

## The Physics of Quantum Mechanics

### Solutions to starred problems

**3.9\*** By expressing the annihilation operator  $A$  of the harmonic oscillator in the momentum representation, obtain  $\langle p|0\rangle$ . Check that your expression agrees with that obtained from the Fourier transform of

$$\langle x|0\rangle = \frac{1}{(2\pi\ell^2)^{1/4}} e^{-x^2/4\ell^2}, \quad \text{where } \ell \equiv \sqrt{\frac{\hbar}{2m\omega}}. \quad (3.1)$$

**Soln:** In the momentum representation  $x = i\hbar\partial/\partial p$  so  $[x, p] = i\hbar\partial p/\partial p = i\hbar$ . Thus from Problem 3.7

$$A = \left( \frac{x}{2\ell} + i\frac{\ell}{\hbar}p \right) = i \left( \frac{\ell p}{\hbar} + \frac{\hbar}{2\ell} \frac{\partial}{\partial p} \right)$$

$$0 = Au_0 \Rightarrow \frac{\ell p}{\hbar}u_0 = -\frac{\hbar}{2\ell} \frac{\partial u_0}{\partial p} \Rightarrow u_0(p) \propto e^{-p^2\ell^2/\hbar^2}$$

Alternatively, transforming  $u_0(x)$ :

$$\langle p|0\rangle = \int dx \langle p|x\rangle \langle x|0\rangle = \frac{1}{\sqrt{h}} \int_{-\infty}^{\infty} dx e^{-ipx/\hbar} \frac{e^{-x^2/4\ell^2}}{(2\pi\ell^2)^{1/4}}$$

$$= \frac{1}{(2\pi\ell^2\hbar^2)^{1/4}} \int_{-\infty}^{\infty} dx \exp\left(-\left\{\frac{x}{2\ell} + \frac{ip\ell}{\hbar}\right\}^2\right) e^{-p^2\ell^2/\hbar^2} = \frac{2\ell\sqrt{\pi}}{(2\pi\ell^2\hbar^2)^{1/4}} e^{-p^2\ell^2/\hbar^2}$$

**3.11\*** A Fermi oscillator has Hamiltonian  $H = f^\dagger f$ , where  $f$  is an operator that satisfies

$$f^2 = 0 \quad ; \quad f f^\dagger + f^\dagger f = 1. \quad (3.2)$$

Show that  $H^2 = H$ , and thus find the eigenvalues of  $H$ . If the ket  $|0\rangle$  satisfies  $H|0\rangle = 0$  with  $\langle 0|0\rangle = 1$ , what are the kets (a)  $|a\rangle \equiv f|0\rangle$ , and (b)  $|b\rangle \equiv f^\dagger|0\rangle$ ?

In quantum field theory the vacuum is pictured as an assembly of oscillators, one for each possible value of the momentum of each particle type. A boson is an excitation of a harmonic oscillator, while a fermion is an excitation of a Fermi oscillator. Explain the connection between the spectrum of  $f^\dagger f$  and the Pauli principle.

**Soln:**

$$H^2 = f^\dagger f f^\dagger f = f^\dagger (1 - f^\dagger f) f = f^\dagger f = H$$

Since eigenvalues have to satisfy any equations satisfied by their operators, the eigenvalues of  $H$  must satisfy  $\lambda^2 = \lambda$ , which restricts them to the numbers 0 and 1. The Fermi exclusion principle says there can be no more than one particle in a single-particle state, so each such state is a Fermi oscillator that is either excited once or not at all.

$$||a\rangle|^2 = \langle 0|f^\dagger f|0\rangle = 0 \quad \text{so this ket vanishes.}$$

$$||b\rangle|^2 = \langle 0|f f^\dagger|0\rangle = \langle 0|(1 - f^\dagger f)|0\rangle = 1 \quad \text{so } |b\rangle \text{ is more interesting.}$$

Moreover,

$$H|b\rangle = f^\dagger f f^\dagger|0\rangle = f^\dagger (1 - f^\dagger f)|0\rangle = f^\dagger|0\rangle = |b\rangle$$

so  $|b\rangle$  is the eigenket with eigenvalue 1.

**3.13\***  $P$  is the probability that at the end of the experiment described in Problem 3.12, the oscillator is in its second excited state. Show that when  $f = \frac{1}{2}$ ,  $P = 0.144$  as follows. First show that the annihilation operator of the original oscillator

$$A = \frac{1}{2} \{ (f^{-1} + f)A' + (f^{-1} - f)A'^\dagger \}, \quad (3.3)$$

where  $A'$  and  $A'^\dagger$  are the annihilation and creation operators of the final oscillator. Then writing the ground-state ket of the original oscillator as a sum  $|0\rangle = \sum_n c_n |n'\rangle$  over the energy eigenkets of the final oscillator, impose the condition  $A|0\rangle = 0$ . Finally use the normalisation of  $|0\rangle$  and the

orthogonality of the  $|n'\rangle$ . What value do you get for the probability of the oscillator remaining in the ground state?

Show that at the end of the experiment the expectation value of the energy is  $0.2656\hbar\omega$ . Explain physically why this is less than the original ground-state energy  $\frac{1}{2}\hbar\omega$ .

This example contains the physics behind the inflationary origin of the Universe: gravity explosively enlarges the vacuum, which is an infinite collection of harmonic oscillators (Problem 3.11). Excitations of these oscillators correspond to elementary particles. Before inflation the vacuum is unexcited so every oscillator is in its ground state. At the end of inflation, there is non-negligible probability of many oscillators being excited and each excitation implies the existence of a newly created particle.

**Soln:** From Problem 3.6 we have

$$\begin{aligned} A &\equiv \frac{m\omega x + ip}{\sqrt{2m\hbar\omega}} & A' &\equiv \frac{mf^2\omega x + ip}{\sqrt{2m\hbar f^2\omega}} \\ &= \frac{x}{2\ell} + \frac{i\ell}{\hbar}p & &= \frac{fx}{2\ell} + \frac{i\ell}{f\hbar}p \end{aligned}$$

Hence

$$\begin{aligned} A' + A'^{\dagger} &= \frac{f}{\ell}x & A' - A'^{\dagger} &= f\frac{2i\ell}{f\hbar}p & \text{so } A &= \frac{1}{2f}(A' + A'^{\dagger}) + \frac{f}{2}(A' - A'^{\dagger}) \\ 0 = A|0\rangle &= \frac{1}{2} \sum_k \left\{ (f^{-1} + f)c_k A'|k'\rangle + (f^{-1} - f)c_k A'^{\dagger}|k'\rangle \right\} \\ &= \frac{1}{2} \sum_k \left\{ (f^{-1} + f)\sqrt{k}c_k|k-1'\rangle + (f^{-1} - f)\sqrt{k+1}c_k|k+1'\rangle \right\} \end{aligned}$$

Multiply through by  $\langle n'|$ :

$$0 = (f^{-1} + f)\sqrt{n+1}c_{n+1} + (f^{-1} - f)\sqrt{n}c_{n-1},$$

which is a recurrence relation from which all non-zero  $c_n$  can be determined in terms of  $c_0$ . Put  $c_0 = 1$  and solve for the  $c_n$ . Then evaluate  $S \equiv |c_n|^2$  and renormalise:  $c_n \rightarrow c_n/\sqrt{S}$ .

The probability of remaining in the ground state is  $|c_0|^2 = 0.8$ .  $\langle E \rangle = \sum_n |c_n|^2 (n + \frac{1}{2})\hbar f^2\omega$ . It is less than the original energy because of the chance that energy is in the spring when the stiffness is reduced.

**3.14\*** In terms of the usual ladder operators  $A$ ,  $A^{\dagger}$ , a Hamiltonian can be written

$$H = \mu A^{\dagger}A + \lambda(A + A^{\dagger}). \quad (3.4)$$

What restrictions on the values of the numbers  $\mu$  and  $\lambda$  follow from the requirement for  $H$  to be Hermitian?

Show that for a suitably chosen operator  $B$ ,  $H$  can be rewritten

$$H = \mu B^{\dagger}B + \text{constant}. \quad (3.5)$$

where  $[B, B^{\dagger}] = 1$ . Hence determine the spectrum of  $H$ .

**Soln:** Hermiticity requires  $\mu$  and  $\lambda$  to be real. Defining  $B = A + a$  with  $a$  a number, we have  $[B, B^{\dagger}] = 1$  and

$$H = \mu(B^{\dagger} - a^*)(B - a) + \lambda(B - a + B^{\dagger} - a^*) = \mu B^{\dagger}B + (\lambda - \mu a^*)B + (\lambda - \mu a)B^{\dagger} + (|a|^2\mu - \lambda(a + a^*)).$$

We dispose of the terms linear in  $B$  by setting  $a = \lambda/\mu$ , a real number. Then  $H = \mu B^{\dagger}B - \lambda^2/\mu$ . From the theory of the harmonic oscillator we know that the spectrum of  $B^{\dagger}B$  is  $0, 1, \dots$ , so the spectrum of  $H$  is  $n\mu - \lambda^2/\mu$ .

**3.15\*** Numerically calculate the spectrum of the anharmonic oscillator shown in Figure 3.2. From it estimate the period at a sequence of energies. Compare your quantum results with the equivalent classical results.

**Soln:**

**3.16\*** Let  $B = cA + sA^\dagger$ , where  $c \equiv \cosh \theta$ ,  $s \equiv \sinh \theta$  with  $\theta$  a real constant and  $A, A^\dagger$  are the usual ladder operators. Show that  $[B, B^\dagger] = 1$ .

Consider the Hamiltonian

$$H = \epsilon A^\dagger A + \frac{1}{2} \lambda (A^\dagger A^\dagger + AA), \quad (3.6)$$

where  $\epsilon$  and  $\lambda$  are real and such that  $\epsilon > \lambda > 0$ . Show that when

$$\epsilon c - \lambda s = E c \quad ; \quad \lambda c - \epsilon s = E s \quad (3.7)$$

with  $E$  a constant,  $[B, H] = EB$ . Hence determine the spectrum of  $H$  in terms of  $\epsilon$  and  $\lambda$ .

**Soln:**

$$[B, B^\dagger] = [cA + sA^\dagger, cA^\dagger + sA] = (c^2 - s^2)[A, A^\dagger] = 1$$

$$\begin{aligned} [B, H] &= [cA + sA^\dagger, \epsilon A^\dagger A + \frac{1}{2} \lambda (A^\dagger A^\dagger + AA)] = c[A, \epsilon A^\dagger A + \frac{1}{2} \lambda A^\dagger A^\dagger] + s[A^\dagger, \epsilon A^\dagger A + \frac{1}{2} \lambda AA] \\ &= c(\epsilon A + \lambda A^\dagger) - s(\epsilon A^\dagger + \lambda A) = cEA + sEA^\dagger = EB \end{aligned}$$

as required. Let  $H|E_0\rangle = E_0|E_0\rangle$ . Then multiplying through by  $B$

$$E_0 B|E_0\rangle = BH|E_0\rangle = (HB + [B, H])|E_0\rangle = (HB + EB)|E_0\rangle$$

So  $H(B|E_0\rangle) = (E_0 - E)(B|E_0\rangle)$ , which says the  $B|E_0\rangle$  is an eigenket for eigenvalue  $E_0 - E$ .

We assume that the sequence of eigenvalues  $E_0, E_0 - E, E_0 - 2E, \dots$  terminates because  $B|E_{\min}\rangle = 0$ . Mod-squaring this equation we have

$$\begin{aligned} 0 &= \langle E_{\min} | B^\dagger B | E_{\min} \rangle = \langle E_{\min} | (cA^\dagger + sA)(cA + sA^\dagger) | E_{\min} \rangle \\ &= \langle E_{\min} | \{ (c^2 + s^2) A^\dagger A + s^2 + cs(A^\dagger A^\dagger + AA) \} | E_{\min} \rangle \\ &= cs \langle E_{\min} | \{ (c/s + s/c) A^\dagger A + s/c + (A^\dagger A^\dagger + AA) \} | E_{\min} \rangle \end{aligned}$$

But eliminating  $E$  from the given equations, we find  $\lambda(c/s + s/c) = 2\epsilon$ . Putting this into the last equation

$$0 = \langle E_{\min} | \left\{ \frac{2\epsilon}{\lambda} A^\dagger A + s/c + (A^\dagger A^\dagger + AA) \right\} | E_{\min} \rangle$$

Multiplying through by  $\lambda/2$  this becomes

$$0 = \langle E_{\min} | \{ H + s\lambda/2c \} | E_{\min} \rangle$$

so  $E_{\min} = -s\lambda/2c$ . Finally,  $x = s/c$  satisfies the quadratic

$$x^2 - 2\frac{\epsilon}{\lambda}x + 1 = 0 \quad \Rightarrow \quad x = \frac{\epsilon}{\lambda} \pm \sqrt{\frac{\epsilon^2}{\lambda^2} - 1}.$$

Also from the above  $E = \epsilon - \lambda x$  so the general eigenenergy is

$$\begin{aligned} E_n &= E_{\min} + nE = -\frac{1}{2}\lambda x + n\epsilon - n\lambda x = n\epsilon - (n + \frac{1}{2})\lambda x = n\epsilon - (n + \frac{1}{2}) \left( \epsilon \pm \sqrt{\epsilon^2 - \lambda^2} \right) \\ &= -\frac{1}{2}\epsilon \mp (n + \frac{1}{2}) \sqrt{\epsilon^2 - \lambda^2} \end{aligned}$$

We have to choose the plus sign in order to achieve consistency with our previously established value of  $E_{\min}$ ; thus finally

$$E_n = -\frac{1}{2}\epsilon + (n + \frac{1}{2}) \sqrt{\epsilon^2 - \lambda^2}$$

**3.17\*** This problem is all classical emag, but it gives physical insight into quantum physics. It is hard to do without a command of Cartesian tensor notation. A point charge  $Q$  is placed at the origin in the magnetic field generated by a spatially confined current distribution. Given that

$$\mathbf{E} = \frac{Q}{4\pi\epsilon_0} \frac{\mathbf{r}}{r^3} \quad (3.8)$$

and  $\mathbf{B} = \nabla \times \mathbf{A}$  with  $\nabla \cdot \mathbf{A} = 0$ , show that the field's momentum

$$\mathbf{P} \equiv \epsilon_0 \int d^3\mathbf{x} \mathbf{E} \times \mathbf{B} = Q\mathbf{A}(0). \quad (3.9)$$

Write down the relation between the particle's position and momentum and interpret this relation physically in light of the result you have just obtained.

*Hint:* write  $\mathbf{E} = -(Q/4\pi\epsilon_0)\nabla r^{-1}$  and  $\mathbf{B} = \nabla \times \mathbf{A}$ , expand the vector triple product and integrate each of the resulting terms by parts so as to exploit in one  $\nabla \cdot \mathbf{A} = 0$  and in the other  $\nabla^2 r^{-1} = -4\pi\delta^3(\mathbf{r})$ . The tensor form of Gauss's theorem states that  $\int d^3\mathbf{x} \nabla_i \mathbf{T} = \oint d^2 S_i \mathbf{T}$  no matter how many indices the tensor  $\mathbf{T}$  may carry.

**Soln:** In tensor notation with  $\partial_i \equiv \partial/\partial x_i$

$$\mathbf{P} = -\frac{Q}{4\pi} \int d^3\mathbf{x} \nabla r^{-1} \times (\nabla \times \mathbf{A})$$

becomes

$$\begin{aligned} P_i &= -\frac{Q}{4\pi} \int d^3\mathbf{x} \sum_{jklm} \epsilon_{ijk} \partial_j r^{-1} \epsilon_{klm} \partial_l A_m \\ &= -\frac{Q}{4\pi} \int d^3\mathbf{x} \sum_{jklm} \epsilon_{kij} \epsilon_{klm} \partial_j r^{-1} \partial_l A_m \\ &= -\frac{Q}{4\pi} \int d^3\mathbf{x} \sum_{jlm} (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) \partial_j r^{-1} \partial_l A_m \\ &= -\frac{Q}{4\pi} \int d^3\mathbf{x} \sum_j (\partial_j r^{-1} \partial_i A_j - \partial_j r^{-1} \partial_j A_i) \end{aligned}$$

In the first integral we use the divergence theorem to move  $\partial_j$  from  $r^{-1}$  to  $\partial_i A_j$  and in the second integral we move the  $\partial_j$  from  $A_j$  to  $\partial_j r^{-1}$ . We argue that the surface integrals over some bounding sphere of radius  $R$  that arise in this process vanish as  $R \rightarrow \infty$  because their integrands have explicit  $R^{-2}$  scaling, so they will tend to zero as  $R \rightarrow \infty$  so long as  $A \rightarrow 0$  no matter how slowly. After this has been done we have

$$P_i = -\frac{Q}{4\pi} \left( - \int d^3\mathbf{x} (r^{-1} \partial_j \partial_i A_j + \int d^3\mathbf{x} \partial_j \partial_j r^{-1} A_i) \right)$$

The first integral vanishes because  $\partial_j A_j = \nabla \cdot \mathbf{A} = 0$  and in the second integral we note that  $\partial_j \partial_j r^{-1} = \nabla^2 r^{-1} = -4\pi\delta^3(\mathbf{x})$ , so evaluation of the integral is trivial and yields the required expression.

The physical interpretation is that when we accelerate a charge, we have to inject momentum into the emag field that moves with the charge. So the conserved momentum  $\mathbf{p}$  associated with the particle's motion includes both the momentum in the particle and that in the field, which we have just shown to be  $Q\mathbf{A}(\mathbf{x})$ , where  $\mathbf{x}$  is the particle's location. Thus  $\mathbf{p} = m\dot{\mathbf{x}} + Q\mathbf{A}$ . The particle's kinetic energy is  $H = \frac{1}{2}m\dot{\mathbf{x}}^2 = (\mathbf{p} - Q\mathbf{A})^2/2m$ .

**3.18\*** From equation (3.58) show that the the normalised wavefunction of a particle of mass  $m$  that is in the  $n^{\text{th}}$  Landau level of a uniform magnetic field  $B$  is

$$\langle \mathbf{x} | n \rangle = \frac{r^n e^{-r^2/4r_B^2} e^{-in\phi}}{2^{(n+1)/2} \sqrt{n!} \pi r_B^{n+1}}, \quad (3.10)$$

where  $r_B = \sqrt{\hbar/QB}$ . Hence show that the expectation of the particle's gyration radius is

$$\langle r \rangle_n \equiv \langle n | r | n \rangle = \sqrt{2} \{ (n + \frac{1}{2})(n - \frac{1}{2}) \times \dots \times \frac{1}{2} \} \frac{r_B}{n!}. \quad (3.11)$$

Show further that

$$\frac{\delta \ln \langle r \rangle_n}{\delta n} \simeq \frac{1}{2n} \quad (3.12)$$

and thus show that in the limit of large  $n$ ,  $\langle r \rangle \propto \sqrt{E}$ , where  $E$  is the energy of the level. Show that this result is in accordance with the correspondence principle.

**Soln:** We obtain the required expression for  $\langle \mathbf{x} | n \rangle$  by evaluating  $\int dr r r^{2n} e^{-r^2/2r_B^2} (n+r^2/2r_B^2) \int d\phi$  with the help of the definition  $z! = \int_0^\infty dx x^z e^{-x}$ . Then

$$\langle r \rangle_n = \frac{\int dr r^2 r^{2n} e^{-r^2/2r_B^2} 2\pi}{2^{n+1} n! \pi r_B^{2n+2}} = \frac{2^{3/2} r_B}{n!} \int_0^\infty \frac{dz}{2} z^{n+1/2} e^{-z} = \frac{\sqrt{2} r_B}{n!} (n + \frac{1}{2})!$$

where  $z \equiv r/\sqrt{2}r_B$ .

$$\frac{\delta \ln \langle r \rangle_n}{\delta n} = \langle r \rangle_{n+1} - \langle r \rangle_n = \ln \left( \frac{(n + \frac{3}{2})! n!}{(n + \frac{1}{2})! (n+1)!} \right) = \ln \left( \frac{n + \frac{3}{2}}{n+1} \right) = \ln \left( \frac{1 + \frac{3}{2n}}{1 + \frac{1}{n}} \right) \simeq \frac{1}{2n}$$

Summing this expression over several increments we have that the overall change  $\Delta \ln \langle r \rangle_n = \Delta \ln(n^{1/2})$ , so for  $n \gg 1$ ,  $\langle r \rangle_n \sim n^{1/2} \sim E^{1/2}$ . Classically

$$\frac{mv^2}{r} = QvB \quad \Rightarrow \quad E = \frac{1}{2}mv^2 = \frac{1}{2}m \left( \frac{QB}{m} \right)^2 r^2$$

so  $r \propto E^{1/2}$  as in QM.

**3.20\*** Equation (2.106) gives the probability current density associated with a wavefunction. Show that the flux given by this expression changes when we make a gauge change  $\psi \rightarrow \psi' = e^{iQ\Lambda/\hbar} \psi$ . Why is this state of affairs physically unacceptable?

Show that in Dirac's notation equation (2.83) is

$$\mathbf{J}(\mathbf{x}) = \frac{1}{m} \Re (\langle \psi | \mathbf{x} | \mathbf{x} | \mathbf{p} | \psi \rangle). \quad (3.13)$$

Modify this expression to obtain a gauge-invariant definition of  $\mathbf{J}$ . Explain why your new expression makes good physical sense given the form that the kinetic-energy operator takes in the presence of a magnetic field. Show that in terms of the amplitude and phase  $\theta$  of  $\psi$  your expression reads

$$\mathbf{J} = \frac{|\psi|^2}{m} (\hbar \nabla \theta - Q\mathbf{A}). \quad (3.14)$$

Explicitly check that this formula makes  $\mathbf{J}$  invariant under a gauge transformation.

Using cylindrical polar coordinates  $(r, \phi, z)$ , show that the probability current density associated with the wavefunction (3.10) of the  $n^{\text{th}}$  Landau level is

$$\mathbf{J}(r) = -\frac{\hbar r^{2n-1} e^{-r^2/2r_B^2}}{2^{n+1} \pi n! m r_B^{2n+2}} \left( n + \frac{r^2}{2r_B^2} \right) \hat{\mathbf{e}}_\phi, \quad (3.15)$$

where  $r_B \equiv \sqrt{\hbar/QB}$ . Plot  $\mathbf{J}$  as a function of  $r$  and interpret your plot physically.

**Soln:** The gauge transformation changes the phase of the wavefunction  $\theta \rightarrow \theta + Q\Lambda/\hbar$  so it changes the current by  $(|\psi|^2 Q/m) \nabla \Lambda$ . This is unacceptable because nothing physical should be changed by a gauge transformation.

$$\frac{1}{m} \Re (\langle \psi | \mathbf{x} | \mathbf{x} | \mathbf{p} | \psi \rangle) = \frac{1}{2m} (\langle \psi | \mathbf{x} | \mathbf{x} | \mathbf{p} | \psi \rangle + \langle \mathbf{x} | \psi \rangle (\langle \mathbf{x} | \mathbf{p} | \psi \rangle)^*) = \frac{1}{2m} (\psi^2 (-i\hbar \nabla \psi) + \psi^* (-i\hbar \nabla \psi)^*)$$

which agrees with the definition of  $\mathbf{J}$ . The principle of minimal coupling requires us to replace  $\mathbf{p}$  by  $\mathbf{p} - Q\mathbf{A}$ , so we redefine  $\mathbf{J}$  to be

$$\mathbf{J}(\mathbf{x}) = \frac{1}{m} \Re (\langle \psi | \mathbf{x} | \mathbf{x} | (\mathbf{p} - Q\mathbf{A}) | \psi \rangle).$$

From  $H$  we recognise  $(\mathbf{p} - Q\mathbf{A})/m$  as the particle's velocity, and clearly this is what determines the current. Converting back to the position representation, we find

$$\begin{aligned}\mathbf{J} &= \frac{1}{2m} (\langle \psi | \mathbf{x} \rangle \langle \mathbf{x} | (\mathbf{p} - Q\mathbf{A}) | \psi \rangle + \langle \mathbf{x} | \psi \rangle \langle (\mathbf{x} | (\mathbf{p} - Q\mathbf{A}) | \psi \rangle)^*) \\ &= \frac{1}{2m} (\psi^* (-i\hbar \nabla \psi - Q\mathbf{A}\psi) + \psi (-i\hbar \nabla \psi - Q\mathbf{A}\psi)^*) \\ &= \frac{1}{2m} (-i\hbar (\psi^* \nabla \psi - \psi \nabla \psi^*) - 2Q\mathbf{A}|\psi|^2)\end{aligned}$$

In amplitude-phase format we now have

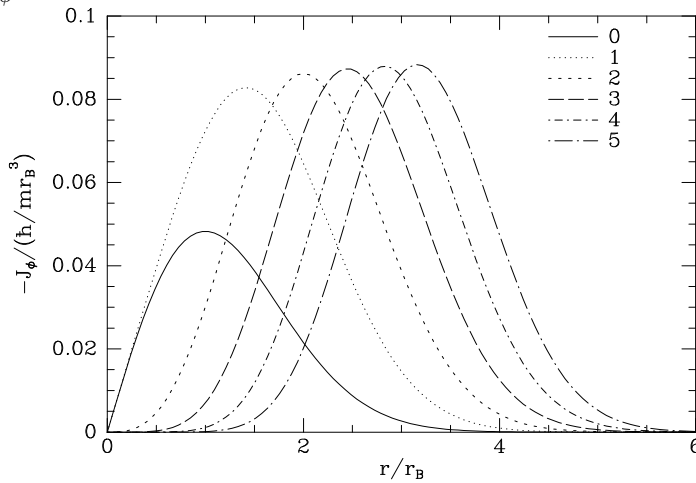
$$\mathbf{J} = \frac{|\psi|^2}{m} (\hbar \nabla \theta - Q\mathbf{A}).$$

This is clearly invariant when we add  $Q\Lambda/\hbar$  to  $\theta$  and  $Q\nabla\Lambda$  to  $\mathbf{A}$ .

In plane polars,

$$\nabla = \left( \frac{\partial}{\partial r}, \frac{1}{r} \frac{\partial}{\partial \phi} \right),$$

so we obtain the required expression for  $\mathbf{J}$  of the Landau level when we take  $|\psi|$  and  $\theta$  from (3.10) and use  $\mathbf{A} = \frac{1}{2}Br\hat{\mathbf{e}}_\phi$ .



The figure shows the current density as a function of radius for the first six Landau levels. The ground state is in a class by itself. For the excited states the characteristic radius  $r$  increases with  $n$  roughly as  $\sqrt{n}$  as predicted by classical physics, while the peak magnitude of the flow is almost independent of  $n$  because  $J \propto \omega|\psi|^2$  and  $\omega \sim \text{constant}$  and  $|\psi|^2 \simeq 1/r$  as expected from classical mechanics.

**3.21\*** Determine the probability current density associated with the  $n^{\text{th}}$  Landau ground-state wavefunction (3.67) (which for  $n = 4$  is shown on the front cover). Use your result to explain in as much detail as you can why this state can be interpreted as a superposition of states in which the electron gyrates around different gyrocentres. Hint: adapt equation (3.15).

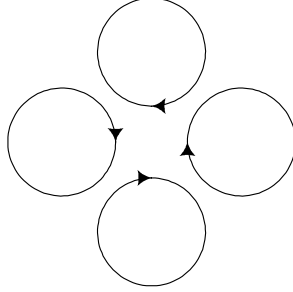
Why is the energy of a gyrating electron incremented if we multiply the wavefunction  $e^{-(m\omega/4\hbar)r^2}$  by  $v^n = (x - iy)^n$  but not if we multiply it by  $u^n = (x + iy)^n$ ?

**Soln:** The wavefunction of the  $n^{\text{th}}$  state in the ground-state level differs from that of the first state of the  $n^{\text{th}}$  excited level only in having  $u^n$  instead of  $v^n$  in front of  $e^{-uv/4r_B^2}$ . Consequently these wavefunctions have the same amplitudes but where the phase of the  $n^{\text{th}}$  excited state is  $\theta = -n\phi$ , that of the  $n^{\text{th}}$  ground state is  $\theta = n\phi$ . Since  $\mathbf{J} \propto (\hbar \nabla \theta - Q\mathbf{A})$  it follows that the probability current is given by equation (3.15) with a minus sign in front of the  $n$ :

$$\mathbf{J}(r) = -\frac{\hbar r^{2n-1} e^{-r^2/2r_B^2}}{2^{n+1} \pi n! m r_B^{2n+2}} \left( \frac{r^2}{2r_B^2} - n \right) \hat{\mathbf{e}}_\phi,$$

$J$  now changes sign at  $r = \sqrt{2nr_B}$ : at small  $r$  it flows in the opposite sense to the current of the  $n^{\text{th}}$  excited level (and the opposite sense to that of classical gyrations), but flows in the same sense at

large  $r$ . This behaviour arises naturally if you arrange clockwise vortices of radius  $\sim r_B$  around a circle of radius  $\sqrt{2nr_B}$ . So whereas in the  $n^{\text{th}}$  excited level the particle is moving counter-clockwise around a path of radius  $\sim \sqrt{nr_B}$ , in this state it is moving on a circle of radius  $\sim r_B$  that is offset from the centre by  $\sim \sqrt{nr_B}$ . The direction of the offset is completely uncertain, so we have to imagine a series of offset circles. These clearly generate an anti-clockwise flow around the origin:



When the ground-state  $\psi(\mathbf{r})$  is multiplied by either  $u^n$  or  $v^n$ , a factor  $r^n e^{\pm in\phi}$  is added. This factor moves outwards the radius  $r_m$  at which  $|\psi|^2$  peaks in the same way regardless of whether we multiply by  $u^n$  or  $v^n$ . But our expressions for  $\mathbf{J}(r)$  show that when we multiply by  $u^n$  we shift  $r_m$  out to the radius near which  $\mathbf{J} = 0$  so there is not much kinetic energy. Had we multiplied by  $v^n$ ,  $\mathbf{J}$  and the kinetic energy would have been large at  $r_m$ . This asymmetry between the effects of multiplying by  $e^{in\phi}$  or  $e^{-in\phi}$  arises because  $\mathbf{A}$  always points in the direction  $\hat{\mathbf{e}}_\phi$ .

**3.22\*** In classical electromagnetism the magnetic moment of a planar loop of wire that has area  $A$ , normal  $\hat{\mathbf{n}}$  and carries a current  $I$  is defined to be

$$\boldsymbol{\mu} = IA\hat{\mathbf{n}}. \quad (3.16)$$

Use this formula and equation (3.15) to show that the magnetic moment of a charge  $Q$  that is in a Landau level of a magnetic field  $B$  has magnitude  $\mu = E/B$ , where  $E$  is the energy of the level. Rederive this formula from classical mechanics.

**Soln:** Eq. (3.15) gives the probability current density  $J$ . We multiply it by  $Q$  to get the electrical current density  $QJ$ . The current  $dI = QJ(r)dr$  through the annulus of radius  $r$  contributes magnetic moment  $d\mu = \pi r^2 dI$ . Summing over annuli we obtain

$$\begin{aligned} \mu &= Q\pi \int_0^\infty dr r^2 J(r) = -\frac{Q\hbar}{2^{n+1}n!mr_B^{2n+2}} \int_0^\infty dr r^{2n+1} e^{-r^2/2r_B^2} \left( n + \frac{r^2}{2r_B^2} \right) \\ &= -\frac{\hbar Q}{2n!m} \int_0^\infty dz z^n e^{-z} (n+z) = -\frac{\hbar Q}{2n!m} [n n! + (n+1)!] = (n + \frac{1}{2}) \frac{\hbar Q}{m} \end{aligned}$$

But  $E = (n + \frac{1}{2})\hbar Q B/m$  so  $\mu E/B$ .

Classically,  $I = Q/\tau = Q\omega/2\pi = Q^2 B/2\pi m$  and  $r^2 = 2mE/Q^2 B^2$ , so  $\mu = \pi r^2 I = E/B$ .

**4.2\*** Show that the vector product  $\mathbf{a} \times \mathbf{b}$  of two classical vectors transforms like a vector under rotations. Hint: A rotation matrix  $\mathbf{R}$  satisfies the relations  $\mathbf{R} \cdot \mathbf{R}^T = \mathbf{I}$  and  $\det(\mathbf{R}) = 1$ , which in tensor notation read  $\sum_p R_{ip} R_{tp} = \delta_{it}$  and  $\sum_{ijk} \epsilon_{ijk} R_{ir} R_{js} R_{kt} = \epsilon_{rst}$ .

**Soln:** Let the rotated vectors be  $\mathbf{a}' = \mathbf{R}\mathbf{a}$  and  $\mathbf{b}' = \mathbf{R}\mathbf{b}$ . Then

$$\begin{aligned} (\mathbf{a}' \times \mathbf{b}')_i &= \sum_{jklm} \epsilon_{ijk} R_{jl} a_l R_{km} b_m \\ &= \sum_{tjklm} \delta_{it} \epsilon_{tjk} R_{jl} R_{km} a_l b_m \\ &= \sum_{ptjklm} R_{ip} R_{tp} \epsilon_{tjk} R_{jl} R_{km} a_l b_m \\ &= \sum_{plm} R_{ip} \epsilon_{plm} a_l b_m = (\mathbf{R}\mathbf{a} \times \mathbf{b})_i. \end{aligned}$$

**4.3\*** We have shown that  $[v_i, J_j] = i \sum_k \epsilon_{ijk} v_k$  for any operator whose components  $v_i$  form a vector. The expectation value of this operator relation in any state  $|\psi\rangle$  is then  $\langle \psi | [v_i, J_j] | \psi \rangle =$

$i \sum_k \epsilon_{ijk} \langle \psi | v_k | \psi \rangle$ . Check that with  $U(\boldsymbol{\alpha}) = e^{-i\boldsymbol{\alpha} \cdot \mathbf{J}}$  this relation is consistent under a further rotation  $|\psi\rangle \rightarrow |\psi'\rangle = U(\boldsymbol{\alpha})|\psi\rangle$  by evaluating both sides separately.

**Soln:** Under the further rotation the LHS  $\rightarrow \langle \psi | U^\dagger [v_i, J_j] U | \psi \rangle$ . Now

$$\begin{aligned} U^\dagger [v_i, J_j] U &= U^\dagger v_i J_j U - U^\dagger J_j v_i U = (U^\dagger v_i U)(U^\dagger J_j U) - (U^\dagger J_j U)(U^\dagger v_i U) \\ &= \sum_{kl} [R_{ik} v_k, R_{jl} J_l] = \sum_{kl} R_{ik} R_{jl} [v_k, J_l]. \end{aligned}$$

Similar  $|\psi\rangle \rightarrow U|\psi\rangle$  on the RHS yields

$$i \sum_{km} R_{km} \epsilon_{ijk} \langle \psi | v_m | \psi \rangle.$$

We now multiply each side by  $R_{is} R_{jt}$  and sum over  $i$  and  $j$ . On the LHS this operation yields  $[v_s, J_t]$ . On the right it yields

$$i \sum_{ijkm} R_{is} R_{jt} R_{km} \epsilon_{ijk} \langle \psi | v_m | \psi \rangle = i \sum_m \epsilon_{stm} \langle \psi | v_m | \psi \rangle,$$

which is what our original equation would give for  $[v_s, J_t]$ .

**4.4\*** The matrix for rotating an ordinary vector by  $\phi$  around the  $z$  axis is

$$\mathbf{R}(\phi) \equiv \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (4.1)$$

By considering the form taken by  $\mathbf{R}$  for infinitesimal  $\phi$  calculate from  $\mathbf{R}$  the matrix  $\mathbf{J}_z$  that appears in  $\mathbf{R}(\phi) = \exp(-i\mathbf{J}_z \phi)$ . Introduce new coordinates  $u_1 \equiv (-x + iy)/\sqrt{2}$ ,  $u_2 = z$  and  $u_3 \equiv (x + iy)/\sqrt{2}$ . Write down the matrix  $\mathbf{M}$  that appears in  $\mathbf{u} = \mathbf{M} \cdot \mathbf{x}$  [where  $\mathbf{x} \equiv (x, y, z)$ ] and show that it is unitary. Then show that

$$\mathbf{J}'_z \equiv \mathbf{M} \cdot \mathbf{J}_z \cdot \mathbf{M}^\dagger. \quad (4.2)$$

is identical with  $S_z$  in the set of spin-one Pauli analogues

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (4.3)$$

Write down the matrix  $\mathbf{J}_x$  whose exponential generates rotations around the  $x$  axis, calculate  $\mathbf{J}'_x$  by analogy with equation (4.2) and check that your result agrees with  $S_x$  in the set (4.3). Explain as fully as you can the meaning of these calculations.

**Soln:** For an infinitesimal rotation angle  $\delta\phi$  to first order in  $\delta\phi$  we have

$$1 - i\mathbf{J}_z \delta\phi = \mathbf{R}(\delta\phi) = \begin{pmatrix} 1 & -\delta\phi & 0 \\ \delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

comparing coefficients of  $\delta\phi$  we find

$$\mathbf{J}_z = i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

In components  $\mathbf{u} = \mathbf{M} \cdot \mathbf{x}$  reads

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

so  $\mathbf{M}$  is the matrix above. We show that  $\mathbf{M}$  is unitary by calculating the product  $\mathbf{M}\mathbf{M}^\dagger$ . Now we have

$$\begin{aligned}\mathcal{J}'_z &= \frac{1}{2} \begin{pmatrix} -1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 1 \\ -i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} -1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & -1 \\ -i & 0 & i \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix}\end{aligned}$$

Similarly, we have

$$\mathcal{J}_x = i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

so

$$\begin{aligned}\mathcal{J}'_x &= \frac{1}{2} \begin{pmatrix} -1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 1 \\ -i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} -1 & i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & -i\sqrt{2} & 0 \\ 1 & 0 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}\end{aligned}$$

These results show that the only difference between the generators of rotations of ordinary 3d vectors and the spin-1 representations of the angular-momentum operators, is that for conventional vectors we use a different coordinate system than we do for spin-1 amplitudes. Apart from this, the three amplitudes for the spin of a spin-1 particle to point in various directions are equivalent to the components of a vector, and they transform among themselves when the particle is reoriented for the same reason that the rotation of a vector changes its Cartesian components.

**4.6\*** Show that if  $\alpha$  and  $\beta$  are non-parallel vectors,  $\alpha$  is not invariant under the combined rotation  $\mathbf{R}(\alpha)\mathbf{R}(\beta)$ . Hence show that  $\mathbf{R}^\dagger(\beta)\mathbf{R}^\dagger(\alpha)\mathbf{R}(\beta)\mathbf{R}(\alpha)$  is not the identity operation. Explain the physical significance of this result.

**Soln:**  $\mathbf{R}(\alpha)\alpha = \alpha$  because a rotation leaves its axis invariant. But the only vectors that are invariant under  $\mathbf{R}(\beta)$  are multiples of the rotation axis  $\beta$ . So  $\mathbf{R}(\beta)\alpha$  is not parallel to  $\alpha$ .

If  $\mathbf{R}^\dagger(\beta)\mathbf{R}^\dagger(\alpha)\mathbf{R}(\beta)\mathbf{R}(\alpha)$  were the identity, we would have

$$\mathbf{R}^\dagger(\beta)\mathbf{R}^\dagger(\alpha)\mathbf{R}(\beta)\mathbf{R}(\alpha)\alpha = \alpha \quad \Rightarrow \quad \mathbf{R}(\beta)\mathbf{R}(\alpha)\alpha = \mathbf{R}(\alpha)\mathbf{R}(\beta)\alpha \quad \Rightarrow \quad \mathbf{R}(\beta)\alpha = \mathbf{R}(\alpha)(\mathbf{R}(\beta)\alpha)$$

which would imply that  $\mathbf{R}(\beta)\alpha$  is invariant under  $\mathbf{R}(\alpha)$ . Consequently we would have  $\mathbf{R}(\beta)\alpha = \alpha$ . But this is true only if  $\alpha$  is parallel to  $\beta$ . So our original hypothesis that  $\mathbf{R}^\dagger(\beta)\mathbf{R}^\dagger(\alpha)\mathbf{R}(\beta)\mathbf{R}(\alpha) = \mathbf{I}$  is wrong. This demonstrates that when you rotate about two non-parallel axes and then do the reverse rotations in the same order, you always finish with a non-trivial rotation.

**4.7\*** In this problem you derive the wavefunction

$$\langle \mathbf{x} | \mathbf{p} \rangle = e^{i\mathbf{p} \cdot \mathbf{x} / \hbar} \quad (4.4)$$

of a state of well defined momentum from the properties of the translation operator  $U(\mathbf{a})$ . The state  $|\mathbf{k}\rangle$  is one of well-defined momentum  $\hbar\mathbf{k}$ . How would you characterise the state  $|\mathbf{k}'\rangle \equiv U(\mathbf{a})|\mathbf{k}\rangle$ ? Show that the wavefunctions of these states are related by  $u_{\mathbf{k}'}(\mathbf{x}) = e^{-i\mathbf{a} \cdot \mathbf{k}} u_{\mathbf{k}}(\mathbf{x})$  and  $u_{\mathbf{k}'}(\mathbf{x}) = u_{\mathbf{k}}(\mathbf{x} - \mathbf{a})$ . Hence obtain equation (4.4).

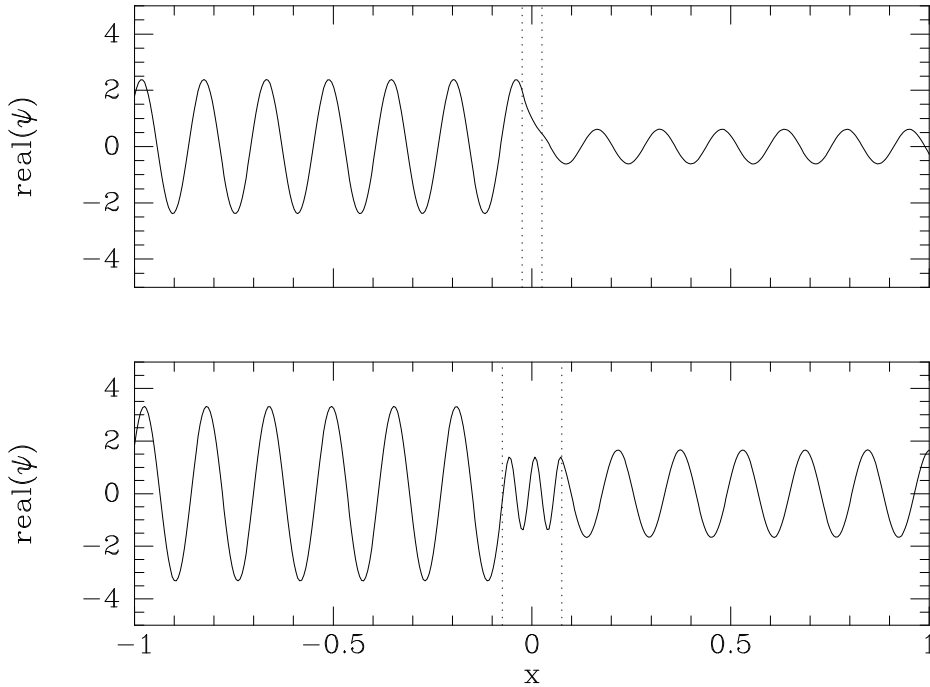
**Soln:**  $U(\mathbf{a})|\mathbf{k}\rangle$  is the result of translating a state of well-defined momentum by  $\mathbf{k}$ . Moving to the position representation

$$u_{\mathbf{k}'}(\mathbf{x}) = \langle \mathbf{x} | U(\mathbf{a}) | \mathbf{k} \rangle = \langle \mathbf{k} | U^\dagger(\mathbf{a}) | \mathbf{x} \rangle^* = \langle \mathbf{k} | \mathbf{x} - \mathbf{a} \rangle^* = u_{\mathbf{k}}(\mathbf{x} - \mathbf{a})$$

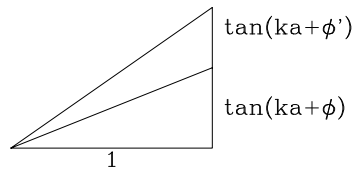
Also

$$\langle \mathbf{x} | U(\mathbf{a}) | \mathbf{k} \rangle = \langle \mathbf{x} | e^{-i\mathbf{a} \cdot \mathbf{p} / \hbar} | \mathbf{k} \rangle = e^{-i\mathbf{a} \cdot \mathbf{k}} \langle \mathbf{x} | \mathbf{k} \rangle = e^{-i\mathbf{a} \cdot \mathbf{k}} u_{\mathbf{k}}(\mathbf{x})$$

Putting these results together we have  $u_{\mathbf{k}}(\mathbf{x} - \mathbf{a}) = e^{-i\mathbf{a} \cdot \mathbf{k}} u_{\mathbf{k}}(\mathbf{x})$ . Setting  $\mathbf{a} = \mathbf{x}$  we find  $u_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} u_{\mathbf{k}}(0)$ , as required.



**Figure 5.0** The real part of the wavefunction when a free particle of energy  $E$  is scattered by a classically forbidden square barrier (top) and a potential well (bottom). The upper panel is for a barrier of height  $V_0 = E/0.7$  and half width  $a$  such that  $2mEa^2/\hbar^2 = 1$ . The lower panel is for a well of depth  $V_0 = E/0.2$  and half width  $a$  such that  $2mEa^2/\hbar^2 = 9$ . In both panels  $(2mE/\hbar^2)^{1/2} = 40$ .



**Figure 5.1** A triangle for Problem 5.9

**5.12\*** In this problem you investigate the interaction of ammonia molecules with electromagnetic waves in an ammonia maser. Let  $|+\rangle$  be the state in which the  $N$  atom lies above the plane of the  $H$  atoms and  $|-\rangle$  be the state in which the  $N$  lies below the plane. Then when there is an oscillating electric field  $\mathcal{E} \cos \omega t$  directed perpendicular to the plane of the hydrogen atoms, the Hamiltonian in the  $|\pm\rangle$  basis becomes

$$H = \begin{pmatrix} \bar{E} + q\mathcal{E}s \cos \omega t & -A \\ -A & \bar{E} - q\mathcal{E}s \cos \omega t \end{pmatrix}. \quad (5.1)$$

Transform this Hamiltonian from the  $|\pm\rangle$  basis to the basis provided by the states of well-defined parity  $|e\rangle$  and  $|o\rangle$  (where  $|e\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$ , etc). Writing

$$|\psi\rangle = a_e(t)e^{-iE_e t/\hbar}|e\rangle + a_o(t)e^{-iE_o t/\hbar}|o\rangle, \quad (5.2)$$

show that the equations of motion of the expansion coefficients are

$$\begin{aligned} \frac{da_e}{dt} &= -i\Omega a_o(t) \left( e^{i(\omega - \omega_0)t} + e^{-i(\omega + \omega_0)t} \right) \\ \frac{da_o}{dt} &= -i\Omega a_e(t) \left( e^{i(\omega + \omega_0)t} + e^{-i(\omega - \omega_0)t} \right), \end{aligned} \quad (5.3)$$

where  $\Omega \equiv q\mathcal{E}s/2\hbar$  and  $\omega_0 = (E_o - E_e)/\hbar$ . Explain why in the case of a maser the exponentials involving  $\omega + \omega_0$  can be neglected so the equations of motion become

$$\frac{da_e}{dt} = -i\Omega a_o(t)e^{i(\omega - \omega_0)t} \quad ; \quad \frac{da_o}{dt} = -i\Omega a_e(t)e^{-i(\omega - \omega_0)t}. \quad (5.4)$$

Solve the equations by multiplying the first equation by  $e^{-i(\omega-\omega_0)t}$  and differentiating the result. Explain how the solution describes the decay of a population of molecules that are initially all in the higher energy level. Compare your solution to the result of setting  $\omega = \omega_0$  in (5.4).

**Soln:** We have

$$\begin{aligned}\langle e|H|e\rangle &= \frac{1}{2}(\langle +| + \langle -|)H(|+ \rangle + |- \rangle) \\ &= \frac{1}{2}(\langle +|H|+ \rangle + \langle -|H|- \rangle + \langle -|H|+ \rangle + \langle +|H|- \rangle) \\ &= \bar{E} - A = E_e \\ \langle o|H|o\rangle &= \frac{1}{2}(\langle +| - \langle -|)H(|+ \rangle - |- \rangle) \\ &= \frac{1}{2}(\langle +|H|+ \rangle + \langle -|H|- \rangle - \langle -|H|+ \rangle - \langle +|H|- \rangle) \\ &= \bar{E} + A = E_o \\ \langle o|H|e\rangle &= \langle e|H|o\rangle = \frac{1}{2}(\langle +| + \langle -|)H(|+ \rangle - |- \rangle) \\ &= \frac{1}{2}(\langle +|H|+ \rangle - \langle -|H|- \rangle + \langle -|H|+ \rangle - \langle +|H|- \rangle) \\ &= q\mathcal{E}s \cos(\omega t)\end{aligned}$$

Now we use the TDSE to calculate the evolution of  $|\psi\rangle = a_e e^{-iE_e t/\hbar}|e\rangle + a_o e^{-iE_o t/\hbar}|o\rangle$ :

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = i\hbar \dot{a}_e e^{-iE_e t/\hbar}|e\rangle + a_e E_e e^{-iE_e t/\hbar}|e\rangle + i\hbar \dot{a}_o e^{-iE_o t/\hbar}|o\rangle + a_o E_o e^{-iE_o t/\hbar}|o\rangle = a_e e^{-iE_e t/\hbar} H|e\rangle + a_o e^{-iE_o t/\hbar} H|o\rangle$$

We now multiply through by first  $\langle e|$  and then  $\langle o|$ . After dividing through by some exponential factors to simplify, we get

$$\begin{aligned}i\hbar \dot{a}_e + a_e E_e &= a_e \langle e|H|e\rangle + a_o e^{i(E_e - E_o)t/\hbar} \langle e|H|o\rangle \\ i\hbar \dot{a}_o + a_o E_o &= a_e e^{i(E_o - E_e)t/\hbar} \langle o|H|e\rangle + a_o \langle o|H|o\rangle\end{aligned}$$

With the results derived above

$$\begin{aligned}i\hbar \dot{a}_e + a_e E_e &= a_e E_e + a_o e^{i(E_e - E_o)t/\hbar} q\mathcal{E}s \cos(\omega t) \\ i\hbar \dot{a}_o + a_o E_o &= a_e e^{i(E_o - E_e)t/\hbar} q\mathcal{E}s \cos(\omega t) + a_o E_o\end{aligned}$$

After cancelling terms in each equation, we obtain the desired equations of motion on expressing the cosines in terms of exponentials and using the new notation.

The exponential with frequency  $\omega + \omega_0$  oscillates so rapidly that it effectively averages to zero, so we can drop it. Multiplying the first eqn through by  $e^{-i(\omega-\omega_0)t}$  and differentiating gives

$$\frac{d}{dt} \left( e^{-i(\omega-\omega_0)t} \dot{a}_e \right) = e^{-i(\omega-\omega_0)t} [-i(\omega - \omega_0)\dot{a}_e + \ddot{a}_e] = -\Omega^2 a_e e^{-i(\omega-\omega_0)t}$$

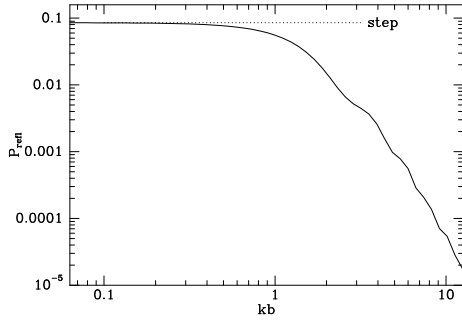
The exponentials cancel leaving a homogeneous second-order o.d.e. with constant coefficients. Since initially all molecules are in the higher-energy state  $|o\rangle$ , we have to solve subject to the boundary condition  $a_e(0) = 0$ . With  $a_o(0) = 1$  we get from the original equations the second initial condition  $\dot{a}_e(0) = -i\Omega$ . For trial solution  $a_e \propto e^{\alpha t}$  the auxiliary eqn is

$$\alpha^2 - i(\omega - \omega_0)\alpha + \Omega^2 = 0 \quad \Rightarrow \quad \alpha = \frac{1}{2} \left[ i(\omega - \omega_0) \pm \sqrt{-(\omega - \omega_0)^2 - 4\Omega^2} \right] = i\omega_{\pm}$$

with  $\omega_{\pm} = \frac{1}{2} \left[ (\omega - \omega_0) \pm \sqrt{(\omega - \omega_0)^2 + 4\Omega^2} \right]$ . When  $\omega \simeq \omega_0$ , these frequencies both lie close to  $\Omega$ . From the condition  $a_e(0) = 0$ , the required solution is  $a_e(t) \propto (e^{i\omega_+ t} - e^{i\omega_- t})$  and the constant of proportionality follows from the second initial condition, so finally

$$a_e(t) = \frac{-\Omega}{\sqrt{(\omega - \omega_0)^2 + 4\Omega^2}} (e^{i\omega_+ t} - e^{i\omega_- t}) \quad (*)$$

The probability oscillates between the odd and even states. First the oscillating field stimulates emission of radiation and decay from  $|o\rangle$  to  $|e\rangle$ . Later the field excites molecules in the ground state to move back up to the first-excited state  $|o\rangle$ .



**Figure 5.2** The symbols show the ratio of the probability of reflection to the probability of transmission when particles move from  $x = -\infty$  in the potential (5.69) with energy  $E = \hbar^2 k^2/2m$  and  $V_0 = 0.7E$ . The dotted line is the value obtained for a step change in the potential

If we solve the original equations (1) exactly on resonance ( $\omega = \omega_0$ ), the relevant solution is

$$a_e(t) = \frac{1}{2}(e^{-i\Omega t} - e^{i\Omega t}),$$

which is what our general solution (\*) reduces to as  $\omega \rightarrow \omega_0$ .

**5.14\*** Particles of mass  $m$  and momentum  $\hbar k$  at  $x < -a$  move in the potential

$$V(x) = V_0 \begin{cases} 0 & \text{for } x < -a \\ \frac{1}{2}[1 + \sin(\pi x/2a)] & \text{for } |x| < a \\ 1 & \text{for } x > a, \end{cases} \quad (5.5)$$

where  $V_0 < \hbar^2 k^2/2m$ . Numerically reproduce the reflection probabilities plotted Figure 5.20 as follows. Let  $\psi_i \equiv \psi(x_j)$  be the value of the wavefunction at  $x_j = j\Delta$ , where  $\Delta$  is a small increment in the  $x$  coordinate. From the TISE show that

$$\psi_j \simeq (2 - \Delta^2 k^2)\psi_{j+1} - \psi_{j+2}, \quad (5.6)$$

where  $k \equiv \sqrt{2m(E - V)}/\hbar$ . Determine  $\psi_j$  at the two grid points with the largest values of  $x$  from a suitable boundary condition, and use the recurrence relation (5.6) to determine  $\psi_j$  at all other grid points. By matching the values of  $\psi$  at the points with the smallest values of  $x$  to a sum of sinusoidal waves, determine the probabilities required for the figure. Be sure to check the accuracy of your code when  $V_0 = 0$ , and in the general case explicitly check that your results are consistent with equal fluxes of particles towards and away from the origin.

Equation (11.40) gives an analytical approximation for  $\psi$  in the case that there is negligible reflection. Compute this approximate form of  $\psi$  and compare it with your numerical results for larger values of  $a$ .

**Soln:**

We discretise the TISE

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V\psi = E\psi \quad \text{by} \quad -\frac{\hbar^2}{2m} \frac{\psi_{j+1} + \psi_{j-1} - 2\psi_j}{\Delta^2} + V_j \psi_j = E\psi_j$$

which readily yields the required recurrence relation. At the right-hand boundary we require a pure outgoing wave, so  $\psi_j = \exp(ijK\Delta)$  gives  $\psi$  at the two last grid points. From the recurrence relation we obtain  $\psi$  elsewhere. At the left boundary we solve for  $A_+$  and  $A_-$  the equations

$$A_+ \exp(i0k\Delta) + A_- \exp(-i0k\Delta) = \psi_0$$

$$A_+ \exp(i1k\Delta) + A_- \exp(-i1k\Delta) = \psi_1$$

The transmission probability is  $(K/k)/|A_+|^2$ . The code must reproduce the result of Problem 5.4 in the appropriate limit.

**5.15\*** In this problem we obtain an analytic estimate of the energy difference between the even- and odd-parity states of a double square well. Show that for large  $\theta$ ,  $\coth \theta - \tanh \theta \simeq 4e^{-2\theta}$ . Next letting  $\delta k$  be the difference between the  $k$  values that solve

$$\tan[r\pi - k(b-a)] \sqrt{\frac{W^2}{(ka)^2} - 1} = \begin{cases} \coth\left(\sqrt{W^2 - (ka)^2}\right) & \text{even parity} \\ \tanh\left(\sqrt{W^2 - (ka)^2}\right) & \text{odd parity,} \end{cases} \quad (5.7a)$$

where

$$W \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}} \quad (5.7b)$$

for given  $r$  in the odd- and even-parity cases, deduce that

$$\left\{ \left[ \left( \frac{W^2}{(ka)^2} - 1 \right)^{1/2} + \left( \frac{W^2}{(ka)^2} - 1 \right)^{-1/2} \right] (b-a) + \frac{1}{k} \left( 1 - \frac{(ka)^2}{W^2} \right)^{-1} \right\} \delta k \quad (5.8)$$

$$\simeq -4 \exp \left[ -2\sqrt{W^2 - (ka)^2} \right].$$

Hence show that when  $W \gg 1$  the fractional difference between the energies of the ground and first excited states is

$$\frac{\delta E}{E} \simeq \frac{-8a}{W(b-a)} e^{-2W\sqrt{1-E/V_0}}. \quad (5.9)$$

**Soln:** First

$$\coth \theta - \tanh \theta = \frac{e^\theta + e^{-\theta}}{e^\theta - e^{-\theta}} - \frac{e^\theta - e^{-\theta}}{e^\theta + e^{-\theta}} = \frac{1 + e^{-2\theta}}{1 - e^{-2\theta}} - \frac{1 - e^{-2\theta}}{1 + e^{-2\theta}} \simeq (1 + 2e^{-2\theta}) - (1 - 2e^{-2\theta}) = 4e^{-2\theta}$$

So when  $W \gg 1$  the difference in the right side of the equations for  $k$  in the cases of even and odd parity is small and we may estimate the difference in the left side by its derivative w.r.t.  $k$  times the difference  $\delta k$  in the solutions. That is

$$-s^2[r\pi - k(b-a)](b-a)\delta k \sqrt{\frac{W^2}{(ka)^2} - 1} + \tan[r\pi - k(b-a)] \frac{-W^2/(ka)^2 \delta k/k}{\sqrt{\frac{W^2}{(ka)^2} - 1}} \simeq 4e^{-2\sqrt{W^2 - (ka)^2}}$$

In the case of interest the right side of the original equation is close to unity, so we can simplify the last equation by using

$$\tan[r\pi - k(b-a)] \sqrt{\frac{W^2}{(ka)^2} - 1} \simeq 1$$

With the help of the identity  $s^2\theta = 1 + \tan^2\theta$  we obtain the required relation. We now approximate the left side for  $W \gg ka$ . This yields

$$\frac{W}{ka}(b-a)\delta k \simeq -4e^{-2W\sqrt{1-(ka/W)^2}} \quad (\$)$$

Since  $E = \hbar^2 k^2/2m$ ,  $\delta E/E = 2\delta k/k$  and

$$(ka/W)^2 = \frac{2mEa^2}{\hbar^2} \times \frac{\hbar^2}{2mV_0a^2} = E/V_0.$$

The required relation follows when we use these relations in (\$).

**6.10\*** Show that when the density operator takes the form  $\rho = |\psi\rangle\langle\psi|$ , the expression  $\bar{Q} = \text{Tr } Q\rho$  for the expectation value of an observable can be reduced to  $\langle\psi|Q|\psi\rangle$ . Explain the physical significance of this result. For the given form of the density operator, show that the equation of motion of  $\rho$  yields

$$|\phi\rangle\langle\psi| = |\psi\rangle\langle\phi| \quad \text{where} \quad |\phi\rangle \equiv i\hbar \frac{\partial|\psi\rangle}{\partial t} - H|\psi\rangle. \quad (6.1)$$

Show from this equation that  $|\phi\rangle = a|\psi\rangle$ , where  $a$  is real. Hence determine the time evolution of  $|\psi\rangle$  given that at  $t = 0$   $|\psi\rangle = |E\rangle$  is an eigenket of  $H$ . Explain why  $\rho$  does not depend on the phase of  $|\psi\rangle$  and relate this fact to the presence of  $a$  in your solution for  $|\psi, t\rangle$ .

**Soln:**

$$\text{Tr}(Q\rho) = \sum_n \langle n|Q|\psi\rangle\langle\psi|n\rangle$$

We choose a basis that  $|\psi\rangle$  is a member. Then there is only one non-vanishing term in the sum, when  $|n\rangle = |\psi\rangle$ , and the right side reduces to  $\langle\psi|Q|\psi\rangle$  as required. This result shows that density operators recover standard experimental predictions when the system is in a pure state.

Differentiating the given  $\rho$  we have

$$\frac{d\rho}{dt} = \frac{\partial|\psi\rangle}{\partial t}\langle\psi| + |\psi\rangle\frac{\partial\langle\psi|}{\partial t} = \frac{1}{i\hbar}(H|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|H)$$

Gathering the terms proportional to  $\langle\psi|$  on the left and those proportional to  $|\psi\rangle$  on the right we obtain the required expression. Now

$$|\phi\rangle\langle\psi| = |\psi\rangle\langle\phi| \Rightarrow |\phi\rangle\langle\psi|\phi\rangle = |\psi\rangle\langle\phi|\phi\rangle,$$

which establishes that  $|\phi\rangle \propto |\psi\rangle$ . We define  $a$  as the constant of proportionality. Using  $|\phi\rangle = a|\psi\rangle$  in  $|\phi\rangle\langle\psi| = |\psi\rangle\langle\phi|$  we learn that  $a = a^*$  so  $a$  is real.

Returning to the definition of  $|\phi\rangle$  we now have

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = (H - a)|\psi\rangle.$$

This differs from the TDSE in having the term in  $a$ . If  $|\psi\rangle$  is an eigenfunction of  $H$ , we find that its time dependence is  $|\psi, t\rangle = |\psi, 0\rangle e^{-i(E-a)t/\hbar}$  rather than the expected result  $|\psi, t\rangle = |\psi, 0\rangle e^{-iEt/\hbar}$ . We cannot determine  $a$  from the density-matrix formalism because  $\rho$  is invariant under the transformation  $|\psi\rangle \rightarrow e^{-i\chi}|\psi\rangle$ , where  $\chi$  is any real number.

**7.3\*** We have that

$$L_+ \equiv L_x + iL_y = e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right). \quad (7.1)$$

From the Hermitian nature of  $L_z = -i\partial/\partial\phi$  we infer that derivative operators are anti-Hermitian. So using the rule  $(AB)^\dagger = B^\dagger A^\dagger$  on equation (7.1), we infer that

$$L_- \equiv L_+^\dagger = \left(-\frac{\partial}{\partial\theta} + i\frac{\partial}{\partial\phi}\cot\theta\right)e^{-i\phi}.$$

This argument and the result it leads to is wrong. Obtain the correct result by integrating by parts  $\int d\theta \sin\theta \int d\phi (f^* L_+ g)$ , where  $f$  and  $g$  are arbitrary functions of  $\theta$  and  $\phi$ . What is the fallacy in the given argument?

**Soln:**

$$\begin{aligned} \int d\theta \sin\theta \int d\phi (f^* L_+ g) &= \int d\theta \sin\theta \int d\phi f^* e^{i\phi} \left(\frac{\partial g}{\partial\theta} + i\cot\theta\frac{\partial g}{\partial\phi}\right) \\ &= \int d\phi e^{i\phi} \int d\theta \sin\theta f^* \frac{\partial g}{\partial\theta} + i \int d\theta \cos\theta \int d\phi f^* e^{i\phi} \frac{\partial g}{\partial\phi} \\ &= \int d\phi e^{i\phi} \left([\sin\theta f^* g] - \int d\theta g \frac{\partial(\sin\theta f^*)}{\partial\theta}\right) \\ &\quad + i \int d\theta \cos\theta \left([f^* e^{i\phi} g] - \int d\phi g \frac{\partial(f^* e^{i\phi})}{\partial\phi}\right) \end{aligned}$$

The square brackets vanish so long  $f, g$  are periodic in  $\phi$ . Differentiating out the products we get

$$\begin{aligned} \int d\theta \sin\theta \int d\phi (f^* L_+ g) &= - \int d\phi e^{i\phi} \left(\int d\theta \sin\theta g \frac{\partial f^*}{\partial\theta} + \int d\theta \cos\theta g f^*\right) \\ &\quad - i \int d\theta \cos\theta \left(\int d\phi e^{i\phi} g \frac{\partial f^*}{\partial\phi} + i \int d\phi e^{i\phi} g f^*\right) \end{aligned}$$

The two integrals containing  $f^* g$  cancel as required leaving us with

$$\int d\theta \sin\theta \int d\phi (f^* L_+ g) = - \int d\theta \sin\theta \int d\phi g e^{i\phi} \left(\frac{\partial f^*}{\partial\theta} + i\cot\theta\frac{\partial f^*}{\partial\phi}\right) = \int d\theta \sin\theta \int d\phi g (L_- f)^*$$

where

$$L_- = -e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\right).$$

The fallacy is the proposition that  $\partial/\partial\theta$  is anti-Hermitian: the inclusion of the factor  $\sin\theta$  in the integral prevents this being so.

**7.4\*** By writing  $\hbar^2 L^2 = (\mathbf{x} \times \mathbf{p}) \cdot (\mathbf{x} \times \mathbf{p}) = \sum_{ijklm} \epsilon_{ijk} x_j p_k \epsilon_{ilm} x_l p_m$  show that

$$p^2 = \frac{\hbar^2 L^2}{r^2} + \frac{1}{r^2} \{(\mathbf{r} \cdot \mathbf{p})^2 - i\hbar \mathbf{r} \cdot \mathbf{p}\}. \quad (7.2)$$

By showing that  $\mathbf{p} \cdot \hat{\mathbf{r}} - \hat{\mathbf{r}} \cdot \mathbf{p} = -2i\hbar/r$ , obtain  $\mathbf{r} \cdot \mathbf{p} = rp_r + i\hbar$ . Hence obtain

$$p^2 = p_r^2 + \frac{\hbar^2 L^2}{r^2}. \quad (7.3)$$

Give a physical interpretation of one over  $2m$  times this equation.

**Soln:** From the formula for the product of two epsilon symbols we have

$$\begin{aligned} \hbar^2 L^2 &= \sum_{jklm} (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}) x_j p_k x_l p_m \\ &= \sum_{jk} (x_j p_k x_j p_k - x_j p_k x_k p_j). \end{aligned}$$

The first term is

$$\begin{aligned} \sum_{jk} x_j p_k x_j p_k &= \sum_{jk} x_j (x_j p_k + [p_k, x_j]) p_k = \sum_{jk} x_j (x_j p_k - i\hbar \delta_{jk}) p_k \\ &= r^2 p^2 - i\hbar \mathbf{r} \cdot \mathbf{p}. \end{aligned}$$

The second term is

$$\begin{aligned} \sum_{jk} x_j p_k x_k p_j &= \sum_{jk} x_j (x_k p_k - i\hbar) p_j \\ &= \sum_{jk} x_j (p_j x_k p_k + i\hbar \delta_{jk} p_k) - 3i\hbar \sum_j x_j p_j \\ &= (\mathbf{r} \cdot \mathbf{p})(\mathbf{r} \cdot \mathbf{p}) - 2i\hbar (\mathbf{r} \cdot \mathbf{p}). \end{aligned}$$

When these relations are substituted above, the required result follows.

Using the position representation

$$\mathbf{p} \cdot \hat{\mathbf{r}} - \hat{\mathbf{r}} \cdot \mathbf{p} = -i\hbar \nabla \cdot (\mathbf{r}/r) = -\frac{3i\hbar}{r} - i\hbar \mathbf{r} \cdot \nabla(1/r) = -\frac{3i\hbar}{r} - i\hbar r \frac{\partial r^{-1}}{\partial r} = -\frac{3i\hbar}{r} + i\hbar r \frac{1}{r^2}$$

Using this relation and the definition of  $p_r$

$$rp_r = \frac{r}{2} (\hat{\mathbf{r}} \cdot \mathbf{p} + \mathbf{p} \cdot \hat{\mathbf{r}}) = \frac{r}{2} \left( 2\hat{\mathbf{r}} \cdot \mathbf{p} - \frac{2i\hbar}{r} \right) = \mathbf{r} \cdot \mathbf{p} - i\hbar$$

Substituting this into our expression for  $p^2$  we have

$$p^2 = \frac{\hbar^2 L^2}{r^2} + \frac{1}{r^2} ((rp_r + i\hbar)(rp_r + i\hbar) - i\hbar(rp_r + i\hbar))$$

When we multiply out the bracket, we encounter  $rp_r rp_r = r^2 p_r^2 + r[p_r, r]p_r = r^2 p_r^2 - i\hbar rp_r$ . Now when we clean up we find that all terms in the bracket that are proportional to  $\hbar$  cancel and we have desired result.

This equation divided by  $2m$  expresses the kinetic energy as a sum of tangential and radial KE.

**7.18\*** Repeat the analysis of Problem 7.15 for spin-one particles coming on filters aligned successively along  $+z$ ,  $45^\circ$  from  $z$  towards  $x$  [i.e. along  $(1,0,1)$ ], and along  $x$ .

Use classical electromagnetic theory to determine the outcome in the case that the spin-one particles were photons and the filters were polaroid. Why do you get a different answer? Which answer is correct?

**Soln:** We adapt the calculation of Problem 7.15 by replacing the matrix for  $J_x$  by that for  $\mathbf{n} \cdot \mathbf{J} = (J_x + J_z)/\sqrt{2}$ . So if now  $(a, b, c)$  is  $|+\mathbf{n}\rangle$  in the usual basis, we have

$$\begin{pmatrix} 2^{-1/2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & -2^{-1/2} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{cases} a = \frac{b}{2 - \sqrt{2}} \\ c = \frac{b}{2 + \sqrt{2}} \end{cases}$$

The normalisation yields  $b = \frac{1}{2}$ , so  $a = \frac{1}{2}/(2 - \sqrt{2})$  and the required probability is the square of this,  $0.25/(6 - 4\sqrt{2}) \simeq 0.73$ . So the probability of getting through all three filters is  $\frac{1}{3} \times (0.73)^2 \simeq 0.177$ .

In electromagnetism just one of two polarisations gets through the first filter, so we must say that a photon has a probability of half of passing the first filter. Then we resolve its  $\mathcal{E}$  field along the direction of the second filter and find that the amplitude of  $\mathcal{E}$  falls by  $1/\sqrt{2}$  on passing the second filter, so half the energy and therefore photons that pass the first filter pass the second. Of these just a half pass the third filter. Hence in total  $\frac{1}{8} = 0.125$  of the photons get right through.

Although photons are spin-one particles, there are two major difference between the two cases. Most obviously, polaroid selects for linear polarisation rather than circular polarisation, and a photon with well-defined angular momentum is circularly polarised. The other difference is that a photon can be in the state  $|+z\rangle$  or  $|-z\rangle$  but not the state  $|0z\rangle$ , where the  $z$ -axis is parallel to the photon's motion. This fact arises because emag waves are transverse so they do not drive motion in the direction of propagation  $\mathbf{k}$ ; an angular momentum vector perpendicular to  $\mathbf{k}$  would require motion along  $\mathbf{k}$ . Our theory does not allow for this case because it is non-relativistic, whereas a photon, having zero rest mass, is an inherently relativistic object; we cannot transform to a frame in which a photon is at rest so all three directions would be equivalent.

**7.19\*** Show that  $l$  excitations can be divided amongst the  $x, y$  or  $z$  oscillators of a three-dimensional harmonic oscillator in  $(\frac{1}{2}l + 1)(l + 1)$  ways. Verify in the case  $l = 4$  that this agrees with the number of states of well defined angular momentum and the given energy.

**Soln:** If we assign  $n_x$  of the  $l$  excitations to the  $x$  oscillator, we can assign  $0, 1, \dots, l - n_x$  excitations to the  $y$  oscillator [ $(l - n_x + 1)$  possibilities], and the remaining excitations go to  $z$ . So the number of ways is

$$S \equiv \sum_{n_x=0}^l (l - n_x + 1) = \sum_{n_x=0}^l (l + 1) - \sum_{n_x=1}^l n_x = (l + 1)^2 - \frac{1}{2}l(l + 1) = (l + 1)(\frac{1}{2}l + 1)$$

In the case of 4 excitations, the possible values of  $l$  are 4, 2 and 0, so the number of states is  $(2 * 4 + 1) + (2 * 2 + 1) + 1 = 15$ , which is indeed equal to  $(4 + 1) * (2 + 1)$ .

**7.20\*** Let

$$A_l \equiv \frac{1}{\sqrt{2m\hbar\omega}} \left( ip_r - \frac{(l + 1)\hbar}{r} + m\omega r \right). \quad (7.4)$$

be the ladder operator of the three-dimensional harmonic oscillator and  $|E, l\rangle$  be the oscillator's stationary state of energy  $E$  and angular-momentum quantum number  $l$ . Show that if we write  $A_l|E, l\rangle = \alpha_-|E - \hbar\omega, l + 1\rangle$ , then  $\alpha_- = \sqrt{\mathcal{L} - l}$ , where  $\mathcal{L}$  is the angular-momentum quantum number of a circular orbit of energy  $E$ . Show similarly that if  $A_{l-1}^\dagger|E, l\rangle = \alpha_+|E + \hbar\omega, l - 1\rangle$ , then  $\alpha_+ = \sqrt{\mathcal{L} - l + 2}$ .

**Soln:** Taking the mod-square of each side of  $A_l|E, l\rangle = \alpha_-|E - \hbar\omega, l + 1\rangle$  we find

$$|\alpha_-|^2 = \langle E, l | A_l^\dagger A_l | E, l \rangle = \langle E, l | \left( \frac{H_l}{\hbar\omega} - (l + \frac{3}{2}) \right) | E, l \rangle = \frac{E}{\hbar\omega} - (l + \frac{3}{2}).$$

In the case  $l = \mathcal{L}$ ,  $|\alpha_-|^2 = 0$ , so  $\mathcal{L} = (E/\hbar\omega) - \frac{3}{2}$  and therefore  $|\alpha_-|^2 = \mathcal{L} - l$  as required. We can choose the phase of  $\alpha_-$  at our convenience.

Similarly

$$\begin{aligned} \alpha_+^2 &= \langle E, l | A_{l-1}^\dagger A_{l-1} | E, l \rangle = \langle E, l | (A_{l-1}^\dagger A_{l-1} + [A_{l-1}, A_{l-1}^\dagger]) | E, l \rangle \\ &= \langle E, l | \left( \frac{H_{l-1}}{\hbar\omega} - (l + \frac{1}{2}) + \frac{H_l - H_{l-1}}{\hbar\omega} + 1 \right) | E, l \rangle = \frac{E}{\hbar\omega} - l + \frac{1}{2} = \mathcal{L} - l + 2 \end{aligned}$$

**7.21\*** Show that the probability distribution in radius of a particle that orbits in the three-dimensional harmonic-oscillator potential on a circular orbit with angular-momentum quantum number  $l$  peaks at  $r/a = \sqrt{l+1}$ , where

$$a \equiv \sqrt{\frac{\hbar}{m\omega}}. \quad (7.5)$$

Derive the corresponding classical result.

**Soln:** The radial wavefunctions of circular orbits are annihilated by  $A_l$ , so  $A_l|E, l\rangle = 0$ . In the position representation this is

$$\left(\frac{\partial}{\partial r} + \frac{1}{r} - \frac{l+1}{r} + \frac{r}{a^2}\right)u(r) = 0$$

Using the integrating factor,

$$\exp\left\{\int dr\left(-\frac{l}{r} + \frac{r}{a^2}\right)\right\} = r^{-l} \exp(r^2/2a^2), \quad (7.6)$$

to solve the equation, we have  $u \propto r^l e^{-r^2/2a^2}$ . The radial distribution is  $P(r) \propto r^2|u|^2 = r^{2(l+1)}e^{-r^2/a^2}$ . Differentiating to find the maximum, we have

$$2(l+1)r^{2l+1} - r^{2(l+1)}2r/a^2 = 0 \Rightarrow r = (l+1)^{1/2}a$$

For the classical result we have

$$mrv = l\hbar \quad \text{and} \quad \frac{mv^2}{r} = m\omega^2 r \Rightarrow r = v/\omega = \frac{l\hbar}{mr\omega}$$

so  $r = (l\hbar/m\omega)^{1/2} = l^{1/2}a$  in agreement with the QM result when  $l \gg 1$ .

**7.22\*** A particle moves in the three-dimensional harmonic oscillator potential with the second largest angular-momentum quantum number possible at its energy. Show that the radial wavefunction is

$$u_1 \propto x^l \left(x - \frac{l+\frac{1}{2}}{x}\right) e^{-x^2/2} \quad \text{where } x \equiv r/a \quad \text{with } a \equiv \sqrt{\frac{\hbar}{m\omega}}. \quad (7.7)$$

How many radial nodes does this wavefunction have?

**Soln:** From Problem 7.21 we have that the wavefunction of the circular orbit with angular momentum  $l$  is  $\langle r|E, l\rangle \propto r^l e^{-r^2/2a^2}$ . So the required wavefunction is

$$\begin{aligned} \langle r|E + \hbar\omega, l-1\rangle &\propto \langle r|A_{l-1}^\dagger|E, l\rangle \\ &\propto \left(-\frac{\partial}{\partial r} - \frac{l+1}{r} + \frac{r}{a^2}\right) r^l e^{-r^2/2a^2} = \left(-lr^{l-1} + \frac{r^{l+1}}{a^2} - (l+1)r^{l-1} + \frac{r^{l+1}}{a^2}\right) e^{-r^2/2a^2} \\ &= r^l e^{-r^2/2a^2} \left(\frac{2r}{a^2} - \frac{2l+1}{r}\right) \propto x^l e^{-x^2/2} \left(x - \frac{l+\frac{1}{2}}{x}\right) \end{aligned}$$

This wavefunction clearly has one node at  $x = \sqrt{l + \frac{1}{2}}$ .

**7.23\*** The interaction between neighbouring spin-half atoms in a crystal is described by the Hamiltonian

$$H = K \left( \frac{\mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)}}{a} - 3 \frac{(\mathbf{S}^{(1)} \cdot \mathbf{a})(\mathbf{S}^{(2)} \cdot \mathbf{a})}{a^3} \right), \quad (7.8)$$

where  $K$  is a constant,  $\mathbf{a}$  is the separation of the atoms and  $\mathbf{S}^{(1)}$  is the first atom's spin operator. Explain what physical idea underlies this form of  $H$ . Show that  $S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} = \frac{1}{2}(S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)})$ . Show that the mutual eigenkets of the total spin operators  $S^2$  and  $S_z$  are also eigenstates of  $H$  and find the corresponding eigenvalues.

At time  $t = 0$  particle 1 has its spin parallel to  $\mathbf{a}$ , while the other particle's spin is antiparallel to  $\mathbf{a}$ . Find the time required for both spins to reverse their orientations.

**Soln:** This Hamiltonian recalls the mutual potential energy  $V$  of two classical magnetic dipoles  $\boldsymbol{\mu}^{(i)}$  that are separated by the vector  $\mathbf{a}$ , which we can calculate by evaluating the magnetic field  $\mathbf{B}$  that the first dipole creates at the location of the second and then recognising that  $V = -\boldsymbol{\mu} \cdot \mathbf{B}$ .

$$S_+^{(1)}S_-^{(2)} = (S_x^{(1)} + iS_y^{(1)})(S_x^{(2)} - iS_y^{(2)}) = S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} + i(S_y^{(1)}S_x^{(2)} - S_x^{(1)}S_y^{(2)})$$

Similarly,

$$S_-^{(1)}S_+^{(2)} = S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} - i(S_y^{(1)}S_x^{(2)} - S_x^{(1)}S_y^{(2)})$$

Adding these expressions we obtain the desired relation.

We choose to orient the  $z$ -axis along  $\mathbf{a}$ . Then  $H$  becomes

$$H = \frac{K}{a} \left( \frac{1}{2}(S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)}) + S_z^{(1)}S_z^{(2)} - 3S_z^{(1)}S_z^{(2)} \right). \quad (7.9)$$

The eigenkets of  $S^2$  and  $S_z$  are the three spin-one kets  $|1, 1\rangle$ ,  $|1, 0\rangle$  and  $|1, -1\rangle$  and the single spin-zero ket  $|0, 0\rangle$ . We multiply each of these kets in turn by  $H$ :

$$\begin{aligned} H|1, 1\rangle &= H|+\rangle|+\rangle = \frac{K}{a} \left( \frac{1}{2}(S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)}) - 2S_z^{(1)}S_z^{(2)} \right) |+\rangle|+\rangle \\ &= -\frac{K}{2a}|1, 1\rangle \end{aligned}$$

which uses the fact that  $S_+^{(i)}|+\rangle = 0$ . Similarly  $H|1, -1\rangle = H|-\rangle|-\rangle = -(K/2a)|1, -1\rangle$ .

$$\begin{aligned} H|1, 0\rangle &= H \frac{1}{\sqrt{2}}(|+\rangle|-\rangle + |-\rangle|+\rangle) = \frac{K}{\sqrt{2}a} \left( \frac{1}{2}(S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)}) - 2S_z^{(1)}S_z^{(2)} \right) (|+\rangle|-\rangle + |-\rangle|+\rangle) \\ &= \frac{K}{\sqrt{2}a} \left( \frac{1}{2} + 1 \right) (|+\rangle|-\rangle + |-\rangle|+\rangle) = \frac{K}{a}|1, 0\rangle \end{aligned}$$

where we have used  $S_+|-\rangle = |+\rangle$ , etc. Finally

$$\begin{aligned} H|0, 0\rangle &= H \frac{1}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle) = \frac{K}{\sqrt{2}a} \left( \frac{1}{2}(S_+^{(1)}S_-^{(2)} + S_-^{(1)}S_+^{(2)}) - 2S_z^{(1)}S_z^{(2)} \right) (|+\rangle|-\rangle - |-\rangle|+\rangle) \\ &= \frac{K}{\sqrt{2}a} \left( -\frac{1}{2} + \frac{1}{2} \right) (|+\rangle|-\rangle - |-\rangle|+\rangle) = 0 \end{aligned}$$

The given initial condition

$$|\psi\rangle = |+\rangle|-\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle + |0, 0\rangle),$$

which is a superposition of two stationary states of energies that differ by  $K/a$ . By analogy with the symmetrical-well problem, we argue that after time  $\pi\hbar/\Delta E = \pi\hbar a/K$  the particle spins will have reversed.

**7.24\*** Show that  $[J_i, L_j] = i\sum_k \epsilon_{ijk}L_k$  and  $[J_i, L^2] = 0$  by eliminating  $L_i$  using its definition  $\mathbf{L} = \hbar^{-1}\mathbf{x} \times \mathbf{p}$ , and then using the commutators of  $J_i$  with  $\mathbf{x}$  and  $\mathbf{p}$ .

**Soln:**

$$\begin{aligned} \hbar[J_i, L_j] &= \epsilon_{jkl}[J_i, x_k p_l] = \epsilon_{jkl}([J_i, x_k]p_l + x_k[J_i, p_l]) \\ &= \epsilon_{jkl}(i\epsilon_{ikm}x_m p_l + i\epsilon_{iln}x_k p_n) = i(\epsilon_{klj}\epsilon_{kmi}x_m p_l + \epsilon_{ljk}\epsilon_{lni}x_k p_n) \\ &= i(\delta_{lm}\delta_{ji} - \delta_{li}\delta_{jm})x_m p_l + i(\delta_{jn}\delta_{ki} - \delta_{ji}\delta_{kn})x_k p_n \\ &= i(\mathbf{x} \cdot \mathbf{p}\delta_{ij} - x_j p_i + x_i p_j - \mathbf{x} \cdot \mathbf{p}\delta_{ij}) = i(x_i p_j - x_j p_i) \end{aligned}$$

But

$$i\hbar\epsilon_{ijk}L_k = i\epsilon_{ijk}\epsilon_{klm}x_l p_m = i\epsilon_{kij}\epsilon_{klm}x_l p_m = i(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})x_l p_m = i(x_i p_j - x_j p_i)$$

**7.25\*** In this problem you show that many matrix elements of the position operator  $\mathbf{x}$  vanish when states of well defined  $l, m$  are used as basis states. These results will lead to selection rules for electric dipole radiation. First show that  $[L^2, x_i] = i \sum_{jk} \epsilon_{jik} (L_j x_k + x_k L_j)$ . Then show that  $\mathbf{L} \cdot \mathbf{x} = 0$  and using this result derive

$$[L^2, [L^2, x_i]] = i \sum_{jk} \epsilon_{jik} (L_j [L^2, x_k] + [L^2, x_k] L_j) = 2(L^2 x_i + x_i L^2). \quad (7.10)$$

By squeezing this equation between angular-momentum eigenstates  $\langle l, m |$  and  $| l', m' \rangle$  show that

$$0 = \{(\beta - \beta')^2 - 2(\beta + \beta')\} \langle l, m | x_i | l', m' \rangle,$$

where  $\beta \equiv l(l+1)$  and  $\beta' \equiv l'(l'+1)$ . By equating the factor in front of  $\langle l, m | x_i | l', m' \rangle$  to zero, and treating the resulting equation as a quadratic equation for  $\beta$  given  $\beta'$ , show that  $\langle l, m | x_i | l', m' \rangle$  must vanish unless  $l + l' = 0$  or  $l = l' \pm 1$ . Explain why the matrix element must also vanish when  $l = l' = 0$ .

**Soln:**

$$\begin{aligned} \sum_j [L_j^2, x_i] &= \sum_j (L_j [L_j, x_i] + [L_j, x_i] L_j) = i \sum_{jk} \epsilon_{jik} (L_j x_k + x_k L_j) \\ \hbar \mathbf{L} \cdot \mathbf{x} &= \sum_{ijk} \epsilon_{ijk} x_j p_k x_i = \sum_{ijk} \epsilon_{ijk} (x_j x_i p_k + x_j [p_k, x_i]) = \sum_{ijk} \epsilon_{ijk} (x_j x_i p_k - i \hbar x_j \delta_{ki}) \end{aligned}$$

Both terms on the right side of this expression involve  $\sum_{ik} \epsilon_{ijk} S_{ik}$  where  $S_{ik} = S_{ki}$  so they vanish by Problem 7.1. Hence  $\mathbf{x} \cdot \mathbf{L} = 0$  as in classical physics.

Now

$$\begin{aligned} [L^2, [L^2, x_i]] &= i \sum_{jk} \epsilon_{jik} [L^2, (L_j x_k + x_k L_j)] = i \sum_{jk} \epsilon_{jik} (L_j [L^2, x_k] + [L^2, x_k] L_j) \\ &= - \sum_{jklm} \epsilon_{jik} \epsilon_{lkm} (L_j \{L_l x_m + x_m L_l\} + \{L_l x_m + x_m L_l\} L_j) \\ &= - \sum_{jlm} (\delta_{jm} \delta_{il} - \delta_{jl} \delta_{im}) (L_j \{L_l x_m + x_m L_l\} + \{L_l x_m + x_m L_l\} L_j) \\ &= - \sum_j (L_j \{L_i x_j + x_j L_i\} + \{L_i x_j + x_j L_i\} L_j - L_j \{L_j x_i + x_i L_j\} - \{L_j x_i + x_i L_j\} L_j) \\ &= - \left\{ \sum_j (L_j L_i x_j + x_j L_i L_j) - L^2 x_i - \sum_j (L_j x_i L_j + L_j x_i L_j) - x_i L^2 \right\} \end{aligned}$$

where to obtain the last line we have identified occurrences of  $\mathbf{L} \cdot \mathbf{x}$  and  $\mathbf{x} \cdot \mathbf{L}$ . Now

$$\sum_j L_j L_i x_j = \sum_j (L_j x_j L_i + L_j [L_i, x_j]) = i \sum_{jk} \epsilon_{ijk} L_j x_k$$

Similarly,  $\sum_j x_j L_i L_j = i \sum_{jk} \epsilon_{jik} x_k L_j$ . Moreover

$$\begin{aligned} \sum_j L_j x_i L_j &= \sum_j ([L_j, x_i] L_j + x_i L_j L_j) = i \sum_{jk} \epsilon_{jik} x_k L_j + x_i L^2 \\ &= \sum_j (L_j [x_i, L_j] + L_j L_j x_i) = i \sum_{jk} \epsilon_{ijk} L_j x_k + L^2 x_i \end{aligned}$$

Assembling these results we find

$$\begin{aligned} [L^2, [L^2, x_i]] &= - \left\{ i \sum_{jk} \epsilon_{ijk} [L_j, x_k] - L^2 x_i - i \sum_{jk} \epsilon_{jik} [x_k, L_j] - x_i L^2 - L^2 x_i - x_i L^2 \right\} \\ &= 2(L^2 x_i + x_i L^2) \end{aligned}$$

as required. The relevant matrix element is

$$\langle lm|[L^2, [L^2, x_i]]|l'm'\rangle = \langle lm|(L^2L^2x_i - 2L^2x_iL^2 + x_iL^2L^2)|l'm'\rangle = 2\langle lm|(L^2x_i + x_iL^2)|l'm'\rangle$$

which implies

$$\beta^2 \langle lm|x_i|l'm'\rangle - 2\beta \langle lm|x_i|l'm'\rangle \beta' + \langle lm|x_i|l'm'\rangle \beta'^2 = 2\beta \langle lm|x_i|l'm'\rangle + 2\langle lm|x_i|l'm'\rangle \beta'$$

Taking out the common factor we obtain the required result.

The quadratic for  $\beta(\beta')$  is

$$\beta^2 - 2(\beta' + 1)\beta + \beta'(\beta' - 2) = 0$$

so

$$\begin{aligned} \beta &= \beta' + 1 \pm \sqrt{(\beta' + 1)^2 - \beta'(\beta' - 2)} = \beta' + 1 \pm \sqrt{4\beta' + 1} \\ &= l'(l' + 1) + 1 \pm \sqrt{4l'^2 + 4l' + 1} = l'(l' + 1) + 1 \pm (2l' + 1) \\ &= l'^2 + 3l' + 2 \quad \text{or} \quad l'^2 - l' \end{aligned}$$

We now have two quadratic equations to solve

$$\begin{aligned} l^2 + l - (l'^2 + 3l' + 2) &= 0 \quad \Rightarrow \quad l = \frac{1}{2}[-1 \pm (2l' + 3)] \\ l^2 + l - (l'^2 - l') &= 0 \quad \Rightarrow \quad l = \frac{1}{2}[-1 \pm (2l' - 1)] \end{aligned}$$

Since  $l, l' \geq 0$ , the only acceptable solutions are  $l + l' = 0$  and  $l = l' \pm 1$  as required. However, when  $l = l' = 0$  the two states have the same (even) parity so the matrix element vanishes by the proof given in eq (4.41) of the book.

**8.9\*** A spherical potential well is defined by

$$V(r) = \begin{cases} 0 & \text{for } r < a \\ V_0 & \text{otherwise,} \end{cases} \quad (8.1)$$

where  $V_0 > 0$ . Consider a stationary state with angular-momentum quantum number  $l$ . By writing the wavefunction  $\psi(\mathbf{x}) = R(r)Y_l^m(\theta, \phi)$  and using  $p^2 = p_r^2 + \hbar^2 L^2/r^2$ , show that the state's radial wavefunction  $R(r)$  must satisfy

$$-\frac{\hbar^2}{2m} \left( \frac{d}{dr} + \frac{1}{r} \right)^2 R + \frac{l(l+1)\hbar^2}{2mr^2} R + V(r)R = ER. \quad (8.2)$$

Show that in terms of  $S(r) \equiv rR(r)$ , this can be reduced to

$$\frac{d^2 S}{dr^2} - l(l+1) \frac{S}{r^2} + \frac{2m}{\hbar^2} (E - V)S = 0. \quad (8.3)$$

Assume that  $V_0 > E > 0$ . For the case  $l = 0$  write down solutions to this equation valid at (a)  $r < a$  and (b)  $r > a$ . Ensure that  $R$  does not diverge at the origin. What conditions must  $S$  satisfy at  $r = a$ ? Show that these conditions can be simultaneously satisfied if and only if a solution can be found to  $k \cot ka = -K$ , where  $\hbar^2 k^2 = 2mE$  and  $\hbar^2 K^2 = 2m(V_0 - E)$ . Show graphically that the equation can only be solved when  $\sqrt{2mV_0}a/\hbar > \pi/2$ . Compare this result with that obtained for the corresponding one-dimensional potential well.

The deuteron is a bound state of a proton and a neutron with zero angular momentum. Assume that the strong force that binds them produces a sharp potential step of height  $V_0$  at interparticle distance  $a = 2 \times 10^{-15}$  m. Determine in MeV the minimum value of  $V_0$  for the deuteron to exist. *Hint: remember to consider the dynamics of the reduced particle.*

**Soln:** In the position representation  $p_r = -i\hbar(\partial/\partial r + r^{-1})$ , so in this representation and for an eigenfunction of  $L^2$  we get the required form of  $E|E\rangle = H|E\rangle = (p^2/2m + V)|E\rangle$ . Writing  $R = S/r$  we have

$$\left( \frac{d}{dr} + \frac{1}{r} \right) R = \left( \frac{d}{dr} + \frac{1}{r} \right) \frac{S}{r} = \frac{1}{r} \frac{dS}{dr} \quad \Rightarrow \quad \left( \frac{d}{dr} + \frac{1}{r} \right)^2 R = \left( \frac{d}{dr} + \frac{1}{r} \right) \frac{1}{r} \frac{dS}{dr} = \frac{1}{r} \frac{d^2 S}{dr^2}$$

Inserting this into our TISE and multiplying through by  $r$ , we obtain the required expression.

When  $l = 0$  the equation reduces to either exponential decay or shm, so with the given condition on  $E$  we have

$$S \propto \begin{cases} \cos kr & \text{or } \sin kr & \text{at } r < a \\ Ae^{-Kr} & & \text{at } r > a \end{cases}$$

where  $k^2 = 2mE/\hbar^2$  and  $K^2 = 2m(V_0 - E)/\hbar^2$ . At  $r < a$  we must chose  $S \propto \sin kr$  because we require  $R = S/r$  to be finite at the origin. We require  $S$  and its first derivative to be continuous at  $r = a$ , so

$$\begin{aligned} \sin(ka) &= Ae^{-Ka} \\ k \cos(ka) &= -KAe^{-Ka} \end{aligned} \Rightarrow \cot(ka) = -\frac{K}{k} = -\sqrt{W^2/(ka)^2 - 1}$$

with  $W \equiv \sqrt{2mV_0a^2/\hbar^2}$ . In a plot of each side against  $ka$ , the right side starts at  $-\infty$  when  $ka = 0$  and rises towards the  $x$  axis, where it terminates when  $ka = W$ . The left side starts at  $\infty$  and becomes negative when  $ka = \pi/2$ . There is a solution iff the right side has not already terminated, i.e. iff  $W > \pi/2$ .

We obtain the minimum value of  $V_0$  for  $W = (a/\hbar)\sqrt{2mV_0} = \pi/2$ , so

$$V_0 = \frac{\pi^2 \hbar^2}{8ma^2} = \frac{(\pi \hbar/a)^2}{4m_p} = 25.6 \text{ MeV}$$

where  $m \simeq \frac{1}{2}m_p$  is the reduced mass of the proton.

**8.10\*** Given that the ladder operators for hydrogen satisfy

$$A_l^\dagger A_l = \frac{a_0^2 \mu}{\hbar^2} H_l + \frac{Z^2}{2(l+1)^2} \quad \text{and} \quad [A_l, A_l^\dagger] = \frac{a_0^2 \mu}{\hbar^2} (H_{l+1} - H_l), \quad (8.4)$$

where  $H_l$  is the Hamiltonian for angular-momentum quantum number  $l$ , show that

$$A_{l-1} A_{l-1}^\dagger = \frac{a_0^2 \mu}{\hbar^2} H_l + \frac{Z^2}{2l^2}. \quad (8.5)$$

Hence show that

$$A_{l-1}^\dagger |E, l\rangle = \frac{Z}{\sqrt{2}} \left( \frac{1}{l^2} - \frac{1}{n^2} \right)^{1/2} |E, l-1\rangle, \quad (8.6)$$

where  $n$  is the principal quantum number. Explain the physical meaning of this equation and its use in setting up the theory of the hydrogen atom.

**Soln:** Replacing  $l$  with  $l-1$  in the given formulae, we have

$$A_{l-1}^\dagger A_{l-1} = \frac{a_0^2 \mu}{\hbar^2} H_{l-1} + \frac{Z^2}{2l^2} \quad \text{and} \quad [A_{l-1}, A_{l-1}^\dagger] = \frac{a_0^2 \mu}{\hbar^2} (H_l - H_{l-1})$$

So now we can write

$$\begin{aligned} A_{l-1} A_{l-1}^\dagger &= A_{l-1}^\dagger A_{l-1} + [A_{l-1}, A_{l-1}^\dagger] = \frac{a_0^2 \mu}{\hbar^2} H_{l-1} + \frac{Z^2}{2l^2} + \frac{a_0^2 \mu}{\hbar^2} (H_l - H_{l-1}) \\ &= \frac{a_0^2 \mu}{\hbar^2} H_l + \frac{Z^2}{2l^2} \end{aligned} \quad (\dagger)$$

as required.

We multiply  $H_l |E, l\rangle = E |E, l\rangle$  by  $A_{l-1}^\dagger$ :

$$EA_{l-1}^\dagger |E, l\rangle = A_{l-1}^\dagger H_l |E, l\rangle = (H_l A_{l-1}^\dagger + [A_{l-1}^\dagger, H_l]) |E, l\rangle$$

We use  $(\dagger)$  to replace the  $H_l$  in the commutator by a multiple of  $A_{l-1} A_{l-1}^\dagger$  and obtain

$$\begin{aligned} EA_{l-1}^\dagger |E, l\rangle &= (H_l A_{l-1}^\dagger + \frac{\hbar^2}{a_0^2 \mu} [A_{l-1}^\dagger, A_{l-1} A_{l-1}^\dagger]) |E, l\rangle \\ &= (H_l A_{l-1}^\dagger + \frac{\hbar^2}{a_0^2 \mu} [A_{l-1}^\dagger, A_{l-1}] A_{l-1}^\dagger) |E, l\rangle \\ &= (H_l - H_l + H_{l-1}) A_{l-1}^\dagger |E, l\rangle \end{aligned}$$

Rearranging

$$H_{l-1}A_{l-1}^\dagger|E, l\rangle = EA_{l-1}^\dagger|E, l\rangle$$

which establishes that  $A_{l-1}^\dagger|E, l\rangle = C|E, l-1\rangle$  is an eigenket of the Hamiltonian for angular momentum number  $l-1$  and the same energy, as required. To get the proportionality constant  $C$  we take the mod-square of both sides

$$C^2 = \langle E, l|A_{l-1}A_{l-1}^\dagger|E, l\rangle = \langle E, l|\left(\frac{a_0^2\mu}{\hbar^2}H_l + \frac{Z^2}{2l^2}\right)|E, l\rangle = \frac{a_0^2\mu}{\hbar^2}E_l + \frac{Z^2}{2l^2} = -\frac{Z^2}{2n^2} + \frac{Z^2}{2l^2}$$

as required. The equation shows that  $A_{l-1}^\dagger$  creates a state of the same energy but with less angular momentum and more radial motion (a more eccentric orbit).

We obtain the wavefunctions of hydrogen's stationary states by first solving the first-order ode  $A_l|E, l\rangle = 0$ , where  $l$  is the maximum angular momentum at energy  $E$ . This is the wavefunction of the circular orbit. Then we obtain the wavefunctions of non-circular orbits by repeatedly applying  $A_{l-1}^\dagger$  to this wavefunction, which simply involves differentiation.

**8.12\*** From equation (8.44) show that  $l' + \frac{1}{2} = \sqrt{(l + \frac{1}{2})^2 - \beta}$  and that the increment  $\Delta$  in  $l'$  when  $l$  is increased by one satisfies  $\Delta^2 + \Delta(2l' + 1) = 2(l + 1)$ . By considering the amount by which the solution of this equation changes when  $l'$  changes from  $l$  as a result of  $\beta$  increasing from zero to a small number, show that

$$\Delta = 1 + \frac{2\beta}{4l^2 - 1} + O(\beta^2). \quad (8.7)$$

Explain the physical significance of this result.

**Soln:** The given eqn is a quadratic in  $l'$ :

$$l'^2 + l' - l(l+1) + \beta = 0 \quad \Rightarrow \quad l' = \frac{-1 \pm \sqrt{1 + 4l(l+1) - 4\beta}}{2} \quad \Rightarrow \quad l' + \frac{1}{2} = \sqrt{(l + \frac{1}{2})^2 - \beta}, \quad (8.8)$$

where we've chosen the root that makes  $l' > 0$ .

Squaring up this equation, we have

$$(l' + \frac{1}{2})^2 = (l + \frac{1}{2})^2 - \beta \quad \Rightarrow \quad (l' + \Delta + \frac{1}{2})^2 = (l + \frac{3}{2})^2 - \beta$$

Taking the first eqn from the second yields

$$\Delta^2 + 2(l' + \frac{1}{2})\Delta = (l + \frac{3}{2})^2 - (l + \frac{1}{2})^2 = 2(l + 1)$$

This is a quadratic equation for  $\Delta$ , which is solved by  $\Delta = 1$  when  $l' = l$ . We are interested in the small change  $\delta\Delta$  in this solution when  $l'$  changes by a small amount  $\delta l'$ . Differentiating the equation, we have

$$2\Delta\delta\Delta + 2\Delta\delta l' + (2l' + 1)\delta\Delta = 0 \quad \Rightarrow \quad \delta\Delta = -\frac{2\Delta\delta l'}{2\Delta + 2l' + 1}$$

Into this we put  $\Delta = 1$ ,  $l' = l$ , and by binomial expansion of (8.8)

$$\delta l' = -\frac{\beta}{2l + 1}$$

and have finally

$$\delta\Delta = \frac{-2\beta}{(2l + 1)(2l + 3)}$$

Eq (8.49) gives the energy of a circular orbit as

$$E = -\frac{Z_0^2 e^2}{8\pi\epsilon_0 a_0 (l'(l) + k + 1)^2},$$

with  $k$  the number of nodes in the radial wavefunction. This differs from Rydberg's formula in that  $(l'(l) + k + 1)$  is not an integer  $n$ . Crucially  $l'(l) + k$  does not stay the same if  $k$  is decreased by unity

and  $l$  increased by unity – in fact these changes (which correspond to shifting to a more circular orbit) cause  $l'(l) + k$  to increase slightly and therefore  $E$  to decrease slightly: on a more circular orbit, the electron is more effectively screened from the nucleus. So in the presence of screening the degeneracy in H under which at the same  $E$  there are states of different angular momentum is lifted by screening.

**9.7\*** The Hamiltonian of a two-state system can be written

$$H = \begin{pmatrix} A_1 + B_1\epsilon & B_2\epsilon \\ B_2\epsilon & A_2 \end{pmatrix}, \quad (9.1)$$

where all quantities are real and  $\epsilon$  is a small parameter. To first order in  $\epsilon$ , what are the allowed energies in the cases (a)  $A_1 \neq A_2$ , and (b)  $A_1 = A_2$ ?

Obtain the exact eigenvalues and recover the results of perturbation theory by expanding in powers of  $\epsilon$ .

**Soln:** When  $A_1 \neq A_2$ , the eigenvectors of  $H_0$  are  $(1, 0)$  and  $(0, 1)$  so to first-order in  $\epsilon$  the perturbed energies are the diagonal elements of  $H$ , namely  $A_1 + B_1\epsilon$  and  $A_2$ .

When  $A_1 = A_2$  the unperturbed Hamiltonian is degenerate and degenerate perturbation theory applies: we diagonalise the perturbation

$$H_1 = \begin{pmatrix} B_1\epsilon & B_2\epsilon \\ B_2\epsilon & 0 \end{pmatrix} = \epsilon \begin{pmatrix} B_1 & B_2 \\ B_2 & 0 \end{pmatrix}$$

The eigenvalues  $\lambda$  of the last matrix satisfy

$$\lambda^2 - B_1\lambda - B_2^2 = 0 \quad \Rightarrow \quad \lambda = \frac{1}{2} \left( B_1 \pm \sqrt{B_1^2 + 4B_2^2} \right)$$

and the perturbed energies are

$$A_1 + \lambda\epsilon = A_1 + \frac{1}{2}B_1\epsilon \pm \frac{1}{2}\sqrt{B_1^2 + 4B_2^2}\epsilon$$

Solving for the exact eigenvalues of the given matrix we find

$$\begin{aligned} \lambda &= \frac{1}{2}(A_1 + A_2 + B_1\epsilon) \pm \frac{1}{2}\sqrt{(A_1 + A_2 + B_1\epsilon)^2 - 4A_2(A_1 + B_1\epsilon) + 4B_2\epsilon^2} \\ &= \frac{1}{2}(A_1 + A_2 + B_1\epsilon) \pm \frac{1}{2}\sqrt{(A_1 - A_2)^2 + 2(A_1 - A_2)B_1\epsilon + (B_1^2 + 4B_2^2)\epsilon^2} \end{aligned}$$

If  $A_1 = A_2$  this simplifies to

$$\lambda = A_1 + \frac{1}{2}B_1\epsilon + \pm \frac{1}{2}\sqrt{B_1^2 + 4B_2^2}\epsilon$$

in agreement with perturbation theory. If  $A_1 \neq A_2$  we expand the radical to first order in  $\epsilon$

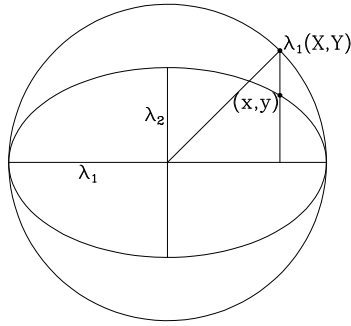
$$\begin{aligned} \lambda &= \frac{1}{2}(A_1 + A_2 + B_1\epsilon) \pm \frac{1}{2}(A_1 - A_2) \left( 1 + \frac{B_1}{A_1 - A_2}\epsilon + O(\epsilon^2) \right) \\ &= \begin{cases} A_1 + B_1\epsilon & \text{if } + \\ A_2 & \text{if } - \end{cases} \end{aligned}$$

again in agreement with perturbation theory

**9.8\*** For the  $P$  states of hydrogen, obtain the shift in energy caused by a weak magnetic field (a) by evaluating the Landé  $g$  factor, and (b) by use equation (9.28) and the Clebsch–Gordan coefficients calculated in §7.5.2.

**Soln:** (a) From  $l = 1$  and  $s = \frac{1}{2}$  we can construct  $j = \frac{3}{2}$  and  $\frac{1}{2}$  so we have to evaluate two values of  $g_L$ . When  $j = \frac{3}{2}$ ,  $j(j+1) = 15/4$ , and when  $j = \frac{1}{2}$ ,  $j(j+1) = 3/4$ , so

$$g_L = \frac{3}{2} - \frac{1}{2} \frac{l(l+1) - s(s+1)}{j(j+1)} = \begin{cases} \frac{4}{3} & \text{for } j = \frac{3}{2} \\ \frac{1}{2} & \text{for } j = \frac{1}{2} \end{cases}$$



**Figure 9.3** The input and output vectors of a  $2 \times 2$  Hermitian matrix are related by a circle with the matrix's largest eigenvalue as radius and the ellipse that has the eigenvalues as semi-axes.

So

$$E_B/(\mu_B B) = mg_L = \begin{cases} 2 & \text{for } j = \frac{3}{2}, m = \frac{3}{2} \\ \frac{2}{3} & \text{for } j = \frac{3}{2}, m = \frac{1}{2} \\ \frac{1}{3} & \text{for } j = \frac{1}{2}, m = \frac{1}{2} \end{cases}$$

with the values for negative  $m$  being minus the values for positive  $m$ .

(b) We have  $|\frac{3}{2}, \frac{3}{2}\rangle = |+\rangle|11\rangle$  so  $\langle \frac{3}{2}, \frac{3}{2} | S_z | \frac{3}{2}, \frac{3}{2} \rangle = \frac{1}{2}$  and  $E_B/(\mu_B B) = m + \langle \psi | S_z | \psi \rangle = \frac{3}{2} + \frac{1}{2} = 2$  in agreement with the Landé factor. Similarly

$$|\frac{3}{2}, \frac{1}{2}\rangle = \sqrt{\frac{1}{3}}|-\rangle|11\rangle + \sqrt{\frac{2}{3}}|+\rangle|10\rangle \Rightarrow \langle \frac{3}{2}, \frac{1}{2} | S_z | \frac{3}{2}, \frac{1}{2} \rangle = \frac{1}{3}(-\frac{1}{2}) + \frac{2}{3}\frac{1}{2} = \frac{1}{6}$$

so  $E_B/(\mu_B B) = \frac{1}{2} + \frac{1}{6} = \frac{2}{3}$  Finally

$$|\frac{1}{2}, \frac{1}{2}\rangle = \sqrt{\frac{2}{3}}|-\rangle|11\rangle - \sqrt{\frac{1}{3}}|+\rangle|10\rangle \Rightarrow \langle \frac{1}{2}, \frac{1}{2} | S_z | \frac{1}{2}, \frac{1}{2} \rangle = \frac{2}{3}(-\frac{1}{2}) + \frac{1}{3}\frac{1}{3} = -\frac{1}{6}$$

so  $E_B/(\mu_B B) = \frac{1}{2} - \frac{1}{6} = \frac{1}{3}$

**9.11\*** Using the result proved in Problem 9.10, show that the trial wavefunction  $\psi_b = e^{-b^2 r^2/2}$  yields  $-8/(3\pi)\mathcal{R}$  as an estimate of hydrogen's ground-state energy, where  $\mathcal{R}$  is the Rydberg constant.

**Soln:** With  $\psi = e^{-b^2 r^2/2}$ ,  $d\psi/dr = -b^2 r e^{-b^2 r^2/2}$ , so

$$\begin{aligned} \langle H \rangle &= \left( \frac{\hbar^2 b^4}{2m} \int dr r^4 e^{-b^2 r^2} - \frac{e^2}{4\pi\epsilon_0} \int dr r e^{-b^2 r^2} \right) / \int dr r^2 e^{-b^2 r^2} \\ &= \left( \frac{\hbar^2}{2mb} \int dx x^4 e^{-x^2} - \frac{e^2}{4\pi\epsilon_0 b^2} \int dx x e^{-x^2} \right) / \frac{1}{b^3} \int dx x^2 e^{-x^2} \end{aligned}$$

Now

$$\begin{aligned} \int dx x e^{-x^2} &= \left[ \frac{e^{-x^2}}{-2} \right]_0^\infty = \frac{1}{2} \\ \int dx x^2 e^{-x^2} &= \left[ \frac{x e^{-x^2}}{-2} \right]_0^\infty + \frac{1}{2} \int dx e^{-x^2} = \frac{\sqrt{\pi}}{4} \\ \int dx x^4 e^{-x^2} &= \left[ \frac{x^3 e^{-x^2}}{-2} \right]_0^\infty + \frac{3}{2} \int dx x^2 e^{-x^2} = \frac{3\sqrt{\pi}}{8} \end{aligned}$$

so

$$\langle H \rangle = \left( \frac{\hbar^2}{2mb} \frac{3\sqrt{\pi}}{8} - \frac{e^2}{4\pi\epsilon_0 b^2} \frac{1}{2} \right) / \frac{\sqrt{\pi}}{4b^3} = \frac{3\hbar^2 b^2}{4m} - \frac{e^2 b}{2\pi^{3/2}\epsilon_0}$$

At the stationary point of  $\langle H \rangle$   $b = me^2/(3\pi^{3/2}\epsilon_0\hbar^2)$ . Plugging this into  $\langle H \rangle$  we find

$$\langle H \rangle = \frac{3\hbar^2}{4m} \frac{m^2 e^4}{9\pi^3 \epsilon_0^2 \hbar^4} - \frac{e^2}{2\pi^{3/2}\epsilon_0} \frac{me^2}{3\pi^{3/2}\epsilon_0\hbar^2} = -\frac{8}{3\pi} \frac{m}{2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 = \frac{8}{3\pi} \mathcal{R}$$

**9.13\*** A particle travelling with momentum  $p = \hbar k > 0$  from  $-\infty$  encounters the steep-sided potential well  $V(x) = -V_0 < 0$  for  $|x| < a$ . Use the Fermi golden rule to show that the probability that a particle will be reflected by the well is

$$P_{\text{reflect}} \simeq \frac{V_0^2}{4E^2} \sin^2(2ka),$$

where  $E = p^2/2m$ . Show that in the limit  $E \gg V_0$  this result is consistent with the exact reflection probability derived in Problem 5.9. Hint: adopt periodic boundary conditions so the wavefunctions of the in and out states can be normalised.

**Soln:** We consider a length  $L$  of the  $x$  axis where  $L \gg a$  and  $k = 2n\pi/L$ , where  $n \gg 1$  is an integer. Then correctly normalised wavefunctions of the in and out states are

$$\psi_{\text{in}}(x) = \frac{1}{\sqrt{L}} e^{ikx} \quad ; \quad \psi_{\text{out}}(x) = \frac{1}{\sqrt{L}} e^{-ikx}$$

The required matrix element is

$$\frac{1}{L} \int_{-L/2}^{L/2} dx e^{ikx} V(x) e^{ikx} = -V_0 \int_{-a}^a dx e^{2ikx} = -V_0 \frac{\sin(2ka)}{Lk}$$

so the rate of transitions from the in to the out state is

$$\dot{P} = \frac{2\pi}{\hbar} g(E) \langle \text{out} | V | \text{in} \rangle = \frac{2\pi}{\hbar} g(E) V_0^2 \frac{\sin^2(2ka)}{L^2 k^2}$$

Now we need the density of states  $g(E)$ .  $E = p^2/2m = \hbar^2 k^2/2m$  is just kinetic energy. Eliminating  $k$  in favour of  $n$ , we have

$$n = \frac{L}{2\pi\hbar} \sqrt{2mE}$$

As  $n$  increases by one, we get one extra state to scatter into, so

$$g = \frac{dn}{dE} = \frac{L}{4\pi\hbar} \sqrt{\frac{2m}{E}}.$$

Substituting this value into our scattering rate we find

$$\dot{P} = \frac{V_0^2}{2\hbar^2} \sqrt{\frac{2m}{E}} \frac{\sin^2(2ka)}{Lk^2}$$

This vanishes as  $L \rightarrow \infty$  because the fraction of the available space that is occupied by the scattering potential is  $\sim 1/L$ . If it is not scattered, the particle covers distance  $L$  in a time  $\tau = L/v = L/\sqrt{2E/m}$ . So the probability that it is scattered on a single encounter is

$$\dot{P}\tau = \frac{V_0^2 m \sin^2(2ka)}{E\hbar^2 k^2} = \frac{V_0^2}{4E^2} \sin^2(2ka)$$

Equation (5.78) gives the reflection probability as

$$P = \frac{(K/k - k/K)^2 \sin^2(2Ka)}{(K/k + k/K)^2 \sin^2(2Ka) + 4 \cos^2(2Ka)}$$

When  $V_0 \ll E$ ,  $K^2 - k^2 = 2mV_0 \ll k^2$ , so we approximate  $Ka$  with  $ka$  and then the reflection probability becomes

$$P \simeq \left( \frac{K^2 - k^2}{2kK} \right)^2 \sin^2(2ka)$$

which agrees with the value we obtained from Fermi's rule.

**9.14\*** Show that the number states  $g(E) dE d^2\Omega$  with energy in  $(E, E + dE)$  and momentum in the solid angle  $d^2\Omega$  around  $\mathbf{p} = \hbar\mathbf{k}$  of a particle of mass  $m$  that moves freely subject to periodic boundary conditions on the walls of a cubical box of side length  $L$  is

$$g(E) dE d^2\Omega = \left(\frac{L}{2\pi}\right)^3 \frac{m^{3/2}}{\hbar^3} \sqrt{2E} dE d\Omega^2. \quad (9.2)$$

Hence show from Fermi's golden rule that the cross section for elastic scattering of such particles by a weak potential  $V(\mathbf{x})$  from momentum  $\hbar\mathbf{k}$  into the solid angle  $d^2\Omega$  around momentum  $\hbar\mathbf{k}'$  is

$$d\sigma = \frac{m^2}{(2\pi)^2 \hbar^4} d^2\Omega \left| \int d^3\mathbf{x} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} V(\mathbf{x}) \right|^2. \quad (9.3)$$

Explain in what sense the potential has to be “weak” for this **Born approximation** to the scattering cross section to be valid.

**Soln:** We have  $k_x = 2n_x\pi/L$ , where  $n_x$  is an integer, and similarly for  $k_y, k_z$ . So each state occupies volume  $(2\pi/L)^3$  in  $k$ -space. So the number of states in the volume element  $k^2 dk d^2\Omega$  is

$$g(E) dE d^2\Omega = \left(\frac{L}{2\pi}\right)^3 k^2 dk d^2\Omega$$

Using  $k^2 = 2mE/\hbar^2$  to eliminate  $k$  we obtain the required expression.

From the Fermi rule the probability of making the transition  $\mathbf{k} \rightarrow \mathbf{k}'$  is

$$\dot{P} = \frac{2\pi}{\hbar} g(E) d^2\Omega |\langle \text{out} | V | \text{in} \rangle|^2 = \frac{2\pi}{\hbar} \left(\frac{L}{2\pi}\right)^3 k^2 \frac{dk}{dE} d^2\Omega |\langle \text{out} | V | \text{in} \rangle|^2$$

The matrix element is

$$\langle \text{out} | V | \text{in} \rangle = \frac{1}{L^3} \int d^3\mathbf{x} e^{-i\mathbf{k}'\cdot\mathbf{x}} V(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}}$$

Now the cross section  $d\sigma$  is defined by  $\dot{P} = d\sigma \times \text{incoming flux} = (v/L^3) d\sigma = (\hbar k/mL^3) d\sigma$ . Putting everything together, we find

$$\begin{aligned} \frac{\hbar k}{mL^3} d\sigma &= \frac{1}{L^6} \left| \int d^3\mathbf{x} e^{-i\mathbf{k}'\cdot\mathbf{x}} V(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} \right|^2 \frac{2\pi}{\hbar} \left(\frac{L}{2\pi}\right)^3 k^2 \frac{dk}{dE} d^2\Omega \\ &\Rightarrow d\sigma = \frac{mk dk/dE}{(2\pi)^2 \hbar^2} \left| \int d^3\mathbf{x} e^{-i\mathbf{k}'\cdot\mathbf{x}} V(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} \right|^2. \end{aligned}$$

Eliminating  $k$  with  $\hbar^2 k dk = m dE$  we obtain the desired expression.

The Born approximation is valid providing the unperturbed wavefunction is a reasonable approximation to the true wavefunction throughout the scattering potential. That is, we must be able to neglect “shadowing” by the scattering potential.

**10.5\*** Assume that a LiH molecule comprises a  $\text{Li}^+$  ion electrostatically bound to an  $\text{H}^-$  ion, and that in the molecule's ground state the kinetic energies of the ions can be neglected. Let the centres of the two ions be separated by a distance  $b$  and calculate the resulting electrostatic binding energy under the assumption that they attract like point charges. Given that the ionisation energy of Li is  $0.40\mathcal{R}$  and using the result of Problem 10.4, show that the molecule has less energy than that of well separated hydrogen and lithium atoms for  $b < 4.4a_0$ . Does this calculation suggest that LiH is a stable molecule? Is it safe to neglect the kinetic energies of the ions within the molecule?

**Soln:** When the Li and H are well separated, the energy required to strip an electron from the Li and park it on the  $\text{H}^-$  is  $E = (0.4 + 1 - 0.955)\mathcal{R} = 0.445\mathcal{R}$ . Now we recover some of this energy by letting the  $\text{Li}^+$  and  $\text{H}^-$  fall towards each other. When they have reached distance  $b$  the energy released is

$$\frac{e^2}{4\pi\epsilon_0 b} = 2\mathcal{R} \frac{a_0}{b}$$

This energy equals our original outlay when  $b = (2/0.445)a_0 = 4.49a_0$ , which establishes the required proposition.

In LiH the Li-H separation will be  $\lesssim 2a_0$ , because only at a radius of this order will the electron clouds of the two ions generate sufficient repulsion to balance the electrostatic attraction we have been calculating. At this separation the energy will be decidedly less than that of isolated Li and H, so yes the molecule will be stable.

In its ground state the molecule will have zero angular momentum, so there is no rotational kinetic energy to worry about. However the length of the Li-H bond will oscillate around its equilibrium value, roughly as a harmonic oscillator, so there will be zero-point energy. However, this energy will suffice only to extend the bond length by a fraction of its equilibrium value, so it does not endanger the stability of the molecule.

**10.6\*** *Two spin-one gyros are a box. Express that states  $|j, m\rangle$  in which the box has definite angular momentum as linear combinations of the states  $|1, m\rangle|1, m'\rangle$  in which the individual gyros have definite angular momentum. Hence show that*

$$|0, 0\rangle = \frac{1}{\sqrt{3}}(|1, -1\rangle|1, 1\rangle - |1, 0\rangle|1, 0\rangle + |1, 1\rangle|1, -1\rangle)$$

*By considering the symmetries of your expressions, explain why the ground state of carbon has  $l = 1$  rather than  $l = 2$  or  $0$ . What is the total spin angular momentum of a C atom?*

**Soln:** We have that  $J_-|2, 2\rangle = 2|2, 1\rangle$ ,  $J_-|2, 1\rangle = \sqrt{6}|2, 0\rangle$ ,  $J_-|1, 1\rangle = \sqrt{2}|1, 0\rangle$ ,  $J_-|1, 0\rangle = \sqrt{2}|1, -1\rangle$ . We start from

$$|2, 2\rangle = |1, 1\rangle|1, 1\rangle$$

and apply  $J_-$  to both sides, obtaining

$$2|2, 1\rangle = \sqrt{2}(|1, 0\rangle|1, 1\rangle + |1, 1\rangle|1, 0\rangle) \Rightarrow |2, 1\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle|1, 1\rangle + |1, 1\rangle|1, 0\rangle)$$

Applying  $J_-$  again we find

$$|2, 0\rangle = \frac{1}{\sqrt{6}}(|1, -1\rangle|1, 1\rangle + 2|1, 0\rangle|1, 0\rangle + |1, 1\rangle|1, -1\rangle)$$

Next we identify  $|1, 1\rangle$  as the linear combination of  $|1, 1\rangle|1, 0\rangle$  and  $|1, 0\rangle|1, 1\rangle$  that's orthogonal to  $|2, 1\rangle$ . It clearly is

$$|1, 1\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle|1, 1\rangle - |1, 1\rangle|1, 0\rangle)$$

We obtain  $|1, 0\rangle$  by applying  $J_-$  to this

$$|1, 0\rangle = \frac{1}{\sqrt{2}}(|1, -1\rangle|1, 1\rangle - |1, 1\rangle|1, -1\rangle)$$

and applying  $J_-$  again we have

$$|1, -1\rangle = \frac{1}{\sqrt{2}}(|1, -1\rangle|1, 0\rangle - |1, 0\rangle|1, -1\rangle)$$

Finally we have that  $|0, 0\rangle$  is the linear combination of  $|1, -1\rangle|1, 1\rangle$ ,  $|1, 1\rangle|1, -1\rangle$  and  $|1, 0\rangle|1, 0\rangle$  that's orthogonal to both  $|2, 0\rangle$  and  $|1, 0\rangle$ . By inspection it's the given expression.

The kets for  $j = 2$  and  $j = 0$  are symmetric under interchange of the  $m$  values of the gyros, while that for  $j = 1$  is antisymmetric under interchange. Carbon has two valence electrons both in an  $l = 1$  state, so each electron maps to a gyro and the box to the atom. When the atom is in the  $|1, 1\rangle$  state, for example, from the above the part of the wavefunction that described the locations of the two valence electrons is

$$\langle \mathbf{x}_1, \mathbf{x}_2 | 1, 1 \rangle = \frac{1}{\sqrt{2}}(\langle \mathbf{x}_1 | 1, 0 \rangle \langle \mathbf{x}_2 | 1, 1 \rangle - \langle \mathbf{x}_1 | 1, 1 \rangle \langle \mathbf{x}_2 | 1, 0 \rangle)$$

This function is antisymmetric in its arguments so vanishes when  $\mathbf{x}_1 = \mathbf{x}_2$ . Hence in this state of the atom, the electrons do a good job of keeping out of each other's way and we can expect the electron-electron repulsion to make this state (and the other two  $l = 1$  states) lower-lying than the  $l = 2$  or  $l = 0$  states, which lead to wavefunctions that are symmetric functions of  $\mathbf{x}_1$  and  $\mathbf{x}_2$ .

Since the wavefunction has to be antisymmetric overall, for the  $l = 1$  state it must be symmetric in the spins of the electrons, so the total spin has to be 1.

**10.7\*** Suppose we have three spin-one gyros in a box. Express the state  $|0, 0\rangle$  of the box in which it has no angular momentum as a linear combination of the states  $|1, m\rangle|1, m'\rangle|1, m''\rangle$  in which the individual gyros have well-defined angular momenta. Hint: start with just two gyros in the box, giving states  $|j, m\rangle$  of the box, and argue that only for a single value of  $j$  will it be possible to get  $|0, 0\rangle$  by adding the third gyro; use results from Problem 10.6.

Explain the relevance of your result to the fact that the ground state of nitrogen has  $l = 0$ . Deduce the value of the total electron spin of an N atom.

**Soln:** Since when we add gyros with spins  $j_1$  and  $j_2$  the resulting  $j$  satisfies  $|j_1 - j_2| \leq j \leq j_1 + j_2$ , we will be able to construct the state  $|0, 0\rangle$  on adding the third gyro to the box, only if the box has  $j = 1$  before adding the last gyro. From Problem 10.6 we have that

$$|0, 0\rangle = \frac{1}{\sqrt{3}}(|1, -1\rangle|1, 1\rangle - |1, 0\rangle|1, 0\rangle + |1, 1\rangle|1, -1\rangle),$$

where we can consider the first ket in each product is for the combination of 2 gyros and the second ket is for the third gyro. We use Problem 10.6 again to express the kets of the 2-gyro box as linear combinations of the kets of individual gyros:

$$\begin{aligned} |0, 0\rangle &= \frac{1}{\sqrt{3}} \left( \frac{1}{\sqrt{2}}(|1, -1\rangle|1, 0\rangle - |1, 0\rangle|1, -1\rangle)|1, 1\rangle - \frac{1}{\sqrt{2}}(|1, -1\rangle|1, 1\rangle - |1, 1\rangle|1, -1\rangle)|1, 0\rangle \right. \\ &\quad \left. + \frac{1}{\sqrt{2}}(|1, 0\rangle|1, 1\rangle - |1, 1\rangle|1, 0\rangle)|1, -1\rangle \right), \\ &= \frac{1}{\sqrt{6}} \left( |1, -1\rangle|1, 0\rangle|1, 1\rangle - |1, 0\rangle|1, -1\rangle|1, 1\rangle - |1, -1\rangle|1, 1\rangle|1, 0\rangle \right. \\ &\quad \left. + |1, 1\rangle|1, -1\rangle|1, 0\rangle + |1, 0\rangle|1, 1\rangle|1, 0\rangle - |1, 1\rangle|1, 0\rangle|1, 0\rangle \right) \end{aligned}$$

This state is totally antisymmetric under exchange of the  $m$  values of the gyros.

When we interpret the gyros as electrons and move to the position representation we find that the wavefunction of the valence electrons is a totally antisymmetric function of their coordinates,  $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ . Hence the electrons do an excellent job of keeping out of each other's way, and this will be the ground state. To be totally antisymmetric overall, the state must be symmetric in the spin labels of the electrons, so the spin states will be  $|+\rangle|+\rangle|+\rangle$  and the states obtained from this by application of  $J_-$ . Thus the total spin will be  $s = \frac{3}{2}$ .

**10.8\*** Consider a system made of three spin-half particles with individual spin states  $|\pm\rangle$ . Write down a linear combination of states such as  $|+\rangle|+\rangle|-\rangle$  (with two spins up and one down) that is symmetric under any exchange of spin eigenvalues  $\pm$ . Write down three other totally symmetric states and say what total spin your states correspond to.

Show that it is not possible to construct a linear combination of products of  $|\pm\rangle$  which is totally antisymmetric.

What consequences do these results have for the structure of atoms such as nitrogen that have three valence electrons?

**Soln:** There are just three of these product states to consider because there are just three places to put the single minus sign. The sum of these states is obviously totally symmetric:

$$|\psi\rangle = \frac{1}{\sqrt{3}}(|+\rangle|+\rangle|-\rangle + |+\rangle|-\rangle|+\rangle + |-\rangle|+\rangle|+\rangle)$$

Three other totally symmetric state are clearly  $|+\rangle|+\rangle|+\rangle$  and what you get from this ket and the one given by everywhere interchanging  $+$  and  $-$ . These four kets are the kets  $|\frac{3}{2}, m\rangle$ .

A totally antisymmetric state would have to be constructed from the same three basis kets used above, so we write it as

$$|\psi'\rangle = a|+\rangle|+\rangle|-\rangle + b|+\rangle|-\rangle|+\rangle + c|-\rangle|+\rangle|+\rangle$$

On swapping the spins of the first and the third particles, the first and third kets would interchange, and this would have to generate a change of sign. So  $a = -c$  and  $b = 0$ . Similarly, by swapping the

spins on the first and second particles, we can show that  $a = 0$ . Hence  $|\psi\rangle = 0$ , and we have shown that no nonzero ket has the required symmetry.

States that satisfy the exchange principle can be constructed by multiplying a spatial wavefunction that is totally antisymmetric in its arguments by a totally symmetric spin function. Such states have maximum total spin. In contrast to the situation with helium, conforming states cannot be analogously constructed by multiplying a symmetric wavefunction by an antisymmetric spin function.