle reflected or transmitted at a discrete potential step. Suppose the particle moves in the  $z$  direction under the influence of a potential such that

$$V(z) = 0 \quad \text{for } z < 0, \quad V(z) = +V_0 \quad \text{for } z > 0, \quad (1)$$

where we assume,  $V_0 > 0$ . The solution will be independent of the spin of the electron. Let us therefore choose an electron with spin projection in the  $+z$  direction. We shall choose a positive-energy solution. In region I, for  $z < 0$ , we expect plane waves moving both to the left and to the right. Therefore, for  $z \leq 0$ ,

$$\psi = A \begin{pmatrix} 1 \\ 0 \\ \frac{cp}{E+mc^2} \\ 0 \end{pmatrix} e^{\frac{i}{\hbar}(pz-Et)} + B \begin{pmatrix} 1 \\ 0 \\ -\frac{cp}{E+mc^2} \\ 0 \end{pmatrix} e^{-\frac{i}{\hbar}(pz+Et)}, \quad (2)$$

with  $E > 0$ , and  $p = +\sqrt{(\frac{E^2}{c^2} - m^2 c^2)}$ , where  $A$  gives the amplitude of the incident wave traveling to the right, and  $B$  gives the amplitude of the reflected wave traveling to the left. From  $S_z = c\psi^\dagger \alpha_z \psi$ , we have

$$\begin{aligned} (S_z)_{\text{inc.}} &= cAA^*(1 \ 0 \ \frac{cp}{E+mc^2} \ 0) \begin{pmatrix} \frac{cp}{E+mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix} \\ &= \frac{2c^2 p}{E+mc^2} |A|^2 = \frac{c^2 p}{E} \psi_{\text{inc.}}^\dagger \psi_{\text{inc.}} = +v \psi_{\text{inc.}}^\dagger \psi_{\text{inc.}}. \end{aligned} \quad (3)$$

Similarly,

$$(S_z)_{\text{refl.}} = -\frac{2c^2 p}{E + mc^2} |B|^2 = -v \psi_{\text{refl.}}^\dagger \psi_{\text{refl.}}. \quad (4)$$

In region II, we would expect

$$\psi = C \begin{pmatrix} 1 \\ 0 \\ \frac{cp}{E - V_0 + mc^2} \\ 0 \end{pmatrix} e^{\frac{i}{\hbar}(\bar{p}z - Et)}, \quad (5)$$

so here

$$(S_z)_{\text{transm.}} = \frac{2c^2 \bar{p}}{(E - V_0 + mc^2)} |C|^2 = \frac{c^2 \bar{p}}{(E - V_0)} \psi_{\text{transm.}}^\dagger \psi_{\text{transm.}}, \quad (6)$$

where, now,

$$c^2 \bar{p}^2 = (E - V_0)^2 - m^2 c^4, \quad (7)$$

and

$$c \bar{p} = \pm \sqrt{(E - V_0)^2 - m^2 c^2} = \pm \sqrt{(E - V_0 - mc^2)(E - V_0 + mc^2)}. \quad (8)$$

Now, at the boundary,  $z = 0$ , the continuity of both the probability density and the probability current density,  $S_z$ , are satisfied by the continuity of  $\psi$ , but now this means all components of  $\psi$ . Therefore, this requires

$$(A - B) \frac{cp}{E + mc^2} = C \frac{c \bar{p}}{(E - V_0 + mc^2)}, \quad (9)$$

leading to

$$2A = \left[ 1 + \frac{c \bar{p}}{cp} \frac{(E + mc^2)}{(E - V_0 + mc^2)} \right] C, \\ 2B = \left[ 1 - \frac{c \bar{p}}{cp} \frac{(E + mc^2)}{(E - V_0 + mc^2)} \right] C, \quad (10)$$

leading to a reflection coefficient

$$R = \left| \frac{B}{A} \right|^2 = \left| \frac{\left[ 1 - \frac{c \bar{p}}{cp} \frac{(E + mc^2)}{(E - V_0 + mc^2)} \right]}{\left[ 1 + \frac{c \bar{p}}{cp} \frac{(E + mc^2)}{(E - V_0 + mc^2)} \right]} \right|^2. \quad (11)$$

Now, we must consider various cases, depending on the relative magnitudes of  $E$  and  $V_0$  (see Fig. 75.1).

Case 1.

$$V_0 < E - mc^2.$$

In this case, we would certainly expect a transmitted wave, with a kinetic energy in region II that is somewhat less than that in region I, and a momentum,  $\bar{p} > 0$ , and,

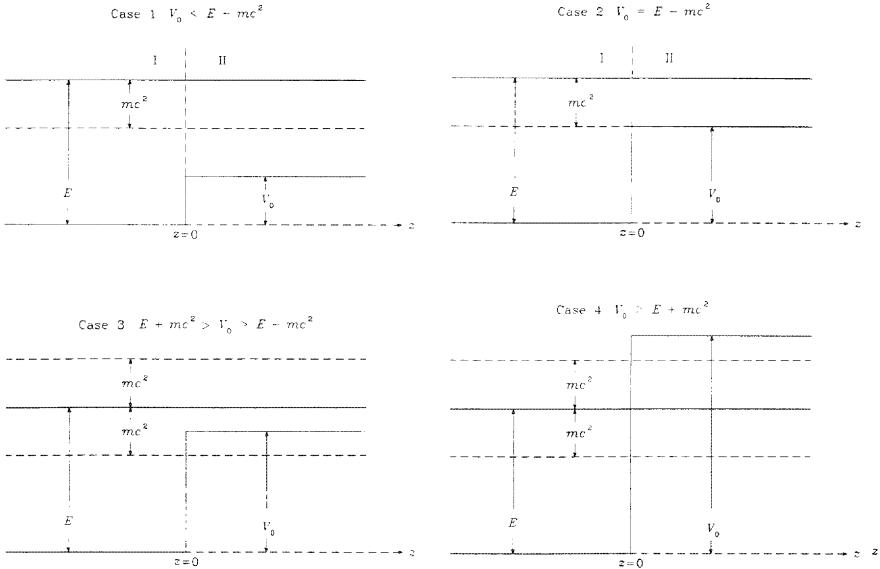


FIGURE 75.1. The four cases for free Dirac particle transmission and reflection at a potential step.

hence, a positive probability density current for  $z > 0$ , hence electrons moving to the right in region II. The reflection coefficient,  $R < 1$ , as expected.

Case 2.

$$V_0 = E - mc^2.$$

In this case,  $\bar{p} = 0$ . The reflection coefficient is  $R = 1$ , and hence the transmission coefficient,  $T = 0$ . Again, no surprises!

Case 3.

$$E + mc^2 > V_0 > E - mc^2.$$

In this case,  $\bar{p}$  is pure imaginary. The reflection coefficient,  $R = 1$ . The wave function in region II has an exponential decay, so  $\psi_{II} \rightarrow 0$  as  $z \rightarrow \infty$ . Still no surprises!

Case 4.

$$V_0 > E + mc^2.$$

In this case,  $\bar{p}$  is again real, but because  $(E - V_0 + mc^2)$  is a negative quantity and now

$$(S_z)_{\text{transm.}} = -\frac{2c^2 \bar{p}}{(V_0 - E - mc^2)} |C|^2. \quad (12)$$

Klein chose the negative root for  $\bar{p}$  [see eq. (8)], so

$$\frac{c\bar{p}}{(E - V_0 + mc^2)} = \sqrt{\frac{(V_0 - E + mc^2)}{(V_0 - E - mc^2)}}. \quad (13)$$

Klein thought (naturally for the time!)  $S_z$  had to be positive in the region  $z > 0$ . Thus, with

$$\frac{(E + mc^2)}{cp} = \sqrt{\frac{(E + mc^2)}{(E - mc^2)}}, \quad (14)$$

he obtained a reflection coefficient

$$R = \left[ \frac{1 - \sqrt{\frac{(V_0 - E + mc^2)(E + mc^2)}{(V_0 - E - mc^2)(E - mc^2)}}}{1 + \sqrt{\frac{(V_0 - E + mc^2)(E + mc^2)}{(V_0 - E - mc^2)(E - mc^2)}}} \right]^2. \quad (15)$$

In the limit in which  $V_0$  becomes large (let  $V_0 \rightarrow \infty$ ),

$$R \rightarrow \left[ \frac{1 - \frac{cp}{(E - mc^2)}}{1 + \frac{cp}{(E - mc^2)}} \right]^2 = \left[ \frac{1 - \frac{2cp}{E - mc^2} + \frac{E + mc^2}{E - mc^2}}{1 + \frac{2cp}{E - mc^2} + \frac{E + mc^2}{E - mc^2}} \right] = \frac{E - cp}{E + cp}. \quad (16)$$

Thus, in the limit of large  $V_0$ , Klein predicted reflection and transmission coefficients

$$R \rightarrow \frac{E - cp}{E + cp}, \quad T \rightarrow \frac{2cp}{E + cp}. \quad (17)$$

In particular, for  $v/c = \sqrt{\frac{1}{2}}$ , and therefore  $E = 1.1547mc^2$ , the transmission coefficient is  $T = .83$ . Klein of course expected no transmission and complete reflection in the limit of large potential barrier  $V_0$ . This "Klein Paradox" and similarly paradoxical situations bothered physicists in the earliest days of Dirac theory. Dirac came up with the solution: In the normal vacuum, all negative-energy states are completely filled. However, if one electron is taken out of a normally filled negative-energy state, the missing electron, a hole in the normally filled negative-energy sea, makes for a missing charge in a normally electrically neutral vacuum and thus behaves like a particle of charge  $+|e|$ . In this way, Dirac was led to the prediction of the existence of the positron.

## A Modern Hole Analysis of the Klein Barrier Reflection

According to Dirac's final interpretation, the Klein experiment must be understood in the following way. In region I, for  $z < 0$ , an electron with positive energy

$E = +\sqrt{(m^2c^4 + c^2p^2)}$  is placed in a level normally empty. However, if this  $E$  is such that  $E < V_0 - mc^2$ , in region II, for  $z > 0$ , all such levels are normally filled. The normal vacuum in this region thus consists of an infinite number of filled states with  $E$  negative relative to the reference energy  $V_0$ , with  $E < V_0 - mc^2$ . Now, if an electron from the beam in region I reaches the potential barrier at  $z = 0$ , it can knock an electron out of this filled sea, creating a hole in this negative-energy sea. This hole at  $z = 0$ , however, can be filled by an electron at  $z > 0$  with the same energy. When this electron has moved into the hole at  $z = 0$ , the hole at  $z > 0$  can be filled by another electron with this same  $E$  but at still greater values of  $z$ . Thus, an electron current from right to left exists, i.e., in a direction such that  $S_z$  is negative. Thus, with

$$S_z = \frac{2c\bar{p}}{(E - V_0 + mc^2)} |C|^2, \quad \text{and with } (E - V_0 + mc^2) < 0, \quad (18)$$

we need the *positive* root for  $\bar{p}$ ; that is,

$$c\bar{p} = +\sqrt{(V_0 - E + mc^2)(V_0 - E - mc^2)},$$

$$\text{so } \frac{c\bar{p}}{(E - V_0 + mc^2)} = -\sqrt{\frac{(V_0 - E + mc^2)}{(V_0 - E - mc^2)}}. \quad (19)$$

Substituting this equation into eq. (11), we get

$$R = \left[ \frac{1 + \sqrt{\frac{(V_0 - E + mc^2)(E + mc^2)}{(V_0 - E - mc^2)(E - mc^2)}}}{1 - \sqrt{\frac{(V_0 - E + mc^2)(E + mc^2)}{(V_0 - E - mc^2)(E - mc^2)}}} \right]^2. \quad (20)$$

Now, in the limit,  $V_0 \rightarrow \infty$ , we have

$$R \rightarrow \left[ \frac{1 + \frac{cp}{(E - mc^2)}}{1 - \frac{cp}{(E - mc^2)}} \right]^2 = \frac{E + cp}{E - cp} > 1. \quad (21)$$

This reflection coefficient is now greater than unity because the electrons knocked out of the filled negative-energy sea at  $z = 0$  can join the electrons reflected at the barrier, so the number of electrons in the reflected beam is greater than the number of electrons in the incident beam. In region II, however, for every electron that has joined the incident electrons in the reflected beam, there is a hole moving to the right. This appears to us like a positron moving to the right in region II. The electron current in region II, however, is from right to left, as electrons from further to the right fill holes to the left. Note, in particular, for  $v/c = \sqrt{\frac{1}{2}}$ ,

$$\lim_{V_0 \rightarrow \infty} R = \frac{\sqrt{2} + 1}{\sqrt{2} - 1} = 5.8. \quad (22)$$

Before justifying this perhaps surprisingly large number, a remark about sharp potential rises is in order. Our potential rises sharply from a value of zero to a large value at  $z = 0$ . This idealization of a realistic potential rise would be a good approximation if the actual distance,  $d$ , over which the rise occurs (see Fig. 75.2)

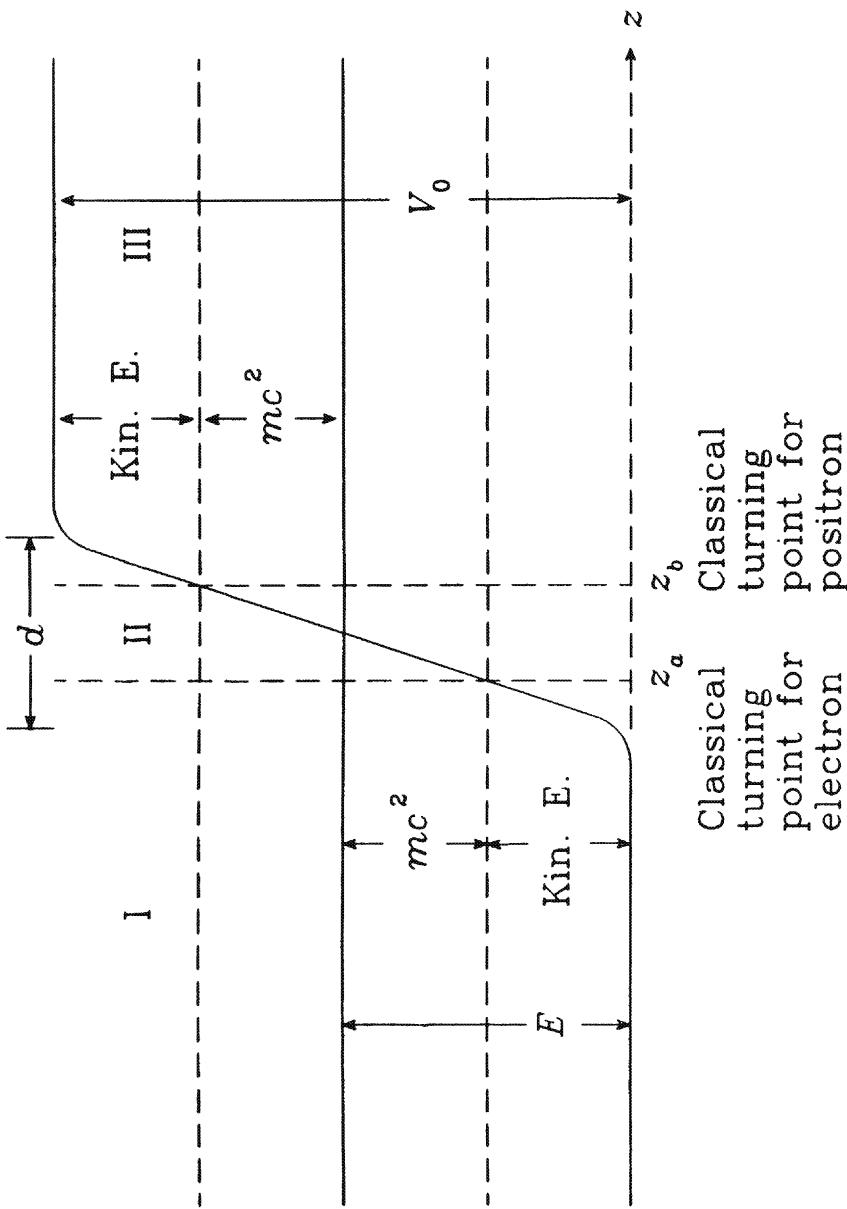


FIGURE 75.2. The tunneling of Dirac particles from the filled negative-energy sea for a potential step of finite width and height  $> 2mc^2$ .

is small compared with the relevant length parameter for the problem. This would be the Compton wavelength of the electron. Thus, our potential would be realistic, if

$$d \ll \frac{\hbar}{mc} = 4 \times (10)^{-11} \text{ cm}. \quad (23)$$

This result would be hard to achieve in a realistic setup!! In an actual experimental setup, the potential rise would look more like that shown in Fig. 75.2. Now, for an energy  $E$ , such that  $E + mc^2 < V_0$ , we need to consider three regions. In region I, we have the situation of case 1, considered above; i.e.,  $V(z) < E - mc^2$ . In region II between the points  $z = z_a$  and  $z = z_b$ , we have case 3, considered above; i.e.,  $E - mc^2 < V(z) < E + mc^2$ . In region II, therefore,  $\bar{p}(z)$  is pure imaginary. An exponential falloff with  $z$  exists in the wave function, starting at  $z = z_a$  and ending at  $z = z_b$ . In region III, with  $z > z_b$ , we have case 4, considered above. Here, we have oscillatory solutions, with holes (positrons) traveling to the right, but with an electron current to the left. Before the electrons knocked out of the filled negative-energy sea for  $z > z_b$  can reach to region I to join the reflected electrons from the incident beam, however, they must tunnel through a barrier, between  $z = z_a$  and  $z = z_b$ . This tunneling related to the exponential falloff in the wave function in this region will reduce the reflection coefficient from the large value exhibited above.

## Problems

45. If the 16  $\Gamma^A$  are defined as  $\mathbf{1}, \gamma^\mu, i\gamma^\mu\gamma^\nu, i\gamma^5\gamma^\mu, \gamma^5$  (note the extra factor  $i$  in the definition of  $i\gamma^5\gamma^\mu$ ), and if lower index  $\gamma$ 's are given by  $\gamma_0 = \gamma^0, \gamma_i = -\gamma^i$  for  $i = 1, 2, 3$ , but  $\gamma_5 = \gamma^5$ , show

$$\Gamma^A \Gamma_A = +\mathbf{1}$$

for all 16 cases, and

$$\text{trace}(\Gamma^A \Gamma_B) = 4\delta_B^A.$$

Use these two properties to show a general  $4 \times 4$  matrix  $\Gamma$  can be expanded by

$$\Gamma = \sum_{A=1}^{16} c_A \Gamma^A = \frac{1}{4} \sum_{A=1}^{16} \text{trace}(\Gamma \Gamma_A) \Gamma^A,$$

and show a specific matrix element,  $\Gamma_{ik}$ , can be written

$$\Gamma_{ik} = \frac{1}{4} \sum_{A=1}^{16} \sum_{l=1}^4 \sum_{m=1}^4 \Gamma_{lm} (\Gamma^A)_{ml} (\Gamma_A)_{ik},$$

with  $i, k$  fixed,  $i, k = 1, \dots, 4$ . (These Latin indices are here used to specify particular matrix elements of the  $4 \times 4$  matrices.) Use this property to show

$$(\bar{\psi}(a)\mathbf{1}\psi(b))(\bar{\psi}(c)\mathbf{1}\psi(d)) = \frac{1}{4} \sum_{A=1}^{16} (\bar{\psi}(a)\Gamma^A\psi(d))(\bar{\psi}(c)\Gamma_A\psi(b)),$$

where  $\psi(a), \psi(b), \psi(c), \psi(d)$  are four different four-component  $\psi$ 's. Also, show

$$\begin{aligned} & 4 \sum_{\mu=0}^3 (\bar{\psi}(a)\gamma^\mu\psi(b))(\bar{\psi}(c)\gamma_\mu\psi(d)) \\ &= 4(\bar{\psi}(a)\mathbf{1}\psi(d))(\bar{\psi}(c)\mathbf{1}\psi(b)) - 4(\bar{\psi}(a)\gamma^5\psi(d))(\bar{\psi}(c)\gamma_5\psi(b)) \\ &+ 2 \sum_{\mu=0}^3 (\bar{\psi}(a)i\gamma^5\gamma^\mu\psi(d))(\bar{\psi}(c)i\gamma_5\gamma_\mu\psi(b)) \\ &- 2 \sum_{\mu=0}^3 (\bar{\psi}(a)\gamma^\mu\psi(d))(\bar{\psi}(c)\gamma_\mu\psi(b)). \end{aligned}$$

To do the calculations, let  $\Gamma_{ik} = (\psi(b))_i(\bar{\psi}(c))_k$  in the above.

**46.** Show the operator

$$\Lambda_+(p) = \frac{\gamma^\mu p_\mu + mc}{2mc}$$

is a projection operator for positive-energy states with the properties:

$$(\Lambda_+(p))^2 = \Lambda_+(p),$$

$$\Lambda_+(p)u^{(r)}(\vec{p}) = u^{(r)}(\vec{p}) \quad \text{for } r = 1, 2,$$

$$\Lambda_+(p)u^{(r)}(\vec{p}) = 0 \quad \text{for } r = 3, 4.$$

**47.** For the Dirac Hamiltonian of a particle in an outside electromagnetic field, with

$$H = \beta mc^2 + c(\vec{\alpha} \cdot \vec{\Pi}) + e\Phi,$$

which can be ordered as

$$H^{(0)} + H^{(1)} + H^{(2)} = H^{(0)} \left( 1 + \text{Order} \frac{p}{mc} + \text{Order} \left( \frac{p}{mc} \right)^2 \right)$$

in the nonrelativistic limit,  $p/mc \equiv \lambda \ll 1$ ; show that the transformed Hamiltonian, through fourth order, obtained via the transformation

$$H' = UHU^\dagger = e^{i\lambda G}He^{-i\lambda G},$$

with

$$i\lambda G = \frac{\beta(\vec{\alpha} \cdot \vec{\Pi})}{2mc}$$

leads to the Pauli approximation terms of the Dirac equation.

(Surviving third-order terms that only make connections of the type  $\psi_A \leftrightarrow \psi_B$  can be transformed into fifth and higher order terms, diagonal in  $\psi_A$ , via a further transformation, but therefore they do not contribute through fourth order.)

Also recall, with  $\lambda \ll 1$ ,

$$\begin{aligned} & e^{i\lambda G} H^{(n)} e^{-i\lambda G} \\ &= H^{(n)} + i\lambda[G, H^{(n)}] + \cdots + \frac{(i\lambda)^k}{k!} [G, [G, [G, \cdots [G, H^{(n)}] \cdots]]] + \cdots, \end{aligned}$$

where the  $k$ th term involves  $k$  commutators of  $G$  with  $H^{(n)}$ .

**48.** A relativistic electron beam polarized such that the longitudinal polarization is  $P_z = +1$ , where the  $z$  axis is chosen parallel to the initial momentum vector,  $\vec{p}_0$ , is scattered by a point nucleus of charge  $Ze$  (Mott scattering) into an angle  $\theta$ , with  $\vec{p}_{\text{scatt.}}$  parallel to a  $z'$  axis, lying in the  $x-z$  plane. If the detector is set so it accepts only longitudinally polarized electrons, with  $P_{z'} = +1$ , i.e., electrons with spin parallel to  $\vec{p}_{\text{scatt.}}$ , find the differential cross section as a function of  $\theta$  for this experimental setup. It may be useful to first find the normalized plane wave eigenstates of  $\Sigma_{z'} = (\cos \theta \Sigma_z + \sin \theta \Sigma_x)$ , or to make an active rotation about the  $y$  axis through an angle  $\theta$  of the plane wave state,  $u^{(1)}(\vec{p})$ .

**49.** An unpolarized relativistic electron beam is scattered from a finite-sized nucleus of charge  $Ze$ . Assume the nucleus can be described by the liquid drop model with a uniform charge distribution spread over a sphere of radius  $a$ , with

$$V(r) = -\frac{Ze^2}{r} \quad \text{for } r \geq a, \quad V(r) = -\frac{Ze^2}{a} \left( \frac{3}{2} - \frac{r^2}{2a^2} \right) \quad \text{for } r \leq a.$$

Find the differential cross section as a function of  $\theta$  and  $\beta = v/c$  of the incident electron beam.

**50.** The Dirac equation with Hamiltonian

$$H = \gamma^0 mc^2 + c(\gamma^0 \vec{\gamma} \cdot \vec{p} + im\omega \vec{\gamma} \cdot \vec{r})$$

has been named the “Dirac equation for the harmonic oscillator.”

(a) Justify this name by using the two-component  $\psi_A$  and  $\psi_B$  defined by

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} e^{-\frac{i}{\hbar} mc^2 t}$$

and by finding the wave equation for  $\psi_A$  in the nonrelativistic limit in which  $\frac{\hbar}{i} \frac{\partial \psi_B}{\partial t}$  can be neglected compared with  $2mc^2 \psi_B$ .

(b) Show the three components of  $\vec{J}$

$$\vec{J} = \vec{L} + \frac{1}{2}\hbar \Sigma$$

commute with this Hamiltonian.

- (c) Find the exact relativistic-energy eigenvalues for this Hamiltonian.  
 (d) Why is the Dirac equation

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = (\gamma^0 mc^2 + c \gamma^0 \vec{\gamma} \cdot \vec{p} + V(r)) \quad \text{with } V(r) = \frac{1}{2} m \omega^2 r^2$$

perhaps not suitable as a relativistic harmonic oscillator equation?

**51.** A nucleus with a ground state of angular momentum and parity,  $0^+$ , with nuclear wave function,  $\psi_{g.st.}$ , has a first excited state also with angular momentum and parity,  $0^+$ , and nuclear wave function,  $\psi_{exc.}$ . Show the excited state cannot decay to the ground state via the emission of a  $\gamma$  photon. If the excited state energy is greater than  $2mc^2$  ( $E_{exc.}^{nucl.} - E_{g.st.}^{nucl.} > 2mc^2 = 1.022 \text{ MeV}$ ), the nuclear deexcitation can occur via the emission of an electron–positron pair.

Calculate the probability per second for  $e^+, e^-$  emission in this case. In particular, calculate the probability per second the positron is emitted with energy between  $E_+$  and  $E_+ + dE_+$ , with no measurements made on the  $e^-$  energy. Assume the nuclear mass is big enough that the nuclear recoil energy  $P^2/2M_{\text{nucleus}}$  is negligible, so

$$E_{exc.}^{nucl.} - E_{g.st.}^{nucl.} = E_+ + E_- + P^2/2M_{\text{nucleus}} = E_+ + E_-,$$

where  $\vec{P} = -(\vec{p}_+ + \vec{p}_-)$ . Assume, however,  $P = |\vec{p}_+ + \vec{p}_-|$  is such that  $(Pr_{\text{nuc.}}/\hbar) \ll 1$ , where  $r_{\text{nuc.}}$  is a typical nuclear distance, of order 1–6 fm. Show in this limit the above probability depends on the nuclear states only through the square of the following nuclear matrix element

$$e \int \cdots \int d\vec{r}_1 \cdots d\vec{r}_A \psi_{g.st.}^{nucl.*} \sum_{j=1}^Z r_j^2 \psi_{exc.}^{nucl.} = e \langle r^2 \rangle_{fi},$$

where the sum is over the  $Z$  protons of the nucleus;  $r_j$  is the distance of the  $j^{\text{th}}$  proton from the center of mass of the nucleus. The interaction for the transition is the Coulomb interaction between the protons in the nucleus and the electron that makes a transition from the filled negative-energy state with  $E = -|E| = -E_+$ , and  $\vec{p}_i = -\vec{p}_+$ , to a positive-energy state with  $E = +E_-$ , and  $\vec{p}_f = \vec{p}_-$ . That is,

$$H_{\text{int.}} = - \sum_{j=1}^Z \frac{e^2}{|\vec{r} - \vec{r}_j|},$$

where  $\vec{r}$  without subscript refers to the position of the electron that makes the transition from the filled negative-energy state to the open positive-energy state. In doing some of the radial integrals, you may have to regularize Coulomb divergent integrals with a screening factor,  $b$ , e.g.,

$$\int_{r_i}^{\infty} dr \sin\left(\frac{Pr}{\hbar}\right) \rightarrow \lim_{b \rightarrow 0} \int_{r_i}^{\infty} dr \sin\left(\frac{Pr}{\hbar}\right) e^{-br} = \frac{\hbar}{P} \cos\left(\frac{Pr_i}{\hbar}\right).$$

Assume  $(E_{exc.}^{nucl.} - E_{g.st.}^{nucl.})$  is large enough or  $Z$  is small enough so the electron and positron wave functions can be approximated by Dirac plane waves. Calculate first the probability the electron is emitted into a  $d\Omega_-$  about the direction  $\theta_-, \phi_-$ ,

and the positron is emitted into a  $d\Omega_+$  about the direction  $\theta_+, \phi_+$  and integrate over all possible directions.

The nucleus  $^{16}O$  has a first excited state at 6.05 MeV that is a  $0^+$  state. Make an educated guess for the order of magnitude of the nuclear matrix element,  $\langle r^2 \rangle_{if}$ , and thus an order of magnitude estimate of the meanlife of this excited state.

# Exact Solutions for the Dirac Equation for Spherically Symmetric Potentials

Having discussed the plane-wave solutions to the Dirac equation in some detail, let us now look at solutions to the Dirac equation with a spherically symmetric  $V(r)$ . In particular, two cases are of special interest as follows.

Case 1.

$$V(r) = -\frac{Ze^2}{r}.$$

The hydrogenic atom is of particular interest, especially for inner atomic shells in a high  $Z$  atom, where relativistic effects may become important (e.g., in  $K$ -shell or  $L$ -shell X-ray spectra).

Case 2.

The quark model with  $V(r) = 0$  for  $r < a$ ,

and boundary conditions at  $r = a$  such that the quarks are confined to the spherical region with  $r < a$ . (Note: Our discussion of the Klein paradox indicates this confinement might not be achievable with a potential that is  $\infty$  for  $r > a$ .) This quark model is known as the MIT Bag model.

Let us first look at the general case of the Dirac equation with a spherically symmetric  $V(r)$ , i.e., the Dirac equation with Hamiltonian

$$H = c(\vec{\alpha} \cdot \vec{p}) + \beta mc^2 + V(r)\mathbf{1}. \quad (1)$$

We have already proved the three components of  $\vec{J}$ , with

$$\vec{J} = \vec{L} + \frac{\hbar}{2}\vec{\Sigma}, \quad \text{with } \Sigma_j = \frac{i}{2}\epsilon_{jkl}\gamma^k\gamma^l, \quad (2)$$

commutes with this  $H$ . Thus, we can diagonalize the operators,  $H$ ,  $\vec{J}^2$ , and  $J_z$  simultaneously, and the eigenvalues of  $H$  will have good  $j$ , and  $m_j$ . (We use the standard convention that lowercase letters are used for the eigenvalues of single-electron atoms.) The question arises: Are there other operators that commute with both  $H$  and  $\vec{J}$ ? The answer is yes. The operator, denoted by  $K$ , which is defined by

$$K = \beta(\vec{\Sigma} \cdot \vec{J} - \frac{\hbar}{2}), \quad (3)$$

commutes with both  $H$  and  $\vec{J}$ . To prove this, only the  $c(\vec{\alpha} \cdot \vec{p}) = c\gamma^0(\vec{\gamma} \cdot \vec{p})$  term of the above  $H$  needs to be considered, so we need to calculate

$$\begin{aligned} [H, K] &= [c\gamma^0(\vec{\gamma} \cdot \vec{p}), \gamma^0(\vec{\Sigma} \cdot \vec{J} - \frac{\hbar}{2})] \\ &= c[\gamma^0(\vec{\gamma} \cdot \vec{p}), \gamma^0](\vec{\Sigma} \cdot \vec{J} - \frac{\hbar}{2}) + c\gamma^0[\gamma^0(\vec{\gamma} \cdot \vec{p}), (\vec{\Sigma} \cdot \vec{J})] \\ &= -2c(\vec{\gamma} \cdot \vec{p})(\vec{\Sigma} \cdot \vec{J} - \frac{\hbar}{2}) + c\gamma^0[\gamma^0(\vec{\gamma} \cdot \vec{p}), \Sigma_j]J^j, \end{aligned} \quad (4)$$

where we have used the fact that  $\gamma^0(\vec{\gamma} \cdot \vec{p})$  commutes with all components of  $\vec{J}$ . If we further use the fact that  $\gamma^0$  commutes with  $\Sigma_j$ , the second term can be evaluated through

$$\begin{aligned} c\gamma^0[\gamma^0(\vec{\gamma} \cdot \vec{p}), \Sigma_j]J^j &= c(\gamma^0)^2[(\vec{\gamma} \cdot \vec{p}), \Sigma_j]J^j \\ &= \frac{ic}{2}\epsilon_{jmk}[\gamma^l, \gamma^m\gamma^k]p_lJ^j = \frac{ic}{2}\epsilon_{jmk}(2g^{lm}\gamma^k - 2g^{lk}\gamma^m)p_lJ^j \\ &= i\epsilon_{jmk}(-\gamma^k p^m J^j + \gamma^m p^k J^j) \\ &= 2i\epsilon_{mkj}\gamma^m p^k J^j = 2ic\vec{\gamma} \cdot [\vec{p} \times \vec{J}] \\ &= 2ic \begin{pmatrix} 0 & \vec{\sigma} \cdot [\vec{p} \times \vec{J}] \\ -\vec{\sigma} \cdot [\vec{p} \times \vec{J}] & 0 \end{pmatrix}. \end{aligned} \quad (5)$$

The first term of eq. (4), except for the factor  $-2c$ , can be evaluated by

$$\begin{aligned} (\vec{\gamma} \cdot \vec{p})(\vec{\Sigma} \cdot \vec{J} - \frac{\hbar}{2}) &= \\ \begin{pmatrix} 0 & \vec{\sigma} \cdot \vec{p} \\ -\vec{\sigma} \cdot \vec{p} & 0 \end{pmatrix} \begin{pmatrix} (\vec{\sigma} \cdot \vec{J} - \frac{\hbar}{2}) & 0 \\ 0 & (\vec{\sigma} \cdot \vec{J} - \frac{\hbar}{2}) \end{pmatrix} &= \\ \begin{pmatrix} 0 & (\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{J} - \frac{\hbar}{2}) \\ -(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{J} - \frac{\hbar}{2}) & 0 \end{pmatrix} &= \\ \begin{pmatrix} 0 & (\vec{p} \cdot \vec{J}) + i\vec{\sigma} \cdot [\vec{p} \times \vec{J}] - \frac{\hbar}{2}(\vec{p} \cdot \vec{\sigma}) \\ -(\vec{p} \cdot \vec{J}) - i\vec{\sigma} \cdot [\vec{p} \times \vec{J}] + \frac{\hbar}{2}(\vec{p} \cdot \vec{\sigma}) & 0 \end{pmatrix} \end{aligned} \quad (6)$$

Now, combining the results of eqs. (5) and (6), we get

$$[H, K] = -2c\gamma^0\gamma^5\left((\vec{p} \cdot \vec{J}) - \frac{\hbar}{2}(\vec{p} \cdot \vec{\Sigma})\right) = -2c\gamma^0\gamma^5(\vec{p} \cdot \vec{L}) = 0, \quad (7)$$

because  $\vec{p} \cdot [\vec{r} \times \vec{p}] \equiv 0$ .

We also see the operator,  $K$ , commutes with all components of  $\vec{J}$ :

$$\begin{aligned} [K, J^i] &= [\gamma^0 \left( \vec{\Sigma} \cdot \vec{J} - \frac{\hbar}{2} \right), J^i] = \gamma^0 \left( \Sigma_j [J^j, J^i] + [\Sigma^j, J^i] J_j \right) \\ &= \gamma^0 \left( i\hbar \Sigma_j \epsilon^{jik} J_k + [\Sigma^j, \frac{\hbar}{2} \Sigma^i] J_j \right) = \gamma^0 \left( i\hbar \epsilon^{jik} \Sigma_j J_k + i\hbar \epsilon^{jik} \Sigma_k J_j \right) \\ &= i\hbar \gamma^0 (\epsilon^{jik} + \epsilon^{kij}) \Sigma_j J_k = i\hbar \gamma^0 (\epsilon^{jik} - \epsilon^{jik}) \Sigma_j J_k = 0. \end{aligned} \quad (8)$$

Now, to evaluate the eigenvalue of the operator,  $K$ ,

$$\begin{aligned} K &= \beta \left( \vec{\Sigma} \cdot \vec{J} - \frac{\hbar}{2} \right) = \beta \left( \vec{\Sigma} \cdot \vec{L} + \frac{\hbar}{2} (\vec{\Sigma} \cdot \vec{\Sigma} - 1) \right) \\ &= \beta \left( \vec{\Sigma} \cdot \vec{L} + \frac{\hbar}{2} (3 - 1) \right) = \beta \left( \vec{\Sigma} \cdot \vec{L} + \hbar \right). \end{aligned} \quad (9)$$

Therefore,

$$\begin{aligned} K^2 &= \beta \left( \vec{\Sigma} \cdot \vec{L} + \hbar \right) \beta \left( \vec{\Sigma} \cdot \vec{L} + \hbar \right) = (\vec{\Sigma} \cdot \vec{L} + \hbar)(\vec{\Sigma} \cdot \vec{L} + \hbar) \\ &= (\vec{\Sigma} \cdot \vec{L})(\vec{\Sigma} \cdot \vec{L}) + 2\hbar(\vec{\Sigma} \cdot \vec{L}) + \hbar^2 \\ &= \vec{L} \cdot \vec{L} + i\vec{\Sigma} \cdot (i\hbar \vec{L}) + 2\hbar(\vec{\Sigma} \cdot \vec{L}) + \hbar^2 \\ &= \vec{L} \cdot \vec{L} + \hbar(\vec{\Sigma} \cdot \vec{L}) + \frac{3}{4}\hbar^2 + \frac{1}{4}\hbar^2 \\ &= \left( \vec{L} + \frac{1}{2}\hbar \vec{\Sigma} \right)^2 + \frac{1}{4}\hbar^2 = \hbar^2 \left( j(j+1) + \frac{1}{4} \right). \end{aligned} \quad (10)$$

Thus,  $K^2$  has the eigenvalue

$$K_{\text{eigen}}^2 = \hbar^2 \left( j + \frac{1}{2} \right)^2. \quad (11)$$

Essentially, only the sign of  $K$  gives us a new quantum number, because the magnitude of  $K$  is given by the total angular-momentum quantum number,  $j$ . We shall introduce the new quantum number,  $\kappa$ , defined by

$$K = -\hbar\kappa, \quad \text{so } \kappa = \pm \left( j + \frac{1}{2} \right). \quad (12)$$

The minus sign in this defining relation is included to agree with the conventional definition of this new quantum number (see, e.g., J. J. Sakurai, *Advanced Quantum Mechanics*, Reading, MA: Addison-Wesley, 1967). Now let us find solutions to the Dirac equation for a spherically symmetric  $V(r)$ , with eigenfunctions of good  $j$ ,  $m_j$ , and  $\kappa$ . Again, introduce two component functions,  $\psi_A$  and  $\psi_B$ , with

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} e^{-\frac{i}{\hbar} Et}, \quad (13)$$

so

$$\begin{aligned} (E - mc^2 - V(r))\psi_A &= c(\vec{\sigma} \cdot \vec{p})\psi_B, \\ (E + mc^2 - V(r))\psi_B &= c(\vec{\sigma} \cdot \vec{p})\psi_A. \end{aligned} \quad (14)$$

Now, introduce vector-coupled spherical harmonics of the type introduced in conjunction with scattering theory of spin- $\frac{1}{2}$  nonrelativistic particles.

$$\mathcal{Y}_{[l\frac{1}{2}]jm_j} \equiv \sum_{m_s, (m_l)} \langle lm_l | \frac{1}{2} m_s | jm_j \rangle i^l Y_{lm_l}(\theta, \phi) \chi_{\frac{1}{2} m_s}$$

$$= \begin{pmatrix} \langle l(m_j - \frac{1}{2})\frac{1}{2} + \frac{1}{2}|jm_j\rangle i^l Y_{l(m_j - \frac{1}{2})}(\theta, \phi) \\ \langle l(m_j + \frac{1}{2})\frac{1}{2} - \frac{1}{2}|jm_j\rangle i^l Y_{l(m_j + \frac{1}{2})}(\theta, \phi) \end{pmatrix}. \quad (15)$$

We now let

$$\begin{aligned} \psi_A &= g(r)\mathcal{Y}_{[l_A \frac{1}{2}]jm_j}, \\ \psi_B &= f(r)\mathcal{Y}_{[l_B \frac{1}{2}]jm_j}, \end{aligned} \quad (16)$$

and using

$$(\vec{\sigma} \cdot \frac{\vec{r}}{r})(\vec{\sigma} \cdot \frac{\vec{r}}{r}) = 1, \quad (17)$$

we are led to the simple identity

$$\begin{aligned} (\vec{\sigma} \cdot \vec{p}) &= \frac{(\vec{\sigma} \cdot \vec{r})}{r^2} ((\vec{\sigma} \cdot \vec{r})(\vec{\sigma} \cdot \vec{p})) = \frac{(\vec{\sigma} \cdot \vec{r})}{r^2} ((\vec{r} \cdot \vec{p}) + i\vec{\sigma} \cdot [\vec{r} \times \vec{p}]) \\ &= \frac{(\vec{\sigma} \cdot \vec{r})}{r^2} \left( -i\hbar r \frac{\partial}{\partial r} + i(\vec{\sigma} \cdot \vec{L}) \right). \end{aligned} \quad (18)$$

Therefore, we can replace  $(\vec{\sigma} \cdot \vec{p})$  by

$$(\vec{\sigma} \cdot \vec{p}) = \left( \vec{\sigma} \cdot \frac{\vec{r}}{r} \right) \frac{1}{i} \left( \hbar \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) - \frac{1}{r} ((\vec{\sigma} \cdot \vec{L}) + \hbar) \right). \quad (19)$$

Finally, we shall need the relation

$$\begin{aligned} \left( \vec{\sigma} \cdot \frac{\vec{r}}{r} \right) \mathcal{Y}_{[l \frac{1}{2}]j=(l+\frac{1}{2})m_j} &= c_+ \mathcal{Y}_{[(l+1)\frac{1}{2}]l(l+\frac{1}{2})m_j}, \\ \left( \vec{\sigma} \cdot \frac{\vec{r}}{r} \right) \mathcal{Y}_{[l \frac{1}{2}]j=(l-\frac{1}{2})m_j} &= c_- \mathcal{Y}_{[(l-1)\frac{1}{2}]l(l-\frac{1}{2})m_j}, \\ \text{with } c_+ &= +i, \quad c_- = -i, \end{aligned} \quad (20)$$

where eq. (17) leads to  $c_-c_+ = c_+c_- = 1$ , and  $c_+$  can be evaluated most easily by specific calculation, using

$$\left( \vec{\sigma} \cdot \frac{\vec{r}}{r} \right) = \sum_q (-1)^q \sigma_{-q} Y_{1,+q}(\theta, \phi) \sqrt{\frac{4\pi}{3}}. \quad (21)$$

This equation is a scalar operator whose matrix elements are therefore diagonal in  $j$  and independent of  $m_j$ . Thus, we can choose  $m_j$  judiciously, as always in applying the Wigner-Eckart theorem.

$$\begin{aligned} \left( \vec{\sigma} \cdot \frac{\vec{r}}{r} \right) \mathcal{Y}_{[l \frac{1}{2}]l(l+\frac{1}{2}), m_j=l+\frac{1}{2}} &= i^l \sqrt{\frac{4\pi}{3}} \left[ Y_{10} Y_{ll} \chi_{m_s=+\frac{1}{2}} - Y_{1+1} Y_{ll} \frac{2}{\sqrt{2}} \chi_{m_s=-\frac{1}{2}} \right] \\ &= i^l \sqrt{\frac{(2l+1)}{(2l+3)}} \langle l010|l+10\rangle \left[ \langle ll10|l+1l\rangle Y_{(l+1),l} \chi_{+\frac{1}{2}} \right. \\ &\quad \left. - \sqrt{\frac{1}{2}} \langle ll11|l+1l+1\rangle Y_{l+1,l+1} \chi_{-\frac{1}{2}} \right] \end{aligned}$$

$$\begin{aligned}
&= i^l \left[ \frac{1}{\sqrt{(2l+3)}} Y_{l+1,l} \chi_{+\frac{1}{2}} - \sqrt{\frac{2(l+1)}{(2l+3)}} Y_{l+1,l+1} \chi_{-\frac{1}{2}} \right] \\
&= -i^l \left[ (l+1) \frac{1}{2} |l + \frac{1}{2} l + \frac{1}{2} \rangle Y_{l+1,l} \chi_{+\frac{1}{2}} \right. \\
&\quad \left. + (l+1) l + 1 \frac{1}{2} - \frac{1}{2} |l + \frac{1}{2} l + \frac{1}{2} \rangle Y_{l+1,l+1} \chi_{-\frac{1}{2}} \right] \\
&= +i \mathcal{Y}_{[(l+1)\frac{1}{2}](l+\frac{1}{2})(l+\frac{1}{2})}.
\end{aligned} \tag{22}$$

Thus, we see specifically  $c_+ = +i$ , and therefore  $c_- = -i$ .

It will also prove convenient to choose the radial functions,  $g(r)$  and  $f(r)$ , such that

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} g(r) \mathcal{Y}_{[l+\frac{1}{2}](l+\frac{1}{2})m_j} \\ f(r) \mathcal{Y}_{[(l+1)\frac{1}{2}](l+\frac{1}{2})m_j} \end{pmatrix} \quad \text{for } j = (l_A + \frac{1}{2}), \tag{23}$$

and

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} g(r) \mathcal{Y}_{[l+\frac{1}{2}](l-\frac{1}{2})m_j} \\ -f(r) \mathcal{Y}_{[(l-1)\frac{1}{2}](l-\frac{1}{2})m_j} \end{pmatrix} \quad \text{for } j = (l_A - \frac{1}{2}), \tag{24}$$

where these two states have different eigenvalues  $\kappa$ . To see this, use eq. (9) to express  $K$  as  $K = \hbar \beta (\vec{\Sigma} \cdot \vec{l} + 1)$ , where  $\vec{l}$  is the dimensionless orbital angular-momentum operator,  $\vec{L} = \hbar \vec{l}$ , and use the eigenvalue  $(\vec{\sigma} \cdot \vec{l}) = [j(j+1) - l(l+1) - \frac{3}{4}]$ . With this, we get

$$\begin{aligned}
\frac{K}{\hbar} \begin{pmatrix} g(r) \mathcal{Y}_{[l+\frac{1}{2}](l+\frac{1}{2})m_j} \\ f(r) \mathcal{Y}_{[(l+1)\frac{1}{2}](l+\frac{1}{2})m_j} \end{pmatrix} &= +(l+1) \begin{pmatrix} g(r) \mathcal{Y}_{[l+\frac{1}{2}](l+\frac{1}{2})m_j} \\ f(r) \mathcal{Y}_{[(l+1)\frac{1}{2}](l+\frac{1}{2})m_j} \end{pmatrix}, \\
\frac{K}{\hbar} \begin{pmatrix} g(r) \mathcal{Y}_{[l+\frac{1}{2}](l-\frac{1}{2})m_j} \\ -f(r) \mathcal{Y}_{[(l-1)\frac{1}{2}](l-\frac{1}{2})m_j} \end{pmatrix} &= -l \begin{pmatrix} g(r) \mathcal{Y}_{[l+\frac{1}{2}](l-\frac{1}{2})m_j} \\ -f(r) \mathcal{Y}_{[(l-1)\frac{1}{2}](l-\frac{1}{2})m_j} \end{pmatrix}.
\end{aligned} \tag{25}$$

The eigenvalue  $\kappa$  is negative for  $j = (l_A + \frac{1}{2})$ ; i.e.,  $\kappa = -(j + \frac{1}{2})$  in this case, whereas  $\kappa$  is positive for  $j = (l_A - \frac{1}{2})$ ; i.e.,  $\kappa = +(j + \frac{1}{2})$  in this case.

Substituting eqs. (23) and (24) into eqs. (14), and using the results of eqs. (19) and (20), as well as the orthonormality of the  $\mathcal{Y}_{[l+\frac{1}{2}]jm_j}$ , we get the two coupled equations

$$\begin{aligned}
(E - mc^2 - V(r))g(r) &= -\hbar c \left( \frac{\partial}{\partial r} + \frac{(1 - \kappa)}{r} \right) f(r), \\
(E + mc^2 - V(r))f(r) &= +\hbar c \left( \frac{\partial}{\partial r} + \frac{(1 + \kappa)}{r} \right) g(r),
\end{aligned} \tag{26}$$

valid for both eigenvalues  $\kappa$ . It will also be convenient to one-dimensionalize these radial equations by introducing,  $G(r)$  and  $F(r)$ , via

$$rg(r) = G(r), \quad rf(r) = F(r), \tag{27}$$

to lead to the radial equations

$$\begin{aligned}
(E - mc^2 - V(r))G(r) &= -\hbar c \left( \frac{dF}{dr} - \frac{\kappa}{r} F \right), \\
(E + mc^2 - V(r))F(r) &= +\hbar c \left( \frac{dG}{dr} + \frac{\kappa}{r} G \right).
\end{aligned} \tag{28}$$

## A The Relativistic Hydrogen Atom

Let us first solve the radial equations for a hydrogenic atom, with

$$V(r) = -\frac{Ze^2}{r}. \quad (29)$$

Introduce relativistic coordinates, with energies measured in units of  $mc^2$  and distances measured in units of the Compton wavelength,  $\hbar/mc$ , with dimensionless energies,  $\epsilon$ , and dimensionless radial coordinate,  $\bar{r}$ , such that

$$E = mc^2\epsilon, \quad r = \frac{\hbar}{mc}\bar{r}. \quad (30)$$

This process transforms eq. (28) to

$$\begin{aligned} \left(\epsilon - 1 + \frac{Z\alpha}{\bar{r}}\right)G &= -\left(\frac{dF}{d\bar{r}} - \frac{\kappa}{\bar{r}}F\right), \\ \left(\epsilon + 1 + \frac{Z\alpha}{\bar{r}}\right)F &= +\left(\frac{dG}{d\bar{r}} + \frac{\kappa}{\bar{r}}G\right), \end{aligned} \quad (31)$$

where  $\alpha = e^2/\hbar c$  is the fine structure constant. It will be even more convenient to convert to the dimensionless variable,  $\rho$ , defined by

$$\rho = \sqrt{(1 - \epsilon^2)}\bar{r} = \sqrt{(1 - \epsilon^2)}\frac{mc}{\hbar}r. \quad (32)$$

In terms of this variable, the radial equations are

$$\begin{aligned} \left(-\sqrt{\frac{1 - \epsilon}{1 + \epsilon}} + \frac{Z\alpha}{\rho}\right)G &= -\frac{dF}{d\rho} + \frac{\kappa}{\rho}F, \\ \left(+\sqrt{\frac{1 + \epsilon}{1 - \epsilon}} + \frac{Z\alpha}{\rho}\right)F &= +\frac{dG}{d\rho} + \frac{\kappa}{\rho}G. \end{aligned} \quad (33)$$

In particular,  $\epsilon < 1$  for the bound positive-energy states with  $E < mc^2$ .

Of the many possible methods of solution, let us use the Fuchsian differential equation method. First, look at the form of the asymptotic solutions. As  $\rho \rightarrow \infty$ , the differential equations can be approximated by

$$-\sqrt{\frac{1 - \epsilon}{1 + \epsilon}}G = -\frac{dF}{d\rho}, \quad \sqrt{\frac{1 + \epsilon}{1 - \epsilon}}F = \frac{dG}{d\rho}, \quad (34)$$

leading to

$$\frac{d^2F}{d\rho^2} - F = 0, \quad \frac{d^2G}{d\rho^2} - G = 0, \quad \text{as } \rho \rightarrow \infty. \quad (35)$$

This equation has the solutions  $e^{\pm\rho}$  for both  $F$  and  $G$ , but only the solution,  $e^{-\rho}$ , can lead to square-integrable wave functions. Next, as  $\rho \rightarrow 0$ , the equations collapse to

$$\frac{Z\alpha}{\rho}G = -\frac{dF}{d\rho} + \frac{\kappa}{\rho}F,$$

$$\frac{Z\alpha}{\rho} F = + \frac{dG}{d\rho} + \frac{\kappa}{\rho} G. \quad (36)$$

If we try solutions of the form

$$F = A\rho^s, \quad G = B\rho^s, \quad \text{as } \rho \rightarrow 0,$$

we are led to the linear equations

$$\begin{aligned} (s - \kappa)A + Z\alpha B &= 0, \\ -Z\alpha A + (s + \kappa)B &= 0, \end{aligned} \quad (37)$$

with solutions, other than  $A = B = 0$ , only for  $s^2 - \kappa^2 + (Z\alpha)^2 = 0$ , so  $s = \pm\sqrt{\kappa^2 - (Z\alpha)^2}$ . To have solutions regular at  $\rho = 0$ , and thus square-integrable, we can only retain the positive root. Thus,

$$s = +\sqrt{\kappa^2 - (Z\alpha)^2} = +\sqrt{(j + \frac{1}{2})^2 - (Z\alpha)^2}. \quad (38)$$

We shall therefore try solutions to the full equations in the form

$$\begin{aligned} F &= \rho^s e^{-\rho} \sum_{m=0}^{\infty} a_m \rho^m, \\ G &= \rho^s e^{-\rho} \sum_{m=0}^{\infty} b_m \rho^m. \end{aligned} \quad (39)$$

Substituting back into eq. (33) and shifting indices appropriately, this process leads to recursive equations

$$\begin{aligned} -\sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{m-1} + (Z\alpha)b_m &= [\kappa - (m+s)]a_m + a_{m-1}, \\ +\sqrt{\frac{1+\epsilon}{1-\epsilon}} a_{m-1} + (Z\alpha)a_m &= [\kappa + (m+s)]b_m - b_{m-1}. \end{aligned} \quad (40)$$

In the limit in which  $m \rightarrow \infty$ , with  $\kappa \pm s \ll m$ , so  $\kappa \pm s$  can be neglected, we have

$$b_m \rightarrow \frac{b_{m-1}}{m} c_B, \quad a_m \rightarrow \frac{a_{m-1}}{m} c_A, \quad (41)$$

where we will choose  $c_B = c_A = c$ , so the functions  $F(\rho)$  and  $G(\rho)$  have the same asymptotic behavior as  $\rho \rightarrow \infty$ . With this large  $m$  limit, we then have

$$\begin{aligned} -\sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{m-1} + \text{Order}\left(\frac{1}{m}\right) &= a_{m-1}(1-c), \\ +\sqrt{\frac{1+\epsilon}{1-\epsilon}} a_{m-1} + \text{Order}\left(\frac{1}{m}\right) &= -b_{m-1}(1-c), \end{aligned} \quad (42)$$

or

$$a_{m-1}(1-c) + \sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{m-1} = 0,$$

$$a_{m-1} \sqrt{\frac{1+\epsilon}{1-\epsilon}} + b_{m-1}(1-c) = 0, \quad (43)$$

leading to a solution only if  $(c^2 - 2c) = 0$ . Thus, the only nonzero solution gives  $c = 2$ , but with this solution the infinite series implied by eq. (41) would lead to

$$\sum_m a_m \rho^m \rightarrow e^{+2\rho}, \quad \sum_m b_m \rho^m \rightarrow e^{+2\rho}.$$

The infinite series would therefore overpower the  $e^{-\rho}$  term of eq. (39) and give the unacceptable asymptotic behavior  $e^{+\rho}$  that must be ruled out. Thus, the series solutions of eq. (39) can lead to square-integrable wave functions only if the series terminate, say, at the  $n'^{th}$  terms, so both  $a_{n'+1} = 0$  and  $b_{n'+1} = 0$ . With this assumption, eq. (40), with  $m = n' + 1$ , leads to

$$\begin{aligned} -\sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{n'} &= a_{n'}, \\ +\sqrt{\frac{1+\epsilon}{1-\epsilon}} a_{n'} &= -b_{n'}, \end{aligned} \quad (44)$$

leading to

$$\frac{a_{n'}}{b_{n'}} = -\sqrt{\frac{1-\epsilon}{1+\epsilon}}. \quad (45)$$

Using this ratio, and choosing  $m = n'$  in eq. (40), we get

$$-\sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{n'-1} + (Z\alpha)b_{n'} = -(\kappa - n' - s)\sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{n'} + a_{n'-1}, \quad (46)$$

$$+\sqrt{\frac{1+\epsilon}{1-\epsilon}} a_{n'-1} - (Z\alpha)\sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{n'} = (\kappa + n' + s)b_{n'} - b_{n'-1}. \quad (47)$$

Solving eq. (46) for  $a_{n'-1}$  and substituting into eq. (47), we get an equation independent of  $b_{n'-1}$ :

$$\left( \frac{2\epsilon}{\sqrt{1-\epsilon^2}} (Z\alpha) - 2(n' + s) \right) b_{n'} = 0, \quad (48)$$

or

$$\frac{\epsilon}{\sqrt{1-\epsilon^2}} = \frac{(n' + s)}{Z\alpha} = \frac{(n' + \sqrt{[\kappa^2 - (Z\alpha)^2]})}{Z\alpha}, \quad \text{with } n' = 0, 1, \dots, \quad (49)$$

giving us the relativistic energy

$$\frac{E}{mc^2} = \epsilon = \frac{1}{\sqrt{1 + \frac{(Z\alpha)^2}{(n'+s)^2}}} = \frac{1}{\sqrt{1 + \frac{(Z\alpha)^2}{[n'+\sqrt{(j+\frac{1}{2})^2-(Z\alpha)^2}]^2}}}. \quad (50)$$

Now, for  $(Z\alpha) \ll 1$ , we can expand this result to get (through terms of order  $(Z\alpha)^4$ )

$$\frac{E}{mc^2} = 1$$

$$\begin{aligned}
&= -\frac{1}{2} \frac{(Z\alpha)^2}{[n' + \sqrt{(j + \frac{1}{2})^2 - (Z\alpha)^2}]^2} + \frac{3}{8} \frac{(Z\alpha)^4}{[n' + \sqrt{(j + \frac{1}{2})^2 - (Z\alpha)^2}]^4} + \dots \\
&= -\frac{1}{2} \frac{(Z\alpha)^2}{(n' + j + \frac{1}{2})^2} \left[ 1 + \frac{(Z\alpha)^2}{(j + \frac{1}{2})(n' + j + \frac{1}{2})} + \dots \right] + \frac{3}{8} \frac{(Z\alpha)^4}{(n' + j + \frac{1}{2})^4} + \dots \\
&= -\frac{(Z\alpha)^2}{2n^2} - \frac{(Z\alpha)^4}{2n^3} \left[ \frac{1}{(j + \frac{1}{2})} - \frac{3}{4n} \right] + \dots , \tag{51}
\end{aligned}$$

where we have renamed  $(n' + j + \frac{1}{2}) = n$  in the last step to get the conventional principal quantum number  $n$  of the hydrogen atom. (We obtained this last result by applying perturbation theory to the nonrelativistic hydrogen atom, after incorporating the magnetic spin-orbit term, the Thomas precession term, and the relativistic mass correction term into the theory. See problem 36 following Chapter 26.)

To obtain the radial functions,  $F(\rho)$  and  $G(\rho)$ , let us return to eq. (40). By eliminating the quantity

$$a_{m-1} + \sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{m-1},$$

from these two equations, we can solve for the ratio

$$\frac{a_m}{b_m} = \frac{(Z\alpha)[(\kappa + m - n') - \sqrt{(Z\alpha)^2 + (n' + s)^2}]}{[(Z\alpha)^2 + (m + s - \kappa)[(n' + s) + \sqrt{(Z\alpha)^2 + (n' + s)^2}]]}. \tag{52}$$

Using this relation, we can also rewrite the first of eq. (40) as

$$\begin{aligned}
a_{m-1} + \sqrt{\frac{1-\epsilon}{1+\epsilon}} b_{m-1} &= \\
\frac{(Z\alpha)m(2s+m)}{[(Z\alpha)^2 + (m+s-\kappa)[(n'+s) + \sqrt{(Z\alpha)^2 + (n'+s)^2}]]} b_m, \tag{53}
\end{aligned}$$

where we have used the relation

$$(Z\alpha)^2 + (m + s)^2 - \kappa^2 = m^2 + 2ms.$$

Now, we use

$$\sqrt{\frac{1-\epsilon}{1+\epsilon}} = \frac{(Z\alpha)}{[(n'+s) + \sqrt{(Z\alpha)^2 + (n'+s)^2}]}$$

and the ratio,  $a_{m-1}/b_{m-1}$  via eq. (52) to substitute into eq. (53) to obtain

$$\frac{b_{m-1}}{b_m} = \frac{m(2s+m)}{2(m-1-n')} \frac{[(m-1-n'-\kappa) + \sqrt{(Z\alpha)^2 + (n'+s)^2}]}{[(m-n'-\kappa) + \sqrt{(Z\alpha)^2 + (n'+s)^2}]}, \tag{54}$$

or, defining,

$$\gamma \equiv \sqrt{(Z\alpha)^2 + (n'+s)^2} - \kappa, \quad \text{with } s = \sqrt{\kappa^2 - (Z\alpha)^2}, \tag{55}$$

the ratio becomes

$$\frac{b_{m-1}}{b_m} = -\frac{m(2s+m)}{2(n'+1-m)} \frac{(m-1-n')+\gamma}{(m-n')+\gamma}, \quad (56)$$

so

$$\frac{b_{n'-k}}{b_{n'}} = (-1)^k \frac{n'(n'-1)\cdots(n'-k+1)}{2^k(1\cdot 2\cdots k)} \frac{(\gamma-1)(\gamma-2)\cdots(\gamma-k+1)(\gamma-k)}{\gamma(\gamma-1)\cdots(\gamma-k+1)} \quad (57)$$

or

$$\frac{b_{n'-k}}{b_{n'}} = (-1)^k \frac{(n')!}{2^k k!(n'-k)!} \frac{(\gamma-k)}{\gamma}, \quad k = 1, \dots, n'. \quad (58)$$

Also, from eq. (52),

$$\frac{a_{n'-k}}{b_{n'-k}} = -\frac{(Z\alpha)(\gamma+k)}{(\gamma-k)[(n'+s) + \sqrt{(Z\alpha)^2 + (n'+s)^2}]} \quad k = 0, \dots, n'. \quad (59)$$

As a very specific example, let us look at the ground-state wave function. In this case,

$$n' = 0, \quad \kappa = -1, \quad s = \sqrt{1 - (Z\alpha)^2}, \quad \epsilon = \sqrt{1 - (Z\alpha)^2}.$$

Recalling

$$\rho = \sqrt{1 - \epsilon^2} \frac{mc}{\hbar} r, \quad \text{so } \rho = \frac{Zr}{a_0},$$

we have in this case

$$\begin{aligned} G(\rho) &= \rho^s e^{-\rho} b_0, \\ F(\rho) &= -\frac{(Z\alpha)}{1+s} \rho^s e^{-\rho} b_0. \end{aligned} \quad (60)$$

Also recall  $rg(r) = G(r)$  and  $rf(r) = F(r)$ . With  $\kappa = -1$ , eq. (23) then gives

$$\psi = \mathcal{N} \left( \frac{Zr}{a_0} \right)^{[\sqrt{1-(Z\alpha)^2}-1]} e^{-\frac{Zr}{a_0}} \left( -\frac{\mathcal{Y}_{[0\frac{1}{2}]\frac{1}{2}m_J}}{\frac{(Z\alpha)}{[1+\sqrt{1-(Z\alpha)^2}]}\mathcal{Y}_{[1\frac{1}{2}]\frac{1}{2}m_J}} \right), \quad (61)$$

where the normalization constant is

$$\mathcal{N} = \left( \frac{Z}{a_0} \right)^{\frac{1}{2}} 2^{\sqrt{1-(Z\alpha)^2}} \frac{\sqrt{[1 + \sqrt{1 - (Z\alpha)^2}]}}{\sqrt{\Gamma(1 + 2\sqrt{1 - (Z\alpha)^2})}}. \quad (62)$$

# The MIT Bag Model: The Dirac Equation for a Quark Confined to a Spherical Region

Quarks, like the leptons (electrons,  $\mu$  and  $\tau$  mesons) are Dirac  $s = \frac{1}{2}$  particles. Unlike the leptons, quarks have additional internal degrees of freedom, specified by “flavor” (including isospin that determines their charge) and “color.” They come in three colors and three generations of isospin doublets ( $u, d$ ; up and down quarks;  $s, c$ ; strange and charmed quarks; and  $b, t$ ; bottom and top quarks). They appear in nature only in “colorless” combinations corresponding to the scalar irreducible representations of the color symmetry SU(3) [the analogue of  $S = 0$  multiparticle spin states, corresponding to the scalar irreducible representations of SU(2)]. The “colorless” combinations can arise either from quark–antiquark combinations or combinations of three quarks. Protons, e.g., are made of two up quarks, each with charge of  $+\frac{2}{3}e$ , and one down quark with charge  $-\frac{1}{3}e$ , whereas neutrons are made of one up quark and two down quarks, total charge  $= (+\frac{2}{3} - \frac{1}{3} - \frac{1}{3})e = 0$ . These three-quark systems have a total spin,  $S = \frac{1}{2}$ , and isospin,  $I = \frac{1}{2}$ , with  $M_I = \pm \frac{1}{2}$ . The quark aggregates are confined to finite regions of space, for the three-quark aggregates of the nucleon, to a region of approximately 1.2 fm. The confinement mechanism is not at all understood. One of the most successful phenomenological models for quark confinement is the “MIT bag model,” named after the institution of the inventors of the model. In this model, it is simply assumed the quarks are confined to a spherical region of space, with a radius,  $r = a$ , and  $V(r) = 0$  for  $r < a$ . The rest mass of the  $u$  and  $d$  quarks, however, is so small their motion in the region with  $r < a$  must be treated by the Dirac equation. In a sense, the MIT bag model is the quark analogue of the nuclear shell model. In one extreme version of the nuclear shell model, the potential is assumed to have the form:  $V(r) = 0$  for  $r < a$ , and  $V = +\infty$  for  $r > a$ . Our discussion of the Klein paradox, however,

should convince us an infinite potential is unable to confine a relativistic particle. It may be enough to solve a model in which the quark is in free particle motion inside the region for  $r < a$ , but is subject to boundary conditions at  $r = a$  that simply dictate the confinement.

We shall therefore find solutions to the Dirac equation with  $V(r) = 0$  for  $r < a$ ; i.e.,

$$H = c(\vec{\alpha} \cdot \vec{p}) + \beta mc^2, \quad \text{for } r < a, \quad (1)$$

and boundary conditions (which insure the confinement)

$$1. \quad \int \int r^2 d\Omega \vec{S} \cdot \left( \frac{\vec{r}}{r} \right) = c \int \int r^2 d\Omega \bar{\psi} \left( \vec{\gamma} \cdot \frac{\vec{r}}{r} \right) \psi = 0 \quad \text{at } r = a \quad (2)$$

and

$$1. \quad \int \int r^2 d\Omega \bar{\psi} \mathbf{1} \psi = 0 \quad \text{at } r = a. \quad (3)$$

Relation 1. insures no net outward (radial) component of the probability density current through the sphere of radius  $a$  exists. Relation 2. insures the same for the Lorentz scalar quantity,  $\bar{\psi} \mathbf{1} \psi$ , over the surface of the sphere of radius  $a$ .

In the region,  $r < a$ , the solutions  $\psi$  are of the form

$$\psi = \begin{pmatrix} g(r) \mathcal{Y}_{[l_A \frac{1}{2}]jm_j} \\ \pm f(r) \mathcal{Y}_{[l_B \frac{1}{2}]jm_j} \end{pmatrix} \quad \text{for } \kappa = \mp(j + \frac{1}{2}), \quad (4)$$

where again  $j = (l_A + \frac{1}{2})$ ;  $l_B = (l_A + 1)$ , for the negative value of  $\kappa$  (upper sign), and  $j = (l_A - \frac{1}{2})$ ;  $l_B = (l_A - 1)$ , for the positive value of  $\kappa$  (lower sign). Again, defining the one-dimensionalized radial functions,  $G(r) = rg(r)$ , and  $F(r) = rf(r)$ , the radial equations for the region  $r < a$ , where  $V(r) = 0$  are then given by

$$\begin{aligned} \left( \frac{E - mc^2}{\hbar c} \right) G(r) &= \left( -\frac{d}{dr} + \frac{\kappa}{r} \right) F(r), \\ \left( \frac{E + mc^2}{\hbar c} \right) F(r) &= \left( +\frac{d}{dr} + \frac{\kappa}{r} \right) G(r), \end{aligned} \quad (5)$$

which lead to

$$\begin{aligned} \left( -\frac{d}{dr} + \frac{\kappa}{r} \right) \left( \frac{d}{dr} + \frac{\kappa}{r} \right) G &= \frac{E^2 - m^2 c^4}{(\hbar c)^2} G, \\ \left( \frac{d}{dr} + \frac{\kappa}{r} \right) \left( -\frac{d}{dr} + \frac{\kappa}{r} \right) F &= \frac{E^2 - m^2 c^4}{(\hbar c)^2} F, \end{aligned} \quad (6)$$

or

$$\begin{aligned} \left( -\frac{d}{dr^2} + \frac{\kappa(\kappa + 1)}{r^2} - q^2 \right) G &= 0, \\ \left( -\frac{d}{dr^2} + \frac{\kappa(\kappa - 1)}{r^2} - q^2 \right) F &= 0, \end{aligned}$$

$$\text{with } q^2 = \left(\frac{E}{\hbar c}\right)^2 - \left(\frac{mc}{\hbar}\right)^2. \quad (7)$$

With  $j = (l_A \pm \frac{1}{2})$ , i.e., with  $\kappa = \mp(j + \frac{1}{2})$ , we have

$$\begin{aligned} &\text{with } \kappa = -(l_A + 1) : \\ &\kappa(\kappa + 1) = l_A(l_A + 1); \quad \kappa(\kappa - 1) = (l_A + 1)(l_A + 2) = l_B(l_B + 1), \\ &\text{with } \kappa = +l_A : \\ &\kappa(\kappa + 1) = l_A(l_A + 1); \quad \kappa(\kappa - 1) = l_A(l_A - 1) = (l_B + 1)l_B, \end{aligned} \quad (8)$$

so, with

$$\rho = qr, \quad (9)$$

both entries of eq. (7) have the form

$$\left(-\frac{d}{d\rho^2} + \frac{l(l+1)}{\rho^2} - 1\right)u_l = 0, \quad (10)$$

with  $u_{l_A} = G$ , and  $u_{l_B} = F$ , where  $u_l$  is the one-dimensionalized radial equation for the spherical Bessel functions; see eqs. (36)–(43) of Chapter 41. Because we need solutions regular at the origin, we have  $G(\rho)/\rho = j_{l_A}(\rho)$ . The second of eqs. (5) then leads to

$$\begin{aligned} F(\rho) &= \sqrt{\frac{(E - mc^2)}{(E + mc^2)}} \left( \frac{d}{d\rho} + \frac{\kappa}{\rho} \right) u_{l_A}(\rho) \\ &= \begin{cases} -\sqrt{\frac{(E - mc^2)}{(E + mc^2)}} \left( -\frac{d}{d\rho} + \frac{(l_A + 1)}{\rho} \right) u_{l_A}(\rho) \\ +\sqrt{\frac{(E - mc^2)}{(E + mc^2)}} \left( \frac{d}{d\rho} + \frac{l_A}{\rho} \right) u_{l_A}(\rho) \end{cases} \\ &= \begin{cases} -\sqrt{\frac{(E - mc^2)}{(E + mc^2)}} u_{(l_A + 1)}(\rho) \\ +\sqrt{\frac{(E - mc^2)}{(E + mc^2)}} u_{(l_A - 1)}(\rho) \end{cases} = \mp \sqrt{\frac{(E - mc^2)}{(E + mc^2)}} u_{l_B}(\rho), \end{aligned} \quad (11)$$

where the upper (and lower) entries are for  $\kappa = -(l_A + 1)$  (and  $\kappa = +l_A$ ) and we have used the stepup and down operators,  $O_+(l_A + 1)$  and  $O_-(l_A)$ , of eq. (37) of Chapter 41. Remembering  $\rho g(\rho) = G(\rho)$  and  $\rho f(\rho) = F(\rho)$ , and the signs in eq. (4), we have for  $r < a$ ,

$$\psi = \mathcal{N} \begin{pmatrix} j_{l_A}(qr) \mathcal{Y}_{[l_A \frac{1}{2}]jm_j} \\ -\sqrt{\frac{(E - mc^2)}{(E + mc^2)}} j_{l_B}(qr) \mathcal{Y}_{[l_B \frac{1}{2}]jm_j} \end{pmatrix}. \quad (12)$$

These solutions must satisfy the boundary conditions of eqs. (2) and (3) at  $r = a$ . For eq. (2), it is useful to recast the radial component of  $\vec{S}$  (using  $\vec{r}/r \equiv \vec{n}$ ) in the form

$$c\bar{\psi}_{r=a}(\vec{\gamma} \cdot \vec{n})\psi_{r=a} = c\bar{\psi}_{r=a} \begin{pmatrix} 0 & (\vec{\sigma} \cdot \vec{n}) \\ -(\vec{\sigma} \cdot \vec{n}) & 0 \end{pmatrix} \begin{pmatrix} \psi_A(r = a) \\ \psi_B(r = a) \end{pmatrix}$$

$$\begin{aligned}
&= c \bar{\psi}_{r=a} \left( -\sqrt{\frac{E-mc^2}{E+mc^2}} j_{l_B}(qa) (\vec{\sigma} \cdot \vec{n}) \mathcal{Y}_{[l_B \frac{1}{2}]jm_j} \right. \\
&\quad \left. - j_{l_A}(qa) (\vec{\sigma} \cdot \vec{n}) \mathcal{Y}_{[l_A \frac{1}{2}]jm_j} \right) \\
&= c \bar{\psi}_{r=a} (\pm i) \left( +\sqrt{\frac{E-mc^2}{E+mc^2}} j_{l_B}(qa) \mathcal{Y}_{[l_A \frac{1}{2}]jm_j} \right. \\
&\quad \left. - j_{l_A}(qa) \mathcal{Y}_{[l_B \frac{1}{2}]jm_j} \right), \quad (13)
\end{aligned}$$

where we have used eq. (20) of Chapter 76 for the action of  $(\vec{\sigma} \cdot \vec{n})$  on  $\mathcal{Y}_{[l \frac{1}{2}]jm_j}$ . The upper sign refers to  $\kappa = -(j + \frac{1}{2})$  and the lower sign to  $\kappa = +(j + \frac{1}{2})$ , respectively. The boundary condition 1. at  $r = a$  therefore leads to

$$\pm i \sqrt{\frac{E-mc^2}{E+mc^2}} ca^2 j_{l_A}(qa) j_{l_B}(qa) \int \int d\Omega \left( |\mathcal{Y}_{[l_A \frac{1}{2}]jm_j}|^2 - |\mathcal{Y}_{[l_B \frac{1}{2}]jm_j}|^2 \right) = 0. \quad (14)$$

This relation is satisfied automatically from the orthonormality of the  $\mathcal{Y}_{[l \frac{1}{2}]jm_j}$ . Conversely, boundary condition 2. at  $r = a$  leads to

$$\begin{aligned}
&\int \int a^2 d\Omega \left( (j_{l_A}(qa))^2 |\mathcal{Y}_{[l_A \frac{1}{2}]jm_j}|^2 - \frac{E-mc^2}{E+mc^2} (j_{l_B}(qa))^2 |\mathcal{Y}_{[l_B \frac{1}{2}]jm_j}|^2 \right) \\
&= \left( (j_{l_A}(qa))^2 - \frac{E-mc^2}{E+mc^2} (j_{l_B}(qa))^2 \right) = 0. \quad (15)
\end{aligned}$$

This boundary condition is satisfied if

$$j_{l_A}(qa) = \pm \sqrt{\frac{E-mc^2}{E+mc^2}} j_{l_B}(qa). \quad (16)$$

Here, the sign is related to the sign of  $\kappa$

$$j_{l_A}(qa) = -\frac{\kappa}{|\kappa|} \sqrt{\frac{E-mc^2}{E+mc^2}} j_{l_B}(qa). \quad (17)$$

One way to see the  $\kappa$  dependence of this sign is to assume the mass term in the Dirac equation has different values in the interior and exterior regions,  $r < a$  and  $r > a$ . The quark mass in the exterior region,  $r > a$ , will be named  $M$ , and we assume  $M \rightarrow \infty$ . This is the confinement condition (rather than  $V \rightarrow \infty$ ). In this limit, the radial equations given by the first of eqs. (7) and the second of eqs. (5) collapse to

$$\left( -\frac{d^2}{dr^2} + \left( \frac{Mc}{\hbar} \right)^2 \right) G(r) = 0, \quad (18)$$

$$F(r) = \frac{\hbar}{Mc} \frac{d}{dr} G(r), \quad (19)$$

with solutions

$$G(r) = e^{-\frac{Mc}{\hbar} r}, \quad F(r) = -G(r), \quad M \rightarrow \infty. \quad (20)$$

At the boundary,  $r = a$ , we must therefore have  $f(a) = -g(a)$ . Eq. (17) therefore follows from eq. (12) and eq. (4). The difference in sign arises through the differences in sign in the  $f(r)$  piece of eq. (4). The magnitude follows from eq. (12).

Eq. (17) leads to a transcendental equation for the allowed values of  $q$ . If the  $n^{th}$  solution of this transcendental equation is named  $x_{n,\kappa}$ , the energies are determined by

$$x_{n,\kappa} = (q_{n,\kappa}a) = \frac{\hbar c}{\hbar c} \sqrt{E_{n,\kappa}^2 - mc^2}. \quad (21)$$

The masses of the up and down quarks are believed to be very small ( $\ll$  than the nucleon mass), so it may be a good approximation to set the quark mass equal to zero. With  $m = 0$ , we have

$$E_{n,\kappa} = \frac{\hbar c}{a} x_{n,\kappa}, \quad \text{where } j_{l_A}(x_{n,\kappa}) = -\frac{\kappa}{|\kappa|} j_{l_B}(x_{n,\kappa}). \quad (22)$$

For example, with  $\kappa = -1$ , i.e.,  $j = \frac{1}{2}$ ,  $l_A = 0$ ,  $l_B = 1$ :

$$j_0(x_{n,-1}) = j_1(x_{n,-1}). \quad (23)$$

With  $\kappa = +1$ , i.e.,  $j = \frac{1}{2}$ ,  $l_A = 1$ ,  $l_B = 0$ :

$$j_1(x_{n,+1}) = -j_0(x_{n,+1}), \quad (24)$$

leading to

$$\frac{\sin(x_{n,\mp 1})}{x_{n,\mp 1}} = \pm \left( \frac{\sin(x_{n,\mp 1})}{x_{n,\mp 1}^2} - \frac{\cos(x_{n,\mp 1})}{x_{n,\mp 1}} \right), \quad (25)$$

or

$$\tan(x_{n,\mp 1}) = \mp \frac{x_{n,\mp 1}}{(x_{n,\mp 1} \mp 1)}, \quad \text{for } \kappa = \mp 1. \quad (26)$$

Similarly,

$$\tan(x_{n,\mp 2}) = \pm \frac{(x_{n,\mp 2}^2 \mp 3x_{n,\mp 2})}{(x_{n,\mp 2}^2 \pm x_{n,\mp 2} - 3)}, \quad (27)$$

where these transcendental equations have solutions

$$\begin{aligned} x_{1,-1} &= 2.043, & x_{2,-1} &= 5.40, \dots \\ x_{1,+1} &= 3.81, & x_{2,+1} &= 7.00, \dots \\ x_{1,-2} &= 3.20, \dots \\ x_{1,+2} &= 5.12, \dots \\ &\dots \end{aligned} \quad (28)$$

In particular, the lowest allowed energy, with  $\kappa = -1$ ,  $j = \frac{1}{2}$ ,  $l_A = 0$ ,  $l_B = 1$ , is

$$E_{1,-1} = \frac{\hbar c}{a} 2.043. \quad (29)$$

Thus, for the three-quark system of the nucleon, taking  $a = 1.25$  fm, we get a zeroth-order energy in the MIT bag model of

$$3 \left( \frac{197.3 \text{ MeV fm}}{1.25 \text{ fm}} \right) 2.043 = 967 \text{ MeV}.$$

This equation is not far from the observed nucleon mass. The gluon interaction among the three quarks will make additional contributions, but on the whole the MIT bag model with zero rest-mass quarks gives a good account not only of the nucleon mass, but, also, of additional nucleon properties, such as the “anomalous” magnetic moments of the nucleon.

# Introduction to Many-Body Theory

# Many-Body Formalism

## A Occupation Number Representation

As already noted in Chapter 39, systems of many identical particles, either bosons or fermions, form an important part of nature and, because of the required overall symmetry or antisymmetry of the many-particle wave function, these form not only important, but also very special, types of quantum-mechanical systems. Examples we have met are the many-electron system of an atom, or the many-electron system of condensed matter physics, the many nucleon-system of a nucleus, and the many-quark system of particle physics. All of these involve identical spin  $\frac{1}{2}$  particles and, hence, fermions. All of these identical particles have besides their orbital degrees of freedom, internal degrees of freedom such as their spin degree of freedom, but in the case of identical nucleons, an additional charge or isospin internal degree of freedom, and in the case of quarks, additional flavor (including isospin) and color degrees of freedom. Systems of identical bosons include the system of many  $^4\text{He}$  atoms, an example of a many-particle system where we may be dealing with a huge number of identical particles. Other examples of many-boson systems would include more complicated atoms, provided the identical atoms have an electron plus nucleon number that is an even number so the total atomic spin is an integer. Such systems are of particular recent interest in connection with the Bose–Einstein condensation of such atomic gases.

For the many-boson system, the total many-particle wave function must be totally symmetric under any permutation of particle indices, where the permutation operator must exchange the particle indices on *all* particle variables, orbital, spin, and any additional internal variables, such as isospin or flavor and color

variables of the single-particle system. For the many-fermion system, the total many-particle wave function must be totally antisymmetric; that is, it must change sign under any odd permutation of particle indices, involving an odd number of pair exchanges, whereas it must remain unchanged under any even permutation, involving an even number of pair exchanges. For the two-particle system, it was easy to construct two-particle wave functions with the appropriate symmetry from products of single-particle wave functions. Moreover, it was easy to factor the products of two-particle functions into products of their two-particle orbital functions, two-particle spin functions, two-particle isospin functions, and possibly two-particle functions of additional internal degrees of freedom, if applicable. The construction of the two-particle total wave function of the appropriate symmetry is then still very straightforward, because the products of two-particle symmetric functions with two-particle antisymmetric (or symmetric) functions automatically leads to two-particle antisymmetric (or symmetric) functions. For  $N \geq 3$ , however, this factoring of the  $N$ -particle functions into orbital, spin, and possibly other factors becomes more complicated, because of the existence of more complicated intermediate symmetries. For  $N = 3$ , three types of three-particle symmetries exist. Three-particle functions can be totally symmetric (completely unchanged by any permutation operator), totally antisymmetric, with a change of sign under any odd permutation and no change of sign under any even permutation, but the possibility of more complicated intermediate symmetries exist. Such symmetries are described by Young tableaux, pictures of  $N$  squares arranged in rows and columns. A tableau with all  $N$  squares in the same row represents a totally symmetric wave function. A tableau with all squares in the same column represents a totally antisymmetric wave function. For  $N = 3$ , a possible intermediate symmetry exists, involving a tableau with two squares in one row and a third square placed in the first column, as shown in Fig. 78.1(a). Such a tableau represents a three-particle function that can be made symmetric in one pair or antisymmetric in one pair, but is patently such that it cannot be made more symmetric or more antisymmetric. That is, an attempt to make such a function totally symmetric, by acting on it with the full symmetrization operator, will destroy this wave function; i.e., it will simply yield a result that is identically zero, similarly, for an attempt to make such a function totally antisymmetric. Clearly, totally antisymmetric wave functions could be constructed from products of totally symmetric spin functions with totally antisymmetric orbital functions or totally antisymmetric spin functions with totally symmetric orbital functions. As already mentioned in Chapter 39, for electrons or any other  $s = \frac{1}{2}$  system, it is impossible to make three-particle spin functions totally antisymmetric, because the single-particle spin function has only two possible quantum states;  $m_s = \pm \frac{1}{2}$ . Thus, three-particle  $s = \frac{1}{2}$  spin functions can only be totally symmetric, with  $S = \frac{3}{2}$  (see Chapter 39), or have intermediate symmetry, of type [21] (two squares in the first row of the tableau, one square in the second row), with  $S = \frac{1}{2}$ . These must be combined with orbital functions also of [21] symmetry to yield total wave functions which are totally antisymmetric. The process of finding the proper linear combination of spin and orbital functions

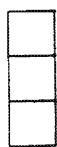
with these symmetries, however, is already somewhat complicated for this simple case with  $N = 3$ , two independent functions of intermediate [21] symmetry exist, and the two independent spin functions must be combined with appropriate "conjugate" orbital functions to make the required three-particle totally antisymmetric total wave function. For  $N = 4$ , the combinations of possible symmetries is even richer. We can now have totally symmetric wave functions with all four squares of the tableau in the same row, to be designated by [4] [see Fig. 78.1(b)]. In addition, three independent functions of intermediate symmetry, [31], exist that can be made symmetric in one group of three particles, but cannot be made more symmetric and can be made antisymmetric in one pair of particles, but cannot be made antisymmetric in more than one pair. The other four-particle symmetries include two independent functions of symmetry [22] that can be made symmetric in two different pairs, corresponding to the two rows of the tableau, or antisymmetric in two different pairs, corresponding to the two columns of the tableau; three independent functions of symmetry [211] that can be made antisymmetric in one group of three but symmetric in at most one pair; and finally the totally antisymmetric function, [1111], corresponding to a tableau with a single column. Because four-particle  $s = \frac{1}{2}$  spin functions cannot be antisymmetrized in groups of three, these can only have symmetries [4], with  $S = 2$ , [31] with  $S = 1$ , and [22] with  $S = 0$ . To make the totally antisymmetric total wave function, these four types of spin functions must be combined with the orbital functions of the appropriate "conjugate" symmetry, involving Young tableaux in which the role of rows and columns has been interchanged. Thus, totally symmetric spin functions of spin symmetry, [4], must be combined with totally antisymmetric orbital functions of symmetry, [1111]. Three independent spin functions of spin symmetry, [31], must be combined in the proper linear combination with three orbital functions of the appropriate conjugate functions of symmetry, [211], to make a totally antisymmetric total wave function. Similarly, two independent spin functions of intermediate spin symmetry, [22], exist that must be combined in the proper linear combination with the appropriately matched orbital functions, now also of symmetry, [22], to make a totally antisymmetric total four-particle wave function.

For an  $N$ -electron atom, where it might be advantageous to factor the  $N$ -particle wave function into a product of an  $N$ -particle spin function and an  $N$ -particle orbital function, the process of antisymmetrization of the total wave function becomes rather complicated for  $N \geq 3$ . It will therefore in general be better to antisymmetrize the full  $N$ -particle wave function in terms of products of single-particle wave functions involving all variables, orbital plus internal, of the type

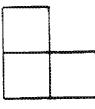
$$\psi_{\alpha_n}(\vec{\xi}_k); \quad \text{with } k = 1, \dots, N,$$

where  $\vec{\xi}_k$  stands for *all* variables of the particle labeled number,  $k$ ; e.g.,  $\vec{\xi}_k = \vec{r}_k, \vec{\sigma}_k, \vec{t}_k, \dots$ , where  $\vec{r}_k$  gives the three orbital variables that give the position of particle, labeled  $k$ , in the quantum system,  $\vec{\sigma}_k$ , stands for the internal spin degree of freedom of particle labeled  $k$ ,  $\vec{t}_k$  stands for the internal isospin degree of freedom, etc., where the  $\dots$  may stand for additional internal degrees of freedom, such as those of color, if applicable. In addition,  $\alpha_n$  stands for *all* single-particle quan-

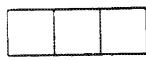
[3]



[21]



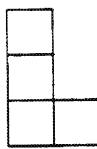
[111]



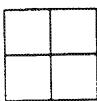
[4]



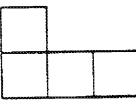
[31]



[22]



[211]



[1111]

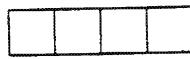


FIGURE 78.1. Young tableaux showing the possible symmetries for three-particle systems (a) and four-particle systems (b).

tum numbers, such as  $nlm_l, m_s, m_i, \dots$  for the  $n^{\text{th}}$  single-particle quantum state, numbered according to some order starting with  $n = 1$ . In terms of products of  $N$  such single-particle functions, it is fairly simple to construct an  $N$ -particle wave function totally symmetric for the  $N$ -boson sysystem, or totally antisymmetric for the  $N$ -fermion system.

For the  $N$ -boson system, the totally symmetric  $N$ -particle wave function can be given by

$$\begin{aligned} \psi(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}_3, \dots, \vec{\xi}_N) &= \mathcal{N} \sum_P P \left( \psi_{\alpha_1}(\vec{\xi}_1) \cdots \psi_{\alpha_1}(\vec{\xi}_{n_1}) \psi_{\alpha_2}(\vec{\xi}_{n_1+1}) \cdots \psi_{\alpha_2}(\vec{\xi}_{n_1+n_2}) \right. \\ &\quad \times \left. \psi_{\alpha_3}(\vec{\xi}_{n_1+n_2+1}) \cdots \psi_{\alpha_3}(\vec{\xi}_{n_1+n_2+n_3}) \cdots \psi_{\alpha_k}(\vec{\xi}_{N-n_k+1}) \cdots \psi_{\alpha_k}(\vec{\xi}_N) \right), \end{aligned} \quad (1)$$

where  $\sum_P$  includes a sum over the

$$\frac{N!}{n_1! n_2! n_3! \cdots n_k!}$$

permutations that exchange particles between groups of particles, e.g., between the group of  $n_1$  particles in the same quantum state,  $\alpha_1$ , and particles from the group with  $n_2$  particles in quantum state  $\alpha_2$  or particles in still other groups in higher quantum states. Permutations,  $P$ , which exchange particles with labels 1 through  $n_1$  are excluded from the sum, because the product of single-particle functions in the same quantum state,  $\alpha_1$ , are already symmetric in the first group of  $n_1$  particles. The normalization constant is then given by the squareroot of the inverse of the number of terms in this sum.

$$\mathcal{N} = \left[ \frac{\prod_{i=1}^k n_i!}{N!} \right]^{\frac{1}{2}}.$$

For the  $N$ -fermion system, the antisymmetrization will require that all  $n_i$  be either  $n_i = 1$  or  $n_i = 0$ , and the sum over permutations will require all  $N!$  terms with the appropriate sign

$$\psi(\vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_N) = \frac{1}{\sqrt{N!}} \sum_P^{N!} P (-1)^{\sigma(P)} \psi_{\alpha_1}(\vec{\xi}_1) \psi_{\alpha_2}(\vec{\xi}_2) \psi_{\alpha_3}(\vec{\xi}_3) \cdots \psi_{\alpha_N}(\vec{\xi}_N), \quad (2)$$

where  $\sigma(P)$  is an odd integer for all odd permutations, whereas it is an even integer for all even permutations. We have seen that such a totally antisymmetric  $N$ -particle function can be written in terms of an  $N \times N$  Slater determinant

$$\psi(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}_3, \dots, \vec{\xi}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{\alpha_1}(\vec{\xi}_1) & \psi_{\alpha_1}(\vec{\xi}_2) & \cdots & \psi_{\alpha_1}(\vec{\xi}_N) \\ \psi_{\alpha_2}(\vec{\xi}_1) & \psi_{\alpha_2}(\vec{\xi}_2) & \cdots & \psi_{\alpha_2}(\vec{\xi}_N) \\ \psi_{\alpha_3}(\vec{\xi}_1) & \psi_{\alpha_3}(\vec{\xi}_2) & \cdots & \psi_{\alpha_3}(\vec{\xi}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{\alpha_N}(\vec{\xi}_1) & \psi_{\alpha_N}(\vec{\xi}_2) & \cdots & \psi_{\alpha_N}(\vec{\xi}_N) \end{vmatrix}. \quad (3)$$

Wave functions of the type given by eqs. (1) or (3) are by themselves acceptable solutions for the  $N$ -particle system only if the interactions between particles are

“turned off.” For an  $N$ -electron atom, e. g., where the single particle quantum numbers,  $nlm_l m_s$ , specify the single-particle wave functions in the central Coulomb field of the nucleus, the  $N$ -particle wave function of eq. (3) would be an eigenfunction of the  $N$ -particle Hamiltonian with the Coulomb repulsion between electrons and all other electron-electron interactions “turned off.” We will therefore need linear combinations of such basis functions. In addition, despite the compact Slater determinant notation of eq. (3), each such wave function will be composed of  $N!$  terms. A better description of such  $N$ -particle state vectors would be through the occupation number representation, rather than the coordinate representations of eqs. (1) or (3). With the proper total symmetry for boson systems, or the proper total antisymmetry for fermion systems built in, we simply specify the occupation numbers,  $n_1, n_2, n_3, \dots, n_i, \dots$ , of quantum states labeled according to the index  $i$ , which includes all necessary single-particle quantum numbers, usually for the noninteracting  $N$ -particle system, which of course must be ordered according to some specific prescription, and with

$$\sum_{i=1}^{\infty} n_i = N, \quad (4)$$

where the  $n_i$  may be  $> 1$  for the boson systems, although of course many  $n_i$  will be zero, whereas for fermion systems,  $n_i = 1$  or  $n_i = 0$ , are the only possibilities.

Thus, for boson systems, we have state vectors of the type

$$|n_1 n_2 n_3 \cdots n_i \cdots \rangle$$

with  $n_i \geq 0$  and  $\sum_i n_i = N$ .

For fermion systems, we have state vectors of the type

$$|1101011100 \cdots \rangle$$

with  $N$  occupation numbers of 1, and the rest all 0.

To express arbitrary operators in this type of basis, it will be convenient to introduce operators acting only on the  $i^{\text{th}}$  single-particle state, ordered according to a definite prescription, where the index  $i$  is then also specified by the complete set of single-particle quantum numbers, such as  $nlm_l m_s \dots$  with specific index  $i$ , and where these operators annihilate or create one particle with specific index  $i$ , i.e., operators,  $a_i$  and  $a_i^\dagger$ , with nonzero matrix elements:

For the boson case:

$$\begin{aligned} \langle n_1 n_2 \cdots (n_i - 1) \cdots | a_i | n_1 n_2 \cdots n_i \cdots \rangle &= \sqrt{n_i}, \\ \langle n_1 n_2 \cdots n_i \cdots | a_i^\dagger | n_1 n_2 \cdots (n_i - 1) \cdots \rangle &= \sqrt{n_i}. \end{aligned} \quad (5)$$

For the fermion case:

$$\begin{aligned} |\langle \cdots n_i = 0 \cdots | a_i | \cdots n_i = 1 \cdots \rangle| &= 1, \\ |\langle \cdots n_i = 1 \cdots | a_i^\dagger | \cdots n_i = 0 \cdots \rangle| &= 1, \end{aligned} \quad (6)$$

all other matrix elements being zero for both bosons and fermions. Note the similarity of the boson case with that of an  $\infty$ -dimensional harmonic oscillator. Also, the sign of the fermion matrix elements may depend on the number of occupied states,

with  $i' < i$ , in our state vector prescription. Recall in the coordinate representation, the phase of the wave function depends on the ordering of the single-particle states with index  $i$ . Imagine that, in the ket of the matrix element of the annihilation operator,  $a_i$ , the occupied state with index  $i$ , and  $n_i = 1$  is shifted to the left through the occupied states, lower than  $i$  in our ordering scheme. A shift through each such occupied state will lead to a change in sign of the ket (cf., the coordinate representation Slater determinant), so

$$\langle \cdots n_i = 0 \cdots | a_i | \cdots n_i = 1 \cdots \rangle = (-1)^{\sum_{\mu=1}^{i-1} n_{\mu}}. \quad (7)$$

Similarly,

$$\langle \cdots n_i = 1 \cdots | a_i^{\dagger} | \cdots n_i = 0 \cdots \rangle = (-1)^{\sum_{\mu=1}^{i-1} n_{\mu}}. \quad (8)$$

Let us next look at matrix elements of products of two operators, such as  $a_i$  and  $a_r^{\dagger}$ , or  $a_i$  and  $a_r$ , in both the boson and fermion cases.

For the boson case, with index  $r \neq i$ ,

$$\begin{aligned} \langle \cdots n_i - 1 \cdots n_r \cdots | a_r^{\dagger} a_i | \cdots n_i \cdots n_r - 1 \cdots \rangle &= \sqrt{n_i n_r}, \\ \langle \cdots n_i - 1 \cdots n_r \cdots | a_i a_r^{\dagger} | \cdots n_i \cdots n_r - 1 \cdots \rangle &= \sqrt{n_i n_r}, \end{aligned} \quad (9)$$

leading to

$$\langle \cdots n_i - 1 \cdots n_r \cdots | (a_i a_r^{\dagger} - a_r^{\dagger} a_i) | \cdots n_i \cdots n_r - 1 \cdots \rangle = 0 \quad (10)$$

for all state vectors of the type shown and for  $r \neq i$ . Conversely, if the indices on the operators are the same,  $r = i$ , we have, as follows.

For the boson case:

$$\begin{aligned} \langle \cdots n_i \cdots | a_i^{\dagger} a_i | \cdots n_i \cdots \rangle &= n_i, \\ \langle \cdots n_i \cdots | a_i a_i^{\dagger} | \cdots n_i \cdots \rangle &= n_i + 1, \end{aligned} \quad (11)$$

leading in this case to

$$\langle \cdots n_i \cdots | (a_i a_i^{\dagger} - a_i^{\dagger} a_i) | \cdots n_i \cdots \rangle = +1. \quad (12)$$

Because these relations must hold for all indices and all state vectors, the operators,  $a_i$  and  $a_i^{\dagger}$ , must satisfy the commutation relation

$$[a_i, a_r^{\dagger}] = \delta_{ir}, \quad [a_i, a_r] = 0, \quad [a_i^{\dagger}, a_r^{\dagger}] = 0, \quad (13)$$

where the last two relations follow from the general matrix elements in similar fashion. The boson annihilation and creation operators therefore satisfy the same commutation relations as the annihilation and creation operators for an  $\infty$ -dimensional harmonic oscillator.

For fermions, conversely, with  $r < i$ ,

$$\begin{aligned} &\langle \cdots n_r = 1 \cdots n_i = 0 \cdots | a_r^{\dagger} a_i | \cdots n_r = 0 \cdots n_i = 1 \cdots \rangle \\ &= \langle \cdots n_r = 1 \cdots n_i = 0 \cdots | a_r^{\dagger} | \cdots n_r = 0 \cdots n_i = 0 \cdots \rangle \\ &\times \langle \cdots n_r = 0 \cdots n_i = 0 \cdots | a_i | \cdots n_r = 0 \cdots n_i = 1 \cdots \rangle \\ &= (-1)^{\sum_{\mu=1}^{i-1} n_{\mu} (\text{with } n_r = 0)} (-1)^{\sum_{v=1}^{r-1} n_v}, \end{aligned} \quad (14)$$

whereas

$$\begin{aligned} & \langle \cdots n_r = 1 \cdots n_i = 0 \cdots | a_i a_r^\dagger | \cdots n_r = 0 \cdots n_i = 1 \cdots \rangle \\ &= \langle \cdots n_r = 1 \cdots n_i = 0 \cdots | a_i | \cdots n_r = 1 \cdots n_i = 1 \cdots \rangle \\ &\times \langle \cdots n_r = 1 \cdots n_i = 1 \cdots | a_r^\dagger | \cdots n_r = 0 \cdots n_i = 1 \cdots \rangle \\ &= (-1)^{\sum_{k=1}^{i-1} n_k (\text{with } n_r=1)} (-1)^{\sum_{v=i+1}^r n_v}. \end{aligned} \quad (15)$$

Because of the extra  $n_r = 1$  in the phase factor for the second relation, we have, with  $r \neq i$ ,

$$\langle \cdots n_r = 1 \cdots n_i = 0 \cdots | (a_i a_r^\dagger + a_r^\dagger a_i) | \cdots n_r = 0 \cdots n_i = 1 \cdots \rangle = 0. \quad (16)$$

Conversely, with  $r = i$ , we have

$$\langle \cdots n_i \cdots | a_i^\dagger a_i | \cdots n_i \cdots \rangle = \begin{cases} 1 & \text{for } n_i = 1 \\ 0 & \text{for } n_i = 0 \end{cases} = n_i, \quad (17)$$

and

$$\langle \cdots n_i \cdots | a_i a_i^\dagger | \cdots n_i \cdots \rangle = \begin{cases} 1 & \text{for } n_i = 0 \\ 0 & \text{for } n_i = 1 \end{cases} = 1 - n_i, \quad (18)$$

leading to

$$\langle \cdots n_i \cdots | (a_i a_i^\dagger + a_i^\dagger a_i) | \cdots n_i \cdots \rangle = 1. \quad (19)$$

Combining the two cases,  $r \neq i$  and  $r = i$ , we have

$$\langle \text{arbitrary state} | (a_i a_r^\dagger + a_r^\dagger a_i) | \text{arbitrary state} \rangle = \delta_{ri}, \quad (20)$$

leading to the anticommutation relation

$$\{a_i, a_r^\dagger\}_+ = a_i a_r^\dagger + a_r^\dagger a_i = \delta_{ir}. \quad (21)$$

Similarly,

$$\{a_i, a_r\}_+ = 0, \quad \{a_i^\dagger, a_r^\dagger\}_+ = 0. \quad (22)$$

In particular, with  $i = r$ , the last relation gives

$$a_r^\dagger a_r^\dagger = 0. \quad (23)$$

We cannot create two identical fermions in the same quantum state. Similarly,

$$a_r a_r = 0. \quad (24)$$

For fermions, in general, the boson commutation relations are converted to fermion anticommutation relations, and for fermions, we need to deal with an anticommutator rather than a commutator algebra.

## B State Vectors

We shall now write both state vectors and operators representing physical quantities in terms of the above creation and annihilation operators. For both bosons and

fermions, we start with the vacuum state, the state of zero particles, i.e., no particles whatsoever.

$$|0\rangle = |00\cdots 0\cdots\rangle, \quad \text{with } a_i|0\rangle = 0 \quad \text{for all } i. \quad (25)$$

**Single-particle states:** For both the boson and fermion systems, single-particle states are given by

$$a_i^\dagger |0\rangle, \quad (26)$$

where the quantum number index,  $i$ , is shorthand for a specific set of values of all single-particle quantum numbers, orbital, spin, and quantum numbers with other internal degrees of freedom, if applicable.

**$N$ -particle states:** For boson systems, we have

$$\prod_i \frac{(a_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0\rangle, \quad \text{with } \sum_i n_i = N. \quad (27)$$

For fermion systems, we have

$$a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_N}^\dagger |0\rangle. \quad (28)$$

In particular, the action of a creation operator on such an  $N$ -particle state to make an  $(N+1)$ -particle state will in general add a phase factor to make a state with the conventional ordering of states dictated by our particular prescription.

$$a_{i_s}^\dagger (a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_N}^\dagger) |0\rangle = (-1)^{\sum_{\mu=1}^{s-1} n_\mu} (a_{i_1}^\dagger a_{i_2}^\dagger \cdots a_{i_s}^\dagger \cdots a_{i_N}^\dagger) |0\rangle. \quad (29)$$

## C One-Body Operators

Let us now construct the dynamical operators that we shall need and see how they can be expressed in terms of single-particle creation and annihilation operators. The simplest class of operators are the one-body operators. In coordinate representation, they can be expressed through

$$F_{\text{op.}} = \sum_{i=1}^N f_i, \quad \text{with } f_i = f(\vec{r}_i, \vec{\nabla}_i, \vec{\sigma}_i, \vec{\tau}_i, \dots), \quad (30)$$

where  $\dots$  will stand for additional internal variables, with index  $i$ , if needed for additional internal degrees of freedom. Examples would be the kinetic energy term in a nonrelativistic  $N$ -particle Hamiltonian

$$T = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m_i}, \quad (31)$$

or the potential terms of the  $N$ -particle system in an external field, e.g., the potential of the  $N$ -electron atomic system in the field of the central nucleus of charge,  $Ze$ ,

$$V = \sum_{i=1}^N \left( \frac{-Ze^2}{r_i} \right). \quad (32)$$

Other examples would be electric or magnetic multipole transition operators, e.g., the three components of the electric dipole moment vector,

$$F = \sum_{i=1}^N e_i \vec{r}_i, \quad (33)$$

or the spherical components of the magnetic  $2^L$ -pole operator,

$$F = \sum_{i=1}^N e_i \left[ r_i^{L-1} Y_{L-1}(\theta_i, \phi_i) \times \left( \frac{2}{L+1} \vec{l}_i^1 + g_s \vec{s}_i^1 \right) \right]_M^L. \quad (34)$$

To transcribe such operators from their coordinate representation to the occupation number representation, let us now use  $\vec{r}_i$  as shorthand for *all* variables, both orbital and intrinsic, with particle index  $i$ ; i.e.,  $\vec{r}_i \equiv \vec{r}_i, \vec{\sigma}_i, \vec{t}_i, \dots$ . In this shorthand notation,  $\int d\vec{r}_i$ , will then stand for an integral over all orbital variables and over all internal variables, or alternatively a matrix-element-taking over spin, isospin, . . . , quantum numbers, if the internal variables cannot be specified through specific coordinates. A one-body operator can then be expressed through

$$F_{\text{op.}} = \sum_{\alpha_s} \sum_{\alpha'_s} |\alpha'_1 \alpha'_2 \cdots \alpha'_N\rangle \langle \alpha'_1 \alpha'_2 \cdots \alpha'_N| F |\alpha_1 \alpha_2 \cdots \alpha_N\rangle \langle \alpha_1 \alpha_2 \cdots \alpha_N|, \quad (35)$$

where the sums over  $\alpha_s$  and  $\alpha'_s$  are infinite sums over all possible sets of  $N$ -particle quantum numbers in their canonical ordering. We can convert this expression in occupation number representation into coordinate representation, via

$$\begin{aligned} F_{\text{op.}} &= \int d\vec{r}'_1 \cdots d\vec{r}'_N \int d\vec{r}_1 \cdots d\vec{r}_N \sum_{\alpha_s} \sum_{\alpha'_s} |\alpha'_1 \alpha'_2 \cdots \alpha'_N\rangle \langle \alpha'_1 \alpha'_2 \cdots \alpha'_N| \vec{r}'_1 \cdots \vec{r}'_N \\ &\times \langle \vec{r}'_1 \cdots \vec{r}'_N | \sum_{i=1}^N f(\vec{r}_i, \vec{\nabla}_i, \dots) | \vec{r}_1 \cdots \vec{r}_N \rangle \langle \vec{r}_1 \cdots \vec{r}_N | \alpha_1 \alpha_2 \cdots \alpha_N \rangle \langle \alpha_1 \alpha_2 \cdots \alpha_N|. \end{aligned} \quad (36)$$

Let us now specialize to the fermion case. (The boson case is very similar, except for the additional phase factors that come into play for fermions.) In coordinate representation, we have

$$\begin{aligned} &\langle \vec{r}'_1 \cdots \vec{r}'_N | \sum_{i=1}^N f(\vec{r}_i, \vec{\nabla}_i, \dots) | \vec{r}_1 \cdots \vec{r}_N \rangle \\ &= \left( \sum_{i=1}^N f(\vec{r}_i, \vec{\nabla}_i, \dots) \delta(\vec{r}_i - \vec{r}'_i) \right) \prod_{j \neq i}^N \delta(\vec{r}_j - \vec{r}'_j), \end{aligned} \quad (37)$$

and the coordinate representations of the fully antisymmetrized  $N$ -particle states can be expressed in the form of eq. (2) or eq. (3),

$$\langle \alpha_1 \cdots \alpha_N | \vec{r}_1 \cdots \vec{r}_N \rangle = \Psi_{\alpha_1 \cdots \alpha_N}(\vec{r}_1, \dots, \vec{r}_N). \quad (38)$$

Eq. (36) can therefore be transcribed into

$$F_{\text{op.}} = \sum_{\alpha_s} \sum_{\alpha'_s} |\alpha'_1 \alpha'_2 \cdots \alpha'_N\rangle \int d\vec{r}_1 \cdots d\vec{r}_N \Psi_{\alpha'_1 \cdots \alpha'_N}^*(\vec{r}_1, \dots, \vec{r}_N) \langle \vec{r}'_1 \cdots \vec{r}'_N | \sum_{i=1}^N f(\vec{r}_i, \vec{\nabla}_i, \dots) | \vec{r}_1 \cdots \vec{r}_N \rangle \langle \vec{r}_1 \cdots \vec{r}_N | \alpha_1 \alpha_2 \cdots \alpha_N \rangle \langle \alpha_1 \alpha_2 \cdots \alpha_N|.$$

$$\times \sum_{i=1}^N f(\vec{r}_i, \vec{\nabla}_i, \dots) \Psi_{\alpha_1 \dots \alpha_N} \langle \alpha_1 \alpha_2 \dots \alpha_N |. \quad (39)$$

We now use the antisymmetry of the  $N$ -particle functions,  $\Psi_{\alpha_1 \dots \alpha_N}$ , viz.,

$$P_{1i} \Psi_{\alpha_1 \dots \alpha_N} = -\Psi_{\alpha_1 \dots \alpha_N},$$

to rewrite

$$\begin{aligned} & \int d\vec{r}_1 \dots d\vec{r}_N \Psi_{\alpha'_1 \dots \alpha'_N}^* f(\vec{r}_i, \vec{\nabla}_i, \dots) \Psi_{\alpha_1 \dots \alpha_N} \\ &= \int d\vec{r}_1 \dots d\vec{r}_N \Psi_{\alpha'_1 \dots \alpha'_N}^* \left( P_{1i}^{-1} f(\vec{r}_1, \vec{\nabla}_1, \dots) P_{1i} \right) \Psi_{\alpha_1 \dots \alpha_N} \\ &= \int d\vec{r}_1 \dots d\vec{r}_N \Psi_{\alpha'_1 \dots \alpha'_N}^* f(\vec{r}_1, \vec{\nabla}_1, \dots) \Psi_{\alpha_1 \dots \alpha_N}. \end{aligned} \quad (40)$$

Repeating this process  $N$  times, for  $i = 1 \rightarrow N$ , we get

$$F_{\text{op.}} = N \int d\vec{r}_1 \dots d\vec{r}_N \Psi_{\alpha'_1 \dots \alpha'_N}^* f_1 \Psi_{\alpha_1 \dots \alpha_N}, \quad (41)$$

where we have used the shorthand notation of eq. (30)

$$f_1 = f(\vec{r}_1, \vec{\nabla}_1, \dots). \quad (42)$$

If we now expand the fully antisymmetrized  $N$ -particle functions in this expression in terms of fully antisymmetrized  $(N-1)$ -particle functions, we get

$$\begin{aligned} F_{\text{op.}} &= \frac{N}{\sqrt{N} \sqrt{N}} \left( \int d\vec{r}_1 \Psi_{\alpha'_1}^* f_1 \Psi_{\alpha_1} \int d\vec{r}_2 \dots d\vec{r}_N \Psi_{\alpha'_2 \dots \alpha'_N}^* \Psi_{\alpha_2 \dots \alpha_N} \right. \\ &\quad - \int d\vec{r}_1 \Psi_{\alpha'_1}^* f_1 \Psi_{\alpha_2} \int d\vec{r}_2 \dots d\vec{r}_N \Psi_{\alpha'_2 \dots \alpha'_N}^* \Psi_{\alpha_1 \alpha_3 \dots \alpha_N} \\ &\quad + \int d\vec{r}_1 \Psi_{\alpha'_1}^* f_1 \Psi_{\alpha_3} \int d\vec{r}_2 \dots d\vec{r}_N \Psi_{\alpha'_2 \dots \alpha'_N}^* \Psi_{\alpha_1 \alpha_2 \alpha_4 \dots \alpha_N} \\ &\quad - \dots \\ &\quad + (-1)^{N-1} \int d\vec{r}_1 \Psi_{\alpha'_1}^* f_1 \Psi_{\alpha_N} \int d\vec{r}_2 \dots d\vec{r}_N \Psi_{\alpha'_2 \dots \alpha'_N}^* \Psi_{\alpha_1 \alpha_2 \dots \alpha_{N-1}} \\ &\quad - \int d\vec{r}_1 \Psi_{\alpha'_1}^* f_1 \Psi_{\alpha_2} \int d\vec{r}_2 \dots d\vec{r}_N \Psi_{\alpha'_1 \alpha'_3 \dots \alpha'_N}^* \Psi_{\alpha_2 \dots \alpha_N} \\ &\quad + \dots \\ &\quad \left. + \int d\vec{r}_1 \Psi_{\alpha'_N}^* f_1 \Psi_{\alpha_N} \int d\vec{r}_2 \dots d\vec{r}_N \Psi_{\alpha'_1 \alpha'_2 \dots \alpha'_{N-1}}^* \Psi_{\alpha_1 \alpha_2 \dots \alpha_{N-1}} \right), \end{aligned} \quad (43)$$

where  $N^2$  terms in this expansion exist altogether, but where the  $(N-1)$ -particle overlap integrals in the particles labeled 2 through  $N$  will all be zero unless the primed and unprimed quantum numbers in the  $(N-1)$ -particle functions are all the same, i.e., unless  $(\alpha'_2 \dots \alpha'_N) = (\alpha_2 \dots \alpha_N)$  in the first term of this expansion. Hence, the full matrix element of the one-body operator,  $F_{\text{op.}}$ , will be different from zero only in two cases as follows.

Case (1), if the  $\alpha'_1 \dots \alpha'_N$  differ from the  $\alpha_1 \dots \alpha_N$  in only *one* of the  $\alpha_s$ .

Case (2), if all  $\alpha'_s = \alpha_s$ .

For case (1), we have

$$\begin{aligned} |\alpha_1 \cdots \alpha_N\rangle &= |\alpha_1 \alpha_2 \cdots \alpha_r \cdots \alpha_{s-1} \alpha_{s+1} \cdots \alpha_N\rangle, \\ |\alpha'_1 \cdots \alpha'_N\rangle &= |\alpha_1 \alpha_2 \cdots \alpha_{r-1} \alpha_{r+1} \cdots \alpha_s \cdots \alpha_N\rangle. \end{aligned} \quad (44)$$

For case (2), we have

$$|\alpha'_1 \cdots \alpha'_N\rangle = |\alpha_1 \cdots \alpha_N\rangle. \quad (45)$$

For case (1), the  $N$ -particle matrix element of  $F_{\text{op.}}$  is

$$\begin{aligned} &\langle \alpha'_1 \cdots \alpha'_N | F_{\text{op.}} | \alpha_1 \cdots \alpha_N \rangle \\ &= (-1)^{\sum_{\mu=1}^{r-1} n_\mu} (-1)^{\sum_{v=1}^{s-1} n'_v} \int d\vec{r}_1 \psi_{\alpha_r}^*(\vec{r}_1) f(\vec{r}_1, \vec{\nabla}_1, \dots) \psi_{\alpha_r}(\vec{r}_1) \\ &= (-1)^{\sum_{\mu=1}^{r-1} n_\mu} (-1)^{\sum_{v=1}^{s-1} n'_v} \langle s | f | r \rangle, \end{aligned} \quad (46)$$

where we have used an obvious shorthand notation for the single-particle matrix element of the single-particle operator in the last step.

For case (2), conversely, we have

$$\begin{aligned} \langle \alpha'_1 \cdots \alpha'_N | F_{\text{op.}} | \alpha_1 \cdots \alpha_N \rangle &= \sum_{\substack{\alpha_i = \alpha_N \\ \alpha_i = \alpha_1}}^{\alpha_i = \alpha_N} \int d\vec{r}_1 \psi_{\alpha_r}^*(\vec{r}_1) f(\vec{r}_1, \vec{\nabla}_1, \dots) \psi_{\alpha_r}(\vec{r}_1) \\ &= \sum_{i=1}^{N_{\text{occ}}} \langle i | f | i \rangle, \end{aligned} \quad (47)$$

where the sum is over the  $N$  occupied states. Now, if we use the matrix elements

$$\begin{aligned} &a_r |\alpha_1 \alpha_2 \cdots \alpha_r \cdots \alpha_{s-1} \alpha_{s+1} \cdots \alpha_N\rangle \\ &= (-1)^{\sum_{\mu=1}^{r-1} n_\mu} |\alpha_1 \alpha_2 \cdots \cdots \alpha_{s-1} \alpha_{s+1} \cdots \alpha_N\rangle, \\ &\langle \alpha_1 \alpha_2 \cdots \alpha_{r-1} \alpha_{r+1} \cdots \alpha_{s-1} \alpha_{s+1} \cdots \alpha_N | a_s^\dagger \\ &= \langle \alpha_1 \alpha_2 \cdots \alpha_{r-1} \alpha_{r+1} \cdots \alpha_{s-1} \alpha_s \alpha_{s+1} \cdots \alpha_N | (-1)^{\sum_{v=1}^{s-1} n'_v}, \\ &\langle \alpha_1 \alpha_2 \cdots \alpha_N | a_i^\dagger a_i | \alpha_1 \alpha_2 \cdots \alpha_N \rangle = n_i, \\ &\text{with } n_i = 1 \text{ for occ. states, } n_i = 0 \text{ otherwise,} \end{aligned} \quad (48)$$

the matrix elements for cases (1) and (2) will be obtained if the one-body operator is expressed in terms of single-particle creation and annihilation operators, via

$$F_{\text{op.}} = \sum_{r,s} \langle s | f | r \rangle a_s^\dagger a_r. \quad (49)$$

## D Examples of One-Body Operators

Before proceeding to two-body operators, let us look at a few specific examples of simple one-body operators in this new language.

1. The number operator.

One of the simplest one-body operators is the simple number operator that counts the total number of particles. In the coordinate representation, it is simply a sum of  $N$  unit operators

$$F = \sum_{i=1}^N 1 = N. \quad (50)$$

With  $f_i = 1$ , the single-particle matrix elements are simply

$$\langle s | f | r \rangle = \langle s | 1 | r \rangle = \delta_{sr}, \quad (51)$$

so

$$F_{\text{op.}} \equiv N_{\text{op.}} = \sum_s a_s^\dagger a_s. \quad (52)$$

### 2. Total angular momentum operator.

In this case, we may want the three components,  $J_z$ ,  $J_x$ ,  $J_y$ , where

$$J_z = \sum_{i=1}^N j_{z,i}, \quad (53)$$

where capital letters are used for the operator acting in the  $N$ -particle system and the lowercase letter indicates the operator acts in the space of the single-particle labeled with index  $i$ . If the total angular momentum vector is built from orbital and spin angular momenta,  $\vec{J} = \vec{L} + \vec{S}$ , it will be useful to employ an  $|nlsjm_j\rangle$  single-particle basis, with  $|r\rangle = |n_r l_r s_r j_r m_{j_r}\rangle$ , rather than a  $|nlm_l sm_s\rangle$  basis, so  $J_z = J_0$  is diagonal in this basis:

$$\begin{aligned} J_0 &= \sum_{i,k} \langle i | j_0 | k \rangle a_i^\dagger a_k \\ &= \sum_{i,k} \langle n_i l_i s_i j_i m_{j_i} | j_0 | n_k l_k s_k j_k m_{j_k} \rangle a_i^\dagger a_k \\ &= \sum_{i,k} m_j \delta_{ik} a_i^\dagger a_k \\ &= \sum_{nlsj} \sum_{m_j} m_j a_{nlsjm_j}^\dagger a_{nlsjm_j}. \end{aligned} \quad (54)$$

The perpendicular components of  $\vec{J}$  are best expressed in terms of  $J_\pm = (J_x \pm i J_y)$ , via

$$\begin{aligned} J_\pm &= \sum_{i,k} \langle i | j_\pm | k \rangle a_i^\dagger a_k \\ &= \sum_{nlsj} \sum_{m_j} \sqrt{(j \mp m_j)(j \pm m_j + 1)} a_{nlsj(m_j \pm 1)}^\dagger a_{nlsj m_j}. \end{aligned} \quad (55)$$

### 3. Electric dipole moment operator.

In this case, let us look first at the  $m = +1$  spherical component of the electric dipole moment vector of the  $N$  electron system in an atom, where

$$\mu_{+1}^{(\text{el.})} = \sum_{i=1}^N e_i (\vec{r}_i)_{+1} = -|e| \sum_{i=1}^N r_i Y_{1,+1}(\theta_i, \phi_i) \sqrt{\frac{4\pi}{3}}, \quad (56)$$

where  $\vec{r}_i$  measures the position of the electron with particle index  $i$  relative to the nucleus at the origin. It will now be advantageous to use a  $|nlm_lsm_s\rangle$  basis, so in our new language

$$|k\rangle \equiv |n_k l_k m_{l_k} s_k m_{s_k}\rangle.$$

In the new language, we then have

$$\begin{aligned} \mu_{+1}^{(\text{el.})} &= \sum_{n'l'} \sum_{nl} \sum_{m_l m_s} \langle n'l'(m_l + 1) \frac{1}{2} m_s | \mu_{+1}^{(\text{el.})} | nlm_l \frac{1}{2} m_s \rangle a_{n'l'(m_l+1)m_s}^\dagger a_{nlm_l m_s} \\ &= -|e| \sum_{n'l'} \sum_{nl} \sum_{m_l m_s} (r)_{n'l',nl} \sqrt{\frac{(2l+1)}{(2l'+1)}} \langle l010 | l'0 \rangle \\ &\quad \times \langle lm_l 11 | l'(m_l + 1) \rangle a_{n'l'(m_l+1)m_s}^\dagger a_{nlm_l m_s}, \end{aligned} \quad (57)$$

where  $(r)_{n'l',nl}$  is the radial integral

$$(r)_{n'l',nl} = \int_0^\infty dr r^2 R_{n'l'}^*(r) r R_{nl}(r).$$

For a system of  $A$  nucleons in a nucleus, we can write the charge of the  $i^{\text{th}}$  nucleon as

$$e_i = |e| \frac{1}{2} (1 - \tau_{z,i}),$$

and use a  $|nlm_lsm_s m_i\rangle$  basis in a convention in which the neutron has isospin quantum number  $m_i = +\frac{1}{2}$ , with  $\tau_z$ -eigenvalue of +1, whereas the proton has  $m_i = -\frac{1}{2}$ , with  $\tau_z$ -eigenvalue of -1. In this  $A$ -particle system, we have

$$\begin{aligned} \mu_{+1}^{(\text{el.})} &= \sum_{i=1}^A |e| \frac{1}{2} (1 - \tau_{z,i}) r_i Y_{1,+1}(\theta_i, \phi_i) \sqrt{\frac{4\pi}{3}} \\ &= |e| \sum_{n'l'} \sum_{nl} \sum_{m_l m_s} \sum_{m_i} \left( \frac{1}{2} - m_i \right) (r)_{n'l',nl} \sqrt{\frac{(2l+1)}{(2l'+1)}} \langle l010 | l'0 \rangle \\ &\quad \times \langle lm_l 11 | l'(m_l + 1) \rangle a_{n'l'(m_l+1)m_s m_i}^\dagger a_{nlm_l m_s m_i}, \end{aligned} \quad (58)$$

where the isospin quantum number,  $m_i$ , has the values  $m_i = +\frac{1}{2}$  for neutrons,  $m_i = -\frac{1}{2}$  for protons. (The subscript,  $i$ , on  $m_i$  stands for isospin.)

#### 4. Magnetic dipole moment operator.

For the magnetic dipole moment operator in the  $N$ -electron atom, we have

$$\mu_{+1}^{(\text{magn.})} = \sum_{i=1}^N \frac{e\hbar}{2mc} \left[ (\vec{l}_i)_{+1} + g_s (\vec{s}_i)_{+1} \right], \quad (59)$$

with  $g_s = 2$ , where we have neglected the nuclear magnetic moment because of the small electron to nucleus mass ratio,  $m/M_{\text{nuc.}}$ . In the new language, we would then have

$$\begin{aligned} \mu_{+1}^{(\text{magn.})} = & -\frac{1}{\sqrt{2}} \frac{e\hbar}{2mc} \sum_{nl} \sum_{m_l} \sum_{m_s} \\ & \left[ \sqrt{(l-m_l)(l+m_l+1)} a_{nl(m_l+1)m_s}^\dagger a_{nlm_lm_s} \right. \\ & \left. + g_s \sqrt{\left(\frac{1}{2}-m_s\right)\left(\frac{1}{2}+m_s+1\right)} a_{nlm_l(m_s+1)}^\dagger a_{nlm_lm_s} \right]. \end{aligned} \quad (60)$$

## E Two-Body Operators

In coordinate representation, two-body operators can be written as a sum over  $\frac{1}{2}N(N-1)$  terms

$$G_{\text{op.}} = \sum_{i < k}^N g_{ik}, \quad (61)$$

where

$$g_{ik} = g(\vec{r}_i, \vec{r}_k) = g(\vec{r}_k, \vec{r}_i), \quad (62)$$

and we again use the shorthand notation: Let  $\vec{r}_i$  stand for all coordinates, both orbital and internal, for particle labeled with particle index,  $i$ . A simple example would be the Coulomb repulsion potential between electrons in an  $N$ -electron atom,

$$g_{ik} = \frac{e^2}{r_{ik}} = \frac{e^2}{|\vec{r}_i - \vec{r}_k|}. \quad (63)$$

Now, using the antisymmetry of the  $N$ -particle wave functions,  $\Psi_{\alpha_1\alpha_2\dots\alpha_N}$ , we can reduce the matrix element of  $G_{\text{op.}}$  to a matrix element of  $g_{12}$ .

$$\begin{aligned} & \int d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_N \Psi_{\alpha'_1\alpha'_2\dots\alpha'_N}^* G_{\text{op.}} \Psi_{\alpha_1\alpha_2\dots\alpha_N} \\ &= \frac{1}{2}N(N-1) \int d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_N \Psi_{\alpha'_1\alpha'_2\dots\alpha'_N}^* g_{12} \Psi_{\alpha_1\alpha_2\dots\alpha_N}, \end{aligned} \quad (64)$$

where this is the analogue of eq. (41) for the one-body operator,  $F_{\text{op.}}$ . In addition, it will be useful to expand the totally antisymmetric  $N$ -particle functions,  $\Psi_{\alpha_1\alpha_2\dots\alpha_N}$ , in terms of totally antisymmetric  $(N-2)$ -particle functions, via [see eq. (3)],

$$\begin{aligned} \Psi_{\alpha_1\alpha_2\dots\alpha_N}(\vec{r}_1, \dots, \vec{r}_N) = & \frac{1}{\sqrt{N(N-1)}} \left[ \left( \psi_{\alpha_1}(\vec{r}_1) \psi_{\alpha_2}(\vec{r}_2) - \psi_{\alpha_2}(\vec{r}_1) \psi_{\alpha_1}(\vec{r}_2) \right) \Psi_{\alpha_3\alpha_4\dots\alpha_N}(\vec{r}_3, \dots, \vec{r}_N) \right. \\ & - \left. \left( \psi_{\alpha_1}(\vec{r}_1) \psi_{\alpha_3}(\vec{r}_2) - \psi_{\alpha_3}(\vec{r}_1) \psi_{\alpha_1}(\vec{r}_2) \right) \Psi_{\alpha_2\alpha_4\dots\alpha_N}(\vec{r}_3, \dots, \vec{r}_N) \right. \\ & \left. + \dots \right. \end{aligned}$$

$$\begin{aligned}
& + (-1)^{\chi_{ij}} \left( \psi_{\alpha_i}(\vec{r}_1) \psi_{\alpha_j}(\vec{r}_2) - \psi_{\alpha_j}(\vec{r}_1) \psi_{\alpha_i}(\vec{r}_2) \right) \Psi_{\alpha_1 \dots \alpha_N}(\vec{r}_3, \dots, \vec{r}_N) \\
& + \dots \\
& + \left. \left( \psi_{\alpha_{N-1}}(\vec{r}_1) \psi_{\alpha_N}(\vec{r}_2) - \psi_{\alpha_N}(\vec{r}_1) \psi_{\alpha_{N-1}}(\vec{r}_2) \right) \Psi_{\alpha_1 \alpha_2 \dots \alpha_{N-2}}(\vec{r}_3, \dots, \vec{r}_N) \right], \\
\text{with } \chi_{ij} = & \sum_{\mu=1}^{i-1} n_{\mu} + \sum_{v=1}^{j-1} n_v - 1,
\end{aligned} \tag{65}$$

where we have assumed  $i < j$  in fixing the phase of the generic term in this expansion. Now, three classes of nonzero matrix elements exist, as follows.

Case (1): The  $\alpha'_1 \dots \alpha'_N$  differ from the  $\alpha_1 \dots \alpha_N$  in two quantum numbers: Suppose  $\alpha_i$  and  $\alpha_j$ , with  $i < j$ , are present in the  $N$ -particle state with unprimed  $\alpha$ 's, but absent in the state with primed  $\alpha$ 's, whereas  $\alpha_r$  and  $\alpha_s$ , with  $r < s$ , are present in the state with primed  $\alpha$ 's, but missing in the state with unprimed  $\alpha$ 's. The remaining  $(N-2)$   $\alpha'_k$  are the same as the remaining  $(N-2)$   $\alpha_k$ . In that case,

$$\begin{aligned}
\langle \alpha'_1 \dots \alpha'_N | G_{\text{op.}} | \alpha_1 \dots \alpha_N \rangle = & \frac{1}{2} (-1)^{\sum_{\mu=1}^{i-1} n_{\mu} + \sum_{v=1}^{j-1} n_v - 1 + \sum_{\mu=1}^{r-1} n'_{\mu} + \sum_{v=1}^{s-1} n'_v - 1} \\
\times & \left[ \langle rs | g_{12} | ij \rangle - \langle rs | g_{12} | ji \rangle + \langle sr | g_{12} | ji \rangle - \langle sr | g_{12} | ij \rangle \right].
\end{aligned} \tag{66}$$

Case (2): The  $\alpha'_1 \dots \alpha'_N$  differ from the  $\alpha_1 \dots \alpha_N$  in one quantum number. Suppose  $\alpha_i$  is present in the  $N$ -particle state with unprimed  $\alpha$ 's, but absent in the state with primed  $\alpha$ 's, whereas  $\alpha_r$  is present in the state with primed  $\alpha$ 's, but missing in the state with unprimed  $\alpha$ 's. The remaining  $(N-1)$   $\alpha'_k$  are the same as the remaining  $(N-1)$   $\alpha_k$ . In that case,

$$\begin{aligned}
\langle \alpha'_1 \dots \alpha'_N | G_{\text{op.}} | \alpha_1 \dots \alpha_N \rangle = & \frac{1}{2} (-1)^{\sum_{\mu=1}^{i-1} n_{\mu}} (-1)^{\sum_{v=1}^{r-1} n'_v} \\
\times & \sum_{\substack{\text{occ.} \\ k \neq i, r}} \left[ \langle rk | g_{12} | ik \rangle - \langle rk | g_{12} | ki \rangle + \langle kr | g_{12} | ki \rangle - \langle kr | g_{12} | ik \rangle \right].
\end{aligned} \tag{67}$$

The sum over  $k$  is a sum over the  $(N-1)$  occupied states other than  $k = i$  of the ket and  $k = r$  in the bra.

Case (3): Diagonal matrix elements. The  $\alpha'_s$  are all equal to the  $\alpha_s$ :  $\alpha'_1 \alpha'_2 \dots \alpha'_N = \alpha_1 \alpha_2 \dots \alpha_N$ . In this case,

$$\begin{aligned}
\langle \alpha_1 \dots \alpha_N | G_{\text{op.}} | \alpha_1 \dots \alpha_N \rangle = & \\
\frac{1}{2} \sum_{i < k}^{\text{occ.}} & \left[ \langle ik | g_{12} | ik \rangle - \langle ik | g_{12} | ki \rangle + \langle ki | g_{12} | ki \rangle - \langle ki | g_{12} | ik \rangle \right],
\end{aligned} \tag{68}$$

where the sum is now over all  $N$  occupied states.

In eqs. (66), (67), and (68), the two-particle matrix elements, such as

$$\langle rs | g_{12} | ij \rangle = \int d\vec{r}_1 d\vec{r}_2 \psi_{\alpha_r}^*(\vec{r}_1) \psi_{\alpha_s}^*(\vec{r}_2) g(\vec{r}_1, \vec{r}_2) \psi_{\alpha_i}(\vec{r}_1) \psi_{\alpha_j}(\vec{r}_2),$$

can be related to the two-particle matrix elements

$$\langle sr | g_{12} | ji \rangle$$

by a renaming of the dummy integration variables  $\vec{r}_1 \leftrightarrow \vec{r}_2$ , and by making use of the symmetry of  $g_{12}$

$$g(\vec{r}_2, \vec{r}_1) = g(\vec{r}_1, \vec{r}_2)$$

to obtain

$$\begin{aligned} \langle rs|g_{12}|ij\rangle &= \langle sr|g_{12}|ji\rangle, \\ \langle rs|g_{12}|ji\rangle &= \langle sr|g_{12}|ij\rangle. \end{aligned} \quad (69)$$

In eqs. (66)–(68), we have purposely left off this simplification to facilitate the transition to the new language in terms of annihilation and creation operators. To make this transition,

$$\begin{aligned} a_j a_i \left( a_{k_1}^\dagger a_{k_2}^\dagger \cdots a_i^\dagger \cdots a_j^\dagger \cdots a_{k_N}^\dagger \right) |0\rangle \\ = (-1)^{\sum_{\mu=1}^{i-1} n_\mu} (-1)^{\sum_{v=1}^{j-1} n_v - 1} \left( a_{k_1}^\dagger a_{k_2}^\dagger \cdots \cdots \cdots a_{k_N}^\dagger \right) |0\rangle, \end{aligned} \quad (70)$$

where we have assumed,  $i < j$ , in our prescription for ordering the states. To obtain eq. (70), we use the anticommutation relations for the fermion annihilation and creation operators, and first “anticommute  $a_i$  through to the right,” obtaining a factor (-1) for every occupied state with index  $\mu < i$ . The resultant  $a_i a_i^\dagger$  is then rewritten as  $(1 - a_i^\dagger a_i)$ . Because the  $a_i$  sitting to the right of the creation operator  $a_i^\dagger$  can no longer meet an  $a_i^\dagger$  in its action to the right, it will simply annihilate the vacuum state and yield zero. Subsequently,  $a_j$  is “anticommutated through to the right,” yielding a factor (-1) for every occupied state with index  $v < j$  except the state with  $v = i$ , because this state was already eliminated by the prior action with  $a_i$ . Similarly, we have, with  $r < s$ ,

$$\begin{aligned} a_r^\dagger a_s^\dagger \left( a_{k_1}^\dagger a_{k_2}^\dagger \cdots \cdots \cdots a_{k_N}^\dagger \right) |0\rangle \\ = (-1)^{\sum_{v=1}^{s-1} n_v - 1} (-1)^{\sum_{\mu=1}^{r-1} n_\mu} \left( a_{k_1}^\dagger a_{k_2}^\dagger \cdots a_r^\dagger \cdots a_s^\dagger \cdots a_{k_N}^\dagger \right) |0\rangle, \end{aligned} \quad (71)$$

where the occupation numbers,  $n_v$  and  $n_\mu$ , are the occupation numbers of the final  $N$ -particle state. In particular,  $a_s^\dagger$  does not meet the state with  $v = r$  as it is “anticommutated through to the right” into its proper position according to our prescription for the indices.

Now, using eqs. (70) and (71), the general two-body operator can be expressed in the new language through

$$G_{\text{op.}} = \frac{1}{2} \sum_{a,b,c,d} \langle ab|g|cd\rangle a_a^\dagger a_b^\dagger a_d a_c, \quad (72)$$

yielding the required phases for the  $N$ -particle matrix elements of eqs. (66)–(68). In particular, the order of the annihilation operators  $a_d$  and  $a_c$  is the reverse of the order of the states  $c$  and  $d$  in the ket of the two-particle matrix elements.

We have derived eqs. (49) and (72) for the case of  $N$ -fermion systems. The derivation for the  $N$ -boson systems parallels that of the  $N$ -fermion system, except for the extra phase factors of (-1), which arise through the anticommutation processes of the fermion systems. These phase factors are missing for the boson

systems, where the anticommutation process is replaced by a commutation process. Because these fermion phase factors drop out of the final expressions of eq. (49) for one-body operators and eq. (72) for two-body operators, these expressions are valid for both bosons and fermions. [In the fermion case, however, a term with  $a = b$ , or with  $c = d$  is automatically missing in eq. (72), because  $a_a^\dagger a_a^\dagger \equiv 0$ , similarly  $a_c a_c \equiv 0$ , in the fermion case.]

## F Examples of Two-Body Operators

Let us return to the fermion case and examine first the simplest two-body operator, the two-body unit operator, which merely counts the number of pairs in the  $N$ -body system. In coordinate representation,

$$G_{\text{op.}} = \sum_{i < k}^N 1 = \frac{1}{2} N(N - 1). \quad (73)$$

In the new language,

$$\begin{aligned} G_{\text{op.}} &= \frac{1}{2} \sum_{a,b,c,d} \langle ab | cd \rangle a_a^\dagger a_b^\dagger a_d a_c = \frac{1}{2} \sum_{a,b,c,d} \delta_{ac} \delta_{bd} a_a^\dagger a_b^\dagger a_d a_c \\ &= \frac{1}{2} \sum_{a,b} a_a^\dagger a_b^\dagger a_b a_a = -\frac{1}{2} \sum_{a,b} a_a^\dagger a_b^\dagger a_a a_b = -\frac{1}{2} \sum_{a,b} a_a^\dagger (-a_a a_b^\dagger + \delta_{ab}) a_b \\ &= \frac{1}{2} \sum_a a_a^\dagger a_a \sum_b a_b^\dagger a_b - \frac{1}{2} \sum_a a_a^\dagger a_a = \frac{1}{2} (N_{\text{op.}}^2 - N_{\text{op.}}) = \frac{1}{2} N(N - 1). \end{aligned} \quad (74)$$

As an example of a simple two-body interaction, let us write the electron pairing interaction for a condensed matter system where the three orbital quantum numbers are given by the  $\vec{k}$  vector, with a finely spaced (effectively continuous) spectrum of allowed  $\vec{k}$  values, where

$$\begin{aligned} V &= \sum_{i < k}^N v_{ik}^{\text{pairing}} \\ &= \frac{1}{2} \sum_{\vec{k}} \sum_{\vec{k}'} \sum_{m_s} \sum_{m'_s} v_{\vec{k}\vec{k}'} a_{\vec{k}m_s}^\dagger a_{-\vec{k}-m_s}^\dagger a_{-\vec{k}'-m'_s} a_{\vec{k}'m'_s}, \end{aligned} \quad (75)$$

where the coefficients,  $v_{\vec{k}\vec{k}'}$ , are independent of the sign of  $\vec{k}$  or of  $\vec{k}'$ . The interaction thus acts only on electron pairs with zero two-particle momentum and two-particle spin,  $S = 0$ . In the next chapter, we shall examine in more detail a similar nuclear pairing interaction.

# Many-Body Techniques: Some Simple Applications

## A Construction of All Pauli-Allowed States of a $(d_{5/2})^{N=3}$ Fermion Configuration

As a first simple application, let us construct all allowed states of a  $(d_{5/2})^{N=3}$  configuration of identical fermions. The fermions could be electrons in a valence shell of an atom for which the  $j - j$  coupling scheme is valid, or they could be identical nucleons, either all protons or all neutrons, in a nuclear shell model valence orbit of a nucleus. Let us first consider the possible states for a system of three distinguishable particles, each with a single-particle angular momentum with  $j = 5/2$ . They could be distinguishable because they are different particles, e.g., one proton, one neutron, and one electron, or they could be identical particles, say, all neutrons in a nucleus, but with different principal and orbital angular momentum quantum numbers; i.e.  $n_1 l_1 \neq n_2 l_2 \neq n_3 l_3$ . For this case of three distinguishable particles, each with  $j = 5/2$ , there are  $6 \times 6 \times 6 = 216$  allowed states with total angular momenta,  $J$ , given by

$$J = \left(\frac{1}{2}\right)^2, \left(\frac{3}{2}\right)^4, \left(\frac{5}{2}\right)^6, \left(\frac{7}{2}\right)^5, \left(\frac{9}{2}\right)^4, \left(\frac{11}{2}\right)^3, \left(\frac{13}{2}\right)^2, \left(\frac{15}{2}\right)^1,$$

where the superscripts give the number of occurrences of each listed  $J$  value. The two independent  $J = \frac{1}{2}$  states could be obtained from the two states with  $J_{12} = 2$  and  $J_{12} = 3$  coupled with the third  $j = 5/2$ -particle. In general, we have

$$J = [J_{12} \times \frac{5}{2}] = [(0 + 1 + 2 + 3 + 4 + 5) \times \frac{5}{2}].$$

For three identical  $j = \frac{5}{2}$  fermions, however, the set of allowed total  $J$  values is much more restricted. Because the three fermions are assumed to have the same values for the quantum numbers,  $nlsj$ , with  $s = \frac{1}{2}$  and  $j = \frac{5}{2}$ , let us use the abbreviation

$$a_{nlsj=\frac{5}{2}m}^\dagger \equiv a_m^\dagger;$$

i.e., for economy of writing the common quantum numbers,  $nlsj$ , will be quietly understood. A three-particle state can thus be expressed in our new language by

$$a_{m_1}^\dagger a_{m_2}^\dagger a_{m_3}^\dagger |0\rangle,$$

where the “vacuum” state,  $|0\rangle$ , could be the true vacuum state, with particle number zero, or a closed shell state with  $(N - 3)$  particles filling lower shell model orbits, which satisfy the condition,  $a_{m_k}|0\rangle = 0$ , where  $a_{m_k}$  is the shorthand notation for the annihilation operator for the  $nlsjm$  single-particle state under consideration. Because the above

$$a_{m_1}^\dagger a_{m_2}^\dagger a_{m_3}^\dagger |0\rangle$$

will be identically equal to zero, if  $m_1 = m_2$ , or if any two  $m_k$  are the same, there will be six possible choices for  $m_1$ , but once  $m_1$  has been chosen, there are only five possible choices for  $m_2$ , and once both  $m_1$  and  $m_2$  have been chosen, only four possible choices for  $m_3$  remain. In addition, any of the possible  $3!$  permutations of the quantum numbers  $m_k$  can at most change the sign of the above three-fermion state. Therefore, only

$$\frac{6 \cdot 5 \cdot 4}{3!} = 20$$

independent states exist in a configuration of three identical  $j = 5/2$  fermions, in place of the 216 states with  $J$  values ranging from  $\frac{1}{2}$  to  $\frac{15}{2}$  listed above. What are the possible  $J, M_J$  values of these 20 states? It will be worthwhile to answer this question through a specific construction of these states. This process will then permit us to make calculations involving such states. The requirement  $m_1 \neq m_2 \neq m_3$  shows us the highest possible value of  $M_J = m_1 + m_2 + m_3$  is

$$M_J = \frac{5}{2} + \frac{3}{2} + \frac{1}{2} = \frac{9}{2}.$$

Moreover, the state

$$a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger |0\rangle = |J = \frac{9}{2}, M_J = \frac{9}{2}\rangle; \quad (1)$$

i.e., this state has both  $M_J = \frac{9}{2}$ , and  $J = \frac{9}{2}$ . This result can be seen by noting

$$J_+ \left( a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger |0\rangle \right) = 0, \quad (2)$$

where the operator,  $J_+$ , see eq. (55) of Chapter 78,

$$J_+ = \sqrt{5}a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}} + \sqrt{8}a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}} + 3a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}} + \sqrt{8}a_{-\frac{1}{2}}^\dagger a_{-\frac{3}{2}} + \sqrt{5}a_{-\frac{3}{2}}^\dagger a_{-\frac{5}{2}}, \quad (3)$$

when acting on the above three-particle state with  $M_J = \frac{9}{2}$  can only convert the single-particle creation operator with  $m = \frac{3}{2}$  into a single-particle creation operator with  $m = \frac{5}{2}$ , making a state with  $a_{m_1}^\dagger = a_{m_2}^\dagger$ , which is identically equal to zero, or it could convert the single-particle creation operator with  $m = \frac{1}{2}$  into one with  $m = \frac{3}{2}$ , again creating a state identically equal to zero.

Now, starting with the state of eq. (1), we can create states with  $J = \frac{9}{2}$  and lower values of  $M_J$  by successive actions with the operator,  $J_-$ , with

$$J_- = \sqrt{5}a_{\frac{3}{2}}^\dagger a_{\frac{5}{2}} + \sqrt{8}a_{\frac{1}{2}}^\dagger a_{\frac{3}{2}} + 3a_{-\frac{1}{2}}^\dagger a_{\frac{1}{2}} + \sqrt{8}a_{-\frac{3}{2}}^\dagger a_{-\frac{1}{2}} + \sqrt{5}a_{-\frac{5}{2}}^\dagger a_{-\frac{3}{2}}. \quad (4)$$

Note,

$$J_- |\frac{9}{2} + \frac{9}{2}\rangle = \sqrt{9 \cdot 1} |\frac{9}{2} + \frac{7}{2}\rangle = 3a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{1}{2}}^\dagger |0\rangle, \quad (5)$$

so the normalized state is

$$|\frac{9}{2} + \frac{7}{2}\rangle = a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{1}{2}}^\dagger |0\rangle. \quad (6)$$

In particular, just one combination of  $m_1, m_2, m_3$ , with  $\sum_i m_i = +\frac{7}{2}$  and  $m_1 \neq m_2 \neq m_3$  exists. Further action with  $J_-$  on this state yields

$$J_- |\frac{9}{2} + \frac{7}{2}\rangle = \sqrt{16} |\frac{9}{2} + \frac{5}{2}\rangle = \sqrt{8}a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger |0\rangle + \sqrt{8}a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{3}{2}}^\dagger |0\rangle, \quad (7)$$

so

$$|\frac{9}{2} + \frac{5}{2}\rangle = \frac{1}{\sqrt{2}} (a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger + a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{3}{2}}^\dagger) |0\rangle. \quad (8)$$

Because this state with  $M_J = \frac{5}{2}$  is a linear combination of two independent states, two independent states with  $M_J = \frac{5}{2}$  must now exist, but with different values of  $J$ . The state orthogonal to the above  $|\frac{9}{2} + \frac{5}{2}\rangle$  is a state with  $J = \frac{5}{2}$ ,

$$|\frac{5}{2} + \frac{5}{2}\rangle = \frac{1}{\sqrt{2}} (a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger - a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{3}{2}}^\dagger) |0\rangle. \quad (9)$$

The  $J = \frac{5}{2}$  character of this state can be seen by noting the operator  $J_+$  acting on this state yields zero,  $J_+ |\frac{5}{2} + \frac{5}{2}\rangle = 0$ . Further action with  $J_-$  on the states of eqs. (8) and (9) yields the two states with  $M_J = +\frac{3}{2}$  and  $J = \frac{9}{2}, J = \frac{5}{2}$ , respectively.

$$|\frac{9}{2} + \frac{3}{2}\rangle = \left[ \sqrt{\frac{5}{42}} (a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger + a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{5}{2}}^\dagger) + \frac{4}{\sqrt{21}} a_{\frac{5}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger \right] |0\rangle, \quad (10)$$

$$|\frac{5}{2} + \frac{3}{2}\rangle = \frac{1}{\sqrt{2}} (a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger - a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{5}{2}}^\dagger) |0\rangle. \quad (11)$$

Because these states are linear combinations of three independent states, a third state with  $M_J = +\frac{3}{2}$  must exist, orthogonal to the above two. Using this orthogonality, we can construct the state with  $J = \frac{3}{2}$  and  $M_J = +\frac{3}{2}$ ,

$$|\frac{3}{2} + \frac{3}{2}\rangle = \left[ \sqrt{\frac{8}{21}} (a_{\frac{3}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger + a_{\frac{5}{2}}^\dagger a_{\frac{3}{2}}^\dagger a_{-\frac{5}{2}}^\dagger) - \sqrt{\frac{5}{21}} a_{\frac{5}{2}}^\dagger a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger \right] |0\rangle, \quad (12)$$

where action with  $J_+$  on this state again yields zero. We have thus been able to create states with  $J = \frac{9}{2}$ ,  $J = \frac{5}{2}$ ,  $J = \frac{3}{2}$ , accounting for the  $10 + 6 + 4 = 20$  allowed states of the  $(\frac{5}{2})^3$  configuration of identical  $j = \frac{5}{2}$  fermions. States with  $M_J$ -values  $< +\frac{3}{2}$  could now be created by further action with  $J_-$ . Note, however, that judicious use of the Wigner–Eckart theorem may make it unnecessary to construct states with all possible values of  $M_J$ . Also, this method of giving a very explicit construction of the states of good  $J$  and  $M_J$  automatically gives normalized states through the known matrix elements of  $J_-$ . Alternatively, we could have constructed states of good  $J$  and  $M_J$  via angular momentum coupling techniques, by coupling first two particles to a particular value of  $J_{12}$  and then coupling this state with the third particle of  $j = \frac{5}{2}$  to resultant total  $J$ . As a very specific example, the state with  $J = M_J = \frac{5}{2}$  could have been obtained by coupling a two-particle state with  $J_{12} = 0$  to the third state with  $j = m_j = \frac{5}{2}$ . Using the Clebsch–Gordan coefficient,

$$\langle jmj - m | 00 \rangle = \frac{(-1)^{j-m}}{\sqrt{(2j+1)}},$$

we have

$$\begin{aligned} |J_{12} = 0, M_{12} = 0\rangle &= \sum_m \frac{(-1)^{j-m}}{\sqrt{(2j+1)}} a_m^\dagger a_{-m}^\dagger |0\rangle \\ &= \frac{1}{\sqrt{6}} (a_{\frac{5}{2}}^\dagger a_{-\frac{5}{2}}^\dagger - a_{\frac{3}{2}}^\dagger a_{-\frac{3}{2}}^\dagger + a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger - a_{-\frac{1}{2}}^\dagger a_{\frac{1}{2}}^\dagger + a_{-\frac{3}{2}}^\dagger a_{\frac{3}{2}}^\dagger - a_{-\frac{5}{2}}^\dagger a_{\frac{5}{2}}^\dagger) |0\rangle \\ &= \frac{2}{\sqrt{6}} (a_{\frac{5}{2}}^\dagger a_{-\frac{5}{2}}^\dagger - a_{\frac{3}{2}}^\dagger a_{-\frac{3}{2}}^\dagger + a_{\frac{1}{2}}^\dagger a_{-\frac{1}{2}}^\dagger) |0\rangle, \end{aligned} \quad (13)$$

where we have used  $a_{-m}^\dagger a_m^\dagger = -a_m^\dagger a_{-m}^\dagger$  via the fermion anticommutation relation. This state, however, is now not normalized and would have to be multiplied by an additional factor of  $\frac{1}{\sqrt{2}}$  to yield the *normalized* state with  $J_{12} = M_{12} = 0$ ,

$$|J_{12} = 0, M_{12} = 0\rangle = \sum_{m>0} \frac{(-1)^{j-m}}{\sqrt{(j+\frac{1}{2})}} a_m^\dagger a_{-m}^\dagger |0\rangle. \quad (14)$$

Coupling this  $J_{12} = 0$  two-particle state to a third state with  $j = m_j = \frac{5}{2}$ , we get the three-particle state

$$\begin{aligned} |J = \frac{5}{2}, M_J = +\frac{5}{2}\rangle &= a_{\frac{5}{2}}^\dagger \sum_{m>0} \frac{(-1)^{j-m}}{\sqrt{(j+\frac{1}{2})}} a_m^\dagger a_{-m}^\dagger |0\rangle \\ &= \frac{1}{\sqrt{3}} a_{\frac{5}{2}}^\dagger (-a_{\frac{5}{2}}^\dagger a_{-\frac{5}{2}}^\dagger + a_{\frac{3}{2}}^\dagger a_{-\frac{3}{2}}^\dagger) |0\rangle, \end{aligned} \quad (15)$$

where the relation  $a_{\frac{5}{2}}^\dagger a_{\frac{5}{2}}^\dagger \equiv 0$  has eliminated one of the terms in the above sum.

Note, in particular, that a renormalization factor of  $\sqrt{3/2}$  is therefore needed to convert this state into the normalized state given by eq. (9). States with  $J = \frac{9}{2}$  and  $J = \frac{3}{2}$  could be constructed by similar angular momentum coupling techniques.

Also, if we attempt to construct a three-identical-fermion state with  $J = \frac{1}{2}$  or  $J = \frac{7}{2}$ , say, the latter by coupling a two-particle state with  $J_{12} = 2$  with a third particle with  $j = \frac{5}{2}$  to resultant  $J = \frac{7}{2}$ , we would discover this state is identically zero and, hence, Pauli-forbidden. We could therefore also discover which states are Pauli-forbidden by this technique, using the anticommutation relations of the  $a_m^\dagger$ .

## B Calculation of an Electric Dipole Transition Probability

To show how the three-particle states of the last section can be used in an actual application, let us calculate the electric dipole transition probability for the transitions from the three-particle configurations

$$(nd_{\frac{5}{2}})^2 J=0 (n' p_{\frac{3}{2}})^1 J=\frac{3}{2} \longrightarrow (nd_{\frac{5}{2}})^3 J=\frac{3}{2}, \quad \text{with } J = \frac{5}{2} \text{ and } \frac{3}{2}.$$

The transition to the final state with  $J = \frac{9}{2}$  is forbidden by an angular-momentum selection rule.

To get the needed reduced matrix element for the transition  $J = \frac{3}{2} \rightarrow \frac{5}{2}$ , it will be sufficient to calculate

$$\langle (nd_{\frac{5}{2}})^3 J = \frac{5}{2}, M_J = \frac{5}{2} | \mu_{+1}^{(\text{el.})} | (nd_{\frac{5}{2}})^2 J=0 (n' p_{\frac{3}{2}})^1 J = \frac{3}{2}, M_J = \frac{3}{2} \rangle.$$

Using the expansion of the one-body operator,  $\mu_{+1}^{(\text{el.})}$ , in the form

$$\mu_{+1}^{(\text{el.})} = \sum_{n'l'j'm'nlmj} \langle n[l\frac{1}{2}]jm_j | \mu_{+1}^{(\text{el.})} | n'[l'\frac{1}{2}]j'm'_j \rangle a_{n[l\frac{1}{2}]jm_j}^\dagger a_{n'[l'\frac{1}{2}]j'm'_j}, \quad (16)$$

only the term with the above value of  $n', l' = 1, j' = m'_j = \frac{3}{2}$  and the above value of  $n, l = 2$ , and  $j = m_j = \frac{5}{2}$  can contribute to the above three-particle matrix element, so, effectively,

$$\mu_{+1}^{(\text{el.})} = \dots + \langle (nd_{\frac{5}{2}})m_j = \frac{5}{2} | \mu_{+1}^{(\text{el.})} | (n' p_{\frac{3}{2}})m'_j = \frac{3}{2} \rangle a_{n[2\frac{1}{2}]\frac{5}{2}\frac{5}{2}}^\dagger a_{n'[1\frac{1}{2}]\frac{3}{2}\frac{3}{2}} + \dots, \quad (17)$$

i.e., terms indicated by  $\dots$  can make no contribution to the needed three-particle matrix element. Using eq. (14) for the two-particle state with  $J_{12} = 0$ , we have

$$\begin{aligned} & \langle (nd_{\frac{5}{2}})^2 J=0 (n' p_{\frac{3}{2}})^1 J = \frac{3}{2}, M_J = \frac{3}{2} \rangle = \frac{1}{\sqrt{3}} a_{n[2\frac{1}{2}]\frac{5}{2}\frac{5}{2}}^\dagger \\ & \times \left( a_{n[2\frac{1}{2}]\frac{5}{2}\frac{5}{2}}^\dagger a_{n[2\frac{1}{2}]\frac{5}{2}-\frac{5}{2}}^\dagger - a_{n[2\frac{1}{2}]\frac{5}{2}\frac{3}{2}}^\dagger a_{n[2\frac{1}{2}]\frac{5}{2}-\frac{3}{2}}^\dagger + a_{n[2\frac{1}{2}]\frac{5}{2}\frac{1}{2}}^\dagger a_{n[2\frac{1}{2}]\frac{5}{2}-\frac{1}{2}}^\dagger \right), \end{aligned} \quad (18)$$

and, using eq. (17), we get

$$\begin{aligned} & \mu_{+1}^{(\text{el.})} | (nd_{\frac{5}{2}})^2 J=0 (n' p_{\frac{3}{2}})^1 J = \frac{3}{2}, M_J = \frac{3}{2} \rangle \\ & = \frac{1}{\sqrt{3}} a_{n[2\frac{1}{2}]\frac{5}{2}\frac{5}{2}}^\dagger \left( -a_{n[2\frac{1}{2}]\frac{5}{2}\frac{5}{2}}^\dagger a_{n[2\frac{1}{2}]\frac{5}{2}-\frac{5}{2}}^\dagger + a_{n[2\frac{1}{2}]\frac{5}{2}\frac{1}{2}}^\dagger a_{n[2\frac{1}{2}]\frac{5}{2}-\frac{1}{2}}^\dagger \right) \end{aligned}$$

$$\times \langle (nd_{\frac{5}{2}})m_j = \frac{5}{2} | \mu_{+1}^{(\text{el.})} | (n' p_{\frac{3}{2}})m'_j = \frac{3}{2} \rangle, \\ + \dots, \quad (19)$$

where we have again used  $a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} \equiv 0$ . Thus, comparing eq. (19) with eq. (9) (in abbreviated form), we have

$$\mu_{+1}^{(\text{el.})} |(nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}})^1 J = \frac{3}{2}, M_J = \frac{3}{2} \rangle = \sqrt{\frac{2}{3}} |(nd_{\frac{5}{2}})^3 J = M_J = \frac{5}{2} \rangle \\ \times \langle (nd_{\frac{5}{2}})m_j = \frac{5}{2} | \mu_{+1}^{(\text{el.})} | (n' p_{\frac{3}{2}})m'_j = \frac{3}{2} \rangle + \dots, \quad (20)$$

so

$$\langle (nd_{\frac{5}{2}})^3 J = M_J = \frac{5}{2} | \mu_{+1}^{(\text{el.})} | (nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}})^1 J = M_J = \frac{3}{2} \rangle \\ = \sqrt{\frac{2}{3}} \langle (nd_{\frac{5}{2}})m_j = \frac{5}{2} | \mu_{+1}^{(\text{el.})} | (n' p_{\frac{3}{2}})m'_j = \frac{3}{2} \rangle, \quad (21)$$

and the three-particle reduced matrix element is related to the single-particle reduced matrix element by the same factor

$$\langle (nd_{\frac{5}{2}})^3 J = \frac{5}{2} | \mu^{(\text{el.})} | (nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}})^1 J = \frac{3}{2} \rangle = \sqrt{\frac{2}{3}} \langle (nd_{\frac{5}{2}}) | \mu^{(\text{el.})} | (n' p_{\frac{3}{2}}) \rangle. \quad (22)$$

Because the transition probabilities are proportional to the squares of the electric dipole moment reduced matrix elements, the transition probability for the  $J = \frac{3}{2} \rightarrow \frac{5}{2}$  transition in the three-particle system is related to the corresponding transition in the single-particle system via

$$\left[ \frac{1}{\tau_{\mathcal{E}1}} \right]_{(nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}}) \rightarrow (nd_{\frac{5}{2}})^3 J = \frac{5}{2}} = \frac{2}{3} \left[ \frac{1}{\tau_{\mathcal{E}1}} \right]_{n' p_{\frac{3}{2}} \rightarrow nd_{\frac{5}{2}}} \frac{\omega_{3,p.}^3}{\omega_{s,p.}^3}, \quad (23)$$

where we have taken account of the fact that the transition frequencies,  $\omega$ , will be different in the three-particle and single-particle systems.

Finally, to calculate the transition probability for the transition

$$(nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}})^1 J = \frac{1}{2} \longrightarrow (nd_{\frac{5}{2}})^3 J = \frac{1}{2},$$

it will be sufficient to calculate

$$\langle (nd_{\frac{5}{2}})^3 J = \frac{1}{2}, M_J = \frac{1}{2} | \mu_{+1}^{(\text{el.})} | (nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}})^1 J = \frac{1}{2}, M_J = \frac{1}{2} \rangle.$$

Now, we have

$$\mu_{+1}^{(\text{el.})} |(nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}})^1 J = \frac{1}{2}, M_J = \frac{1}{2} \rangle \\ = \frac{1}{\sqrt{3}} a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} \left( a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} + a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}-\frac{1}{2}}}^{\dagger} \right) |0\rangle \\ \times \langle (nd_{\frac{5}{2}})m_j = \frac{1}{2} | \mu_{+1}^{(\text{el.})} | (n' p_{\frac{3}{2}})m'_j = \frac{1}{2} \rangle + \dots, \quad (24)$$

where we have now used  $a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} a_{n[2\frac{1}{2}]_{\frac{5}{2}\frac{3}{2}}}^{\dagger} \equiv 0$ . Comparing the right-hand side with eq. (11), we have

$$\mu_{+1}^{(\text{el.})} |(nd_{\frac{5}{2}})_{J=0}^2 (n' p_{\frac{3}{2}})^1 J = \frac{1}{2}, M_J = \frac{1}{2} \rangle$$

$$= \sqrt{\frac{2}{3}} |(nd_{\frac{5}{2}})^3 J = \frac{5}{2}, M_J = \frac{3}{2}\rangle \\ \times \langle (nd_{\frac{5}{2}})m_j = \frac{3}{2} | \mu_{+1}^{(\text{el.})} | (n' p_{\frac{3}{2}})^1 m'_j = \frac{1}{2} \rangle + \dots \quad (25)$$

Now, however, the states

$$|(nd_{\frac{5}{2}})^3 J = \frac{5}{2}, M_J = \frac{3}{2}\rangle$$

and

$$|(nd_{\frac{5}{2}})^3 J = \frac{3}{2}, M_J = \frac{3}{2}\rangle$$

are orthogonal to each other, [cf. eqs. (11) and (12)]. Thus,

$$\langle (nd_{\frac{5}{2}})^3 J = \frac{3}{2}, M_J = \frac{3}{2} | \mu_{+1}^{(\text{el.})} | (nd_{\frac{5}{2}})^2_{J=0} (n' p_{\frac{3}{2}})^1 J = \frac{3}{2}, M_J = \frac{1}{2} \rangle = 0. \quad (26)$$

Thus, the transition

$$(nd_{\frac{5}{2}})^2_{J=0} (n' p_{\frac{3}{2}})^1_{J=\frac{3}{2}} \longrightarrow (nd_{\frac{5}{2}})^3_{J=\frac{3}{2}}$$

is forbidden, even though it is not ruled out by an angular momentum selection rule, and even though the single-particle transition

$$n' p_{\frac{3}{2}} \longrightarrow nd_{\frac{5}{2}}$$

is allowed.

## C Pairing Forces in Nuclei

Two-particle states coupled to angular momentum,  $J = 0$ , are of particular relevance in nuclear physics, especially in configurations of identical nucleons, because the nucleon–nucleon interaction is a short-range attractive interaction. Because identical nucleons with the same  $n$  and  $l$  in states  $|jm\rangle$  and  $|j-m\rangle$  have the same spatial distribution, two identical nucleons coupled to two-particle  $J = 0$  have a large probability of being within the range of the attractive nucleon–nucleon interaction. Low-lying states of nuclei thus have a larger probability of containing  $J = 0$  pairs compared with pairs coupled to  $J > 0$ . In particular, the ground states of all known stable even–even nuclei (with even neutron and proton numbers) are observed to have spin and parity  $0^+$ . States of two identical nucleons, either both neutrons or both protons in a shell model state with the same  $nl$ , coupled to  $J = 0$ , are given by eq. (14). It will therefore be useful to define nucleon pair creation operators

$$A_j^\dagger = \sum_{m>0} (-1)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger, \quad (27)$$

where we have omitted the common quantum numbers  $nl$  in the single nucleon creation operators (for the sake of brevity of notation) and we have left off the two-particle normalization factor,  $[(j + \frac{1}{2})]^{-\frac{1}{2}}$ , to simplify the anticommutator algebra

of such operators. We also define the pair annihilation operators

$$A_j = (A_j^\dagger)^\dagger = \sum_{m>0} (-1)^{j-m} a_{j-m} a_{jm}. \quad (28)$$

Normalized states of  $p$  pairs of  $J = 0$ -coupled identical nucleon pairs are given by

$$\sqrt{\frac{(j + \frac{1}{2} - p)!}{(j + \frac{1}{2})! p!}} (A_j^\dagger)^p |0\rangle. \quad (29)$$

The overall normalization factor can be understood as follows: For one pair coupled to  $J = 0$ ,  $(j + \frac{1}{2})$  terms of the type  $(-1)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger$  exist. For  $p = 2$ , once one of these terms is fixed at some specific  $m = m_1 > 0$ , the second pair operator can multiply this term with only  $(j - \frac{1}{2})$  terms with  $m_2 \neq m_1$ , but the two terms with  $m_1$  and  $m_2$  interchanged are identical, because the anticommutation relations of the fermion operators yield

$$a_{jm_1}^\dagger a_{j-m_1}^\dagger a_{jm_2}^\dagger a_{j-m_2}^\dagger = a_{jm_2}^\dagger a_{j-m_2}^\dagger a_{jm_1}^\dagger a_{j-m_1}^\dagger,$$

so that there are  $\frac{1}{2}(j + \frac{1}{2})(j - \frac{1}{2})$  independent terms but each appears with a factor of 2 for the case of two pairs,  $p = 2$ . For higher  $p$ , by the same arguments, there will be  $(j + \frac{1}{2})(j - \frac{1}{2}) \cdots (j + \frac{3}{2} - p)/p!$  independent terms, but each will appear with a factor of  $p!$ , requiring a normalization factor of

$$\frac{1}{p!} \sqrt{\frac{p!(j + \frac{1}{2} - p)!}{(j + \frac{1}{2})!}}.$$

In rough approximation, the nucleon-nucleon interaction could be replaced by an attractive pairing interaction that acts only when nucleons are coupled in pairs to  $J = 0$ . Although a realistic interaction will have finite terms involving nucleon pairs coupled to  $J \neq 0$ , the highly simplified pairing interaction will give a qualitative account of the nuclear spectra involving the lowest energy states. A general pairing interaction would be given by a Hamiltonian of the form

$$H_{\text{pairing}} = \frac{1}{2} \sum_{j,j'} g_{jj'} A_j^\dagger A_{j'}. \quad (30)$$

Moreover, the strength factors,  $g_{jj'}$ , can be taken approximately  $j$  independent and negative (attractive interaction), so

$$\begin{aligned} H_{\text{pairing}} &= -\frac{1}{2} G \sum_{jj'} A_j^\dagger A_{j'} \\ &= -\frac{1}{2} G \sum_{jj'} \sum_{m>0} \sum_{m'>0} (-1)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger (-1)^{j'-m'} a_{j'-m'}^\dagger a_{j'm'}. \end{aligned} \quad (31)$$

Let us examine the eigenvalues of such a Hamiltonian in a single  $j$  shell, by adding a one-body operator dependent on the single-particle shell-model energy,  $\epsilon_j$ , of this shell, so

$$H = \epsilon_j \sum_m a_{jm}^\dagger a_{jm} - \frac{1}{2} G \sum_{m>0} \sum_{m'>0} (-1)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger (-1)^{j'-m'} a_{j'-m'}^\dagger a_{j'm'}$$

$$= \epsilon_j N_{\text{op.}} - \frac{1}{2} G A^\dagger A, \quad (32)$$

where we have left off the subscript  $j$  on  $A^\dagger$  and  $A$  for brevity of notation in the single  $j$  shell. It will be useful to calculate the commutator,  $[A, A^\dagger]$ . Using the anticommutation relations of the single-particle creation and annihilation operators to move the two  $a$ 's through to the right in the first term of this commutator, we have

$$\begin{aligned} [A, A^\dagger] &= \left[ \sum_{m>0} a_{j-m} a_{jm} (-1)^{j-m}, \sum_{m'>0} a_{jm'}^\dagger a_{j-m'}^\dagger (-1)^{j-m'} \right] \\ &= \sum_{m>0} (a_{j-m} a_{j-m}^\dagger - a_{jm}^\dagger a_{jm}) = \sum_{m>0} (-a_{j-m}^\dagger a_{j-m} - a_{jm}^\dagger a_{jm} + 1) \\ &= - \sum_{\text{all } m} a_{jm}^\dagger a_{jm} + (j + \frac{1}{2}) = - \left( N_{\text{op.}} - (j + \frac{1}{2}) \right) \equiv -N_{\text{op.}}. \end{aligned} \quad (33)$$

We want to calculate the eigenvalue of the simplified Hamiltonian of eq. (32) for the state of eq. (29) built from  $p J = 0$ -pairs. For this purpose, we need to calculate  $-GA^\dagger A(A^\dagger)^p |0\rangle$ . Using the commutator result of eq. (33), we have

$$\begin{aligned} &-GA^\dagger A(A^\dagger)^p |0\rangle \\ &= +GA^\dagger \left( N_{\text{op.}} (A^\dagger)^{p-1} + A^\dagger N_{\text{op.}} (A^\dagger)^{p-2} + \dots \right. \\ &\quad \left. + (A^\dagger)^k N_{\text{op.}} (A^\dagger)^{p-k-1} + \dots + (A^\dagger)^{p-1} N_{\text{op.}} \right) |0\rangle \\ &= +G \sum_{k=0}^{p-1} [2(p-k-1) - (j + \frac{1}{2})] (A^\dagger)^p |0\rangle \\ &= +G \left( [2(p-1) - (j + \frac{1}{2})] p - 2\frac{1}{2}p(p-1) \right) (A^\dagger)^p |0\rangle \\ &= -Gp(j + \frac{3}{2} - p)(A^\dagger)^p |0\rangle. \end{aligned} \quad (34)$$

With  $p = \frac{1}{2}n$ , where  $n$  is the number of nucleons in the  $p$ -pair state with  $J = 0$ , the full Hamiltonian of eq. (32) thus yields

$$H \sqrt{\frac{(j + \frac{1}{2} - p)!}{(j + \frac{1}{2})! p!}} (A_j^\dagger)^p |0\rangle = E_{j,n} \sqrt{\frac{(j + \frac{1}{2} - p)!}{(j + \frac{1}{2})! p!}} (A_j^\dagger)^p |0\rangle, \quad (35)$$

where

$$E_{j,n} = n\epsilon_j - G \frac{n}{4} (2j + 3 - n). \quad (36)$$

It will be interesting to compare this energy for the  $J = 0$  ground state for an even number of nucleons, with the corresponding energy for an odd number of nucleons, where one nucleon must be in the state with angular momentum  $j$ , so the total angular momentum of the ground state for  $n = \text{odd}$  must be  $J = j$ . Such a state can be approximated by

$$\sqrt{\frac{(j - \frac{1}{2} - p)!}{p!(j - \frac{1}{2})!}} (A^\dagger)^p a_{jm_0}^\dagger |0\rangle, \quad (37)$$

where the single-particle creation operator with  $m = m_0$  “blocks” this  $m_0$  value from the pair creation operators; i.e., the first operator  $A^\dagger$  acting on the single particle state will have only  $(j - \frac{1}{2})$  possible  $|m|$ -values, whereas terms with  $p > 1$  will now lead to a state with  $[(j - \frac{1}{2})! / p!(j - \frac{1}{2} - p)!]$  independent pair terms, each appearing with a factor of  $p!$ , leading to the new normalization factor of eq. (37). For this state, we need

$$\begin{aligned} & -GA^\dagger A(A^\dagger)^p a_{jm_0}^\dagger |0\rangle \\ &= +GA^\dagger \left( \sum_{k=0}^{p-1} (A^\dagger)^k N_{\text{op.}} (A^\dagger)^{p-1-k} \right) a_{jm_0}^\dagger |0\rangle \\ &= +G \sum_{k=0}^{p-1} [2(p-1-k) + 1 - (j + \frac{1}{2})] (A^\dagger)^p a_{jm_0}^\dagger |0\rangle \\ &= -Gp(j + \frac{1}{2} - p) (A^\dagger)^p a_{jm_0}^\dagger |0\rangle. \end{aligned} \quad (38)$$

Now, we have  $p = \frac{1}{2}(n - 1)$ , with  $n = \text{odd}$ , leading to the eigenvalue

$$E_{j,n} = n\epsilon_j - G \frac{(n-1)}{4} (2j + 2 - n) \quad (39)$$

for the ground state of an odd- $n$  nucleus with  $J = j$ .

The excited states of an even- $n$  nucleus with  $J \neq 0$  would be expected to have the structure

$$\sum_{m_1, m_2} \langle jm_1 jm_2 | JM_J \rangle \sqrt{\frac{(j - \frac{3}{2} - p)!}{p!(j - \frac{3}{2})!}} (A^\dagger)^p a_{jm_1}^\dagger a_{jm_2}^\dagger |0\rangle. \quad (40)$$

Because the energy of this state is independent of  $M_J$ , we can choose  $M_J \neq 0$  so  $m_2 \neq -m_1$ . The two single-particle creation operators thus “block” two  $m$  values from the pair operators, leading to the new normalization factor. Now, we need

$$\begin{aligned} & -GA^\dagger A(A^\dagger)^p a_{jm_1}^\dagger a_{jm_2}^\dagger |0\rangle \\ &= +GA^\dagger \left( \sum_{k=0}^{p-1} (A^\dagger)^k N_{\text{op.}} (A^\dagger)^{p-k-1} \right) a_{jm_1}^\dagger a_{jm_2}^\dagger |0\rangle \\ &= +G \sum_{k=0}^{p-1} [2(p - k - 1) + 2 - (j + \frac{1}{2})] (A^\dagger)^p a_{jm_1}^\dagger a_{jm_2}^\dagger |0\rangle \\ &= -Gp(j - \frac{1}{2} - p) (A^\dagger)^p a_{jm_1}^\dagger a_{jm_2}^\dagger |0\rangle, \end{aligned} \quad (41)$$

where we now have  $p = \frac{1}{2}(n - 2)$ , with  $n = \text{even}$ , so for such  $J \neq 0$  states in the even nucleus

$$E_{j,n} = n\epsilon_j - G \frac{(n-2)}{4} (2j + 1 - n). \quad (42)$$

Comparing with eq. (36), the energy of the  $J = 0$  ground state, these  $J \neq 0$  states lie at an excitation energy of  $\frac{1}{2}G(2j + 1)$  above the  $J = 0$  ground state. In a configuration  $j^n$  of identical nucleons, either all neutrons or all protons, with  $n = \text{even}$ , the Pauli-allowed states with  $J \neq 0$  have  $J = 2, 4, \dots, (2j - 1)$ . For our

simplified interaction, these excited states would all be degenerate at an energy  $\frac{1}{2}G(2j+1)$  above the  $J=0$  ground state. In a real nucleus, this degeneracy is lifted, but the energy differences between the different levels with  $J \neq 0$  are in general small compared with the energy difference between the average energy of the  $J \neq 0$  levels and the  $J=0$  ground state.

## D The Coulomb Repulsion Term in the $Z$ -Electron Atom

The Hamiltonian for the  $Z$ -electron atom consists of a one-body and a two-body term

$$H = \sum_{i=1}^Z \left( \frac{\vec{p}_i^2}{2m} - \frac{Ze^2}{r_i} \right) + \sum_{i < k} \frac{e^2}{r_{ik}} = \sum_{i=1}^Z h_i + \sum_{i < k} V_{ik}. \quad (43)$$

In the language of many-body theory, this can now be written as

$$H = \sum_{nlmm_s} \epsilon_n a_{nlmm_s}^\dagger a_{nlmm_s} + \frac{1}{2} \sum_{a,b,c,d} \langle ab | \frac{e^2}{r_{12}} | cd \rangle a_a^\dagger a_b^\dagger a_d a_c, \quad (44)$$

where  $a$  is shorthand for  $n_a l_a m_a m_{s_a}$ . Because the Coulomb repulsion potential is a scalar operator, a spherical tensor of rank 0, and is spin independent, it will be useful to transform the two-particle states to states of good two-particle angular momentum,  $L$  and  $S$ ,

$$\begin{aligned} |ab\rangle &= |n_a l_a m_a m_{s_a} n_b l_b m_b m_{s_b}\rangle = \\ &\sum_{L,S} \langle l_a m_a l_b m_b | LM \rangle \langle \frac{1}{2} m_{s_a} \frac{1}{2} m_{s_b} | SM_S \rangle | [n_a l_a n_b l_b] LM, SM_S \rangle, \end{aligned} \quad (45)$$

where  $M$  is fixed by  $m_a + m_b$ , similarly for  $M_S$ . It will now be useful to define pair-creation operators for electron pairs coupled to general  $L$  and  $S$

$$A_{ab,LMSM_S}^\dagger =$$

$$\sum_{m_a, (m_b)} \sum_{(m_{s_a}, m_{s_b})} \langle l_a m_a l_b m_b | LM \rangle \langle \frac{1}{2} m_{s_a} \frac{1}{2} m_{s_b} | SM_S \rangle a_{n_a l_a m_a m_{s_a}}^\dagger a_{n_b l_b m_b m_{s_b}}^\dagger, \quad (46)$$

where these are the generalizations of the  $J=0$  pair creation operators of the last section. In terms of these operators, we then have

$$\begin{aligned} H &= \sum_{nlmm_s} \epsilon_n a_{nlmm_s}^\dagger a_{nlmm_s} + \frac{1}{2} \sum_{n_a l_a n_b l_b n_c l_c n_d l_d} \\ &\times \sum_L \langle [n_a l_a n_b l_b] L | \frac{e^2}{r_{12}} | [n_c l_c n_d l_d] L \rangle \sum_M \sum_{S, M_S} A_{ab,LMSM_S}^\dagger A_{cd,LMSM_S} \end{aligned} \quad (47)$$

where the two-particle matrix element of the scalar operator,  $e^2/r_{12}$ , is independent of  $M$  via the Wigner–Eckart theorem. It could be evaluated by expanding  $1/r_{12}$  in

spherical harmonics [see, e.g., eqs. (22)–(24) of Chapter 38 and eq. (32) of Chapter 30] and by choosing a particular (convenient) value of  $M$ . Thus,

$$\begin{aligned}
 & \langle [n_a l_a n_b l_b] LM | \frac{e^2}{r_{12}} | [n_c l_c n_d l_d] LM \rangle \\
 &= \sum_{k=0}^{\infty} \sqrt{\frac{(2l_c + 1)(2l_d + 1)}{(2l_a + 1)(2l_b + 1)}} \langle l_c 0k0 | l_a 0 \rangle \langle l_d 0k0 | l_b 0 \rangle \\
 &\times \sum_q \sum_{m_a, (m_b) m_c, (m_d)} \langle l_a m_a l_b m_b | LM \rangle \langle l_c m_c l_d m_d | LM \rangle \\
 &\quad \langle l_c m_c k q | l_a m_a \rangle \langle l_d m_d k - q | l_b m_b \rangle (-1)^q \\
 &\times \int_0^{\infty} dr_1 r_1^2 R_{n_a l_a}^*(r_1) R_{n_c l_c}(r_1) \left[ \int_0^{r_1} dr_2 r_2^2 R_{n_b l_b}^*(r_2) \frac{r_2^k}{r_1^{k+1}} R_{n_d l_d}(r_2) \right. \\
 &\quad \left. + \int_{r_1}^{\infty} dr_2 r_2^2 R_{n_b l_b}^*(r_2) \frac{r_1^k}{r_2^{k+1}} R_{n_d l_d}(r_2) \right]. \quad (48)
 \end{aligned}$$

The sum over the magnetic quantum numbers  $q, m_a, (m_b), m_c, (m_d)$  of the product of four Clebsch–Gordan coefficients [including the phase factor  $(-1)^q$ ] could be evaluated directly. Alternatively (see Chapter 34 on recoupling coefficients), it can be expressed through a single recoupling coefficient of the  $6\text{-}j$  type and has the value

$$(-1)^{l_b + l_c + L} \sqrt{(2l_a + 1)(2l_b + 1)} \left\{ \begin{array}{ccc} l_c & k & l_a \\ l_b & L & l_d \end{array} \right\}.$$

So far, in this section, it has been assumed the radial functions are hydrogenic, valid for the  $Z$  of the atom under consideration, i.e., that the  $\psi_{nlmm_s}(\vec{r}_i)$  are the eigenfunctions of the hydrogenic single-particle Hamiltonian,  $h_i$ , of eq. (43). In a heavy atom, however, it may be very useful to add a screening potential,  $V_{\text{screening}}(r_i)$ , to the central Coulomb potential,  $-Ze^2/r_i$ , of  $h_i$ , where  $V_{\text{screening}}(r_i)$  gives the average of the Coulomb repulsion terms of the  $(Z - 1)$  remaining electrons on the electron labeled with index  $i$ . The inner shell electrons, in particular, will screen the full charge  $Z$  of the atomic nucleus, and this screening will depend on the quantum numbers  $nl$ . The full Hamiltonian could then be written

$$\begin{aligned}
 H &= \sum_{i=1}^Z h_i + \sum_{i < k}^Z V_{ik}, \quad \text{with} \\
 h_i &= \frac{p_i^2}{2m} - \frac{Ze^2}{r_i} + V_{\text{scr.}}(r_i), \quad \text{and} \quad V_{ik} = \frac{e^2}{r_{ik}} - V_{\text{scr.}}(r_i), \quad (49)
 \end{aligned}$$

where the eigenfunctions of  $h_i$  would be improved single-particle functions for the many-body problem and might be expanded in the form,

$$\sum_n c_n \psi_{nlmm_s}(\vec{r}_i),$$

where the  $c_n$  might be determined by the variational technique.

## E Hartree–Fock Theory for Atoms: A Brief Introduction

In the language of many-body theory, the atomic Hamiltonian of eq. (49) is

$$H = \sum_{m,j} \langle m | h_1 | j \rangle a_m^\dagger a_j + \frac{1}{2} \sum_{abcd} \langle ab | V_{12} | cd \rangle a_a^\dagger a_b^\dagger a_d a_c. \quad (50)$$

Here the single-particle Hamiltonian,  $h_i$ , may not be diagonal in the chosen single-particle basis,  $|j\rangle$ , so off-diagonal terms have been included in the matrix,  $\langle m | h_1 | j \rangle$ . If the screening potential,  $V_{\text{scr.}}(r_i)$ , which is now included in  $h_i$ , has been well chosen, however, it may be possible to approximate the full Hamiltonian by an effective single-particle Hamiltonian. That is, of the three types of nonzero  $Z$ -particle matrix elements of the two-body operator,  $V_{ik}$  [see eqs. (66)–(68) of Chapter 78], only those with

$$(1) : \quad \alpha'_1 \alpha'_2 \cdots \alpha'_Z = \alpha_1 \alpha_2 \cdots \alpha_Z$$

and with

$$(2) : \quad \alpha'_1 \alpha'_2 \cdots \alpha'_Z = \alpha_1 \alpha_2 \cdots \alpha_m \cdots \alpha_Z$$

$$\alpha_1 \alpha_2 \cdots \alpha_Z = \alpha_1 \alpha_2 \cdots \alpha_j \cdots \alpha_Z, \quad \text{with } j \neq m,$$

will be retained, and matrix elements, (3), in which the  $\alpha'_k$  differ from the  $\alpha_k$  in *two* quantum numbers will be assumed to be negligible. Because the occupied states,  $\alpha_k$ , with  $k \neq j, k \neq m$ , of the  $Z$ -particle system have an eigenvalue of 1 for  $a_k^\dagger a_k$ , we can write the effective single-particle Hamiltonian, the so-called Hartree–Fock Hamiltonian, as

$$\begin{aligned} H_{\text{H.F.}} &= \sum_{j,m} \left( \langle m | h_1 | j \rangle + \sum_k^{\text{occ.}} [\langle mk | V_{12} | jk \rangle - \langle mk | V_{12} | kj \rangle] \right) a_m^\dagger a_j \\ &= \sum_{j,m} \langle m | H_{\text{H.F.}} | j \rangle a_m^\dagger a_j, \end{aligned} \quad (51)$$

where we have used eq. (69) of Chapter 78 to eliminate the factor  $\frac{1}{2}$  for both the direct and exchange matrix elements of  $V_{12}$ . The sum over  $j$  and  $m$  includes a sum over all possible single-particle quantum states. This effective one-body Hamiltonian will lead to an  $\infty$ -dimensional Hamiltonian matrix. We will try to diagonalize this matrix by the Ritz variational technique by introducing improved single-particle states,

$$\begin{aligned} a_v^\dagger &= \sum_t c_t a_t^\dagger \quad \text{or} \\ a_{n_v l m m_s}^\dagger &= \sum_{n_t} c_t a_{n_t l m m_s}^\dagger, \end{aligned} \quad (52)$$

where the  $c_t$  are chosen such that the new improved single-particle states diagonalize  $H_{\text{H.F.}}$  approximately with a finite number of terms in the sum. That is, we

try to find  $c_t$  such that

$$\begin{aligned} \sum_{j,m} \langle m | H_{\text{H.F.}} | j \rangle a_m^\dagger a_j \left( \sum_t c_t a_t^\dagger \right) | 0 \rangle &= \epsilon \left( \sum_t c_t a_t^\dagger \right) | 0 \rangle \quad \text{or} \\ \sum_{j,m} \langle m | H_{\text{H.F.}} | j \rangle a_m^\dagger c_j | 0 \rangle &= \epsilon \left( \sum_t c_t a_t^\dagger \right) | 0 \rangle. \end{aligned} \quad (53)$$

If we act on this equation with the annihilation operator,  $a_{m_1}, a_{m_2}, \dots, a_{m_k}$ , in turn, we get the equations

$$\sum_j \left( \langle m_k | H_{\text{H.F.}} | j \rangle - \epsilon \delta_{m_k j} \right) c_j = 0, \quad (54)$$

with  $k = 1, 2, \dots$ , where we have a system of an infinite number of linear equations with an infinite number of terms in the unknown  $c_j$ , and a truncation at a finite number of terms hopefully gives us improved single-particle energies,  $\epsilon_1, \epsilon_2, \dots, \epsilon_v, \dots$  with improved single-particle creation operators

$$a_v^\dagger = \sum_t c_t^{(v)} a_t^\dagger.$$

The final  $Z$  particle energy for the state in which the  $Z$  electrons fill the  $Z$  lowest states,  $v_1, v_2, \dots, v_Z$ , would then be approximated by

$$\begin{aligned} E_{\text{H.F.}} &= \langle v_1 v_2 \cdots v_Z | H_{\text{H.F.}} | v_1 v_2 \cdots v_Z \rangle \\ &= \sum_{v_k}^{\text{occ.}} \langle v_k | h | v_k \rangle + \sum_{v_k < \mu_k} \left[ \langle v_k \mu_k | V | v_k \mu_k \rangle - \langle v_k \mu_k | V | \mu_k v_k \rangle \right]. \end{aligned} \quad (55)$$

This approximation method may require some iteration because the matrix elements of  $V$  involve occupied states from the very beginning. Also, we have assumed that there is one lowest, i.e., effectively nondegenerate,  $Z$ -particle state with filled single-particle states,  $v_1 v_2 \cdots v_Z$ . The method therefore works simply only for atoms with filled electron shells, with  $L = S = 0$ , or with filled shells  $\pm$  one-valence electron. In the latter case, the electron configuration has  $J = j$ , where  $j$  is one of the fine-structure components of the valence shell and the final energy must be independent of  $m_j$ , so the  $(2j + 1)$ -fold degeneracy of the level plays no role.

# Index

- D* matrix, 278, 285, 292  
*S* matrix, 503  
*T* matrix, 505  
*U* coefficient, 314  
*W* coefficient, 314  
 $\alpha$ - $\alpha$  scattering, 465, 469  
 $\alpha$ -nucleus scattering, 465, 469  
 $\bar{\psi} \Gamma^A \psi$ , 672  
 $\gamma$  matrices, 671  
 $\mu^-$  nucleus scattering, 474  
 $e^-$  nucleus scattering, 474  
*g* factor, 240, 304, 553  
 $g_s$ -factor, 683  
*n*-particle system, 34, 389, 719  
3-j symbol, 271  
6-j coefficient, 319  
6-j symbol, 312, 319  
9-j symbol, 321, 323
- Accidental degeneracy, 229  
accidental near degeneracy, 229  
action variable, 364  
active point of view, 169, 273  
Adams, B. G., 352  
addition theorem for spherical harmonics, 286  
adiabatic approximations, 561
- adjoint operator, 28  
Aharonov, Y., 236  
alkali atoms, 238, 243  
ammonia molecule, 45, 365  
angular momentum, 31, 93, 136, 145,  
    147, 148, 261, 312, 584, 683  
angular momentum coherent states,  
    187, 282  
angular momentum coupling, 263  
angular momentum coupling coefficients, 247, 263, 271  
angular momentum operators, 93, 147,  
    148  
angular momentum recoupling, 312  
anharmonic oscillator, 118, 215  
annihilation operators, 177, 179, 391,  
    580, 726  
anomalous *g* factor, 304, 553  
anticommutation relations, 391, 728  
antilinear, 28, 141  
antisymmetric, 382  
antisymmetrizer, 389  
antisymmetry, 721  
asymmetric rotator, 37, 158, 249  
Auger effect, 629  
average values, 23

- Baker–Campbell–Hausdorff relation,** 279  
**band of continuum states,** 378  
**bands of allowed energies,** 56  
**bands of condensed matter physics,** 56, 371  
**Bargmann transform,** 65, 183  
**base vectors,** 143  
**Berestetskii,** 575  
**Bessel equation** 359, 409  
**beta decay of tritium,** 562, 571  
**Beta function,** 192  
**Bethe, H. A.,** 649  
**bilinear covariants,** 671  
**Bivins, R.,** 271  
**Bjorken, J. D.,** 657  
**Bohm, David,** 236  
**Bohr correspondence principle,** 204  
**Bohr frequency relation,** 3, 80, 205  
**Bohr, Niels,** 3, 4  
**Born approximation,** 462, 547, 678  
  first, 462  
**Bose–Einstein,** 382  
**Bose–Einstein condensation,** 721  
**boson,** 382, 721  
**boson commutation relations,** 728  
**box normalization,** 408, 548  
**bra,** 141  
**Brillouin, L.,** 354  
**Brink, D. M.,** 271
- Carbon dioxide molecule,** 233  
**Casimir operator**  
   $\text{SO}(2,1)$ , 338  
**center of mass coordinates,** 34, 402  
**channel index,** 425  
**charmed quark-charmed antiquark,** 346  
**charmonium,** 346  
**circularly polarized photons,** 585, 586  
**Cizek, J.,** 352  
**classical electron radius,** 634  
**classical radiation Hamiltonian,** 579  
**Clebsch–Gordon coefficients,** 247, 261, 265, 269  
**Clebsch–Gordon series,** 285  
**closure relation,** 142, 167  
**color,** 713  
**color symmetry  $\text{SU}(3)$ ,** 713  
**commutation relations,** 391, 727  
**commutator,** 29  
**commutator algebra,** 136, 147, 178, 192, 334, 338, 350  
**complementary experimental setup,** 6  
**completeness,** 66  
**completeness condition,** 167  
**completeness relation,** 139, 142  
**composite projectile,** 477  
**Condon and Shortley phase convention,** 267  
**confined quark,** 713  
**confluent hypergeometric function,** 428, 470  
**conservation theorem,** 31  
**contact term,** 304  
**continuity equation,** 22, 663  
**continuous spectra,** 167  
**continuum Coulomb states,** 332  
**continuum solutions for the Coulomb problem,** 426  
**coordinate representation,** 144  
**Coulomb modified plane waves,** 467  
**Coulomb parameter,** 426, 469  
**Coulomb problems**  
  perturbed, 332  
**Coulomb repulsion,** 381  
**Coulomb repulsion term,** 385, 749  
**Coulomb scattering,** 465, 468  
**Coulomb scattering of relativistic electrons,** 678  
**coupled harmonic oscillators,** 232  
**coupled tensor operator,** 325  
**creation operators,** 177, 179, 391, 580, 726  
**cross section,** 402, 420, 421, 523, 610, 634, 639, 680  
  resonance fluorescence, 640  
**crystalline lattice,** 48, 377  
**curvilinear coordinates,** 35  
**cyclic interchange,** 390
- D matrix or D function,** 278, 285, 291  
**Darboux method,** 130  
**Darboux, G.,** 130  
**Darstellung,** 278  
**Darwin term,** 689  
**deBroglie relation,** 3  
**degenerate levels,** 221  
**degree of polarization,** 651

- density matrices, 522, 557  
 deuteron, 44, 446, 497, 614, 626  
 diamagnetic term, 240  
 diatomic molecule, 119, 152, 206, 215,  
     247, 310, 650  
 diatomic molecule rigid rotator, 224,  
     249  
 dilation property, 339  
 Dirac  $\gamma$ , 662  
 Dirac  $\alpha$  and  $\beta$  matrices, 659  
 Dirac delta function, 11  
 Dirac equation, 659, 661  
 Dirac equation for the harmonic  
     oscillator, 700  
 Dirac notation, 141  
 Dirac particle in an electromagnetic  
     field, 681  
 Dirac theory, 657  
 direct integral, 386  
 directional correlation, 630  
 disentangle, 280  
 dispersion law, 15  
 distorted wave Born approximation, 501  
 double scattering, 525  
 double-barred matrix element, 299  
 double-minimum potential problem, 45,  
     76, 135, 365  
 Drell, S. D., 657  
 dual vector, 141  
  
**E**dmonds, A. R., 271  
 effective spin-dependent Hamiltonian,  
     386  
 Ehrenfest theorem, 26, 30  
 eigenfunctions, 40, 60  
 eigenvalue problem, 60, 84  
 eigenvalues, 40, 82, 145, 203  
 eigenvectors, 145, 203  
 Einstein  $A$ , 205, 218  
 Einstein  $B$ , 206, 219  
 Eisenberg, Judah, M., 575  
 elastic scattering, 425  
 electric  $2^L$  pole radiation field, 591  
 electric and magnetic multipole  
     radiation, 615  
 electric dipole approximation, 598  
 electric dipole moment, 204  
 electric multipole radiation, 617  
 electromagnetic field, 33  
  
 electromagnetic radiation field, 576  
 electron  
     in a uniform external magnetic field,  
     293  
 electron spin, 240  
 electron–positron pair emission, 701  
 electron–hydrogen atom scattering, 492  
 emission of photons by atoms, 206, 207,  
     598  
 energy gaps, 56  
 Euler angles, 276  
 even permutations, 390  
 exchange integral, 386  
  
**F**actorization method, 84  
 Fermi, 211, 233, 545  
 Fermi resonance, 233  
 Fermi’s golden rule, 211, 546, 551  
 Fermi–Dirac, 382  
 fermion, 382, 721,  
     fermion anticommutation relations, 728  
 fine structure, 243  
 fine structure constant, 242, 304  
 flavor, 713  
 flux, 43, 402, 407  
 Foldy–Wouthuysen transformation, 690  
 forbidden, 206  
 form factor, 500  
 four-dimensional notation, 661  
 four-vector space-time formulation, 657  
 Fourier analysis, 8  
 Fourier transform, 11, 15, 23  
 free particle motion, 36, 674  
 functional, 393  
  
**G**alilean transformation, 22  
 Gamow penetrability factor, 48, 368  
 gauge invariant, 37  
 gauge transformation, 236  
 general oscillator, 78  
 general rotations, 276  
 generalized coherent states, 191  
 generator, 161  
 geometrical shadow, 439  
 Gerlach, 163  
 Glauber, R. J., 180  
 Golden Rule, 211, 545, 551  
 golden rule II, 546  
 Goudsmit, S., 147, 240

- Greiner, Walter, 575  
 group SO(4,2), 350  
 gyromagnetic factor, 240, 303
- H**amiltonian, 19, 30, 31, 33, 35, 175  
 hard sphere, 436  
 Hartree–Fock theory, 751  
 Hecht, K. T., 191  
 Heisenberg algebra, 178  
 Heisenberg commutation relations, 29  
 Heisenberg equation, 176  
 Heisenberg matrix element, 205  
 Heisenberg matrix mechanics, 80  
 Heisenberg picture, 80  
 Heisenberg uncertainty relations, 20  
 Heisenberg, Werner, 3  
 helium atom, 395  
 Hellmann–Feynmann theorem, 135  
 Hermite polynomial, 64  
 Hermitian Operator, 28  
 Herzberg, G., 120  
 Hilbert space, 28, 141  
 hindered internal rotation, 49, 370  
 hole, 695  
 Hull, T. E., 84  
 Hulthén wave function, 497  
 Hund’s rule, 386  
 hydrogen atom, 136, 198, 206, 227,  
     257, 310, 332, 340, 364, 606,  
     613, 626  
 hydrogen ground state, 350  
 hydrogen maser, 626  
 hydrogenic atom, 105, 703  
 Hylleraas, 397  
 hyperfine splitting, 303, 310, 329  
 hypergeometric function, 428
- I**dentical particle Coulomb scattering,  
     465  
 identical particles, 381, 465  
 impact parameter, 421  
 induced absorption, 206  
 induced absorption processes, 219  
 inelastic collision, 477  
 inelastic scattering, 425, 481  
 Infeld, L., 84  
 integral equation, 450  
 interaction of electromagnetic radiation  
     with atomic systems, 575
- interaction picture, 542  
 internal conversion process, 628  
 intrinsic or internal coordinates, 147  
 isospin, 529, 713  
 isotropic harmonic oscillator, 291
- J**Jackson, J. D., 304, 657
- K**epler frequencies, 205  
 ket, 141  
 Klauder, John R., 181  
 Klein paradox, 692  
 Klein–Gordon equation, 20, 36, 658  
 Kramers connection formulae, 357  
 Kramers, H. A., 354
- L**aboratory coordinates, 402  
 ladder operators, 84  
 Lamb shift, 649  
 Larmor formula, 204  
 Larmor frequency, 239  
 left-right asymmetry, 525  
 Legendre polynomials, 411  
 level shift, 648  
 level width, 648  
 lifetime, 206  
 Lifshitz, 575  
 linear, 28, 141  
 linear confining potential, 346, 368  
 linear operators, 27, 142  
 Lippmann–Schwinger equation, 479  
 liquid drop model of the nucleus, 700  
 longitudinal part of the vector potential,  
     591  
 Lorentz covariance, 664  
 Lorentz transformation, 241, 664  
 Lyman  $\alpha$  radiation, 652
- M**agnetic  $2^L$ -pole radiation field, 591  
 magnetic field perturbations, 235  
 magnetic moment, 552, 553, 683  
 magnetic moment-magnetic moment  
     interaction, 304  
 magnetic multipole radiation, 622  
 magnetic resonance, 553  
 magnetization vector, 557  
 many-body formalism, 721  
 many-body theory, 721  
 matrix, 67, 79

- mean lifetime, 621  
 Metropolis, N., 271  
 minimum, 68, 151, 184,  
 minimum uncertainties, 25, 68, 185  
 MIT bag model, 703, 713  
 momentum representation, 144, 167  
 Morse potential, 118  
 Mott formula, 678  
 muon-hydrogen atom scattering, 491  
 Møller operator, 505
- N-identical particle states, 389  
 natural line width, 645  
 nearly degenerate levels, 229  
 neutron nucleus scattering, 474  
 neutron-proton system, 446  
 $\text{NH}_3$  molecule, 45, 76, 365  
 nondegenerate state, 209  
 normal order, 181  
 nuclear electric quadrupole moment, 309  
 nuclear hyperfine interaction, 329  
 nuclear hyperfine structure, 303  
 nuclear magnetic moment, 303
- Occupation number representation**, 721, 726  
 odd permutations, 390  
 one-body operators, 729  
 one-dimensional Green's functions, 458  
 one-dimensional harmonic oscillator, 62, 121, 177, 198, 364  
 one-electron atom, 238, 309, 329, 562  
 operator form of scattering Green's function, 477  
 optical coherent states, 180  
 Optical Theorem, 421  
 orbital angular momentum, 92  
 ortho-helium, 384  
 orthogonal, 28  
 orthogonality, 8, 60  
 orthogonality relations, 160, 167, 266, 665  
 orthonormality, 11  
 oscillating magnetic field, 552, 553  
 oscillator coherent states, 180  
 overcomplete, 182
- Pöschl-Teller potential, 114  
 pair exchange, 382  
 pairing forces in nuclei, 745  
 pairing interaction, 738  
 Paldus, J., 352  
 para-helium, 384  
 parabolic coordinates, 38, 469  
 paramagnetic term, 240  
 parity, 27  
 parity operator, 32  
 Parseval's theorem, 24  
 partial wave, 420  
 Paschen-Back effect, 238  
 passive point of view, 169, 273  
 Pauli  $\sigma$  matrices, 516, 520, 564  
 Pauli  $\vec{\sigma}$  operator, 553  
 Pauli  $\vec{\sigma}$  vector, 509  
 Pauli approximation to the Dirac equation, 686  
 Pauli spin matrices, 151, 164  
 Pauli spin operator, 164  
 Perelomov, A., 191  
 periodic permutation, 550  
 periodic potential, 48  
 periodic square well potential, 48  
 permutation group, 392  
 permutation operators, 389  
 perturbation theory, 203  
 perturbed hydrogenic atom, 344  
 phase shift, 419, 420  
 photo dissociation, 626  
 photoelectric effect, 606  
 photon energy, 582  
 photon linear momentum, 583  
 photon rest mass, 584  
 photon scattering, 631  
 photon spin, 584  
 photons, 575, 582  
 Pitaevskii, 575  
 Planck quantization rule, 364  
 plane wave Born approximation, 501  
 plane wave solutions, 674  
 polarizability tensor, 642, 650  
 polarization, 510  
 polarization filter, 163  
 polarization vector, 518, 577  
 polyatomic molecule, 37, 153  
 positron, 676, 692  
 potential resonances, 443  
 potential scattering, 401

- precession, 240  
 probability density, 21  
 probability density current, 22  
 projectile, 401, 402  
 projection operator, 142, 210  
 proper, 255  
 proper zeroth-order basis, 221  
 proper zeroth-order eigenvectors, 222  
 proton, 493  
 proton–nucleus, 469  
 proton–proton Coulomb scattering, 467  
 pure state, 523
- Quantized radiation field**, 579  
**quark confinement**, 713  
**quark models**, 368, 703
- Racah coefficient**, 312, 314  
**radiative capture process**, 613, 614  
**Raman scattering**, 631, 636  
 Raman scattering from diatomic molecules, 651  
 Ramsauer–Townsend effect, 448  
 Rayleigh scattering, 631, 636  
 Rayleigh–Faxen–Holtzman partial wave expansion, 419  
 Rayleigh–Schrödinger expansion, 203, 208  
 rearrangement collision, 425, 477, 481  
 recoupling, 312  
 recoupling of four angular momenta, 321  
 reduced matrix element, 299  
 relative, 34  
 relative coordinates, 402  
 relativistic electron beam, 700  
 relativistic hydrogen atom, 708  
 relativistic mass correction, 242, 689  
 representations, 138  
 resonance fluorescence cross section, 652  
 reversal of magnetic field, 562  
 rigid rotator, 37, 152, 153, 206  
 Ritz variational method, 397  
 Rodrigues formula, 64, 411  
 Rose, M. E., 271  
 Rosen–Morse potential, 120  
 rotation group, 278  
 rotation matrices, 279
- rotation operators, 274  
 rotations, 273  
 Rotenberg, M., 271  
 Runge–Lenz vector, 32, 73, 136, 334  
 Rutherford, 465
- Sakurai, J. J., 575, 649  
 Satchler, G. R., 271  
 scalar potential, 33, 36, 575, 681  
 scalar product, 28, 141  
 scattering amplitude, 407, 463  
 scattering cross section, 402, 407, 420, 421, 441, 444, 468, 488, 523, 680  
 scattering from spherical potentials, 436  
 scattering Green’s functions, 450  
 scattering length, 444  
 scattering theory, 401, 547  
 Schrödinger, 84  
 Schrödinger equation, 19, 34, 35, 82, 407  
 Schrödinger picture, 176, 541  
 Schrödinger theory, 39  
 screened Coulomb potential, 464  
 semiclassical approximation, 204  
 shape-invariant potentials, 108  
 similarity transformation  
     perturbation theory by, 229  
 single-particle, 729  
 Skagerstam, Bo-Sture, 181  
 Slater determinant, 391, 725  
 SO(2,1), 193, 199  
 $\text{SO}(2,1) \times \text{SO}(2,1)$ , 352  
 SO(2,1) algebra, 193, 332, 338  
 SO(3), 193, 278  
 SO(4) algebra, 334  
 SO(4) group, 334  
 SO(4,2) group, 350  
 solid harmonics, 102  
 Sommerfeld, A., 363  
 space inversion, 32, 670  
 space-inversion operator, 27  
 special Lorentz transformation, 665  
 spherical Bessel functions, 409, 412  
 spherical drop model of the nucleus, 474  
 spherical Hänkel functions, 413  
 spherical harmonics, 92, 408  
 spherical Neumann functions, 409, 412

- spherical tensors, 295  
 spin, 147, 509  
 spin magnetic moment, 240, 303  
 spin-lattice interactions, 559  
 spin-lattice relaxation, 559  
 spin-spin interactions, 559  
 spin-spin relaxation, 559  
 spin-orbit coupling, 240  
 spontaneous emission, 204, 615  
 spontaneous emission of photons, 575  
 square well, 40, 436  
 square well problems, 45  
 stabilized zeroth-order eigenvectors, 222  
 Stark effect, 224, 227, 257, 332, 350  
 Stark energy, 249  
 stationary value, 393  
 stationary-state perturbation theory, 208  
 statistical distribution of spin states, 523  
 Stern, 163  
 stimulated absorption, 207  
 stretched parabolic coordinates, 38, 198, 257, 352  
 stretched states, 340  
 $SU(2)$ , 193, 278  
 $SU(2)$  groups, 335  
 successively emitted  $\gamma$  photons, 630  
 sudden approximations, 561  
 supersymmetric partner potentials, 130, 134,  
 symmetric, 382  
 symmetric gauge, 239  
 symmetric rotator, 37  
 symmetric top rigid rotator, 128  
 symmetrizer, 389  
 symmetry, 721  
 symmetry properties, 269, 323  
 symmetry transformations, 319  
 symmetry-adapted basis, 222  
 symmetry-adapted eigenfunctions, 255
- T**arget, 401, 402  
 target particles, 477  
 tensor interaction, 305  
 Thomas, L. T., 240  
 Thomson scattering, 631, 634  
 three-dimensional harmonic oscillator, 123, 196, 365  
 time evolution, 175, 541
- time evolution operator, 541  
 time-dependent perturbation expansion, 541  
 time-independent Schrödinger equation, 39  
 time-translation, 175  
 transformation properties, 672  
 transformation theory, 159, 167  
 transition probabilities, 204  
 transition probability, 546, 602, 617, 621, 623  
 translation operator, 168  
 tunneling, 76  
 two-body operators, 735  
 two-dimensional harmonic oscillator, 239  
 two-electron atoms, 381  
 two-minimum problem, 365
- U**hlenbeck, G. E., 147, 240  
 uncertainty, 151, 184  
 uncertainty principle, 24  
 unit flux normalization, 407, 425  
 unitary, 541  
 unitary 9-j transformation coefficients, 323  
 unitary group, 278  
 unitary operator, 161, 175  
 unitary transformation, 160, 229
- V**acuum state, 181, 580, 729  
 variation parameters, 394  
 variational methods, 204  
 variational technique, 393  
 vector, 36  
 vector coherent state method, 191  
 vector coupling coefficient, 265  
 vector potential, 33, 575, 681  
 vector space, 138  
 vector spherical harmonics, 587  
 vector-coupled orbital-spin function, 511  
 virtually bound states, 46, 60
- W**entzel, G., 354  
 Wick inequality, 421  
 Wigner coefficient, 265  
 Wigner-Brillouin expansion, 203, 213  
 Wigner-Eckart theorem, 299

- Wigner–Weisskopf treatment, 645  
Wilson, W., 363  
Wilson–Sommerfeld quantization rules,  
    363  
WKB, 204  
WKB approximation, 354  
Wooten, J. K., 271
- Young double slit, 4  
Young tableaux, 392  
Yukawa potential, 464
- Zeeman effect, 238  
Zeeman perturbations, 243