

Solutions to Lectures on Quantum Mechanics, First Edition

Steven Weinberg

The University of Texas at Austin

Prepared by Dr Joel Meyers.

Chapter 1 Problem Set Solutions

1. Consider a non-relativistic particle of mass M in one dimension, confined in a potential that vanishes for $-a \leq x \leq a$, and becomes infinite at $x = \pm a$, so that the wave function must vanish at $x = \pm a$.
 - Find the energy values of states with definite energy, and the corresponding normalized wave functions.
 - Suppose that the particle is placed in a state with a wave function proportional to $a^2 - x^2$. If the energy of the particle is measured, what is the probability that the particle will be found in the state of lowest energy?

The states of definite energy are those which are solutions of the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2M} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x).$$

The potential for the infinite square well is given by

$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ \infty & \text{for } |x| \geq a. \end{cases}$$

This potential requires that the wave function vanishes outside the well

$$\psi(x) = 0 \quad \text{for } |x| \geq a,$$

while inside the well the Schrödinger equation becomes

$$\frac{d^2}{dx^2} \psi(x) = -\frac{2ME}{\hbar^2} \psi(x) \quad \text{for } |x| < a.$$

The solution of this differential equation takes the form

$$\psi(x) = A \sin(kx) + B \cos(kx),$$

where we have defined

$$k \equiv \frac{\sqrt{2ME}}{\hbar}.$$

Continuity of the wave function requires that we impose the boundary conditions

$$\psi(x = \pm a) = 0,$$

and so

$$\begin{aligned} 0 &= A \sin(ka) + B \cos(ka), \\ 0 &= -A \sin(ka) + B \cos(ka). \end{aligned}$$

Adding these two equations gives

$$0 = 2B \cos(ka),$$

which requires that

$$B = 0 \text{ or } k = \frac{n\pi}{2a} \text{ where } n = 2, 4, 6, \dots,$$

and subtracting the equations gives

$$0 = 2A \sin(ka),$$

which requires that

$$A = 0 \text{ or } k = \frac{n\pi}{2a} \text{ where } n = 1, 3, 5, \dots$$

In either case, the energy levels are given by

$$E_n = \frac{\hbar^2 k^2}{2M} = \frac{n^2 \hbar^2 \pi^2}{8Ma}.$$

Next, we need to normalize the wave functions in the sense of Eq. (1.5.4), such that

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1.$$

For n odd, we have

$$\int_{-a}^a \left| B \cos\left(\frac{n\pi x}{2a}\right) \right|^2 dx = |B|^2 \int_{-a}^a \cos^2\left(\frac{n\pi x}{2a}\right) dx = |B|^2 a = 1,$$

which requires that

$$B = \frac{1}{\sqrt{a}},$$

where we have fixed the arbitrary complex phase for convenience. For n even, the normalization condition takes the form

$$\int_{-a}^a \left| A \sin\left(\frac{n\pi x}{2a}\right) \right|^2 dx = |A|^2 \int_{-a}^a \sin^2\left(\frac{n\pi x}{2a}\right) dx = |A|^2 a = 1,$$

which requires that

$$A = \frac{1}{\sqrt{a}},$$

where we have again fixed the arbitrary complex phase for convenience. Summarizing our results, the normalized wave functions of states with definite energy are

$$\psi_n(x) = \begin{cases} \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi x}{2a}\right) & \text{for } |x| < a \text{ and } n = 1, 3, 5, \dots \\ \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right) & \text{for } |x| < a \text{ and } n = 2, 4, 6, \dots \\ 0 & \text{for } |x| \geq a \end{cases}$$

and the energy levels are

$$E_n = \frac{n^2 \hbar^2 \pi^2}{8Ma}.$$

Since these states are normalized and the energy level is determined by n , the argument below Eq. (1.4.26) proves that the states of definite energy are orthonormal

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = \delta_{mn}.$$

Let us define a state which vanishes for $|x| \geq a$, while for $|x| < a$ it is given by

$$\Phi(x, t = 0) = C(a^2 - x^2).$$

We must normalize this state in order to determine C .

$$\int_{-a}^a |C(a^2 - x^2)|^2 dx = |C|^2 \left[\frac{x^5}{5} - \frac{2a^2 x^3}{3} + a^4 x \right]_{-a}^a = \frac{16a^5}{15} |C|^2 = 1,$$

and so we find (after fixing an arbitrary phase)

$$C = \sqrt{\frac{15}{16a^5}},$$

which then gives

$$\Phi(x, t = 0) = \sqrt{\frac{15}{16a^5}} (a^2 - x^2).$$

Since the states of definite energy that we found above form a complete orthonormal set on the interval $-a < x < a$, we can express Φ in terms of those states

$$\Phi(x, t = 0) = \sum_n c_n \psi_n(x),$$

and the probability of measuring the state Φ to have energy E_m , following Eq. (1.5.18), is given by

$$P(\Phi(x, t = 0) \rightarrow \psi_m(x)) = |c_m|^2 = \left| \int_{-a}^a \psi_m^*(x) \Phi(x, t = 0) dx \right|^2.$$

For the state of lowest energy this gives

$$\begin{aligned}
 c_1 &= \int_{-a}^a \frac{1}{\sqrt{a}} \cos\left(\frac{\pi x}{2a}\right) \sqrt{\frac{15}{16a^5}} (a^2 - x^2) dx \\
 &= \sqrt{\frac{15}{16}} \frac{1}{a^3} \left[\frac{2a^3}{\pi} \sin\left(\frac{\pi x}{2a}\right) - \frac{8xa^2}{\pi^2} \cos\left(\frac{\pi x}{2a}\right) - \frac{\frac{\pi^2 x^2}{4a^2} - 2}{\frac{\pi^3}{8a^3}} \sin\left(\frac{\pi x}{2a}\right) \right]_{-a}^a \\
 &= \sqrt{\frac{15}{16}} \frac{1}{a^3} \left[\frac{4a^3}{\pi} - \frac{4a^3}{\pi} + \frac{32a^3}{\pi^3} \right] \\
 &= \frac{8\sqrt{15}}{\pi^3},
 \end{aligned}$$

and so the probability of finding Φ in the lowest energy state is

$$P(\Phi(x, t = 0) \rightarrow \psi_1(x)) = |c_1|^2 = \frac{960}{\pi^6} \approx 0.9986.$$

2. Consider a non-relativistic particle of mass M in three dimensions, described by a Hamiltonian

$$H = \frac{\mathbf{P}^2}{2M} + \frac{M\omega_0^2}{2} \mathbf{X}^2.$$

- Find the energy values of states with definite energy, and the number of states for each energy.
- Find the rate at which a state of next-to-lowest energy decays by photon emission into the state of lowest energy.

Hint: You can express the Hamiltonian as a sum of three Hamiltonians for one-dimensional oscillators, and use the results given in Section 1.4 for the energy levels and x -matrix elements for one-dimensional oscillators.

First, we will rewrite the Hamiltonian in components

$$\begin{aligned}
 H &= \frac{\mathbf{p}^2}{2M} + \frac{M\omega_0^2}{2} \mathbf{x}^2 \\
 &= \left(\frac{p_1^2}{2M} + \frac{M\omega_0^2}{2} x_1^2 \right) + \left(\frac{p_2^2}{2M} + \frac{M\omega_0^2}{2} x_2^2 \right) + \left(\frac{p_3^2}{2M} + \frac{M\omega_0^2}{2} x_3^2 \right) \\
 &= H_1 + H_2 + H_3,
 \end{aligned}$$

where H_1 , H_2 , and H_3 are the one-dimensional harmonic oscillator Hamiltonians for x_1 , x_2 , and x_3 , respectively. Now, we will assume a separable solution of the form

$$\psi(\mathbf{x}) = \psi_1(x_1)\psi_2(x_2)\psi_3(x_3),$$

where

$$H_1 \psi_1(x_1) = E_{n_1} \psi_1(x_1)$$

$$H_2 \psi_2(x_2) = E_{n_2} \psi_2(x_2)$$

$$H_3 \psi_3(x_3) = E_{n_3} \psi_3(x_3)$$

$$H_1 \psi_2(x_2) = 0$$

$$H_1 \psi_3(x_3) = 0$$

⋮

and the E_n are given by the energies of the one-dimensional harmonic oscillator, Eq. (1.4.15)

$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega_0,$$

where $n = 0, 1, 2, \dots$. We therefore find for the three-dimensional harmonic oscillator

$$\begin{aligned} H \psi(\mathbf{x}) &= E_N \psi(\mathbf{x}) \\ &= H_1 \psi_1(x_1) \psi_2(x_2) \psi_3(x_3) + \psi_1(x_1) H_2 \psi_2(x_2) \psi_3(x_3) \\ &\quad + \psi_1(x_1) \psi_2(x_2) H_3 \psi_3(x_3) \\ &= E_{n_1} \psi_1(x_1) \psi_2(x_2) \psi_3(x_3) + \psi_1(x_1) E_{n_2} \psi_2(x_2) \psi_3(x_3) \\ &\quad + \psi_1(x_1) \psi_2(x_2) E_{n_3} \psi_3(x_3), \end{aligned}$$

and so

$$E_N = E_{n_1} + E_{n_2} + E_{n_3} = \left(n_1 + n_2 + n_3 + \frac{3}{2} \right) \hbar \omega_0,$$

where n_1, n_2 , and n_3 are each non-negative integers. If we define

$$N = n_1 + n_2 + n_3,$$

then the energy levels for states of definite energy are

$$E_N = \left(N + \frac{3}{2} \right) \hbar \omega_0,$$

where $N = 0, 1, 2, \dots$

Now we must count the number of states with each energy. For a definite value of N , the integer n_1 can take values $0, 1, \dots, N$, then n_2 will take values $0, 1, \dots, N - n_1$ (which represents $N - n_1 + 1$ possibilities), and n_3 is fixed to be $N - n_1 - n_2$. Then for each energy E_N there is a degeneracy

$$g_N = \sum_{n_1=0}^N (N - n_1 + 1) = N(N+1) - \frac{1}{2}N(N+1) + N + 1 = \frac{1}{2}(N+1)(N+2).$$

The rate of spontaneous emission of photons carrying energy $\hbar\omega_{nm} = E_m - E_n$ is given by Eq. (1.4.5) to be

$$A_m^n = \frac{4e^2\omega_{nm}^3}{3c^3\hbar} |[\mathbf{x}]_{nm}|^2.$$

In three dimensions, we have $E_1 = \frac{5}{2}\hbar\omega_0$ and $E_0 = \frac{3}{2}\hbar\omega_0$, so $\omega_{01} = \omega_0$. The relevant matrix elements for the one-dimensional harmonic oscillator are given by Eq. (1.4.15) to be

$$[x]_{n+1,n}^* = [x]_{n,n+1} = e^{-i\omega_0 t} \sqrt{\frac{(n+1)\hbar}{2m_e\omega_0}}.$$

Since the wave function for the three-dimensional harmonic oscillator is just a product of three one-dimensional harmonic oscillator wave functions, we can also take these matrix elements to represent the matrix elements of a single spatial component x_1 , x_2 , or x_3

$$[x_i]_{mn} = [x]_{mn}.$$

The first excited state has n_1 , n_2 , or n_3 equal to 1 with the others equal to zero, and so the rate of spontaneous emission from the first excited state to the ground state for the three-dimensional harmonic oscillator is given by

$$A_1^0 = \frac{4e^2\omega_{01}^3}{3c^3\hbar} \left(\frac{\hbar}{2m_e\omega_0} \right) = \frac{2e^2\omega_0^2}{3c^3m_e}.$$

3. Suppose the photon had three polarization states rather than two. What difference would that make in the relations between Einstein's A and B coefficients?

For black-body radiation in a cubical box with side L , the frequency of a normal mode is given by Eq. (1.1.2) as $\nu = |\mathbf{n}|c/L$. The number of normal modes $N(\nu)d\nu$ in a range of frequencies between ν and $\nu + d\nu$ is three times the volume of a spherical shell in frequency space (the factor of three here comes from the assumed three polarization states of the photon)

$$N(\nu) d\nu = 3 \times 4\pi |\mathbf{n}|^2 d|\mathbf{n}| = 12\pi \left(\frac{L}{c} \right)^3 \nu^2 d\nu.$$

Assuming that the energies of the light quanta are integer multiples of $h\nu$, the mean energy is

$$\bar{E} = \frac{\sum_n \exp\left(\frac{-nh\nu}{k_B T}\right) nh\nu}{\sum_n \exp\left(\frac{-nh\nu}{k_B T}\right)} = \frac{h\nu}{\exp\left(\frac{h\nu}{k_B T}\right) - 1}.$$

Then the energy density in radiation between ν and $\nu + d\nu$ is given by

$$\rho(\nu) d\nu = \frac{\bar{E} N(\nu) d\nu}{L^3} = \frac{12\pi h}{c^3} \frac{\nu^3 d\nu}{\exp\left(\frac{h\nu}{k_B T}\right) - 1}.$$

Now assume that we have black-body radiation in equilibrium with atoms at a temperature T . The transition rate for atoms to go from state m to state n must equal the rate for the transition from state n to state m , so

$$N_m [A_m^n + B_m^n \rho(\nu_{nm}, T)] = N_n B_n^m \rho(\nu_{nm}, T).$$

Using the Boltzmann distribution for the atoms gives

$$\frac{N_m}{N_n} = \exp\left(-\frac{(E_m - E_n)}{k_B T}\right) = \exp\left(\frac{-h\nu_{nm}}{k_B T}\right).$$

We can then rearrange the condition of equilibrium to give

$$A_m^n = \frac{12\pi h}{c^3} \frac{\nu^3 d\nu}{\exp\left(\frac{h\nu}{k_B T}\right) - 1} \left[\exp\left(\frac{-h\nu_{nm}}{k_B T}\right) B_n^m - B_m^n \right].$$

Requiring that the Einstein coefficients A and B are temperature independent then gives

$$B_m^n = B_n^m,$$

and

$$A_m^n = \left(\frac{12\pi h \nu_{nm}^3}{c^3} \right) B_m^n.$$

This conclusion gives a value for A which is larger than the usual expression Eq. (1.2.16) by a factor of 3/2.

4. Show that the solution $\psi(\mathbf{x}, t)$ of the time-dependent Schrödinger equation for a particle in a real potential has the property that $\partial|\psi|^2/\partial t$ is the divergence of a three-vector.

We wish to calculate

$$\frac{\partial}{\partial t} |\psi(x, t)|^2,$$

for some $\psi(x, t)$ which is a solution of the time-dependent Schrödinger equation, which reads

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \frac{-\hbar^2}{2M} \nabla^2 \psi(x, t) + V(x, t) \psi(x, t).$$

Taking the complex conjugate of the Schrödinger equation gives

$$-i\hbar \frac{\partial}{\partial t} \psi^*(x, t) = \frac{-\hbar^2}{2M} \nabla^2 \psi^*(x, t) + V(x, t) \psi^*(x, t).$$

Recall that $|\psi(x, t)|^2$ can be rewritten as $\psi(x, t)\psi^*(x, t)$, and so we have

$$\frac{\partial}{\partial t}|\psi(x, t)|^2 = \psi^*(x, t)\frac{\partial}{\partial t}\psi(x, t) + \psi(x, t)\frac{\partial}{\partial t}\psi^*(x, t).$$

Using the Schrödinger equation to replace the time derivatives (now dropping space and time arguments), this becomes

$$\begin{aligned} \frac{\partial}{\partial t}|\psi|^2 &= \psi^* \left(\frac{i\hbar}{2M} \nabla^2 \psi - \frac{i}{\hbar} V \psi \right) + \psi \left(\frac{-i\hbar}{2M} \nabla^2 \psi^* + \frac{i}{\hbar} V \psi^* \right) \\ &= \frac{i\hbar}{2M} \psi^* \nabla^2 \psi - \frac{i\hbar}{2M} \psi \nabla^2 \psi^* - \frac{i}{\hbar} V |\psi|^2 + \frac{i}{\hbar} V |\psi|^2 \\ &= \frac{i\hbar}{2M} (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*) \\ &= \frac{i\hbar}{2M} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*). \end{aligned}$$

We see that we can identify a three-vector

$$\mathbf{j} \equiv \frac{-i\hbar}{2M} (\psi^* \nabla \psi - \psi \nabla \psi^*),$$

such that

$$\frac{\partial}{\partial t}|\psi|^2 = -\nabla \cdot \mathbf{j}.$$

Notice that this is a continuity equation which implies that probability is conserved in quantum mechanics. The time rate of change of probability density $|\psi|^2$ in some infinitesimal volume is equal to the rate at which the probability current \mathbf{j} flows into the same infinitesimal volume.

Chapter 2 Problem Set Solutions

1. Use the method described in Section 2.2 to calculate the spherical harmonics (aside from constant factors) for $\ell = 3$.

As discussed in Section 2.2, Y_ℓ^m is given by a sum of terms, each of which contains ν_\pm factors of \hat{x}_\pm such that $m = \nu_+ - \nu_-$, and the total number of factors of \hat{x}_+ , \hat{x}_- , and \hat{x}_3 in each term is ℓ . The unit vectors are defined as in Eq. (2.2.4)

$$\begin{aligned}\hat{x}_\pm &\equiv \hat{x}_1 \pm i\hat{x}_2 = r \sin \theta e^{\pm i\phi}, \\ \hat{x}_3 &= r \cos \theta.\end{aligned}$$

Also, the spherical harmonics satisfy

$$\nabla^2 (r^\ell Y_\ell^m) = 0,$$

and the condition

$$\int d^2\Omega Y_\ell^{m*}(\hat{x}) Y_{\ell'}^{m'}(\hat{x}) = \delta_{\ell\ell'} \delta_{mm'}.$$

We will now fix $\ell = 3$ and compute the spherical harmonics for each value of m . Beginning with $m = 3$, we must have $\nu_+ = 3$ and $\nu_- = 0$, so

$$Y_3^3 \propto (\hat{x}_1 + i\hat{x}_2)^3 = \sin^3 \theta e^{3i\phi}.$$

For $m = 2$, we have $\nu_+ = 2$ and $\nu_- = 0$, which gives

$$Y_3^2 \propto (\hat{x}_1 + i\hat{x}_2)^2 \hat{x}_3 = \sin^2 \theta \cos \theta e^{2i\phi}.$$

For $m = 1$, we must have either $\nu_+ = 2$ and $\nu_- = 1$, or $\nu_+ = 1$ and $\nu_- = 0$, so

$$Y_3^1 \propto A (\hat{x}_1 + i\hat{x}_2)^2 (\hat{x}_1 - i\hat{x}_2) + B (\hat{x}_1 + i\hat{x}_2) \hat{x}_3^2.$$

We can find A and B by requiring that $\nabla^2 (r^3 Y_3^m) = 0$, which in this case gives

$$\begin{aligned}\nabla^2 (r^3 Y_3^1) &\propto \nabla^2 [A (x_1^3 + ix_1^2 x_2 + x_1 x_2^2 + ix_2^3) + B (x_1 x_3^2 + ix_2 x_3^2)] \\ &= A (6x_1 + 2ix_2 + 2x_1 + 6ix_2) + B (2x_1 + 2ix_2) \\ &= 8A (x_1 + ix_2) + 2B (x_1 + ix_2) \\ &= 0,\end{aligned}$$

and so we find that $B = -4A$. Therefore, we can write

$$\begin{aligned}Y_3^1 &\propto (\hat{x}_1 + i\hat{x}_2)^2 (\hat{x}_1 - i\hat{x}_2) - 4 (\hat{x}_1 + i\hat{x}_2) \hat{x}_3^2 \\ &= (\sin^3 \theta - 4 \sin \theta \cos^2 \theta) e^{i\phi} \\ &= (1 - 5 \cos^2 \theta) \sin \theta e^{i\phi}.\end{aligned}$$

For $m = 0$, we must have either $\nu_+ = 1$ and $\nu_- = 1$, or $\nu_+ = 0$ and $\nu_- = 0$, so we find

$$Y_3^0 \propto C (\hat{x}_1 + i\hat{x}_2) (\hat{x}_1 - i\hat{x}_2) \hat{x}_3 + D\hat{x}_3^3.$$

We can find C and D by the same method as above

$$\begin{aligned} \nabla^2 (r^3 Y_3^0) &\propto \nabla^2 [C (x_1^2 + x_2^2) x_3 + D x_3^3] \\ &= 4C x_3 + 6D x_3 \\ &= 0, \end{aligned}$$

and so we find $D = -\frac{2}{3}C$. Therefore, we can write

$$\begin{aligned} Y_3^0 &\propto (\hat{x}_1 + i\hat{x}_2) (\hat{x}_1 - i\hat{x}_2) \hat{x}_3 - \frac{2}{3}\hat{x}_3^3 \\ &= \sin^2 \theta \cos \theta - \frac{2}{3} \cos^3 \theta \\ &= \left(1 - \frac{5}{3} \cos^2 \theta\right) \cos \theta. \end{aligned}$$

For $m = -1$, we must have either $\nu_+ = 1$ and $\nu_- = 2$, or $\nu_+ = 0$ and $\nu_- = 1$, so

$$Y_3^{-1} \propto E (\hat{x}_1 + i\hat{x}_2) (\hat{x}_1 - i\hat{x}_2)^2 + F (\hat{x}_1 - i\hat{x}_2) \hat{x}_3^2.$$

We again find the coefficients by imposing the Laplace equation

$$\begin{aligned} \nabla^2 (r^3 Y_3^{-1}) &\propto \nabla^2 [E (x_1^3 - i x_1^2 x_2 + x_1 x_2^2 - i x_2^3) + F (x_1 x_3^2 - i x_2 x_3^2)] \\ &= E (6x_1 - 2i x_2 + 2x_1 - 6i x_2) + F (2x_1 - 2i x_2) \\ &= 8E (x_1 - i x_2) + 2F (x_1 - i x_2) \\ &= 0, \end{aligned}$$

and so we find that $F = -4E$. Therefore, we can write

$$\begin{aligned} Y_3^{-1} &\propto (\hat{x}_1 + i\hat{x}_2) (\hat{x}_1 - i\hat{x}_2)^2 - 4 (\hat{x}_1 - i\hat{x}_2) \hat{x}_3^2 \\ &= (\sin^3 \theta - 4 \sin \theta \cos^2 \theta) e^{-i\phi} \\ &= (1 - 5 \cos^2 \theta) \sin \theta e^{-i\phi}. \end{aligned}$$

For $m = -2$, we have $\nu_+ = 0$ and $\nu_- = 2$, which gives

$$Y_3^{-2} \propto (\hat{x}_1 - i\hat{x}_2)^2 \hat{x}_3 = \sin^2 \theta \cos \theta e^{-2i\phi}.$$

Finally, for $m = -3$, we must have $\nu_+ = 0$ and $\nu_- = 3$, so

$$Y_3^{-3} \propto (\hat{x}_1 - i\hat{x}_2)^3 = \sin^3 \theta e^{-3i\phi}.$$

Now, we must impose the normalization condition which reads

$$\int d^2\Omega |Y_l^m(\hat{x})|^2 = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi |Y_l^m(\hat{x})|^2 = 1.$$

For $\ell = 3$, we will need to make use of the following integrals

$$\begin{aligned} \int_0^\pi (\sin\theta)^7 d\theta &= \frac{32}{35} \\ \int_0^\pi (\sin\theta)^5 (\cos\theta)^2 d\theta &= \frac{16}{105} \\ \int_0^\pi (\sin\theta)^3 (1 - 5\cos^2\theta)^2 d\theta &= \frac{32}{21} \\ \int_0^\pi \sin\theta (\cos\theta)^2 (3 - 5\cos^2\theta)^2 d\theta &= \frac{8}{7}. \end{aligned}$$

Finally, we arrive at the spherical harmonics for $\ell = 3$

$$\begin{aligned} Y_3^3 &= -\sqrt{\frac{35}{64\pi}} (\hat{x}_1 + i\hat{x}_2)^3 = -\sqrt{\frac{35}{64\pi}} \sin^3\theta e^{3i\phi} \\ Y_3^2 &= \sqrt{\frac{105}{32\pi}} (\hat{x}_1 + i\hat{x}_2)^2 \hat{x}_3 = \sqrt{\frac{105}{32\pi}} \sin^2\theta \cos\theta e^{2i\phi} \\ Y_3^1 &= -\sqrt{\frac{21}{64\pi}} \left[4(\hat{x}_1 + i\hat{x}_2) \hat{x}_3^2 - (\hat{x}_1 + i\hat{x}_2)^2 (\hat{x}_1 - i\hat{x}_2) \right] \\ &= -\sqrt{\frac{21}{64\pi}} (5\cos^2\theta - 1) \sin\theta e^{i\phi} \\ Y_3^0 &= \sqrt{\frac{7}{16\pi}} [2\hat{x}_3^3 - 3(\hat{x}_1 + i\hat{x}_2)(\hat{x}_1 - i\hat{x}_2)\hat{x}_3] \\ &= \sqrt{\frac{7}{16\pi}} (5\cos^2\theta - 3) \cos\theta \\ Y_3^{-1} &= \sqrt{\frac{21}{64\pi}} \left[4(\hat{x}_1 - i\hat{x}_2) \hat{x}_3^2 - (\hat{x}_1 + i\hat{x}_2)(\hat{x}_1 - i\hat{x}_2)^2 \right] \\ &= \sqrt{\frac{21}{64\pi}} (5\cos^2\theta - 1) \sin\theta e^{-i\phi} \\ Y_3^{-2} &= \sqrt{\frac{105}{32\pi}} (\hat{x}_1 - i\hat{x}_2)^2 \hat{x}_3 = \sqrt{\frac{105}{32\pi}} \sin^2\theta \cos\theta e^{-2i\phi} \\ Y_3^{-3} &= \sqrt{\frac{35}{64\pi}} (\hat{x}_1 - i\hat{x}_2)^3 = \sqrt{\frac{35}{64\pi}} \sin^3\theta e^{-3i\phi}. \end{aligned}$$

We have fixed the arbitrary phases here to match the convention used in Section 2.2, a convention which will be explained in Chapter 4.

2. Derive a formula for the rate of single photon emission from the $2p$ to the $1s$ state of hydrogen.

The rate of single photon emission is given in the dipole approximation by Eq. (1.4.5) as

$$A_m^n = \frac{4e^2\omega_{mn}^3}{3c^3\hbar} |[\mathbf{x}]_{nm}|^2,$$

where the matrix element $[\mathbf{x}]_{nm}$ is defined as

$$[\mathbf{x}]_{nm} = \int d^3x \psi_n^*(\mathbf{x}) \mathbf{x} \psi_m(\mathbf{x}).$$

In order to calculate the relevant matrix element for the hydrogen atom, we need to work out the hydrogen wave functions using the method described in Sections 2.1–2.3. We begin as in Section 2.3 with the wave function in the form

$$\psi(x) \propto \frac{u(r)}{r} Y_\ell^m(\theta, \phi),$$

where

$$u = \rho^{\ell+1} e^{-\rho} F(\rho),$$

and we have defined

$$\rho \equiv \kappa r.$$

According to Eq. (2.3.17) $F = 1$ for the $2p$ state, since $\ell = 1$ and $n = 2$. We also have $F = 1$ for the $1s$ state, since $\ell = 0$ and $n = 1$. Using Eqs. (2.3.18) and (2.3.19), we have

$$\kappa_n = \frac{\mu Z e^2}{n\hbar^2} = \frac{1}{na},$$

where the Bohr radius a appearing in the second equality is given by

$$a = \frac{\hbar^2}{\mu Z e^2},$$

and we have included the effect of the finite mass of the nucleus by using the reduced mass in place of the electron mass as discussed in Section 2.4

$$\mu = \frac{m_N m_e}{m_N + m_e}.$$

For the case of hydrogen, we have $Z = 1$ and $m_N = m_p$. Putting this together, the wave functions take the form

$$\begin{aligned} \psi_{1s} &\propto \frac{1}{a} e^{-r/a} Y_0^0(\theta, \phi) \\ \psi_{2p} &\propto \frac{r}{4a^2} e^{-r/2a} Y_1^m(\theta, \phi). \end{aligned}$$

We need to normalize these wave functions so that

$$\int d^3x |\psi(x)|^2 = 1.$$

For the $1s$ state this gives

$$\begin{aligned} 1 &= \int d^3x |\psi_{1s}(\mathbf{x})| \\ &= \int dr r^2 \left| N_1 \frac{1}{a} e^{-r/a} \right|^2 \int d^2\Omega |Y_0^0(\theta, \phi)|^2 \\ &= \frac{|N_1|^2}{a^2} \int_0^\infty dr r^2 e^{-2r/a} \\ &= \frac{|N_1|^2}{a^2} \left(\frac{a^3}{4} \right) \\ &= \frac{a|N_1|^2}{4}, \end{aligned}$$

where in the third line, we used the fact that the spherical harmonics are normalized. We find that the normalization constant N_1 is given, up to an arbitrary phase, by

$$N_1 = \frac{2}{a}.$$

Recalling from Section 2.2 that

$$Y_0^0 = \sqrt{\frac{1}{4\pi}},$$

we find for the normalized $1s$ wave function

$$\psi_{1s} = \sqrt{\frac{1}{\pi}} \frac{1}{a^{3/2}} e^{-r/a}.$$

Following the same procedure for the $2p$ state gives

$$\begin{aligned} 1 &= \int d^3x |\psi_{2p}(\mathbf{x})| \\ &= \int dr r^2 \left| N_2 \frac{r}{4a^2} e^{-r/2a} \right|^2 \int d^2\Omega |Y_1^m(\theta, \phi)|^2 \\ &= \frac{|N_2|^2}{16a^4} \int_0^\infty dr r^4 e^{-r/a} \\ &= \frac{|N_2|^2}{16a^4} (24a^5) \\ &= \frac{3a|N_2|^2}{2}, \end{aligned}$$

which gives up to an arbitrary phase factor

$$N_2 = \sqrt{\frac{2}{3a}},$$

and so

$$\psi_{2p} = \frac{1}{\sqrt{24}} \frac{r}{a^{5/2}} e^{-r/2a} Y_1^m(\theta, \phi).$$

Using the definition of the spherical harmonics from Section 2.2

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta$$

$$Y_1^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi},$$

we find for the normalized $2p$ wave functions

$$\psi_{2p}^{m=0} = \frac{1}{\sqrt{32\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \cos \theta$$

$$\psi_{2p}^{m=\pm 1} = \mp \frac{1}{8\sqrt{\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \sin \theta e^{\pm i\phi}.$$

We are now in a position to calculate the matrix elements appearing in the transition rate. Let us begin by calculating the matrix element for the transition beginning in the $2p$ state of hydrogen with $m = 0$

$$\begin{aligned} [\mathbf{x}]_{(1s)(2p)} &= \int r^2 \sin \theta \, d\theta \, d\phi \, dr \left(\sqrt{\frac{1}{\pi}} \frac{1}{a^{3/2}} e^{-r/a} \right) \\ &\quad \times (\hat{x}_1 r \sin \theta \cos \phi + \hat{x}_2 r \sin \theta \sin \phi + \hat{x}_3 \cos \theta) \\ &\quad \times \left(\frac{1}{\sqrt{32\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \cos \theta \right) \\ &= \frac{1}{\sqrt{32\pi} a^4} \int d\theta \, d\phi \, dr \, r^4 e^{-3r/2a} \sin \theta \cos \theta \\ &\quad \times (\hat{x}_1 r \sin \theta \cos \phi + \hat{x}_2 r \sin \theta \sin \phi + \hat{x}_3 \cos \theta) \\ &= \frac{\hat{x}_3}{\sqrt{8} a^4} \int d\theta \, dr \, r^4 e^{-3r/2a} \sin \theta \cos^2 \theta \\ &= \frac{\hat{x}_3}{\sqrt{18} a^4} \int_0^\infty dr \, r^4 e^{-3r/2a} \\ &= \frac{256}{243\sqrt{2}} a \hat{x}_3. \end{aligned}$$

We will now repeat the calculation beginning from the $2p$ state of hydrogen with $m = \pm 1$

$$\begin{aligned}
 [\mathbf{x}]_{(1s)(2p)} &= \int r^2 \sin \theta \, d\theta \, d\phi \, dr \left(\sqrt{\frac{1}{\pi}} \frac{1}{a^{3/2}} e^{-r/a} \right) \\
 &\quad \times (\hat{x}_1 r \sin \theta \cos \phi + \hat{x}_2 r \sin \theta \sin \phi + \hat{x}_3 \cos \theta) \\
 &\quad \times \left(\mp \frac{1}{8\sqrt{\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \sin \theta e^{\pm i\phi} \right) \\
 &= \mp \frac{1}{8\pi a^4} \int d\theta \, d\phi \, dr \, r^4 e^{-3r/2a} \sin^2 \theta \\
 &\quad \times (\hat{x}_1 r \sin \theta \cos \phi + \hat{x}_2 r \sin \theta \sin \phi + \hat{x}_3 \cos \theta) \\
 &= \mp \frac{1}{8a^4} \int d\theta \, dr \, r^4 e^{-3r/2a} \sin^3 \theta (\hat{x}_1 \pm i\hat{x}_2) \\
 &= \mp \frac{1}{6a^4} \int_0^\infty dr \, r^4 e^{-3r/2a} (\hat{x}_1 \pm i\hat{x}_2) \\
 &= \mp \frac{128}{243} a (\hat{x}_1 \pm i\hat{x}_2).
 \end{aligned}$$

Squaring these matrix elements, we see that for any m , we have

$$|[\mathbf{x}]_{(1s)(2p)}|^2 = \frac{2^{15}}{3^{10}} a^2.$$

To calculate the transition rate, we also need the frequency of the emitted photon, which is given by

$$\omega_{(1s)(2p)} = \frac{E_{(2p)} - E_{(1s)}}{\hbar}.$$

According to Eq. (2.3.20), the energy levels of the hydrogen atom are given by

$$E_n = -\frac{\hbar^2}{2\mu a^2 n^2},$$

and so we see that

$$\omega_{(1s)(2p)} = \frac{3\hbar}{8\mu a^2}.$$

Putting everything together, we arrive at the rate of single photon emission from the $2p$ to the $1s$ state of hydrogen

$$\begin{aligned}
 A_{(2p)}^{(1s)} &= \frac{2^2 e^2}{3c^3 \hbar} \times \frac{3^3 \hbar^3}{2^9 \mu^3 a^6} \times \frac{2^{15} a^2}{3^{10}} \\
 &= \frac{2^8 e^2 \hbar^2}{3^8 c^3 \mu^3 a^4} \\
 &= \frac{2^8 e^{10} \mu}{3^8 \hbar^6 c^3}.
 \end{aligned}$$

3. Calculate the expectation values of the kinetic and potential energies in the 1s state of hydrogen.

For a given state ψ , the expectation value of the kinetic energy in that state is given by

$$\langle K \rangle_\psi = \int d^3x \psi^*(\mathbf{x}) \left(-\frac{\hbar^2}{2M} \nabla^2 \right) \psi(\mathbf{x}),$$

and the expectation value of the potential energy in that state is given by

$$\langle V \rangle_\psi = \int d^3x \psi^*(\mathbf{x}) (V(\mathbf{x})) \psi(\mathbf{x}).$$

In the previous problem, we derived the normalized wave function for the 1s state of hydrogen

$$\psi_{1s} = \sqrt{\frac{1}{\pi}} \frac{1}{a^{3/2}} e^{-r/a}.$$

The expectation value of the kinetic energy in the 1s state of hydrogen is given by

$$\begin{aligned}
 \langle K \rangle_{(1s)} &= \int d^3x \psi_{(1s)}^*(\mathbf{x}) \left(-\frac{\hbar^2}{2\mu} \nabla^2 \right) \psi_{(1s)}(\mathbf{x}) \\
 &= -\frac{\hbar^2}{2\pi a^3 \mu} \int d\theta d\phi dr r^2 \sin\theta e^{-r/a} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} e^{-r/a} \right) \\
 &= -\frac{2\hbar^2}{\mu a^3} \int_0^\infty dr \left(-\frac{1}{a} \right) \left(2a - \frac{r}{a^2} \right) e^{-2r/a} \\
 &= \frac{2\hbar^2}{\mu a^4} \left(\frac{a^2}{2} - \frac{a^2}{4} \right) \\
 &= \frac{\hbar^2}{2\mu a^2} \\
 &= \frac{\mu e^4}{2\hbar^2}.
 \end{aligned}$$

In the second line we have used the Laplacian operator in the form of Eq. (2.1.16), and we used the fact that $\ell = 0$ in the 1s state of hydrogen. The expectation value of the potential energy in the 1s state of hydrogen is given by

$$\begin{aligned}
\langle V \rangle_{(1s)} &= \int d^3x \psi_{(1s)}^*(\mathbf{x}) \left(-\frac{e^2}{r} \right) \psi_{(1s)}(\mathbf{x}) \\
&= -\frac{e^2}{\pi a^3} \int d\theta d\phi dr r^2 \sin\theta \left(\frac{1}{r} \right) e^{-2r/a} \\
&= -\frac{4e^2}{a^3} \int_0^\infty dr r e^{-2r/a} \\
&= -\frac{e^2}{a} \\
&= -\frac{\mu e^4}{\hbar^2} \\
&= -2\langle K \rangle_{(1s)}.
\end{aligned}$$

Notice that this is a special case of the virial theorem, which states that for any potential of the form $V(r) = Cr^n$, we have the relation

$$\langle V \rangle = \frac{2}{n} \langle K \rangle.$$

4. Calculate the expectation values of the kinetic and potential energies in the lowest energy state of the three-dimensional harmonic oscillator, using the algebraic methods that were used in Section 2.5 to find the energy levels in this system.

In order to calculate the expectation values of the kinetic and potential energy for the harmonic oscillator using the algebraic methods of Section 2.5, we will first need to write the position and momentum operators in terms of the raising and lowering operators defined in Eq. (2.5.7)

$$\begin{aligned}
a_i &\equiv \frac{1}{\sqrt{2M\hbar\omega}} \left(-i\hbar \frac{\partial}{\partial x_i} - iM\omega x_i \right), \\
a_i^\dagger &\equiv \frac{1}{\sqrt{2M\hbar\omega}} \left(-i\hbar \frac{\partial}{\partial x_i} + iM\omega x_i \right).
\end{aligned}$$

Solving these expressions for x_i and $\partial/\partial x_i$, we find

$$\begin{aligned}
x_i &= \frac{i\sqrt{\hbar}}{\sqrt{2M\omega}} (a_i - a_i^\dagger), \\
\frac{\partial}{\partial x_i} &= \frac{i\sqrt{M\omega}}{\sqrt{2\hbar}} (a_i + a_i^\dagger).
\end{aligned}$$

Recall the commutation relations for the raising and lowering operators given in Eqs. (2.5.8) and (2.5.9)

$$\begin{aligned}
[a_i, a_i^\dagger] &= \delta_{ij}, \\
[a_i, a_i] &= [a_i^\dagger, a_i^\dagger] = 0.
\end{aligned}$$

We will work with the normalized wave function for the lowest energy state ψ_0 , so that

$$\int d^3x \psi_0^* \psi_0 = 1.$$

Recall also that the lowest energy state is annihilated by the lowering operators

$$a_i \psi_0 = 0.$$

The expectation value of the kinetic energy in the lowest energy state is given by

$$\begin{aligned} \langle K \rangle_0 &= \int d^3x \psi_0^* \left(-\frac{\hbar^2}{2M} \nabla^2 \right) \psi_0 \\ &= \int d^3x \psi_0^* \left(\frac{\hbar\omega}{4} \sum_i (a_i + a_i^\dagger) (a_i + a_i^\dagger) \right) \psi_0 \\ &= \frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* \left(a_i^2 \psi_0 + a_i a_i^\dagger \psi_0 + a_i^\dagger a_i \psi_0 + a_i^{\dagger 2} \psi_0 \right). \end{aligned}$$

The first and third terms vanish because the lowering operator annihilates the lowest energy state. The fourth term can be rewritten by using the definition of the adjoint as

$$\frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* a_i^{\dagger 2} \psi_0 = \frac{\hbar\omega}{4} \sum_i \int d^3x (a_i^2 \psi_0)^* \psi_0 = 0,$$

which vanishes because the lowering operator annihilates the lowest energy state. The only remaining term in the expression for the expectation value of the kinetic energy can be rewritten in terms of a commutator

$$\begin{aligned} \langle K \rangle_0 &= \frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* a_i a_i^\dagger \psi_0 \\ &= \frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* \left([a_i, a_i^\dagger] \psi_0 + a_i^\dagger a_i \psi_0 \right) \\ &= \frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* \psi_0 \\ &= \frac{3}{4} \hbar\omega, \end{aligned}$$

where the second term in the second line vanishes because the lowering operator annihilates the lowest energy state, and we have used the commutation relation of the raising and lowering operators in the first term. Proceeding in the same way for the expectation value of the potential energy gives

$$\begin{aligned}
\langle V \rangle_0 &= \int d^3x \psi_0^* \left(\sum_i \frac{M\omega^2}{2} x_i \right) \psi_0 \\
&= -\frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* (a_i - a_i^\dagger) (a_i - a_i^\dagger) \psi_0 \\
&= -\frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* (a_i^2 \psi_0 - a_i a_i^\dagger \psi_0 - a_i^\dagger a_i \psi_0 + a_i^{\dagger 2} \psi_0) \\
&= -\frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* \left(-[a_i, a_i^\dagger] \psi_0 - a_i^\dagger a_i \psi_0 \right) \\
&= \frac{\hbar\omega}{4} \sum_i \int d^3x \psi_0^* \psi_0 \\
&= \frac{3}{4} \hbar\omega \\
&= \langle K \rangle_0.
\end{aligned}$$

Notice that like the previous problem this gives a specific case of the virial theorem.

5. *Derive the formula for the energy levels of the three-dimensional harmonic oscillator by using the power-series method (with suitable modifications) that was used in Section 2.3 for the hydrogen atom.*

For the harmonic oscillator, the potential takes the form

$$V(r) = \frac{M\omega^2 r^2}{2}.$$

We begin with a wave function of the form given by Eqs. (2.1.21) and (2.1.28),

$$\psi(\mathbf{x}) = \frac{u(r)}{r} Y_\ell^m(\theta, \phi),$$

where $u(r)$ is a solution of Eq. (2.1.29)

$$-\frac{\hbar^2}{2M} \frac{d^2 u(r)}{dr^2} + \left[\frac{M\omega^2 r^2}{2} + \frac{\ell(\ell+1)\hbar^2}{2Mr^2} \right] u(r) = E u(r).$$

Following closely the steps of Section 2.3, this can be rewritten in the form

$$-\frac{d^2 u(r)}{dr^2} + \left[\frac{M^2 \omega^2 r^2}{\hbar^2} + \frac{\ell(\ell+1)}{r^2} \right] u(r) = -\kappa^2 u(r),$$

where κ is defined by

$$E = -\frac{\hbar^2 \kappa^2}{2M}.$$

After defining

$$\rho \equiv \kappa r,$$

and dividing by κ^2 , the equation for u becomes

$$-\frac{d^2u}{d\rho^2} + \left[\xi\rho^2 + \frac{\ell(\ell+1)}{\rho^2} \right] u = -u,$$

where we have also defined

$$\xi \equiv \frac{M^2\omega^2}{\hbar^2\kappa^4}.$$

In the limit $\rho \rightarrow 0$, the differential equation for u becomes

$$\frac{d^2u}{d\rho^2} \approx \ell(\ell+1)\rho^{-2}u,$$

which implies that in this limit, we must have $u \sim \rho^{\ell+1}$. In the limit $\rho \rightarrow \infty$, the equation for u becomes

$$\frac{d^2u}{d\rho^2} \approx \xi\rho^2u,$$

which implies that in this limit, we must have $u \sim e^{\pm\sqrt{\xi}\rho^2/2}$. The requirement that the wave function be normalizable eliminates the exponentially growing solution, and so we keep only the exponentially decaying solution. We can then write u in the form

$$u = \rho^{\ell+1} \exp\left(-\frac{1}{2}\sqrt{\xi}\rho^2\right) F(\rho).$$

In order to plug this into the Schrödinger equation, we must find the second derivative of u . The first derivative is

$$\frac{du}{d\rho} = \rho^{\ell+1} \exp\left(-\frac{1}{2}\sqrt{\xi}\rho^2\right) \left[\left(\frac{\ell+1}{\rho} - \sqrt{\xi}\rho\right) F + \frac{dF}{d\rho} \right],$$

and the second derivative is

$$\begin{aligned} \frac{d^2u}{d\rho^2} &= \rho^{\ell+1} \exp\left(-\frac{1}{2}\sqrt{\xi}\rho^2\right) \\ &\times \left[\left(\frac{\ell(\ell+1)}{\rho^2} - \sqrt{\xi}(2\ell+3) + \xi\rho^2\right) F + 2\left(\frac{\ell+1}{\rho} - \sqrt{\xi}\rho\right) \frac{dF}{d\rho} + \frac{d^2F}{d\rho^2} \right]. \end{aligned}$$

Plugging this into the Schrödinger equation and dividing out common factors gives a differential equation for F

$$\frac{d^2F}{d\rho^2} - 2\left(\sqrt{\xi}\rho - \frac{\ell+1}{\rho}\right) \frac{dF}{d\rho} - \left(\sqrt{\xi}(2\ell+3) - 1\right) F = 0.$$

We can simplify this equation further if we make the identification

$$\rho = \sqrt{\sigma},$$

so that we have

$$\begin{aligned}\frac{d}{d\rho} &= \frac{d\sigma}{d\rho} \frac{d}{d\sigma} = 2\rho \frac{d}{d\sigma} = 2\sqrt{\sigma} \frac{d}{d\sigma}, \\ \frac{d^2}{d\rho^2} &= 4\sigma \frac{d}{d\sigma^2} + 2\frac{d}{d\sigma}.\end{aligned}$$

The differential equation for F now becomes

$$4\sigma \frac{d^2 F}{d\sigma^2} + 2\frac{dF}{d\sigma} - 4\left(\sqrt{\xi}\sigma - (\ell + 1)\right) \frac{dF}{d\sigma} - \left(\sqrt{\xi}(2\ell + 3) - 1\right) F = 0,$$

which can be simplified slightly to read

$$\frac{d^2 F}{d\sigma^2} - \left(\sqrt{\xi} - \frac{\ell + \frac{3}{2}}{\sigma}\right) \frac{dF}{d\sigma} - \frac{\sqrt{\xi}(2\ell + 3) - 1}{4\sigma} F = 0.$$

We now look for a series solution of the form

$$F = \sum_{s=0}^{\infty} a_s \sigma^s,$$

where we require that $a_0 \neq 0$ in order to maintain the behavior of the wave function in the limit $\rho \rightarrow 0$ that we found above. Using this ansatz in the equation for F gives

$$\begin{aligned}\sum_{s=0}^{\infty} a_s \left[s(s-1)\sigma^{s-2} - s\sqrt{\xi}\sigma^{s-1} + s\left(\ell + \frac{3}{2}\right)\sigma^{s-2} \right. \\ \left. - \frac{1}{4}\left(\sqrt{\xi}(2\ell + 3) - 1\right)\sigma^{s-1} \right] = 0.\end{aligned}$$

In the first and third terms, we will make the replacement $s \mapsto s + 1$. This does not affect the limits of the sum, because initially, the $s = 0$ contribution of the first and third term vanishes. After this replacement, the equation becomes

$$\begin{aligned}\sum_{s=0}^{\infty} \left[a_{s+1}s(s+1) - a_s s\sqrt{\xi} + a_{s+1}(s+1)\left(\ell + \frac{3}{2}\right) \right. \\ \left. - \frac{1}{4}\left(\sqrt{\xi}(2\ell + 3) - 1\right) \right] \sigma^{s-1} = 0.\end{aligned}$$

This expression must vanish for values of σ , and therefore the sum must vanish term by term. This results in a recurrence relation for the coefficients of the series solution

$$a_{s+1}(s+1) \left(\ell + \frac{3}{2} + s \right) = a_s \left(s\sqrt{\xi} + \frac{\sqrt{\xi}(2\ell+3)-1}{4} \right).$$

For large values of s , this expression gives $a_{s+1}/a_s \rightarrow \sqrt{\xi}/s$ and so

$$a_s \rightarrow \frac{a\sqrt{\xi}^s}{(s+b)!},$$

which gives for F at large s

$$F \rightarrow a \sum_s \frac{(\sqrt{\xi}\sigma)^s}{(s+b)!} = a \left(\sqrt{\xi}\sigma \right)^{-b} e^{\sqrt{\xi}\sigma} = a \left(\sqrt{\xi}\rho^2 \right)^{-b} e^{\sqrt{\xi}\rho^2},$$

which is the exponentially growing solution we threw out above in order to require normalizability of the wave function. In order to avoid this exponentially growing solution, we require that the power series must terminate at some finite $s = s_{max}$. We therefore require that

$$s_{max}\sqrt{\xi} + \frac{\sqrt{\xi}(2\ell+3)-1}{4} = 0,$$

which we can rearrange to read

$$\frac{1}{\sqrt{\xi}} = 2\ell + 3 + 4s_{max}.$$

Since ℓ and s_{max} are both non-negative integers, we find that $1/\sqrt{\xi}$ must be an odd integer greater than or equal to 3

$$\frac{1}{\sqrt{\xi}} = 2n + 3 \quad \text{for } n = 0, 1, 2, \dots$$

Returning to the definition of ξ we find

$$\xi = \frac{M^2\omega^2}{\hbar^2\kappa^4} = \frac{1}{(2n+3)^2},$$

and so

$$\kappa_n^4 = (2n+3)^2 \frac{M^2\omega^2}{\hbar^2} = \frac{4M^2}{\hbar^4} E_n^2.$$

Finally, we arrive at the expression for the energy levels

$$E_n = \left(n + \frac{3}{2} \right) \hbar\omega.$$

This is exactly what we expect based on the fact that a three-dimensional harmonic oscillator behaves just like three one-dimensional harmonic oscillators. As a side note, we have also arrived at an expression for the wave functions of the three-dimensional harmonic oscillator

$$\psi_n \propto r^\ell \exp\left(-\frac{M\omega}{2\hbar}r^2\right) L_{\frac{1}{2}(n-\ell)}^{(\ell+\frac{1}{2})}\left(\frac{M\omega}{\hbar}r^2\right) Y_\ell^m(\theta, \phi),$$

where the $L_k^{(\alpha)}(y)$ are called generalized Laguerre polynomials, and are generated by the recurrence relation derived above.

6. Find the difference in the energies of the Lyman α transitions in hydrogen and deuterium.

The Lyman α transition refers to the transition from $n = 2$ to $n = 1$. The only relevant difference between hydrogen and deuterium for the Lyman α transition is the reduced mass of the system. For hydrogen, the reduced mass is

$$\mu_H = \frac{m_p m_e}{m_p + m_e},$$

while for deuterium the reduced mass is slightly higher

$$\mu_D = \frac{2m_p m_e}{2m_p + m_e}.$$

According to Eq. (2.3.20), the energy levels of hydrogenic atoms are given by

$$E_n = -\frac{\hbar^2}{2\mu a^2 n^2} = -\frac{\mu Z^2 e^4}{2\hbar^2 n^2}.$$

The energy of a Lyman α photon is given by

$$E_\alpha = E_2 - E_1 = \frac{3\mu Z^2 e^4}{8\hbar^2}.$$

The isotopic shift is given by

$$\begin{aligned} \Delta E_\alpha &= \frac{3Z^2 e^4}{8\hbar^2} (\mu_D - \mu_H) = \frac{3Z^2 e^4}{8\hbar^2} \left(\frac{m_p m_e^2}{(2m_p + m_e)(m_p + m_e)} \right) \\ &\approx 2.77644085 \times 10^{-3} \text{ eV}. \end{aligned}$$

This is to be compared with the energy of a Lyman α photon emitted from a hydrogen atom

$$E_\alpha^{(H)} = \frac{3\mu_H Z^2 e^4}{8\hbar^2} \approx 5.21153244 \text{ eV},$$

and so the isotopic shift represents about a 0.05% shift in the energy of the emitted photon. This shift in energy is large enough to be detected with modern spectroscopic equipment, which allows hydrogen and deuterium to be distinguished by their emission spectra.

7. Calculate the wave function (aside from normalization) of the 3s state of the hydrogen atom.

The 3s state of hydrogen has $n = 3$, $\ell = 0$, and $m = 0$. In order to find the wave function for the 3s state of hydrogen, we begin with the form given by Eq. (2.1.21)

$$\psi(\mathbf{x}) = R(r)Y_\ell^m(\theta, \phi),$$

where $R(r)$ can be put in the form of Eq. (2.1.28)

$$R(r) = \frac{u(r)}{r}.$$

As discussed in Section 2.2, Y_0^0 is just a constant, and since we are not concerned with the normalization here, we can simply include it in the undetermined normalization constant for the purposes of this problem. For the hydrogen atom, u takes a form given by Eq. (2.3.7)

$$u = \rho^{\ell+1} \exp(-\rho)F(\rho),$$

where we have introduced the notation

$$\rho \equiv \kappa r,$$

where κ is defined by Eqs. (2.3.3) and (2.3.18) to be

$$\kappa = \frac{\sqrt{-2\mu E}}{\hbar} = \frac{1}{na},$$

and $a = \hbar^2/\mu Ze^2$ is the Bohr radius. According to Eq. (2.3.9), $F(\rho)$ takes the form of a power series

$$F(\rho) = \sum_s^\infty a_s \rho^s,$$

where the coefficients a_s satisfy a recurrence relation, which is given by Eq. (2.1.12)

$$a_{s+1} = \frac{-2n + 2s + 2\ell + 2}{(s + 2\ell + 2)(s + 1)} a_s.$$

For the 3s state of hydrogen, this gives

$$\begin{aligned} a_1 &= -2a_0 \\ a_2 &= -\frac{1}{3}a_1 = \frac{2}{3}a_0 \\ a_k &= 0 \quad \text{for } k \geq 3. \end{aligned}$$

Therefore, $F(\rho)$ takes the form

$$F = a_0 \left(1 - 2\rho + \frac{2}{3}\rho^2 \right),$$

and so u takes the form

$$u = a_0 \rho \exp(-\rho) \left(1 - 2\rho + \frac{2}{3}\rho^2 \right) = a_0 \left(\frac{r}{3a} - \frac{2r^2}{9a^2} + \frac{2r^3}{81a^3} \right) \exp\left(-\frac{r}{3a}\right).$$

Putting this together, we find the wave function for the 3s state of hydrogen

$$\psi(\mathbf{x}) = N \left(\frac{1}{3a} - \frac{2r}{9a^2} + \frac{2r^2}{81a^3} \right) \exp\left(-\frac{r}{3a}\right),$$

where N is the normalization constant.

Chapter 3 Problem Set Solutions

1. Consider a system with a pair of observable quantities A and B , whose commutation relations with the Hamiltonian take the form $[H, A] = iwB$, $[H, B] = -iwA$, where w is some real constant. Suppose that the expectation values of A and B are known at time $t = 0$. Give formulas for the expectation values of A and B as a function of time.

According to Eq. (3.6.7), for any Heisenberg picture operator $\mathcal{O}_H(t)$, the time derivative is given by

$$\dot{\mathcal{O}}_H(t) = \frac{i}{\hbar} [H, \mathcal{O}_H(t)].$$

In this case, this gives

$$\begin{aligned}\dot{A}_H(t) &= \frac{i}{\hbar} [H, A_H(t)] = -\frac{w}{\hbar} B_H(t), \\ \dot{B}_H(t) &= \frac{i}{\hbar} [H, B_H(t)] = \frac{w}{\hbar} A_H(t).\end{aligned}$$

Taking another time derivative, we find

$$\begin{aligned}\ddot{A}_H(t) &= -\frac{w}{\hbar} \dot{B}_H(t) = -\frac{w^2}{\hbar^2} A_H(t), \\ \ddot{B}_H(t) &= \frac{w}{\hbar} \dot{A}_H(t) = -\frac{w^2}{\hbar^2} B_H(t).\end{aligned}$$

These differential equations have a well-known solution of the form

$$\begin{aligned}A_H(t) &= C_1 \sin\left(\frac{w}{\hbar}t\right) + C_2 \cos\left(\frac{w}{\hbar}t\right), \\ B_H(t) &= C_3 \sin\left(\frac{w}{\hbar}t\right) + C_4 \cos\left(\frac{w}{\hbar}t\right).\end{aligned}$$

Now we must impose the condition that $\dot{A}_H(t) = -\frac{w}{\hbar} B_H(t)$, which for this solution takes the form

$$\frac{w}{\hbar} C_1 \cos\left(\frac{w}{\hbar}t\right) - \frac{w}{\hbar} C_2 \sin\left(\frac{w}{\hbar}t\right) = -\frac{w}{\hbar} C_3 \sin\left(\frac{w}{\hbar}t\right) - \frac{w}{\hbar} C_4 \cos\left(\frac{w}{\hbar}t\right).$$

In order for this to be satisfied for all times, we require

$$C_4 = -C_1, \quad C_3 = C_2.$$

Evaluating these solutions at $t = 0$, we find

$$C_2 = A_H(0), \quad C_1 = -B_H(0),$$

and so we can write the operators as

$$\begin{aligned} A_H(t) &= -B_H(0) \sin\left(\frac{w}{\hbar}t\right) + A_H(0) \cos\left(\frac{w}{\hbar}t\right), \\ B_H(t) &= A_H(0) \sin\left(\frac{w}{\hbar}t\right) + B_H(0) \cos\left(\frac{w}{\hbar}t\right). \end{aligned}$$

Now if we define

$$\langle A_H(0) \rangle \equiv a, \quad \langle B_H(0) \rangle \equiv b,$$

then we find for the expectation values

$$\begin{aligned} \langle A_H(t) \rangle &= -b \sin\left(\frac{w}{\hbar}t\right) + a \cos\left(\frac{w}{\hbar}t\right), \\ \langle B_H(t) \rangle &= a \sin\left(\frac{w}{\hbar}t\right) + b \cos\left(\frac{w}{\hbar}t\right). \end{aligned}$$

2. Consider a normalized initial state Ψ at $t = 0$ with a spread ΔE in energy, defined by

$$\Delta E \equiv \sqrt{\left\langle \left(H - \langle H \rangle_{\Psi} \right)^2 \right\rangle_{\Psi}}.$$

Calculate the probability $|\langle \Psi(\delta t), \Psi \rangle|^2$ that after a very short time δt the system is still in the state Ψ . Express the result in terms of ΔE , \hbar and δt , to second order in δt .

We can use Eq. (3.6.3) to write

$$\Psi(\delta t) = \exp(-iH\delta t/\hbar) \Psi,$$

where we have defined $\Psi \equiv \Psi(0)$, and we will assume that Ψ is normalized so that $\langle \Psi, \Psi \rangle = 1$. Now let us expand $\Psi(\delta t)$ to second order in δt

$$\Psi(\delta t) = \Psi - \frac{i}{\hbar} H \delta t \Psi - \frac{1}{2\hbar^2} H^2 \delta t^2 \Psi + \mathcal{O}(\delta t^3).$$

We can then calculate the probability that the system remains in the initial state

$$\begin{aligned} |\langle \Psi(\delta t), \Psi \rangle|^2 &= \left| \langle \Psi, \Psi \rangle + \frac{i}{\hbar} \delta t \langle H \Psi, \Psi \rangle - \frac{1}{2\hbar^2} \delta t^2 \langle H^2 \Psi, \Psi \rangle \right|^2 \\ &= |\langle \Psi, \Psi \rangle|^2 + \frac{i}{\hbar} \delta t \langle H \Psi, \Psi \rangle \langle \Psi, \Psi \rangle - \frac{i}{\hbar} \delta t \langle H \Psi, \Psi \rangle \langle \Psi, \Psi \rangle \\ &\quad + \frac{1}{\hbar^2} \delta t^2 |\langle H \Psi, \Psi \rangle|^2 - \frac{1}{\hbar^2} \delta t^2 \langle H^2 \Psi, \Psi \rangle \langle \Psi, \Psi \rangle + \mathcal{O}(\delta t^3) \\ &= 1 + \frac{\delta t^2}{\hbar^2} \langle H \rangle_{\Psi}^2 - \frac{\delta t^2}{\hbar^2} \langle H^2 \rangle_{\Psi} + \mathcal{O}(\delta t^3). \end{aligned}$$

Now we note that

$$\begin{aligned}\Delta_\Psi E &\equiv \sqrt{\langle (H - \langle H \rangle_\Psi)^2 \rangle_\Psi} \\ &= \sqrt{\langle H^2 \rangle_\Psi - 2\langle H \langle H \rangle_\Psi \rangle_\Psi + \langle \langle H \rangle_\Psi^2 \rangle_\Psi} \\ &= \sqrt{\langle H^2 \rangle_\Psi - \langle H \rangle_\Psi^2},\end{aligned}$$

and so we can rewrite the inner product above as

$$|(\Psi(\delta t), \Psi)|^2 = 1 - \frac{(\Delta_\Psi E)^2 \delta t^2}{\hbar^2} + \mathcal{O}(\delta t^3).$$

3. Suppose that the Hamiltonian is a linear operator with

$$H\Psi = g\Phi, \quad H\Phi = g^*\Psi, \quad H\Upsilon_n = 0,$$

where g is an arbitrary constant, Ψ and Φ are a pair of normalized independent (but not necessarily orthogonal) state vectors, and Υ_n runs over all state vectors orthogonal to both Ψ and Φ . What are the conditions that Φ and Ψ must satisfy in order for this Hamiltonian to be Hermitian? With these conditions satisfied, find the states with definite energy, and the corresponding energy values.

In order for H to be Hermitian, we must have

$$(\Psi, H\Psi) = (H\Psi, \Psi).$$

Using the relation $H\Psi = g\Phi$, we can rewrite the left-hand side as

$$(\Psi, H\Psi) = (\Psi, g\Phi) = g(\Psi, \Phi),$$

and the right-hand side as

$$(H\Psi, \Psi) = (g\Phi, \Psi) = g^*(\Phi, \Psi) = g^*(\Psi, \Phi)^* = [g(\Psi, \Phi)]^*.$$

We find that the condition for H to be Hermitian is that the product $g(\Psi, \Phi)$ must be real.

We will now look for states $\chi_i = a_i\Psi + b_i\Phi + \sum_n c_{in}\Upsilon_n$ such that $H\chi_i = E_i\chi_i$. Applying the Hamiltonian to such a state χ_i , we find

$$\begin{aligned}H\chi_i &= H\left(a_i\Psi + b_i\Phi + \sum_n c_{in}\Upsilon_n\right) = ga_i\Phi + g^*b_i\Psi + 0 \\ &= E_i\left(a_i\Psi + b_i\Phi + \sum_n c_{in}\Upsilon_n\right) = E_i\chi_i.\end{aligned}$$

First, we notice that either $c_{in} = 0$ or $E_i = a_i = b_i = 0$. We will set $c_{in} = 0$ and look for states with non-zero energy. We find that for $E_i \neq 0$, we must have

$$E_i a_i = g^* b_i, \quad E_i b_i = g a_i,$$

which we can combine to find that

$$E_i^2 = |g|^2.$$

Let us distinguish two states which we will call χ_+ and χ_- such that

$$E_+ = |g|, \quad E_- = -|g|.$$

We then find that the states are given by

$$\chi_{\pm} = N_{\pm} \left(\Psi \pm \frac{g}{|g|} \Phi \right),$$

where N_{\pm} is a normalization constant, which we can determine by the condition that

$$1 = (\chi_{\pm}, \chi_{\pm}) = |N_{\pm}|^2 \left[(\Psi, \Psi) + (\Phi, \Phi) \pm 2 \frac{g}{|g|} (\Psi, \Phi) \right].$$

So we find, up to an arbitrary overall phase the normalized states of definite energy are given by

$$\chi_{\pm} = \left[2 \pm 2 \frac{g}{|g|} (\Psi, \Phi) \right]^{-1/2} \left(\Psi \pm \frac{g}{|g|} \Phi \right),$$

and these states satisfy the condition

$$H \chi_{\pm} = \pm |g| \chi_{\pm},$$

and of course there are the states of zero energy

$$H \Upsilon_n = 0.$$

4. *Suppose that a linear operator A , though not Hermitian, satisfies the condition that it commutes with its adjoint. What can be said about the relation between the eigenvalues of A and of A^\dagger ? What can be said about the scalar product of two eigenstates of A with unequal eigenvalues?*

We are told that the operator A commutes with its adjoint $[A, A^\dagger] = 0$, and so there exists a state Ψ , which we will take to be normalized $(\Psi, \Psi) = 1$, which is an eigenstate of both A and A^\dagger

$$A \Psi = a \Psi, \quad A^\dagger \Psi = b \Psi.$$

Now let us calculate the expectation value of the product AA^\dagger in the state Ψ

$$\begin{aligned} (\Psi, AA^\dagger \Psi) &= ba = (A^\dagger \Psi, A^\dagger \Psi) = |b|^2 = (\Psi, A^\dagger A \Psi) \\ &= ab = (A \Psi, A \Psi) = |a|^2. \end{aligned}$$

We can see from this that we must have $a = b^*$.

If we now define a second state Ψ' such that

$$A\Psi' = a'\Psi', \quad A^\dagger\Psi' = b'\Psi',$$

we can use the definition of the adjoint to write

$$0 = (\Psi', A\Psi) - (A^\dagger\Psi', \Psi) = a(\Psi', \Psi) - b'^*(\Psi', \Psi).$$

We see that this equation implies that either $a = b'^*$ or $(\Psi', \Psi) = 0$. Since $b'^* = a'$ because A commutes with its adjoint, we find that for $a \neq a'$, we must have $(\Psi', \Psi) = 0$.

5. *Suppose the state vectors Ψ and Ψ' are eigenvectors of a unitary operator with eigenvalues λ and λ' , respectively. What relation must λ and λ' satisfy if Ψ is not orthogonal to Ψ' ?*

We have two states Ψ and Ψ' such that

$$U\Psi = \lambda\Psi, \quad U\Psi' = \lambda'\Psi',$$

with U a unitary operator $U^\dagger U = 1$. Let us first consider the inner product of Ψ with itself

$$(\Psi, \Psi) = (\Psi, U^\dagger U\Psi) = (U\Psi, U\Psi) = (\lambda\Psi, \lambda\Psi) = \lambda^*\lambda(\Psi, \Psi),$$

which implies that $\lambda^*\lambda = 1$. The same procedure applied to Ψ' requires that $\lambda'^*\lambda' = 1$. Now let us consider the inner product of Ψ with Ψ'

$$(\Psi, \Psi') = (\Psi, U^\dagger U\Psi') = (U\Psi, U\Psi') = (\lambda\Psi, \lambda'\Psi') = \lambda^*\lambda'^*(\Psi, \Psi'),$$

which implies that $\lambda^*\lambda' = 1$ or $(\Psi, \Psi') = 0$. Putting this together we find that for Ψ and Ψ' not orthogonal, we must have

$$\lambda = \lambda'^* = e^{i\phi}$$

for some real constant ϕ .

6. *Show that the product of the uncertainties in position and momentum takes its minimum value $\hbar/2$ for a Gaussian wave packet of free particle wave functions.*

We wish to show that

$$\Delta_\Psi X \Delta_\Psi P = \frac{\hbar}{2}$$

for a Gaussian wave packet, where the spread of any observable corresponding to an operator A in a state Ψ is defined as in Eq. (3.3.23)

$$\Delta_\Psi A \equiv \sqrt{\langle (A - \langle A \rangle_\Psi)^2 \rangle_\Psi}.$$

A Gaussian wave packet can be written in a coordinate representation as

$$\psi(x) = \frac{\exp(-ip_0x/\hbar)}{(2\pi a^2)^{1/4}} \exp\left(-\frac{(x-x_0)^2}{4a^2}\right).$$

Let us begin by calculating $\langle X \rangle_\psi$ for the Gaussian wave packet

$$\begin{aligned} \langle X \rangle_\psi &= \int_{-\infty}^{\infty} \psi^*(x)x\psi(x) dx \\ &= \frac{1}{(2\pi a^2)^{1/2}} \int_{-\infty}^{\infty} x \exp\left(-\frac{(x-x_0)^2}{2a^2}\right) dx \\ &= x_0. \end{aligned}$$

We follow a similar procedure to calculate $\langle X^2 \rangle_\psi$

$$\begin{aligned} \langle X^2 \rangle_\psi &= \int_{-\infty}^{\infty} \psi^*(x)x^2\psi(x) dx \\ &= \frac{1}{(2\pi a^2)^{1/2}} \int_{-\infty}^{\infty} x^2 \exp\left(-\frac{(x-x_0)^2}{2a^2}\right) dx \\ &= x_0^2 + a^2. \end{aligned}$$

This gives for the spread in position

$$\begin{aligned} \Delta_\psi X &= \sqrt{\langle (X - \langle X \rangle_\psi)^2 \rangle_\psi} = \sqrt{\langle X^2 \rangle_\psi - \langle X \rangle_\psi^2} \\ &= \sqrt{(x_0^2 + a^2) - (x_0)^2} = a. \end{aligned}$$

Next, we will calculate $\langle P \rangle_\psi$ for the Gaussian wave packet

$$\begin{aligned} \langle P \rangle_\psi &= \int_{-\infty}^{\infty} \psi^*(x)i\hbar\frac{d}{dx}\psi(x) dx \\ &= \frac{1}{(2\pi a^2)^{1/2}} \int_{-\infty}^{\infty} \left(p_0 - i\hbar\frac{x-x_0}{2a^2}\right) \exp\left(-\frac{(x-x_0)^2}{2a^2}\right) dx \\ &= p_0. \end{aligned}$$

For $\langle P^2 \rangle_\psi$ we find

$$\begin{aligned} \langle P^2 \rangle &= \int_{-\infty}^{\infty} \psi^*(x) \left(-\hbar^2\frac{d^2}{dx^2}\right) \psi(x) dx \\ &= \frac{1}{(2\pi a^2)^{1/2}} \int_{-\infty}^{\infty} \left[\left(p_0 - i\hbar\frac{x-x_0}{2a^2}\right)^2 + \frac{\hbar^2}{2a^2} \right] \exp\left(-\frac{(x-x_0)^2}{2a^2}\right) dx \\ &= p_0^2 + \frac{\hbar^2}{4a^2}. \end{aligned}$$

This gives for the spread in momentum

$$\begin{aligned}\Delta_{\psi}P &= \sqrt{\langle (P - \langle P \rangle_{\psi})^2 \rangle_{\psi}} = \sqrt{\langle P^2 \rangle_{\psi} - \langle P \rangle_{\psi}^2} \\ &= \sqrt{\left(p_0^2 + \frac{\hbar^2}{4a^2}\right) - (p_0)^2} = \frac{\hbar}{2a}.\end{aligned}$$

Now, calculating the product of the spread in position and momentum, we find

$$\Delta_{\psi}X \Delta_{\psi}P = \frac{\hbar}{2},$$

which saturates the bound from the Heisenberg uncertainty principle.

Chapter 4 Problem Set Solutions

1. Suppose that an electron is in a state of orbital angular momentum $\ell = 2$. Show how to construct the state vectors with total angular momentum $j = 5/2$ and corresponding 3-components $m = 5/2$ and $m = 3/2$ as linear combinations of state vectors with definite values of S_3 and L_3 . Then find the state vector with $j = 3/2$ and $m = 3/2$. (All state vectors here should be properly normalized.) Summarize your results by giving values for the Clebsch–Gordan coefficients $C_{\frac{1}{2}2}(jm; m_s m_\ell)$ in the cases $(j, m) = (5/2, 5/2)$, $(5/2, 3/2)$ and $(3/2, 3/2)$.

We would like to construct eigenstates of the operators \mathbf{J}^2 , J_3 , \mathbf{L}^2 , and \mathbf{S}^2 which are linear combinations of eigenstates of the operators \mathbf{L}^2 , L_3 , \mathbf{S}^2 , and S_3 , just as in Eq. (4.3.18)

$$\Psi_{\ell s j}^m = \sum_{m_\ell, m_s} C_{\ell s}(j m; m_\ell m_s) \psi_{\ell s}^{m_\ell m_s}.$$

The state with the maximum values of j and m is given simply by the state with the maximum values of m_ℓ and m_s , as shown in Eq. (4.3.20), and so in the case $\ell = 2$, $s = 1/2$, this reads

$$\Psi_{2 \frac{1}{2} \frac{5}{2}}^{\frac{5}{2}} = \psi_{2 \frac{1}{2}}^{2 \frac{1}{2}}.$$

To find the state with $m = 3/2$, we can apply the lowering operator with proper normalization as given in Eq. (4.2.16)

$$\begin{aligned} \Psi_{2 \frac{1}{2} \frac{5}{2}}^{\frac{3}{2}} &= \frac{1}{\hbar} \left[\frac{5}{2} \left(\frac{5}{2} + 1 \right) - \left(\frac{5}{2} \right)^2 + \frac{5}{2} \right]^{-1/2} (J_1 - iJ_2) \Psi_{2 \frac{1}{2} \frac{5}{2}}^{\frac{5}{2}} \\ &= \frac{1}{\hbar\sqrt{5}} (L_1 - iL_2 + S_1 - iS_2) \psi_{2 \frac{1}{2}}^{2 \frac{1}{2}} \\ &= \frac{1}{\hbar\sqrt{5}} \left(\hbar [2(2+1) - (2)^2 + 2]^{1/2} \psi_{2 \frac{1}{2}}^{1 \frac{1}{2}} \right. \\ &\quad \left. + \hbar \left[\frac{1}{2} \left(\frac{1}{2} + 1 \right) - \left(\frac{1}{2} \right)^2 + \frac{1}{2} \right]^{1/2} \psi_{2 \frac{1}{2}}^{2 - \frac{1}{2}} \right) \\ &= \sqrt{\frac{4}{5}} \psi_{2 \frac{1}{2}}^{1 \frac{1}{2}} + \sqrt{\frac{1}{5}} \psi_{2 \frac{1}{2}}^{2 - \frac{1}{2}}. \end{aligned}$$

The properly normalized state vector constructed from $\psi_{2 \frac{1}{2}}^{2 - \frac{1}{2}}$ and $\psi_{2 \frac{1}{2}}^{2 - \frac{1}{2}}$ which is orthogonal to $\Psi_{2 \frac{1}{2} \frac{5}{2}}^{\frac{3}{2}}$ must be $\Psi_{2 \frac{1}{2} \frac{3}{2}}^{\frac{3}{2}}$, as in Eq. (4.3.23), and so we find

$$\Psi_{2\frac{1}{2} \ 2\frac{3}{2}} = -\sqrt{\frac{1}{5}}\psi_{2\frac{1}{2}}^{1\frac{1}{2}} + \sqrt{\frac{4}{5}}\psi_{2\frac{1}{2}}^{2-\frac{1}{2}},$$

up to an arbitrary overall phase factor. We can read off the Clebsch–Gordan coefficients by comparing with the first equation above, and we find for the non-vanishing coefficients

$$C_{2\frac{1}{2}}\left(\frac{5}{2} \ \frac{5}{2}; 2 \ \frac{1}{2}\right) = 1$$

$$C_{2\frac{1}{2}}\left(\frac{5}{2} \ \frac{3}{2}; 2 \ -\frac{1}{2}\right) = \sqrt{\frac{1}{5}}$$

$$C_{2\frac{1}{2}}\left(\frac{5}{2} \ \frac{5}{2}; 1 \ \frac{1}{2}\right) = \sqrt{\frac{4}{5}}$$

$$C_{2\frac{1}{2}}\left(\frac{5}{2} \ \frac{3}{2}; 2 \ -\frac{1}{2}\right) = \sqrt{\frac{4}{5}}$$

$$C_{2\frac{1}{2}}\left(\frac{5}{2} \ \frac{5}{2}; 1 \ \frac{1}{2}\right) = -\sqrt{\frac{1}{5}}$$

2. Suppose that \mathbf{A} and \mathbf{B} are vector operators, in the sense that

$$[J_i, A_j] = i\hbar \sum_k \epsilon_{ijk} A_k, \quad [J_i, B_j] = i\hbar \sum_k \epsilon_{ijk} B_k.$$

Show that the cross-product $\mathbf{A} \times \mathbf{B}$ is a vector in the same sense. Given that

$$[J_i, A_j] = i\hbar \sum_k \epsilon_{ijk} A_k, \quad [J_i, B_j] = i\hbar \sum_k \epsilon_{ijk} B_k,$$

we wish to show that

$$[J_i, (\mathbf{A} \times \mathbf{B})_j] = i\hbar \sum_k \epsilon_{ijk} (\mathbf{A} \times \mathbf{B})_k.$$

First, we note that the cross-product can be written as

$$(\mathbf{A} \times \mathbf{B})_i = \sum_{\ell m} \epsilon_{i\ell m} A_\ell B_m,$$

and so we can write the right-hand side of the desired result as

$$\begin{aligned} i\hbar \sum_k \epsilon_{ijk} (\mathbf{A} \times \mathbf{B})_k &= \sum_{k\ell m} \epsilon_{ijk} \epsilon_{k\ell m} A_\ell B_m \\ &= i\hbar \sum_{\ell m} (\delta_{i\ell} \delta_{jm} - \delta_{im} \delta_{j\ell}) A_\ell B_m \\ &= i\hbar (A_i B_j - A_j B_i), \end{aligned}$$

where we have used the well-known relation for the Levi–Civita symbols

$$\sum_k \epsilon_{kij} \epsilon_{k\ell m} = \delta_{i\ell} \delta_{jm} - \delta_{im} \delta_{j\ell}.$$

Now we can calculate the commutator of J_i with the cross-product $(\mathbf{A} \times \mathbf{B})_j$

$$\begin{aligned} [J_i, (\mathbf{A} \times \mathbf{B})_j] &= \sum_{\ell m} \epsilon_{j\ell m} ([J_i, A_\ell] B_m + A_\ell [J_i, B_m]) \\ &= \sum_{\ell m} \epsilon_{j\ell m} \left(i\hbar \sum_k \epsilon_{i\ell k} A_k B_m + A_\ell i\hbar \sum_k \epsilon_{imk} B_k \right) \\ &= i\hbar \left[\sum_{km} \left(\sum_\ell \epsilon_{j\ell m} \epsilon_{i\ell k} \right) A_k B_m + \sum_{k\ell} \left(\sum_m \epsilon_{j\ell m} \epsilon_{imk} \right) A_\ell B_k \right] \\ &= i\hbar \left[\sum_{km} (\delta_{mk} \delta_{ji} - \delta_{mi} \delta_{jk}) A_k B_m + \sum_{k\ell} (\delta_{jk} \delta_{i\ell} - \delta_{ij} \delta_{k\ell}) A_\ell B_k \right] \\ &= i\hbar \left[\delta_{ij} \sum_k A_k B_k - A_j B_i + A_i B_j - \delta_{ij} \sum_k A_k B_k \right] \\ &= i\hbar [A_i B_j - A_j B_i] \\ &= i\hbar \sum_k \epsilon_{ijk} (\mathbf{A} \times \mathbf{B})_k. \end{aligned}$$

We find that if \mathbf{A} and \mathbf{B} are vector operators, then $(\mathbf{A} \times \mathbf{B})$ is also a vector operator.

3. What is the minimum value of the total angular momentum \mathbf{J}^2 that a state must have in order to have a non-zero expectation value for an operator \mathcal{O}_j^m of spin j .

Let us define a state

$$\Omega_{j j'}^{m m'} \equiv \mathcal{O}_j^m \Psi_{j'}^{m'},$$

which as shown in Eq. (4.4.10) acts as a state vector describing two particles with spins j and j' and spin 3-components m and m' . We can express this state vector as a sum over states with total angular momentum J and 3-component M as in Eq. (4.4.11)

$$\Omega_{j j'}^{m m'} = \sum_{j'', m''} C_{j j'}(j'' m''; m m') \omega_{j j'}^{m''}.$$

As discussed in Section 4.3, the range of j'' is

$$j'' = |j - j'|, |j - j'| + 1, \dots, j + j'.$$

We are interested in the inner product $(\Psi_{j'}^{m'}, \omega_{j' j''}^{m''})$. Note that because \mathbf{J}^2 is an Hermitian, this inner product vanishes unless $j' = j''$

$$(\Psi_{j'}^{m'}, \mathbf{J}^2 \omega_{j' j''}^{m''}) = \hbar^2 j''(j''+1) (\Psi_{j'}^{m'}, \omega_{j' j''}^{m''}) = \hbar^2 j'(j'+1) (\Psi_{j'}^{m'}, \omega_{j' j''}^{m''}).$$

A non-vanishing inner product therefore requires that j' is in the range spanned by j'' , and so the minimum value that j' can take is given by

$$j'_{\min} = |j - j'_{\min}| = j - j'_{\min},$$

where we have taken $j - j'_{\min}$ to be positive because for $j < j'$ there is always a smaller value of j' for which the inner product does not vanish. Solving this equation for j'_{\min} we find

$$j'_{\min} = \frac{1}{2}j.$$

We therefore conclude that

$$(\Psi_{j'}^{m'}, \mathcal{O}_j^m \Psi_{j'}^{m'}) \neq 0 \quad \text{for } j' \geq \frac{1}{2}j,$$

where j is restricted to be an integer. For half-integer j , one of $\Psi_{j'}^{m'}$ and $\mathcal{O}_j^m \Psi_{j'}^{m'}$ will be bosonic while the other is fermionic, and so will always have a vanishing inner product.

4. *The Hamiltonian for a free particle of mass M and spin \mathbf{S} placed in a magnetic field \mathbf{B} in the 3-direction is*

$$H = \frac{\mathbf{p}^2}{2M} - g|\mathbf{B}|S_3,$$

where g is a constant (proportional to the particle's magnetic moment). Give the equations that govern the time dependence of the expectation values of all three components of \mathbf{S} .

We can find the time derivative of $\mathbf{S}(t)$ in the Heisenberg picture by taking the commutator with the Hamiltonian

$$\begin{aligned} \dot{S}_i &= \frac{i}{\hbar} [H, S_i] = \frac{i}{\hbar} \left[\frac{\mathbf{p}^2}{2M}, S_i \right] - \frac{i\mu B}{\hbar} [S_3, S_i] \\ &= -\frac{i\mu B}{\hbar} \left(i\hbar \sum_k \epsilon_{3ik} S_k \right) \\ &= \mu B (\delta_{i1} S_2 - \delta_{i2} S_1). \end{aligned}$$

Therefore, the individual components of the spin have time derivatives

$$\dot{S}_1 = \mu B S_2, \quad \dot{S}_2 = -\mu B S_1, \quad \dot{S}_3 = 0.$$

We can take second time derivatives of S_1 and S_2 to find

$$\begin{aligned}\ddot{S}_1 &= \mu B \dot{S}_2 = -\mu^2 B^2 S_1, \\ \ddot{S}_2 &= \mu B \dot{S}_1 = -\mu^2 B^2 S_2.\end{aligned}$$

These differential equations have well-known solutions of the form

$$\begin{aligned}S_1(t) &= A_1 \cos(\mu B t) + A_2 \sin(\mu B t), \\ S_2(t) &= A_3 \cos(\mu B t) + A_4 \sin(\mu B t).\end{aligned}$$

Imposing the condition that $\dot{S}_1(t) = \mu B S_2(t)$, we find that

$$-A_1 \mu B \sin(\mu B t) + A_2 \mu B \cos(\mu B t) = A_3 \mu B \cos(\mu B t) + A_4 \mu B \sin(\mu B t),$$

which must be true for all times, and so this requires

$$-A_4 = A_1, \quad A_2 = A_3.$$

Evaluating these solutions at $t = 0$, we find

$$A_1 = S_1(0), \quad A_3 = S_2(0),$$

and so we find

$$\begin{aligned}\langle S_1(t) \rangle &= \langle S_1(0) \rangle \cos(\mu B t) + \langle S_2(0) \rangle \sin(\mu B t), \\ \langle S_2(t) \rangle &= \langle S_2(0) \rangle \cos(\mu B t) - \langle S_1(0) \rangle \sin(\mu B t), \\ \langle S_3(t) \rangle &= \langle S_3(0) \rangle.\end{aligned}$$

5. *A particle of spin 3/2 decays into a nucleon and pion. Show how the angular distribution in the final state (with spins not measured) can be used to determine the parity of the decaying particle.*

First, we note that nucleons have spin 1/2 and pions have spin 0. In order for the decay of a spin-3/2 particle (which we will call X) into a nucleon and pion to conserve angular momentum, the final state must have orbital angular momentum $\ell = 1$ or $\ell = 2$. Assuming that the decay conserves parity, we can write

$$\eta_X = (-1)^\ell \eta_N \eta_\pi.$$

According to Section 4.7, nucleons have intrinsic parity $\eta_N = +1$ while pions have intrinsic parity $\eta_\pi = -1$ and so we find

$$\eta_X = (-1)^{\ell+1}.$$

Now, if the angular distribution of the final state can be used to determine the orbital angular momentum ℓ , we can use this expression to find the intrinsic parity of the spin-3/2 particle. To be specific, we find

$$\eta_X = \begin{cases} +1 & \text{if } \ell = 1 \\ -1 & \text{if } \ell = 2 \end{cases}.$$

6. A particle X of isospin 1 and charge zero decays into a K and a \bar{K} . What is the ratio of the rates of the processes $X^0 \rightarrow K^+ + \bar{K}^-$ and $X^0 \rightarrow K^0 + \bar{K}^0$? First, we note that the isospin of all of the kaons is $T = 1/2$. The T_3 quantum number for each of the kaons is given below

$$\begin{aligned} K^+ & T_3 = +1/2 \\ \bar{K}^- & T_3 = -1/2 \\ K^0 & T_3 = -1/2 \\ \bar{K}^0 & T_3 = +1/2. \end{aligned}$$

Because the particle X decays into a K and a \bar{K} , the conservation of T_3 in strong interactions requires that the particle X has $T_3 = 0$. If we label the T_3 quantum numbers of the final state particles as m and m' , the amplitudes of these decays will be proportional to Clebsch–Gordan coefficients of the form

$$M(0, m, m') = M_0 C_{\frac{1}{2} \frac{1}{2}} \left(1 0; m m' \right).$$

In both cases the relevant Clebsch–Gordan coefficient is

$$C_{\frac{1}{2} \frac{1}{2}} \left(1 0; +\frac{1}{2} -\frac{1}{2} \right) = \sqrt{\frac{1}{2}}.$$

We therefore find for the ratio of the decay rates

$$\frac{\Gamma(X \rightarrow K^+ + \bar{K}^-)}{\Gamma(X \rightarrow K^0 + \bar{K}^0)} = \frac{|M(0 + \frac{1}{2} - \frac{1}{2})|^2}{|M(0 + \frac{1}{2} - \frac{1}{2})|^2} = \frac{|M_0|^2 (\frac{1}{2})}{|M_0|^2 (\frac{1}{2})} = 1.$$

7. Imagine that the electron has spin 3/2 instead of 1/2, but assume that the one-particle states with definite values of n and l in atoms are filled, as the atomic number increases, in the same order as in the real world. What elements with atomic numbers in the range from 1 to 21 would have chemical properties similar to those of noble gases, alkali metals, halogens, and alkali earths in the real world?

The values taken by the 3-component of spin range from $-s$ to s in integer steps giving $2s + 1$ values. There are four values taken by m_s for a spin-3/2 particle

$$m_s = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}.$$

As a result, for multi-electron atoms constructed from spin-3/2 electrons there will be $4(2l + 1)$ distinct states for each value of the principal quantum number n and the orbital angular momentum l . Then if atoms are filled in the order described by Eq. (4.5.11), we can count states as

1s	4 states
2s, 2p	4 + 12 = 16 states
3s, 3p	4 + 12 = 16 states
⋮	⋮

Noble gases are those which have a full outer shell of electrons, and in this case are atoms with atomic number $Z = 2, 10, 18, 36, 54, 86$. Alkali metals are those which have only one electron in the outermost shell, and here are atoms with $Z = 1, 3, 11, 19, 27, 35, 53, 81, 89$. Halogens are elements having an outermost shell which is one electron short of being full, and in this case are atoms with $Z = 5, 17, 35, 53, 85, 87$. Finally alkali earths have two electrons in their outer shell, and here are the atoms with $Z = 4, 12, 20, 28, 36, 54, 82, 90$.

8. *What is the commutator of the angular momentum operator \mathbf{J} with the generator \mathbf{K} of Galilean transformations?*

Since the generator of Galilean transformations \mathbf{K} is a vector operator, we expect that

$$[J_i, K_j] = i\hbar \sum_k \epsilon_{ijk} K_k,$$

according to Eq. (4.1.13). To be more explicit, we may write the generator of Galilean transformations as

$$\mathbf{K} = \frac{1}{\hbar} \left(\mathbf{P}t - \sum_n m_n \mathbf{X}_n \right),$$

which satisfies the commutation relations given by Eqs. (3.6.18) and (3.6.20). Now, using the commutation relations of the angular momentum operator with \mathbf{X}_n and \mathbf{P} given in Eq. (4.1.22), we may compute the commutator directly

$$\begin{aligned} [J_i, K_j] &= \left[J_i, \frac{1}{\hbar} \left(P_j t - \sum_n m_n X_{nj} \right) \right] = i \sum_k \epsilon_{ijk} \left(P_k t - \sum_n m_n X_{nk} \right) \\ &= i\hbar \sum_k \epsilon_{ijk} K_k. \end{aligned}$$

9. *Consider an electron in a state of zero orbital angular momentum in an atom whose nucleus has spin (that is, internal angular momentum) $3/2$. Express the states of the atom with total angular momentum z -component $m = 1$ (of electron plus nucleus) and each possible definite value of the total angular momentum as linear combinations of states with definite values of the z -components of the nuclear and electron spins.*

We would like to construct eigenstates of the operators \mathbf{J}^2 , J_3 , \mathbf{I}^2 , and \mathbf{S}^2 which are linear combinations of eigenstates of the operators \mathbf{I}^2 , I_3 , \mathbf{S}^2 , and S_3 , just as in Eq. (4.3.18)

$$\Psi_{I_s j}^m = \sum_{m_I, m_s} C_{I_s}(j m; m_I m_s) \psi_{I_s}^{m_I m_s},$$

where we are labeling the nuclear spin quantum number as I and its three-component as m_I . The state with $j = 2$ and $m = 1$ is given by

$$\Psi_{\frac{3}{2} \frac{1}{2} 2}^1 = C_{\frac{3}{2} \frac{1}{2}} \left(2 \ 1; \frac{3}{2} \ -\frac{1}{2} \right) \psi_{\frac{3}{2} \frac{1}{2}}^{\frac{3}{2} \ -\frac{1}{2}} + C_{\frac{3}{2} \frac{1}{2}} \left(2 \ 1; \frac{1}{2} \ \frac{1}{2} \right) \psi_{\frac{3}{2} \frac{1}{2}}^{\frac{1}{2} \ \frac{1}{2}},$$

and the state with $j = 1$ and $m = 1$ is given by

$$\Psi_{\frac{3}{2} \frac{1}{2} 1}^1 = C_{\frac{3}{2} \frac{1}{2}} \left(1 \ 1; \frac{1}{2} \ \frac{1}{2} \right) \psi_{\frac{3}{2} \frac{1}{2}}^{\frac{1}{2} \ \frac{1}{2}} + C_{\frac{3}{2} \frac{1}{2}} \left(1 \ 1; -\frac{1}{2} \ \frac{1}{2} \right) \psi_{\frac{3}{2} \frac{1}{2}}^{-\frac{1}{2} \ \frac{1}{2}}.$$

Now all that remains is to find the relevant Clebsch–Gordan coefficients. The first two coefficients can be read off from Eqs. (4.3.24) and (4.3.25), and the others can be obtained by requiring the orthogonality of the two states. We therefore find

$$\begin{aligned} \Psi_{\frac{3}{2} \frac{1}{2} 2}^1 &= \frac{1}{2} \psi_{\frac{3}{2} \frac{1}{2}}^{\frac{3}{2} \ -\frac{1}{2}} + \sqrt{\frac{3}{4}} \psi_{\frac{3}{2} \frac{1}{2}}^{\frac{1}{2} \ \frac{1}{2}}, \\ \Psi_{\frac{3}{2} \frac{1}{2} 1}^1 &= \sqrt{\frac{3}{4}} \psi_{\frac{3}{2} \frac{1}{2}}^{\frac{3}{2} \ -\frac{1}{2}} - \frac{1}{2} \psi_{\frac{3}{2} \frac{1}{2}}^{\frac{1}{2} \ \frac{1}{2}}. \end{aligned}$$

Chapter 5 Problem Set Solutions

1. Suppose that the interaction of the electron with the proton in the hydrogen atom produces a change in the potential energy of the electron of the form

$$\Delta V(r) = V_0 \exp(-r/R),$$

where R is much smaller than the Bohr radius a . Calculate the shift in the energies of the $2s$ and $2p$ states of hydrogen, to first order in V_0 .

The first-order shift in energy due to a perturbation is given by Eq. (5.1.6) as

$$\delta_1 E_a = (\Psi_a, \delta H \Psi_a).$$

In this case the perturbation is given by

$$\Delta V(r) = V_0 \exp(-r/R),$$

where R is much smaller than the Bohr radius a . In order to calculate this energy shift for the $2s$ and $2p$ states of hydrogen, we need to work out the form of the unperturbed wave functions. Recall from Section 2.3 that these wave functions are given by

$$\begin{aligned}\psi_{2s} &= R_{20}(r)Y_0^0, \\ \psi_{2p} &= R_{21}(r)Y_0^m,\end{aligned}$$

where the radial part of the wave function is

$$R_{n\ell} \propto r^\ell \exp(-r/na) F_{n\ell}(r/na).$$

According to Eq. (2.3.17) in this case we have

$$\begin{aligned}F_{20} &= 1 - \frac{r}{2a}, \\ F_{21} &= 1,\end{aligned}$$

and so the radial parts of the wave functions take the form

$$\begin{aligned}R_{20} &= A \exp(-r/2a) \left(1 - \frac{r}{2a}\right), \\ R_{21} &= Br \exp(-r/2a).\end{aligned}$$

We can normalize the wave functions to determine A and B . For A we find

$$\begin{aligned}\int d^3x \psi_{2s}^* \psi_{2s} &= \int_0^\infty dr r^2 (R_{20})^2 \int d^2\Omega Y_0^{0*} Y_0^0 \\ &= |A|^2 \int_0^\infty dr r^2 \left(1 - \frac{r}{2a}\right)^2 \exp(-r/a) \\ &= 2a^3 |A|^2 \\ A &= (2a^3)^{-1/2},\end{aligned}$$

and for B we find

$$\begin{aligned}\int d^3x \psi_{2p}^* \psi_{2p} &= \int_0^\infty dr r^2 (R_{21})^2 \int d^2\Omega Y_1^{m*} Y_1^m \\ &= |B|^2 \int_0^\infty dr r^4 \exp(-r/a) \\ &= 24a^5 |B|^2 \\ B &= (24a^5)^{-1/2}.\end{aligned}$$

We find for the $2s$ and $2p$ hydrogen wave functions

$$\begin{aligned}\psi_{2s} &= (2a)^{-3/2} \left(2 - \frac{r}{a}\right) \exp(-r/2a) Y_0^0, \\ \psi_{2p} &= (2a)^{-3/2} \frac{r}{\sqrt{3}a} \exp(-r/2a) Y_0^m.\end{aligned}$$

We can now calculate the first-order shift in energy of the $2s$ state as

$$\begin{aligned}\delta_1 E_{2s} &= \int d^3x \psi_{2s}^* V_0 \exp(-r/R) \psi_{2s} \\ &= V_0 \int_0^\infty dr r^2 (2a)^{-3} \left(2 - \frac{r}{a}\right)^2 \exp\left(-\frac{r}{a} - \frac{r}{R}\right) \int d^2\Omega Y_0^{0*} Y_0^0 \\ &= V_0 \frac{R^3 (a^2 - aR + R^2)}{(a + R)^5},\end{aligned}$$

and for the $2p$ state we find

$$\begin{aligned}\delta_1 E_{2p} &= \int d^3x \psi_{2p}^* V_0 \exp(-r/R) \psi_{2p} \\ &= V_0 \int_0^\infty dr r^2 (2a)^{-3} \frac{r^2}{3a^2} \exp\left(-\frac{r}{a} - \frac{r}{R}\right) \int d^2\Omega Y_1^{m*} Y_1^m \\ &= V_0 \frac{R^5}{a^5}.\end{aligned}$$

In the limit $R \ll a$, we find for the energy shifts

$$\begin{aligned}\delta_1 E_{2s} &\rightarrow V_0 \frac{R^3}{a^3}, \\ \delta_1 E_{2p} &\rightarrow V_0 \frac{R^5}{a^5}.\end{aligned}$$

2. It is sometimes assumed that the electrostatic potential felt by an electron in a multi-electron atom can be approximated by a shielded Coulomb potential, of the form

$$V(r) = -\frac{Ze^2}{r} \exp(-r/R),$$

where R is the estimated radius of the atom. Use the variational method to give an approximate formula for the energy of an electron in the state of lowest energy in this potential, taking as the trial wave function

$$\psi(\mathbf{x}) \propto \exp\left(-r/\rho\right),$$

with ρ a free parameter.

Given that the potential takes the form

$$V(r) = -\frac{Ze^2}{r} \exp(-r/R),$$

we will try to minimize the ground state energy by taking an ansatz for the wave function of the form

$$\psi(\mathbf{x}) \propto \exp(-r/\rho) Y_\ell^m(\hat{x}),$$

by varying the parameter ρ . The Hamiltonian takes the form

$$H = \frac{\mathbf{p}^2}{2M} - \frac{Ze^2}{r} \exp(-r/R),$$

which can be written in the form

$$H = -\frac{\hbar^2}{2Mr^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{2Mr^2} \mathbf{L}^2 - \frac{Ze^2}{r} \exp(-r/R),$$

as was done in Chapter 2. Since we are examining the ground state, we will take $\ell = 0$, because non-zero values of ℓ will have higher energy. First, we will normalize our wave function

$$\begin{aligned} 1 &= \int d^3x \psi^*(\mathbf{x}) \psi(\mathbf{x}) = \int_0^\infty dr r^2 |A|^2 \exp(-2r/\rho) \int d^2\Omega Y_0^{0*} Y_0^0 \\ &= |A|^2 \frac{\rho^3}{4} \\ A &= \frac{2}{\rho^{3/2}}. \end{aligned}$$

We find for our normalized trial wave function

$$\psi(\mathbf{x}) = \frac{2}{\rho^{3/2}} \exp(-r/\rho) Y_0^0 = \frac{1}{\sqrt{\pi} \rho^{3/2}} \exp(-r/\rho).$$

The expectation value of the energy in this state is given by

$$\begin{aligned} \langle H \rangle_\psi &= \int d^3x \psi^*(\mathbf{x}) H \psi(\mathbf{x}) \\ &= \int_0^\infty dr r^2 \frac{4}{\rho^3} \exp(-r/\rho) \left(-\frac{\hbar^2}{2Mr^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{Ze^2}{r} \exp(-r/R) \right) \\ &\quad \times \exp(-r/\rho) \int d^2\Omega Y_0^{0*} Y_0^0 \end{aligned}$$

$$\begin{aligned}
&= \frac{4}{\rho^3} \int_0^\infty dr \left[-\frac{\hbar^2}{2M} \left(-\frac{2r}{\rho} + \frac{r^2}{\rho^2} \right) \exp(-2r/\rho) \right. \\
&\quad \left. - Ze^2 r \exp\left(-\frac{2r}{\rho} - \frac{r}{R} \right) \right] \\
&= \frac{4}{\rho^3} \left[-\frac{\hbar^2}{2M} \left(-\frac{\rho}{2} + \frac{\rho}{4} \right) - \frac{Ze^2}{\left(\frac{2}{\rho} + \frac{1}{R} \right)^2} \right] \\
&= \frac{\hbar^2}{2M\rho^2} - \frac{4Ze^2 R^2}{(2R + \rho)^2 \rho}.
\end{aligned}$$

We can find the value of ρ that will minimize the energy by setting the derivative with respect to ρ equal to zero

$$0 = \frac{\partial}{\partial \rho} \langle H \rangle_\psi = -\frac{\hbar^2}{M\rho^3} + \frac{8Ze^2 R^2}{(2R + \rho)^3 \rho} + \frac{4Ze^2 R^2}{(2R + \rho)^2 \rho^2}.$$

We can simplify this expression slightly by multiplying both sides by $-\frac{M}{\hbar^2(2R+\rho)^3\rho^3}$ and using the definition of the Bohr radius $a = \hbar^2/Me^2$

$$0 = \rho^3 + \left(6R - 12\frac{ZR^2}{a} \right) \rho^2 + \left(12R^2 - 8\frac{ZR^3}{a} \right) \rho + 8R^3.$$

Solving this equation for ρ , we find that the only real root is given by

$$\begin{aligned}
\rho_0 &\equiv -\frac{2R}{a}(a - 2RZ) + \frac{2R^3Z(-5a + 6RZ)}{a} \\
&\times \left[\frac{27}{4}R^4Z(a - 4RZ)(a - RZ) + \frac{3}{4}\sqrt{3a^2R^8Z^2(27a^2 - 20aRZ - 9R^2Z^2)} \right]^{-1/3} \\
&+ \frac{2}{a} \left[2R^4Z(a - 4RZ)(a - RZ) + \frac{2}{9}\sqrt{3a^2R^8Z^2(27a^2 - 20aRZ - 9R^2Z^2)} \right]^{1/3}.
\end{aligned}$$

This gives the energy in the ground state as

$$\langle H \rangle_\psi = \frac{\hbar^2}{2M\rho_0^2} - \frac{4Ze^2 R^2}{(2R + \rho_0)^2 \rho_0}.$$

3. Calculate the shift in energy of the $2p_{3/2}$ state of hydrogen in a very weak static electric field E , to second order in E , assuming that E is small enough so that this shift is much less than the fine-structure splitting between the $2p_{1/2}$ and $2p_{3/2}$ states. In using second-order perturbation theory here, you can consider only the intermediate state for which the energy-denominator is smallest.

The perturbation to the Hamiltonian in this case takes the form

$$\delta H = -e\mathbf{E} \cdot \mathbf{X},$$

and for convenience, we will define our coordinate system so that \mathbf{E} points in the 3-direction $\mathbf{E} = |\mathbf{E}|\hat{x}_3$, and so the perturbation becomes

$$\delta H = -e|\mathbf{E}|X_3.$$

Notice first that the first-order perturbation to the energy vanishes for $n = 2$ and $j = 3/2$ because

$$\left(\Psi_{n\ell'j}^{m'}, \delta H \Psi_{n\ell j}^m \right) = -e|\mathbf{E}| \delta_{m'm} \left(\Psi_{n\ell'j}^m, X_3 \Psi_{n\ell j}^m \right),$$

and due to the fact that X_3 changes sign under space inversion this must vanish unless $(-1)^{\ell'}(-1)^\ell = -1$. For the $n = 2, j = 3/2$ state, we must have $\ell = 1$, and so this inner product vanishes. The second-order shift in the energy is given by Eq. (5.4.5) as

$$\delta_2 E_a = \sum_{b \neq a} \frac{|\langle \Psi_b, \delta H \Psi_a \rangle|^2}{E_a - E_b}.$$

The largest contribution to this sum comes from states Ψ_b for which $|E_a - E_b|$ is the smallest. For the $2p_{3/2}$ state of hydrogen, the states nearest in energy are the $2s_{1/2}$ and $2p_{1/2}$ states which would be degenerate with the $2p_{3/2}$ state in the absence of fine-structure splitting. The relevant matrix element for the $2p_{1/2}$ state is given by

$$-e|\mathbf{E}| \delta_{m'm} \left(\Psi_{21\frac{1}{2}}^{m'}, X_3 \Psi_{21\frac{3}{2}}^m \right) = 0,$$

which vanishes due to the behavior of X_3 under space inversion because $(-1)^1(-1)^1 = 1$. This leaves only the $2s_{1/2}$ intermediate state. The operator X_3 acts on orbital angular momentum, but not on spin, so we need to express the state vectors in terms of state vectors with definite values for the m_ℓ and m_s quantum numbers

$$\Psi_{n\ell j}^m = \sum_{m_\ell m_s} C_{\ell \frac{1}{2}} \left(j m; m_\ell m_s \right) \psi_{n\ell}^{m_\ell m_s}.$$

After making this change of basis, we can write the matrix elements as

$$\begin{aligned} \left(\psi_{n\ell}^{m_\ell m_s}, X_3 \psi_{n'\ell'}^{m'_\ell m'_s} \right) &= \delta_{m_s m'_s} \int d^3x R n \ell(r) Y_\ell^{m_\ell*}(\theta, \phi) r \cos \theta \\ &\quad \times R_{n'; \ell'}(r) Y_{\ell'}^{m'_\ell}(\theta, \phi), \end{aligned}$$

as in Eq. (5.3.5). The state vector $\Psi_{20\frac{1}{2}}^m$ must have $m_\ell = 0$ so the matrix elements of X_3 between $\Psi_{20\frac{1}{2}}^m$ and $\Psi_{21\frac{1}{2}}^m$ receive contributions only from the $m_\ell = 0$ components of both wave functions. The relevant matrix element then takes the form

$$\left(\Psi_{20\frac{1}{2}}^{\pm\frac{1}{2}}, X_3 \Psi_{21\frac{1}{2}}^{\pm\frac{1}{2}} \right) = C_{0\frac{1}{2}} \left(\frac{1}{2} \pm \frac{1}{2}; 0 \pm \frac{1}{2} \right) C_{1\frac{1}{2}} \left(\frac{3}{2} \pm \frac{1}{2}; 0 \pm \frac{1}{2} \right) \mathcal{I},$$

where we have defined

$$\mathcal{I} \equiv \int d^3x r \cos \theta R_{20}(r) Y_0^0(\theta, \phi) R_{21}(r) Y_1^0(\theta, \phi),$$

as in Eq. (5.3.15). This integral was evaluated in Eq. (5.3.15), which gives

$$\mathcal{I} = -3a.$$

The relevant Clebsch–Gordan coefficients are

$$C_{0\frac{1}{2}} \left(\frac{1}{2} \pm \frac{1}{2}; 0 \pm \frac{1}{2} \right) = 1$$

$$C_{1\frac{1}{2}} \left(\frac{3}{2} \pm \frac{1}{2}; 0 \pm \frac{1}{2} \right) = \sqrt{\frac{2}{3}},$$

and so we find

$$\left(\Psi_{20\frac{1}{2}}^{\pm\frac{1}{2}}, X_3 \Psi_{21\frac{1}{2}}^{\pm\frac{1}{2}} \right) = -\sqrt{6}a.$$

Putting this together, we find for the second-order shift in the energy of the $2p_{3/2}$ state of hydrogen

$$\delta_2 E_{(2p_{3/2})} = \frac{\left| -e|\mathbf{E}| \left(\Psi_{20\frac{1}{2}}^{\pm\frac{1}{2}}, X_3 \Psi_{21\frac{1}{2}}^{\pm\frac{1}{2}} \right) \right|^2}{E_{(2p_{3/2})} - E_{(2s_{1/2})}} = \frac{6e^2 |\mathbf{E}|^2 a^2}{E_{(2p_{3/2})} - E_{(2s_{1/2})}}.$$

The fine-structure splitting gives an energy difference of

$$E_{(2p_{3/2})} - E_{(2s_{1/2})} = \frac{mZ^4 e^8}{16\hbar^4 c^2} \left(\frac{1}{2} - 1 \right) = -\frac{mZ^4 e^8}{32\hbar^4 c^2} = -\frac{Z^4 e^6}{32a\hbar^2 c^2},$$

and so we find for the second-order energy shift

$$\delta_2 E_{(2p_{3/2})} = -\frac{192\hbar^2 c^2 a^3 |\mathbf{E}|^2}{Z^4 e^4}.$$

4. *The spin-orbit coupling of the electron in hydrogen produces a term in the Hamiltonian of the form*

$$\Delta H = \xi(r) \mathbf{L} \cdot \mathbf{S},$$

where $\xi(r)$ is some small function of r . Give a formula for the contribution of ΔV to the fine-structure splitting between the $2p_{1/2}$ and $2p_{3/2}$ states in hydrogen, to first order in $\xi(r)$.

The first-order shift in energy is given by

$$\delta_1 E = \left(\Psi_{n\ell j}^m, \Delta H \Psi_{n\ell j}^m \right),$$

where $\Delta H = \xi(r)\mathbf{L} \cdot \mathbf{S}$. First, we recall that because $[\mathbf{L}, \mathbf{S}] = 0$, we may write

$$\mathbf{J}^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{L} \cdot \mathbf{S},$$

and so

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2} [\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2].$$

We can therefore write the first-order energy shift as

$$\begin{aligned} \delta_1 E &= \left(\Psi_{n\ell j}^m, \frac{1}{2} \xi(r) (\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) \Psi_{n\ell j}^m \right) \\ &= \frac{\hbar^2}{2} \left(j(j+1) - \ell(\ell+1) - \frac{3}{4} \right) (\Psi_{n\ell j}^m, \xi(r) \Psi_{n\ell j}^m) \\ &= \frac{\hbar^2}{2} \left(j(j+1) - \ell(\ell+1) - \frac{3}{4} \right) \int dr r^2 \xi(r) (R_{n\ell}(r))^2. \end{aligned}$$

For both the $2p_{1/2}$ and $2p_{3/2}$ states of hydrogen, the radial integral takes the form

$$\begin{aligned} \int dr r^2 \xi(r) (R_{21}(r))^2 &= \int dr r^2 \xi(r) \left(\frac{1}{\sqrt{3}} \left(\frac{1}{2a} \right)^{3/2} \left(\frac{r}{a} \right) \exp(-r/2a) \right)^2 \\ &= \int dr \xi(r) \frac{r^4}{24a^5} \exp(-r/a). \end{aligned}$$

The energy shift for the $2p_{3/2}$ state is given by

$$\begin{aligned} \delta_1 E_{(2p_{3/2})} &= \frac{\hbar^2}{2} \left(\frac{3}{2} \left(\frac{3}{2} + 1 \right) - 1(1+1) - \frac{3}{4} \right) \int dr \xi(r) \frac{r^4}{24a^5} \exp(-r/a) \\ &= \frac{\hbar^2}{2} \int dr \xi(r) \frac{r^4}{24a^5} \exp(-r/a), \end{aligned}$$

and the energy shift for the $2p_{1/2}$ state is given by

$$\begin{aligned} \delta_1 E_{(2p_{1/2})} &= \frac{\hbar^2}{2} \left(\frac{1}{2} \left(\frac{1}{2} + 1 \right) - 1(1+1) - \frac{3}{4} \right) \int dr \xi(r) \frac{r^4}{24a^5} \exp(-r/a) \\ &= -\frac{\hbar^2}{2} \int dr \xi(r) \frac{r^4}{24a^5} \exp(-r/a). \end{aligned}$$

This gives a splitting between the states of

$$\delta_1 E_{(2p_{3/2})} - \delta_1 E_{(2p_{1/2})} = \frac{\hbar^2}{16a^5} \int dr \xi(r) r^4 \exp(-r/a).$$

5. Using the WKB approximation, derive a formula for the energies of the bound states of a particle of mass m in a potential $V(r) = -V_0 e^{-r/R}$, with V_0 and R both positive.

Eq. (5.7.33) gives the condition for a bound state for a central potential with $\ell = 0$ as

$$\int_0^{b_E} k(r') dr' = \left(n + \frac{3}{4}\right) \pi,$$

where the function $k(r)$ is defined as in Eq. (5.7.2)

$$k(r) = \sqrt{\frac{2m}{\hbar^2} (E - U(r))},$$

where $U(r)$ is given by

$$U(r) = V(r) + \frac{\hbar^2 \ell(\ell + 1)}{2m r^2},$$

and b_E is the turning point, defined by the condition that $U(b_E) = E$. In this case, we are considering only states with $\ell = 0$ and a potential given by

$$V(r) = -V_0 \exp(-r/R).$$

We find that b_E is given by

$$b_E = -R \ln \left(-\frac{E}{V_0} \right),$$

and $k(r)$ is

$$k(r) = \sqrt{\frac{2m}{\hbar^2} (E + V_0 \exp(-r/R))}.$$

The integral appearing in the condition for a bound state becomes

$$\begin{aligned} \int_0^{b_E} k(r) dr &= \int_0^{b_E} dr \sqrt{\frac{2m}{\hbar^2} (E + V_0 \exp(-r/R))} \\ &= -2R \sqrt{\frac{2m V_0}{\hbar^2}} \left[\sqrt{\frac{E}{V_0} + \exp(-r/R)} + \sqrt{-\frac{E}{V_0}} \sin^{-1} \left(\sqrt{-\frac{E}{V_0} \exp(-r/R)} \right) \right]_0^{b_E} \\ &= 2R \sqrt{\frac{2m}{\hbar^2}} \left[\sqrt{E + V_0} + \sqrt{-E} \left(\sin^{-1} \left(\sqrt{-\frac{E}{V_0}} \right) - \sin^{-1} \left(\frac{|E|}{V_0} \right) \right) \right]. \end{aligned}$$

The condition for a bound state is then a transcendental equation for E which reads

$$2R\sqrt{\frac{2m}{\hbar^2}} \left[\sqrt{E + V_0} + \sqrt{-E} \left(\sin^{-1} \left(\sqrt{-\frac{E}{V_0}} \right) - \sin^{-1} \left(\frac{|E|}{V_0} \right) \right) \right] \\ = \left(n + \frac{3}{4} \right) \pi,$$

whose solutions give the values of the energy levels.

Chapter 6 Problem Set Solutions

1. Consider a time-dependent Hamiltonian $H = H_0 + H'(t)$, with

$$H'(t) = U \exp(-t/T),$$

where H_0 and U are time-independent operators, and T is a constant. What is the probability to lowest order in U that the perturbation will produce a transition from one eigenstate n of H_0 to a different eigenstate m of H_0 during a time interval from $t = 0$ to a time $t \gg T$?

If we expand the solution of the full Hamiltonian H in terms of eigenstates of the unperturbed Hamiltonian H_0 as in Eq. (6.1.4)

$$\Psi(t) = \sum_n c_n(t) \exp(-i E_n(t)/\hbar) \Psi_n,$$

then the coefficients in this expansion can be found to first order in the perturbation $H'(t)$ as in Eq. (6.1.6)

$$c_j(t) \approx c_j(0) - \frac{i}{\hbar} \sum_k c_k(0) \int_0^t dt' H'_{jk}(t') \exp(i(E_j - E_k)t'/\hbar),$$

where $H'_{jk}(t') \equiv (\Psi_j, H'(t')\Psi_k)$. To find the probability of a transition from a state n to a state m , we set $c_n(0) = 1$ and $c_k(0) = 0$ for all $k \neq n$, so the state is described at time $t = 0$ by Ψ_n . If we take $H'(t) = U \exp(-t/T)$, we can then calculate the coefficient of the state Ψ_m after a time t as

$$\begin{aligned} c_m(t) &\approx -\frac{i}{\hbar} \int_0^t dt' H'_{mn}(t') \exp(i(E_m - E_n)t'/\hbar) \\ &= -\frac{i}{\hbar} \int_0^t dt' U_{mn} \exp(-t'/T) \exp(i(E_m - E_n)t'/\hbar), \end{aligned}$$

where we have defined $U_{mn} = (\Psi_m, U\Psi_n)$. In the limit where $t \gg T$, this becomes

$$\begin{aligned} c_m(t) &= -\frac{i}{\hbar} U_{mn} \int_0^\infty dt' \exp\left[\left(i\frac{E_m - E_n}{\hbar} - \frac{1}{T}\right)t'\right] \\ &= -\frac{i}{\hbar} U_{mn} \left[\frac{-1}{i\frac{E_m - E_n}{\hbar} - \frac{1}{T}} \right] \\ &= \frac{iU_{mn}}{i(E_m - E_n) - \frac{\hbar}{T}}. \end{aligned}$$

The probability of finding the system in the state m is then given in the limit of large t by

$$|(\Psi_m, \Psi(t))|^2 = |c_m(t)|^2 \rightarrow \frac{|U_{mn}|^2}{(E_m - E_n)^2 + \frac{\hbar^2}{T^2}}.$$

2. Calculate the rate of ionization of a hydrogen atom in the $2p$ state in a monochromatic external electric field, averaged over the component of angular momentum in the direction of the field. (Ignore spin.)

Without loss of generality, we can choose our coordinate system such that the electric field lies along the z -direction so that the perturbation in the Hamiltonian takes the form of Eq. (6.3.2)

$$H'(t) = -e\mathcal{E}X_3 \exp(-i\omega t) - e\mathcal{E}^*X_3 \exp(i\omega t),$$

where X is the operator for the electron position. This means that the operator U appearing in Eq. (6.2.1) is

$$U = -e\mathcal{E}X_3.$$

We need to calculate the matrix element of this perturbation between the normalized wave function describing the $2p$ state of hydrogen and the free electron wave function, given by Eq. (3.5.12)

$$\psi_{\mathbf{k}}(\mathbf{x}) = (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{x}),$$

where the momentum of the electron is $\hbar\mathbf{k}$ which we take to be much larger than the hydrogen binding energy such that we may ignore the effect of the Coulomb field of the proton in the final state. Recall the form of the wave functions for the $2p$ state of hydrogen

$$\begin{aligned} \psi_{2p}^{m=0} &= \frac{1}{\sqrt{32\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \cos \theta \\ \psi_{2p}^{m=\pm 1} &= \mp \frac{1}{8\sqrt{\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \sin \theta e^{\pm i\phi}, \end{aligned}$$

which were worked out for the Chapter 2 problem set. The relevant matrix elements are then

$$\begin{aligned} U_{\mathbf{k}2p^{m=0}} &= -\frac{e\mathcal{E}}{(2\pi)^{3/2}\sqrt{32\pi}a^5} \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} x_3 r e^{-r/2a} \cos \theta \\ U_{\mathbf{k}2p^{m=\pm 1}} &= \pm \frac{e\mathcal{E}}{(2\pi)^{3/2}\sqrt{64\pi}a^5} \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} x_3 r e^{-r/2a} \sin \theta e^{\pm i\phi}. \end{aligned}$$

We can rewrite these integrals as

$$\begin{aligned} U_{\mathbf{k}2p^{m=0}} &= -\frac{e\mathcal{E}}{(2\pi)^{3/2}\sqrt{32\pi}a^5} \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} x_3^2 e^{-r/2a} \\ U_{\mathbf{k}2p^{m=\pm 1}} &= \pm \frac{e\mathcal{E}}{(2\pi)^{3/2}\sqrt{64\pi}a^5} \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} x_3(x_1 \pm ix_2) e^{-r/2a}, \end{aligned}$$

and then we can perform the angular integral by recalling that

$$\int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} f(r) = \frac{1}{k} \int_0^\infty dr 4\pi r f(r) \sin kr.$$

Differentiating both sides twice with respect to k_3 , we find

$$-\int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} f(r) x_3^2 = \frac{1}{k^3} \int_0^\infty dr 4\pi r f(r) \\ \times \left[-\sin kr + kr \cos kr + 3\frac{k_3^2}{k^2} \sin kr - 3\frac{k_3^2 r}{k} \cos kr - k_3^2 r^2 \sin kr \right],$$

or applying $\frac{\partial}{\partial x_3} \left(\frac{\partial}{\partial x_1} \pm i \frac{\partial}{\partial x_2} \right)$ to both sides, we find

$$-\int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} f(r) x_3 (x_1 \pm i x_2) = \frac{1}{k^3} \int_0^\infty dr 4\pi r f(r) \\ \times \left[3\frac{k_3(k_1 \pm ik_2)}{k^2} \sin kr - 3\frac{k_3(k_1 \pm ik_2)r}{k} \cos kr - k_3(k_1 \pm ik_2)r^2 \sin kr \right].$$

Using these expressions in the matrix elements gives

$$U_{\mathbf{k}2p^m=0} = \frac{4\pi e\mathcal{E}}{(2\pi)^{3/2} k^3 \sqrt{32\pi a^5}} \int_0^\infty dr r e^{-r/2a} \left[-\sin kr + kr \cos kr \right. \\ \left. + 3\frac{k_3^2}{k^2} \sin kr - 3\frac{k_3^2 r}{k} \cos kr - k_3^2 r^2 \sin kr \right], \\ U_{\mathbf{k}2p^m=\pm 1} = \mp \frac{4\pi e\mathcal{E}}{(2\pi)^{3/2} k^3 \sqrt{64\pi a^5}} \int_0^\infty dr r e^{-r/2a} \left[3\frac{k_3(k_1 \pm ik_2)}{k^2} \sin kr \right. \\ \left. - 3\frac{k_3(k_1 \pm ik_2)r}{k} \cos kr - k_3(k_1 \pm ik_2)r^2 \sin kr \right].$$

The radial integrals can be evaluated to give

$$\int_0^\infty dr r e^{-r/2a} \left[-\sin kr + kr \cos kr + 3\frac{k_3^2}{k^2} \sin kr \right. \\ \left. - 3\frac{k_3^2 r}{k} \cos kr - k_3^2 r^2 \sin kr \right] = -\frac{256a^5 k^3 (1 + 4a^2(k^2 - 6k_3^2))}{(1 + 4a^2 k^2)^4}, \\ \int_0^\infty dr r e^{-r/2a} \left[3\frac{k_3(k_1 \pm ik_2)}{k^2} \sin kr - 3\frac{k_3(k_1 \pm ik_2)r}{k} \cos kr \right. \\ \left. - k_3(k_1 \pm ik_2)r^2 \sin kr \right] = \pm i \frac{6144a^7 k^3 k_3 (k_1 \mp ik_2)}{(1 + 4a^2 k^2)^4}.$$

Plugging these into the matrix elements, we find

$$U_{\mathbf{k}2p^m=0} = \frac{64a^{5/2} e\mathcal{E} (1 + 4a^2(k^2 - 6k_3^2))}{\pi (1 + 4a^2 k^2)^4}, \\ U_{\mathbf{k}2p^m=\pm 1} = -i \frac{768\sqrt{2} a^{9/2} e\mathcal{E} k_3 (k_1 \mp k_2)}{\pi (1 + 4a^2 k^2)^4}.$$

Using Eq. (6.2.6), the differential ionization rate is

$$d\Gamma(2p \rightarrow \mathbf{k}) = \frac{2\pi}{\hbar} |U_{\mathbf{k}2p}|^2 \delta(-B_{2p} + \hbar\omega - E(\mathbf{k})) k^2 dk d\Omega,$$

where $B_{2p} \approx 3.4$ eV is the binding energy of the $2p$ state of hydrogen, $d\Omega$ is the differential element of solid angle of the final electron direction, and $E(\mathbf{k}) = \hbar^2 \mathbf{k}^2 / 2m_e$. Now, $dk = m_e dE / \hbar^2 k$, and the effect of the factor $dE \delta(-B_{2p} + \hbar\omega - E(\mathbf{k}))$ in the integral over k is just to set k equal to the value fixed by the conservation of energy

$$k = \sqrt{2m_e(\hbar\omega - B_{2p})} / \hbar,$$

and so the differential ionization rate is

$$\frac{d\Gamma(2p \rightarrow \mathbf{k})}{d\Omega} = \frac{2\pi m_e k}{\hbar^3} |U_{\mathbf{k}2p}|^2,$$

with k given by the expression above. In order to calculate the rate averaged over the component of angular momentum in the direction of the field, we need to average the squares of the matrix elements we calculated above. The norm square matrix elements are given by

$$|U_{\mathbf{k}2p^{m=0}}|^2 = \frac{2^{12} a^5 e^2 \mathcal{E}^2 (1 + 4a^2(k^2 - 6k^2 \cos^2 \theta))^2}{\pi^2 (1 + 4a^2 k^2)^8},$$

$$|U_{\mathbf{k}2p^{m=\pm 1}}|^2 = \frac{2^{17} 3^2 a^9 e^2 \mathcal{E}^2 k^4 \cos^2 \theta \sin^2 \theta}{\pi^2 (1 + 4a^2 k^2)^8}.$$

These formulas only apply in the limit of large k , and so we may drop the terms which are suppressed by k^2 to find

$$|U_{\mathbf{k}2p^{m=0}}|^2 = \frac{e^2 \mathcal{E}^2 (1 - 6 \cos^2 \theta)^2}{\pi^2 a^7 k^{12}},$$

$$|U_{\mathbf{k}2p^{m=\pm 1}}|^2 = \frac{18 e^2 \mathcal{E}^2 \cos^2 \theta \sin^2 \theta}{\pi^2 a^7 k^{12}},$$

and so the average for large k is

$$|U_{\mathbf{k}2p}|^2 = \frac{1}{3} (|U_{\mathbf{k}2p^{m=0}}|^2 + |U_{\mathbf{k}2p^{m=1}}|^2 + |U_{\mathbf{k}2p^{m=-1}}|^2)$$

$$= \frac{e^2 \mathcal{E}^2 (1 + 24 \cos^2 \theta)}{3\pi^2 a^7 k^{12}}.$$

Finally, we find for the differential ionization rate

$$\frac{d\Gamma(2p \rightarrow \mathbf{k})}{d\Omega} = \frac{2m_e e^2 \mathcal{E}^2 (1 + 24 \cos^2 \theta)}{3\pi \hbar^3 a^7 k^{11}}.$$

3. Consider a Hamiltonian $H[s]$ that depends on a number of slowly varying parameters collectively called $s(t)$. What is the effect on the Berry phase

$\gamma_n[C]$ for a given closed curve C , if $H[s]$ is replaced with $f[s]H[s]$, where $f[s]$ is an arbitrary real numerical function of the s ?

We begin with the formula for the Berry phase given in Eq. (6.7.8)

$$\begin{aligned} \gamma_n[C] &= i \iint_{A[C]} \sum_{ij} dA_{ij} \sum_{m \neq n} \\ &\times \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_i} \right] \Phi_m[s] \right)^* \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_j} \right] \Phi_m[s] \right) (E_m[s] - E_n[s])^{-2}. \end{aligned}$$

If we replace $H[s]$ by $f[s]H[s]$, the Schrödinger equation appearing in Eq. (6.6.1) is modified to

$$f[s]H[s]\Phi_n[s] = f[s]E_n[s]\Phi_n[s],$$

and the derivatives appearing in the Berry phase become

$$\frac{\partial f[s]H[s]}{\partial s_i} = \frac{\partial f[s]}{\partial s_i} H[s] + \frac{\partial H[s]}{\partial s_i} f[s].$$

The relevant matrix elements are then

$$\begin{aligned} \left(\Phi_n[s], \left[\frac{\partial f[s]H[s]}{\partial s_i} \right] \Phi_m[s] \right) &= \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_j} \right] \Phi_m[s] \right) f[s] \\ &\quad + \left(\Phi_n[s], H[s] \Phi_m[s] \right) \frac{\partial f[s]}{\partial s_i} \\ &= \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_j} \right] \Phi_m[s] \right) f[s] \\ &\quad + \left(\Phi_n[s], \Phi_m[s] \right) E_m \frac{\partial f[s]}{\partial s_i} \\ &= \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_j} \right] \Phi_m[s] \right) f[s] \\ &\quad + \delta_{nm} E_m \frac{\partial f[s]}{\partial s_i}. \end{aligned}$$

Using this to calculate the Berry phase, we find

$$\begin{aligned} \gamma_n[C] &= i \iint_{A[C]} \sum_{ij} dA_{ij} \\ &\times \sum_{m \neq n} \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_i} \right] \Phi_m[s] \right)^* \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_j} \right] \Phi_m[s] \right) \\ &\times f[s]^2 (f[s]E_m[s] - f[s]E_n[s])^{-2} \end{aligned}$$

$$\begin{aligned}
&= i \int \int_{A[C]} \sum_{ij} dA_{ij} \sum_{m \neq n} \\
&\quad \times \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_i} \right] \Phi_m[s] \right)^* \left(\Phi_n[s], \left[\frac{\partial H[s]}{\partial s_j} \right] \Phi_m[s] \right) \\
&\quad \times (E_m[s] - E_n[s])^{-2},
\end{aligned}$$

where the terms involving $\partial f[s]/\partial s_i$ have gone away because the sum excludes the term $n = m$, and the factors of $f[s]$ cancel due to the fact that both the Hamiltonian and the energy eigenvalues are rescaled. We therefore find that the Berry phase is unchanged by the transformation $H[s] \rightarrow f[s]H[s]$ for a real function $f[s]$.

Chapter 7 Problem Set Solutions

1. Use the Born approximation to give a formula for the s -wave scattering length a_s for scattering of a particle of mass μ and wave number k by an arbitrary central potential $V(r)$ of finite range R , in the limit $kR \ll 1$. Use this result and the optical theorem to calculate the imaginary part of the forward scattering amplitude to second order in the potential.

In the Born approximation, Eq. (7.4.2) gives the scattering amplitude for a central potential

$$f_{\mathbf{k}}(\hat{x}) = -\frac{2\mu}{\hbar^2} \int_0^\infty dr r^2 V(r) \frac{\sin qr}{qr},$$

where q is defined as in Eq. (7.4.3)

$$q \equiv |\mathbf{k} - k\hat{x}| = 2k \sin(\theta/2).$$

For $kR \ll 1$ where R is the range of the potential, we can expand

$$\sin qr \approx 2kr \sin(\theta/2) + \mathcal{O}((kr)^3),$$

and in this limit the scattering amplitude becomes

$$\begin{aligned} f_{\mathbf{k}}(\hat{x}) &\approx -\frac{2\mu}{\hbar^2} \int_0^\infty dr r^2 V(r) \frac{2kr \sin(\theta/2) + \mathcal{O}((kr)^3)}{2kr \sin(\theta/2)} \\ &= -\frac{2\mu}{\hbar^2} \int_0^\infty dr r^2 V(r) + \mathcal{O}((kR)^2). \end{aligned}$$

We can also expand the scattering amplitude in Legendre polynomials as in Eq. (7.5.10)

$$f_{\mathbf{k}}(\hat{x}) \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell + 1) P_\ell(\cos \theta) (e^{2i\delta_\ell} - 1).$$

For $k \rightarrow 0$, the quantity $\tan \delta_\ell$ vanishes as $k^{2\ell+1}$, so δ_0 dominates, and so in this limit,

$$\begin{aligned} k \cot \delta_0 &\rightarrow -\frac{1}{a_s} + \mathcal{O}(k^2), \\ \tan \delta_0 &\approx \delta_0 \rightarrow -a_s k. \end{aligned}$$

We can therefore write the scattering amplitude in terms of the scattering length a_s

$$f_{\mathbf{k}}(\hat{x}) \approx \frac{1}{2ik} (2 \times 0 + 1) P_0(\cos \theta) (1 + 2i\delta_0 - 1) = \frac{\delta_0}{k} \approx -a_s.$$

Comparing this with the expression above, we find that in the Born approximation the s -wave scattering length for a central potential is given by

$$a_s \approx \frac{2\mu}{\hbar^2} \int_0^\infty dr r^2 V(r) + \mathcal{O}((kR)^2).$$

The cross-section is given by

$$\sigma = \int d\Omega |f_{\mathbf{k}}(\hat{x})|^2,$$

which in this limit goes to

$$\sigma \rightarrow 4\pi a_s^2 = \frac{16\mu^2}{\hbar^4} \left[\int_0^\infty dr r^2 V(r) \right]^2.$$

Then, according to Eq. (7.3.8) the optical theorem gives

$$\text{Im} f_{\mathbf{k}}(0) = \frac{k}{4\pi} \sigma = \frac{4k\mu^2}{\hbar^4} \left[\int_0^\infty dr r^2 V(r) \right]^2.$$

2. Suppose that in the scattering of a spinless non-relativistic particle of mass μ by an unknown potential, a resonance is observed at energy E_R for which the elastic cross section at the peak of the resonance is σ_{\max} . Show how to use this data to give a value for the orbital angular momentum of the resonant state.

We begin with the Breit–Wigner formula given in Eq. (7.6.12)

$$\sigma_{\text{scat}} = \frac{\pi(2\ell_0 + 1)}{k^2} \frac{\Gamma^2}{(E - E_R)^2 + \Gamma^2/4}.$$

Setting $E = E_R$, we find

$$\sigma_{\max} = \frac{4\pi(2\ell_0 + 1)}{k_R^2},$$

where we have defined

$$k_R^2 = \frac{2\mu E_R}{\hbar^2}.$$

We can rearrange this equation to solve for ℓ_0 , which gives

$$\ell_0 = \frac{1}{2} \left(\frac{\mu E_R \sigma_{\max}}{2\pi \hbar^2} - 1 \right).$$

3. Give a formula for the tangent of the $\ell = 0$ phase shift for scattering by a potential

$$V(r) = \begin{cases} -V_0 & r < R \\ 0 & r \geq R \end{cases},$$

for all $E > 0$, and to all orders in $V_0 > 0$.

We are dealing here with a central potential of the form

$$V(r) = \begin{cases} -V_0 & r < R \\ 0 & R \geq R \end{cases}$$

We will use Eq. (7.5.17) which reads

$$\tan \delta_\ell(k) = \frac{kj'_\ell(kR) - \Delta_\ell(k)j_\ell(kR)}{kn'_\ell(kR) - \Delta_\ell(k)n_\ell(kR)},$$

where $\Delta_\ell(k)$ is defined in Eq. (7.5.16)

$$\Delta_\ell(k) = \frac{R'_\ell(R)}{R_\ell(R)},$$

and $R_\ell(r)$ is the radial wave function. For $u(r) = rR(r)$, the radial part of the Schrödinger equation for $r < R$ takes the form

$$\frac{d^2u}{dr^2} - \frac{\ell(\ell+1)}{r^2}u + \frac{2\mu}{\hbar^2}V_0u + k^2u = 0.$$

Setting $\ell = 0$ this gives

$$\frac{d^2u}{dr^2} = -\left(k^2 + \frac{2\mu}{\hbar^2}V_0\right)u = -\frac{2\mu}{\hbar^2}(E + V_0)u \equiv -\tilde{k}^2u.$$

We can then solve for $u(r)$ which gives

$$u(r) = A \sin \tilde{k}r + B \cos \tilde{k}r,$$

and so $R_0(r)$ is

$$R_0(r) = \frac{A}{r} \sin \tilde{k}r + \frac{B}{r} \cos \tilde{k}r.$$

The radial wave function must be finite at $r = 0$, and so we must set $B = 0$. We therefore find for the radial wave function for $\ell = 0$ in the range $r < R$

$$R_0(r) = \frac{A}{r} \sin \tilde{k}r,$$

and for its derivative we get

$$R'_0(r) = \frac{A}{r} \tilde{k} \cos \tilde{k}r - \frac{A}{r^2} \sin \tilde{k}r.$$

We can then calculate $\Delta_0(k)$

$$\Delta_0(k) = \frac{R'_0(R)}{R_0(R)} = \tilde{k} \cot \tilde{k}R - \frac{1}{R}.$$

The relevant Bessel functions and their derivatives are

$$j_0(z) = \frac{\sin z}{z}$$

$$\begin{aligned}
 j'_0(z) &= \frac{\cos z}{z} - \frac{\sin z}{z^2} \\
 n_0(z) &= -\frac{\cos z}{z} \\
 n'_0(z) &= \frac{\sin z}{z} + \frac{\cos z}{z^2}.
 \end{aligned}$$

Putting this together, we find for the tangent of the $\ell = 0$ phase shift

$$\begin{aligned}
 \tan \delta_0(k) &= \frac{\left(\frac{\cos kR}{R} - \frac{\sin kR}{kR^2}\right) - \left(\tilde{k} \cot \tilde{k}R - \frac{1}{R}\right) \frac{\sin kR}{kR}}{\left(\frac{\sin kR}{R} + \frac{\cos kR}{kR^2}\right) + \left(\tilde{k} \cot \tilde{k}R - \frac{1}{R}\right) \frac{\cos kR}{kR}} \\
 &= \frac{k \cos kR - \tilde{k} \cot \tilde{k}R \sin kR}{k \sin kR + \tilde{k} \cot \tilde{k}R \cos kR},
 \end{aligned}$$

where $\tilde{k} \equiv \sqrt{\frac{2\mu(E+V_0)}{\hbar^2}}$.

4. Suppose that the eigenstates of an unperturbed Hamiltonian include not only continuum states of a free particle with momentum \mathbf{p} and unperturbed energy $E = \mathbf{p}^2/2\mu$, but also a discrete state of angular momentum ℓ with a negative unperturbed energy. Suppose that when we turn on the interaction, the continuum states feel a local potential, but remain in the continuum, while also the discrete state moves to positive energy, thereby becoming unstable. What is the change in the phase shift $\delta_\ell(k)$ as the wave number k increases from $k = 0$ to $k = \infty$?

If we place the system in a sphere of radius R , the number of states with angular momentum ℓ and energies between 0 and E is given by Eq. (7.8.2)

$$N_\ell(E) = \frac{1}{\pi}(kR + \delta_\ell(E) - \delta_\ell(0)).$$

The change in the number of scattering states with energy between 0 and E due to the interaction is given by Eq. (7.8.3)

$$\Delta N_\ell(E) = \frac{1}{\pi}(\delta_\ell(E) - \delta_\ell(0)).$$

Because one bound state becomes a positive energy scattering state when the interaction is turned on, we must have

$$\Delta N_\ell(\infty) = \frac{1}{\pi}(\delta_\ell(\infty) - \delta_\ell(0)) = 1,$$

and as a result we must have

$$\delta_\ell(\infty) - \delta_\ell(0) = \pi.$$

5. Find an upper bound on the elastic scattering cross section in the case where the scattering amplitude f is independent of angles θ and ϕ .

The scattering cross-section is given by

$$\sigma_{\text{scattering}} \equiv \int_0^\pi \sin \theta \, d\theta \int_0^{2\pi} d\phi |f_{\mathbf{k}}(\theta, \phi)|^2,$$

which by the optical theorem Eq. (7.3.8) is equal to

$$\sigma_{\text{scattering}} = \frac{4\pi}{k} \text{Im} f_{\mathbf{k}}(0).$$

In the case where the scattering amplitude is independent of angle, we have

$$f_{\mathbf{k}}(\theta, \phi) = f_{\mathbf{k}}(0),$$

and so the scattering cross-section is

$$\begin{aligned} \sigma_{\text{scattering}} &= \int_0^\pi \sin \theta \, d\theta \int_0^{2\pi} d\phi |f_{\mathbf{k}}(0)|^2 \\ &= 4\pi |f_{\mathbf{k}}(0)|^2, \end{aligned}$$

and since the absolute value square of any function is always greater than the absolute value square of its imaginary part, we may write

$$4\pi |f_{\mathbf{k}}(0)|^2 \geq 4\pi |\text{Im} f_{\mathbf{k}}(0)|^2 = 4\pi \left(\frac{k^2}{16\pi^2} \sigma_{\text{scattering}}^2 \right),$$

where we have again used the optical theorem. We therefore find that

$$\sigma_{\text{scattering}} \geq \frac{k^2}{4\pi} \sigma_{\text{scattering}}^2,$$

and so we find an upper bound on the scattering cross-section

$$\sigma_{\text{scattering}} \leq \frac{4\pi}{k^2}.$$

6. *Use the eikonal approximation to calculate the phase of the scattering amplitude for the scattering of a non-relativistic charged particle by a Coulomb potential.*

We are interested in calculating the phase of the scattering amplitude for the scattering of a non-relativistic particle by a Coulomb potential. We begin with Eq. (7.10.3) which in this case reads

$$\frac{(\nabla S)^2}{2m} + \frac{Z_1 Z_2 e^2}{r} = E.$$

We imagine starting with a particle very far from the scattering center with energy $\frac{\hbar^2 k^2}{2m}$ moving in the z -direction toward the scattering center with an impact parameter b . Since the eikonal approximation is only valid where the wave function $\psi(\mathbf{x})$ varies much more rapidly with \mathbf{x} than the potential, we require that $E \gg V$. In this limit, the deflection of the particle will be

small, and we can approximate the classical trajectory of the particle as a straight line. We can then solve the above expression for the phase of the wave function as

$$\frac{S}{\hbar} = \int_{-\infty}^z \left[k^2 - \frac{2m}{\hbar^2} \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} \right]^{1/2} dz' + S_0.$$

In the case when the particle is uncharged, this expression should give $S = \hbar k z$, and so we can choose the constant S_0 such that

$$\frac{S}{\hbar} = \int_{-\infty}^z \left[\left[k^2 - \frac{2m}{\hbar^2} \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} \right]^{1/2} - k \right] dz' + k z.$$

Since we are working in the regime where $\hbar^2 k^2 / 2m \gg Z_1 Z_2 e^2 / \sqrt{b^2 + z'^2}$, we can expand the square root to get

$$\frac{S}{\hbar} \approx k z - \frac{m}{\hbar^2 k} \int_{-\infty}^z \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} dz'.$$

Now, recalling Eq. (7.10.2) we find that the wave function takes the form

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} e^{i k z} \exp \left(-\frac{i m}{\hbar^2 k} \int_{-\infty}^z \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} dz' \right),$$

where we have neglected the spatial variation of $N(\mathbf{x})$ at this order of approximation. Now recall that the scattering amplitude is given in Eq. (7.2.6) as

$$f_{\mathbf{k}}(\hat{x}) = -\frac{m}{2\pi \hbar^2} (2\pi \hbar)^{3/2} \int d^3 y e^{-i \mathbf{k} \hat{x} \cdot \mathbf{y}} V(\mathbf{y}) \psi_{\mathbf{k}}(\mathbf{y}).$$

In this case, the expression for the scattering amplitude takes the form

$$f_{\mathbf{k}}(\hat{x}) = -\frac{m}{2\pi \hbar^2} \int d^3 x' e^{-i \mathbf{k} \hat{x} \cdot \mathbf{x}'} \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} e^{i \mathbf{k} \cdot \mathbf{x}'} \\ \times \exp \left[-\frac{i m}{\hbar^2 k} \int_{-\infty}^{z'} \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z''^2}} dz'' \right].$$

Now we will use cylindrical coordinates to do the integral over \mathbf{x}' for which $d^3 x' = b db d\phi dz'$. Let us examine the factor $(\mathbf{k} - k\hat{x}) \cdot \mathbf{x}'$ appearing in the exponential, which here becomes

$$(\mathbf{k} - k\hat{x}) \cdot \mathbf{x}' = (\mathbf{k} - k\hat{x}) \cdot (\mathbf{b} + z'\hat{z}) \approx (\mathbf{k} - k\hat{x}) \cdot \mathbf{b},$$

because $(\mathbf{k} - k\hat{x}) \cdot \hat{z}$ is negligible for small deflection angle. We can then express this in cylindrical coordinates as

$$(\mathbf{k} - k\hat{x}) \cdot \mathbf{x}' \approx -2kb \sin \left(\frac{\theta}{2} \right) \cos \phi,$$

where we have used the fact that $\mathbf{k} - k\hat{x} = \mathbf{q}$ where $q = 2k \sin(\frac{\theta}{2})$. Our expression for the scattering amplitude now becomes

$$f_{\mathbf{k}}(\hat{x}) = -\frac{m}{2\pi\hbar^2} \int_0^\infty b db \int_0^{2\pi} e^{-iqb \cos \phi} d\phi \\ \times \int_{-\infty}^\infty dz' \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} \exp \left[-\frac{im}{\hbar^2 k} \int_{-\infty}^{z'} \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z''^2}} dz'' \right].$$

Next, we notice that we can write

$$\int_{-\infty}^\infty dz' \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} \exp \left[-\frac{im}{\hbar^2 k} \int_{-\infty}^{z'} \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z''^2}} dz'' \right] \\ = \frac{i\hbar^2 k}{m} \exp \left[-\frac{im}{\hbar^2 k} \int_{-\infty}^{z'} \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z''^2}} dz'' \right] \Big|_{z'=-\infty}^{z'=\infty},$$

and the integral over ϕ can be done to give

$$\int_0^{2\pi} d\phi e^{-iqb \cos \phi} = 2\pi J_0(qb).$$

The scattering amplitude then takes the form

$$f_{\mathbf{k}}(\theta) = -ik \int_0^\infty db b J_0(qb) [e^{i\chi(b)} - 1],$$

where we have defined the Eikonal phase

$$\chi(b) = -\frac{m}{\hbar^2 k} \int_{-\infty}^\infty \frac{Z_1 Z_2 e^2}{\sqrt{b^2 + z'^2}} dz'.$$

This integral is logarithmically divergent, but it can be computed by introducing a screening radius and then taking the limit in which the screening radius tends to infinity. The result is

$$\chi(b) = -\frac{2mZ_1 Z_2 e^2}{\hbar^2 k} \ln(kb).$$

The scattering amplitude is then

$$f_{\mathbf{k}}(\theta) = -ik \int_0^\infty db b J_0(qb) [e^{i\chi(b)} - 1] \\ = -\frac{ik}{q^2} \int_0^\infty J_0(x) \left[\left(\frac{kx}{q} \right)^{2i\xi} - 1 \right] x dx \\ = -\frac{ik}{q^2} \left[\left(\frac{k}{q} \right)^{2i\xi} \int_0^\infty J_0(x) x^{2i\xi+1} dx - \int_0^\infty J_0(x) x dx \right],$$

where we have defined ξ as in Eq. (7.9.5)

$$\xi \equiv \frac{mZ_1Z_2e^2}{\hbar^2k}.$$

We can then evaluate these integrals by using the identity

$$\int x J_0(x) dx = x J_1(x),$$

and integrating by parts in the first term, and so we find

$$\begin{aligned} f_{\mathbf{k}}(\theta) &= -\frac{ik}{q^2} \left(\frac{k}{q}\right)^{2i\xi} x^{2i\xi+1} J_1(x) \Big|_0^\infty + 2i\xi \left(\frac{k}{q}\right)^{2i\xi} \int_0^\infty x^{2i\xi} J_1(x) dx + x J_1(x) \Big|_0^\infty \\ &= -\frac{ik}{q^2} \left[x J_1(x) (e^{2i\xi \ln(kx/q)} - 1) \Big|_0^\infty - 2i\xi \left(\frac{k}{q}\right)^{2i\xi} 2^{2i\xi} \frac{\Gamma(1+i\xi)}{\Gamma(1-i\xi)} \right] \\ &= -\frac{2k\xi}{q^2} \left(\frac{2k}{q}\right)^{2i\xi} \frac{\Gamma(1+i\xi)}{\Gamma(1-i\xi)} \\ &= -\frac{2mZ_1Z_2}{\hbar^2q^2} \frac{\Gamma(1+i\xi)}{\Gamma(1-i\xi)} \exp \left[-i\xi \ln \left(\sin^2 \left(\frac{\theta}{2} \right) \right) \right]. \end{aligned}$$

Now, comparing with Eqs. (7.9.13) and (7.9.14), in the limit of large r where we can neglect the logarithmic term in the exponential, we find that the eikonal approximation has reproduced the exact expression for the scattering amplitude valid at all angles. This is a bit surprising considering that we approximated the classical path as a straight line, but it should be noted that this feature is specific to the Coulomb potential, and the eikonal approximation does not give the exact scattering amplitude for general potentials.

Chapter 8 Problem Set Solutions

1. Consider a general Hamiltonian $H_0 + V$, where H_0 is the free-particle energy. Define a state Ψ_α^0 by the modified Lippmann–Schwinger equation

$$\Psi_\alpha^0 = \Phi_\alpha + \frac{(E_\alpha - H_0)}{(E_\alpha - H_0)^2 + \epsilon^2} V \Psi_\alpha^0,$$

where Φ_α is an eigenstate of H_0 with eigenvalue E_α , and ϵ is a positive infinitesimal quantity. Define

$$A_{\beta\alpha} \equiv (\Phi_\beta, V \Psi_\alpha^0).$$

(a) Show that $A_{\beta\alpha} = A_{\alpha\beta}^*$ for $E_\beta = E_\alpha$.

(b) For the simple case of a non-relativistic particle with energy $\mathbf{k}^2 \hbar^2 / 2\mu$ in a local potential $V(\mathbf{x})$, calculate the asymptotic behavior of the coordinate-space wave function $(\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0)$ of the state $\Psi_{\mathbf{k}}^0$ for $\mathbf{x} \rightarrow \infty$. Express the result in terms of matrix elements of A .

(a) We begin with the definition

$$\Psi_\alpha^0 = \Phi_\alpha + \frac{(E_\alpha - H_0)}{(E_\alpha - H_0)^2 + \epsilon^2} V \Psi_\alpha^0,$$

where Φ_α is an eigenstate of the free-particle Hamiltonian H_0 with eigenvalue E_α and ϵ is a positive infinitesimal quantity. We will find it useful to rearrange this equation to get an expression for Φ_α in terms of Ψ_α^0

$$\Phi_\alpha = \Psi_\alpha^0 - \frac{(E_\alpha - H_0)}{(E_\alpha - H_0)^2 + \epsilon^2} V \Psi_\alpha^0.$$

The quantity $A_{\beta\alpha}$ is defined as

$$A_{\beta\alpha} \equiv (\Phi_\beta, V \Psi_\alpha^0).$$

We can then write

$$\begin{aligned} A_{\alpha\beta}^* &= (\Phi_\alpha, V \Psi_\beta^0)^* = (V \Psi_\beta^0, \Phi_\alpha) \\ &= \left(V \Psi_\beta^0, \left[\Psi_\alpha^0 - \frac{(E_\alpha - H_0)}{(E_\alpha - H_0)^2 + \epsilon^2} V \Psi_\alpha^0 \right] \right) \\ &= (V \Psi_\beta^0, \Psi_\alpha^0) - \left(V \Psi_\beta^0, \frac{(E_\alpha - H_0)}{(E_\alpha - H_0)^2 + \epsilon^2} V \Psi_\alpha^0 \right) \\ &= (\Psi_\beta^0, V \Psi_\alpha^0) - \left(\frac{(E_\alpha - H_0)}{(E_\alpha - H_0)^2 + \epsilon^2} V \Psi_\beta^0, V \Psi_\alpha^0 \right), \end{aligned}$$

where in the last line we have used the fact that V and H_0 are Hermitian, and that E_α and ϵ are real. We can now combine these inner products and use the fact that $E_\alpha = E_\beta$ to find

$$\begin{aligned}
A_{\alpha\beta}^* &= \left(\left[\Psi_\beta^0 - \frac{(E_\alpha - H_0)}{(E_\alpha - H_0)^2 + \epsilon^2} V \Psi_\beta^0 \right], V \Psi_\alpha^0 \right) \\
&= (\Phi_\beta, V \Psi_\alpha^0) \\
&= A_{\beta\alpha}.
\end{aligned}$$

- (b) We are interested in calculating the coordinate-space wave function $(\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0)$ for a non-relativistic particle with energy $\mathbf{k}^2 \hbar^2 / 2\mu$ in a local potential $V(\mathbf{x})$. We will use the modified Lippmann–Schwinger equation to write

$$(\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0) = (\Phi_{\mathbf{x}}, \Phi_{\mathbf{k}}) + \left(\Phi_{\mathbf{x}}, \frac{\left(\frac{\hbar^2 \mathbf{k}^2}{2\mu} - H_0 \right)}{\left(\frac{\hbar^2 \mathbf{k}^2}{2\mu} - H_0 \right)^2 + \epsilon^2} V \Psi_{\mathbf{k}}^0 \right).$$

The first inner product is just the free-particle wave function given in Eq. (3.5.12), and we will insert a complete set of states $\Phi_{\mathbf{p}}$ in the second inner product which gives

$$\begin{aligned}
(\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0) &= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} + \int d^3 p (\Phi_{\mathbf{x}}, \Phi_{\mathbf{p}}) \left(\Phi_{\mathbf{p}}, \frac{\left(\frac{\hbar^2 \mathbf{k}^2}{2\mu} - H_0 \right)}{\left(\frac{\hbar^2 \mathbf{k}^2}{2\mu} - H_0 \right)^2 + \epsilon^2} V \Psi_{\mathbf{k}}^0 \right) \\
&= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} + \int d^3 p (\Phi_{\mathbf{x}}, \Phi_{\mathbf{p}}) \frac{\left(\frac{\hbar^2 \mathbf{k}^2}{2\mu} - \frac{\hbar^2 \mathbf{p}^2}{2\mu} \right)}{\left(\frac{\hbar^2 \mathbf{k}^2}{2\mu} - \frac{\hbar^2 \mathbf{p}^2}{2\mu} \right)^2 + \epsilon^2} (\Phi_{\mathbf{p}}, V \Psi_{\mathbf{k}}^0) \\
&= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} + \frac{2\mu}{\hbar^2} \int d^3 p (\Phi_{\mathbf{x}}, \Phi_{\mathbf{p}}) \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} (\Phi_{\mathbf{p}}, V \Psi_{\mathbf{k}}^0),
\end{aligned}$$

where in the second expression, we have defined $\epsilon' = \frac{2\mu}{\hbar^2} \epsilon$ which is also a real positive infinitesimal quantity. Now we insert another complete set of states $\Phi_{\mathbf{y}}$ in the second term, and we find

$$\begin{aligned}
(\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0) &= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} + \frac{2\mu}{\hbar^2} \int d^3 p d^3 y (\Phi_{\mathbf{x}}, \Phi_{\mathbf{p}}) \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} \\
&\quad \times (\Phi_{\mathbf{p}}, \Phi_{\mathbf{y}}) (\Phi_{\mathbf{y}}, V \Psi_{\mathbf{k}}^0) \\
&= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} + \frac{2\mu}{\hbar^2} \int \frac{d^3 p}{(2\pi)^3} d^3 y e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} (\Phi_{\mathbf{y}}, V \Psi_{\mathbf{k}}^0).
\end{aligned}$$

Now we can perform the integral over \mathbf{p} by the same method used in Eq. (7.4.2), that is

$$\begin{aligned}
\int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} &= \int_0^\infty \frac{4\pi p^2 dp}{(2\pi)^3} \frac{\sin(p|\mathbf{x}-\mathbf{y}|)}{p|\mathbf{x}-\mathbf{y}|} \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} \\
&= \frac{-i}{4\pi^2|\mathbf{x}-\mathbf{y}|} \int_0^\infty dp p \left(e^{ip|\mathbf{x}-\mathbf{y}|} - e^{-ip|\mathbf{x}-\mathbf{y}|} \right) \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} \\
&= \frac{-i}{4\pi^2|\mathbf{x}-\mathbf{y}|} \int_{-\infty}^\infty dp p e^{ip|\mathbf{x}-\mathbf{y}|} \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2},
\end{aligned}$$

where in going to the third line we have taken $p \rightarrow -p$ in the second term in parentheses in order to combine the integrals. Now we can write

$$\frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} = \frac{(k^2 - p^2)}{(k^2 - p^2 - i\epsilon')(k^2 - p^2 + i\epsilon')},$$

and then we can do the integral by closing the contour in the upper half complex plane and calculating the contribution of the residues at $p = k + i\epsilon'$ and $p = -k + i\epsilon'$. This gives

$$\begin{aligned}
\int \frac{d^3 p}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \frac{(k^2 - p^2)}{(k^2 - p^2)^2 + \epsilon'^2} &= \frac{-i}{4\pi^2|\mathbf{x}-\mathbf{y}|} (-2\pi i) \left[\frac{ke^{ik|\mathbf{x}-\mathbf{y}|}}{2k} - \frac{ke^{-ik|\mathbf{x}-\mathbf{y}|}}{-2k} \right] \\
&= \frac{-1}{4\pi|\mathbf{x}-\mathbf{y}|} \left[e^{ik|\mathbf{x}-\mathbf{y}|} + e^{-ik|\mathbf{x}-\mathbf{y}|} \right],
\end{aligned}$$

which we can plug into the coordinate-space wave function to get

$$(\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} - \int d^3 y (\Phi_{\mathbf{y}}, V\Psi_{\mathbf{k}}^0) \frac{2\mu}{\hbar^2} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} \left[e^{ik|\mathbf{x}-\mathbf{y}|} + e^{-ik|\mathbf{x}-\mathbf{y}|} \right].$$

Now we can insert another complete set of states $\Phi_{\mathbf{q}}$ to get

$$\begin{aligned}
(\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0) &= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} - \int d^3 y d^3 q (\Phi_{\mathbf{y}}, \Phi_{\mathbf{q}}) (\Phi_{\mathbf{q}}, V\Psi_{\mathbf{k}}^0) \frac{2\mu}{\hbar^2} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} \\
&\quad \times \left[e^{ik|\mathbf{x}-\mathbf{y}|} + e^{-ik|\mathbf{x}-\mathbf{y}|} \right] \\
&= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} - \int d^3 y d^3 q \frac{e^{i\mathbf{q}\cdot\mathbf{y}}}{(2\pi)^{3/2}} A_{\mathbf{qk}} \frac{2\mu}{\hbar^2} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} \\
&\quad \times \left[e^{ik|\mathbf{x}-\mathbf{y}|} + e^{-ik|\mathbf{x}-\mathbf{y}|} \right].
\end{aligned}$$

In the limit of large \mathbf{x} , we can expand $|\mathbf{x}-\mathbf{y}|$ to get

$$|\mathbf{x}-\mathbf{y}| = r|\hat{\mathbf{x}} - \frac{\mathbf{y}}{r}| \rightarrow r\sqrt{1 - \frac{2\mathbf{y}\cdot\hat{\mathbf{x}}}{r}} \approx r - \mathbf{y}\cdot\hat{\mathbf{x}},$$

where $r \equiv |\mathbf{x}|$. In this limit, the wave function takes the form

$$\begin{aligned}
 (\Phi_{\mathbf{x}}, \Psi_{\mathbf{k}}^0) &= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} - \int d^3y d^3q \frac{e^{i\mathbf{q}\cdot\mathbf{y}}}{(2\pi)^{3/2}} A_{\mathbf{q}\mathbf{k}} \frac{2\mu}{\hbar^2} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} \\
 &\quad \times \left[e^{i\mathbf{k}r} e^{-i\mathbf{k}\hat{x}\cdot\mathbf{y}} + e^{-i\mathbf{k}r} e^{i\mathbf{k}\hat{x}\cdot\mathbf{y}} \right] \\
 &= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} - \int d^3q \frac{\sqrt{2\pi}\mu}{\hbar^2 r} \\
 &\quad \times \left[\delta^3(\mathbf{q}-\mathbf{k}\hat{x}) e^{i\mathbf{k}r} A_{\mathbf{q}\mathbf{k}} + \delta^3(\mathbf{q}+\mathbf{k}\hat{x}) e^{-i\mathbf{k}r} A_{\mathbf{q}\mathbf{k}} \right] \\
 &= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} - \frac{\sqrt{2\pi}\mu}{\hbar^2 r} \left[e^{i\mathbf{k}r} A_{+\mathbf{k}\hat{x}\mathbf{k}} + e^{-i\mathbf{k}r} A_{-\mathbf{k}\hat{x}\mathbf{k}} \right].
 \end{aligned}$$

2. Consider a separable interaction, whose matrix elements between free-particle states have the form

$$(\Phi_{\beta}, V\Phi_{\alpha}) = f(\alpha) f^*(\beta),$$

where $f(\alpha)$ is some general function of the momenta and other quantum numbers characterizing the free-particle state Φ_{α} .

(a) Find an exact solution of the Lippmann–Schwinger equation for the “in” state in this theory.

(b) Use the result of (a) to calculate the S -matrix.

(c) Verify the unitarity of the S -matrix.

- (a) The Lippmann–Schwinger equation is given in Eq. (8.1.6) which reads

$$\Psi_{\alpha}^{+} = \Phi_{\alpha} + (E_{\alpha} - H_0 + i\epsilon)^{-1} V \Psi_{\alpha}^{+},$$

where Φ_{α} is an eigenstate of H_0 with eigenvalue E_{α} . We can insert a complete set of states Φ_{α_1} in the second term and then expand using the Lippmann–Schwinger equation again to find

$$\begin{aligned}
 \Psi_{\alpha}^{+} &= \Phi_{\alpha} + \int d\alpha_1 \Psi_{\alpha_1} (\Psi_{\alpha_1}, (E_{\alpha} - H_0 + i\epsilon)^{-1} V \Psi_{\alpha}^{+}) \\
 &= \Phi_{\alpha} + \int d\alpha_1 \Phi_{\alpha_1} (E_{\alpha} - E_{\alpha_1} + i\epsilon)^{-1} \\
 &\quad \times [(\Phi_{\alpha_1}, V\Phi_{\alpha}) + (\Phi_{\alpha_1}, V(E_{\alpha} - H_0 + i\epsilon)^{-1} V \Psi_{\alpha}^{+})].
 \end{aligned}$$

We can then use the fact that $(\Phi_{\beta}, V\Phi_{\alpha}) = f(\alpha) f^*(\beta)$ in the first term in brackets, and insert another complete set of states Φ_{α_2} in the second term in brackets to get

$$\begin{aligned}
 \Psi_{\alpha}^{+} &= \Phi_{\alpha} + \int d\alpha_1 \frac{f(\alpha) f^*(\alpha_1)}{(E_{\alpha} - E_{\alpha_1} + i\epsilon)} \Phi_{\alpha_1} \\
 &\quad + \int d\alpha_1 d\alpha_2 \frac{(\Phi_{\alpha_1}, V(E_{\alpha} - H_0 + i\epsilon)^{-1} \Phi_{\alpha_2})}{E_{\alpha} - E_{\alpha_1} + i\epsilon} (\Phi_{\alpha_2}, V\Psi_{\alpha}^{+}) \Phi_{\alpha_1}
 \end{aligned}$$

$$\begin{aligned}
&= \Phi_\alpha + \int d\alpha_1 \frac{f(\alpha) f^*(\alpha_1)}{(E_\alpha - E_{\alpha_1} + i\epsilon)} \Phi_{\alpha_1} \\
&\quad + \int d\alpha_1 d\alpha_2 \frac{f(\alpha_2) f^*(\alpha_1) f(\alpha) f^*(\alpha_2)}{(E_\alpha - E_{\alpha_1} + i\epsilon)(E_\alpha - E_{\alpha_2} + i\epsilon)} \Phi_{\alpha_1} \\
&\quad + \int d\alpha_1 d\alpha_2 \frac{f(\alpha) f^*(\alpha_1) (\Phi_{\alpha_2}, V(E_\alpha - H_0 + i\epsilon)^{-1} V \Psi_\alpha^+)}{(E_\alpha - E_{\alpha_1} + i\epsilon)(E_\alpha - E_{\alpha_2} + i\epsilon)} \Phi_{\alpha_1}.
\end{aligned}$$

We can then iterate this process of inserting complete sets of states and using the Lippmann–Schwinger equation to get

$$\begin{aligned}
\Psi_\alpha^+ &= \Phi_\alpha + \int d\alpha_1 \frac{f(\alpha) f^*(\alpha_1)}{(E_\alpha - E_{\alpha_1} + i\epsilon)} \Phi_{\alpha_1} \\
&\quad + \int d\alpha_1 d\alpha_2 \frac{f(\alpha) f^*(\alpha_1) |f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_1} + i\epsilon)(E_\alpha - E_{\alpha_2} + i\epsilon)} \Phi_{\alpha_1} \\
&\quad + \int d\alpha_1 d\alpha_2 d\alpha_3 \frac{f(\alpha) f^*(\alpha_1) |f(\alpha_2)|^2 |f(\alpha_3)|^2}{(E_\alpha - E_{\alpha_1} + i\epsilon)(E_\alpha - E_{\alpha_2} + i\epsilon)(E_\alpha - E_{\alpha_3} + i\epsilon)} \Phi_{\alpha_1} + \dots \\
&= \Phi_\alpha + \int d\alpha_1 \frac{f(\alpha) f^*(\alpha_1)}{(E_\alpha - E_{\alpha_1} + i\epsilon)} \Phi_{\alpha_1} \\
&\quad \times \left[1 + \int d\beta \frac{|f(\beta)|^2}{(E_\alpha - E_\beta + i\epsilon)} + \left(\int d\beta \frac{|f(\beta)|^2}{(E_\alpha - E_\beta + i\epsilon)} \right)^2 + \dots \right].
\end{aligned}$$

The term in square brackets is just an infinite power series which we can sum to get an explicit expression for Ψ_α^+

$$\Psi_\alpha^+ = \Phi_\alpha + \frac{\int d\alpha_1 \frac{f(\alpha) f^*(\alpha_1)}{(E_\alpha - E_{\alpha_1} + i\epsilon)} \Phi_{\alpha_1}}{1 - \int d\beta \frac{|f(\beta)|^2}{(E_\alpha - E_\beta + i\epsilon)}}.$$

(b) The S-matrix is given by Eq. (8.1.10) as

$$S_{\beta\alpha} = \delta(\beta - \alpha) - 2\pi i \delta(E_\alpha - E_\beta) T_{\beta\alpha},$$

where $T_{\beta\alpha}$ is defined in Eq. (8.1.11) as

$$T_{\beta\alpha} \equiv (\Phi_\beta, V \Psi_\alpha^+).$$

Using our expression for Ψ_α^+ from above, we can calculate $T_{\beta\alpha}$ in this case to be

$$\begin{aligned}
T_{\beta\alpha} &= (\Phi_\beta, V \Phi_\alpha) + \frac{\int d\alpha_1 \frac{f(\alpha) f^*(\alpha_1)}{(E_\alpha - E_{\alpha_1} + i\epsilon)} (\Phi_\beta, V \Phi_{\alpha_1})}{1 - \int d\gamma \frac{|f(\gamma)|^2}{(E_\alpha - E_\gamma + i\epsilon)}} \\
&= f(\alpha) f^*(\beta) + \frac{\int d\alpha_1 \frac{f(\alpha) f^*(\alpha_1) f(\alpha_1) f^*(\beta)}{(E_\alpha - E_{\alpha_1} + i\epsilon)}}{1 - \int d\gamma \frac{|f(\gamma)|^2}{(E_\alpha - E_\gamma + i\epsilon)}}
\end{aligned}$$

$$\begin{aligned}
&= f(\alpha)f^*(\beta) \left[1 + \frac{\int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} + i\epsilon)}}{1 - \int d\gamma \frac{|f(\gamma)|^2}{(E_\alpha - E_\gamma + i\epsilon)}} \right] \\
&= \frac{f(\alpha)f^*(\beta)}{1 - \int d\gamma \frac{|f(\gamma)|^2}{(E_\alpha - E_\gamma + i\epsilon)}}.
\end{aligned}$$

We can then plug this into the expression for the S-matrix to find

$$S_{\beta\alpha} = \delta(\beta - \alpha) - 2\pi i \delta(E_\alpha - E_\beta) \frac{f(\alpha)f^*(\beta)}{1 - \int d\gamma \frac{|f(\gamma)|^2}{(E_\alpha - E_\gamma + i\epsilon)}}.$$

(c) In order to verify unitarity of the S-matrix, we must show that

$$\int d\gamma S_{\gamma\beta}^* S_{\gamma\alpha} = \delta(\alpha - \beta).$$

Using our expression for the S-matrix from part (b), we can write this out as

$$\begin{aligned}
&\int d\gamma S_{\gamma\beta}^* S_{\gamma\alpha} \\
&= \int d\gamma \left[\delta(\gamma - \beta)\delta(\gamma - \alpha) + 2\pi i \delta(E_\gamma - E_\beta)\delta(\gamma - \alpha) \frac{f^*(\beta)f(\gamma)}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\beta - E_{\alpha_1} - i\epsilon)}} \right. \\
&\quad - 2\pi i \delta(E_\gamma - E_\alpha)\delta(\gamma - \beta) \frac{f(\alpha)f^*(\gamma)}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} + i\epsilon)}} \\
&\quad \left. + 4\pi^2 \delta(E_\gamma - E_\alpha)\delta(E_\gamma - E_\beta) \frac{f(\alpha)f^*(\beta)|f(\gamma)|^2}{\left(1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\beta - E_{\alpha_1} - i\epsilon)}\right) \left(1 - \int d\alpha_2 \frac{|f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_2} + i\epsilon)}\right)} \right].
\end{aligned}$$

We can use the δ -functions in the first three terms to do the integral over γ , and so this expression becomes

$$\begin{aligned}
&\int d\gamma S_{\gamma\beta}^* S_{\gamma\alpha} \\
&= \delta(\beta - \alpha) \\
&\quad + 2\pi i \delta(E_\alpha - E_\beta) f(\alpha) f^*(\beta) \left[\frac{1}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\beta - E_{\alpha_1} - i\epsilon)}} - \frac{1}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} + i\epsilon)}} \right] \\
&\quad + 4\pi^2 f(\alpha) f^*(\beta) \int d\gamma \frac{\delta(E_\gamma - E_\alpha)\delta(E_\gamma - E_\beta)|f(\gamma)|^2}{\left(1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\beta - E_{\alpha_1} - i\epsilon)}\right) \left(1 - \int d\alpha_2 \frac{|f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_2} + i\epsilon)}\right)}.
\end{aligned}$$

We can set the energies equal in the terms in square brackets on the second line because they are multiplied by $\delta(E_\alpha - E_\beta)$, and then these terms can be combined to give

$$\begin{aligned}
& \left[\frac{1}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} - i\epsilon)}} - \frac{1}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} + i\epsilon)}} \right] \\
&= \frac{\int d\gamma |f(\gamma)|^2 \left(\frac{-1}{E_\alpha - E_\gamma + i\epsilon} + \frac{1}{E_\alpha - E_\gamma - i\epsilon} \right)}{\left(1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} - i\epsilon)} \right) \left(1 - \int d\alpha_2 \frac{|f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_2} + i\epsilon)} \right)} \\
&= \frac{\int d\gamma |f(\gamma)|^2 \left(\frac{2i\epsilon}{(E_\alpha - E_\gamma)^2 + \epsilon^2} \right)}{\left(1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} - i\epsilon)} \right) \left(1 - \int d\alpha_2 \frac{|f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_2} + i\epsilon)} \right)}.
\end{aligned}$$

As discussed in the text above Eq. (8.1.15), for infinitesimal ϵ , the function $\epsilon/(x^2 + \epsilon^2)$ is negligible away from $x = 0$, while its integral over all x is π , and so it can be replaced in any integral by $\pi\delta(x)$. The above expression then becomes

$$\begin{aligned}
& \left[\frac{1}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} - i\epsilon)}} - \frac{1}{1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} + i\epsilon)}} \right] \\
&= 2\pi i \int d\gamma \frac{\delta(E_\alpha - E_\gamma) |f(\gamma)|^2}{\left(1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\alpha - E_{\alpha_1} - i\epsilon)} \right) \left(1 - \int d\alpha_2 \frac{|f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_2} + i\epsilon)} \right)}.
\end{aligned}$$

We therefore see that

$$\begin{aligned}
& \int d\gamma S_{\gamma\beta}^* S_{\gamma\alpha} \\
&= \delta(\beta - \alpha) \\
&\quad - 4\pi^2 f(\alpha) f^*(\beta) \int d\gamma \frac{\delta(E_\gamma - E_\alpha) \delta(E_\gamma - E_\beta) |f(\gamma)|^2}{\left(1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\beta - E_{\alpha_1} - i\epsilon)} \right) \left(1 - \int d\alpha_2 \frac{|f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_2} + i\epsilon)} \right)} \\
&\quad + 4\pi^2 f(\alpha) f^*(\beta) \int d\gamma \frac{\delta(E_\gamma - E_\alpha) \delta(E_\gamma - E_\beta) |f(\gamma)|^2}{\left(1 - \int d\alpha_1 \frac{|f(\alpha_1)|^2}{(E_\beta - E_{\alpha_1} - i\epsilon)} \right) \left(1 - \int d\alpha_2 \frac{|f(\alpha_2)|^2}{(E_\alpha - E_{\alpha_2} + i\epsilon)} \right)} \\
&= \delta(\beta - \alpha),
\end{aligned}$$

and so we see that the S-matrix is indeed unitary.

3. *The scattering of π^+ on protons at energies less than a few hundred MeV is purely elastic, and receives appreciable contributions only from orbital angular momenta $\ell = 0$ and $\ell = 1$.*

(a) *List all the phase shifts that enter in the amplitude for π^+ -proton scattering at these low energies. (Recall that the spins of the pion and proton are zero and 1/2, respectively.)*

(b) *Give a formula for the differential scattering cross-section in terms of these phase shifts.*

- (a) As discussed in Chapter 4, when adding two angular momenta ℓ and s , the values taken by the resulting angular momentum J ranges from $|\ell - s|$ to $\ell + s$ in integer steps. For $\ell = 0$ and $s = 1/2$, the only possibility is that $J = 1/2$. For $\ell = 1$ and $s = 1/2$, we may have $J = 1/2$ or $J = 3/2$. If we adopt the notation $\delta_{J\ell s}$ for the phase shifts, then the phase shifts that contribute to the amplitude for low energy π^+ -proton scattering are

$$\delta_{\frac{1}{2}0\frac{1}{2}}, \delta_{\frac{1}{2}1\frac{1}{2}}, \text{ and } \delta_{\frac{3}{2}1\frac{1}{2}}.$$

- (b) Using Eq. (8.2.14), we can write a formula for the differential cross-section as

$$d\sigma(\alpha \rightarrow \beta) = (2\pi\hbar)^2 \left(\frac{p_\beta}{p_\alpha} \right) \mu_\alpha \mu_\beta |M_{\beta\alpha}|^2 d\Omega_\beta,$$

where $\mu = E_1 E_2 / c^2 (E_1 + E_2)$. If we work in the center of momentum frame in a coordinate system in which the initial state π^+ momentum is in the three-direction, we have an a matrix element like that given in Eq. (8.4.12)

$$\begin{aligned} M_{\mathbf{p}'_\pi, 0, -\mathbf{p}'_\pi, \sigma'_p; \mathbf{p}_\pi, 0, -\mathbf{p}_\pi, \sigma_p} &= \frac{1}{\sqrt{\mu' |\mathbf{p}'_\pi|}} \frac{1}{\sqrt{\mu |\mathbf{p}_\pi|}} \\ &\times \sum_{JM} \sum_{\ell' m' s' \sigma'} Y_{\ell'}^{m'}(\hat{\mathbf{p}}'_\pi) C_{0\frac{1}{2}}(s' \sigma'; 0 \sigma'_p) C_{s' \ell'}(JM; \sigma' m') \\ &\times \sum_{\ell s \sigma} \sqrt{\frac{2\ell + 1}{4\pi}} C_{0\frac{1}{2}}(s \sigma; 0 \sigma_p) C_{s \ell}(JM; \sigma 0) [S^J(E) - 1]_{\ell' s'; \ell s}, \end{aligned}$$

where

$$[S^J(E)]_{\ell' s'; \ell s} = \exp(2i\delta_{J\ell s}(E)) \delta_{\ell' \ell} \delta_{s' s}.$$

The relevant Clebsch–Gordan coefficients take the form

$$\begin{aligned} C_{0\frac{1}{2}}(s' \sigma'; 0 \sigma'_p) &= \delta_{\frac{1}{2} s'} \delta_{\sigma' \sigma'_p} \\ C_{0\frac{1}{2}}(s \sigma; 0 \sigma_p) &= \delta_{\frac{1}{2} s} \delta_{\sigma \sigma_p}, \end{aligned}$$

and so the matrix element simplifies to

$$\begin{aligned} M_{\mathbf{p}'_\pi, 0, -\mathbf{p}'_\pi, \sigma'_p; \mathbf{p}_\pi, 0, -\mathbf{p}_\pi, \sigma_p} &= \frac{1}{\sqrt{\mu' |\mathbf{p}'_\pi|}} \frac{1}{\sqrt{\mu |\mathbf{p}_\pi|}} \\ &\times \sum_{JM} \sum_{\ell' m'} Y_{\ell'}^{m'}(\hat{\mathbf{p}}'_\pi) C_{\frac{1}{2} \ell'}(JM; \sigma'_p m') \\ &\times \sqrt{\frac{2\ell + 1}{4\pi}} C_{\frac{1}{2} \ell}(JM; \sigma_p 0) \left[\exp(2i\delta_{J\ell \frac{1}{2}}(E)) - 1 \right]. \end{aligned}$$

When the initial and final proton spin 3-components are both $+1/2$ this becomes

$$\begin{aligned}
M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},+\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},+\frac{1}{2}} &= \frac{1}{\sqrt{\mu'|\mathbf{p}'_{\pi}|}} \frac{1}{\sqrt{\mu|\mathbf{p}_{\pi}|}} \\
&\times \left[Y_0^0(\hat{\mathbf{p}}'_{\pi}) C_{\frac{1}{2}0}\left(\frac{1}{2} + \frac{1}{2}; +\frac{1}{2}0\right) \sqrt{\frac{1}{4\pi}} C_{\frac{1}{2}0}\left(\frac{1}{2} + \frac{1}{2}; +\frac{1}{2}0\right) \left[\exp(2i\delta_{\frac{1}{2}0\frac{1}{2}}(E)) - 1 \right] \right. \\
&+ Y_0^1(\hat{\mathbf{p}}'_{\pi}) C_{\frac{1}{2}1}\left(\frac{1}{2} + \frac{1}{2}; +\frac{1}{2}0\right) \sqrt{\frac{3}{4\pi}} C_{\frac{1}{2}1}\left(\frac{1}{2} + \frac{1}{2}; +\frac{1}{2}0\right) \left[\exp(2i\delta_{\frac{1}{2}1\frac{1}{2}}(E)) - 1 \right] \\
&\left. + Y_0^1(\hat{\mathbf{p}}'_{\pi}) C_{\frac{1}{2}1}\left(\frac{3}{2} + \frac{1}{2}; +\frac{1}{2}0\right) \sqrt{\frac{3}{4\pi}} C_{\frac{1}{2}1}\left(\frac{3}{2} + \frac{1}{2}; +\frac{1}{2}0\right) \left[\exp(2i\delta_{\frac{3}{2}1\frac{1}{2}}(E)) - 1 \right] \right].
\end{aligned}$$

Plugging in the relevant Clebsch–Gordan coefficients and spherical harmonics, this gives

$$\begin{aligned}
M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},+\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},+\frac{1}{2}} &= \frac{1}{\sqrt{\mu'|\mathbf{p}'_{\pi}|}} \frac{1}{\sqrt{\mu|\mathbf{p}_{\pi}|}} \\
&\times \left[\frac{1}{4\pi} \left[\exp(2i\delta_{\frac{1}{2}0\frac{1}{2}}(E)) - 1 \right] + \frac{1}{4\pi} \cos\theta' \left[\exp(2i\delta_{\frac{1}{2}1\frac{1}{2}}(E)) - 1 \right] \right. \\
&\left. + \frac{1}{2\pi} \cos\theta' \left[\exp(2i\delta_{\frac{3}{2}1\frac{1}{2}}(E)) - 1 \right] \right],
\end{aligned}$$

which is the same expression for the case when the initial and final proton spin are both $-1/2$

$$M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},-\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},-\frac{1}{2}} = M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},+\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},+\frac{1}{2}}.$$

For the case when the initial and final proton spins are $-1/2$ and $+1/2$, respectively, we find

$$\begin{aligned}
M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},+\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},-\frac{1}{2}} &= \frac{1}{\sqrt{\mu'|\mathbf{p}'_{\pi}|}} \frac{1}{\sqrt{\mu|\mathbf{p}_{\pi}|}} \\
&\times \left[Y_1^{-1}(\hat{\mathbf{p}}'_{\pi}) C_{\frac{1}{2}1}\left(\frac{1}{2} - \frac{1}{2}; +\frac{1}{2} - 1\right) \sqrt{\frac{e}{4\pi}} C_{\frac{1}{2}1}\left(\frac{1}{2} - \frac{1}{2}; -\frac{1}{2}0\right) \left[\exp(2i\delta_{\frac{1}{2}1\frac{1}{2}}(E)) - 1 \right] \right. \\
&\left. + Y_1^{-1}(\hat{\mathbf{p}}'_{\pi}) C_{\frac{1}{2}1}\left(\frac{3}{2} - \frac{1}{2}; +\frac{1}{2} - 1\right) \sqrt{\frac{3}{4\pi}} C_{\frac{1}{2}1}\left(\frac{3}{2} - \frac{1}{2}; -\frac{1}{2}0\right) \left[\exp(2i\delta_{\frac{3}{2}1\frac{1}{2}}(E)) - 1 \right] \right],
\end{aligned}$$

and plugging in the relevant Clebsch–Gordan coefficients and spherical harmonics gives

$$\begin{aligned}
M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},+\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},-\frac{1}{2}} &= \frac{1}{\sqrt{\mu'|\mathbf{p}'_{\pi}|}} \frac{1}{\sqrt{\mu|\mathbf{p}_{\pi}|}} \left[\frac{-1}{4\pi} \sin\theta' e^{-i\phi'} \right. \\
&\left. \times \left[\exp(2i\delta_{\frac{1}{2}1\frac{1}{2}}(E)) - 1 \right] + \frac{1}{4\pi} \sin\theta' e^{-i\phi'} \left[\exp(2i\delta_{\frac{3}{2}1\frac{1}{2}}(E)) - 1 \right] \right].
\end{aligned}$$

The matrix element is identical up to a minus sign for the case when the initial and final proton spins are $+1/2$ and $-1/2$, respectively

$$M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},+\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},-\frac{1}{2}} = -M_{\mathbf{p}'_{\pi},0,-\mathbf{p}'_{\pi},-\frac{1}{2};\mathbf{p}_{\pi},0,-\mathbf{p}_{\pi},+\frac{1}{2}}.$$

Finally, we can use these matrix elements to find the differential cross-sections by using Eq. (8.2.14)

$$\begin{aligned} d\sigma \left(\sigma_p = +\frac{1}{2} \rightarrow \sigma'_p = +\frac{1}{2} \right) &= \frac{\hbar^2}{|\mathbf{p}_{\pi}|^2} \left| \frac{1}{2} \left[\exp(2i\delta_{\frac{1}{2}0\frac{1}{2}}(E)) - 1 \right] \right. \\ &\quad \left. + \frac{1}{2} \cos \theta' \left[\exp(2i\delta_{\frac{1}{2}1\frac{1}{2}}(E)) - 1 \right] + \cos \theta' \left[\exp(2i\delta_{\frac{3}{2}1\frac{1}{2}}(E)) - 1 \right] \right|^2 d\Omega' \\ &= d\sigma \left(\sigma_p = -\frac{1}{2} \rightarrow \sigma'_p = -\frac{1}{2} \right), \end{aligned}$$

and

$$\begin{aligned} d\sigma \left(\sigma_p = -\frac{1}{2} \rightarrow \sigma'_p = +\frac{1}{2} \right) &= \frac{\hbar^2}{|\mathbf{p}_{\pi}|^2} \left| -\frac{1}{2} \sin \theta' \left[\exp(2i\delta_{\frac{1}{2}1\frac{1}{2}}(E)) - 1 \right] \right. \\ &\quad \left. + \frac{1}{2} \sin \theta' \left[\exp(2i\delta_{\frac{3}{2}1\frac{1}{2}}(E)) - 1 \right] \right|^2 d\Omega' \\ &= d\sigma \left(\sigma_p = +\frac{1}{2} \rightarrow \sigma'_p = -\frac{1}{2} \right). \end{aligned}$$

4. Let $T_{\beta\alpha}^{(1)}$ be the term in $T_{\beta\alpha}$ including contributions of all orders in V_s but only of first order in V_w , where the total interaction is $V_s + V_w$. Show that the complex conjugate of $T_{\beta\alpha}^{(1)}$ satisfies a relation of the form

$$T_{\beta\alpha}^{(1)*} = \int d\beta' d\alpha' c_{\beta\alpha\beta'\alpha'} T_{\beta'\alpha'}^{(1)}.$$

Give a formula for the coefficients $c_{\beta\alpha\beta'\alpha'}$ in terms of S -matrix elements, including contributions of all orders in V_s but zeroth order in V_w .

We begin by writing the Lippmann–Schwinger equation for the in and out states in the absence of V_w as in Eq. (8.6.16)

$$\Psi_{s\alpha}^{\pm} = \Phi_{\alpha} + (E_{\alpha} - H_0 \pm i\epsilon)^{-1} V_s \Psi_{s\alpha}^{\pm},$$

where Φ_{α} is an eigenstate of H_0 with eigenvalue E_{α} . We can then write the T -matrix as in Eq. (8.6.17)

$$T_{\beta\alpha} = (\Psi_{s\beta}^{-}, V_w \Psi_{\alpha}^{+}) + (\Psi_{s\beta}^{-}, V_s \Phi_{\alpha}),$$

and we will assume that the process $\alpha \rightarrow \beta$ cannot occur in the absence of V_w , so that the second term vanishes. In this case we can write

$$T_{\beta\alpha} = (\Psi_{s\beta}^{-}, V_w \Psi_{\alpha}^{+}),$$

and to first order in V_w , we can neglect the difference between Ψ_α^+ and $\Psi_{s\alpha}^+$ and so the T-matrix at first order in V_w is given by

$$T_{\beta\alpha}^{(1)} = (\Psi_{s\beta}^-, V_w \Psi_{s\alpha}^+).$$

We can write the complex conjugate as

$$T_{\beta\alpha}^{(1)*} = (V_w \Psi_{s\beta}^+, \Psi_{s\alpha}^-) = (\Psi_{s\beta}^+, V_w \Psi_{s\alpha}^-),$$

where we have used the fact that V_w is Hermitian. Now, because $\Psi_{s\alpha}^+$ and $\Psi_{s\alpha}^-$ each form a complete set of states, we may expand each in terms of the other

$$\begin{aligned} \Psi_{s\alpha}^+ &= \int d\beta' \Psi_{s\beta'}^- (\Psi_{s\beta'}^-, \Psi_{s\alpha}^+) = \int d\beta' \Psi_{s\beta'}^- S_{\beta'\alpha}^{(0)} \\ \Psi_{s\beta}^- &= \int d\alpha' \Psi_{s\alpha'}^+ (\Psi_{s\alpha'}^+, \Psi_{s\beta}^-) = \int d\alpha' \Psi_{s\alpha'}^+ S_{\beta\alpha'}^{(0)*}, \end{aligned}$$

where $S_{\alpha\beta}^{(0)}$ is the S-matrix evaluated to all orders in V_s , but to zeroth order in V_w . Using these expressions in our formula above we find

$$\begin{aligned} T_{\beta\alpha}^{(1)*} &= \int d\beta' d\alpha' (\Psi_{s\beta'}^- S_{\beta'\alpha}^{(0)}, V_w S_{\beta\alpha'}^{(0)*} \Psi_{s\alpha'}^+) \\ &= \int d\beta' d\alpha' S_{\beta'\alpha}^{(0)*} S_{\beta\alpha'}^{(0)*} (\Psi_{s\beta'}^-, V_w \Psi_{s\alpha'}^+) \\ &= \int d\beta' d\alpha' S_{\beta'\alpha}^{(0)*} S_{\beta\alpha'}^{(0)*} T_{\beta'\alpha'}^{(1)*} \\ &= \int d\beta' d\alpha' c_{\beta\alpha\beta'\alpha'} T_{\beta'\alpha'}^{(1)*}, \end{aligned}$$

where $c_{\beta\alpha\beta'\alpha'} = S_{\beta'\alpha}^{(0)*} S_{\beta\alpha'}^{(0)*}$.

5. By direct calculation, show that the terms of first and second order in the interaction in time-dependent perturbation theory give the same results for the S-matrix as the first- and second-order terms in old-fashioned perturbation theory.

In old-fashioned perturbation theory, the S-matrix is given up to second order in V by plugging Eq. (8.6.1) into Eq. (8.1.10)

$$\begin{aligned} S_{\beta\alpha} &= \delta(\beta - \alpha) - 2\pi i \delta(E_\alpha - E_\beta) T_{\beta\alpha} \\ &= \delta(\beta - \alpha) - 2\pi i \delta(E_\alpha - E_\beta) (\Phi_\beta, V \Psi_\alpha^+) \\ &= \delta(\beta - \alpha) - 2\pi i \delta(E_\alpha - E_\beta) \\ &\quad \times [(\Phi_\beta, V \Phi_\alpha^+) + (\Phi_\beta, V(E_\alpha - H_0 + i\epsilon)^{-1} V \Phi_\alpha) + \dots], \end{aligned}$$

where the dots represent terms of higher order in V . In time-dependent perturbation theory, the S-matrix is given by Eq. (8.7.4), which we can write up to second order as

$$S_{\beta\alpha} = \left(\Phi_\beta, \left[1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} d\tau V_I(\tau) + \left(\frac{-i}{\hbar} \right)^2 \int_{-\infty}^{+\infty} d\tau_1 \right. \right. \\ \left. \left. \times \int_{-\infty}^{\tau_1} d\tau_2 V_I(\tau_1) V_I(\tau_2) + \cdots \right] \Phi_\alpha \right),$$

where $V_I(\tau)$ is defined in Eq. (8.7.8)

$$V_I(t) \equiv e^{iH_0 t/\hbar} V e^{-iH_0 t/\hbar}.$$

The term of zeroth order in V is simply given by

$$(\Phi_\beta, \Phi_\alpha) = \delta(\beta - \alpha).$$

The term of first order in V is

$$\begin{aligned} \left(\Phi_\beta, -\frac{i}{\hbar} \int_{-\infty}^{+\infty} d\tau V_I(\tau) \Phi_\alpha \right) &= -\frac{i}{\hbar} \int_{-\infty}^{+\infty} d\tau \left(\Phi_\beta, e^{iH_0\tau/\hbar} V e^{-iH_0\tau/\hbar} \Phi_\alpha \right) \\ &= -\frac{i}{\hbar} \int_{-\infty}^{+\infty} d\tau e^{iE_\beta\tau/\hbar} e^{-iE_\alpha\tau/\hbar} (\Phi_\beta, V \Phi_\alpha) \\ &= -2\pi i \delta(E_\beta - E_\alpha) (\Phi_\beta, V \Phi_\alpha), \end{aligned}$$

where in the second line we have used the fact that Φ_α is an eigenstate of H_0 with eigenvalue E_α . The term which is second order in V is given by

$$\begin{aligned} &\left(\Phi_\beta, \left(\frac{-i}{\hbar} \right)^2 \int_{-\infty}^{+\infty} d\tau_1 \int_{-\infty}^{\tau_1} d\tau_2 V_I(\tau_1) V_I(\tau_2) \Phi_\alpha \right) \\ &= -\frac{1}{\hbar^2} \int_{-\infty}^{+\infty} d\tau_1 \int_{-\infty}^{\tau_1} d\tau_2 \left(\Phi_\beta, e^{iH_0\tau_1/\hbar} V e^{-iH_0\tau_1/\hbar} e^{iH_0\tau_2/\hbar} V e^{-iH_0\tau_2/\hbar} \Phi_\alpha \right) \\ &= -\frac{1}{\hbar^2} \int_{-\infty}^{+\infty} d\tau_1 \int_{-\infty}^{\tau_1} d\tau_2 e^{iE_\beta\tau_1/\hbar} e^{-iE_\alpha\tau_2/\hbar} \left(\Phi_\beta, V e^{-iH_0\tau_1/\hbar} e^{iH_0\tau_2/\hbar} V \Phi_\alpha \right) \\ &= -\frac{1}{\hbar^2} \int_{-\infty}^{+\infty} d\tau_1 e^{iE_\beta\tau_1/\hbar} \left(\Phi_\beta, V e^{-iH_0\tau_1/\hbar} \int_{-\infty}^{\tau_1} d\tau_2 e^{-i(E_\alpha - H_0)\tau_2/\hbar} V \Phi_\alpha \right). \end{aligned}$$

Now, we can do the integral over τ_2 by noticing that

$$\begin{aligned} \int_{-\infty}^{\tau_1} d\tau_2 e^{-i(E_\alpha - H_0)\tau_2/\hbar} &= \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{\tau_1} d\tau_2 e^{-i(E_\alpha - H_0 + i\epsilon)\tau_2/\hbar} \\ &= \frac{\hbar}{-i} (E_\alpha - H_0 + i\epsilon)^{-1} e^{-i(E_\alpha - H_0)\tau_1/\hbar}, \end{aligned}$$

where ϵ is taken to be a positive infinitesimal in the second line. Using this result in the expression above, we find

$$\begin{aligned}
 & \left(\Phi_\beta, \left(\frac{-i}{\hbar} \right)^2 \int_{-\infty}^{+\infty} d\tau_1 \int_{-\infty}^{\tau_1} d\tau_2 V_I(\tau_1) V_I(\tau_2) \Phi_\alpha \right) \\
 &= -\frac{1}{\hbar^2} \int_{-\infty}^{+\infty} d\tau_1 e^{iE_\beta \tau_1 / \hbar} \\
 & \quad \times \left(\Phi_\beta, V e^{-iH_0 \tau_1 / \hbar} \frac{\hbar}{-i} (E_\alpha - H_0 + i\epsilon)^{-1} e^{-i(E_\alpha - H_0) \tau_1 / \hbar} V \Phi_\alpha \right) \\
 &= -\frac{i}{\hbar} \int_{-\infty}^{+\infty} d\tau_1 e^{i(E_\beta - E_\alpha) \tau_1 / \hbar} (\Phi_\beta, (E_\alpha - H_0 + i\epsilon)^{-1} V \Phi_\alpha) \\
 &= -2\pi i \delta(E_\beta - E_\alpha) (\Phi_\beta, V (E_\alpha - H_0 + i\epsilon)^{-1} \Phi_\alpha).
 \end{aligned}$$

Putting these results together, we find for S-matrix calculated to second order in V in time-dependent perturbation theory

$$\begin{aligned}
 S_{\beta\alpha} = & \delta(\beta - \alpha) - 2\pi i \delta(E_\beta - E_\alpha) (\Phi_\beta, V \Phi_\alpha) \\
 & - 2\pi i \delta(E_\beta - E_\alpha) (\Phi_\beta, V (E_\alpha - H_0 + i\epsilon)^{-1} V \Phi_\alpha) + \dots,
 \end{aligned}$$

which matches the result we found for old-fashioned perturbation theory.

6. Assume isospin conservation, and suppose that the only appreciable phase shift in the scattering of pions on nucleons is the one with quantum numbers $J = 3/2$, $\ell = 1$, and $T = 3/2$. Calculate the differential cross-sections for the reactions $\pi^+ + p \rightarrow \pi^+ + p$, $\pi^+ + n \rightarrow \pi^+ + n$, $\pi^+ + n \rightarrow \pi^0 + p$, and $\pi^- + n \rightarrow \pi^- + n$ in terms of this phase shift.

The differential cross-section of each process will be very similar to that worked out in Problem 3 above, but we will need to work with phase shifts for states with definite J , ℓ , s , and T , which we will denote $\delta_{J\ell s T}$. For pion–nucleon scattering, assuming the conservation of isospin, Eq. (8.4.12) is modified to

$$\begin{aligned}
 M_{\mathbf{p}'_\pi, 0, T'_{3\pi}, -\mathbf{p}'_\pi, \sigma'_N, T'_{3N}; \mathbf{p}_\pi, 0, T_{3\pi}, -\mathbf{p}_\pi, \sigma_N, T_{3N}} &= \frac{1}{\sqrt{\mu' |\mathbf{p}'_\pi|}} \frac{1}{\sqrt{\mu |\mathbf{p}_\pi|}} \\
 & \times \sum_{JM} \sum_{\ell' m' s' \sigma'} Y_{\ell' m'}^{m'}(\hat{\mathbf{p}}'_\pi) C_{0\frac{1}{2}}(s' \sigma'; 0 \sigma'_p) C_{s' \ell'}(JM; \sigma' m') \\
 & \times \sum_{\ell s \sigma} \sqrt{\frac{2\ell + 1}{4\pi}} C_{0\frac{1}{2}}(s \sigma; 0 \sigma_p) C_{s \ell}(JM; \sigma 0) \\
 & \times \sum_T C_{1\frac{1}{2}}(T T_3; T'_{3\pi} T'_{3N}) C_{1\frac{1}{2}}(T T_3; T_{3\pi} T_{3N}) [S^{JT}(E) - 1]_{\ell' s'; \ell s},
 \end{aligned}$$

where

$$[S^{JT}(E)]_{\ell' s'; \ell s} = \exp(2i\delta_{J\ell s T}(E)) \delta_{\ell' \ell} \delta_{s' s}.$$

In the case when only $\delta_{\frac{3}{2} 1 \frac{1}{2} \frac{3}{2}}$ is appreciable, this becomes

$$\begin{aligned} M_{\mathbf{p}'_{\pi}, 0, T'_{3\pi}, -\mathbf{p}'_{\pi}, +\frac{1}{2}, T'_{3N}; \mathbf{p}_{\pi}, 0, T_{3\pi}, -\mathbf{p}_{\pi}, +\frac{1}{2}, T_{3N}} &= \frac{1}{\sqrt{|\mu'| |\mathbf{p}'_{\pi}|}} \frac{1}{\sqrt{|\mu| |\mathbf{p}_{\pi}|}} \\ &\times \left[\frac{1}{2\pi} \cos \theta' \left[\exp(2i \delta_{\frac{3}{2} 1 \frac{1}{2} \frac{3}{2}}(E)) - 1 \right] \right] C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T'_{3\pi} T'_{3N} \right) \\ &\times C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T_{3\pi} T_{3N} \right) \\ &= M_{\mathbf{p}'_{\pi}, 0, T'_{3\pi}, -\mathbf{p}'_{\pi}, -\frac{1}{2}, T'_{3N}; \mathbf{p}_{\pi}, 0, T_{3\pi}, -\mathbf{p}_{\pi}, -\frac{1}{2}, T_{3N}} \end{aligned}$$

when the initial and final nucleon spin 3-components are equal and

$$\begin{aligned} M_{\mathbf{p}'_{\pi}, 0, T'_{3\pi}, -\mathbf{p}'_{\pi}, +\frac{1}{2}, T'_{3N}; \mathbf{p}_{\pi}, 0, T_{3\pi}, -\mathbf{p}_{\pi}, -\frac{1}{2}, T_{3N}} &= \frac{1}{\sqrt{|\mu'| |\mathbf{p}'_{\pi}|}} \frac{1}{\sqrt{|\mu| |\mathbf{p}_{\pi}|}} \\ &\times \left[\frac{1}{4\pi} \sin \theta' e^{-i\phi'} \left[\exp(2i \delta_{\frac{3}{2} 1 \frac{1}{2} \frac{3}{2}}(E)) - 1 \right] \right] C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T'_{3\pi} T'_{3N} \right) \\ &\times C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T_{3\pi} T_{3N} \right) \\ &= M_{\mathbf{p}'_{\pi}, 0, T'_{3\pi}, -\mathbf{p}'_{\pi}, -\frac{1}{2}, T'_{3N}; \mathbf{p}_{\pi}, 0, T_{3\pi}, -\mathbf{p}_{\pi}, +\frac{1}{2}, T_{3N}} \end{aligned}$$

when the initial and final nucleon spin 3-components are opposite. We can then write the differential cross-sections in this case by using Eq. (8.2.14) which gives

$$\begin{aligned} d\sigma (\pi N \rightarrow \pi' N'; \sigma_N = \sigma'_N) &= \frac{\hbar^2}{|\mathbf{p}_{\pi}|^2} \left| \cos \theta' \left[\exp(2i \delta_{\frac{3}{2} 1 \frac{1}{2} \frac{3}{2}}(E)) - 1 \right] \right|^2 \\ &\times \left[C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T'_{3\pi} T'_{3N} \right) C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T_{3\pi} T_{3N} \right) \right]^2 d\Omega', \end{aligned}$$

when the initial and final nucleon spins are equal, and

$$\begin{aligned} d\sigma (\pi N \rightarrow \pi' N'; \sigma_N = -\sigma'_N) &= \frac{\hbar^2}{4|\mathbf{p}_{\pi}|^2} \left| \sin \theta' \left[\exp(2i \delta_{\frac{3}{2} 1 \frac{1}{2} \frac{3}{2}}(E)) - 1 \right] \right|^2 \\ &\times \left[C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T'_{3\pi} T'_{3N} \right) C_{1 \frac{1}{2}} \left(\frac{3}{2} T_3; T_{3\pi} T_{3N} \right) \right]^2 d\Omega', \end{aligned}$$

when the initial and final nucleon spins are opposite. The isospin quantum numbers for each of the relevant particles are given by the following table.

	T	T_3
π^+	1	1
π^0	1	0
π^-	1	-1
p	1/2	1/2
n	1/2	-1/2

The differential cross-section for the process $\pi^+ + p \rightarrow \pi^+ + p$ is then given by

$$d\sigma (\pi^+ + p \rightarrow \pi^+ + p; \sigma_p = \sigma'_p) = \frac{\hbar^2 \cos^2 \theta'}{|\mathbf{p}_\pi|^2} \sin^2 \delta_{\frac{3}{2} 1 \frac{1}{2} \frac{3}{2}}(E) d\Omega' \\ \equiv d\sigma (\sigma_N = \sigma'_N),$$

when the initial and final proton spins are equal, and

$$d\sigma (\pi^+ + p \rightarrow \pi^+ + p; \sigma_p = -\sigma'_p) = \frac{\hbar^2 \sin^2 \theta'}{4|\mathbf{p}_\pi|^2} \sin^2 \delta_{\frac{3}{2} 1 \frac{1}{2} \frac{3}{2}}(E) d\Omega' \\ \equiv d\sigma (\sigma_N = -\sigma'_N),$$

when the initial and final proton spins are opposite. The differential cross-sections for each of the pion–nucleon processes are then just multiples of these expressions, given by the appropriate Clebsch–Gordan coefficients associated with isospin

$$d\sigma (\pi^+ + n \rightarrow \pi^+ + n; \sigma_n = \sigma'_n) = \frac{1}{9} d\sigma (\sigma_N = \sigma'_N), \\ d\sigma (\pi^+ + n \rightarrow \pi^0 + p; \sigma_n = \sigma'_p) = \frac{2}{9} d\sigma (\sigma_N = \sigma'_N), \\ d\sigma (\pi^- + n \rightarrow \pi^- + n; \sigma_n = \sigma'_n) = d\sigma (\sigma_N = \sigma'_N),$$

and similarly for the processes where the initial and final nucleon spin are opposite

$$d\sigma (\pi^+ + n \rightarrow \pi^+ + n; \sigma_n = -\sigma'_n) = \frac{1}{9} d\sigma (\sigma_N = -\sigma'_N), \\ d\sigma (\pi^+ + n \rightarrow \pi^0 + p; \sigma_n = -\sigma'_p) = \frac{2}{9} d\sigma (\sigma_N = -\sigma'_N), \\ d\sigma (\pi^- + n \rightarrow \pi^- + n; \sigma_n = -\sigma'_n) = d\sigma (\sigma_N = -\sigma'_N).$$

Chapter 9 Problem Set Solutions

1. Consider the theory of a single particle with Lagrangian

$$L = \frac{m}{2} \dot{\mathbf{x}}^2 + \dot{\mathbf{x}} \cdot \mathbf{f}(\mathbf{x}) - V(\mathbf{x}),$$

where $\mathbf{f}(\mathbf{x})$ and $V(\mathbf{x})$ are arbitrary vector and scalar functions of position.

- Find the equation of motion satisfied by \mathbf{x} .
- Find the Hamiltonian, as a function of \mathbf{x} and its canonical conjugate \mathbf{p} .
- What is the Schrödinger equation satisfied by the coordinate-space wave function $\psi(\mathbf{x}, t)$?

The equations of motion may be derived from Eq. (9.1.3), which in this case reads

$$\frac{\partial L(\mathbf{x}(t), \dot{\mathbf{x}}(t))}{\partial x_i} = \frac{d}{dt} \frac{\partial L(\mathbf{x}(t), \dot{\mathbf{x}}(t))}{\partial \dot{x}_i}.$$

Taking the appropriate derivatives of L , the equations of motion are

$$\dot{\mathbf{x}} \times (\nabla \times \mathbf{f}(\mathbf{x})) + (\dot{\mathbf{x}} \cdot \nabla) \mathbf{f}(\mathbf{x}) - \nabla V(\mathbf{x}) = m\ddot{\mathbf{x}} + (\dot{\mathbf{x}} \cdot \nabla) \mathbf{f}(\mathbf{x}),$$

which can be simplified to read

$$\dot{\mathbf{x}} \times (\nabla \times \mathbf{f}(\mathbf{x})) - \nabla V(\mathbf{x}) = m\ddot{\mathbf{x}}.$$

Notice that this is very similar to the equation of motion of a charged particle in an external magnetic field, given by Eq. (10.1.1) with vanishing electric field.

The canonical conjugate of \mathbf{x} is defined in Eq. (9.3.3) as

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i + f_i(x),$$

and the Hamiltonian is given in Eq. (9.3.4) as

$$H = \dot{\mathbf{x}}(\mathbf{x}, \mathbf{p}) \cdot \mathbf{p} - L(\mathbf{x}, \dot{\mathbf{x}}(\mathbf{x}, \mathbf{p})),$$

which in this case gives

$$\begin{aligned} H &= \frac{1}{m} (\mathbf{p} - \mathbf{f}(\mathbf{x})) \cdot \mathbf{p} - \frac{1}{2m} (\mathbf{p} - \mathbf{f}(\mathbf{x}))^2 - \frac{1}{m} (\mathbf{p} - \mathbf{f}(\mathbf{x})) \cdot \mathbf{f}(\mathbf{x}) + V(\mathbf{x}) \\ &= \frac{1}{2m} (\mathbf{p} - \mathbf{f}(\mathbf{x}))^2 + V(\mathbf{x}). \end{aligned}$$

Notice that this is very similar to the Hamiltonian for a charged particle in an external magnetic field, given by Eq. (10.1.9) with vanishing scalar potential.

The Schrödinger equation satisfied by the coordinate-space wave function $\psi(\mathbf{x}, t)$ is given by

$$H\psi(\mathbf{x}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t),$$

where the operator \mathbf{p} acts on the coordinate-space wave function as $-i\hbar\nabla$. The Schrödinger equation therefore takes the form

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = & -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t) + \frac{i\hbar}{m} \mathbf{f}(\mathbf{x}) \cdot \nabla \psi(\mathbf{x}, t) \\ & + \frac{i\hbar}{2m} (\nabla \cdot \mathbf{f}(\mathbf{x})) \psi(\mathbf{x}, t) + \frac{\mathbf{f}^2(\mathbf{x})}{2m} \psi(\mathbf{x}, t) + V(\mathbf{x}) \psi(\mathbf{x}, t). \end{aligned}$$

2. Show that Poisson brackets and Dirac brackets both satisfy the Jacobi identity.

The Poisson bracket is defined in Eq. (9.4.19)

$$[f(q, p), g(q, p)]_P \equiv \sum_N \left[\frac{\partial f(p, q)}{\partial q_N} \frac{\partial g(p, q)}{\partial p_N} - \frac{\partial g(p, q)}{\partial q_N} \frac{\partial f(p, q)}{\partial p_N} \right],$$

which we will write in a slightly more compact notation as

$$[f, g]_P = \sum_N [\partial_{q_N} f \partial_{p_N} g - \partial_{q_N} g \partial_{p_N} f].$$

We wish to show by direct calculation that the Poisson bracket satisfies the Jacobi identity, which is given in Eq. (9.4.22)

$$[f, [g, h]_P]_P + [g, [h, f]_P]_P + [h, [f, g]_P]_P = 0.$$

Let us first work out just one of the terms appearing in the Jacobi identity

$$\begin{aligned} [f, [g, h]_P]_P &= \left[f, \sum_N (\partial_{q_N} g \partial_{p_N} h - \partial_{q_N} h \partial_{p_N} g) \right]_P \\ &= \sum_{MN} \left(\partial_{q_M} f \partial_{p_M} (\partial_{q_N} g \partial_{p_N} h - \partial_{q_N} h \partial_{p_N} g) \right. \\ &\quad \left. - \partial_{q_M} (\partial_{q_N} g \partial_{p_N} h - \partial_{q_N} h \partial_{p_N} g) \partial_{p_M} f \right) \\ &= \sum_{MN} \left(\partial_{q_M} f \partial_{p_M} \partial_{q_N} g \partial_{p_N} h + \partial_{q_M} f \partial_{q_N} g \partial_{p_M} \partial_{p_N} h \right. \\ &\quad - \partial_{q_M} f \partial_{p_M} \partial_{q_N} h \partial_{p_N} g - \partial_{q_M} f \partial_{q_N} h \partial_{p_M} \partial_{p_N} g \\ &\quad - \partial_{q_M} \partial_{q_N} g \partial_{p_N} h \partial_{p_M} f - \partial_{q_N} g \partial_{q_M} \partial_{p_N} h \partial_{p_M} f \\ &\quad \left. - \partial_{q_M} \partial_{q_N} h \partial_{p_N} g \partial_{p_M} f - \partial_{q_N} h \partial_{q_M} \partial_{p_N} g \partial_{p_M} f \right). \end{aligned}$$

Now, putting this together to calculate the combination appearing in the Jacobi identity, we find

$$\begin{aligned}
& [f, [g, h]_P]_P + [g, [h, f]_P]_P + [h, [f, g]_P]_P \\
&= \sum_{MN} \left[\left(\partial_{q_M} f \partial_{p_M} \partial_{q_N} g \partial_{p_N} h + \partial_{q_M} f \partial_{q_N} g \partial_{p_M} \partial_{p_N} h \right. \right. \\
&\quad - \partial_{q_M} f \partial_{p_M} \partial_{q_N} h \partial_{p_N} g - \partial_{q_M} f \partial_{q_N} h \partial_{p_M} \partial_{p_N} g \\
&\quad - \partial_{q_M} \partial_{q_N} g \partial_{p_N} h \partial_{p_M} f - \partial_{q_N} g \partial_{q_M} \partial_{p_N} h \partial_{p_M} f \\
&\quad \left. \left. - \partial_{q_M} \partial_{q_N} h \partial_{p_N} g \partial_{p_M} f - \partial_{q_N} h \partial_{q_M} \partial_{p_N} g \partial_{p_M} f \right) \right. \\
&\quad + \left(\partial_{q_M} g \partial_{p_M} \partial_{q_N} h \partial_{p_N} f + \partial_{q_M} g \partial_{q_N} h \partial_{p_M} \partial_{p_N} f \right. \\
&\quad - \partial_{q_M} g \partial_{p_M} \partial_{q_N} f \partial_{p_N} h - \partial_{q_M} g \partial_{q_N} f \partial_{p_M} \partial_{p_N} h \\
&\quad - \partial_{q_M} \partial_{q_N} h \partial_{p_N} f \partial_{p_M} g - \partial_{q_N} h \partial_{q_M} \partial_{p_N} f \partial_{p_M} g \\
&\quad \left. \left. - \partial_{q_M} \partial_{q_N} f \partial_{p_N} h \partial_{p_M} g - \partial_{q_N} f \partial_{q_M} \partial_{p_N} h \partial_{p_M} g \right) \right. \\
&\quad \left. + \left(\partial_{q_M} h \partial_{p_M} \partial_{q_N} f \partial_{p_N} g + \partial_{q_M} h \partial_{q_N} f \partial_{p_M} \partial_{p_N} g \right. \right. \\
&\quad - \partial_{q_M} h \partial_{p_M} \partial_{q_N} g \partial_{p_N} f - \partial_{q_M} h \partial_{q_N} g \partial_{p_M} \partial_{p_N} f \\
&\quad - \partial_{q_M} \partial_{q_N} f \partial_{p_N} g \partial_{p_M} h - \partial_{q_N} f \partial_{q_M} \partial_{p_N} g \partial_{p_M} h \\
&\quad \left. \left. - \partial_{q_M} \partial_{q_N} g \partial_{p_N} f \partial_{p_M} h - \partial_{q_N} g \partial_{q_M} \partial_{p_N} f \partial_{p_M} h \right) \right].
\end{aligned}$$

Now, due to the fact that partial derivatives commute and also that we can relabel the summation variables, we can begin canceling terms. The pairs of terms which cancel are the 1st and 22nd, 2nd and 12th, 3rd and 16th, 4th and 18th, 5th and 23rd, 6th and 9th, 7th and 13th, 8th and 19th, 10th and 20th, 11th and 24th, 14th and 17th, and finally the 15th and 21st. We see that all terms in the sum cancel, and we have

$$[f, [g, h]_P]_P + [g, [h, f]_P]_P + [h, [f, g]_P]_P = 0,$$

and so the Poisson bracket satisfies the Jacobi identity.

The Dirac bracket is defined in Eq. (9.5.16) as

$$[f, g]_D \equiv [f, g]_P - \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [\chi_s, g]_P,$$

where the matrix C_{rs} is defined in Eq. (9.5.12)

$$C_{rs} \equiv [\chi_r, \chi_s]_P.$$

We will now work out $[f, [g, h]_D]_D$ in terms of Poisson brackets

$$\begin{aligned}
[f, [g, h]_D]_D &= [f, [g, h]_P]_D - \left[f, \sum_{rs} [g, \chi_r]_P C_{rs}^{-1} [\chi_s, h]_P \right]_D \\
&= [f, [g, h]_P]_P - \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [\chi_s, [g, h]_P]_P - \left[f, \sum_{rs} [g, \chi_r]_P C_{rs}^{-1} [\chi_s, h]_P \right]_P \\
&\quad + \sum_{tu} [f, \chi_t]_P C_{tu}^{-1} \left[\chi_u, \sum_{rs} [g, \chi_r]_P C_{rs}^{-1} [\chi_s, h]_P \right]_P \\
&= [f, [g, h]_P]_P - \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [\chi_s, [g, h]_P]_P - \sum_{rs} [f, [g, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad - \sum_{rs} [g, \chi_r]_P \left[f, C_{rs}^{-1} \right]_P [\chi_s, h]_P - \sum_{rs} [g, \chi_r]_P C_{rs}^{-1} [f, [\chi_s, h]_P]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_u, [g, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P \left[\chi_u, C_{rs}^{-1} \right]_P [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, h]_P]_P.
\end{aligned}$$

Using the Jacobi identity for Poisson brackets, which we proved above, we can rewrite the 6th term in this last expression as

$$\begin{aligned}
&\sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_u, [g, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&= - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, [\chi_r, \chi_u]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, g]_P]_P C_{rs}^{-1} [\chi_s, h]_P.
\end{aligned}$$

Now we can use the definition of C_{ru} and the fact that $C_{ru} = -C_{ur}$ to simplify the 1st term

$$\begin{aligned}
- \sum_u C_{tu}^{-1} [g, C_{ru}]_P &= - \sum_u [g, C_{tu}^{-1} C_{ru}]_P + \sum_u [g, C_{tu}^{-1}]_P C_{ru} \\
&= - [g, (-\delta_{tr})]_P + \sum_u [g, C_{tu}^{-1}]_P C_{ru} \\
&= \sum_u [g, C_{tu}^{-1}]_P C_{ru}.
\end{aligned}$$

Using this in the expression above gives

$$\begin{aligned}
\sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_u, [g, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, h]_P &= - \sum_{rs} [f, \chi_r]_P \left[g, C_{rs}^{-1} \right]_P [\chi_s, h]_P \\
&\quad - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, g]_P]_P C_{rs}^{-1} [\chi_s, h]_P
\end{aligned}$$

$$\begin{aligned}
&= \sum_{rs} [h, \chi_r]_P [g, C_{rs}^{-1}]_P [\chi_s, f]_P \\
&\quad - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, g]_P]_P C_{rs}^{-1} [\chi_s, h]_P,
\end{aligned}$$

where in the last equality, we have used the antisymmetry of C_{rs}^{-1} and also the antisymmetry of the Poisson bracket to rearrange the first term on the right-hand side. Returning now to $[f, [g, h]_D]_D$, we have

$$\begin{aligned}
[f, [g, h]_D]_D &= [f, [g, h]_P]_P - \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [\chi_s, [g, h]_P]_P \\
&\quad - \sum_{rs} [f, [g, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad - \sum_{rs} [g, \chi_r]_P [f, C_{rs}^{-1}]_P [\chi_s, h]_P - \sum_{rs} [g, \chi_r]_P C_{rs}^{-1} [f, [\chi_s, h]_P]_P \\
&\quad + \sum_{rs} [h, \chi_r]_P [g, C_{rs}^{-1}]_P [\chi_s, f]_P \\
&\quad - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, g]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, h]_P]_P.
\end{aligned}$$

Now, the combination appearing in the Jacobi identity reads

$$\begin{aligned}
&[f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \tag{1} \\
&= [f, [g, h]_P]_P - \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [\chi_s, [g, h]_P]_P \\
&\quad - \sum_{rs} [f, [g, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad - \sum_{rs} [g, \chi_r]_P [f, C_{rs}^{-1}]_P [\chi_s, h]_P - \sum_{rs} [g, \chi_r]_P C_{rs}^{-1} [f, [\chi_s, h]_P]_P \\
&\quad + \sum_{rs} [h, \chi_r]_P [g, C_{rs}^{-1}]_P [\chi_s, f]_P \\
&\quad - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, g]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, h]_P]_P
\end{aligned}$$

$$\begin{aligned}
& + [g, [h, f]_P]_P - \sum_{rs} [g, \chi_r]_P C_{rs}^{-1} [\chi_s, [h, f]_P]_P \\
& - \sum_{rs} [g, [h, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, f]_P \\
& - \sum_{rs} [h, \chi_r]_P [g, C_{rs}^{-1}]_P [\chi_s, f]_P - \sum_{rs} [h, \chi_r]_P C_{rs}^{-1} [g, [\chi_s, f]_P]_P \\
& + \sum_{rs} [f, \chi_r]_P [h, C_{rs}^{-1}]_P [\chi_s, g]_P \\
& - \sum_{iu} \sum_{rs} [g, \chi_t]_P C_{iu}^{-1} [\chi_r, [\chi_u, h]_P]_P C_{rs}^{-1} [\chi_s, f]_P \\
& + \sum_{iu} \sum_{rs} [g, \chi_t]_P C_{iu}^{-1} [h, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, f]_P \\
& + \sum_{iu} \sum_{rs} [g, \chi_t]_P C_{iu}^{-1} [h, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, f]_P]_P \\
& + [h, [f, g]_P]_P - \sum_{rs} [h, \chi_r]_P C_{rs}^{-1} [\chi_s, [f, g]_P]_P \\
& - \sum_{rs} [h, [f, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, g]_P \\
& - \sum_{rs} [f, \chi_r]_P [h, C_{rs}^{-1}]_P [\chi_s, g]_P - \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [h, [\chi_s, g]_P]_P \\
& + \sum_{rs} [g, \chi_r]_P [f, C_{rs}^{-1}]_P [\chi_s, h]_P \\
& - \sum_{iu} \sum_{rs} [h, \chi_t]_P C_{iu}^{-1} [\chi_r, [\chi_u, f]_P]_P C_{rs}^{-1} [\chi_s, g]_P \\
& + \sum_{iu} \sum_{rs} [h, \chi_t]_P C_{iu}^{-1} [f, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, g]_P \\
& + \sum_{iu} \sum_{rs} [h, \chi_t]_P C_{iu}^{-1} [f, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, g]_P]_P.
\end{aligned}$$

We can see immediately that the 1st, 10th, and 19th terms sum to zero because the Poisson brackets obey the Jacobi identity. The 12th term in Eq. (1) can be rewritten as

$$\begin{aligned}
- \sum_{rs} [g, [h, \chi_r]_P]_P C_{rs}^{-1} [\chi_s, f]_P &= - \sum_{rs} [\chi_r, f]_P C_{sr}^{-1} [g, [h, \chi_s]_P]_P \\
&= + \sum_{rs} [f, \chi_r]_P C_{sr}^{-1} [g, [h, \chi_s]_P]_P \\
&= - \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [g, [h, \chi_s]_P]_P,
\end{aligned}$$

and after this rearrangement, we can see that the 2nd, 12th, and 23rd terms of Eq. (1) sum to zero because the Poisson brackets obey the Jacobi identity. Likewise, we can do a similar rearrangement of the 3rd and 21st terms in Eq. (1), and then we see that the 3rd, 13th, and 20th terms of Eq. (1) sum to zero, and also the 5th, 11th, and 21st terms of Eq. (1) sum to zero. We can also see that the 4th and 24th terms of Eq. (1) cancel, as well as the 6th and 13th, and the 15th and 22nd. At this point, we are left with

$$\begin{aligned}
& [f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \tag{2} \\
&= - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, g]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, h]_P \\
&\quad + \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, h]_P]_P \\
&\quad - \sum_{tu} \sum_{rs} [g, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, h]_P]_P C_{rs}^{-1} [\chi_s, f]_P \\
&\quad + \sum_{tu} \sum_{rs} [g, \chi_t]_P C_{tu}^{-1} [h, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, f]_P \\
&\quad + \sum_{tu} \sum_{rs} [g, \chi_t]_P C_{tu}^{-1} [h, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, f]_P]_P \\
&\quad - \sum_{tu} \sum_{rs} [h, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, f]_P]_P C_{rs}^{-1} [\chi_s, g]_P \\
&\quad + \sum_{tu} \sum_{rs} [h, \chi_t]_P C_{tu}^{-1} [f, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, g]_P \\
&\quad + \sum_{tu} \sum_{rs} [h, \chi_t]_P C_{tu}^{-1} [f, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, g]_P]_P.
\end{aligned}$$

We can rewrite the 1st term of Eq. (2) as

$$\begin{aligned}
& - \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [\chi_r, [\chi_u, g]_P]_P C_{rs}^{-1} [\chi_s, h]_P \\
&= - \sum_{tu} \sum_{rs} [f, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, g]_P]_P C_{ut}^{-1} [\chi_t, h]_P \\
&= - \sum_{tu} \sum_{rs} [h, \chi_t]_P C_{tu}^{-1} [f, \chi_r]_P C_{rs}^{-1} [\chi_u, [\chi_s, g]_P]_P,
\end{aligned}$$

and so we can see that the 1st and 9th terms of Eq. (2) cancel. After a similar rewriting of the 4th and 7th terms, we find that the 3rd and 4th terms of Eq. (2) cancel, as well as the 6th and 7th. This leaves only three terms remaining

$$\begin{aligned}
& [f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \quad (3) \\
&= \sum_{tu} \sum_{rs} [f, \chi_t]_P C_{tu}^{-1} [g, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, h]_P \\
&+ \sum_{tu} \sum_{rs} [g, \chi_t]_P C_{tu}^{-1} [h, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, f]_P \\
&+ \sum_{tu} \sum_{rs} [h, \chi_t]_P C_{tu}^{-1} [f, \chi_r]_P [\chi_u, C_{rs}^{-1}]_P [\chi_s, g]_P.
\end{aligned}$$

Next, notice that

$$\begin{aligned}
[\chi_u, C_{rs}^{-1}]_P &= \sum_v [\chi_u, \delta_{rv} C_{vs}^{-1}]_P = \sum_{vw} [\chi_u, C_{rw}^{-1} C_{wv} C_{vs}^{-1}]_P \\
&= \sum_{vw} [\chi_u, C_{rw}^{-1}]_P C_{wv} C_{vs}^{-1} + \sum_{vw} C_{rw}^{-1} [\chi_u, C_{wv}]_P C_{vs}^{-1} \\
&+ \sum_{vw} C_{rw}^{-1} C_{wv} [\chi_u, C_{vs}^{-1}]_P \\
&= \sum_w [\chi_u, C_{rw}^{-1}]_P \delta_{ws} + \sum_{vw} C_{rw}^{-1} [\chi_u, C_{wv}]_P C_{vs}^{-1} + \sum_v \delta_{rv} [\chi_u, C_{vs}^{-1}]_P \\
&= 2 [\chi_u, C_{rs}^{-1}]_P + \sum_{vw} C_{rw}^{-1} [\chi_u, C_{wv}]_P C_{vs}^{-1} \\
[\chi_u, C_{rs}^{-1}]_P &= - \sum_{vw} C_{rw}^{-1} [\chi_u, C_{wv}]_P C_{vs}^{-1} = - \sum_{vw} C_{rw}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P C_{vs}^{-1}.
\end{aligned}$$

Using this identity in each of the terms appearing in Eq. (3), we can rewrite this expression as

$$\begin{aligned}
& [f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \\
&= - \sum_{tu} \sum_{rs} \sum_{vw} [f, \chi_t]_P [g, \chi_r]_P [\chi_s, h]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P \\
&- \sum_{tu} \sum_{rs} \sum_{vw} [g, \chi_t]_P [h, \chi_r]_P [\chi_s, f]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P \\
&- \sum_{tu} \sum_{rs} \sum_{vw} [h, \chi_t]_P [f, \chi_r]_P [\chi_s, g]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P,
\end{aligned}$$

using the antisymmetry of the Poisson bracket this becomes

$$\begin{aligned}
& [f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \\
&= \sum_{tu} \sum_{rs} \sum_{vw} [f, \chi_t]_P [g, \chi_r]_P [h, \chi_s]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P \\
&+ \sum_{tu} \sum_{rs} \sum_{vw} [g, \chi_t]_P [h, \chi_r]_P [f, \chi_s]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P \\
&+ \sum_{tu} \sum_{rs} \sum_{vw} [h, \chi_t]_P [f, \chi_r]_P [g, \chi_s]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P,
\end{aligned}$$

after relabeling summation indices this becomes

$$\begin{aligned}
& [f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \\
&= \sum_{tu} \sum_{rs} \sum_{vw} [f, \chi_t]_P [g, \chi_r]_P [h, \chi_s]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P \\
&+ \sum_{tu} \sum_{rs} \sum_{vw} [g, \chi_r]_P [h, \chi_s]_P [f, \chi_t]_P C_{ru}^{-1} C_{sw}^{-1} C_{vt}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P \\
&+ \sum_{tu} \sum_{rs} \sum_{vw} [h, \chi_s]_P [f, \chi_t]_P [g, \chi_r]_P C_{su}^{-1} C_{tw}^{-1} C_{vr}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P,
\end{aligned}$$

and after some more relabeling this gives

$$\begin{aligned}
& [f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \\
&= \sum_{tu} \sum_{rs} \sum_{vw} [f, \chi_t]_P [g, \chi_r]_P [h, \chi_s]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} [\chi_u, [\chi_w, \chi_v]_P]_P \\
&+ \sum_{tu} \sum_{rs} \sum_{vw} [g, \chi_r]_P [h, \chi_s]_P [f, \chi_t]_P C_{rw}^{-1} C_{sv}^{-1} C_{ut}^{-1} [\chi_w, [\chi_v, \chi_u]_P]_P \\
&+ \sum_{tu} \sum_{rs} \sum_{vw} [h, \chi_s]_P [f, \chi_t]_P [g, \chi_r]_P C_{sv}^{-1} C_{tu}^{-1} C_{wr}^{-1} [\chi_v, [\chi_u, \chi_w]_P]_P,
\end{aligned}$$

and we can use the antisymmetry of C_{rs}^{-1} to express this as

$$\begin{aligned}
& [f, [g, h]_D]_D + [g, [h, f]_D]_D + [h, [f, g]_D]_D \\
&= \sum_{tu} \sum_{rs} \sum_{vw} [f, \chi_t]_P [g, \chi_r]_P [h, \chi_s]_P C_{tu}^{-1} C_{rw}^{-1} C_{vs}^{-1} \\
&\quad \times ([\chi_u, [\chi_w, \chi_v]_P]_P + [\chi_w, [\chi_v, \chi_u]_P]_P + [\chi_v, [\chi_u, \chi_w]_P]_P) \\
&= 0,
\end{aligned}$$

which vanishes because the Poisson brackets obey the Jacobi identity. We have thus shown that the Dirac brackets obey the Jacobi identity.

3. Consider a one-dimensional harmonic oscillator, with Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}.$$

Use the path-integral formalism to calculate the probability amplitude for a transition from a position x at time t to a position x' at time $t' > t$.

The Hamiltonian of the harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2},$$

and since this Hamiltonian is quadratic in the momentum, we can write the path integral in the form given in Eq. (9.6.20)

$$\begin{aligned}
& (\Psi_{x',t'}, \Psi_{x,t}) \\
&= C \int_{x(t)=x; x(t')=x'} \prod_{\tau} dx(\tau) \exp \left[\frac{i}{\hbar} \int_t^{t'} d\tau \left(\frac{m\dot{x}^2(\tau)}{2} - \frac{m\omega^2 x^2(\tau)}{2} \right) \right],
\end{aligned}$$

where we have used the fact that the Lagrangian of the harmonic oscillator is

$$L(x(\tau), \dot{x}(\tau)) = \frac{m\dot{x}^2(\tau)}{2} - \frac{m\omega^2 x^2(\tau)}{2}.$$

The Lagrangian is quadratic in $x(\tau)$ and $\dot{x}(\tau)$, and so we can do the integral by setting $x(\tau)$ equal to the classical solution, which is given by

$$\frac{d}{d\tau} \frac{\partial L(\tau)}{\partial \dot{x}(\tau)} = \frac{\partial L(\tau)}{\partial x(\tau)},$$

with the constraint that $x(t) = x$ and $x(t') = x'$. The equation of motion takes the form

$$m\ddot{x}(\tau) = -m\omega^2 x(\tau),$$

which has a well-known solution of the form

$$x(\tau) = Ae^{i\omega\tau} + Be^{-i\omega\tau}.$$

Imposing the conditions $x(t) = x$ and $x(t') = x'$ we find

$$\begin{aligned}
x &= x(t) = Ae^{i\omega t} + Be^{-i\omega t} \\
x' &= x(t') = Ae^{i\omega t'} + Be^{-i\omega t'},
\end{aligned}$$

and so A and B are given by

$$\begin{aligned}
A &= \frac{xe^{i\omega t} - x'e^{i\omega t'}}{e^{2i\omega t} - e^{2i\omega t'}} \\
B &= \frac{xe^{-i\omega t} - x'e^{-i\omega t'}}{e^{-2i\omega t} - e^{-2i\omega t'}}.
\end{aligned}$$

We can then calculate $\dot{x}(\tau)$ to be

$$\dot{x}(\tau) = i\omega Ae^{i\omega\tau} - i\omega Be^{-i\omega\tau}.$$

Plugging in the classical solution, we can evaluate the integral appearing in the exponential of the path integral

$$\begin{aligned}
\int_t^{t'} d\tau L(\tau) &= \int_t^{t'} d\tau \left(\frac{m\dot{x}^2(\tau)}{2} - \frac{m\omega^2 x^2(\tau)}{2} \right) \\
&= \int_t^{t'} d\tau \left[\frac{m}{2} (-\omega^2 A^2 e^{2i\omega\tau} + 2\omega^2 AB - \omega^2 B^2 e^{-2i\omega\tau}) \right. \\
&\quad \left. - \frac{m\omega^2}{2} (A^2 e^{2i\omega\tau} + 2AB + B^2 e^{2i\omega\tau}) \right]
\end{aligned}$$

$$\begin{aligned}
&= \int_t^{t'} d\tau \left(-m\omega^2 A^2 e^{2i\omega\tau} - m\omega^2 B^2 e^{-2i\omega\tau} \right) \\
&= \frac{im\omega A^2}{2} \left(e^{2i\omega t'} - e^{2i\omega t} \right) - \frac{im\omega B^2}{2} \left(e^{-2i\omega t'} - e^{-2i\omega t} \right).
\end{aligned}$$

Plugging in the expressions for A and B , this becomes

$$\begin{aligned}
\int_t^{t'} d\tau L(\tau) &= \frac{im\omega}{2} \left[\frac{x^2 e^{2i\omega t} - 2xx' e^{i\omega(t+t')} + x'^2 e^{2i\omega t'}}{e^{2i\omega t'} - e^{2i\omega t}} \right. \\
&\quad \left. - \frac{x^2 e^{-2i\omega t} - 2xx' e^{-i\omega(t+t')} + x'^2 e^{-2i\omega t'}}{e^{-2i\omega t'} - e^{-2i\omega t}} \right] \\
&= \frac{im\omega}{2} \left[\frac{1}{(e^{2i\omega t'} - e^{2i\omega t})(e^{-2i\omega t'} - e^{-2i\omega t})} \right] \left[x^2 \left(e^{2i\omega(t-t')} - e^{-2i\omega(t-t')} \right) \right. \\
&\quad \left. + x'^2 \left(e^{2i\omega(t-t')} - e^{-2i\omega(t-t')} \right) - 2xx' \left(2e^{i\omega(t-t')} - 2e^{-i\omega(t-t')} \right) \right] \\
&= \frac{im\omega}{2} \left[\frac{2i(x^2 + x'^2) \sin(2\omega(t-t)) - 8ixx' \sin(\omega(t-t))}{2 - 2\cos(2\omega(t-t))} \right] \\
&= -\frac{m\omega}{2} \left[\frac{2(x^2 + x'^2) \sin(\omega(t-t)) \cos(\omega(t-t)) - 4xx' \sin(\omega(t-t))}{2 \sin^2(\omega(t-t))} \right] \\
&= -\frac{m\omega}{2} \left[\frac{(x^2 + x'^2) \cos(\omega(t-t)) - 2xx'}{\sin(\omega(t-t))} \right].
\end{aligned}$$

The expression for the path integral then becomes

$$(\Psi_{x',t'}, \Psi_{x,t}) = C \exp \left[\frac{im\omega}{2\hbar} \left[\frac{(x^2 + x'^2) \cos(\omega(t' - t)) - 2xx'}{\sin(\omega(t' - t))} \right] \right],$$

where C is a proportionality constant which depends on $t' - t$. We can find C by requiring that

$$\lim_{t' \rightarrow t} (\Psi_{x',t'}, \Psi_{x,t}) \rightarrow \delta(x' - x),$$

or in other words that

$$\lim_{t' \rightarrow t} \int_{-\infty}^{+\infty} dx C \exp \left[\frac{im\omega}{2\hbar} \left[\frac{(x^2 + x'^2) \cos(\omega(t' - t)) - 2xx'}{\sin(\omega(t' - t))} \right] \right] f(x) \rightarrow f(x').$$

In the limit $t' \rightarrow t$, the exponential function oscillates very rapidly, and so the only appreciable contribution to the integral come from the value $x = x'$. It only remains to show that

$$\lim_{t' \rightarrow t} \int_{-\infty}^{+\infty} dx C \exp \left[\frac{im\omega}{2\hbar} \left[\frac{(x^2 + x'^2) \cos(\omega(t' - t)) - 2xx'}{\sin(\omega(t' - t))} \right] \right] \rightarrow 1.$$

We can do this integral by using Eqs. (9.6.17) and (9.6.18) which give

$$\begin{aligned} & \lim_{t' \rightarrow t} \int_{-\infty}^{+\infty} dx C \exp \left[\frac{im\omega}{2\hbar} \left[\frac{(x^2 + x'^2) \cos(\omega(t' - t)) - 2xx'}{\sin(\omega(t' - t))} \right] \right] \\ &= \lim_{t' \rightarrow t} C \sqrt{\frac{2i\pi\hbar \sin(\omega(t' - t))}{m\omega \cos(\omega(t' - t))}} \exp \left[\frac{im\omega}{2\hbar} \left(-\frac{\sin(\omega(t' - t))}{\cos(\omega(t' - t))} \right) x'^2 \right]. \end{aligned}$$

In order for this expression to approach 1 in the limit $t' \rightarrow t$, its absolute value square must also approach 1 in this limit, and so we see that up to an arbitrary overall phase

$$C = \sqrt{\frac{m\omega \cos(\omega(t' - t))}{2i\pi\hbar \sin(\omega(t' - t))}}.$$

We therefore find the probability amplitude for the transition from a position x at t to a position x' at t' to be

$$\begin{aligned} & (\Psi_{x',t'}, \Psi_{x,t}) \\ &= \sqrt{\frac{m\omega \cos(\omega(t' - t))}{2i\pi\hbar \sin(\omega(t' - t))}} \exp \left[\frac{im\omega}{2\hbar} \left[\frac{(x^2 + x'^2) \cos(\omega(t' - t)) - 2xx'}{\sin(\omega(t' - t))} \right] \right]. \end{aligned}$$

Chapter 10 Problem Set Solutions

1. Consider a system in an external electromagnetic field. Suppose that the part of the Lagrangian that depends on the scalar potential ϕ and vector potential \mathbf{A} takes the form

$$L_{\text{int}}(t) = \int d^3x [-\rho(\mathbf{x}, t)\phi(\mathbf{x}, t) + \mathbf{J}(\mathbf{x}, t) \cdot \mathbf{A}(\mathbf{x}, t)],$$

where ρ and \mathbf{J} depend on the matter variables but not on ϕ or \mathbf{A} . What condition must be satisfied by ρ and \mathbf{J} for the action to be gauge-invariant? We will work with an interaction Lagrangian density of the form

$$L_{\text{int}} = \int d^3x [-\rho(\mathbf{x}, t)\phi(\mathbf{x}, t) + \mathbf{J}(\mathbf{x}, t) \cdot \mathbf{A}(\mathbf{x}, t)],$$

and we wish to find the conditions such that the action is invariant under a gauge transformation, defined in Eqs. (10.2.1) and (10.2.2) as

$$\begin{aligned} \mathbf{A}(\mathbf{x}, t) &\mapsto \mathbf{A}'(\mathbf{x}, t) = \mathbf{A}(\mathbf{x}, t) + \nabla\alpha(\mathbf{x}, t) \\ \phi(\mathbf{x}, t) &\mapsto \phi'(\mathbf{x}, t) = \phi(\mathbf{x}, t) - \frac{1}{c} \frac{\partial}{\partial t} \alpha(\mathbf{x}, t). \end{aligned}$$

Under this transformation, the interaction part of the action becomes

$$\begin{aligned} S_{\text{int}} &= \int_{-\infty}^{\infty} dt L_{\text{int}} \\ &\mapsto \int_{-\infty}^{\infty} dt \int d^3x -\rho(\mathbf{x}, t) \left(\phi(\mathbf{x}, t) - \frac{1}{c} \frac{\partial}{\partial t} \alpha(\mathbf{x}, t) \right) + \mathbf{J}(\mathbf{x}, t) \cdot (\mathbf{A}(\mathbf{x}, t) + \nabla\alpha(\mathbf{x}, t)) \\ &= S_{\text{int}} + \int_{-\infty}^{\infty} dt \frac{\partial}{\partial t} \left[\int d^3x \frac{1}{c} \rho(\mathbf{x}, t) \alpha(\mathbf{x}, t) \right] - \int_{-\infty}^{\infty} dt \int d^3x \frac{1}{c} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} \alpha(\mathbf{x}, t) \\ &\quad + \int_{-\infty}^{\infty} dt \int d^3x \nabla \cdot [\mathbf{J}(\mathbf{x}, t) \alpha(\mathbf{x}, t)] - \int_{-\infty}^{\infty} dt \int d^3x \nabla \cdot \mathbf{J} \alpha(\mathbf{x}, t). \end{aligned}$$

The second and fourth terms are both total derivatives which integrate to zero as long as $\alpha(\mathbf{x}, t) \rightarrow 0$ as $t \rightarrow \pm\infty$ and $\mathbf{J}(\mathbf{x}, t) \rightarrow 0$ as $\mathbf{x} \rightarrow \infty$, respectively. The transformation then takes the form

$$S_{\text{int}} \mapsto S_{\text{int}} - \int_{-\infty}^{\infty} dt \int d^3x \left[\frac{1}{c} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{J}(\mathbf{x}, t) \right] \alpha(\mathbf{x}, t),$$

and so in order for the action to be invariant for arbitrary $\alpha(\mathbf{x}, t)$, we require

$$\frac{1}{c} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{J}(\mathbf{x}, t) = 0,$$

which is the continuity equation for electric charge.

2. Consider a homogeneous rectangular slab of metal, with edges L_x , L_y , and L_z . Assume that the electric potential ϕ vanishes within the slab, and that the wave functions of conduction electrons in the slab satisfy periodic boundary

conditions at the slab faces. Suppose that the slab is in a constant magnetic field in the z -direction that is strong enough so that the cyclotron frequency ω is very much larger than $\hbar/m_e L_z^2$. Suppose that there are n_e conduction electrons per unit volume in the slab. Calculate the maximum energy of individual conduction electrons, in the limit $\omega m_e L_z^2/\hbar \rightarrow \infty$.

The Hamiltonian for an electron in a general electromagnetic field is given in Eq. (10.3.1)

$$H = \frac{1}{2m_e} \left(\mathbf{p} + \frac{e}{c} \mathbf{A}(\mathbf{x}, t) \right)^2 - \frac{2\mu_e}{\hbar} \mathbf{s} \cdot \mathbf{H}(\mathbf{x}, t).$$

For a constant magnetic field in the z -direction, the vector potential can be taken to have the form

$$A_y = xH_z, \quad A_x = A_z = 0,$$

and so the Hamiltonian becomes

$$H = \frac{1}{2m_e} \left(p_x^2 + \left(p_y + \frac{exH_z}{c} \right)^2 + p_z^2 \right) - \frac{2\mu_e}{\hbar} s_z H_z.$$

This Hamiltonian commutes with p_y , p_z , and s_z , so there exist states Ψ such that

$$p_y \Psi = \hbar k_y \Psi, \quad p_z \Psi = \hbar k_z \Psi, \quad s_z \Psi = \pm \frac{\hbar}{2} \Psi, \quad H \Psi = E \Psi.$$

The Schrödinger equation can then be written as

$$\frac{1}{2m_e} \left(p_x^2 + \left(\hbar k_y + \frac{eH_z x}{c} \right)^2 \right) \Psi = \left(E - \frac{\hbar^2 k_z^2}{2m_e} \pm \mu_e H_z \right) \Psi,$$

which we can rewrite as

$$\left[\frac{1}{2m_e} p_x^2 + \frac{m_e \omega^2}{2} (x - x_0)^2 \right] \Psi = \left(E - \frac{\hbar^2 k_z^2}{2m_e} \pm \mu_e H_z \right) \Psi,$$

where we have defined $\omega \equiv eH_z/m_e c$ and $x_0 \equiv -\hbar k_y c/eH_z$. In this form, it is clear that this is just the Schrödinger equation for the harmonic oscillator which was discussed in Section 2.5, and so the energy levels are given by

$$E = \frac{\hbar^2 k_z^2}{2m_e} \mp \mu_e H_z + \hbar \omega \left(n + \frac{1}{2} \right) \quad \text{for } n = 0, 1, 2, \dots$$

For electrons in a metal slab with dimensions L_x , L_y , and L_z , we must have

$$-\frac{L_x}{2} \leq x \leq \frac{L_x}{2}, \quad -\frac{L_y}{2} \leq y \leq \frac{L_y}{2}, \quad -\frac{L_z}{2} \leq z \leq \frac{L_z}{2},$$

and as a result we must have

$$\begin{aligned} |x_0| &< \frac{L_x}{2} \\ \left| \frac{\hbar k_y c}{e H_z} \right| &< \frac{L_x}{2} \\ |k_y| &< \frac{e H_z L_x}{2 \hbar c}. \end{aligned}$$

Due to the periodic boundary conditions at the slab faces, we have

$$k_y = \frac{2\pi n_y}{L_y}, \quad k_z = \frac{2\pi n_z}{L_z},$$

where n_x and n_y are integers. The number of states with a given n , $\hbar^2 k_z^2 / 2m_e$, and s_z having $|k_y|$ less than $e H_z L_x / 2 \hbar c$ is the number of positive and negative integers with magnitude less than $(e H_z L_x / 2 \hbar c) (L_y / 2\pi)$ which is

$$\mathcal{N} = \frac{e H_z A}{2\pi \hbar c},$$

where $A = L_x L_y$ is the area of the slab face perpendicular to the magnetic field. In the limit $\omega m_e L_z^2 / \hbar \rightarrow \infty$ all of the conduction electrons will be in the state $n = 0$, and with spin- z component along the direction of the magnetic field, so the energy of individual conduction electrons is $E = \hbar^2 k_z^2 / 2m_e$, where we are neglecting corrections which come from quantum electrodynamics. The Pauli exclusion principle allows one electron in each state, which will be filled in order of increasing energy until \mathcal{N} / V times the number of filled energy states equals the number of conduction electrons per unit volume n_e . The integer n_z will take values $0, \pm 1, \pm 2, \dots, n_{z,\max}$ with one electron for each n_z , or two electrons for each value of $|n_z|$, so that

$$n_e = \frac{2|n_{z,\max}| \mathcal{N}}{L_x L_y L_z}.$$

Solving this expression for $|n_{z,\max}|$ we find

$$|n_{z,\max}| = \frac{n_e L_x L_y L_z}{2} \left(\frac{2\pi \hbar c}{e H_z L_x L_y} \right) = \frac{n_e L_z \pi \hbar c}{e H_z}.$$

Therefore the maximum energy of individual conduction electrons is

$$E_{\max} = \frac{\hbar^2}{2m_e} \left(\frac{2\pi n_{z,\max}}{L_z} \right)^2 = \frac{2\pi^4 \hbar^4 c^2 n_e^2}{m_e e^2 H_z^2}.$$

3. Consider a non-relativistic electron in an external electromagnetic field. Calculate the commutators of different components of its velocity.

Recall that for a non-relativistic electron in an external electromagnetic field, the velocity is given in terms of the canonical momentum as in Eq. (10.1.8)

$$\dot{\mathbf{x}} = \frac{1}{m} \left[\mathbf{p} + \frac{e}{c} \mathbf{A}(\mathbf{x}, t) \right],$$

where we have inserted the charge of the electron $e_n = -e$. The position and its canonical conjugate obey the commutation relations given in Eqs. (10.1.10) and (10.1.11)

$$\begin{aligned} [x_i, p_j] &= i\hbar\delta_{ij} \\ [x_i, x_j] &= [p_i, p_j] = 0. \end{aligned}$$

The commutation relations of two components of the velocity are then given by

$$\begin{aligned} [\dot{x}_i, \dot{x}_j] &= \left[\frac{1}{m} \left(p_i + \frac{e}{c} A_i(\mathbf{x}, t) \right), \frac{1}{m} \left(p_j + \frac{e}{c} A_j(\mathbf{x}, t) \right) \right] \\ &= \frac{1}{m^2} \left[[p_i, p_j] + \left[p_i, \frac{e}{c} A_j(\mathbf{x}, t) \right] + \left[\frac{e}{c} A_i(\mathbf{x}, t), p_j \right] \right. \\ &\quad \left. + \left[\frac{e}{c} A_i(\mathbf{x}, t), \frac{e}{c} A_j(\mathbf{x}, t) \right] \right]. \end{aligned}$$

The first and last terms vanish, and we can calculate the remaining commutators by using the canonical commutation relations

$$\left[\frac{e}{c} A_i(\mathbf{x}, t), p_j \right] = i\hbar \frac{e}{c} \frac{\partial A_i(\mathbf{x}, t)}{\partial x_j},$$

and so we find

$$\begin{aligned} [\dot{x}_i, \dot{x}_j] &= -i\hbar \frac{e}{m^2 c} \left[\frac{\partial A_j(\mathbf{x}, t)}{\partial x_i} - \frac{\partial A_i(\mathbf{x}, t)}{\partial x_j} \right] \\ &= -i\hbar \frac{e}{m^2 c} \sum_k \epsilon_{ijk} (\nabla \times \mathbf{A}(\mathbf{x}, t))_k. \end{aligned}$$

Chapter 11 Problem Set Solutions

1. Calculate the rates for emission of photons in the transitions $3d \rightarrow 2p$ and $2p \rightarrow 1s$ in hydrogen. Give formulas and numerical values. You can use the facts that the proton is much heavier than the electron, and the wavelength of the photon emitted in these processes is much larger than the atomic size, and neglect electron spin.

For the transitions $3d \rightarrow 2p$ and $2p \rightarrow 1s$, assuming that $kr \ll 1$, and ignoring electron spin, we can use the dipole approximation and calculate the rate by using Eq. (11.7.28)

$$\Gamma = \frac{4\omega^2}{3c^3\hbar} \left| \sum_n e_n (b | \bar{\mathbf{x}}_n | a) \right|^2,$$

where the matrix element is given by Eq. (11.7.27)

$$(b | \bar{\mathbf{x}}_n | a) = \int \left(\prod_m d^3 \bar{x}_m \right) \delta^3 \left(\sum_m \frac{m_m \bar{\mathbf{x}}_m}{M} \right) \psi_b^*(\bar{\mathbf{x}}) \bar{\mathbf{x}}_n \psi_a(\bar{\mathbf{x}}).$$

For hydrogen, the delta function becomes

$$\delta^3 \left(\sum_m \frac{m_m \bar{\mathbf{x}}_m}{M} \right) = \delta^3 \left(\frac{m_p \bar{\mathbf{x}}_p + m_e \bar{\mathbf{x}}_e}{m_e + m_p} \right) \approx \delta^3(\bar{\mathbf{x}}_p),$$

since the mass of the proton is much larger than the mass of the electron $m_p \gg m_e$. Therefore, the integral over $\bar{\mathbf{x}}_p$ just sets $\bar{\mathbf{x}}_p = 0$. Now, we need to calculate the matrix elements

$$(b | \bar{\mathbf{x}}_n | a) = \int d^3 \bar{x} \psi_b^*(\bar{\mathbf{x}}) \bar{\mathbf{x}} \psi_a(\bar{\mathbf{x}}),$$

where $\bar{\mathbf{x}}$ is the position of the electron relative to the proton. Clearly, the transition rates will be independent of the m quantum number of the initial state, because the rate cannot depend upon how we choose to orient our coordinate system, but we will show this explicitly below. The relevant wave functions for hydrogen are given by

$$\begin{aligned} \psi_{3d^{\pm 2}} &= \frac{1}{162\sqrt{\pi}} \left(\frac{1}{a} \right)^{3/2} \left(\frac{r}{a} \right)^2 e^{-r/3a} \sin^2 \theta e^{\pm 2i\phi}, \\ \psi_{3d^{\pm 1}} &= \frac{1}{81\sqrt{\pi}} \left(\frac{1}{a} \right)^{3/2} \left(\frac{r}{a} \right)^2 e^{-r/3a} \sin \theta \cos \theta e^{\pm i\phi}, \\ \psi_{3d^0} &= \frac{1}{81\sqrt{6\pi}} \left(\frac{1}{a} \right)^{3/2} \left(\frac{r}{a} \right)^2 e^{-r/3a} (3 \cos^2 \theta - 1), \\ \psi_{2p^{\pm 1}} &= \frac{1}{8\sqrt{\pi}} \left(\frac{1}{a} \right)^{3/2} \left(\frac{r}{a} \right)^2 e^{-r/2a} \sin \theta e^{\pm i\phi}, \end{aligned}$$

$$\psi_{2p^0} = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a}\right)^{3/2} \left(\frac{r}{a}\right)^2 e^{-r/2a} \cos \theta,$$

$$\psi_{1s^0} = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a}\right)^{3/2} e^{-r/a}.$$

The only non-vanishing matrix elements for the transition $3d \rightarrow 2p$ are given by

$$\begin{aligned} (2p^{\pm 1} | \bar{x} | 3d^{\pm 2}) &= \frac{1}{2^4 3^4 \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\ &\quad \times \int_0^\pi d\theta \sin^5 \theta \int_0^{2\pi} d\phi e^{\pm i\phi} \cos \phi \\ &= \frac{2^{11} 3^4}{5^7} a \\ (2p^{\pm 1} | \bar{y} | 3d^{\pm 2}) &= \frac{1}{2^4 3^4 \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\ &\quad \times \int_0^\pi d\theta \sin^5 \theta \int_0^{2\pi} d\phi e^{\pm i\phi} \sin \phi \\ &= \pm i \frac{2^{11} 3^4}{5^7} a \\ (2p^{\pm 1} | \bar{z} | 3d^{\pm 1}) &= \frac{1}{2^3 3^4 \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\ &\quad \times \int_0^\pi d\theta \sin^3 \theta \cos^2 \theta \int_0^{2\pi} d\phi \\ &= \frac{2^{11} 3^4}{5^7} a \\ (2p^0 | \bar{x} | 3d^{\pm 1}) &= \frac{1}{2^{5/2} 3^4 \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\ &\quad \times \int_0^\pi d\theta \sin^3 \theta \cos^2 \theta \int_0^{2\pi} d\phi e^{\pm i\phi} \cos \phi \\ &= \frac{1}{\sqrt{2}} \frac{2^{11} 3^4}{5^7} a \\ (2p^0 | \bar{y} | 3d^{\pm 1}) &= \frac{1}{2^{5/2} 3^4 \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\ &\quad \times \int_0^\pi d\theta \sin^3 \theta \cos^2 \theta \int_0^{2\pi} d\phi e^{\pm i\phi} \sin \phi \\ &= \pm \frac{i}{\sqrt{2}} \frac{2^{11} 3^4}{5^7} a \end{aligned}$$

$$\begin{aligned}
(2p^0|\bar{z}|3d^0) &= \frac{1}{2^3 3^{9/2} \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\
&\quad \times \int_0^\pi d\theta \sin\theta \cos^2\theta (3\cos^2\theta - 1) \int_0^{2\pi} d\phi \\
&= \frac{2}{\sqrt{3}} \frac{2^{11} 3^4}{5^7} a \\
(2p^{\pm 1}|\bar{x}|3d^0) &= \frac{1}{2^{7/2} 3^{9/2} \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\
&\quad \times \int_0^\pi d\theta \sin^3\theta (3\cos^2\theta - 1) \int_0^{2\pi} d\phi e^{\mp i\phi} \cos\phi \\
&= -\frac{1}{\sqrt{6}} \frac{2^{11} 3^4}{5^7} a \\
(2p^{\pm 1}|\bar{y}|3d^0) &= \frac{1}{2^{7/2} 3^{9/2} \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right)^3 e^{-5r/6a} \\
&\quad \times \int_0^\pi d\theta \sin^3\theta (3\cos^2\theta - 1) \int_0^{2\pi} d\phi e^{\mp i\phi} \sin\phi \\
&= \pm \frac{i}{\sqrt{6}} \frac{2^{11} 3^4}{5^7} a,
\end{aligned}$$

and the only non-vanishing matrix elements for the transition $2p \rightarrow 1s$ are

$$\begin{aligned}
(1s^0|\bar{x}|2p^{\pm 1}) &= \frac{1}{2^3 \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right) e^{-3r/2a} \int_0^\pi d\theta \sin^3\theta \int_0^{2\pi} d\phi e^{\pm i\phi} \cos\phi \\
&= \frac{2^7}{3^5} a \\
(1s^0|\bar{y}|2p^{\pm 1}) &= \frac{1}{2^3 \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right) e^{-3r/2a} \int_0^\pi d\theta \sin^3\theta \int_0^{2\pi} d\phi e^{\pm i\phi} \sin\phi \\
&= \pm i \frac{2^7}{3^5} a \\
(1s^0|\bar{x}|2p^0) &= \frac{1}{2^{5/2} \pi a^3} \int_0^\infty dr r^3 \left(\frac{r}{a}\right) e^{-3r/2a} \int_0^\pi d\theta \sin\theta \cos^2\theta \int_0^{2\pi} d\phi \\
&= \sqrt{2} \frac{2^7}{3^5} a.
\end{aligned}$$

Squaring these matrix elements, we find for the $3d \rightarrow 2p$ transition

$$\begin{aligned}
|(2p|\bar{\mathbf{x}}|3d^{\pm 2})|^2 &= |(2p^{\pm 1}|\bar{x}|3d^{\pm 2})|^2 + |(2p^{\pm 1}|\bar{y}|3d^{\pm 2})|^2 \\
&= \frac{2^{23} 3^8}{5^{14}} a^2
\end{aligned}$$

$$\begin{aligned}
|(2p|\bar{x}|3d^{\pm 1})|^2 &= |(2p^{\pm 1}|\bar{z}|3d^{\pm 1})|^2 + |(2p^0|\bar{x}|3d^{\pm 1})|^2 + |(2p^0|\bar{y}|3d^{\pm 1})|^2 \\
&= \frac{2^{23}3^8}{5^{14}}a^2 \\
|(2p|\bar{x}|3d^0)|^2 &= |(2p^0|\bar{z}|3d^0)|^2 + 2|(2p^{\pm 1}|\bar{x}|3d^0)|^2 + 2|(2p^{\pm 1}|\bar{y}|3d^0)|^2 \\
&= \frac{2^{23}3^8}{5^{14}}a^2,
\end{aligned}$$

and for the $2p \rightarrow 1s$ transition

$$\begin{aligned}
|(1s|\bar{x}|2p^{\pm 1})|^2 &= |(1s^0|\bar{x}|2p^{\pm 1})|^2 + |(1s^0|\bar{y}|2p^{\pm 1})|^2 \\
&= \frac{2^{13}}{3^{10}}a^2 \\
|(1s|\bar{x}|2p^0)|^2 &= |(1s^0|\bar{z}|2p^0)|^2 \\
&= \frac{2^{15}}{3^{10}}a^2.
\end{aligned}$$

As stated above, we see that the transition rate does not depend upon the initial value of the m quantum number. Next, we need the frequencies for the emitted photons in the $3d \rightarrow 2p$ and $2p \rightarrow 1s$ transitions of hydrogen. The energy of the n th level is

$$E_n = -\frac{m_e e^4}{2\hbar^2 n^2},$$

and so the frequency is given by

$$\omega = \frac{E_a - E_b}{\hbar} = \frac{m_e e^4}{2\hbar^3} \left(\frac{1}{n_b^2} - \frac{1}{n_a^2} \right).$$

For the $3d \rightarrow 2p$ transition, this gives

$$\omega_{3d \rightarrow 2p} = \frac{5m_e e^4}{62\hbar^3},$$

and for the $2p \rightarrow 1s$ transition, this gives

$$\omega_{2p \rightarrow 1s} = \frac{3m_e e^4}{8\hbar^3}.$$

Putting this together and using the definition of the Bohr radius $a = \hbar^2/m_e e^2$, we find for the rate of the $3d \rightarrow 2p$ transition

$$\begin{aligned}
\Gamma_{3d \rightarrow 2p} &= \frac{4}{3} \left(\frac{5m_e e^4}{72\hbar^2} \right)^3 \frac{e^2}{c^3 \hbar} \frac{2^{23}3^5}{5^{14}} a^2 \\
&= \frac{2^{16}3}{5^{11}} \frac{m_e^2 e^{14}}{c^3 \hbar^{10}} a^2 \\
&= \frac{2^{16}3}{5^{11}} \frac{m_e e^{10}}{c^3 \hbar^6} \\
&= 6.4677 \times 10^7 \text{ s}^{-1},
\end{aligned}$$

and for the rate of the $2p \rightarrow 1s$ transition

$$\begin{aligned}\Gamma_{2p \rightarrow 1s} &= \frac{4}{3} \left(\frac{3m_e e^4}{8\hbar^3} \right)^3 \frac{e^2}{c^3 \hbar} \frac{2^{15}}{3^{10}} a^2 \\ &= \frac{2^8 m_e^3 e^{14}}{3^8 c^3 \hbar^{10}} a^2 \\ &= \frac{2^8 m_e^3}{3^8 c^3 \hbar^6} \\ &= 6.2674 \times 10^8 \text{ s}^{-1}.\end{aligned}$$

2. What power of the photon wave number appears in the rate for single photon emission in the decay of the $4f$ state of hydrogen into the $3s$, $3p$, and $3d$ states?

We will begin by examining Eq. (11.7.18) which gives the differential rate for single photon emission

$$d\Gamma(\hat{k}, \sigma) = \frac{k}{2\pi \hbar} \left| \mathbf{e}^*(\hat{k}, \sigma) \cdot \sum_n \frac{e_n}{m_n c} \mathbf{D}_{nba}(\hat{k}) \right|^2 d\Omega,$$

where \mathbf{D}_{nba} is defined in Eq. (11.7.13)

$$\mathbf{D}_{nba}(\hat{k}) = \int \left(\prod_m d^3 \bar{x}_m \right) \delta^3 \left(\sum_m \frac{m_m \bar{\mathbf{x}}_m}{M} \right) \psi_b^*(\bar{\mathbf{x}}) e^{-i\mathbf{k} \cdot \bar{\mathbf{x}}_n} (-i\hbar \nabla_n) \psi_a(\bar{\mathbf{x}}).$$

In the case when the wavelength of the emitted photon is much larger than the atomic size $kr \gg 1$, we can expand the exponential appearing in \mathbf{D}_{nba} and keep only the leading non-vanishing term

$$e^{-i\mathbf{k} \cdot \bar{\mathbf{x}}_n} \approx 1 - i\mathbf{k} \cdot \bar{\mathbf{x}}_n - \frac{1}{2} (\mathbf{k} \cdot \bar{\mathbf{x}}_n)^2 + \dots$$

The operators \mathbf{P}_n and $\bar{\mathbf{X}}_n$ are spatial vectors, and so they behave as operators with $j = 1$ under rotations. The matrix elements of such operators between states ψ_a and ψ_b vanish unless the angular momentum quantum numbers j_a and j_b satisfy $|j_a - j_b| \leq 1$ with j_a and j_b not both zero. Furthermore, these operators change sign under a spatial reflection, so these matrix elements vanish unless the states ψ_a and ψ_b have opposite parity.

The states $4f$ and $3d$ have opposite parity, and $|3 - 2| = 1 \leq 1$, so for the transition $4f \rightarrow 3d$, we can use the leading term in the expansion of $e^{-i\mathbf{k} \cdot \bar{\mathbf{x}}_n}$. In this case, the transition rate is given by Eq. (11.7.28)

$$\Gamma_{4f \rightarrow 3d} = \frac{4\omega^3}{3c^3 \hbar} \left| \sum_n e_n (3d | \bar{\mathbf{x}}_n | 4f) \right|^2 = \frac{4k^3}{3\hbar} \left| \sum_n e_n (3d | \bar{\mathbf{x}}_n | 4f) \right|^2,$$

and so we find

$$\Gamma_{4f \rightarrow 3d} \propto k^3.$$

The states $4f$ and $3p$ have the same parity, and $|3-1| = 2 \not\leq 1$, so we need to use the second term in the expansion of $e^{-i\mathbf{k}\cdot\bar{\mathbf{x}}_n}$. In this case, the transition rate is given by Eq. (11.7.34)

$$\Gamma_{4f \rightarrow 3p} = \frac{2k^3}{15\hbar} \sum_{im} \left[\frac{3}{4} |(3p|Q_{ij}|4f)|^2 + \frac{5}{4} |(3p|M_{ij}|4f)|^2 \right].$$

The second term, which represents the magnetic dipole contribution vanishes because the operator M_{ij} acts under rotation as an operator with $j = 1$ and therefore vanishes between states ψ_a and ψ_b unless $|j_a - j_b| \leq 1 \leq j_a + j_b$. The first term, which represents the electric quadrupole moment, does not vanish for this transition because the operator Q_{ij} acts as an operator with $j = 2$ under rotation, and therefore the matrix elements $(b|Q_{ij}|a)$ vanish unless $|j_a - j_b| \leq 2 \leq j_a + j_b$. The electric quadrupole matrix element can be written as in Eq. (10.7.38)

$$(b|Q_{ij}|a) = ick \sum_n e_n \left[(b|\bar{x}_{ni}\bar{x}_{nj}|a) - \frac{1}{3} (b|\bar{x}_n^2|a) \right].$$

This means that the rate $\Gamma_{4f \rightarrow 3p}$ will have an additional factor k^2 relative to the rate $\Gamma_{4f \rightarrow 3d}$

$$\Gamma_{4f \rightarrow 3p} = \frac{2k^3}{15\hbar} \sum_{ij} \left[\frac{3}{4} c^2 k^2 \left| i \sum_n e_n \left[(3p|\bar{x}_{ni}\bar{x}_{nj}|4f) - \frac{1}{3} (3p|\bar{x}_n^2|4f) \right] \right|^2 \right],$$

and so we find

$$\Gamma_{4f \rightarrow 3p} \propto k^5.$$

The states $4f$ and $3s$ have opposite parity and $|3-0| = 3$, so we must use the third term in the expansion of the exponential. The matrix element appearing in the rate for the transition $4f \rightarrow 3s$ is then

$$-\frac{1}{2} \sum_{ij} k_i k_j (3s|\bar{x}_{ni}\bar{x}_{nj}\mathbf{p}_n|4f).$$

The product of three spatial vectors contains a term which behaves as an operator with $j = 3$ (and also terms with lower values of j), and so this matrix element will be non-vanishing if $|j_a - j_b| \leq 3$. Following the same logic as above, the rate for the transition $4f \rightarrow 3s$ then has an additional factor k^4 as compared to the rate $\Gamma_{4f \rightarrow 3d}$, and so we find

$$\Gamma_{4f \rightarrow 3s} \propto k^7.$$

3. Consider the theory of a real scalar field $\varphi(\mathbf{x}, t)$, interacting with a set of particles with coordinates $\mathbf{x}_n(t)$. Take the Lagrangian as

$$L(t) = \frac{1}{2} \int d^3x \left[\left(\frac{\partial \varphi(\mathbf{x}, t)}{\partial t} \right)^2 - c^2 (\nabla \varphi(\mathbf{x}, t))^2 - \mu^2 \varphi^2(\mathbf{x}, t) \right] - \sum_n g_n \varphi(\mathbf{x}_n(t), t) + \sum_n \frac{m_n}{2} (\dot{\mathbf{x}}_n(t))^2 - V(\mathbf{x}(t)),$$

where μ , m_n and g_n are real parameters, and V is a real local function of the differences of the particle coordinates.

- Find the field equations and commutation rules for φ .
- Find the Hamiltonian for the whole system.
- Express φ in the interaction picture in terms of operators that create and destroy the quanta of the scalar field.
- Calculate the energy and momentum of these quanta.
- Give a general formula for the rate of emission per solid angle of a single φ quantum in a transition between eigenstates of the matter part of the Hamiltonian (that is, the part of the Hamiltonian involving only the coordinates \mathbf{x}_n and their canonical conjugates).
- Integrate this formula over solid angles in the case where the wavelength of the emitted quanta is much larger than the size of the initial and final particle system. What are the selection rules for these transitions?

We begin with a Lagrangian of the form

$$L(t) = \frac{1}{2} \int d^3x \left[\left(\frac{\partial \varphi(\mathbf{x}, t)}{\partial t} \right)^2 - c^2 (\nabla \varphi(\mathbf{x}, t))^2 - \mu^2 \varphi^2(\mathbf{x}, t) \right] - \sum_n g_n \varphi(\mathbf{x}_n(t), t) + \sum_n \frac{m_n}{2} (\dot{\mathbf{x}}(t))^2 - V(\mathbf{x}(t)).$$

We can rewrite this Lagrangian as

$$L(t) = \int d^3x \mathcal{L}(\mathbf{x}, t) + \sum_n \frac{m_n}{2} (\dot{\mathbf{x}}(t))^2 - V(\mathbf{x}(t)),$$

where we have defined the Lagrangian density for the field φ

$$\mathcal{L}(\mathbf{x}, t) = \frac{1}{2} \left(\frac{\partial \varphi(\mathbf{x}, t)}{\partial t} \right)^2 - \frac{c^2}{2} (\nabla \varphi(\mathbf{x}, t))^2 - \frac{\mu^2}{2} \varphi^2(\mathbf{x}, t) - \sum_n g_n \varphi(\mathbf{x}, t) \delta^3(\mathbf{x} - \mathbf{x}_n(t)).$$

(a) The Euler–Lagrange field equations are given by Eq. (11.1.9)

$$\frac{\partial \mathcal{L}}{\partial \varphi} - \frac{\partial}{\partial x_i} \frac{\partial \mathcal{L}}{\partial (\partial_i \varphi)} = \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\varphi}},$$

which in this case read

$$-\mu^2 \varphi(\mathbf{x}, t) - \sum_n g_n \delta^3(\mathbf{x} - \mathbf{x}_n(t)) + c^2 \nabla^2 \varphi(\mathbf{x}, t) = \ddot{\varphi}(\mathbf{x}, t).$$

We can also find the field equation for $\mathbf{x}_n(t)$ which is given by

$$\frac{\partial}{\partial t} \left(\frac{\delta L}{\delta \dot{x}_{ni}} \right) = \frac{\delta L}{\delta x_{ni}},$$

which gives in this case

$$\ddot{x}_{ni}(t) = -\frac{\partial V(\mathbf{x}_n(t))}{\partial x_{ni}} - g_n \frac{\partial \varphi(\mathbf{x}_n(t), t)}{\partial x_{ni}}.$$

The canonical conjugate to φ is

$$\pi(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} = \dot{\varphi}(\mathbf{x}, t).$$

Since there are no constraints, the field φ and its conjugate π obey canonical commutation relations

$$\begin{aligned} [\varphi(\mathbf{x}, t), \pi(\mathbf{y}, t)] &= i\hbar \delta^3(\mathbf{x} - \mathbf{y}) \\ [\varphi(\mathbf{x}, t), \varphi(\mathbf{y}, t)] &= [\pi(\mathbf{x}, t), \pi(\mathbf{y}, t)] = 0. \end{aligned}$$

(b) The Hamiltonian for the system is

$$H = \int d^3x \pi(\mathbf{x}, t) \dot{\varphi}(\mathbf{x}, t) + \mathbf{p}_n(t) \cdot \dot{\mathbf{x}}_n(t) - L(t),$$

where we have defined the canonical conjugate of \mathbf{x}_n

$$p_{ni}(t) = \frac{\delta L}{\delta \dot{x}_{ni}} = m_n \dot{x}_{ni}(t).$$

The Hamiltonian is then given by

$$\begin{aligned} H &= \frac{1}{2} \int d^3x [\pi^2(\mathbf{x}, t) + c^2 (\nabla \varphi(\mathbf{x}, t))^2 + \mu^2 \varphi^2(\mathbf{x}, t)] \\ &\quad + \sum_n g_n \varphi(\mathbf{x}_n(t), t) + \sum_n \frac{(\mathbf{p}_n(t))^2}{2m_n} + V(\mathbf{x}(t)). \end{aligned}$$

We can rewrite this in terms of a free Hamiltonian and an interaction

$$H = H_{0\varphi} + H_{0\text{mat}} + H_{\text{int}},$$

where we have defined

$$H_{0\varphi} = \frac{1}{2} \int d^3x \left[\pi^2(\mathbf{x}, t) + c^2 (\nabla\varphi(\mathbf{x}, t))^2 + \mu^2\varphi^2(\mathbf{x}, t) \right]$$

$$H_{0\text{mat}} = \sum_n \frac{(\mathbf{p}_n(t))^2}{2m_n} + V(\mathbf{x}(t))$$

$$H_{\text{int}} = \sum_n g_n \varphi(\mathbf{x}_n(t), t).$$

- (c) Now we will introduce the interaction picture field φ_I whose time-dependence is governed by $H_{0\varphi}$

$$\dot{\varphi}_I = \frac{i}{\hbar} [H_{0\varphi}, \varphi_I] = \pi_I$$

$$\dot{\pi}_I = \frac{i}{\hbar} [H_{0\varphi}, \pi_I] = c^2 \nabla^2 \varphi_I - \mu^2 \varphi_I = \ddot{\varphi}_I.$$

The interaction picture field and its canonical conjugate obey the same commutation relations as the Heisenberg picture fields

$$[\varphi_I(\mathbf{x}, t), \pi_I(\mathbf{y}, t)] = i\hbar \delta^3(\mathbf{x} - \mathbf{y})$$

$$[\varphi_I(\mathbf{x}, t), \varphi_I(\mathbf{y}, t)] = [\pi_I(\mathbf{x}, t), \pi_I(\mathbf{y}, t)] = 0.$$

The wave equation for φ_I reads

$$\ddot{\varphi}_I = c^2 \nabla^2 \varphi_I - \mu^2 \varphi_I.$$

This can be solved by writing φ_I as a Fourier integral

$$\varphi_I(\mathbf{x}, t) = \int d^3k \left[e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\omega t} \alpha(\mathbf{k}) + e^{-i\mathbf{k}\cdot\mathbf{x}} e^{i\omega t} \alpha^\dagger(\mathbf{k}) \right].$$

Plugging this expression into the wave equation gives

$$-\omega^2 \varphi_I = -c^2 k^2 \varphi_I - \mu^2 \varphi_I,$$

and so we can solve for ω

$$\omega = \sqrt{c^2 k^2 + \mu^2}.$$

The canonical conjugate for φ can then be expressed as

$$\pi_I(\mathbf{x}, t) = \dot{\varphi}_I = -i \int d^3k \omega \left[e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\omega t} \alpha(\mathbf{k}) - e^{-i\mathbf{k}\cdot\mathbf{x}} e^{i\omega t} \alpha^\dagger(\mathbf{k}) \right].$$

We can work out the commutators of $\alpha(\mathbf{k})$ and $\alpha^\dagger(\mathbf{k})$ by requiring that we recover the correct commutation relations for φ_I and π_I

$$[\varphi_I(\mathbf{x}, t), \pi_I(\mathbf{y}, t)] = -i \int d^3k \int d^3k' \omega' \left[e^{i(\mathbf{k}\cdot\mathbf{x} + \mathbf{k}'\cdot\mathbf{y})} e^{-i(\omega t + \omega' t)} [\alpha(\mathbf{k}), \alpha(\mathbf{k}')] \right. \\ \left. + e^{i(-\mathbf{k}\cdot\mathbf{x} + \mathbf{k}'\cdot\mathbf{y})} e^{i(\omega t - \omega' t)} [\alpha^\dagger(\mathbf{k}), \alpha(\mathbf{k}')] \right]$$

$$\begin{aligned}
& - e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})} e^{i(-\omega t+\omega' t)} [\alpha(\mathbf{k}), \alpha^\dagger(\mathbf{k}')] \\
& - e^{i(-\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})} e^{i(\omega t+\omega' t)} [\alpha^\dagger(\mathbf{k}), \alpha^\dagger(\mathbf{k}')] \Big] \\
& = i\hbar\delta^3(\mathbf{x}-\mathbf{y}).
\end{aligned}$$

This expression is time-independent, so the first and the fourth terms must vanish, which requires

$$[\alpha(\mathbf{k}), \alpha(\mathbf{k}')] = [\alpha^\dagger(\mathbf{k}), \alpha^\dagger(\mathbf{k}')] = 0,$$

and this condition immediately guarantees that

$$[\varphi_I(\mathbf{x}, t), \varphi_I(\mathbf{y}, t)] = [\pi_I(\mathbf{x}, t), \pi_I(\mathbf{y}, t)] = 0.$$

For the remaining terms, we can express $\delta^3(\mathbf{x}-\mathbf{y})$ as a Fourier integral

$$\delta^3(\mathbf{x}-\mathbf{y}) = \frac{1}{(2\pi)^3} \int d^3k e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}.$$

We can now read off the remaining commutator

$$[\alpha(\mathbf{k}), \alpha^\dagger(\mathbf{k}')] = \frac{\hbar}{(2\pi)^3 2\omega} \delta^3(\mathbf{k}-\mathbf{k}').$$

Now, we can rewrite $\alpha(\mathbf{k})$ in terms of $a(\mathbf{k})$ which has simple commutation relations

$$\alpha(\mathbf{k}) = \sqrt{\frac{\hbar}{(2\pi)^3 2\omega}} a(\mathbf{k}).$$

The commutation relations for $a(\mathbf{k})$ and $a^\dagger(\mathbf{k})$ are then

$$\begin{aligned}
[a(\mathbf{k}), a^\dagger(\mathbf{k}')] &= \delta^3(\mathbf{k}-\mathbf{k}') \\
[a(\mathbf{k}), a(\mathbf{k}')] &= [a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')] = 0,
\end{aligned}$$

which we recognize as the commutation relations of creation and annihilation operators. We can then express the interaction picture field and its conjugate in terms of these creation and annihilation operators

$$\begin{aligned}
\varphi_I(\mathbf{x}, t) &= \int d^3k \sqrt{\frac{\hbar}{(2\pi)^3 2\omega}} [e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\omega t} a(\mathbf{k}) + e^{-i\mathbf{k}\cdot\mathbf{x}} e^{i\omega t} a^\dagger(\mathbf{k})] \\
\pi_I(\mathbf{x}, t) &= -i \int d^3k \omega \sqrt{\frac{\hbar}{(2\pi)^3 2\omega}} [e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\omega t} a(\mathbf{k}) - e^{-i\mathbf{k}\cdot\mathbf{x}} e^{i\omega t} a^\dagger(\mathbf{k})].
\end{aligned}$$

- (d) Let us first write out the free part of the Hamiltonian in terms of creation and annihilation operators. The terms appearing in $H_{0\varphi}$ are, after performing the integrals over \mathbf{x} and \mathbf{k}'

$$\begin{aligned}
\int d^3x \pi_I^2(\mathbf{x}, t) &= - \int d^3k \omega^2 \left(\frac{\hbar}{2\omega} \right) \left[e^{-2i\omega t} a(\mathbf{k})a(-\mathbf{k}) + e^{2i\omega t} a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k}) \right. \\
&\quad \left. - a(\mathbf{k})a^\dagger(\mathbf{k}) - a^\dagger(\mathbf{k})a(\mathbf{k}) \right] \\
\int d^3x c^2 (\nabla\varphi_I(\mathbf{x}, t))^2 &= c^2 \int d^3k \left(\frac{\hbar}{2\omega} \right) k^2 \left[e^{-2i\omega t} a(\mathbf{k})a(-\mathbf{k}) \right. \\
&\quad \left. + e^{2i\omega t} a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k}) + a(\mathbf{k})a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k})a(\mathbf{k}) \right] \\
\int d^3x \mu^2 \varphi_I^2(\mathbf{x}, t) &= \mu^2 \int d^3k \left(\frac{\hbar}{2\omega} \right) \left[e^{-2i\omega t} a(\mathbf{k})a(-\mathbf{k}) + e^{2i\omega t} a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k}) \right. \\
&\quad \left. + a(\mathbf{k})a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k})a(\mathbf{k}) \right].
\end{aligned}$$

Using the dispersion relation $\omega^2 = c^2k^2 + \mu^2$, we can see that all of the time-dependent terms in $H_{0\varphi}$ cancel, and we have

$$H_{0\varphi} = \frac{1}{2} \int d^3k \hbar\omega [a(\mathbf{k})a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k})a(\mathbf{k})].$$

Now, we can calculate the commutators of the Hamiltonian $H_{0\varphi}$ with the operators $a^\dagger(\mathbf{k})$ and $a(\mathbf{k})$

$$\begin{aligned}
[H_{0\varphi}, a^\dagger(\mathbf{k})] &= \hbar\omega a^\dagger(\mathbf{k}) = \hbar\sqrt{c^2k^2 + \mu^2} a^\dagger(\mathbf{k}) \\
[H_{0\varphi}, a(\mathbf{k})] &= -\hbar\omega a(\mathbf{k}) = -\hbar\sqrt{c^2k^2 + \mu^2} a(\mathbf{k}).
\end{aligned}$$

This confirms that $a^\dagger(\mathbf{k})$ and $a(\mathbf{k})$ are raising and lowering operators for the energy, so if a state Ψ is an eigenstate of $H_{0\varphi}$ with eigenvalue E , then the state $a^\dagger(\mathbf{k})\Psi$ is an eigenstate of $H_{0\varphi}$ with eigenvalue $E + \hbar\sqrt{c^2k^2 + \mu^2}$ and the state $a(\mathbf{k})\Psi$ is an eigenstate with eigenvalue $E - \hbar\sqrt{c^2k^2 + \mu^2}$. If we define a state Ψ_0 such that $a(\mathbf{k})\Psi_0 = 0$, then we can construct states of the form

$$\Psi_{\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n} \propto a^\dagger(\mathbf{k}_1)a^\dagger(\mathbf{k}_2) \cdots a^\dagger(\mathbf{k}_n)\Psi_0,$$

which have energy (ignoring the infinite constant E_0 like the one appearing in Eq. (11.6.5))

$$\hbar\sqrt{c^2k_1^2 + \mu^2} + \hbar\sqrt{c^2k_2^2 + \mu^2} + \cdots + \hbar\sqrt{c^2k_n^2 + \mu^2}.$$

We interpret this as a state with n scalar field quanta, with energies

$$\hbar\sqrt{c^2k_1^2 + \mu^2}, \hbar\sqrt{c^2k_2^2 + \mu^2}, \dots, \hbar\sqrt{c^2k_n^2 + \mu^2}.$$

By using the general formula given in Eq. (9.4.4) we can construct a momentum operator \mathbf{P}_φ which is given by

$$\mathbf{P}_\varphi = - \int d^3x \pi_I(\mathbf{x}, t) \nabla\varphi_I(\mathbf{x}, t).$$

The commutators of this operator with the scalar field and its conjugate are

$$\begin{aligned} [\mathbf{P}_\varphi, \varphi_I(\mathbf{x}, t)] &= i\hbar\nabla\varphi_I(\mathbf{x}, t) \\ [\mathbf{P}_\varphi, \pi_I(\mathbf{x}, t)] &= i\hbar\pi_I(\mathbf{x}, t). \end{aligned}$$

From these relations, we can calculate the commutators with the creation and annihilation operators

$$\begin{aligned} [\mathbf{P}_\varphi, a^\dagger(\mathbf{k})] &= \hbar\mathbf{k}a^\dagger(\mathbf{k}) \\ [\mathbf{P}_\varphi, a(\mathbf{k})] &= -\hbar\mathbf{k}a(\mathbf{k}). \end{aligned}$$

So we can see that the state $\Psi_{\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n}$ has momentum

$$\hbar\mathbf{k}_1 + \hbar\mathbf{k}_2 + \dots + \hbar\mathbf{k}_n,$$

and thus the quanta of the scalar field have momenta $\hbar\mathbf{k}_1, \hbar\mathbf{k}_2, \dots, \hbar\mathbf{k}_n$. To summarize the quantum of scalar field created by $a^\dagger(\mathbf{k})$ has energy $\hbar\sqrt{c^2k^2 + \mu^2}$ and momentum $\hbar\mathbf{k}$.

- (e) Let us define states Ψ_a and Ψ_b which are eigenstates of the matter Hamiltonian $H_{0\text{mat}}$

$$H_{0\text{mat}}\Psi_a = E_a\Psi_a, \quad H_{0\text{mat}}\Psi_b = E_b\Psi_b,$$

and are annihilated by $a(\mathbf{k})$

$$a(\mathbf{k})\Psi_a = a(\mathbf{k})\Psi_b = 0,$$

for all \mathbf{k} . If we wish to calculate the rate of single φ quantum emission from $b \rightarrow a$, then we need a state $\Psi_{b\varphi} = \hbar^{-3/2}a^\dagger(\mathbf{k})\Psi_b$ which contains a single φ quantum. To first order in the interaction, the S-matrix takes the form

$$\begin{aligned} S_{b\varphi,a} &= -2\pi i\delta(E_a - E_b - \hbar\sqrt{c^2k^2 + \mu^2})(\Psi_{b\varphi}, V(0)\Psi_a) \\ &= -2\pi i\hbar^{-3/2}\delta(E_a - E_b - \hbar\sqrt{c^2k^2 + \mu^2})(\Psi_b, a(\mathbf{k})V(0)\Psi_a), \end{aligned}$$

where the potential is given by

$$V(0) = \sum_n g_n\varphi_I(\mathbf{x}_n).$$

Plugging this in and using the commutation relation of $a(\mathbf{k})$ with φ , we find

$$\begin{aligned} S_{b\varphi,a} &= -2\pi i\hbar^{-3/2}\delta(E_a - E_b - \hbar\sqrt{c^2k^2 + \mu^2})\left(\Psi_b, a(\mathbf{k})\sum_n g_n\varphi_I(\mathbf{x}_n)\Psi_a\right) \\ &= -\frac{2\pi i\sqrt{\hbar}}{\sqrt{(2\pi)^3}2\omega}\delta(E_a - E_b - \hbar\omega)\sum_n g_n(\Psi_b, e^{-i\mathbf{k}\cdot\mathbf{x}_n}\Psi_a). \end{aligned}$$

If we shift to center-of-mass coordinates

$$\mathbf{X} = \sum_n \frac{m_n \mathbf{x}_n}{M}, \quad M \equiv \sum_n m_n, \quad \bar{\mathbf{x}}_n \equiv \mathbf{x} - \mathbf{X},$$

we can rewrite the matrix element

$$(\Psi_b, e^{-i\mathbf{k}\cdot\mathbf{x}_n} \Psi_a) = (\Psi_{\bar{b}}, e^{-i\mathbf{k}\cdot\bar{\mathbf{x}}_n} \Psi_a),$$

where we have defined

$$\Psi_{\bar{b}} = e^{i\mathbf{k}\cdot\mathbf{X}} \Psi_b,$$

which has momentum

$$\mathbf{P}\Psi_{\bar{b}} = (\mathbf{p}_b + \hbar\mathbf{k}) \Psi_b.$$

We can then write

$$(\Psi_{\bar{b}}, e^{-i\mathbf{k}\cdot\bar{\mathbf{x}}_n} \Psi_a) = \delta^3(\mathbf{p}_b + \hbar\mathbf{k} - \mathbf{p}_a) D_{nba}(\hat{k}),$$

and so the S-matrix element becomes

$$S_{b\varphi,a} = \delta(E_a - E_b - \hbar\omega) \delta^3(\mathbf{p}_b + \hbar\mathbf{k} - \mathbf{p}_a) M_{b\varphi,a},$$

where we have defined

$$M_{b\varphi,a} = \frac{-2\pi i \sqrt{\hbar}}{\sqrt{(2\pi\hbar)^3 2\omega}} \sum_n g_n D_{nba}(\hat{k}).$$

The differential rate of single φ emission is then given by

$$d\Gamma = \frac{1}{2\pi\hbar} |M_{b\varphi,a}|^2 \mu_b \hbar k d\Omega,$$

where the quantity μ_b is defined as

$$\mu_b \equiv \frac{E_b \hbar\omega}{c^2(E_b + \hbar\omega)} \approx \frac{\hbar\omega}{c^2},$$

and the approximate equality holds when $E_b \approx \mu c^2 \gg \hbar\omega$. Putting this all together we arrive at an expression for the emission rate per solid angle

$$\begin{aligned} \frac{d\Gamma(\hat{k})}{d\Omega} &= \frac{1}{2\pi\hbar} \frac{4\pi^2\hbar}{(2\pi\hbar)^3 2\omega} \frac{\hbar\omega}{c} \hbar k \left| \sum_n g_n D_{nba}(\hat{k}) \right|^2 \\ &= \frac{k}{8\pi^2\hbar c^2} \left| \sum_n g_n D_{nba}(\hat{k}) \right|^2. \end{aligned}$$

- (f) Assuming that wavelength of the emitted quantum is much larger than the size of the initial and final system, we can expand the exponential that appears in $D_{nba}(\hat{k})$ to get

$$D_{nba}(\hat{k}) = (b|e^{-i\mathbf{k}\cdot\bar{\mathbf{x}}_n}|a) = (b|(1 - i\mathbf{k}\cdot\bar{\mathbf{x}}_n + \dots)|a),$$

where for any operator \mathcal{O} we can write the matrix element of \mathbf{O} as

$$(\Psi_{\bar{b}}, \mathcal{O}\Psi_a) = \delta^3(\mathbf{p}_b - \mathbf{p}_a - \hbar\mathbf{k}) (b|\mathcal{O}|a).$$

The states Ψ_a and $\Psi_{\bar{b}}$ are orthogonal, so the first term in this expansion vanishes, and the leading term is given by

$$D_{nba}(\hat{k}) = (b|-i\mathbf{k}\cdot\bar{\mathbf{x}}_n|a) = -ik \sum_i \hat{k}_i (b|\bar{x}_{ni}|a).$$

The matrix element $(b|\bar{x}_{ni}|a)$ is independent of the direction \hat{k} , so we can integrate the differential rate to find the total decay rate

$$\frac{d\Gamma(\hat{k})}{d\Omega} = \frac{k^3}{8\pi^2\hbar c^2} \sum_{nmij} g_n g_m \hat{k}_i \hat{k}_j (b|\bar{x}_{ni}|a) (b|\bar{x}_{mj}|a)^*.$$

Using the formula $\int d\Omega \hat{k}_i \hat{k}_j = \frac{4\pi}{3} \delta_{ij}$, we find for the total decay rate

$$\Gamma = \frac{k^3}{6\pi\hbar c^2} \left| \sum_n g_n (b|\bar{\mathbf{x}}_n|a) \right|^2.$$

The operator $\bar{\mathbf{x}}_n$ is a spatial vector and so acts as an operator with $j = 1$ under rotations. As a result, matrix elements $(b|\bar{\mathbf{x}}_n|a)$ will vanish unless $|j_a - j_b| \leq 1 \leq j_a + j_b$. Also, $\bar{\mathbf{x}}_n$ changes sign under spatial reflection, so $(b|\bar{\mathbf{x}}_n|a)$ will vanish unless the states Ψ_a and Ψ_b have opposite parity.

4. Express the coherent state $\Phi_{\mathcal{A}}$ as a superposition of states (11.6.7) with definite numbers of photons.

The coherent state is defined in Eq. (11.6.17) as

$$a(\mathbf{k}, \sigma)\Phi_{\mathcal{A}} = \mathcal{A}(\mathbf{k}, \sigma)\Phi_{\mathcal{A}}.$$

As discussed at the end of Section 11.6, the state $\Phi_{\mathcal{A}}$ must contain an infinite number of photons, and so we expect the coherent state to take the form

$$\Phi_{\mathcal{A}} = \sum_{n=0}^{\infty} C_n (a^\dagger(\mathbf{k}, \sigma))^n \Psi_0,$$

where the C_n are normalization constants which we will determine below and Ψ_0 is the state defined in Eq. (11.6.3) as the state which obeys

$$a(\mathbf{k}, \sigma)\Psi_0 = 0.$$

Recall the commutation relations for $a(\mathbf{k}, \sigma)$ given in Eqs. (11.5.24) and (11.5.25)

$$\begin{aligned} [a(\mathbf{k}, \sigma), a^\dagger(\mathbf{k}', \sigma')] &= \delta_{\sigma\sigma'}\delta^3(\mathbf{k} - \mathbf{k}') \\ [a(\mathbf{k}, \sigma), a(\mathbf{k}', \sigma')] &= [a^\dagger(\mathbf{k}, \sigma), a^\dagger(\mathbf{k}', \sigma')] = 0. \end{aligned}$$

We will make the assumption that we can put the system in a large but finite box so that \mathbf{k} takes discrete values and the commutator contains a Kronecker delta function for momenta rather than a Dirac delta function. This means that the commutator for equal momenta is 1 rather than being infinite. The continuum limit can be recovered by taking the volume of the box to infinity. With this subtlety aside, and temporarily dropping the momentum and helicity arguments, the defining equation for the coherent state reads

$$a \sum_{n=0}^{\infty} C_n (a^\dagger)^n \Psi_0 = \mathcal{A} \sum_{n=0}^{\infty} C_n (a^\dagger)^n \Psi_0,$$

and using the commutation relations of a and a^\dagger we find a recursion relation for the C_n

$$nC_n = \mathcal{A}C_{n-1}.$$

We can then write all of the C_n in terms of C_0 as

$$C_n = \frac{\mathcal{A}^n}{n!} C_0.$$

To find C_0 , we require that the coherent state is normalized

$$1 = (\Phi_{\mathcal{A}}, \Phi_{\mathcal{A}}) = |C_0|^2 \left(\Psi_0, \sum_{m=0}^{\infty} \frac{\mathcal{A}^{*m}}{m!} a^m \sum_{n=0}^{\infty} \frac{\mathcal{A}^n}{n!} (a^\dagger)^n \Psi_0 \right).$$

Each term for which $m \neq n$ vanishes in this double sum because $a\Psi_0 = 0$, and so the expression becomes a single sum

$$1 = |C_0|^2 \left(\Psi_0, \sum_{n=0}^{\infty} \frac{|\mathcal{A}|^{2n}}{(n!)^2} a^n (a^\dagger)^n \Psi_0 \right).$$

Now we can move each of the factors of a past all of the factors of a^\dagger picking up commutators and use the fact that a annihilates the state Ψ_0 to replace all of the factors of a and a^\dagger in this expression with $n!$

$$1 = |C_0|^2 \left(\Psi_0, \sum_{n=0}^{\infty} \frac{|\mathcal{A}|^{2n}}{n!} \Psi_0 \right) = |C_0|^2 \sum_{n=0}^{\infty} \frac{|\mathcal{A}|^{2n}}{n!} = |C_0|^2 \exp(|\mathcal{A}|^2).$$

Up to an arbitrary phase, we can then write C_0 as

$$C_0 = \exp(-|\mathcal{A}|^2/2).$$

Now we can express the coherent state (restoring momentum and helicity arguments) as

$$\begin{aligned}\Phi_{\mathcal{A}} &= \exp(-|\mathcal{A}(\mathbf{k}, \sigma)|^2/2) \sum_{n=0}^{\infty} \frac{(\mathcal{A}(\mathbf{k}, \sigma)a^\dagger(\mathbf{k}, \sigma))^n}{n!} \Psi_0 \\ &= \exp(-|\mathcal{A}(\mathbf{k}, \sigma)|^2/2) \exp(\mathcal{A}(\mathbf{k}, \sigma)a^\dagger(\mathbf{k}, \sigma)) \Psi_0.\end{aligned}$$