1. Consider a positively-charged spin-1/2 particle in an external magnetic field, governed by the Hamiltonian:

$$H = H_0\,\mathbf{I} - \gamma\vec{\boldsymbol{B}}\boldsymbol{\cdot}\vec{\boldsymbol{S}}\,,$$

where $\mathbf{I}$ is the identity operator in spin space, $\vec{\boldsymbol{S}}$ is the vector of spin-1/2 spin matrices, and γ is a constant (for a positively-charged particle, $\gamma > 0$). H_0 is spin-independent and is independent of the magnetic field $\vec{\boldsymbol{B}}$. For simplicity, assume that H_0 possesses exactly one eigenvalue, which is denoted by E.

(a) If the magnetic field is given by $\vec{\boldsymbol{B}} = B\hat{\boldsymbol{z}}$ (where $B > 0$), determine the energy eigenstates and eigenvalues of H.

Since H_0 is spin-independent, it follows that the both H_0 and H commute with $\vec{\boldsymbol{S}}^2$ and S_z. Consequently, the eigenstates of H can be chosen to be simultaneous eigenstates of $\vec{\boldsymbol{S}}^2$ and S_z. Under the assumptions of this problem,

$$H_0\left|\tfrac{1}{2}\,m_s\right\rangle = E\left|\tfrac{1}{2}\,m_s\right\rangle\,, \qquad\qquad m_s = -\tfrac{1}{2}\,,\,+\tfrac{1}{2}\,.$$

Using $S_z\left|\tfrac{1}{2}\,m_s\right\rangle = \hbar m_s\left|\tfrac{1}{2}\,m_s\right\rangle$, it follows that:

$$H\left|\tfrac{1}{2}\,m_s\right\rangle = [H_0\mathbf{I} - \gamma B S_z]\left|\tfrac{1}{2}\,m_s\right\rangle = (E - \hbar m_s\gamma B)\left|\tfrac{1}{2}\,m_s\right\rangle$$

In what follows, we shall denote the two possible energy eigenvalues by:

$$E_{m_s} = E - \hbar m_s\gamma B\,, \qquad\qquad m_s = \pm\tfrac{1}{2}\,.$$

In particular, the energy difference of the two states is given by:

$$E_{-1/2} - E_{+1/2} = \hbar\gamma B\,, \tag{1}$$

which implies that $E_{-1/2} > E_{+1/2}$ if $\gamma > 0$.

(b) Assume that the magnetic field is given by $\vec{\boldsymbol{B}} = B\hat{\boldsymbol{z}}$ for time $t < 0$. The system is initially observed to be in a spin-up state. At $t = 0$, a time-dependent perturbation is added by modifying the magnetic field. The new magnetic field for $t > 0$ is given by:

$$\vec{\boldsymbol{B}} = b\,(\hat{\boldsymbol{x}}\cos\omega t - \hat{\boldsymbol{y}}\sin\omega t) + B\hat{\boldsymbol{z}}\,,$$

where $b > 0$. Using first-order time-dependent perturbation theory, derive an expression for the probability that the system will be found in a spin-down state at some later time $t = T$. For what range of values of ω is this result reliable?

We shall denote $c_{m_s}(t)$ as the probability amplitude for the spin-$\frac{1}{2}$ to be in an eigenstate of S_z with eigenvalue $\hbar m_s$ at time t. In particular [cf. eq. (18.2.3) on p. 474 of Shankar],

$$|\psi(t)\rangle = \sum_{m_s} c_{m_s}(t)\, e^{-iE_{m_s}t/\hbar} \left|\tfrac{1}{2}\, m_s\right\rangle ,$$

where the sum runs over the two possible values of $m_s = \pm\frac{1}{2}$. Using first-order time-dependent perturbation theory [cf. eq. (18.2.9) on p. 475 of Shankar],

$$c_{-1/2}(t) = c_{-1/2}(0) - \frac{i}{\hbar}\int_0^t \left\langle \tfrac{1}{2}\ -\tfrac{1}{2}\right| H^{(1)}(t) \left|\tfrac{1}{2}\ \ \tfrac{1}{2}\right\rangle e^{i(E_{-1/2}-E_{+1/2})t'/\hbar}\, dt' , \qquad (2)$$

The time-dependent perturbing Hamiltonian is given by:

$$H^{(1)}(t) = -\gamma b(S_x\cos\omega t - S_y \sin\omega t) = -\tfrac{1}{2}\hbar\gamma b(\sigma_x \cos\omega y - \sigma_y\sin\omega t) = -\tfrac{1}{2}\hbar\gamma b\begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0\end{pmatrix} .$$

Thus,

$$\left\langle \tfrac{1}{2}\ -\tfrac{1}{2}\right| H^{(1)}(t) \left|\tfrac{1}{2}\ \ \tfrac{1}{2}\right\rangle = -\tfrac{1}{2}\gamma b \begin{pmatrix} 0 & 1\end{pmatrix}\begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0\end{pmatrix}\begin{pmatrix} 1 \\ 0\end{pmatrix} = -\tfrac{1}{2}\gamma b e^{-i\omega t} .$$

By assumption, the system is observed in a spin-up state at $t = 0$, so that $c_{-1/2}(0) = 0$. Eqs. (1) and (2) then yield:

$$c_{-1/2}(t) = \tfrac{1}{2}i\gamma b\int_0^t e^{i(\gamma B-\omega)t'}\, dt' = \frac{\gamma b}{2(\gamma B-\omega)}\left[e^{i(\gamma B-\omega)t} - 1\right] .$$

The state is observed at time $t = T$. The probability that the state will be observed as spin-down is $P_{\frac{1}{2}\to-\frac{1}{2}} = |c_{-1/2}(T)|^2$. Explicitly,

$$\begin{aligned} P_{\frac{1}{2}\to-\frac{1}{2}} = |c_{-1/2}(T)|^2 &= \frac{\gamma^2 b^2}{4(\gamma B-\omega)^2}\left[e^{i(\gamma B-\omega)T} - 1\right]\left[e^{-i(\gamma B-\omega)T} - 1\right] \\ &= \frac{\gamma^2 b^2}{2(\gamma B-\omega)^2}\left(1 - \cos(\gamma B-\omega)T\right] \end{aligned}$$

Using the identity $\sin^2(\theta/2) \equiv \frac{1}{2}(1-\cos\theta)$, it follows that:

$$\boxed{P_{\frac{1}{2}\to-\frac{1}{2}} = |c_{-1/2}(T)|^2 = \frac{\gamma^2 b^2}{(\gamma B-\omega)^2}\sin^2\left[\tfrac{1}{2}(\gamma B-\omega)T\right]} \qquad (3)$$

First-order perturbation theory is valid if $P_{\frac{1}{2}\to-\frac{1}{2}} \ll 1$. Since the sine function in eq. (3) can be as large as 1, it follows that the coefficient of the sine must be small. Hence,

$$\left|\frac{\gamma b}{\gamma B-\omega}\right| \ll 1 . \qquad (4)$$

That is, ω cannot be too close in value to γB. Assuming that $|\gamma B - \omega| = \mathcal{O}(\gamma B)$, then one must also satisfy $b \ll B$ to ensure that the first-order perturbative result is reliable.[1]

2. Consider the scattering of spinless particles in an attractive exponential spherically symmetric potential:

$$V(r) = -V_0 \exp(-r/r_0)\,, \tag{5}$$

with $V_0 > 0$. It is convenient to define two dimensionless variables for this problem: $\xi \equiv kr_0$ and $\eta \equiv 2mV_0 r_0^2/\hbar^2$, where $\hbar^2 k^2/(2m)$ is the energy of the incoming beam.

(a) Compute, the scattering amplitude and the differential and total cross sections, in the Born approximation, in terms of the variables ξ, η and r_0. Evaluate the total cross section in the low energy limit.

The scattering amplitude in the Born approximation, in the case of a spherically symmetric potential, depends only on the scattering angle θ, and is given by [cf. eq.(19.3.8) on p. 531 of Shankar]:

$$f(\theta) = \frac{-2m}{\hbar^2}\int_0^\infty \frac{\sin qr}{q}\, V(r) r\, dr\,, \qquad \text{where} \quad q = 2k\sin(\theta/2)\,.$$

Using eq. (5) for $V(r)$ and defining $\eta \equiv 2mV_0 r_0^2/\hbar^2$, it follows that:

$$\begin{aligned}
f(\theta) &= \frac{\eta}{qr_0^2}\int_0^\infty r\, e^{-r/r_0}\, \sin qr\, dr \\
&= \frac{\eta}{qr_0^2}\,\mathrm{Im}\int_0^\infty r\, \exp\left\{-\frac{r}{r_0} + iqr\right\} dr \\
&= \frac{\eta}{qr_0^2}\,\mathrm{Im}\, \exp\left\{-\frac{r}{r_0} + iqr\right\}\left[\frac{r}{iq - \dfrac{1}{r_0}} - \frac{1}{\left(iq - \dfrac{1}{r_0}\right)^2}\right]\Bigg|_0^\infty \\
&= \frac{\eta}{qr_0^2}\,\mathrm{Im}\,\frac{1}{\left(iq - \dfrac{1}{r_0}\right)^2} = \frac{\eta}{qr_0^2}\,\mathrm{Im}\,\frac{\left(iq + \dfrac{1}{r_0}\right)^2}{\left(q^2 + \dfrac{1}{r_0^2}\right)^2} = \frac{2\eta}{r_0^3}\frac{1}{\left(q^2 + \dfrac{1}{r_0^2}\right)^2} \\
&= \frac{2\eta r_0}{(1 + q^2 r_0^2)^2}\,.
\end{aligned}$$

[1]Normally, one might have guessed that the reliability of the first-order perturbation theory result should depend only on the magnitude of b, since the perturbing Hamiltonian is proportional to b. This is true as long as one is far from the resonance condition. As noted above, if $|\gamma B - \omega| \sim \mathcal{O}(\gamma B)$, then the first-order perturbation theory result is reliable if $b \ll B$. However, if the resonance condition is exactly satisfied, then eq. (4) cannot be satisfied no matter how small b is, in which case the first-order perturbation theory result can never be reliable.

Inserting $q^2 = 4k^2 \sin^2(\theta/2) = 2k^2(1 - \cos\theta)$ into the above result yields:

$$\boxed{f(\theta) = \frac{2\eta r_0}{\left[1 + 2\xi^2(1 - \cos\theta)\right]^2}} \tag{6}$$

where $\xi \equiv kr_0$.

Using eq. (6), we can compute the differential cross-section:

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{4\eta^2 r_0^2}{\left[1 + 2\xi^2(1 - \cos\theta)\right]^4}} \tag{7}$$

Integrating over angles,

$$\sigma = 8\pi\eta^2 r_0^2 \int_{-1}^{1} \frac{d\cos\theta}{(1 + 2\xi^2 - 2\xi^2\cos\theta)^4} = \frac{8\pi\eta^2 r_0^2}{6\xi^3(1 + 2\xi^2 - 2\xi^2\cos\theta)^3}\Bigg|_{-1}^{1},$$

which yields

$$\boxed{\sigma = \frac{4\pi\eta^2 r_0^2}{3\xi^2}\left(1 - \frac{1}{(1 + 4\xi^2)^3}\right)}$$

In the low energy limit, $\xi \to 0$ and

$$1 - \frac{1}{(1 + 4\xi^2)^3} = 1 - (1 - 12\xi^2) + \mathcal{O}(\xi^4) \simeq 12\xi^2 .$$

Hence,

$$\boxed{\sigma \simeq 16\pi\eta^2 r_0^2 , \qquad \text{as } \ \xi \to 0} \tag{8}$$

(b) Using the scattering amplitude obtained in part (a), calculate the s-wave and p-wave phase shifts. [*NOTE*: it is sufficient to evaluate $e^{i\delta_\ell}\sin\delta_\ell$ for $\ell = 0,\, 1$.]

The partial wave expansion for $f(\theta)$ is given by eq. (19.5.17) on p. 548 of Shankar:

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell + 1)\, e^{i\delta_\ell}\ \sin\delta_\ell\, P_\ell(\cos\theta) . \tag{9}$$

By using the orthogonality relation of the Legendre polynomials,

$$\int_{-1}^{1} P_\ell(\cos\theta) P_{\ell'}(\cos\theta) d\cos\theta = \frac{2}{2\ell + 1}\,\delta_{\ell\ell'} ,$$

we can project out $e^{i\delta_\ell}\sin\delta_\ell$ from eq. (9) by multiplying both sides of eq. (9) by $P_{\ell'}(\cos\theta)$ and integrating over $\cos\theta$ using the orthogonality relation above. We then obtain:

$$e^{i\delta_\ell}\sin\delta_\ell = \tfrac{1}{2}k\int_{-1}^{1} f(\theta)\, P_\ell(\cos\theta)\, d\cos\theta . \tag{10}$$

Inserting the expression for $f(\theta)$ obtained in eq. (6) for the cases of $\ell = 0$ (s-wave) and $\ell = 1$ (p-wave), we obtain:

$$\begin{aligned} e^{i\delta_0}\sin\delta_0 = \eta\xi\int_{-1}^{1}\frac{d\cos\theta}{(1+2\xi^2-2\xi^2\cos\theta)^2} &= \frac{\eta}{2\xi(1+2\xi^2-2\xi^2\cos\theta)}\bigg|_{-1}^{1} \\ &= \frac{\eta}{2\xi}\left(1-\frac{1}{1+4\xi^2}\right) = \frac{2\xi\eta}{1+4\xi^2}\,, \end{aligned} \tag{11}$$

and

$$\begin{aligned} e^{i\delta_1}\sin\delta_1 &= \eta\xi\int_{-1}^{1}\frac{\cos\theta\, d\cos\theta}{(1+2\xi^2-2\xi^2\cos\theta)^2} \\ &= \frac{\eta}{4\xi^3}\left[\ln(1+2\xi^2-2\xi^2\cos\theta)+\frac{1+2\xi^2}{1+2\xi^2-2\xi^2\cos\theta}\right]\bigg|_{-1}^{1} \\ &= \frac{\eta}{4\xi^3}\left[(1+2\xi^2)\left(1-\frac{1}{1+4\xi^2}\right)-\ln(1+4\xi^2)\right] \\ &= \eta\left[\frac{1+2\xi^2}{\xi(1+4\xi^2)}-\frac{1}{4\xi^3}\,\ln(1+4\xi^2)\right]\,. \end{aligned}$$

In summary, we have obtained:

$$\boxed{e^{i\delta_0}\sin\delta_0 = \frac{2\xi\eta}{1+4\xi^2}} \tag{12}$$

and

$$\boxed{e^{i\delta_1}\sin\delta_1 = \eta\left[\frac{1+2\xi^2}{\xi(1+4\xi^2)}-\frac{1}{4\xi^3}\,\ln(1+4\xi^2)\right]} \tag{13}$$

An alternative method for deriving the above results can be found in Appendices 1 and 2.

(c) Using the results of part (b), compute both the s-wave and p-wave phase shifts in the low energy limit. Do you find the expected behavior at low energies?

In the low energy limit, $\xi \to 0$, eq. (12) reduces to:

$$\boxed{e^{i\delta_0}\sin\delta_0 \simeq \delta_0 \simeq 2\eta\xi\,, \qquad \text{as}\ \ \xi\to 0} \tag{14}$$

For the case of $\ell = 1$, we must expand:

$$\begin{aligned} \frac{1+2\xi^2}{\xi(1+4\xi^2)}-\frac{1}{4\xi^3}\,\ln(1+4\xi^2) &= \frac{1+2\xi^2}{\xi}\left[1-4\xi^2+16\xi^4+\cdots\right]-\frac{1}{4\xi^3}\left[4x^2-\tfrac{1}{2}(4\xi^2)^2+\tfrac{1}{3}(4\xi^2)^3+\cdots\right] \\ &= \left[\frac{1}{\xi}-2\xi+8\xi^3+\cdots\right]-\left[\frac{1}{\xi}-2\xi+\tfrac{16}{3}\xi^3+\cdots\right] \\ &= \tfrac{8}{3}\xi^3+\mathcal{O}(\xi^5)\,. \end{aligned}$$

Hence, eq. (13) yields:

$$\boxed{e^{i\delta_1}\sin\delta_1 \simeq \delta_1 \simeq \tfrac{8}{3}\eta\xi^3\,, \qquad \text{as}\quad \xi\to 0} \tag{15}$$

As expected, $\delta_\ell \propto \xi^{2\ell+1}$ as $\xi \to 0$ so that $\delta_1 \ll \delta_0 \ll 1$ at low-energies, in which case the s-wave scattering dominates.

(d) At low energies, the angular distribution of scattering is approximately given by

$$\frac{d\sigma}{d\Omega} = A + B\cos\theta\,. \tag{16}$$

Using the results of parts (b) and (c), compute the leading behavior of B/A as $k \to 0$. Are your results consistent with the differential cross section obtained in part (a)?

Keeping only the s and p wave contributions to the scattering amplitude, eq. (9) yields

$$f(\theta) \simeq \frac{1}{k}\left[e^{i\delta_0}\sin\delta_0 + 3e^{i\delta_1}\sin\delta_1\cos\theta\right]\,.$$

For a consistent expansion, we need to keep terms up to an including $\mathcal{O}(\xi^3)$. Hence, eq. (11) implies that

$$e^{i\delta_0}\sin\delta_0 \simeq \delta_0 \simeq 2\eta\xi(1-4\xi^2)\,, \qquad \text{as } \xi\to 0\,. \tag{17}$$

Using the results from eqs. (15) and (17), it follows that

$$f(\theta) \simeq \frac{2\eta\xi}{k}\left[1-4\xi^2(1-\cos\theta)\right]\,.$$

Hence,

$$\frac{d\sigma}{d\Omega} = \frac{4\eta^2\xi^2}{k^2}\left[1-8\xi^2(1-\cos\theta)+\mathcal{O}(\xi^4)\right]\,. \tag{18}$$

Noting that $\xi \equiv kr_0$, we see that eq. (18) coincides with the $\mathcal{O}(k^2)$ expansion of eq. (7).

Finally, by comparing with eq. (16), it follows that

$$\frac{B}{A} = \frac{8\xi^2}{1-8\xi^2} \simeq 8k^2r_0^2\,, \qquad \text{as } k\to 0\,.$$

3. Consider the hydrogen atom, where the fine structure and the Lamb shift are included, but the hyperfine structure is neglected. The three lowest energy states (in order of increasing energy) are: $1s_{1/2}$, $2p_{1/2}$, and $2s_{1/2}$, where the notation $n\ell_j$ is used to label the states. The latter two states are separated by the Lamb shift ($\nu = 1057$ MHz).

(a) Using selection rules, determine to which state the $2s_{1/2}$ state can decay via an $E1$ transition.

The selection rules for an E1 decay, $A \to B + \gamma$ are:

$$\Delta j \equiv j_A - j_B = \pm 1 \text{ or } 0 \quad (j_A = j_B = 0 \text{ prohibited})\,, \qquad \text{and} \quad \Pi(A) = -\Pi(B)\,,$$

where j_A is the total angular momentum of the state A and $\Pi(A) = (-1)^{\ell_A}$ is the parity of the state A (which depends on the orbital angular momentum ℓ_A of the state A). The restrictions on the total angular momentum are a consequence of the Wigner-Eckart theorem, since the dipole operator $\vec{\boldsymbol{d}} = \vec{\boldsymbol{x}}$ is a spherical tensor or rank 1. Note that a convenient way to summarize the angular momentum selection rule is:

$$|j_A - j_B| \leq 1 \leq j_A + j_B\,.$$

The parity selection rule follows from the fact that $\vec{\boldsymbol{d}}$ is odd under inversion, $\vec{\boldsymbol{x}} \to -\vec{\boldsymbol{x}}$.

We apply these considerations to the energy levels of hydrogen that lie below the $2s_{1/2}$ state: In both cases, we have $j_A = j_B = \frac{1}{2}$, so the angular momentum selection rule is

Energy level	Parity change?	Δj
$2p_{1/2}$	yes	0
$1s_{1/2}$	no	0

satisfied. Invoking the parity selection rule, we conclude that the only possible E1 decay is $2s_{1/2} \to 2p_{1/2} + \gamma\,.$

(b) Compute the $E1$ transition rate for the decay of the $2s_{1/2}$ state and determine the numerical value of the corresponding lifetime. Compare this result with the lifetime of the $2p$ state of hydrogen computed in class.

In class, we obtained the following expression for the decay rate (or equivalently the inverse lifetime) of an $E1$ transition,

$$\Gamma = \tau^{-1} = \frac{4\omega^3 e^2}{3c^3\hbar}\,\frac{1}{2j_i+1}\sum_{m_i,m_f}|\vec{\boldsymbol{d}}_{if}|^2\,, \tag{19}$$

where we have averaged over the $2j_i + 1$ possible m_i values and summed over the $2j_f + 1$ possible final m_f values. Energy conservation implies that $\hbar\omega = E_f - E_i$, where E_i is the energy of the $2s_{1/2}$ state and E_f is the energy of the $2p_{1/2}$ state.

The calculation of the decay rate for $2s_{1/2} \to 2p_{1/2} + \gamma$ is nearly identical to the one presented in class for the decay $2p_{1/2} \to 1s_{1/2} + \gamma$. In class, we ignored the electron spin, and we shall do so here as well.[2] Then, we can employ the result obtained in class,

$$\sum_{m_i,m_f}|\vec{\boldsymbol{d}}_{if}|^2 = \left|\int_0^\infty R_{n_f\ell_f}(r)R_{n_i\ell_i}(r)r^3\,dr\right|^2 \times \begin{cases} \ell_i + 1\,, & \text{for } \ell_f = \ell_i + 1\,, \\ \ell_i\,, & \text{for } \ell_f = \ell_i - 1\,. \end{cases}$$

[2] In Appendix 3, the following calculation is repeated, where the electron spin is explicitly taken into account.

In the present case, $\ell_i = 0$ and $\ell_f = 1$. The corresponding radial wave functions are

$$R_{20}(r) = \frac{1}{\sqrt{8a_0^3}}\left(2 - \frac{r}{a_0}\right) e^{-r/(2a_0)}\,, \qquad\qquad R_{21}(r) = \frac{1}{\sqrt{24a_0^3}}\,\frac{r}{a_0}\, e^{-r/(2a_0)}\,.$$

Thus,

$$\int_0^\infty r^3 R_{20}(r)R_{21}(r)\,dr = \frac{1}{8a_0^4\sqrt{3}}\int_0^\infty r^4\left(2 - \frac{r}{a_0}\right) e^{-r/a_0}\,dr = \frac{a_0}{8\sqrt{3}}\,[2(4!) - 5!] = -3\sqrt{3}\,a_0\,. \tag{20}$$

It follows that

$$\sum_{m_f=\pm 1,0} |\vec{\boldsymbol{d}}_{if}|^2 = 27a_0^2\,.$$

Since $\ell_i = 0$, no average over initial states is necessary (since we are neglecting spin), so eq. (19) yields

$$\Gamma(2s \to 2p + \gamma) = \frac{36\omega^3 e^2 a_0^2}{c^3\hbar} = \frac{36\omega^3\hbar^2}{(mc^2)^2\alpha}\,, \tag{21}$$

where we have used $a_0 = \hbar^2/(me^2)$ and $\alpha = e^2/(\hbar c)$ to write Γ in a more convenient form.

The transition rate for $2s \to 2p+\gamma$ obtained in Eq. (21) is not the same as transition rate for $2s_{1/2} \to 2p_{1/2} + \gamma$. In particular, the $2p_{3/2}$ state lies above the $2s_{1/2}$ state and therefore does not participate in the actual $2s \to 2p + \gamma$ decay process. Since the $2p$ state consists of four $2p_{3/2}$ states and two $2p_{1/2}$ states, it follows that

$$\Gamma(2s_{1/2} \to 2p_{1/2} + \gamma) = \tfrac{1}{3}\Gamma(2s \to 2p + \gamma)\,, \tag{22}$$

since only 1/3 of the $2p$ states actually participate in this decay process. Hence, we conclude that:[3]

$$\Gamma(2s_{1/2} \to 2p_{1/2} + \gamma) = \frac{12\omega^3\hbar^2}{(mc^2)^2\alpha}\,. \tag{23}$$

If this $E1$ decay is responsible for the $2s_{1/2}$ lifetime, then

$$\tau = \frac{(mc^2)^2\alpha\hbar}{12(\hbar\omega)^3}\,.$$

We can now plug in the numbers. Since $\hbar\omega = E_f - E_i = h\nu$, where $\nu = 1057$ Mhz is the Lamb shift frequency, it follows that

$$\hbar\omega = 2\pi\hbar\nu = (2\pi)(6.6\times 10^{-16}\ \text{eV}\cdot\text{sec})(1.056\times 10^{9}\ \text{sec}^{-1}) = 4.38\times 10^{-6}\ \text{eV}\,.$$

Using $mc^2 = 5.11\times 10^5$ eV and $\alpha \simeq 1/137$, we end up with

$$\tau = \frac{(5.11\times 10^5\ \text{eV})^2(1/137)(6.6\times 10^{-16}\ \text{eV}\cdot\text{sec})}{12(4.38\times 10^{-6}\ \text{eV})^3} = 1.25\times 10^9\ \text{sec} = 39.6\ \text{years}\,.$$

This is considerably longer than $\tau(2p \to 1s + \gamma) = 1.6\times 10^{-9}$ sec, which we computed in class.

[3]As shown in Appendix 3, one can confirm the result of eq. (23) by including the electron spin directly into the calculations.

REMARK: For obvious reasons, the $2s_{1/2}$ state is called "metastable". In fact, the dominant decay mode of this state is into the $1s_{1/2}$ ground state with the simultaneous emission of two photons. This decay rate can be computed by second order perturbation theory, although the calculation is more involved and will not be considered here. The resulting lifetime, $\tau = 0.14$ sec is in good agreement with experiment.[4] As a result, the $E1$ decay into a single photon is never observed in practice, as the decay $2s_{1/2} \to 1s_{1/2} + \gamma\gamma$ will take place long before the $2s_{1/2}$ state has a chance to decay via $2s_{1/2} \to 2p_{1/2} + \gamma$.

(c) Can the $2s_{1/2}$ state decay via an $E2$ transition? Explain.

The selection rules for an E2 decay, $A \to B + \gamma$ are:

$$|j_A - j_B| \leq 2 \leq j_A + j_B \,, \quad \text{and} \quad \Pi(A) = \Pi(B) \,,$$

The restrictions on the total angular momentum is a consequence of the Wigner-Eckart theorem, since the quadrupole operator is a spherical tensor or rank 2. The angular momentum selection rule forbids the decay of the $2s_{1/2}$ state into either the $2p_{1/2}$ or the $1s_{1/2}$ states since $j_A = j_B = \frac{1}{2}$ in both cases. In particular, the electric quadrupole operator imparts two units of angular momentum to the initial state, which implies that the final state can only have total angular momentum $\frac{3}{2}$ or $\frac{5}{2}$.

Indeed, the above argument generalizes to higher multipoles. The $2s_{1/2}$ cannot decay via any 2^ℓ-pole with $\ell \geq 2$.

(d) Using selection rules, determine to which state the $2s_{1/2}$ state can decay via an $M1$ transition. By using explicit wave functions, evaluate the matrix element of the magnetic dipole operator, $\langle f|\vec{\boldsymbol{\mu}}|i\rangle$, and show that the $M1$ transition rate vanishes.

The selection rules for an M1 decay, $A \to B + \gamma$ are:

$$|j_A - j_B| \leq 1 \leq j_A + j_B \,, \quad \text{and} \quad \Pi(A) = \Pi(B) \,,$$

The angular momentum selection rule is the same as for $E1$ decay. The parity selection rule arises since

$$\vec{\boldsymbol{\mu}} = \frac{e}{2mc}\left(\vec{\boldsymbol{L}} + g\vec{\boldsymbol{S}}\right) \,,$$

is even under the inversion of the coordinate system. Thus, the decay

$$2s_{1/2} \to 1s_{1/2} + \gamma \,,$$

satisfies both the angular momentum and parity quantum numbers.

[4]Thus, the lifetime of the $2s_{1/2}$ state of hydrogen is a factor of 10^8 *longer* than the corresponding lifetime of the $2p_{1/2}$ state.

Nevertheless, it turns out that $\langle f|\vec{\boldsymbol{\mu}}|i\rangle = 0$ for the $2s_{1/2} \to 1s_{1/2} + \gamma$ transition. To see this, we note that the initial and final state wave functions are:

$$\big|2s_{1/2}\big\rangle = \frac{1}{\sqrt{4\pi}} R_{20}(r)\chi_i\,, \qquad\qquad \big|1s_{1/2}\big\rangle = \frac{1}{\sqrt{4\pi}} R_{10}(r)\chi_f\,,$$

where χ_i and χ_f are the spin parts of the corresponding hydrogenic wave functions. Thus, using $\vec{\boldsymbol{S}} = \frac{1}{2}\hbar\vec{\boldsymbol{\sigma}}$, it follows that:

$$\begin{aligned}\langle f|\,\vec{\boldsymbol{\mu}}\,|i\rangle = \frac{ge}{2mc}\,\langle f|\,\vec{\boldsymbol{S}}\,|i\rangle &= \frac{ge\hbar}{16\pi mc}\,\langle\chi_f|\,\vec{\boldsymbol{\sigma}}\,|\chi_i\rangle \int d^3x\, R_{10}(r)R_{20}(r) \\ &= \frac{ge\hbar}{4mc}\,\langle\chi_f|\,\vec{\boldsymbol{\sigma}}\,|\chi_i\rangle \int_0^\infty r^2 R_{10}(r)R_{20}(r)\,dr\,. \qquad (24)\end{aligned}$$

Note that $\vec{\boldsymbol{L}}$ does not contribute to $\langle f|\,\vec{\boldsymbol{\mu}}\,|i\rangle$ since both the initial and final states are s-states.

We can now invoke the orthogonality of the radial wave functions, which implies that

$$\int_0^\infty r^2 R_{n\ell}(r)R_{n'\ell'}(r)\,dr = \delta_{nn'}\,\delta_{\ell\ell'}\,.$$

Consequently,

$$\langle f|\,\vec{\boldsymbol{\mu}}\,|i\rangle = 0\,,$$

due to the orthogonality of the $1s_{1/2}$ and $2s_{1/2}$ radial wave functions. Thus, the rate for the $M1$ transition vanishes.

<u>*REMARK:*</u> When relativistic effects are included (via the Dirac equation), one finds that $\langle f|\,\vec{\boldsymbol{\mu}}\,|i\rangle$ is no longer zero, and the $M1$ decay $2s_{1/2} \to 1s_{1/2} + \gamma$ can occur. In fact, the corresponding lifetime is *shorter* than the $E1$ decay obtained in part (b), since $\hbar\omega$ is considerably larger for the $2s_{1/2} \to 1s_{1/2}$ transition as compared with the $2s_{1/2} \to 2p_{1/2}$ transition. Nevertheless, because the $M1$ decay rate is suppressed by a relativistic factor, it turns out that the rate for two-photon decay, $2s_{1/2} \to 1s_{1/2} + \gamma\gamma$ dominates over the one-photon decay $2s_{1/2} \to 1s_{1/2} + \gamma$.

4. Two electrons are in plane wave states in a cubical box of length L and volume $V = L^3$. The Hamiltonian governing this system is

$$H = \frac{\vec{\boldsymbol{p}}_1^{\,2}}{2m} + \frac{\vec{\boldsymbol{p}}_2^{\,2}}{2m} + \frac{e^2}{|\vec{\boldsymbol{x}}_1 - \vec{\boldsymbol{x}}_2|}\,,$$

where the last term above is a result of the Coulomb interactions of the electrons. The second-quantized Hamiltonian for this system in terms of creation and annihilation operators is given by

$$H = \sum_{\vec{\boldsymbol{p}},s} \frac{\vec{\boldsymbol{p}}^{\,2}}{2m}\, a^\dagger_{\vec{\boldsymbol{p}},s} a_{\vec{\boldsymbol{p}},s} + \tfrac{1}{2} \sum_{\vec{\boldsymbol{p}}',\vec{\boldsymbol{q}}',s'} \sum_{\vec{\boldsymbol{p}},\vec{\boldsymbol{q}},s} a^\dagger_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}',s'} a_{\vec{\boldsymbol{q}}',s'} a_{\vec{\boldsymbol{q}},s}\, \big\langle \vec{\boldsymbol{p}}, \vec{\boldsymbol{p}}'\big|\,\mathcal{V}\,\big|\vec{\boldsymbol{q}}', \vec{\boldsymbol{q}}\big\rangle\,,$$

where the spin variables s and s' can take on two possible values ($\pm\frac{1}{2}$) and

$$\left\langle \vec{\boldsymbol{p}}, \vec{\boldsymbol{p}}' \right| \mathcal{V} \left| \vec{\boldsymbol{q}}', \vec{\boldsymbol{q}} \right\rangle = \frac{1}{V^2} \int d^3x\, d^3x' \, \frac{e^2}{|\vec{\boldsymbol{x}}_1 - \vec{\boldsymbol{x}}_2|} \, e^{-i(\vec{\boldsymbol{p}}-\vec{\boldsymbol{q}})\cdot\vec{\boldsymbol{x}}/\hbar} \, e^{-i(\vec{\boldsymbol{p}}'-\vec{\boldsymbol{q}}')\cdot\vec{\boldsymbol{x}}'/\hbar} \,. \tag{25}$$

A two-particle electron state is given by

$$\left| \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right\rangle = a^\dagger_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle \,,$$

where $|0\rangle$ is the state with no electrons.

(a) Compute the expectation value,

$$\left\langle \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right| H \left| \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right\rangle \,,$$

in the case where $e = 0$ (i.e. where the Coulomb interactions are switched off). Explain the behavior of your result in the case of $\vec{\boldsymbol{p}} = \vec{\boldsymbol{p}}'$ and $s = s'$.

In the absence of interactions,

$$\begin{aligned}
\left\langle \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right| H \left| \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right\rangle &= \langle 0|\, a_{\vec{\boldsymbol{p}}',s'} a_{\vec{\boldsymbol{p}},s} H a^\dagger_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle \\
&= \sum_{\vec{\boldsymbol{p}}'',s''} \langle 0|\, a_{\vec{\boldsymbol{p}}',s'} a_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}'',s''} a_{\vec{\boldsymbol{p}}'',s''} a^\dagger_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle \, \frac{\vec{\boldsymbol{p}}''^{\,2}}{2m} \,.
\end{aligned} \tag{26}$$

We can evaluate the matrix element above by employing the anticommutation relations,

$$\{a_{\vec{\boldsymbol{p}},s} \,,\, a^\dagger_{\vec{\boldsymbol{p}}',s'}\} = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}'}\, \delta_{ss'} \,, \tag{27}$$

to push the $a^\dagger_{\vec{\boldsymbol{p}}'',s''}$ to the left and the $a_{\vec{\boldsymbol{p}}'',s''}$ to the right until we can make use of

$$\langle 0|\, a^\dagger_{\vec{\boldsymbol{p}}'',s''} = 0 \,, \qquad\qquad a_{\vec{\boldsymbol{p}}'',s''} \left|0\right\rangle = 0 \,.$$

Using eq. (27) to write

$$a_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}',s'} = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}'}\, \delta_{ss'} - a^\dagger_{\vec{\boldsymbol{p}}',s'} a_{\vec{\boldsymbol{p}},s} \,,$$

it follows that:

$$\begin{aligned}
&\langle 0|\, a_{\vec{\boldsymbol{p}}',s'} a_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}'',s''} a_{\vec{\boldsymbol{p}}'',s''} a^\dagger_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle \\
&\quad = \langle 0|\, a_{\vec{\boldsymbol{p}}',s'} (\delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}''}\, \delta_{ss''} - a^\dagger_{\vec{\boldsymbol{p}}'',s''} a_{\vec{\boldsymbol{p}},s}) (\delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}''}\, \delta_{ss''} - a^\dagger_{\vec{\boldsymbol{p}},s} a_{\vec{\boldsymbol{p}}'',s''}) a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle \\
&\quad = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}''}\, \delta_{ss''} \Big[\langle 0|\, a_{\vec{\boldsymbol{p}}',s'} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle - \langle 0|\, a_{\vec{\boldsymbol{p}}',s'} a^\dagger_{\vec{\boldsymbol{p}}'',s''} a_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle - \langle 0|\, a_{\vec{\boldsymbol{p}}',s'} a^\dagger_{\vec{\boldsymbol{p}},s} a_{\vec{\boldsymbol{p}}'',s''} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle \Big] \\
&\qquad\quad + \langle 0|\, a_{\vec{\boldsymbol{p}}',s'} a^\dagger_{\vec{\boldsymbol{p}}'',s''} a_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}},s} a_{\vec{\boldsymbol{p}}'',s''} a^\dagger_{\vec{\boldsymbol{p}}',s'} \left|0\right\rangle \\
&\quad = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}''}\, \delta_{ss''} \left[1 - 2\delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{p}}''}\, \delta_{s's''} \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}'}\, \delta_{ss'} \right] + \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{p}}''}\, \delta_{s's''} \, \langle 0|\, a_{\vec{\boldsymbol{p}},s} a^\dagger_{\vec{\boldsymbol{p}},s} \left|0\right\rangle \,, \\
&\quad = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}''}\, \delta_{ss''} + \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{p}}''}\, \delta_{s's''} - 2\delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}''}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{p}}''}\, \delta_{ss''}\, \delta_{s's''} \,.
\end{aligned}$$

Inserting this result in eq. (26), it follows that

$$\left\langle \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right| H \left| \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right\rangle = \frac{\vec{\boldsymbol{p}}^{\,2}}{2m} + \frac{\vec{\boldsymbol{p}}'^{\,2}}{2m} - \frac{\vec{\boldsymbol{p}}^{\,2}}{m}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{p}}'}\, \delta_{ss'}\,. \tag{28}$$

In the limit of $\vec{\boldsymbol{p}} = \vec{\boldsymbol{p}}'$ and $s = s'$, eq. (28) yields $\left\langle \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right| H \left| \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right\rangle = 0$, which is a consequence of the Pauli principle, since two identical electrons cannot occupy the same state.

(b) Treating the Coulomb interactions to first-order in perturbation theory, compute the energy difference of the parallel ($s = s'$) and antiparallel ($s \neq s'$) spin alignments of the two electrons. Express your answer as a volume integral over the box.

Using first-order in perturbation theory,

$$E^{(1)} = \left\langle \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right| H^{(1)} \left| \vec{\boldsymbol{p}}, s\,;\, \vec{\boldsymbol{p}}', s' \right\rangle\,,$$

where

$$H^{(1)} = \tfrac{1}{2} \sum_{\vec{\boldsymbol{k}}', \vec{\boldsymbol{q}}', s_2} \sum_{\vec{\boldsymbol{k}}, \vec{\boldsymbol{q}}, s_1} a^\dagger_{\vec{\boldsymbol{k}}, s_1} a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} a_{\vec{\boldsymbol{q}}, s_1} \langle \vec{\boldsymbol{k}}, \vec{\boldsymbol{k}}' | \mathcal{V} | \vec{\boldsymbol{q}}', \vec{\boldsymbol{q}} \rangle\,,$$

Thus, we must evaluate:

$$\begin{aligned}
&\langle 0 |\, a_{\vec{\boldsymbol{p}}', s'} a_{\vec{\boldsymbol{p}}, s} a^\dagger_{\vec{\boldsymbol{k}}, s_1} a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} a_{\vec{\boldsymbol{q}}, s_1} a^\dagger_{\vec{\boldsymbol{p}}, s} a^\dagger_{\vec{\boldsymbol{p}}', s'} \,| 0 \rangle \\
&\quad = \langle 0 |\, a_{\vec{\boldsymbol{p}}', s'} (\delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}}\, \delta_{ss_1} - a^\dagger_{\vec{\boldsymbol{k}}, s_1} a_{\vec{\boldsymbol{p}}, s}) a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} (\delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}}\, \delta_{ss_1} - a^\dagger_{\vec{\boldsymbol{p}}, s} a_{\vec{\boldsymbol{q}}, s_1}) a^\dagger_{\vec{\boldsymbol{p}}', s'} \,| 0 \rangle \\
&\quad = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}}\, \delta_{ss_1} \langle 0 |\, a_{\vec{\boldsymbol{p}}', s'} a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} a^\dagger_{\vec{\boldsymbol{p}}', s'} \,| 0 \rangle - \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}}\, \delta_{ss_1} \langle 0 |\, a_{\vec{\boldsymbol{p}}', s'} a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} a^\dagger_{\vec{\boldsymbol{p}}, s} a_{\vec{\boldsymbol{q}}, s_1} a^\dagger_{\vec{\boldsymbol{p}}', s'} \,| 0 \rangle \\
&\qquad - \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}}\, \delta_{ss_1} \langle 0 |\, a_{\vec{\boldsymbol{p}}', s'} a^\dagger_{\vec{\boldsymbol{k}}, s_1} a_{\vec{\boldsymbol{p}}, s} a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} a^\dagger_{\vec{\boldsymbol{p}}', s'} \,| 0 \rangle + \langle 0 |\, a_{\vec{\boldsymbol{p}}', s'} a^\dagger_{\vec{\boldsymbol{k}}, s_1} a_{\vec{\boldsymbol{p}}, s} a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} a^\dagger_{\vec{\boldsymbol{p}}, s} a_{\vec{\boldsymbol{q}}, s_1} a^\dagger_{\vec{\boldsymbol{p}}', s'} \,| 0 \rangle \\
&\quad = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}}\, \delta_{ss_1} \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}'}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}'}\, \delta_{s's_2} - \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}}\, \delta_{ss_1} \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}'}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}}\, \delta_{s's_1}\, \delta_{s's_2}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}'}\, \delta_{ss_2} \\
&\qquad - \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}}\, \delta_{ss_1} \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}'}\, \delta_{s's_1}\, \delta_{s's_2}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}'}\, \delta_{ss_2} + \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}} \delta_{s's_1}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}'} \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}'}\, \delta_{ss_2}
\end{aligned}$$

Summing over s_1 and s_2 yields

$$\begin{aligned}
&\sum_{s_1, s_2} \langle 0 |\, a_{\vec{\boldsymbol{p}}', s'} a_{\vec{\boldsymbol{p}}, s} a^\dagger_{\vec{\boldsymbol{k}}, s_1} a^\dagger_{\vec{\boldsymbol{k}}', s_2} a_{\vec{\boldsymbol{q}}', s_2} a_{\vec{\boldsymbol{q}}, s_1} a^\dagger_{\vec{\boldsymbol{p}}, s} a^\dagger_{\vec{\boldsymbol{p}}', s'} \,| 0 \rangle \\
&\qquad = \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}'}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}'} + \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}'}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}'} - \delta_{ss'} \left(\delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}'}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}'} + \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{q}}}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{k}}}\, \delta_{\vec{\boldsymbol{p}}'\vec{\boldsymbol{q}}'}\, \delta_{\vec{\boldsymbol{p}}\vec{\boldsymbol{k}}'} \right).
\end{aligned}$$

Hence, we end up with

$$E^{(1)} = \tfrac{1}{2} \Big\{ \langle \vec{\boldsymbol{p}}, \vec{\boldsymbol{p}}' | \mathcal{V} | \vec{\boldsymbol{p}}', \vec{\boldsymbol{p}} \rangle + \langle \vec{\boldsymbol{p}}', \vec{\boldsymbol{p}} | \mathcal{V} | \vec{\boldsymbol{p}}, \vec{\boldsymbol{p}}' \rangle - \delta_{ss'} \left[\langle \vec{\boldsymbol{p}}, \vec{\boldsymbol{p}}' | \mathcal{V} | \vec{\boldsymbol{p}}, \vec{\boldsymbol{p}}' \rangle + \langle \vec{\boldsymbol{p}}', \vec{\boldsymbol{p}} | \mathcal{V} | \vec{\boldsymbol{p}}', \vec{\boldsymbol{p}} \rangle \right] \Big\} \tag{29}$$

Using eq. (25), it follows that $\langle\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'|\mathcal{V}|\vec{\boldsymbol{p}}',\vec{\boldsymbol{p}}\rangle = \langle\vec{\boldsymbol{p}}',\vec{\boldsymbol{p}}|\mathcal{V}|\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'\rangle$ and $\langle\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'|\mathcal{V}|\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'\rangle = \langle\vec{\boldsymbol{p}}',\vec{\boldsymbol{p}}|\mathcal{V}|\vec{\boldsymbol{p}}',\vec{\boldsymbol{p}}\rangle$. Therefore, eq. (29) simplifies to

$$E^{(1)} = \langle\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'|\mathcal{V}|\vec{\boldsymbol{p}}',\vec{\boldsymbol{p}}\rangle - \delta_{ss'}\langle\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'|\mathcal{V}|\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'\rangle\,.$$

It follows that the energy difference between the parallel ($s = s'$) and antiparallel ($s \neq s'$) spin alignments is

$$\begin{aligned}\Delta E = -\langle\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'|\mathcal{V}|\vec{\boldsymbol{p}},\vec{\boldsymbol{p}}'\rangle &= -\frac{1}{V^2}\int d^3x\,d^3x'\,\frac{e^2}{|\vec{\boldsymbol{x}}-\vec{\boldsymbol{x}}'|}e^{i(\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}})\cdot\vec{\boldsymbol{x}}/\hbar}\,e^{-i(\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}})\cdot\vec{\boldsymbol{x}}'/\hbar} \\ &= -\frac{1}{V^2}\int d^3x\,d^3x'\,\frac{e^2}{|\vec{\boldsymbol{x}}-\vec{\boldsymbol{x}}'|}e^{i(\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}})\cdot(\vec{\boldsymbol{x}}-\vec{\boldsymbol{x}}')/\hbar}\,.\end{aligned}$$

To evaluate the above integral, it is convenient to change variables to $\vec{\boldsymbol{R}} \equiv \frac{1}{2}(\vec{\boldsymbol{x}}+\vec{\boldsymbol{x}}')$ and $\vec{\boldsymbol{r}} \equiv \vec{\boldsymbol{x}}-\vec{\boldsymbol{x}}'$. The Jacobian of this transformation is equal to 1. Using

$$\int d^3R = V\,,$$

it follows that

$$\Delta E = -\frac{e^2}{V}\int d^3r\,\frac{e^{i(\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}})\cdot\vec{\boldsymbol{r}}/\hbar}}{r}\,. \tag{30}$$

(c) Calculate the energy difference ΔE of the parallel and antiparallel spin alignments by evaluating the volume integral obtained in part (b) assuming that $|\vec{\boldsymbol{p}}-\vec{\boldsymbol{p}}'|L \gg 1$, where L is the length of a side of the cubical box. How does ΔE depend on V in the limit of $\vec{\boldsymbol{p}} = \vec{\boldsymbol{p}}'$?

Assuming that $|\vec{\boldsymbol{p}}-\vec{\boldsymbol{p}}'|L \gg 1$, we can evaluate the volume integral in eq. (30) to good approximation by taking the volume of the integration region to be infinite (while maintaining the factor of $1/V$ that appears in the coefficient of the integral). In this case, we recognize the volume integral as the Fourier transform of $1/r$, which should be well-known to you. Although the Fourier transform of $1/r$ does not technically exist in the infinite volume limit, it is common practice to insert a convergence factor and evaluate

$$\begin{aligned}\lim_{\epsilon\to 0}\int d^3r\,\frac{e^{-\epsilon r}}{r}\,e^{i(\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}})\cdot\vec{\boldsymbol{r}}/\hbar} &= \lim_{\epsilon\to 0}\,2\pi\int_0^\infty e^{-\epsilon r}r\,dr\int_{-1}^{1} e^{i|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|r\cos\theta/\hbar}\,d\cos\theta \\ &= \lim_{\epsilon\to 0}\,2\pi\int_0^\infty e^{-\epsilon r}r\,dr\frac{\hbar}{i|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|r}\left(e^{i|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|r/\hbar} - e^{-i|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|r/\hbar}\right) \\ &= \lim_{\epsilon\to 0}\frac{2\pi\hbar}{|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|}\int_0^\infty\left[e^{i(|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|+i\epsilon)r/\hbar} - e^{-i(|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|-i\epsilon)r/\hbar}\right]dr \\ &= \lim_{\epsilon\to 0}\frac{2\pi\hbar^2}{|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{k}}|}\left(\frac{1}{|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|+i\epsilon} + \frac{1}{|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|-i\epsilon}\right) \\ &= \frac{4\pi\hbar^2}{|\vec{\boldsymbol{p}}'-\vec{\boldsymbol{p}}|^2}\,.\end{aligned}$$

Inserting this result into eq. (30) yields

$$\Delta E = -\frac{4\pi e^2\hbar^2}{V|\vec{\boldsymbol{p}}' - \vec{\boldsymbol{p}}|^2}\,.$$

In the case of $\vec{\boldsymbol{p}} = \vec{\boldsymbol{p}}'$, the computation above breaks down. In this case, we cannot take the infinite volume limit. To get a sense of the V dependence of ΔE, consider the volume integral given in eq. (30) in the case where the volume is a sphere of radius R. In this case, if $\vec{\boldsymbol{p}} = \vec{\boldsymbol{p}}'$ then

$$\Delta E = -\frac{4\pi e^2}{V}\int_0^R r\,dr = -\frac{2\pi e^2 R^2}{V} = -\frac{3e^2}{2R}\,, \tag{31}$$

after using $V = \frac{4}{3}\pi R^3$. For a cubical box with a side of length L, the volume integral in eq. (30) cannot be performed exactly. However, in light of eq. (31), dimensional analysis suggests that if $\vec{\boldsymbol{p}} = \vec{\boldsymbol{p}}'$, then ΔE must be of the form

$$\Delta E = -\frac{ke^2}{L} = -\frac{ke^2}{V^{1/3}}\,,$$

where k is a constant of order unity.

APPENDICES

:

1. An alternative derivation of the phase shifts in the Born approximation

To solve part (c) of problem 2, one can employ the Born approximation to the phase shifts,

$$e^{i\delta_\ell}\sin\delta_\ell = -\frac{2mk}{\hbar^2}\int_0^\infty [j_\ell(kr)]^2\,V(r)\,r^2\,dr\,.$$

Applying this result to problem 2,

$$e^{i\delta_\ell}\sin\delta_\ell = \frac{\xi\eta}{r_0^3}\int_0^\infty e^{-r/r_0}\,[j_\ell(kr)]^2\,r^2\,dr\,. \tag{32}$$

First, we examine the cases of $\ell = 0$ and $\ell = 1$. Using eq. (12.6.31) on p. 348 of Shankar,

$$j_0(z) = \frac{\sin z}{z}\,, \qquad\qquad j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}\,.$$

It follows that:

$$e^{i\delta_0}\sin\delta_0 = \frac{\xi\eta}{k^2 r_0^3}\int_0^\infty e^{-r/r_0}\,\sin^2(kr)\,dr$$

Defining $x \equiv kr$ and using $\xi = kr_0$,

$$e^{i\delta_0}\sin\delta_0 = \frac{\eta}{\xi^2}\int_0^\infty e^{-x/\xi}\,\sin^2 x\,dx = \frac{2\xi\eta}{1+4\xi^2}\,, \tag{33}$$

after using eq. (44), which is derived in Appendix 2. Thus, we have recovered eq. (12). Likewise,

$$e^{i\delta_1}\sin\delta_1 = \frac{\xi\eta}{r_0^3}\int_0^\infty e^{-r/r_0}\left(\frac{\sin kr}{(kr)^2}-\frac{\cos kr}{kr}\right)^2 r^2\,dr$$

$$= \frac{\eta}{\xi^2}\int_0^\infty e^{-x/\xi}\left(\frac{\sin x}{x}-\cos x\right)^2 dx\,. \tag{34}$$

Integrating by parts,

$$\int_0^\infty \frac{e^{-x/\xi}\,\sin^2 x}{x^2}\,dx = -\frac{1}{\xi}\int_0^\infty \frac{e^{-x/\xi}\,\sin^2 x}{x}\,dx + 2\int_0^\infty \frac{e^{-x/\xi}\,\sin x\cos x}{x}\,dx\,. \tag{35}$$

The second term on the right hand side of eq. (35) cancels the cross-term of eq. (34). We are left with:

$$e^{i\delta_1}\sin\delta_1 = -\frac{\eta}{\xi^3}\int_0^\infty \frac{e^{-x/\xi}\,\sin^2 x}{x}\,dx + \frac{\eta}{\xi^2}\int_0^\infty e^{-x/\xi}\,\cos^2 x\,dx$$

$$= -\frac{\eta}{4\xi^3}\,\ln(1+4\xi^2) + \frac{\eta(1+2\xi^2)}{\xi(1+4\xi^2)}\,, \tag{36}$$

after using eqs. (41) and (42), which are derived in Appendix 2. Thus, we have recovered eq. (13).

It is interesting to note that the integral in eq. (32) can be evaluated in closed form for arbitrary ℓ. We begin with the following integral involving Bessel functions:[5]

$$\int_0^\infty e^{-at}J_\nu(bt)J_\nu(ct)dt = \frac{1}{\pi\sqrt{bc}}\,Q_{\nu-\frac{1}{2}}\left(\frac{a^2+b^2+c^2}{2bc}\right)\,, \tag{37}$$

assuming that $\mathrm{Re}(a \pm ib \pm ic) > 0$ and $\mathrm{Re}(2\nu+1) > 0$. On the right-hand side of eq. (37), $Q_\ell(x)$ is the Legendre function of the second kind.[6] Taking the derivative of this result with respect to a yields:

$$\int_0^\infty e^{-at}J_\nu(bt)J_\nu(ct)\,t\,dt = \frac{-a}{\pi(bc)^{3/2}}\,Q'_{\nu-\frac{1}{2}}\left(\frac{a^2+b^2+c^2}{2bc}\right)\,,$$

where

$$Q'_\ell(x) \equiv \frac{d}{dx}\,Q_\ell(x)\,.$$

We now express the spherical Bessel functions as:

$$j_\ell(kr) = \sqrt{\frac{\pi}{2kr}}J_{\ell+\frac{1}{2}}(kr)\,.$$

[5]See eq. (2) on p. 389 of G.N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, London, 1966).

[6]You are probably more familiar with the Legendre function of the first kind, which for non-negative integer ℓ is the Legendre polynomial, $P_\ell(x)$. For more details on the properties of the Legendre function of the second kind, $Q_\ell(x)$, see see Chapter 7 of N.N. Lebedev, *Special Functions and Their Applications* (Dover Publications, Inc., New York, 1972).

It then follows that:

$$\int_0^\infty e^{-at} j_\ell(bt) j_\ell(ct)\, t^2\, dt = \frac{-a}{2b^2c^2} Q'_\ell\left(\frac{a^2+b^2+c^2}{2bc}\right) .$$

Applying this last result to eq. (32), one immediately obtains:

$$\boxed{e^{i\delta_\ell}\sin\delta_\ell = -\frac{\eta}{2\xi^3} Q'_\ell\left(1+\frac{1}{2\xi^2}\right)} \tag{38}$$

We can again rederive the cases of $\ell = 0$ and $\ell = 1$ by using[7]

$$Q_0(x) = \tfrac{1}{2}\ln\left(\frac{x+1}{x-1}\right) , \qquad Q_1(x) = \tfrac{1}{2}x\ln\left(\frac{x+1}{x-1}\right) - 1 ,$$

which are single-valued real functions for $x > 1$. Taking derivatives with respect to x,

$$Q'_0(x) = \frac{1}{1-x^2} , \qquad Q'_1(x) = \tfrac{1}{2}\ln\left(\frac{x+1}{x-1}\right) + \frac{x}{1-x^2} .$$

Thus,

$$e^{i\delta_0}\sin\delta_0 = -\frac{\eta}{2\xi^3} Q'_0\left(1+\frac{1}{2\xi^2}\right) = \frac{2\eta\xi}{1+4\xi^2} ,$$

$$e^{i\delta_1}\sin\delta_1 = -\frac{\eta}{2\xi^3} Q'_1\left(1+\frac{1}{2\xi^2}\right) = -\frac{\eta}{4\xi^3}\ln(1+4\xi^2) + \frac{2\eta\xi}{1+4\xi^2}\left(1+\frac{1}{2\xi^2}\right) ,$$

which reproduces once again the results of eqs. (12) and (13).

Finally, we can provide one more check of eq. (38) by returning to eqs. (6) and (10), which yields

$$\begin{aligned} e^{i\delta_\ell}\sin\delta_\ell &= \eta\xi \int_{-1}^1 \frac{P_\ell(\cos\theta)\, d\cos\theta}{(1+2\xi^2-2\xi^2\cos\theta)^2} \\ &= \frac{\eta}{4\xi^3}\int_{-1}^1 \frac{P_\ell(\cos\theta)\, d\cos\theta}{(z-\cos\theta)^2} , \qquad \text{where} \quad z = 1+\frac{1}{2\xi^2} . \end{aligned} \tag{39}$$

At this point, we can employ Neumann's integral for $Q_\ell(z)$, which is given by[8]

$$Q_\ell(z) = \tfrac{1}{2}\int_{-1}^1 \frac{P_\ell(t)\, dt}{z-t} ,$$

for non-negative integer ℓ and $|z| > 1$. Taking the derivative of this result with respect to z yields

$$Q'_\ell(z) = -\tfrac{1}{2}\int_{-1}^1 \frac{P_\ell(t)\, dt}{(z-t)^2} , \qquad \text{for non-negative integer } \ell \text{ and } |z| > 1 . \tag{40}$$

[7]See N.N. Lebedev, op. cit., p. 185.

[8]See, e.g. Nico M. Temme, *Special Functions: An Introduction to the Classical Functions of Mathematical Physics* (John Wiley & Sons, Inc., New York, 1996), eq. (8.33) on p. 201.

Comparing eqs. (39) and (40), one immediately obtains:

$$e^{i\delta_\ell}\sin\delta_\ell = -\frac{\eta}{2\xi^3}\,Q'_\ell\left(1+\frac{1}{2\xi^2}\right)\,,$$

which confirms the result obtained in eq. (38).

2. An explicit computation of the integrals in eqs. (33) and (36)

In deriving eqs. (33) and (36), the following integrals were employed:

$$\int_0^\infty e^{-x/\xi}\,\sin^2 x\,\frac{dx}{x} = \tfrac{1}{4}\ln(1+4\xi^2)\,, \tag{41}$$

$$\int_0^\infty e^{-x/\xi}\,\cos^2 x\,dx = \xi - \int_0^\infty e^{-x/\xi}\,\sin^2 x\,dx = \frac{\xi(1+2\xi^2)}{1+4\xi^2}\,. \tag{42}$$

Of course, these integrals can be found in any good table of integrals.[9] Nevertheless, just for the fun of it, I shall provide a derivation of these integrals below.

Our strategy is to make use of the power series expansion for $\sin^2 x$,

$$\sin^2 x = \tfrac{1}{2}(1-\cos 2x) = \tfrac{1}{2}\sum_{k=1}^\infty (-1)^{k+1}\frac{(2x)^{2k}}{(2k)!}\,.$$

Thus,

$$\begin{aligned}\int_0^\infty e^{-x/\xi}\,\sin^2 x\,\frac{dx}{x} &= \tfrac{1}{2}\sum_{k=1}^\infty \frac{(-1)^{k+1}2^{2k}}{(2k)!}\int_0^\infty e^{-x/\xi}\,x^{2k-1}\,dx \\ &= \tfrac{1}{2}\sum_{k=1}^\infty \frac{(-1)^{k+1}(2\xi)^{2k}}{(2k)!}\int_0^\infty e^{-y}\,y^{2k-1}\,dy\,,\end{aligned}$$

after setting $x=\xi y$. The remaining integral is straightforward:

$$\int_0^\infty e^{-y}\,y^{2k-1}\,dy = (2k-1)!$$

Writing $(2k)! = 2k(2k-1)!$, it follows that:

$$\int_0^\infty e^{-x/\xi}\,\sin^2 x\,\frac{dx}{x} = \tfrac{1}{4}\sum_{k=1}^\infty \frac{(-1)^{k+1}(4\xi^2)^k}{k} = \tfrac{1}{4}\ln(1+4\xi^2)\,,$$

after recognizing the well known power series of the logarithm. Thus, eq. (41) is proven.

[9] My reference of choice is I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series and Products* (7th edition), edited by Alan Jeffrey and Daniel Zwillinger (Academic Press, Burlington, MA, 2007).

To prove eq. (42), we write:

$$\int_0^\infty e^{-x/\xi}\,\cos^2 x\,dx = \int_0^\infty e^{-x/\xi}\,(1-\sin^2 x)\,dx = \xi - \int_0^\infty e^{-x/\xi}\,\sin^2 x\,dx\,. \qquad (43)$$

The last integral in eq. (43) can be evaluated by the same technique employed above. Following the same steps as before, we find:

$$\begin{aligned}\int_0^\infty e^{-x/\xi}\,\sin^2 x\,dx &= \tfrac{1}{2}\xi\sum_{k=1}^\infty \frac{(-1)^{k+1}(2\xi)^{2k}}{(2k)!}\int_0^\infty e^{-y}\,y^{2k}\,dy = \tfrac{1}{2}\xi\sum_{k=1}^\infty(-1)^{k+1}(2\xi)^{2k} \\ &= \tfrac{1}{2}\xi\left[1-\sum_{k=0}^\infty(-4\xi^2)^k\right] = \tfrac{1}{2}\xi\left[1-\frac{1}{1+4\xi^2}\right] = \frac{2\xi^3}{1+4\xi^2}\,, \qquad (44)\end{aligned}$$

after summing the geometric series. Inserting this result back into eq. (43) yields:

$$\int_0^\infty e^{-x/\xi}\,\cos^2 x\,dx = \frac{\xi(1+2\xi^2)}{1+4\xi^2}\,,$$

and eq. (42) is proven.

3. Including spin in the computation of the decay rate of $2s_{1/2} \to 2p_{1/2} + \gamma$

In order to include spin in the computation, we must employ the spin spherical harmonics in the hydrogenic wave functions,

$$\psi(r,\theta,\phi) = R_{n\ell}(r)\mathcal{Y}_{jm}^{\ell\,\frac{1}{2}}(\theta,\phi)\,,$$

where the *spin spherical harmonics* are given by

$$\mathcal{Y}^{\ell\,\frac{1}{2}}_{j=\ell\pm\frac{1}{2}\,,\,m}(\theta,\phi) \equiv \langle\theta\,\phi\,|\,j=\ell\pm\tfrac{1}{2}\,,\,m\rangle = \frac{1}{\sqrt{2\ell+1}}\begin{pmatrix}\pm\sqrt{\ell\pm m+\frac{1}{2}}\;Y_{\ell,m-\frac{1}{2}}(\theta,\phi)\\ \sqrt{\ell\mp m+\frac{1}{2}}\;Y_{\ell,m+\frac{1}{2}}(\theta,\phi)\end{pmatrix}. \qquad (45)$$

If $\ell = 0$, there is only one spin spherical harmonic,

$$\mathcal{Y}^{0\,\frac{1}{2}}_{j=\frac{1}{2}\,,\,m}(\theta,\phi) \equiv \langle\theta\,\phi\,|\,j=\tfrac{1}{2}\,,\,m\rangle = \frac{1}{\sqrt{2\ell+1}}\begin{pmatrix}\sqrt{\frac{1}{2}+m}\;Y_{0,m-\frac{1}{2}}(\theta,\phi)\\ \sqrt{\frac{1}{2}-m}\;Y_{0,m+\frac{1}{2}}(\theta,\phi)\end{pmatrix}. \qquad (46)$$

We apply the spin spherical harmonics to the following states:

$$\begin{aligned}2p_{1/2}:&\quad \ell=1\,,\quad j=\ell-\tfrac{1}{2}=\tfrac{1}{2}\,,\\ 2s_{1/2}:&\quad \ell=0\,,\quad j=\ell+\tfrac{1}{2}=\tfrac{1}{2}\,,\end{aligned}$$

The relevant spin spherical harmonics are:

$$\mathcal{Y}^{0\,\frac{1}{2}}_{\frac{1}{2}\,\frac{1}{2}} = \frac{1}{\sqrt{4\pi}}\begin{pmatrix}1\\0\end{pmatrix}\,, \qquad\qquad \mathcal{Y}^{0\,\frac{1}{2}}_{\frac{1}{2}\,,-\frac{1}{2}} = \frac{1}{\sqrt{4\pi}}\begin{pmatrix}0\\1\end{pmatrix}\,,$$

$$\mathcal{Y}^{1\,\frac{1}{2}}_{\frac{1}{2}\,\frac{1}{2}} = \frac{1}{\sqrt{3}}\begin{pmatrix}-Y_{10}(\theta,\phi)\\ \sqrt{2}Y_{11}(\theta,\phi)\end{pmatrix} = -\frac{1}{\sqrt{4\pi}}\begin{pmatrix}\cos\theta\\ e^{i\phi}\sin\theta\end{pmatrix}\,,$$

$$\mathcal{Y}^{1\,\frac{1}{2}}_{\frac{1}{2}\,,-\frac{1}{2}} = \frac{1}{\sqrt{3}}\begin{pmatrix}-\sqrt{2}Y_{1,-1}(\theta,\phi)\\ Y_{10}(\theta,\phi)\end{pmatrix} = \frac{1}{\sqrt{4\pi}}\begin{pmatrix}e^{-i\phi}\sin\theta\\ \cos\theta\end{pmatrix}\,.$$

We shall compute

$$\tfrac{1}{2}\sum_{m_i,m_f}|\vec{\boldsymbol{d}}_{if}|^2\,,$$

where we average over the two possible m_j-values of the initial state and sum over the two possible m_j values of the final state. In the coordinate basis,

$$\sum_{m_i,m_f}|\vec{\boldsymbol{d}}_{if}|^2 = \sum_{m_i,m_f}\int d^3x R_{20}(r)\mathcal{Y}^{\dagger\,0\,\frac{1}{2}}_{\frac{1}{2},m_i}(\hat{\boldsymbol{r}})\,\vec{\boldsymbol{x}}\,R_{21}(r)\mathcal{Y}^{1\,\frac{1}{2}}_{\frac{1}{2},m_f}(\hat{\boldsymbol{r}})\boldsymbol{\cdot}\int d^3x' R_{21}(r')\mathcal{Y}^{\dagger\,1\,\frac{1}{2}}_{\frac{1}{2},m_f}(\hat{\boldsymbol{r}}')\,\vec{\boldsymbol{x}}'\,R_{20}(r')\mathcal{Y}^{0\,\frac{1}{2}}_{\frac{1}{2},m_i}(\hat{\boldsymbol{r}}') \tag{47}$$

Inserting

$$\mathcal{Y}^{0\,\frac{1}{2}}_{\frac{1}{2},m_i} = \begin{pmatrix}\sqrt{\tfrac{1}{2}+m}\,Y_{0,m_i-\frac{1}{2}}(\hat{\boldsymbol{r}})\\ \sqrt{\tfrac{1}{2}-m}\,Y_{0,m_i+\frac{1}{2}}(\hat{\boldsymbol{r}})\end{pmatrix}\,, \qquad\qquad \mathcal{Y}^{1\,\frac{1}{2}}_{\frac{1}{2},m_f} = \begin{pmatrix}-\sqrt{\tfrac{3}{2}-m}\,Y_{1,m_f-\frac{1}{2}}(\hat{\boldsymbol{r}})\\ \sqrt{\tfrac{3}{2}+m}\,Y_{1,m_f+\frac{1}{2}}(\hat{\boldsymbol{r}})\end{pmatrix}\,,$$

into eq. (47), we obtain

$$\begin{aligned}\sum_{m_i,m_f}|\vec{\boldsymbol{d}}_{if}|^2 = \sum_{m_i,m_f}\int d^3x\,d^3x'\,R_{20}(r)R_{20}(r')R_{21}(r)R_{21}(r')\vec{\boldsymbol{x}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}'\\
\times\Big\{\big[(\tfrac{3}{2}+m_f)(\tfrac{1}{2}-m_i)\big]^{1/2}Y^*_{0,m_i+\frac{1}{2}}(\hat{\boldsymbol{r}})Y_{1,m_f+\frac{1}{2}}(\hat{\boldsymbol{r}}) - \big[(\tfrac{3}{2}-m_f)(\tfrac{1}{2}+m_i)\big]^{1/2}Y^*_{0,m_i-\frac{1}{2}}(\hat{\boldsymbol{r}})Y_{1,m_f-\frac{1}{2}}(\hat{\boldsymbol{r}})\Big\}\\
\times\Big\{\big[(\tfrac{3}{2}+m_f)(\tfrac{1}{2}-m_i)\big]^{1/2}Y^*_{1,m_f+\frac{1}{2}}(\hat{\boldsymbol{r}})Y_{0,m_i+\frac{1}{2}}(\hat{\boldsymbol{r}}) - \big[(\tfrac{3}{2}-m_f)(\tfrac{1}{2}+m_i)\big]^{1/2}Y^*_{1,m_f-\frac{1}{2}}(\hat{\boldsymbol{r}})Y_{0,m_i-\frac{1}{2}}(\hat{\boldsymbol{r}})\Big\}.\end{aligned}$$

It is straightforward to perform the sums over m_i and m_f. The product of the two factors in braces above consists of four pieces:

1. $m_i = m_f = \frac{1}{2}$: $\quad \left\{-\frac{1}{4\pi}\cos\theta\right\}\left\{-\frac{1}{4\pi}\cos\theta'\right\}\,,$

2. $m_i = \frac{1}{2}\,,\ m_f = -\frac{1}{2}$: $\quad \left\{-\frac{1}{4\pi}e^{-i\phi}\sin\theta\right\}\left\{-\frac{1}{4\pi}e^{i\phi'}\sin\theta'\right\}\,,$

3. $m_i = -\frac{1}{2}\,,\ m_f = \frac{1}{2}$: $\quad \left\{-\frac{1}{4\pi}e^{i\phi}\sin\theta\right\}\left\{-\frac{1}{4\pi}e^{-i\phi'}\sin\theta'\right\}\,,$

4. $m_i = m_f = -\frac{1}{2}$: $\quad \left\{\frac{1}{4\pi}\cos\theta\right\}\left\{\frac{1}{4\pi}\cos\theta'\right\}\,.$

Summing up the four pieces yields

$$\frac{1}{8\pi^2}\left[\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi')\right] = \frac{1}{8\pi^2}\hat{\boldsymbol{r}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,' ,$$

The last step above follows from the definition of the unit vectors,

$$\hat{\boldsymbol{r}} = (\sin\theta\cos\phi\,,\,\sin\theta\sin\phi\,,\,\cos\theta)\,, \qquad\qquad \hat{\boldsymbol{r}}\,' = (\sin\theta'\cos\phi'\,,\,\sin\theta'\sin\phi'\,,\,\cos\theta')\,.$$

Hence,

$$\sum_{m_i,m_f} |\vec{\boldsymbol{d}}_{if}|^2 = \frac{1}{8\pi^2}\int d^3x\,d^3x' R_{20}(r)R_{20}(r')R_{21}(r)R_{21}(r')rr'(\hat{\boldsymbol{r}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,')^2\,.$$

To perform the integrals above, we employ spherical coordinates and choose the z-axis to lie along $\vec{\boldsymbol{x}}'$. Then, $\hat{\boldsymbol{r}}\boldsymbol{\cdot}\hat{\boldsymbol{r}}\,' = \cos\theta$ and the integral over $d\Omega'$ is free. It follows that

$$\begin{aligned}\sum_{m_i,m_f} |\vec{\boldsymbol{d}}_{if}|^2 &= \frac{1}{2\pi}\int_0^\infty r^3dr\int_0^\infty r'^3dr'\,R_{20}(r)R_{20}(r')R_{21}(r)R_{21}(r')\int d\Omega\cos^2\theta \\ &= \frac{2}{3}\left|\int_0^\infty r^3R_{20}(r)R_{21}(r)\,dr\right|^2 = 18a_0^2\,,\end{aligned}$$

where we have used eq. (20) in the final step. Finally, we average over the two initial m_i values to obtain,

$$\tfrac{1}{2}\sum_{m_i,m_f}|\vec{\boldsymbol{d}}_{if}|^2 = 9a_0^2\,.$$

Inserting this result into eq. (19) yields

$$\Gamma(2s_{1/2}\to 2p_{1/2}+\gamma) = \frac{12\omega^3e^2a_0^2}{c^3\hbar} = \frac{12\omega^3\hbar^2}{(mc^2)^2\alpha}\,,$$

which reproduces the result of eq. (23). Indeed, this computation justifies the factor of $\frac{1}{3}$ that was employed in eq. (22).