The Physics of Quantum Mechanics
Solutions to problems that are not on problem sets

2.10 *Let $\psi(x)$ be a properly normalised wavefunction and Q an operator on wavefunctions. Let $\{q_r\}$ be the spectrum of Q and $\{u_r(x)\}$ be the corresponding correctly normalised eigenfunctions. Write down an expression for the probability that a measurement of Q will yield the value q_r. Show that $\sum_r P(q_r|\psi) = 1$. Show further that the expectation of Q is $\langle Q\rangle \equiv \int_{-\infty}^{\infty} \psi^* \hat{Q}\psi\,\mathrm{d}x$.*[1]
Soln:

$$P_i = \left|\int \mathrm{d}x\, u_i^*(x)\psi(x)\right|^2 \quad \text{where} \quad Qu_i(x) = q_i u_i(x).$$

$$1 = \int \mathrm{d}x\,|\psi|^2 = \int \mathrm{d}x\,\left(\sum_i a_i^* u_i^*\right)\left(\sum_j a_j u_j\right) = \sum_{ij} a_i^* a_j \int \mathrm{d}x\, u_i^* u_j = \sum_i |a_i|^2 = \sum_i P_i$$

Similarly

$$\begin{aligned}\int \mathrm{d}x\,\psi^* Q\psi &= \int \mathrm{d}x\,\left(\sum_i a_i^* u_i^*\right) Q \left(\sum_j a_j u_j\right) = \sum_{ij} a_i^* a_j \int \mathrm{d}x u_i^* Q u_j \\ &= \sum_{ij} a_i^* a_j q_j \int \mathrm{d}x\, u_i^* u_j = \sum_i |a_i|^2 q_i = \sum_i P_i q_i\end{aligned}$$

which is by definition the expectation value of Q.

2.22 *Show that for any three operators A, B and C, the* **Jacobi identity** *holds:*

$$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0. \tag{2.1}$$

Soln: We expand the inner commutator and then use the rule for expanding the commutator of a product:

$$\begin{aligned}[A,[B,C]] + [B,[C,A]] + [C,[A,B]] &= [A,BC] - [A,CB] + [B,CA] - [B,AC] + [C,AB] - [C,BA] \\ &= [A,B]C + B[A,C] - [A,C]B - C[A,B] + [B,C]A + C[B,A] - [B,A]C \\ &\quad - A[B,C] + [C,A]B + A[C,B] - [C,B]A - B[C,A] \\ &= 2\left([A,B]C - C[A,B] - [A,C]B + B[A,C] + [B,C]A - A[B,C]\right) \\ &= 2\big(ABC - BAC - CAB + CBA - ACB + CAB + BAC - BCA + BCA \\ &\quad - CBA - ABC + ACB\big) = 0\end{aligned}$$

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*

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

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

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

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

---

[1] In the most elegant formulation of qantum mechanics, this last result is the basic postulate of the theory, and one *derives* other rules for the physical interpretation of the q_n, a_n etc. from it – see J. von Neumann, *Mathematical Foundations of Quantum Mechanics.*

Alternatively, transforming $u_0(x)$:

$$\langle p|0\rangle = \int \mathrm{d}x\langle p|x\rangle\langle x|0\rangle = \frac{1}{\sqrt{h}}\int_{-\infty}^{\infty}\mathrm{d}x\,\mathrm{e}^{-\mathrm{i}px/\hbar}\frac{\mathrm{e}^{-x^2/4\ell^2}}{(2\pi\ell^2)^{1/4}}$$
$$= \frac{1}{(2\pi\ell^2h^2)^{1/4}}\int_{-\infty}^{\infty}\mathrm{d}x\,\exp\left(-\left\{\frac{x}{2\ell}+\frac{\mathrm{i}p\ell}{\hbar}\right\}^2\right)\mathrm{e}^{-p^2\ell^2/\hbar^2} = \frac{2\ell\sqrt{\pi}}{(2\pi\ell^2h^2)^{1/4}}\,\mathrm{e}^{-p^2\ell^2/\hbar^2}$$

3.10 *Show that for any two $N\times N$ matrices A, B, trace$([A,B])=0$. Comment on this result in the light of the results of Problem 3.7 and the canonical commutation relation $[x,p]=\mathrm{i}\hbar$.*
Soln:

$$\mathrm{trace}(AB)=\sum_j(AB)_{jj}=\sum_{jk}A_{jk}B_{kj}\quad;\quad\mathrm{trace}(BA)=\sum_k(BA)_{kk}=\sum_{kj}B_{kj}A_{jk}=\sum_{kj}A_{jk}B_{kj}$$

These two expressions differ only in the order of the summations over j and k. We can reverse one order and thus show them to be equal iff $\sum_{jk}|A_{jk}B_{kj}|^2$ is finite, which it will be for finite-dimensional matrices with finite elements. Hence x and p can only be represented by infinite matrices with elements that are not square summable, (which the matrices of Problem 3.7 are not).

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

$$f^2=0\qquad;\qquad ff^\dagger+f^\dagger f=1. \tag{3.2}$$

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 in an excitation of a Fermi oscillator. Explain the connection between the spectrum of $f^\dagger f$ and the Pauli principle.
Soln:

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

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.

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

Moreover,

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

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

3.12 *In the time interval $(t+\delta t,t)$ the Hamiltonian H of some system varies in such a way that $|H|\psi\rangle|$ remains finite. Show that under these circumstances $|\psi\rangle$ is a continuous function of time.*

A harmonic oscillator with frequency ω is in its ground state when the stiffness of the spring is instantaneously reduced by a factor $f^4<1$, so its natural frequency becomes $f^2\omega$. What is the probability that the oscillator is subsequently found to have energy $\frac{3}{2}\hbar f^2\omega$? Discuss the classical analogue of this problem.
Soln: From the TDSE $\delta|\psi\rangle=-(\mathrm{i}/\hbar)H|\psi\rangle\delta t$, so $\lim_{\delta t\to 0}|\delta|\psi\rangle|=0$, proving that $|\psi\rangle$ changes continuously no matter how suddenly H changes.

$$P(E=\tfrac{3}{2}f^2\omega)=\left|\int\mathrm{d}x\,u_1'^*(x)u_0(x)\right|^2=0\quad\text{by parity.}$$

Classically the effect of a sudden change in spring stiffness depends on the phase of the oscillation when the spring slackens: if the change happens when the mass is at $x=0$, the mass has all its energy in kinetic form and there is no change in its energy; if the spring slackens when the mass is stationary, all its energy is invested in the spring and the mass suddenly gets poorer. We expect quantum mechanics to yield a probability distribution for the changes in E that is similar to the average of the classical changes over phase. Of course classical mechanics averages probabilities for states of even and odd parity because it doesn't recognise the parity of a state.

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*

$$A = \tfrac{1}{2}\left\{(f^{-1} + f)A' + (f^{-1} - f)A'^\dagger\right\}, \tag{3.3}$$

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

$$A \equiv \frac{m\omega x + \mathrm{i}p}{\sqrt{2m\hbar\omega}} \qquad A' \equiv \frac{mf^2\omega x + \mathrm{i}p}{\sqrt{2m\hbar f^2\omega}}$$
$$= \frac{x}{2\ell} + \frac{\mathrm{i}\ell}{\hbar}p \qquad = \frac{fx}{2\ell} + \frac{\mathrm{i}\ell}{f\hbar}p$$

Hence

$$A' + A'^\dagger = \frac{f}{\ell}x \quad A' - A'^\dagger = f\frac{2\mathrm{i}\ell}{f\hbar}p \quad \text{so} \quad A = \frac{1}{2f}(A' + A'^\dagger) + \frac{f}{2}(A' - A'^\dagger)$$

$$0 = A|0\rangle = \tfrac{1}{2}\sum_k \left\{(f^{-1} + f)c_k A'|k'\rangle + (f^{-1} - f)c_k A'^\dagger|k'\rangle\right\}$$
$$= \tfrac{1}{2}\sum_k \left\{(f^{-1} + f)\sqrt{k}c_k|k - 1'\rangle + (f^{-1} - f)\sqrt{k+1}c_k|k + 1'\rangle\right\}$$

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: $c_n \to c_n/\sqrt{S}$.

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*

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

What restrictions on the values of the numbers μ and λ follow from the requirement for H to be Hermitian?

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

$$H = \mu B^\dagger B + \text{constant}. \tag{3.5}$$

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

Soln: Hermiticity requires μ and λ 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 $0, 1, \ldots$, 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 θ a real constant and A, $A^\dagger$ are the usual ladder operators. Show that $[B, B^\dagger] = 1$.*

Consider the Hamiltonian

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

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

$$\epsilon c - \lambda s = Ec \quad ; \quad \lambda c - \epsilon s = Es \tag{3.7}$$

with E a constant, $[B, H] = EB$. Hence determine the spectrum of H in terms of ϵ and λ.
Soln:

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

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

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 $E_0, E_0 - E, E_0 - 2E, \ldots$ terminates because $B|E_{\rm min}\rangle = 0$. Mod-squaring this equation we have

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

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

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

Multiplying through by $\lambda/2$ this becomes

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

so $E_{\rm min} = -s\lambda/2c$. 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

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

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

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

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*

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

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

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

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 $\int \mathrm{d}^3\mathbf{x}\,\nabla_i\mathbf{T} = \oint \mathrm{d}^2S_i\,\mathbf{T}$ no matter how many indices the tensor $\mathbf{T}$ may carry.

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

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

becomes

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

In the first integral we use the divergence theorem to move ∂_j from r^{-1} to $\partial_i A_j$ and in the second integral we move the ∂_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 $R\to\infty$ because their integrands have explicit R^{-2} scaling, so they will tend to zero as $R\to\infty$ so long as $A\to 0$ no matter how slowly. After this has been done we have

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

The first integral vanishes because $\partial_j A_j = \boldsymbol{\nabla}\cdot\mathbf{A} = 0$ 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 $n^{\rm th}$ Landau level of a uniform magnetic field B is*

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

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

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

Show further that

$$\frac{\delta\ln\langle r\rangle_n}{\delta n} \simeq \frac{1}{2n} \tag{3.12}$$

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 $\int \mathrm{d}r\, r\, r^{2n}\mathrm{e}^{-r^2/2r_B^2}(n+r^2/2r_B^2)\int \mathrm{d}\phi$ with the help of the definition $z! = \int_0^\infty \mathrm{d}x\, x^z\mathrm{e}^{-x}$. Then

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

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

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

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

3.19 *A particle of charge Q is confined to move in the xy plane, with electrostatic potential $\phi = 0$ and vector potential $\mathbf{A}$ satisfying*

$$\boldsymbol{\nabla}\times\mathbf{A} = (0,0,B). \tag{3.13}$$

Consider the operators ρ_x, ρ_y, R_x and R_y, defined by

$$\boldsymbol{\rho} = \frac{1}{QB}\,\hat{\mathbf{e}}_z\times(\mathbf{p}-Q\mathbf{A}) \qquad \textit{and} \qquad \mathbf{R} = \mathbf{r}-\boldsymbol{\rho}, \tag{3.14}$$

where $\mathbf{r}$ and $\mathbf{p}$ are the usual position and momentum operators, and $\hat{\mathbf{e}}_z$ is the unit vector along $\mathbf{B}$. Show that the only non-zero commutators formed from the x- and y-components of these are

$$[\rho_x,\rho_y] = \mathrm{i}r_B^2 \qquad \textit{and} \qquad [R_x,R_y] = -\mathrm{i}r_B^2, \tag{3.15}$$

where $r_B^2 = \hbar/QB$.

The operators a, $a^\dagger$, b and $b^\dagger$ are defined via

$$a = \frac{1}{\sqrt{2}\,r_B}(\rho_x+\mathrm{i}\rho_y) \qquad \textit{and} \qquad b = \frac{1}{\sqrt{2}\,r_B}(R_y+\mathrm{i}R_x). \tag{3.16}$$

Evaluate $[a,a\dagger]$ and $[b,b^\dagger]$. Show that for suitably defined ω, the Hamiltonian can be written

$$H = \hbar\omega\left(a^\dagger a+\tfrac{1}{2}\right). \tag{3.17}$$

Given that there exists a unique state $|\psi\rangle$ satisfying

$$a|\psi\rangle = b|\psi\rangle = 0, \tag{3.18}$$

what conclusions can be drawn about the allowed energies of the Hamiltonian and their degeneracies? What is the physical interpretation of these results?

Soln: We have

$$\rho_x = -\frac{1}{QB}(p_y - QA_y) \quad ; \quad \rho_y = \frac{1}{QB}(p_x - QA_x)$$

so

$$\begin{aligned}[\rho_x, \rho_y] &= -\frac{1}{(QB)^2}[(p_y - QA_y), (p_x - QA_x)] = \frac{1}{QB^2}([p_y, A_x] + [A_y, p_x]) \\ &= \frac{-\mathrm{i}\hbar}{QB^2}\left(\frac{\partial A_x}{\partial y} - \frac{\partial A_y}{\partial x}\right) = \frac{\mathrm{i}\hbar}{QB} = \mathrm{i}r_B^2\end{aligned}$$

Also

$$\begin{aligned}[\rho_x, x] &= -\frac{1}{QB}[p_y, x] = 0 \quad ; \quad [\rho_x, y] = -\frac{1}{QB}[p_y, y] = \frac{\mathrm{i}\hbar}{QB} = \mathrm{i}r_B^2 \\ [\rho_y, x] &= \frac{1}{QB}[p_x, x] = -\mathrm{i}r_B^2 \quad ; \quad [\rho_y, y] = 0\end{aligned}$$

So

$$[\rho_x, R_x] = [\rho_x, x - \rho_x] = 0 \quad ; \quad [\rho_x, R_y] = [\rho_x, y - \rho_y] = \mathrm{i}r_B^2(1-1) = 0$$

and similarly $[\rho_y, R_i] = 0$. Finally

$$[R_x, R_y] = [x - \rho_x, y - \rho_y] = -[\rho_x, y] - [x, \rho_y] + [\rho_x, \rho_y] = -\mathrm{i}r_B^2$$

Now

$$\begin{aligned}[a, a^\dagger] &= \frac{1}{2r_B^2}[\rho_x + \mathrm{i}\rho_y, \rho_x - \mathrm{i}\rho_y] = -\frac{1}{2r_B^2}2\mathrm{i}[\rho_x, \rho_y] = 1 \\ [b, b^\dagger] &= \frac{1}{2r_B^2}[R_y + \mathrm{i}R_x, R_y - \mathrm{i}R_x] = \frac{1}{2r_B^2}2\mathrm{i}[R_x, R_y] = 1 \\ a^\dagger a &= \frac{1}{2r_B^2}(\rho_x - \mathrm{i}\rho_y)(\rho_x + \mathrm{i}\rho_y) = \frac{1}{2r_B^2}(\rho_x^2 + \rho_y^2 + \mathrm{i}[\rho_x, \rho_y]) \\ &= \frac{1}{2r_B^2}\left(\frac{|\mathbf{p} - Q\mathbf{A}|^2}{(QB)^2} - r_B^2\right) = \frac{1}{2\hbar}\frac{|\mathbf{p} - Q\mathbf{A}|^2}{QB} - \tfrac{1}{2}\end{aligned}$$

But

$$H = \frac{|\mathbf{p} - Q\mathbf{A}|^2}{2m} = (a^\dagger a + \tfrac{1}{2})\hbar\frac{QB}{m} = (a^\dagger a + \tfrac{1}{2})\hbar\omega,$$

where $\omega \equiv QB/m$.

Given $a|\psi\rangle = 0$, we have $H|\psi\rangle = (a^\dagger a + \frac{1}{2})\hbar\omega|\psi\rangle = \frac{1}{2}\hbar\omega|\psi\rangle$ so $|\psi\rangle$ is a stationary state of energy $\frac{1}{2}\hbar\omega$. Given any stationary state $|E\rangle$ of energy $|E\rangle$ we have that $a^\dagger|E\rangle$ is a stationary state of energy $E + \hbar\omega$:

$$Ha^\dagger|E\rangle = \hbar\omega a^\dagger(aa^\dagger + \tfrac{1}{2})|E\rangle = \hbar\omega a^\dagger(a^\dagger a + [a, a^\dagger] + \tfrac{1}{2})|E\rangle = a^\dagger(H + \hbar\omega)|E\rangle = (E + \hbar\omega)a^\dagger|E\rangle,$$

so the energies are $\hbar\omega \times (\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots)$.

Since $[\rho_i, R_j] = 0$ we have $[a, b] = [a, b^\dagger] = 0$ etc, and it follows that $[b^\dagger, H] = 0$. Hence $b^\dagger|E\rangle$ is a stationary state of energy E.

To show that it is distinct from $|E\rangle$, we define the number operator $N \equiv b^\dagger b$. $N|\psi\rangle = 0$ because $b|\psi\rangle = 0$. Given that $N|n\rangle = n|n\rangle$, we have that

$$N(b^\dagger|n\rangle) = b^\dagger(bb^\dagger|n\rangle) = b^\dagger(b^\dagger b + [b, b^\dagger])|n\rangle = b^\dagger(N+1)|n\rangle = (n+1)b^\dagger|n\rangle$$

Thus by repeatedly applying $b^\dagger$ to $|\psi\rangle$ we can create distinct states of energy $\frac{1}{2}\hbar\omega$, and by applying it to $a^\dagger|\psi\rangle$ we can make distinct states of energy $\frac{3}{2}\hbar\omega$, etc. Hence all energy levels are infinitely degenerate.

Physically the energy levels are degenerate because there are an infinite number of possible locations of the gyrocentre of a particle that is gyrating with a given energy.

3.20* *Equation (2.87) gives the probability current density associated with a wavefunction. Show that the flux given by this expression changes when we make a gauge change $\psi \to \psi' = \mathrm{e}^{\mathrm{i}Q\Lambda/\hbar}\psi$. Why is this state of affairs physically unacceptable?*

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

$$\mathbf{J}(\mathbf{x}) = \frac{1}{m}\Re\left(\langle\psi|\mathbf{x}\rangle\langle\mathbf{x}|\mathbf{p}|\psi\rangle\right). \tag{3.19}$$

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* θ *of* ψ *your expression reads*

$$\mathbf{J} = \frac{|\psi|^2}{m}(\hbar\boldsymbol{\nabla}\theta - Q\mathbf{A}). \tag{3.20}$$

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

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

$$\mathbf{J}(r) = -\frac{\hbar r^{2n-1}\mathrm{e}^{-r^2/2r_B^2}}{2^{n+1}\pi n! m r_B^{2n+2}}\left(n + \frac{r^2}{2r_B^2}\right)\hat{\mathbf{e}}_\phi, \tag{3.21}$$

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 $\theta \to \theta + Q\Lambda/\hbar$ so it changes the current by $(|\psi|^2 Q/m)\boldsymbol{\nabla}\Lambda$. This is unacceptable because nothing physical should be changed by a gauge transformation.

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

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

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

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

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

In amplitude-phase format we now have

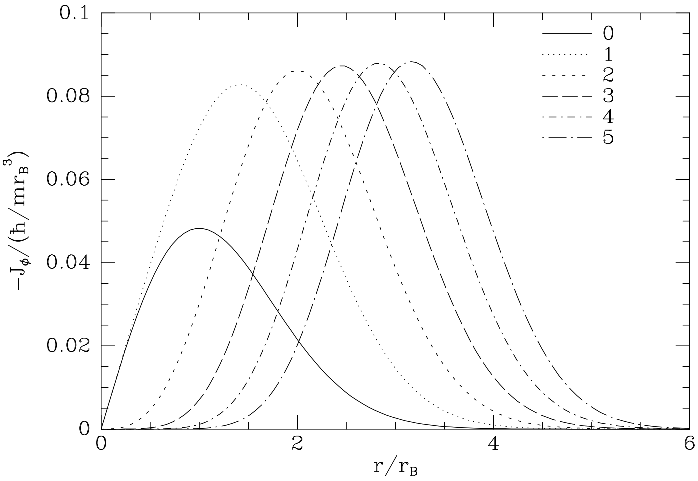
$$\mathbf{J} = \frac{|\psi|^2}{m}(\hbar\boldsymbol{\nabla}\theta - Q\mathbf{A}).$$

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

In plane polars,

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

so we obtain the required expression for $\mathbf{J}$ of the Landau level when we take $|\psi|$ and θ 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 $\omega \sim$ constant and $|\psi|^2 \simeq 1/r$ as expected from classical mechanics.

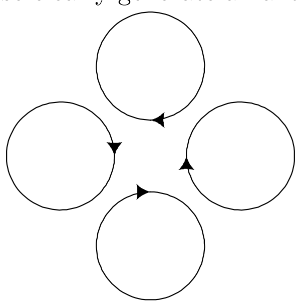
3.21* *Determine the probability current density associated with the* $n^{\rm th}$ *Landau ground-state wavefunction (3.67) (which for* $n=4$ *is shown on the front cover). Use your result to explain in as much detail as you can why this state can be interpreted as a superposition of states in which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

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

Soln: The wavefunction of the $n^{\rm th}$ state in the ground-state level differs from that of the first state of the $n^{\rm th}$ excited level only in having u^n instead of v^n in front of $\mathrm{e}^{-uv/4r_B^2}$. Consequently these wavefunctions have the same amplitudes but where the phase of the $n^{\rm th}$ excited state is $\theta=-n\phi$, that of the $n^{\rm th}$ 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 (3.21) with a minus sign in front of the n:

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

J now changes sign at $r=\sqrt{2n}r_B$: at small r it flows in the opposite sense to the current of the $n^{\rm th}$ 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 $\sqrt{2n}r_B$. So whereas in the $n^{\rm th}$ excited level the particle is moving counter-clockwise around a path of radius $\sim\sqrt{n}r_B$, in this state it is moving on a circle of radius $\sim r_B$ that is offset from the centre by $\sim\sqrt{n}r_B$. 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 $r^n\mathrm{e}^{\pm\mathrm{i}n\phi}$ is added. This factor moves outwards the radius $r_{\rm m}$ 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 $r_{\rm m}$ 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 $r_{\rm m}$. This asymmetry between the effects of multiplying by $\mathrm{e}^{\mathrm{i}n\phi}$ or $\mathrm{e}^{-\mathrm{i}n\phi}$ 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*

$$\boldsymbol{\mu}=IA\hat{\mathbf{n}}.\tag{3.22}$$

Use this formula and equation (3.21) 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. (3.21) gives the probability current density J. We multiply it by Q to get the electrical current density QJ. The current $\mathrm{d}I=QJ(r)\mathrm{d}r$ through the annulus of radius r contributes magnetic moment $\mathrm{d}\mu=\pi r^2\mathrm{d}I$. Summing over annuli we obtain

$$\begin{aligned}\mu&=Q\pi\int_0^\infty\mathrm{d}r\,r^2J(r)=-\frac{Q\hbar}{2^{n+1}n!mr_B^{2n+2}}\int_0^\infty\mathrm{d}r\,r^{2n+1}\mathrm{e}^{-r^2/2r_B^2}\left(n+\frac{r^2}{2r_B^2}\right)\\&=-\frac{\hbar Q}{2n!m}\int_0^\infty\mathrm{d}z\,z^n\mathrm{e}^{-z}(n+z)=-\frac{\hbar Q}{2n!m}[n\,n!+(n+1)!]=(n+\tfrac12)\frac{\hbar Q}{m}\end{aligned}$$

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

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

4.1 *Verify that* $[\mathbf{J},\mathbf{x}\cdot\mathbf{x}]=0$ *and* $[\mathbf{J},\mathbf{x}\cdot\mathbf{p}]=0$ *by using the commutation relations* $[x_i,J_j]=\mathrm{i}\sum_k\epsilon_{ijk}x_k$ *and* $[p_i,J_j]=\mathrm{i}\sum_k\epsilon_{ijk}p_k$.

Soln: It suffices to compute the commutator with the i^{th} component of $\mathbf{J}$

$$[J_i,\mathbf{x}\cdot\mathbf{x}]=\sum_j[J_i,x_jx_j]=\sum_j[J_i,x_j]x_j+\sum_j x_j[J_i,x_j]=\mathrm{i}\sum_{jk}\epsilon_{ijk}(x_kx_j+x_jx_k)=0$$

because the term in brackets is symmetric in ij while ϵ_{ijk} is antisymmetric in ij. Similarly

$$[J_i,\mathbf{x}\cdot\mathbf{p}]=\mathrm{i}\sum_{jk}\epsilon_{ijk}(x_kp_j+x_jp_k)=0$$

for the same reason.

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 $\mathbf{a}'=\mathbf{Ra}$ and $\mathbf{b}'=\mathbf{Rb}$. Then

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

4.3* *We have shown that* $[v_i,J_j]=\mathrm{i}\sum_k\epsilon_{ijk}v_k$ *for any operator whose components* v_i *form a vector. The expectation value of this operator relation in any state* $|\psi\rangle$ *is then* $\langle\psi|[v_i,J_j]|\psi\rangle=\mathrm{i}\sum_k\epsilon_{ijk}\langle\psi|v_k|\psi\rangle$. *Check that with* $U(\boldsymbol{\alpha})=\mathrm{e}^{-\mathrm{i}\boldsymbol{\alpha}\cdot\mathbf{J}}$ *this relation is consistent under a further rotation* $|\psi\rangle\to|\psi'\rangle=U(\boldsymbol{\alpha})|\psi\rangle$ *by evaluating both sides separately.*

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

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

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

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

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

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

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

4.4* *The matrix for rotating an ordinary vector by* ϕ *around the* z *axis is*

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

By considering the form taken by $\mathbf{R}$ *for infinitesimal* ϕ *calculate from* $\mathbf{R}$ *the matrix* $\boldsymbol{\mathcal{J}}_z$ *that appears in* $\mathbf{R}(\phi) = \exp(-\mathrm{i}\boldsymbol{\mathcal{J}}_z\phi)$*. Introduce new coordinates* $u_1 \equiv (-x+\mathrm{i}y)/\sqrt{2}$*,* $u_2 = z$ *and* $u_3 \equiv (x+\mathrm{i}y)/\sqrt{2}$*. 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*

$$\boldsymbol{\mathcal{J}}'_z \equiv \mathbf{M}\cdot\boldsymbol{\mathcal{J}}_z\cdot\mathbf{M}^\dagger. \tag{4.2}$$

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

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

Write down the matrix $\boldsymbol{\mathcal{J}}_x$ *whose exponential generates rotations around the* x *axis, calculate* $\boldsymbol{\mathcal{J}}'_x$ *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

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

comparing coefficients of $\delta\phi$ we find

$$\boldsymbol{\mathcal{J}}_z = \mathrm{i}\begin{pmatrix}0&-1&0\\1&0&0\\0&0&0\end{pmatrix}$$

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

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

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

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

Similarly, we have

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

so

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

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.

4.5 *Determine the commutator* $[\mathcal{J}'_x, \mathcal{J}'_z]$ *of the generators used in Problem 4.4. Show that it is equal to* $-\mathrm{i}\mathcal{J}'_y$*, where* $\mathcal{J}'_y$ *is identical with* S_y *in the set (4.3).*
Soln: This is straightforward extension of the previous problem.

4.6* *Show that if* $\boldsymbol{\alpha}$ *and* $\boldsymbol{\beta}$ *are non-parallel vectors,* $\boldsymbol{\alpha}$ *is not invariant under the combined rotation* $\mathbf{R}(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})$*. Hence show that* $\mathbf{R}^{\mathrm{T}}(\boldsymbol{\beta})\mathbf{R}^{\mathrm{T}}(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})\mathbf{R}(\boldsymbol{\alpha})$ *is not the identity operation. Explain the physical significance of this result.*
Soln: $\mathbf{R}(\boldsymbol{\alpha})\boldsymbol{\alpha} = \boldsymbol{\alpha}$ because a rotation leaves its axis invariant. But the only vectors that are invariant under $\mathbf{R}(\boldsymbol{\beta})$ are multiples of the rotation axis $\boldsymbol{\beta}$. So $\mathbf{R}(\boldsymbol{\beta})\boldsymbol{\alpha}$ is not parallel to $\boldsymbol{\alpha}$.

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

$$\mathbf{R}^{\mathrm{T}}(\boldsymbol{\beta})\mathbf{R}^{\mathrm{T}}(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})\mathbf{R}(\boldsymbol{\alpha})\boldsymbol{\alpha} = \boldsymbol{\alpha} \quad \Rightarrow \quad \mathbf{R}(\boldsymbol{\beta})\mathbf{R}(\boldsymbol{\alpha})\boldsymbol{\alpha} = \mathbf{R}(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})\boldsymbol{\alpha} \quad \Rightarrow \quad \mathbf{R}(\boldsymbol{\beta})\boldsymbol{\alpha} = \mathbf{R}(\boldsymbol{\alpha})(\mathbf{R}(\boldsymbol{\beta})\boldsymbol{\alpha})$$

which would imply that $\mathbf{R}(\boldsymbol{\beta})\boldsymbol{\alpha}$ is invariant under $\mathbf{R}(\boldsymbol{\alpha})$. Consequently we would have $\mathbf{R}(\boldsymbol{\beta})\boldsymbol{\alpha} = \boldsymbol{\alpha}$. But this is true only if $\boldsymbol{\alpha}$ is parallel to $\boldsymbol{\beta}$. So our original hypothesis that $\mathbf{R}^{\mathrm{T}}(\boldsymbol{\beta})\mathbf{R}^{\mathrm{T}}(\boldsymbol{\alpha})\mathbf{R}(\boldsymbol{\beta})\mathbf{R}(\boldsymbol{\alpha}) = \mathbf{I}$ 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*

$$\langle \mathbf{x}|\mathbf{p}\rangle = \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar} \tag{4.4}$$

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* $u_{\mathbf{k}'}(\mathbf{x}) = \mathrm{e}^{-\mathrm{i}\mathbf{a}\cdot\mathbf{k}}u_{\mathbf{k}}(\mathbf{x})$ *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

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

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

4.8 *By expanding the anticommutator on the left and then applying the third rule of the set (2.22), show that any three operators satisfy the identity*

$$[\{A,B\},C] = \{A,[B,C]\} + \{[A,C],B\}. \tag{4.5}$$

Soln:

$$\begin{aligned}[\{A,B\},C] &= [AB,C] + [BA,C] = [A,C]B + A[B,C] + [B,C]A + B[A,C] \\ &= \{A,[B,C]\} + \{[A,C],B\}.\end{aligned}$$

4.9 *Let* P *be the parity operator and* S *an arbitrary scalar operator. Explain why* P *and* S *must commute.*
Soln: A scalar is something that is unaffected by orthogonal transformations of three-dimensional space. These transformations are made up of the rotations and reflections. The parity operator reflects states, so it is a member of the group of transformations under which a scalar is invariant. Consequently S commutes with P.

4.10 *In this problem we consider discrete transformations other than that associated with parity. Let* $\mathcal{S}$ *be a linear transformation on ordinary three-dimensional space that effects a a reflection in a plane. Let* S *be the associated operator on kets. Explain the physical relationship between the kets* $|\psi\rangle$ *and* $|\psi'\rangle \equiv S|\psi\rangle$*. Explain why we can write*

$$\mathcal{S}\langle\psi|\mathbf{x}|\psi\rangle = \langle\psi|S^\dagger \mathbf{x} S|\psi\rangle. \tag{4.6}$$

What are the possible eigenvalues of S*?*

Given that $\mathcal{S}$ reflects in the plane through the origin with unit normal $\hat{\mathbf{n}}$, show, by means of a diagram or otherwise, that its matrix is given by

$$\mathcal{S}_{ij} = \delta_{ij} - 2n_i n_j. \tag{4.7}$$

Determine the form of this matrix in the case that $\mathbf{n} = (1, -1, 0)/\sqrt{2}$. Show that in this case $Sx = yS$ and give an alternative expression for Sy.

Show that a potential of the form

$$V(\mathbf{x}) = f(R) + \lambda xy, \quad \text{where} \quad R \equiv \sqrt{x^2 + y^2} \tag{4.8}$$

satisfies $V(\mathcal{S}\mathbf{x}) = V(\mathbf{x})$ and explain the geometrical significance of this equation. Show that $[S, V] = 0$. Given that E is an eigenvalue of $H = p^2/2m + V$ that has a unique eigenket $|E\rangle$, what equation does $|E\rangle$ satisfy in addition to $H|E\rangle = E|E\rangle$?

Soln: $|\psi'\rangle \equiv S|\psi\rangle$ is the state in which the amplitude to be at the reflected point $\mathbf{x}' = \mathcal{S}\mathbf{x}$ is equal to the amplitude to be at $\mathbf{x}$. The mathematical statement of this fact is

$$\langle \mathbf{x}'|\psi'\rangle = \langle \mathcal{S}\mathbf{x}|\hat{S}|\psi\rangle = \langle \mathbf{x}|\psi\rangle, \tag{4.9}$$

Equation (4.6) states that the expectation value of $\mathbf{x}$ for the reflected state is the reflection of the expectation value of $\mathbf{x}$ for the original state. Since $\mathbf{x} = \mathcal{S}\mathcal{S}\mathbf{x}$ for all $\mathbf{x}$, $S^2 = I$ and the eigenvalues of S have to be ± 1.

$\mathcal{S}$ reverses the component of its target vector that is perpendicular to the plane. Thus we get $\mathbf{x}'$ by taking from $\mathbf{x}$ twice $(\hat{\mathbf{n}} \cdot \mathbf{x})\hat{\mathbf{n}}$:

$$\mathbf{x}' = \mathcal{S}\mathbf{x} = \mathbf{x} - 2(\hat{\mathbf{n}} \cdot \mathbf{x})\mathbf{n} \quad \rightarrow \sum_j \mathcal{S}_{ij} x_j = \sum_j \delta_{ij} x_j - 2(\sum_j n_j x_j) n_i = \sum_j (\delta_{ij} - 2n_i n_j) x_j. \tag{4.10}$$

For the concrete example given, $\hat{\mathbf{n}} = (1, -1, 0)/\sqrt{2}$, so

$$S_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4.11}$$

Since $\mathcal{S}(x, y, z) = (y, x, z)$, we now have

$$\langle x, y, z|Sy|\psi\rangle = \langle y, x, z|y|\psi\rangle = x\langle y, x, z|\psi\rangle, \tag{4.12}$$

where the last equality follows because y, being Hermitian, can be considered to act backwards. But

$$x\langle y, x, z|\psi\rangle = x\langle x, y, z|S|\psi\rangle = \langle x, y, z|xS|\psi\rangle.$$

Consequently, $Sy = xS$. Similarly, $Sx = yS$.

Swapping the x and y coordinates of $\mathbf{x}$ clearly leaves invariant both R and xy and therefore $V(\mathcal{S}\mathbf{x}) = V(\mathbf{x})$. Geometrically a contour plot of V is symmetrical around the line $x = y$, so the potentials at mirrored points are identical.

$$\langle x, y, z|SV|\psi\rangle = \langle y, x, z|V|\psi\rangle = V(y, x, z)\langle y, x, z|\psi\rangle$$

Similarly

$$\langle x, y, z|VS|\psi\rangle = V(x, y, z)\langle x, y, z|S|\psi\rangle = V(x, y, z)\langle y, x, z|\psi\rangle.$$

But $V(x, y, z) = V(y, x, z)$ so for and $|\psi\rangle$ these two expressions are equal, and it follows that $[V, S] = 0$.

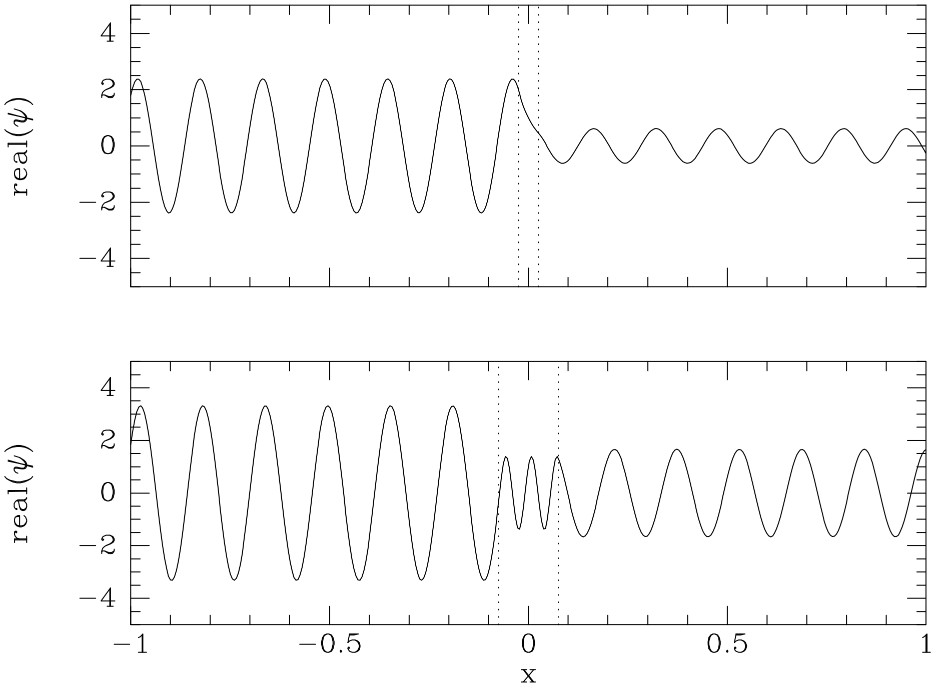


Figure 5.0 The real part of the wavefunction when a free particle of energy E is scattered by a classically forbidden square barrier barrier (top) and a potential well (bottom). The upper panel is for a barrier of height $V_0 = E/0.7$ and half width a such that $2mEa^2/\hbar^2 = 1$. The lower panel is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

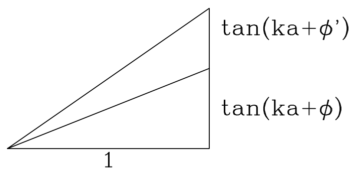


Figure 5.1 A triangle for Problem 5.10

5.7 *Reproduce the plots shown in Figure 5.0 of the wavefunctions of particles that are scattered by a square barrier and a square potential well. Give physical interpretations of as many features of the plots as you can.*

Soln: For the top plot one has to plot the real part of

$$\psi(x) = \begin{cases} B\sin(-kx+\phi) - B'\sin(-kx+\phi') & \text{for } x < -a \\ \cos(Kx) + A\sin(Kx) & \text{for } |x| < a \\ B\sin(kx+\phi) + B'\sin(kx+\phi') & \text{for } x > a \end{cases}$$

where $k = 40$, $a = 1/k$, $K = k\sqrt{1/0.7 - 1}$, $\phi = \arctan((k/K)\coth(Ka)) - ka$, $\phi' = \arctan((k/K)\tanh(Ka)) - ka$, $B = \cosh(Ka)/\sin(ka+\phi)$, $B' = -Be^{i(\phi'-\phi)}$ and $A = B'\sin(ka+\phi')/\sinh(Ka)$. The corresponding equations for the lower panel are $a = 3/k$, $K = k\sqrt{1 + 1/0.2}$, $\phi = -\arctan((k/K)\cot(Ka)) - ka$, $\phi' = \arctan((k/K)\tan(Ka)) - ka$, $B = \cos(Ka)/\sin(ka+\phi)$, $B' = -Be^{i(\phi'-\phi)}$ and $A = B'\sin(ka+\phi')/\sin(Ka)$.

The dotted lines mark the discontinuities in the potential energy. In the barrier we see the exponential decay of the wavefunction through the barrier, which flows into rather a small-amplitude transmitted wave on the right. The profile is close to an exponential because the wave reflected by the right-hand discontinuity is of very low amplitude compared to that transmitted by the left-hand discontinuity. This results in $A \simeq 1$. In the lower panel the shorter wavelength in the well is apparent, indicating that he particle speeds up as it enters the well. Its high speed is also responsible to the wave having lower amplitude in the well than on the right, although the amplitude reduction is modest because in the well particles move in both directions and the flux carried away on the right is only the difference in the fluxes carried each way in the well. In both panels the wave on the left represents particles moving in both senses, but this fact is not apparent from the real part of ψ alone.

5.12 *An electron moves along an infinite chain of potential wells. For sufficiently low energies we can assume that the set $\{|n\rangle\}$ is complete, where $|n\rangle$ is the state of definitely being in the $n^{\rm th}$ well. By analogy with our analysis of the NH_3 molecule we assume that for all n the only non-vanishing matrix elements of the Hamiltonian are $\mathcal{E} \equiv \langle n|H|n\rangle$ and $A \equiv \langle n \pm 1|H|n\rangle$. Give physical interpretations of the numbers A and $\mathcal{E}$.*

Explain why we can write

$$H = \sum_{n=-\infty}^{\infty} \mathcal{E}|n\rangle\langle n| + A\left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right). \tag{5.1}$$

Writing an energy eigenket $|E\rangle = \sum_n a_n|n\rangle$ show that

$$a_m(E-\mathcal{E}) - A\left(a_{m+1} + a_{m-1}\right) = 0. \tag{5.2}$$

Obtain solutions of these equations in which $a_m \propto \mathrm{e}^{ikm}$ and thus find the corresponding energies E_k. Why is there an upper limit on the values of k that need be considered?

Initially the electron is in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|E_k\rangle + |E_{k+\Delta}\rangle\right), \tag{5.3}$$

where $0 < k \ll 1$ and $0 < \Delta \ll k$. Describe the electron's subsequent motion in as much detail as you can.

Soln: $\mathcal{E}$ is the energy of an electron in a well. A is the amplitude for tunnelling through to a neighbouring well. Since the set $\{|n\rangle\}$ may be considered complete, any operator can be written $\sum_{mn} Q_{mn}|m\rangle\langle n|$, where $Q_{mn} = \langle m|Q|n\rangle$ are the operator's matrix elements. In the case of H most of the matrix elements vanish and we are left with the given expression. When $|E\rangle$ is expanded in the $|n\rangle$ basis, the TISE is

$$H|E\rangle = E|E\rangle = E\sum_{n=-\infty}^{\infty} a_n|n\rangle = \sum_{n=-\infty}^{\infty}\left\{\mathcal{E}|n\rangle\langle n| + A\left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right)\right\}\sum_m a_m|m\rangle$$

$$= \sum_{n=-\infty}^{\infty} \mathcal{E}a_n|n\rangle + A\left(a_{n+1}|n\rangle + a_n|n+1\rangle\right)$$

The required recurrence relation is obtained when this eqn is multiplied on the left by $\langle m|$. Substituting in the trial solution $a_m = K\mathrm{e}^{\mathrm{i}km}$ gives

$$0 = \mathrm{e}^{\mathrm{i}km}(E_k - \mathcal{E}) - A\left(\mathrm{e}^{\mathrm{i}k(m+1)} + \mathrm{e}^{\mathrm{i}k(m-1)}\right)$$

Dividing through by $\mathrm{e}^{\mathrm{i}km}$ we find

$$0 = (E_k - \mathcal{E}) - 2A\cos(k)$$

Thus for any k $|k\rangle = K\sum_m \mathrm{e}^{\mathrm{i}km}|m\rangle$ is an energy eigenstate with $E_k = \mathcal{E} + 2A\cos(k)$. However, replacing k with $k' = k + 2r\pi$ changes neither the energy nor the amplitude to be in any well, so it does not provide a physically distinct state. Hence we consider only states with k in the range $(0, 2\pi)$.

Motion is going to be generated by quantum interference between the states $|E_k\rangle$ and $|E_{k+\Delta}\rangle$. The energy difference δE can be estimated by differentiating our expression for E_k:

$$\delta E \simeq -2A\sin(k)\Delta$$

At general time t the state $|\psi\rangle$ is

$$|\psi\rangle = \frac{\mathrm{e}^{-\mathrm{i}E_kt/\hbar}}{\sqrt{2}}\sum_m \mathrm{e}^{\mathrm{i}km}\left(1 + \mathrm{e}^{\mathrm{i}\Delta m - \mathrm{i}\delta Et/\hbar}\right)|m\rangle = \frac{\mathrm{e}^{-\mathrm{i}E_kt/\hbar}}{\sqrt{2}}\sum_m \mathrm{e}^{\mathrm{i}km}\left(1 + \mathrm{e}^{\mathrm{i}\Delta(m+2A\sin(k)t/\hbar)}\right)|m\rangle$$

At some points in the chain, the exponential on the extreme right will cancel on the 1 and the amplitude to be there will vanish. At other points the exponential will be unity so there is a large amplitude to be at these wells. As t increases the points of maximum and minimum amplitude will migrate down the chain as the peaks and troughs of a wave. The speed of this wave is $2A\sin(k)/\hbar$ wells per unit time.

5.13* *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*

$$H = \begin{pmatrix} \overline{E} + q\mathcal{E}s\cos\omega t & -A \\ -A & \overline{E} - q\mathcal{E}s\cos\omega t \end{pmatrix}. \tag{5.4}$$

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

$$|\psi\rangle = a_\mathrm{e}(t)\mathrm{e}^{-\mathrm{i}E_\mathrm{e}t/\hbar}|\mathrm{e}\rangle + a_\mathrm{o}(t)\mathrm{e}^{-\mathrm{i}E_\mathrm{o}t/\hbar}|\mathrm{o}\rangle, \tag{5.5}$$

show that the equations of motion of the expansion coefficients are

$$\begin{aligned} \frac{\mathrm{d}a_\mathrm{e}}{\mathrm{d}t} &= -\mathrm{i}\Omega a_\mathrm{o}(t)\Big(\mathrm{e}^{\mathrm{i}(\omega-\omega_0)t} + \mathrm{e}^{-\mathrm{i}(\omega+\omega_0)t}\Big) \\ \frac{\mathrm{d}a_\mathrm{o}}{\mathrm{d}t} &= -\mathrm{i}\Omega a_\mathrm{e}(t)\Big(\mathrm{e}^{\mathrm{i}(\omega+\omega_0)t} + \mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}\Big), \end{aligned} \tag{5.6}$$

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

$$\frac{\mathrm{d}a_\mathrm{e}}{\mathrm{d}t} = -\mathrm{i}\Omega a_\mathrm{o}(t)\mathrm{e}^{\mathrm{i}(\omega-\omega_0)t} \quad ; \quad \frac{\mathrm{d}a_\mathrm{o}}{\mathrm{d}t} = -\mathrm{i}\Omega a_\mathrm{e}(t)\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}. \tag{5.7}$$

Solve the equations by multiplying the first equation by $\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}$ 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 (5.7).

Soln: We have

$$\begin{aligned} \langle\mathrm{e}|H|\mathrm{e}\rangle &= \tfrac{1}{2}\left(\langle+| + \langle-|\right) H \left(|+\rangle + |-\rangle\right) \\ &= \tfrac{1}{2}\left(\langle+|H|+\rangle + \langle-|H|-\rangle + \langle-|H|+\rangle + \langle+|H|-\rangle\right) \\ &= \overline{E} - A = E_\mathrm{e} \\ \langle\mathrm{o}|H|\mathrm{o}\rangle &= \tfrac{1}{2}\left(\langle+| - \langle-|\right) H \left(|+\rangle - |-\rangle\right) \\ &= \tfrac{1}{2}\left(\langle+|H|+\rangle + \langle-|H|-\rangle - \langle-|H|+\rangle - \langle+|H|-\rangle\right) \\ &= \overline{E} + A = E_\mathrm{o} \\ \langle\mathrm{o}|H|\mathrm{e}\rangle = \langle\mathrm{e}|H|\mathrm{o}\rangle &= \tfrac{1}{2}\left(\langle+| + \langle-|\right) H \left(|+\rangle - |-\rangle\right) \\ &= \tfrac{1}{2}\left(\langle+|H|+\rangle - \langle-|H|-\rangle + \langle-|H|+\rangle - \langle+|H|-\rangle\right) \\ &= q\mathcal{E}s\cos(\omega t) \end{aligned}$$

Now we use the TDSE to calculate the evolution of $|\psi\rangle = a_\mathrm{e}\mathrm{e}^{-\mathrm{i}E_\mathrm{e}t/\hbar}|\mathrm{e}\rangle + a_\mathrm{o}\mathrm{e}^{-\mathrm{i}E_\mathrm{o}t/\hbar}|\mathrm{o}\rangle$:

$$\mathrm{i}\hbar\frac{\partial|\psi\rangle}{\partial t} = \mathrm{i}\hbar\dot{a}_\mathrm{e}\mathrm{e}^{-\mathrm{i}E_\mathrm{e}t/\hbar}|\mathrm{e}\rangle + a_\mathrm{e}E_\mathrm{e}\mathrm{e}^{-\mathrm{i}E_\mathrm{e}t/\hbar}|\mathrm{e}\rangle + \mathrm{i}\hbar\dot{a}_\mathrm{o}\mathrm{e}^{-\mathrm{i}E_\mathrm{o}t/\hbar}|\mathrm{o}\rangle + a_\mathrm{o}E_\mathrm{o}\mathrm{e}^{-\mathrm{i}E_\mathrm{o}t/\hbar}|\mathrm{o}\rangle = a_\mathrm{e}\mathrm{e}^{-\mathrm{i}E_\mathrm{e}t/\hbar}H|\mathrm{e}\rangle + a_\mathrm{o}\mathrm{e}^{-\mathrm{i}E_\mathrm{o}t/\hbar}H|\mathrm{o}\rangle$$

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

$$\begin{aligned} \mathrm{i}\hbar\dot{a}_\mathrm{e} + a_\mathrm{e}E_\mathrm{e} &= a_\mathrm{e}\langle\mathrm{e}|H|\mathrm{e}\rangle + a_\mathrm{o}\mathrm{e}^{\mathrm{i}(E_\mathrm{e}-E_\mathrm{o})t/\hbar}\langle\mathrm{e}|H|\mathrm{o}\rangle \\ \mathrm{i}\hbar\dot{a}_\mathrm{o} + a_\mathrm{o}E_\mathrm{o} &= a_\mathrm{e}\mathrm{e}^{\mathrm{i}(E_\mathrm{o}-E_\mathrm{e})t/\hbar}\langle\mathrm{o}|H|\mathrm{e}\rangle + a_\mathrm{o}\langle\mathrm{o}|H|\mathrm{o}\rangle \end{aligned}$$

With the results derived above

$$\mathrm{i}\hbar\dot a_{\rm e}+a_{\rm e}E_{\rm e}=a_{\rm e}E_{\rm e}+a_{\rm o}\mathrm{e}^{\mathrm{i}(E_{\rm e}-E_{\rm o})t/\hbar}q\mathcal{E}s\cos(\omega t)$$
$$\mathrm{i}\hbar\dot a_{\rm o}+a_{\rm o}E_{\rm o}=a_{\rm e}\mathrm{e}^{\mathrm{i}(E_{\rm o}-E_{\rm e})t/\hbar}q\mathcal{E}s\cos(\omega t)+a_{\rm o}E_{\rm o}$$

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 $\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}$ and differentiating gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}\dot a_{\rm e}\right)=\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}\left[-\mathrm{i}(\omega-\omega_0)\dot a_{\rm e}+\ddot a_{\rm e}\right]=-\Omega^2a_{\rm e}\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}$$

The exponentials cancel leaving a homogeneous second-order o.d.e. with constant coefficients. Since initially all molecules are in the higher-energy state $|\mathrm{o}\rangle$, we have to solve subject to the boundary condition $a_{\rm e}(0)=0$. With $a_0(0)=1$ we get from the original equations the second initial condition $\dot a_{\rm e}(0)=-\mathrm{i}\Omega$. For trial solution $a_{\rm e}\propto\mathrm{e}^{\alpha t}$ the auxiliary eqn is

$$\alpha^2-\mathrm{i}(\omega-\omega_0)\alpha+\Omega^2=0\quad\Rightarrow\quad\alpha=\tfrac12\left[\mathrm{i}(\omega-\omega_0)\pm\sqrt{-(\omega-\omega_0)^2-4\Omega^2}\right]=\mathrm{i}\omega_\pm$$

with $\omega\pm=\frac12\left[(\omega-\omega_0)\pm\sqrt{(\omega-\omega_0)^2+4\Omega^2}\right]$. When $\omega\simeq\omega_0$, these frequencies both lie close to Ω. From the condition $a_{\rm e}(0)=0$, the required solution is $a_{\rm e}(t)\propto(\mathrm{e}^{\mathrm{i}\omega_+t}-\mathrm{e}^{\mathrm{i}\omega_-t})$ and the constant of proportionality follows from the second initial condition, so finally

$$a_{\rm e}(t)=\frac{-\Omega}{\sqrt{(\omega-\omega_0)^2+4\Omega^2}}(\mathrm{e}^{\mathrm{i}\omega_+t}-\mathrm{e}^{\mathrm{i}\omega_-t})\qquad(*)$$

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

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

$$a_{\rm e}(t)=\tfrac12(\mathrm{e}^{-\mathrm{i}\Omega t}-\mathrm{e}^{\mathrm{i}\Omega t}),$$

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

5.14 *^{238}U decays by α emission with a mean lifetime of* 6.4 Gyr. *Take the nucleus to have a diameter $\sim 10^{-14}$ m and suppose that the α particle has been bouncing around within it at speed $\sim c/3$. Modelling the potential barrier that confines the α particle to be a square one of height V_0 and width $2a$, give an order-of-magnitude estimate of $W=(2mV_0a^2/\hbar^2)^{1/2}$. Given that the energy released by the decay is ~ 4 MeV and the atomic number of uranium is $Z=92$, estimate the width of the barrier through which the α particle has to tunnel. Hence give a very rough estimate of the barrier's typical height. Outline numerical work that would lead to an improved estimate of the structure of the barrier.*

Soln: The time between impacts with the wall is $\sim 10^{-14}/10^8$ s, so in 6.4 Gyr $\simeq 2\times10^{17}$ s the α makes $\sim 2\times10^{39}$ escape attempts and the probability of any one attempt succeeding is $\sim 5\times10^{-40}$. This probability is $\sin^2(\Delta\phi)\simeq(4k/K)^2\mathrm{e}^{-4W}$. Taking $4k/K$ to be order unity, we conclude that $W=\frac14\ln(10^{39})=22.5$.

The distance $2a$ from the nucleus at which the α becomes classically allowed is that at which its energy of electrostatic repulsion from the thorium nucleus ($Z=92-2=90$) is 4 MeV: $2a=2\times90e^2/(4\pi\epsilon_0 4\times10^6e)=6.5\times10^{-14}$ m. If the barrier were square rather than wedge shaped, it would not be so thick, so let's adopt $2a=3\times10^{-14}$ m. Then $V_0=(22.5\hbar/a)^2/8m_{\rm p}\simeq1.6\times10^{-12}\,\mathrm{J}\simeq 10$ MeV.

This calculation has two major problems: (a) the assumption of a square barrier instead of a skew and sharply peaked one, and (b) the use of a one-dimensional rather than spherical model given that α becomes allowed at a radius that is significantly greater than the radius of the nucleus. Problem (a) is probably the most serious and could be addressed by numerically solving the one-d TISE as in Problem 5.15. To address problem (b) we would solve the radial wavefunction for a particle with vanishing angular momentum.

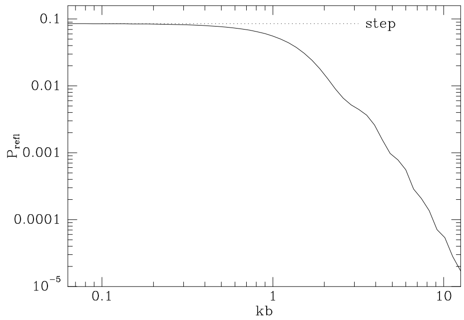


Figure 5.2 The symbols show the ratio of the probability of reflection to the probability of transmission when particles move from $x = -\infty$ in the potential (5.69) with energy $E = \hbar^2k^2/2m$ and $V_0 = 0.7E$. The dotted line is the value obtained for a step change in the potential

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

$$V(x) = V_0 \begin{cases} 0 & \text{for } x < -a \\ \frac{1}{2}[1 + \sin(\pi x/2a)] & \text{for } |x| < a \\ 1 & \text{for } x > a, \end{cases} \tag{5.8}$$

where $V_0 < \hbar^2k^2/2m$. 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 Δ is a small increment in the x coordinate. From the TISE *show that*

$$\psi_j \simeq (2 - \Delta^2k^2)\psi_{j+1} - \psi_{j+2}, \tag{5.9}$$

where $k \equiv \sqrt{2m(E - V)}/\hbar$. Determine ψ_j at the two grid points with the largest values of x from a suitable boundary condition, and use the recurrence relation (5.9) to determine ψ_j at all other grid points. By matching the values of ψ 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 ψ in the case that there is negligible reflection. Compute this approximate form of ψ and compare it with your numerical results for larger values of a.

Soln:

We discretise the TISE

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

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

$$A_+ \exp(\mathrm{i}0k\Delta) + A_- \exp(-\mathrm{i}0k\Delta) = \psi_0$$
$$A_+ \exp(\mathrm{i}1k\Delta) + A_- \exp(-\mathrm{i}1k\Delta) = \psi_1$$

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

5.16* *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 θ, $\coth\theta - \tanh\theta \simeq 4\mathrm{e}^{-2\theta}$. Next letting δk be the difference between the k values that solve*

$$\tan\left[r\pi - k(b-a)\right]\sqrt{\frac{W^2}{(ka)^2} - 1} = \begin{cases} \coth\left(\sqrt{W^2 - (ka)^2}\right) & \text{even parity} \\ \tanh\left(\sqrt{W^2 - (ka)^2}\right) & \text{odd parity,} \end{cases} \tag{5.10a}$$

where

$$W \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}} \tag{5.10b}$$

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

$$\left\{\left[\left(\frac{W^2}{(ka)^2}-1\right)^{1/2}+\left(\frac{W^2}{(ka)^2}-1\right)^{-1/2}\right](b-a)+\frac{1}{k}\left(1-\frac{(ka)^2}{W^2}\right)^{-1}\right\}\delta k \\ \simeq -4\exp\left[-2\sqrt{W^2-(ka)^2}\right]. \tag{5.11}$$

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

$$\frac{\delta E}{E}\simeq\frac{-8a}{W(b-a)}\,\mathrm{e}^{-2W\sqrt{1-E/V_0}}. \tag{5.12}$$

Soln: First

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

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 δk in the solutions. That is

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

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

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

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

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

Since $E=\hbar^2k^2/2m$, $\delta E/E=2\delta k/k$ 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 ($).

6.3 *Given that the state $|\mathrm{AB}\rangle$ of a compound system can be written as a product $|\mathrm{A}\rangle|\mathrm{B}\rangle$ of states of the individual systems, show that when $|\mathrm{AB}\rangle$ is written as $\sum_{ij}c_{ij}|\mathrm{A};i\rangle|\mathrm{B};j\rangle$ in terms of arbitrary basis vectors for the subsystems, every column of the matrix c_{ij} is a multiple of the leftmost column.*
Soln: If $|\mathrm{A}\rangle=\sum_i a_i|\mathrm{A};i\rangle$ and similarly for $|\mathrm{B}\rangle$, $c_{ij}=a_ib_j$, so the ratio of corresponding terms in the j^{th} and k^{th} column is $c_{ij}/c_{ik}=b_j/b_k$ is independent of i as required.

6.6 *Show that when the Hadamard operator U_{H} is applied to every qubit of an n-qubit register that is initially in a member $|m\rangle$ of the computational basis, the resulting state is*

$$|\psi\rangle=\frac{1}{2^{n/2}}\sum_{x=0}^{2^n-1}a_x|x\rangle, \tag{6.1}$$

where $a_x=1$ for all x if $m=0$, but exactly half the $a_x=1$ and the other half the $a_x=-1$ for any other choice of m. Hence show that

$$\frac{1}{2^{n/2}}U_{\mathrm{H}}\sum_x a_x|x\rangle=\begin{cases}|0\rangle & \text{if all } a_x=1\\ |m\rangle\neq|0\rangle & \text{if half the } a_x=1 \text{ and the other } a_x=-1.\end{cases} \tag{6.2}$$

Soln: We are given that the register is in a member of the computational basis, so each of its qubits is in either the state $|0\rangle$ or the state $|1\rangle$. The Hadamard operator puts the $r^{\rm th}$ qubit into the state $(|0\rangle+|1\rangle)/\sqrt{2}$ if it was in the state $|0\rangle$ and $(|0\rangle-|1\rangle)/\sqrt{2}$ if it was in the state $|1\rangle$. So if $|m\rangle = |0\rangle = |0\rangle \times \cdots |0\rangle$ the Hadamard operators produce $U^n|0\rangle = \frac{1}{2^{n/2}}(|0\rangle+|1\rangle)(|0\rangle+|1\rangle)\cdots(|0\rangle+|1\rangle)$. When we multiply this up we get every possible sequence of $|0\rangle$ and $|1\rangle$ exactly once and all added together.

Each original qubit that is $|1\rangle$ gives rise to a factor $(|0\rangle-|1\rangle)$. Multiply all the factors $(|0\rangle+|1\rangle)$ together to get all positive terms. Then multiply in the first factor $(|0\rangle-|1\rangle)$ and half the resulting terms will be positive and half negative from the factor $-|1\rangle$. When we multiply by the next factor $(|0\rangle-|1\rangle)$ half of the existing terms will change sign and half will retain their sign. Hence we will still have half positive and half negative terms. The required result now follows by induction.

6.7 *Show that the trace of every Hermitian operator is real.*
Soln: Since the trace is invariant under unitary transformations, it is equal to the sum of the operator's eigenvalues. But these are all real.

6.8 *Let ρ be the density operator of a two-state system. Explain why ρ can be assumed to have the matrix representation*

$$\rho = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix}, \tag{6.3}$$

where a and b are real numbers. Let E_0 and $E_1 > E_0$ be the eigenenergies of this system and $|0\rangle$ and $|1\rangle$ the corresponding stationary states. Show from the equation of motion of ρ that in the energy representation a and b are time-independent while $c(t) = c(0)\mathrm{e}^{\mathrm{i}\omega t}$ with $\omega = (E_1 - E_0)/\hbar$.

Determine the values of a, b and $c(t)$ for the case that initially the system is in the state $|\psi\rangle = (|0\rangle+|1\rangle)/\sqrt{2}$. Given that the parities of $|0\rangle$ and $|1\rangle$ are even and odd respectively, find the time evolution of the expectation value $\overline{x}$ in terms of the matrix element $\langle 0|x|1\rangle$. Interpret your result physically.
Soln: The density operator is Hermitian and any 2×2 Hermitian matrix can be written thus. With this form of ρ and in the E representation, the equation of motion is

$$\mathrm{i}\hbar\begin{pmatrix} \dot a & \dot c \\ \dot c^* & \dot b \end{pmatrix} = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}\begin{pmatrix} a & c \\ c^* & b \end{pmatrix} - \begin{pmatrix} a & c \\ c^* & b \end{pmatrix}\begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix} = (E_1 - E_0)\begin{pmatrix} 0 & -c \\ c^* & 0 \end{pmatrix}$$

So a and b are constant and c satisfies $\dot c = \mathrm{i}\omega c$, and the required form of $c(t)$ follows trivially.

For the given initial condition

$$\rho(0) = \tfrac12(|0\rangle+|1\rangle)(\langle 0|+\langle 1|) \quad\Rightarrow\quad \rho(0) = \tfrac12\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

We get $\rho(t)$ from our solutions to the equations of motion of a, b and c. From the given parity condition we know that the diagonal elements of the matrix for x vanish, so

$$\overline{x} = \tfrac12\,\mathrm{Tr}\begin{pmatrix} 1 & \mathrm{e}^{\mathrm{i}\omega t} \\ \mathrm{e}^{-\mathrm{i}\omega t} & 1 \end{pmatrix}\begin{pmatrix} 0 & x_{01} \\ x_{01}^* & 0 \end{pmatrix} = x_{01}\mathrm{e}^{\mathrm{i}\omega t} + x_{01}^*\mathrm{e}^{-\mathrm{i}\omega t} = 2|x_{01}|\cos(\omega t + \phi_{01}),$$

where $\phi_{01} = \arg(x_{01})$. We have recovered a result familiar from our study of the harmonic oscillator: oscillations occur at the frequency associated with the energy difference between adjacent stationary states as a result of interference between the amplitudes of these states.

6.9 *In this problem we consider an alternative interpretation of the density operator. Any quantum state can be expanded in the energy basis as*

$$|\psi;\boldsymbol{\phi}\rangle \equiv \sum_{n=1}^{N}\sqrt{p_n}\,\mathrm{e}^{\mathrm{i}\phi_n}|n\rangle, \tag{6.4}$$

where ϕ_n is real and p_n is the probability that a measurement of energy will return E_n. Suppose we know the values of the p_n but not the values of the phases ϕ_n. Then the density operator is

$$\rho = \int_0^{2\pi}\frac{\mathrm{d}^N\boldsymbol{\phi}}{(2\pi)^N}|\psi;\boldsymbol{\phi}\rangle\langle\psi;\boldsymbol{\phi}|. \tag{6.5}$$

Show that this expression reduces to $\sum_n p_n|n\rangle\langle n|$. Contrast the physical assumptions made in this derivation of ρ with those made in §6.3.

Clearly $|\psi;\boldsymbol{\phi}\rangle$ can be expanded in some other basis $\{|q_r\rangle\}$ as

$$|\psi;\boldsymbol{\phi}\rangle \equiv \sum_r \sqrt{P_r}\,\mathrm{e}^{\mathrm{i}\eta_r}|q_r\rangle, \tag{6.6}$$

where P_r is the probability of obtaining q_r on a measurement of the observable Q and the $\eta_r(\boldsymbol{\phi})$ are unknown phases. Why does this second expansion not lead to the erroneous conclusion that ρ is necessarily diagonal in the $\{|q_r\rangle\}$ representation?

Soln: In §6.3 we assumed that the system was in an (unknown) eigenstate $|n\rangle$, which is in practice usually taken to be a stationary state. This is an improbable assumption. Here we assume that the system is in a generic and non-stationary state. So this physical interpretation of the density operator is superior to our earlier one.

In equation (6.5) we assume that all values of the phases ϕ_n are equally likely. Assuming that all values of the phases η_r are equally likely will lead to ρ being diagonal in the $\{|q_r\rangle\}$ representaton. By substituting

$$|n\rangle = \sum_r |\langle q_r|n\rangle|\,\mathrm{e}^{\mathrm{i}\chi_{nr}}|q_r\rangle$$

into (6.4), we can show that

$$\eta_r(\boldsymbol{\phi}) = \frac{1}{\mathrm{i}}\ln\left(\sum_n \sqrt{\frac{p_n}{P_r}}|\langle q_r|n\rangle|\,\mathrm{e}^{\mathrm{i}(\phi_n+\chi_{nr})}\right).$$

Thus the dependence of η_r on the ϕ_n is highly non-linear, and a uniform distribution in the ϕ_n will in general not correspond to a uniform distribution in the η_r.

6.10* *Show that when the density operator takes the form $\rho = |\psi\rangle\langle\psi|$, the expression $\overline{Q} = \mathrm{Tr}\,Q\rho$ 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 ρ yields*

$$|\phi\rangle\langle\psi| = |\psi\rangle\langle\phi| \quad \textit{where} \quad |\phi\rangle \equiv \mathrm{i}\hbar\frac{\partial|\psi\rangle}{\partial t} - H|\psi\rangle. \tag{6.7}$$

Show from this equation that $|\phi\rangle = a|\psi\rangle$, where a is real. Hence determine the time evolution of $|\psi\rangle$ given the at $t=0$ $|\psi\rangle = |E\rangle$ is an eigenket of H. Explain why ρ 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:

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

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 ρ we have

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

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

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

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

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

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 ρ is invariant under the transformation $|\psi\rangle \to e^{-i\chi}|\psi\rangle$, where χ is any real number.

6.11 *The density operator is defined to be $\rho = \sum_\alpha p_\alpha |\alpha\rangle\langle\alpha|$, where p_α is the probability that the system is in the state α. Given an arbitrary basis $\{|i\rangle\}$ and the expansions $|\alpha\rangle = \sum_i a_{\alpha i}|i\rangle$, calculate the matrix elements $\rho_{ij} = \langle i|\rho|j\rangle$ of ρ. Show that the diagonal elements ρ_{ii} are non-negative real numbers and interpret them as probabilities.*
Soln:

$$\rho = \sum_{\alpha ij} p_\alpha a_{\alpha i} a^*_{\alpha j} \rho_{ij} |i\rangle\langle j| \quad \Rightarrow \quad \rho_{ij} = \sum_\alpha p_\alpha a_{\alpha i} a^*_{\alpha j}$$

The diagonal element $\rho_{ii} = \sum_\alpha p_\alpha |a_{\alpha i}|^2$ is the product of two non-negative real numbers so it's real non-negative itself.

Consider the observable $Q = |i\rangle\langle i|$ which is diagonal in the given basis and has eigenvalues 1 and 0: you measure unity if the system is in the state $|i\rangle$ and zero otherwise. $\rho_{ii} = \mathrm{Tr}(Q\rho) = \overline{Q}$ is the expectation value of Q. Consequently it's the probability that if you measure Q you force the system into the state $|i\rangle$. Loosely speaking we can consider ρ_{ii} to be the probability of finding the system in the state $|i\rangle$.

6.12 *Consider the density operator $\rho = \sum_{ij} \rho_{ij}|i\rangle\langle j|$ of a system that is in a pure state. Show that every row of the matrix ρ_{ij} is a multiple of the first row and every column is a multiple of the first column. Given that these relations between the rows and columns of a density matrix hold, show that the system is in a pure state. Hint: exploit the real, non-negativity of ρ_{11} established in Problem 6.11 and the Hermiticity of ρ.*
Soln: Since the system is in a pure state $|\psi\rangle = \sum_i a_i|i\rangle$, $\rho = |\psi\rangle\langle\psi|$. So $\rho_{ij} = a_i a_j^*$. The ratio of the values of the j^{th} elements in the i^{th} and k^{th} rows is

$$\frac{\rho_{ij}}{\rho_{kj}} = \frac{a_i}{a_k}$$

which is independent of j as required. Similarly, the ratio of the i^{th} elements of the j^{th} and k^{th} columns, a_j^*/a_k^* is independent of i.

Conversely, given these relations we recall that the diagonal elements of ρ are real and non-negative so we may define $a_1 = \sqrt{\rho_{11}}$. For $j > 1$ we define $a_j \equiv (\rho_{1j}/a_1)^*$. Then from the condition that each row is a multiple of the top row, there must be numbers b_j such that

$$\rho = \begin{pmatrix} |a_1|^2 & a_1 a_2^* & a_1 a_3^* & \dots \\ b_2|a_1|^2 & b_2 a_1 a_2^* & b_2 a_1 a_3^* & \dots \\ b_3|a_1|^2 & b_3 a_1 a_2^* & b_3 a_1 a_3^* & \dots \end{pmatrix}$$

But ρ is Hermitian, so

$$b_2|a_1|^2 = b_1^* a_1^* a_2 \quad \Rightarrow \quad b_2 = a_2/a_1$$
$$b_3|a_1|^2 = b_1^* a_1^* a_3 \quad \Rightarrow \quad b_3 = a_3/a_1$$

This completes the proof that $\rho_{ij} = a_i a_j^*$, from which it follows that $\rho = |\psi\rangle\langle\psi|$ with $|\psi\rangle = \sum_i a_i|i\rangle$.

6.13 *Consider the rate of change of the expectation of the observable Q when the system is in an impure state. This is*

$$\frac{d\overline{Q}}{dt} = \sum_n p_n \frac{d}{dt}\langle n|Q|n\rangle, \tag{6.8}$$

where p_n is the probability that the system is in the state $|n\rangle$. By using Ehrenfest's theorem to evaluate the derivative on the right of (6.8), derive the equation of motion $i\hbar d\overline{Q}/dt = \mathrm{Tr}(\rho[Q,H])$.
Soln: Using Ehrenfest to replace each derivative of $\langle n|Q|n\rangle$ we get

$$\frac{d\overline{Q}}{dt} = \frac{1}{i\hbar}\sum_n p_n \langle n|[Q,H]|n\rangle, \tag{6.9}$$

But

$$\mathrm{Tr}(\rho[Q,H]) = \sum_{n,i} \langle n|i\rangle p_i \langle i|[Q,H]|n\rangle = \sum_n p_n \langle n|[Q,H]|n\rangle.$$

The result follows on substituting for $\langle n|[Q,H]|n\rangle$ in the previous equation.

6.14 *Find the probability distribution $(p_1,\ldots,p_n)$ for n possible outcomes that maximises the Shannon entropy. Hint: use a Lagrange multiplier.*
Soln: Bearing in mind the requirement for the p_i to be normalised, we set to zero each derivative $\partial/\partial p_j$ of

$$S=\sum_i p_i \ln p_i+\lambda\left(\sum_i p_i-1\right)$$

and obtain

$$0=\ln p_j-1+\lambda \quad \Rightarrow \quad p_j=\mathrm{e}^{1-\lambda}.$$

Thus the p_i are all equal, and from the normalisation condition they must equal $1/n$.

6.15 *Use Lagrange multipliers λ and β to extremise the Shannon entropy of the probability distribution $\{p_i\}$ subject to the constraints (i) $\sum_i p_i=1$ and (ii) $\sum_i p_iE_i=U$. Explain the physical significance of your result.*
Soln: We set to zero each derivative $\partial/\partial p_j$ of

$$S=\sum_i p_i \ln p_i+\lambda\left(\sum_i p_i-1\right)+\beta\left(\sum_i p_iE_i-U\right)$$

and obtain

$$0=\ln p_j-1+\lambda+\beta E_j \quad \Rightarrow \quad p_j=\mathrm{e}^{1-\lambda}\mathrm{e}^{-\beta E_j}.$$

We determine λ from the condition $\sum_i p_i=1$, so $\mathrm{e}^{\lambda-1}$ is the partition function Z. We determine β from the condition that the expectation of the energy is U: β is the inverse temperature $1/k_\mathrm{B}T$ because the smaller it is the higher U is. This calculation establishes that the Gibbs distribution maximises the Shannon entropy of the system subject to the given constraints.

6.16 *A composite system is formed from uncorrelated subsystem A and subsystem B, both in impure states. The numbers $\{p_{\mathrm{A}i}\}$ are the probabilities of the members of the complete set of states $\{|\mathrm{A};i\rangle\}$ for subsystem A, while the numbers $\{p_{\mathrm{B}i}\}$ are the probabilities of the complete set of states $\{|\mathrm{B};i\rangle\}$ for subsystem B. Show that the Shannon entropy of the composite system is the sum of the Shannon entropies of its subsystems. What is the relevance of this result for thermodynamics?*
Soln: The state $|\mathrm{AB};ij\rangle$ of the composite system has probability $p_{ij}=p_{\mathrm{A}i}p_{\mathrm{B}j}$ so the Shannon entropy of the whole system is

$$\begin{aligned}s&=\sum_{ij}p_{ij}\ln(p_{ij})=\sum_{ij}p_{\mathrm{A}i}p_{\mathrm{B}j}\ln(p_{\mathrm{A}i})+\sum_{ij}p_{\mathrm{A}i}p_{\mathrm{B}j}\ln(p_{\mathrm{B}j})=\sum_i p_{\mathrm{A}i}\ln(p_{\mathrm{A}i})+\sum_j p_{\mathrm{B}j}\ln(p_{\mathrm{B}j})\\&=s_\mathrm{A}+s_\mathrm{B}\end{aligned}$$

where we've used the normalisation conditions $\sum_i p_{\mathrm{A}i}=1$, etc. This result establishes that entropy is an "extensive" thermodynamic quantity: the entropy of two litres of water at 20°C is twice the entropy of two one-litre bottles of water at the same temperature.

6.17 *The $|0\rangle$ state of a qubit has energy 0, while the $|1\rangle$ state has energy ϵ. Show that when the qubit is in thermodynamic equilibrium at temperature $T=1/(k_\mathrm{B}\beta)$ the internal energy of the qubit is*

$$U=\frac{\epsilon}{\mathrm{e}^{\beta\epsilon}+1}. \tag{6.10}$$

Show that when $\beta\epsilon\ll 1$, $U\simeq\frac{1}{2}\epsilon$, while for $\beta\epsilon\gg 1$, $U\simeq\epsilon\mathrm{e}^{-\beta\epsilon}$. Interpret these results physically and sketch the specific heat $C=\partial U/\partial T$ as a function of T.
Soln: The partition function is

$$Z=1+\mathrm{e}^{-\beta\epsilon}$$

so the internal energy is

$$U=-\frac{\partial \ln Z}{\partial\beta}=\frac{\epsilon\mathrm{e}^{-\beta\epsilon}}{1+\mathrm{e}^{-\beta\epsilon}}=\frac{\epsilon}{\mathrm{e}^{\beta\epsilon}+1}.$$

When $\beta\epsilon\ll 1$ we can approximate $\mathrm{e}^{\beta\epsilon}\simeq 1+\beta\epsilon$ and then binomial-expand the denominator in U:

$$U\simeq\frac{\epsilon}{2+\beta\epsilon}\simeq\tfrac{1}{2}\epsilon(1-\beta\epsilon+\cdots)$$

When $\beta\epsilon \gg 1$ we neglect unity in the denominator obtaining $U \simeq \epsilon e^{-\beta\epsilon}$.

When $\beta\epsilon \ll 1$ the system is hot and the qubit is nearly as likely to be in either of its two states, so the expectation value of the energy is the average of 0 and ϵ. When $\beta\epsilon \gg 1$, the system is cold and the probability of being in the excited state is $\sim e^{-\beta\epsilon} \ll 1$ so the expectation value of the energy is this probability times ϵ.

6.18 *Show that the partition function of a harmonic oscillator of natural frequency ω is*

$$Z_{\rm ho} = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}. \tag{6.11}$$

Hence show that when the oscillator is at temperature $T = 1/(k_B\beta)$ the oscillator's internal energy is

$$U_{\rm ho} = \hbar\omega\left(\tfrac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right). \tag{6.12}$$

Interpret the factor $(e^{\beta\hbar\omega} - 1)^{-1}$ physically. Show that the specific heat $C = \partial U/\partial T$ is

$$C = k_B \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}(\beta\hbar\omega)^2. \tag{6.13}$$

Show that $\lim_{T\to 0} C = 0$ and obtain a simple expression for C when $k_BT \gg \hbar\omega$.

Soln: The partition function is

$$Z = \sum_{n=0}^{\infty} e^{-(n+1/2)\beta\hbar\omega} = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty} z^n = e^{-\beta\hbar\omega/2}\frac{1}{1-z}$$

where $z \equiv e^{-\beta\hbar\omega}$. Differentiating we obtain

$$U = -\frac{\partial \ln Z}{\partial\beta} = -\frac{\partial}{\partial\beta}\left\{-\tfrac{1}{2}\beta\hbar\omega - \ln(1-z)\right\} = \tfrac{1}{2}\hbar\omega + \frac{\hbar\omega z}{1-z}$$

and the required result follows on dividing through by z.

The factor $(e^{\beta\hbar\omega} - 1)^{-1}$ is the mean number of excitations that the oscillator has. As β becomes small (high T) this number becomes large as expected. Differentiating this factor w.r.t. T we obtain the required expression for C.

As $T \to 0$, $\beta \to \infty$ and we can neglect the unity in the denominator for C, so $C/k_B \to e^{-\beta\hbar\omega}(\beta\hbar\omega)^2$ which goes to zero on account of the exponential. When $k_BT \gg \hbar\omega$, $\beta\hbar\omega \ll 1$ and we can Taylor expand the exponentials in C, finding

$$\frac{C}{k_B} \simeq \frac{1 + \beta\hbar\omega + \cdots}{(1 + \beta\hbar\omega/2 + \cdots)^2} \simeq 1$$

This is in accordance with the classical principle of equipartition under which the oscillator will have $\frac{1}{2}k_BT$ of both kinetic and potential energy.

6.19 *A classical ideal monatomic gas has internal energy $U = \frac{3}{2}Nk_BT$ and pressure $P = Nk_BT/\mathcal{V}$, where N is the number of molecules and $\mathcal{V}$ is the volume they occupy. From these relations, and assuming that the entropy vanishes at zero temperature and volume, show that in general the entropy is*

$$S(T,\mathcal{V}) = Nk_B(\tfrac{3}{2}\ln T + \ln\mathcal{V}). \tag{6.14}$$

A removable wall divides a cylinder into equal parts of volume $\mathcal{V}$. Initially the wall is in place and each half contains N molecules of ideal monatomic gas at temperature T. The wall is removed. Show that equation (6.14) implies that the entropy of the entire body of fluid increases by $2\ln 2\, Nk_B$. Can this result be squared with the principle that $dS = dQ/T$, where dQ is the heat absorbed when the change is made reversibly? What conclusion do you draw from this thought experiment?

Soln: Heating the gas up at constant volume (so $TdS = dU = \frac{3}{2}Nk_BdT$) we conclude that $S(T,V) = \frac{3}{2}Nk_B\ln T + f(V)$, where f is an arbitrary function. Expanding our system at constant temperature (and therefore constant U) we have $0 = TdS - PdV$ which implies $dS = Nk_BdV/V \Rightarrow S = Nk_B\ln V + g(T)$. Using our earlier result to identify g, we obtain the required result.

Initially the total entropy is $S_\mathrm{i} = 2Nk_\mathrm{B}(\frac{3}{2}\ln T + \ln V)$. Since only V changes, it is finally $S_\mathrm{f} = 2Nk_\mathrm{B}[\frac{3}{2}\ln T + \ln(2V)]$, and we obtain the required increase. This result is clearly incompatible with $\mathrm{d}S = \mathrm{d}Q_\mathrm{rev}/T$ because no heat enters the cylinder as the wall is withdrawn. If some molecules could be identified as being initially in the right end of the cylinder, and others as being in the left end, there *would* be a loss of information on withdrawing the wall because with the wall out you would be more uncertain where any *particular* molecule was. Quantum mechanics requires us to treat all molecules as identical and denies the possibility of labelling them as right- or left-molecules.

In a classical universe, in which an ideal gas was possible and molecules could be labelled, entropy would be associated with missing information, but not heat flow. In the real quantum universe an ideal gas satisfies neither $U = \frac{3}{2}Nk_\mathrm{B}T$ nor $PV = Nk_\mathrm{B}T$, molecules cannot be labelled and entropy is both associated with heat flow and missing information.

6.20 *Consider a 'gas' formed by M non-interacting, monatomic molecules of mass m that move in a one-dimensional potential well $V = 0$ for $|x| < a$ and ∞ otherwise. Assume that at sufficiently low temperatures all molecules are either in the ground or first-excited states. Show that in this approximation the partition function is given by*

$$\ln Z = -M\beta E_0 + \mathrm{e}^{-3\beta E_0} - \mathrm{e}^{-3(M+1)\beta E_0} \quad \textit{where} \quad E_0 \equiv \frac{\pi^2\hbar^2}{8ma^2}. \tag{6.15}$$

Show that for M large the internal energy, pressure and specific heat of this gas are given by

$$U = E_0(M + 3\mathrm{e}^{-3\beta E_0}) \; ; \; P = \frac{2E_0}{a}\left(M + 3\mathrm{e}^{-3\beta E_0}\right) \; ; \; C_V = \frac{9E_0^2}{k_\mathrm{B}T^2}\mathrm{e}^{-3\beta E_0}. \tag{6.16}$$

In what respects do these results for a quantum ideal gas differ from the properties of a classical ideal gas? Explain these differences physically.

Soln: The ground-state energy is the kinetic energy of a particle that has de Broglie wavelength $= 4a$ so it can have nodes at $x = \pm a$. Hence $k = 2\pi/4a = \pi/2a$ and $E_0 = (\hbar k)^2/2m = \pi^2\hbar^2/8ma$. The energy of the first excited state is four times the energy of the ground state because for this state k is twice as large. The first excited state may contain 0, 1, ..., M molecules, so

$$Z = \mathrm{e}^{-M\beta E_0} + \mathrm{e}^{-(M-1+4)\beta E_0} + \mathrm{e}^{-(M-2+8)\beta E_0} + \cdots + \mathrm{e}^{-4M\beta E_0} = \mathrm{e}^{-M\beta E_0}\left(1 + \mathrm{e}^{-3\beta E_0} + \cdots + \mathrm{e}^{-3M\beta E_0}\right)$$

Summing this geometrical progression we have

$$Z = \mathrm{e}^{-M\beta E_0}\frac{1 - \mathrm{e}^{-3(M+1)\beta E_0}}{1 - \mathrm{e}^{-3\beta E_0}}$$

Taking logs and using $\ln(1 + x) \simeq x$ yields the required result. We use $M \gg 1$ to simplify Z. Then the internal energy

$$U = -\frac{\partial \ln Z}{\partial \beta} = ME_0 + 3E_0\mathrm{e}^{-3\beta E_0}.$$

The first term on the right is clearly the energy when every molecule is in the ground state, and the second term must give the correction arising from molecules in the first excited state. Remarkably this is *not* proportional to the number of molecules. If we counted states classically, we would have $Z = \mathrm{e}^{-M\beta E_0} + M\mathrm{e}^{-(M+3)\beta E_0} + \cdots$ because there would be a different state of the gas for each molecule we chose to promote to the excited state, and the correction would be proportional to M. Differentiating U w.r.t. T using $\partial/\partial T = -(\beta/T)\partial/\partial\beta$ we obtain the specific heat given. The Helmholtz free energy is $F = -\beta^{-1}\ln Z \simeq ME_0 - \beta^{-1}\mathrm{e}^{-3\beta E_0}$, so $P = -\partial F/\partial a = -(M + 3\mathrm{e}^{-3\beta E_0})(\partial E_0/\partial a)$, from which the required expression follows trivially.

The pressure does not go to zero with T, as does that of a classical gas, on account of zero-point energy. The specific heat vanishes with T, as Nernst's law requires, rather than being independent of temperature, on account of the finite energy required to reach an excited state.

7.3* *We have that*

$$L_+ \equiv L_x + \mathrm{i}L_y = \mathrm{e}^{\mathrm{i}\phi}\Big(\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta\frac{\partial}{\partial\phi}\Big). \tag{7.1}$$

From the Hermitian nature of $L_z = -\mathrm{i}\partial/\partial\phi$ 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

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

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

Soln:

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

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

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

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

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

where

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

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*

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

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

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

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

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

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

The first term is

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

The second term is

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

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

Using the position representaion

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

Using this relation and the definition of p_r

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

Substituting this into our expression for p^2 we have

$$p^2 = \frac{\hbar^2 L_2}{r^2} + \frac{1}{r^2}\left((rp_r + \mathrm{i}\hbar)(rp_r + \mathrm{i}\hbar) - \mathrm{i}\hbar(rp_r + \mathrm{i}\hbar)\right)$$

When we multiply out the bracket, we encounter $rp_r rp_r = r^2p_r^2 + r[p_r, r]p_r = r^2p_r^2 - \mathrm{i}\hbar rp_r$. 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 tangetial and radial KE.

7.8 *A system that has total orbital angular momentum $\sqrt{6}\hbar$ is rotated through an angle ϕ around the z axis. Write down the 5×5 matrix that updates the amplitudes a_m that L_z will take the value m.*

Soln: We need the matrix of $U(\phi) = \exp(-\mathrm{i}\phi L_z)$ when squeezed between the states $|2, m\rangle$, i.e.,

$$U(\phi) = \begin{pmatrix} \mathrm{e}^{-2\mathrm{i}\phi} & 0 & 0 & 0 & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\phi} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\phi} & 0 \\ 0 & 0 & 0 & 0 & \mathrm{e}^{2\mathrm{i}\phi} \end{pmatrix}$$

7.9 *Consider a stationary state $|E, l\rangle$ of a free particle of mass m that has angular-momentum quantum number l. Show that $H_l|E, l\rangle = E|E, l\rangle$, where*

$$H_l \equiv \frac{1}{2m}\left(p_r^2 + \frac{l(l+1)\hbar^2}{r^2}\right). \tag{7.4}$$

Give a physical interpretation of the two terms in the big bracket. Show that $H_l = A_l^\dagger A_l$, where

$$A_l \equiv \frac{1}{\sqrt{2m}}\left(\mathrm{i}p_r - \frac{(l+1)\hbar}{r}\right). \tag{7.5}$$

Show that $[A_l, A_l^\dagger] = H_{l+1} - H_l$. What is the state $A_l|E, l\rangle$? Show that for $E > 0$ there is no upper bound on the angular momentum. Interpret this result physically.

Soln: The Hamiltonian is

$$H = \frac{p^2}{2m} = \frac{1}{2m}\left(p_r^2 + \frac{\hbar^2 L^2}{r^2}\right)$$

For kets $|E, l\rangle$ that are simultaneous eigenkets of l, this expression immediately reduces to the required expression. The second term in the bracket is the kinetic energy of tangential motion (classically $\frac{1}{2}mv_t^2$) and the first term is the radial kinetic energy (classically $\frac{1}{2}mv_r^2$). For the given form of A_l

$$\begin{aligned} A_l^\dagger A_l &= \frac{1}{2m}\left(-\mathrm{i}p_r - \frac{(l+1)\hbar}{r}\right)\left(\mathrm{i}p_r - \frac{(l+1)\hbar}{r}\right) \\ &= \frac{1}{2m}\left(p_r^2 + \frac{(l+1)^2\hbar^2}{r^2} + \mathrm{i}(l+1)\hbar[p_r, r^{-1}]\right) \end{aligned}$$

But $[p_r, r^{-1}] = -r^{-2}[p_r, r] = \mathrm{i}\hbar r^{-2}$ so

$$A_l^\dagger A_l = \frac{1}{2m}\left(p_r^2 + \frac{(l+1)^2\hbar^2}{r^2} - \frac{(l+1)\hbar^2}{r^2}\right) = H_l$$

as required.

Clearly,

$$[A_l, A_l^\dagger] = \frac{1}{2m}\left[\left(\mathrm{i}p_r - \frac{(l+1)\hbar}{r}\right), \left(-\mathrm{i}p_r - \frac{(l+1)\hbar}{r}\right)\right] = -\frac{(l+1)\mathrm{i}\hbar}{m}[p_r, r^{-1}] = \frac{(l+1)\hbar^2}{mr^2}$$

But $H_{l+1} - H_l = \{(l+1)(l+2) - l(l+1)\}\hbar^2/(2mr^2) = (l+1)\hbar^2/mr^2$.

Now

$$A_l H_l = A_l A_l^\dagger A_l = (A_l^\dagger A_l + [A_l, A_l^\dagger])A_l = (H_l + H_{l+1} - H_l)A_l = H_{l+1}A_l$$

So if we multiply both sides of $E|E,l\rangle = H_l|E,l\rangle$ by A_l, we get

$$EA_l|E,l\rangle = A_l H_l|E,l\rangle = H_{l+1}A_l|E,l\rangle,$$

which establishes that $A_l|E,l\rangle \propto |E,l+1\rangle$ is a state with the same energy but more angular momentum. To see whether there is an upper limit on the angular momentum, we evaluate

$$|A_l|E,l\rangle|^2 = \langle E,l|A_l^\dagger A_l|E,l\rangle = E > 0$$

so there is no limit to the angular momentum. Physically, when there is no confining potential, with a given energy the particle can move at a given speed along a path that is as far from the origin as it pleases. Hence its angular momentum is not constrained by its energy.

7.10 *Write down the expression for the commutator $[\sigma_i, \sigma_j]$ of two Pauli matrices. Show that the anticommutator of two Pauli matrices is*

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}. \tag{7.6}$$

Soln: Since $\sigma_i = 2s_i$ is twice the spin operator of a spin-half particle, from the angular-momentum commutation relations we have $[\sigma_i, \sigma_j] = 2\mathrm{i}\epsilon_{ijk}\sigma_k$.

Calculating explicitly

$$\sigma_x^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and similarly $\sigma_y^2 = \sigma_z^2 = I$ so $\{\sigma_i, \sigma_i\} = 2I$ as required. Further

$$\{\sigma_x, \sigma_y\} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} + \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix} + \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix} = 0$$

and similarly for $\{\sigma_y, \sigma_z\}$ and $\{\sigma_x, \sigma_z\}$.

7.13 *Show that a classical top with spin angular momentum $\mathbf{S}$ which is subject to a torque $\mathbf{G} = \mu\mathbf{S}\times\mathbf{B}/|\mathbf{S}|$ precesses at angular velocity $\boldsymbol{\omega} = \mu\mathbf{B}/|\mathbf{S}|$. Explain the relevance of this calculation to nuclear magnetic resonance in general and equation (7.137b) in particular.*

Soln: Since torque is equal to rate of change of angular momentum, we have

$$\frac{\mathrm{d}\mathbf{S}}{\mathrm{d}t} = \mu\mathbf{S}\times\mathbf{B}/|\mathbf{S}|.$$

When a vector $\mathbf{S}$ is rotated with angular velocity $\boldsymbol{\omega}$ its rate of change is (Box 4.3)

$$\frac{\mathrm{d}\mathbf{S}}{\mathrm{d}t} = \boldsymbol{\omega} \times \mathbf{S}.$$

Comparing these equations we see that the torque rotates $\mathbf{S}$ at a rate $\boldsymbol{\omega} = -\mu\mathbf{B}/|\mathbf{S}|$.

The relevance to NMR is that classically the magnetic field would apply a torque $\mu_{\mathrm{p}}\mathbf{S} \times \mathbf{B}/|\mathbf{S}|$ to the proton, and for the proton $|\mathbf{S}| = \frac{1}{2}\hbar$, so classical physics predicts precession of the proton's spin at the angular frequency given by equation (7.137b).

7.14 *For a spin-half particle at rest, the rotation operator* $\mathbf{J}$ *is equal to the spin operator* $\mathbf{S}$*. Use the result of Problem 7.10 to show that in this case the rotation operator* $U(\boldsymbol{\alpha}) \equiv \exp(-\mathrm{i}\boldsymbol{\alpha} \cdot \mathbf{J})$ *is*

$$U(\boldsymbol{\alpha}) = I\cos\left(\frac{\alpha}{2}\right) - \mathrm{i}\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma}\sin\left(\frac{\alpha}{2}\right), \tag{7.7}$$

where $\hat{\boldsymbol{\alpha}}$ *is the unit vector parallel to* $\boldsymbol{\alpha}$*. Comment on the value this gives for* $U(\boldsymbol{\alpha})$ *when* $\alpha = 2\pi$.

Soln:

$$U(\boldsymbol{\alpha}) = \exp(-\tfrac{1}{2}\mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}) = I - \mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}/2 - \frac{(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}/2)^2}{2!} + \mathrm{i}\frac{(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}/2)^3}{3!} + \frac{(\boldsymbol{\alpha} \cdot \boldsymbol{\sigma}/2)^4}{4!} + \cdots$$

Using $\boldsymbol{\alpha} = \alpha\hat{\boldsymbol{\alpha}}$ and $(\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma})^{2n} = I$, and gathering real and imaginary parts, we have

$$U(\boldsymbol{\alpha}) = \left(1 - \frac{(\alpha/2)^2}{2!} + \frac{(\alpha/2)^4}{4!} + \cdots\right)I - \mathrm{i}\left((\alpha/2) - \frac{(\alpha/2)^3}{3!} + \cdots\right)(\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma}).$$

The required result now follows from the power series for $\cos\theta$ and $\sin\theta$. For $\alpha = 2\pi$ we have rotated the system right around but the value of the wavefunction has changed sign because $U = -I$.

7.18* *Repeat the analysis of Problem 7.15 for spin-one particles coming on filters aligned successively along* $+z$*,* $45°$ *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

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

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

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

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*

$$A_l \equiv \frac{1}{\sqrt{2m\hbar\omega}}\left(\mathrm{i}p_r - \frac{(l+1)\hbar}{r} + m\omega r\right). \tag{7.8}$$

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 $A^\dagger_{l-1}|E,l\rangle = \alpha_+|E+\hbar\omega, l-1\rangle$, 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

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

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 α_- at our convenience.

Similarly

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

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 $r/\ell = \sqrt{2(l+1)}$, where*

$$\ell \equiv \sqrt{\frac{\hbar}{2m\omega}}. \tag{7.9}$$

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

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

Using the integrating factor,

$$\exp\left\{\int \mathrm{d}r\,\left(-\frac{l}{r} + \frac{r}{2\ell^2}\right)\right\} = r^{-l}\exp\left(r^2/4\ell^2\right), \tag{7.10}$$

to solve the equation, we have $u \propto r^l \mathrm{e}^{-r^2/4\ell^2}$. The radial distribution is $P(r) \propto r^2|u|^2 = r^{2(l+1)}\mathrm{e}^{-r^2/2\ell^2}$. Differentiating to find the maximum, we have

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

For the classical result we have

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

so $r=(l\hbar/m\omega)^{1/2}=(2l)^{1/2}\ell$ 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*

$$u_1 \propto x^l\left(x-\frac{2l+1}{x}\right)e^{-x^2/4} \quad \text{where} \quad x\equiv r/\ell \quad \text{with} \quad \ell\equiv\sqrt{\frac{\hbar}{2m\omega}}. \tag{7.11}$$

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 $\langle r|E,l\rangle \propto r^l e^{-r^2/4\ell^2}$. So the required radial wavefunction is

$$\begin{aligned}\langle r|E+\hbar\omega, l-1\rangle &\propto \langle r|A^\dagger_{l-1}|E,l\rangle\\ &\propto \left(-\frac{\partial}{\partial r}-\frac{l+1}{r}+\frac{r}{2\ell^2}\right)r^l e^{-r^2/4\ell^2} = \left(-lr^{l-1}+\frac{r^{l+1}}{2\ell^2}-(l+1)r^{l-1}+\frac{r^{l+1}}{2\ell^2}\right)e^{-r^2/4\ell^2}\\ &= r^l e^{-r^2/4\ell^2}\left(\frac{r}{\ell^2}-\frac{2l+1}{r}\right) \propto x^l e^{-x^2/4}\left(x-\frac{2l+1}{x}\right)\end{aligned}$$

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

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

$$H=K\left(\frac{\mathbf{S}^{(1)}\cdot\mathbf{S}^{(2)}}{a}-3\frac{(\mathbf{S}^{(1)}\cdot\mathbf{a})(\mathbf{S}^{(2)}\cdot\mathbf{a})}{a^3}\right), \tag{7.12}$$

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

$$H=\frac{K}{a}\left(\tfrac{1}{2}(S_+^{(1)}S_-^{(2)}+S_-^{(1)}S_+^{(2)})+S_z^{(1)}S_z^{(2)}-3S_z^{(1)}S_z^{(2)}\right). \tag{7.13}$$

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:

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

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

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

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

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

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* $[J_i, L_j] = \mathrm{i}\sum_k \epsilon_{ijk}L_k$ *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:

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

But

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

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* $[L^2, x_i] = \mathrm{i}\sum_{jk}\epsilon_{jik}(L_j x_k + x_k L_j)$. *Then show that* $\mathbf{L}\cdot\mathbf{x} = 0$ *and using this result derive*

$$[L^2, [L^2, x_i]] = \mathrm{i}\sum_{jk}\epsilon_{jik}\left(L_j[L^2, x_k] + [L^2, x_k]L_j\right) = 2(L^2 x_i + x_i L^2). \tag{7.14}$$

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

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

where $\beta \equiv l(l+1)$ *and* $\beta' = l'(l'+1)$. *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* β *given* β', *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:

$$\sum_j [L_j^2, x_i] = \sum_j (L_j[L_j, x_i] + [L_j, x_i]L_j) = \mathrm{i}\sum_{jk}\epsilon_{jik}(L_j x_k + x_k L_j)$$

$$\hbar\mathbf{L}\cdot\mathbf{x} = \sum_{ijk}\epsilon_{ijk}x_j p_k x_i = \sum_{ijk}\epsilon_{ijk}(x_j x_i p_k + x_j[p_k, x_i]) = \sum_{ijk}\epsilon_{ijk}(x_j x_i p_k - \mathrm{i}\hbar x_j\delta_{ki})$$

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

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

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

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

Similarly, $\sum_j x_jL_iL_j = \mathrm{i}\sum_{jk}\epsilon_{jik}x_kL_j$. Moreover

$$\begin{aligned}\sum_j L_jx_iL_j &= \sum_j([L_j,x_i]L_j + x_iL_jL_j) = \mathrm{i}\sum_{jk}\epsilon_{jik}x_kL_j + x_iL^2\\ &= \sum_j(L_j[x_i,L_j] + L_jL_jx_i) = \mathrm{i}\sum_{jk}\epsilon_{ijk}L_jx_k + L^2x_i\end{aligned}$$

Assembling these results we find

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

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

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

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.

8.8 *Tritium, ^{3}H, is highly radioactive and decays with a half-life of 12.3 years to ^{3}He by the emission of an electron from its nucleus. The electron departs with 16 keV of kinetic energy. Explain why its departure can be treated as sudden in the sense that the electron of the original tritium atom barely moves while the ejected electron leaves.*

Calculate the probability that the newly-formed ^{3}He atom is in an excited state. Hint: evaluate $\langle 1,0,0;Z=2|1,0,0;Z=1\rangle$.

Soln: The binding energy of H is just 13.6 eV and by the virial theorem its kinetic energy is half this, so the speed of the ejected electron is larger by a factor $\sqrt{16000/6.8}\simeq 48.5\gg 1$. Hence the orbital electron barely moves in the time required for the ejected electron to get clear of the atom.

After the decay, the orbital electron is still in the ground state of H. The amplitude for it to be in the ground state of the new Hamiltonian is $\langle 100; Z=2|100; Z=1\rangle$. In the position representation this is

$$\begin{aligned}\langle 100; Z=2|100; Z=1\rangle &= \frac{1}{2}\left(\frac{4}{a_0}\frac{2}{a_0}\right)^{3/2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{e}^{-2r/a_0}Y_0^0\mathrm{e}^{-r/a_0}Y_0^0\\ &= 4\frac{2^{3/2}}{a_0^3}\int \mathrm{d}r\, r^2\mathrm{e}^{-3r/a_0} = \frac{4}{3^3}2^{3/2}\int \mathrm{d}x\, x^2\mathrm{e}^{-x} \quad (x\equiv 3r/a_0)\\ &= \frac{4}{3^3}2^{3/2}2!\end{aligned}$$

So the probability of being in an excited state

$$P = 1-\langle 100; Z=2|100; Z=1\rangle^2 = 1-\frac{64\times 8}{27^2} = 0.298$$

8.9* *A spherical potential well is defined by*

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

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

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

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

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

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 $\hbar^2k^2 = 2mE$ and $\hbar^2K^2 = 2m(V_0-E)$. 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 $p_r = -\mathrm{i}\hbar(\partial/\partial r + r^{-1})$, 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

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

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

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

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

$$\begin{aligned}\sin(ka) &= A\mathrm{e}^{-Ka}\\ k\cos(ka) &= -KA\mathrm{e}^{-Ka}\end{aligned} \quad\Rightarrow\quad \cot(ka) = -\frac{K}{k} = -\sqrt{W^2/(ka)^2-1}$$

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 ∞ 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

$$V_0 = \frac{\pi^2\hbar^2}{8ma^2} = \frac{(\pi\hbar/a)^2}{4m_\mathrm{p}} = 25.6\,\mathrm{MeV}$$

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

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

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

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

$$A_l A_l^\dagger = \frac{a_0^2\mu}{\hbar^2}H_{l+1} + \frac{Z^2}{2(l+1)^2}. \tag{8.5}$$

Given that $A_l H_l = H_{l+1}A_l$, show that $H_l A_l^\dagger = A_l^\dagger H_{l+1}$. Hence show that

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

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: We have

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

as required. $H_l A_l^\dagger = A_l^\dagger H_{l+1}$ is just the dagger of the given equation because H_l is Hermitian.

We multiply $H_{l+1}|E, l+1\rangle = E|E, l+1\rangle$ by $A_l^\dagger$:

$$E(A_l^\dagger|E, l+1\rangle) = A_l^\dagger H_{l+1}|E, l+1\rangle = H_l(A_l^\dagger|E, l+1\rangle),$$

which establishes that $A_l^\dagger|E, l+1\rangle = C|E, l\rangle$, where C is a constant. To determine C we take the mod-square of both sides

$$\begin{aligned} C^2 = \langle E, l+1|A_l A_l^\dagger|E, l+1\rangle &= \langle E, l+1|\left(\frac{a_0^2\mu}{\hbar^2}H_{l+1} + \frac{Z^2}{2(l+1)^2}\right)|E, l+1\rangle \\ &= \frac{a_0^2\mu}{\hbar^2}E + \frac{Z^2}{2(l+1)^2} = -\frac{Z^2}{2n^2} + \frac{Z^2}{2(l+1)^2} \end{aligned}$$

as required. The equation shows that $A_l^\dagger$ 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 $A_{n-1}|n, n-1\rangle = 0$. This is the wavefunction of the circular orbit. Then we obtain the wavefunctions of non-circular orbits by applying $A_{n-2}^\dagger$ to this wavefunction, which simply involves differentiation, and then applying $A_{n-3}^\dagger$ to the resulting wavefunction, and so on.

8.12* *From equation (8.46) show that $l' + \frac{1}{2} = \sqrt{(l+\frac{1}{2})^2 - \beta}$ and that the increment Δ 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 β increasing from zero to a small number, show that*

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

Explain the physical significance of this result.

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

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

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

Squaring up this equation, we have

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

Taking the first eqn from the second yields

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

This is a quadratic equation for Δ, 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 (8.51) 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 in 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.

8.13 *Show that Ehrenfest's theorem yields equation (8.70) with $\mathbf{B} = 0$ as the classical equation of motion of the vector $\mathbf{S}$ that is implied by the spin–orbit Hamiltonian (8.71).*

Soln: Bearing in mind that $\mathbf{L}$ commutes with $\mathbf{S}$ and the scalars r and $\mathrm{d}\Phi/\mathrm{d}r$, Ehrenfest's theorem yields

$$\begin{aligned}
\mathrm{i}\hbar \frac{\mathrm{d}\,\langle S_i \rangle}{\mathrm{d}t} = \langle [S_i, H_{\mathrm{SO}}] \rangle &= -\frac{\mathrm{d}\Phi}{\mathrm{d}r} \frac{e\hbar^2}{2rm_{\mathrm{e}}^2 c^2} \sum_j \langle [S_i, S_j L_j] \rangle \\
&= -\frac{\mathrm{d}\Phi}{\mathrm{d}r} \frac{e\hbar^2}{2rm_{\mathrm{e}}^2 c^2} \sum_j \langle [S_i, S_j] L_j + S_j [S_i, L_j] \rangle \\
&= -\frac{\mathrm{d}\Phi}{\mathrm{d}r} \frac{e\hbar^2}{2rm_{\mathrm{e}}^2 c^2} \sum_{jk} \mathrm{i}\epsilon_{ijk} \langle S_k L_j \rangle
\end{aligned}$$

Cancelling i$\hbar$ from each side and using $\sum_{jk} \epsilon_{ijk} S_k L_j = -(\mathbf{S} \times \mathbf{L})_i$ on the right we obtain

$$\frac{\mathrm{d}\,\langle \mathbf{S} \rangle}{\mathrm{d}t} = \frac{\mathrm{d}\Phi}{\mathrm{d}r} \frac{e\hbar}{2rm_\mathrm{e}^2 c^2} \langle \mathbf{S} \times \mathbf{L} \rangle$$

which agrees with (8.70) for $Q = -e$ and $\mathbf{B} = 0$.

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

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

where all quantities are real and ϵ is a small parameter. To first order in ϵ, 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 ϵ.

Soln: When $A_1 \neq A_2$, the eigenvectors of H_0 are $(1,0)$ and $(0,1)$ so to first-order in ϵ 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 λ of the last matrix satisfy

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

and the perturbed energies are

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

Solving for the exact eigenvalues of the given matrix we find

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

If $A_1 = A_2$ this simplifies to

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

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

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

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

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

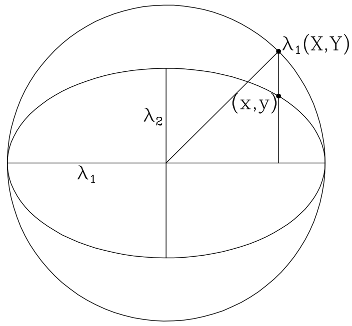


Figure 9.3 The input and output vectors of a 2×2 Hermitian matrix are related by a circle with the matrix's largest eigenvalue as radius and the ellipse that has the eigenvalues as semi-axes.

So

$$E_B/(\mu_\mathrm{B} B) = m g_\mathrm{L} = \begin{cases} 2 & \text{for } j = \frac{3}{2}, m = \frac{3}{2} \\ \frac{2}{3} & \text{for } j = \frac{3}{2}, m = \frac{1}{2} \\ \frac{1}{3} & \text{for } j = \frac{1}{2}, m = \frac{1}{2} \end{cases}$$

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 $E_B/(\mu_\mathrm{B}B) = m + \langle\psi|S_z|\psi\rangle = \frac{3}{2} + \frac{1}{2} = 2$ in agreement with the Landé factor. Similarly

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

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

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

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

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

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

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

Now

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

so

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

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

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

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 5.10. 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

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

The required matrix element is

$$\frac{1}{L}\int_{-L/2}^{L/2}\mathrm{d}x\,\mathrm{e}^{\mathrm{i}kx}V(x)\mathrm{e}^{\mathrm{i}kx} = -V_0\int_{-a}^{a}\mathrm{d}x\,\mathrm{e}^{2\mathrm{i}kx} = -V_0\frac{\sin(2ka)}{Lk}$$

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

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

Now we need the density of states $g(E)$. $E = p^2/2m = \hbar^2k^2/2m$ 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

$$g = \frac{\mathrm{d}n}{\mathrm{d}E} = \frac{L}{4\pi\hbar}\sqrt{\frac{2m}{E}}.$$

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 $L \to \infty$ 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

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

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 $g(E)\,\mathrm{d}E\,\mathrm{d}^2\Omega$ with energy in $(E, E+\mathrm{d}E)$ and momentum in the solid angle $\mathrm{d}^2\Omega$ 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*

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

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 $\mathrm{d}^2\Omega$ around momentum $\hbar\mathbf{k}'$ is

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

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 $k^2\,\mathrm{d}k\mathrm{d}^2\Omega$ is

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

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

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

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

The matrix element is

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

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

$$\frac{\hbar k}{mL^3}\mathrm{d}\sigma = \frac{1}{L^6}\left|\int \mathrm{d}^3\mathbf{x}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}V(\mathbf{x})\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\right|^2 \frac{2\pi}{\hbar}\left(\frac{L}{2\pi}\right)^3 k^2\,\frac{\mathrm{d}k}{\mathrm{d}E}\mathrm{d}^2\Omega$$

$$\Rightarrow\quad \mathrm{d}\sigma = \frac{mk\,\mathrm{d}k/\mathrm{d}E}{(2\pi)^2\hbar^2}\left|\int \mathrm{d}^3\mathbf{x}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}V(\mathbf{x})\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\right|^2.$$

Eliminating k with $\hbar^2k\,\mathrm{d}k = m\mathrm{d}E$ 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 Li^+ ion electrostatically bound to an 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 H^- is $E = (0.4 + 1 - 0.955)\mathcal{R} = 0.445\mathcal{R}$. Now we recover some of this energy by letting the Li^+ and 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

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

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 $|j_1 - j_2| \le j \le j_1 + j_2$, 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:

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

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:

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

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.