1. Consider a two-level system with $E_1 < E_2$. There is a time-dependent potential that connects the two levels as follows:

$$V_{11} = V_{22} = 0, \qquad V_{12} = \gamma e^{i\omega t}, \qquad V_{21} = \gamma e^{-i\omega t} \qquad (\gamma \ \text{ real})\,, \tag{1}$$

where $V_{ij} = \langle i|V|j\rangle$. At time $t = 0$, it is known that only the lower level is populated—that is, $c_1(0) = 1$ and $c_2(0) = 0$. Note that a general state of the system can be expressed as a linear combination of eigenstates of the unperturbed Hamiltonian (in the Schrodinger picture):

$$|\psi(t)\rangle = \sum_{n=1}^{2} c_n(t) e^{-iE_n t/\hbar} \, |n\rangle \ . \tag{2}$$

(a) Starting with the time-dependent Schrodinger equation, derive the following differential equation for $c_k(t)$:

$$i\hbar \frac{dc_k}{dt} = \sum_{n=1}^{2} V_{kn}(t) e^{i\omega_{kn} t} c_n \,, \qquad (k = 1, 2)\,, \tag{3}$$

where $V_{kn}(t) \equiv \langle k|V(t)|n\rangle$ and $\hbar\omega_{kn} \equiv E_k - E_n$. By solving the above system of differential equations *exactly*, find $|c_1(t)|^2$ and $|c_2(t)|^2$ for $t > 0$.

The full Hamiltonian is given by

$$H = H^{(0)} + V \,,$$

where the matrix elements of V are given in eq. (1). The time-dependent Schrodinger equation is given by

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \left[H^{(0)} + V\right] |\psi(t)\rangle \ .$$

Inserting the expansion for $|\psi(t)\rangle$ given in eq. (2) into the above equation, and using $H^{(0)} |n\rangle = E_n |n\rangle$, it follows that[1]

$$\sum_{n=1}^{2} i\hbar \frac{dc_n}{dt} \, e^{-iE_n t/\hbar} \, |n\rangle = \sum_{n=1}^{2} c_n e^{-iE_n t/\hbar} \, V \, |n\rangle \ .$$

Next, multiply on the left by $\langle k|$ and use $\langle k|n\rangle = \delta_{kn}$ to obtain:

$$i\hbar \frac{dc_k}{dt} \, e^{-iE_k t/\hbar} = \sum_{n=1}^{2} c_n e^{-iE_n t/\hbar} \langle k|V|n\rangle \,. \tag{4}$$

[1]For ease in notation, we denote the eigenvalues of the unperturbed Hamiltonian $H^{(0)}$ by E_n rather than $E_n^{(0)}$.

Eq. (4) can be rewritten as:

$$i\hbar\frac{dc_k}{dt} = \sum_{n=1}^{2} V_{kn}(t)e^{i\omega_{kn}t}c_n\,, \qquad (k=1,2)\,,$$

where $V_{kn}(t) \equiv \langle k|V(t)|n\rangle$ and $\hbar\omega_{kn} \equiv E_k - E_n$, which confirms eq. (3). In matrix form,

$$i\hbar\frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t)\end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}e^{i\omega_{12}t} \\ V_{21}e^{i\omega_{21}t} & V_{22}\end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t)\end{pmatrix}\,,$$

where $\omega_{21} = -\omega_{12} = (E_2 - E_1)/\hbar > 0$, and the matrix elements of V are given by eq. (1). That is,

$$i\hbar\frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t)\end{pmatrix} = \begin{pmatrix} 0 & \gamma e^{i(\omega-\omega_{21})t} \\ \gamma e^{-i(\omega-\omega_{21})t} & 0\end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t)\end{pmatrix}\,,$$

Multiplying out the matrix and vector above, one obtains coupled differential equations for $c_1(t)$ and $c_2(t)$:

$$i\hbar\frac{dc_1}{dt} = \gamma e^{i(\omega-\omega_{21})t}\,c_2\,, \qquad\qquad i\hbar\frac{dc_2}{dt} = \gamma e^{-i(\omega-\omega_{21})t}\,c_1\,. \tag{5}$$

At this point, it is convenient to define new coefficients,

$$c_1'(t) \equiv e^{i(\omega_{21}-\omega)t/2}\,c_1(t)\,, \qquad\qquad c_2'(t) \equiv e^{-i(\omega_{21}-\omega)t/2}\,c_2(t)\,. \tag{6}$$

We now can express eq. (5) in terms of $c_1'(t)$ and $c_2'(t)$:

$$i\hbar\frac{d}{dt}\left[e^{-i(\omega_{21}-\omega)t/2}\,c_1'\right] = \gamma e^{i(\omega-\omega_{21})t}\,\left[e^{i(\omega_{21}-\omega)t/2}\,c_2'\right]\,,$$

$$i\hbar\frac{d}{dt}\left[e^{i(\omega_{21}-\omega)t/2}\,c_2'\right] = \gamma e^{-i(\omega-\omega_{21})t}\,\left[e^{-i(\omega_{21}-\omega)t/2}\,c_1'\right]\,.$$

Expanding out the derivatives, one sees that the exponential factors cancel. The resulting equations for $c_1'(t)$ and $c_2'(t)$ are:

$$i\hbar\left[\tfrac{1}{2}i(\omega-\omega_{21})c_1' + \frac{dc_1'}{dt}\right] = \gamma c_2'\,, \qquad\qquad i\hbar\left[-\tfrac{1}{2}i(\omega-\omega_{21})c_2' + \frac{dc_2'}{dt}\right] = \gamma c_1'\,. \tag{7}$$

In matrix form, eq. (7) is given by:

$$i\hbar\frac{d}{dt}\begin{pmatrix} c_1'(t) \\ c_2'(t)\end{pmatrix} = A\begin{pmatrix} c_1'(t) \\ c_2'(t)\end{pmatrix}\,, \tag{8}$$

where A is the *time-independent* 2×2 traceless hermitian matrix,

$$A \equiv \begin{pmatrix} \frac{1}{2}\hbar(\omega-\omega_{21}) & \gamma \\ \gamma & -\frac{1}{2}\hbar(\omega-\omega_{21})\end{pmatrix}\,. \tag{9}$$

Denoting the column vector $\vec{\boldsymbol{c}} \equiv (c_1', c_2')^T$, eq. (8) is of the form

$$\frac{d\vec{\boldsymbol{c}}}{dt} = -\frac{iA}{\hbar}\vec{\boldsymbol{c}}\,. \tag{10}$$

The solution to this equation is:

$$\vec{\boldsymbol{c}}(t) = e^{-iAt/\hbar}\,\vec{\boldsymbol{c}}_0\,, \qquad \text{where} \;\; \vec{\boldsymbol{c}}_0 \equiv \vec{\boldsymbol{c}}(t=0)\,.$$

This is easily verified by inserting the above solution back into eq. (10).

To compute the matrix exponential, a simple strategy is to write writing $A = \vec{\boldsymbol{a}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}$, where the vector $\vec{\boldsymbol{a}}$ is uniquely determined. Such a relation holds for *any* 2×2 traceless hermitian matrix. It is easy to see that for A given by eq. (9),

$$A = \gamma\sigma_x + \tfrac{1}{2}\hbar(\omega-\omega_{21})\sigma_z\,.$$

Using the well-known result:[2]

$$\exp\left(\tfrac{1}{2}i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}\right) = \mathbf{I}\cos(\theta/2) + i\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}\sin(\theta/2) = \begin{pmatrix} \cos(\theta/2)+in_z\sin(\theta/2) & (in_x+n_y)\sin(\theta/2) \\ (in_x-n_y)\sin(\theta/2) & \cos(\theta/2)-in_z\sin(\theta/2)\end{pmatrix},$$

where $\mathbf{I}$ is the 2×2 identity matrix, we can identify

$$\exp(-iAt/\hbar) = \exp\left\{-\frac{it}{\hbar}\left(\gamma\sigma_x + \tfrac{1}{2}\hbar(\omega-\omega_{21})\sigma_z\right)\right\} = \exp\left(\tfrac{1}{2}i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}\right)\,, \tag{11}$$

where[3]

$$\hat{\boldsymbol{n}} = \frac{1}{\sqrt{\hbar^2(\omega-\omega_{21})^2+4\gamma^2}}\bigl(2\gamma\,,\,0\,,\,\hbar(\omega-\omega_{21})\bigr)\,, \tag{12}$$

and

$$\theta = -\frac{t}{\hbar}\sqrt{\hbar^2(\omega-\omega_{21})^2+4\gamma^2}\,. \tag{13}$$

We conclude that

$$\begin{pmatrix} c_1'(t) \\ c_2'(t)\end{pmatrix} = \begin{pmatrix} \cos(\theta/2)+in_z\sin(\theta/2) & in_x\sin(\theta/2) \\ in_x\sin(\theta/2) & \cos(\theta/2)-in_z\sin(\theta/2)\end{pmatrix}\begin{pmatrix} c_1'(0) \\ c_2'(0)\end{pmatrix},$$

where θ is defined by eq. (13) and

$$n_x \equiv \frac{2\gamma}{\sqrt{\hbar^2(\omega-\omega_{21})^2+4\gamma^2}}\,, \qquad n_z = \frac{\hbar(\omega-\omega_{21})}{\sqrt{\hbar^2(\omega-\omega_{21})^2+4\gamma^2}}\,. \tag{14}$$

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[2]If this result is not well-known to you, please derive it as follows. First note that for any non-negative integer k, $(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}})^{2k} = \mathbf{I}$ and $(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}})^{2k+1} = \hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}$, where $\hat{\boldsymbol{n}}$ is a unit vector and $\mathbf{I}$ is the 2×2 identity matrix. Then, using the Taylor series definition of the matrix exponential,

$$\exp\left(\tfrac{1}{2}i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}\right) = \sum_{k=0}^{\infty}\frac{\left(\tfrac{1}{2}i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}\right)^k}{k!} = \mathbf{I}\sum_{k\ \text{even}}\frac{\left(\tfrac{1}{2}i\theta\right)^k}{k!} + \hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}\sum_{k\ \text{odd}}\frac{\left(\tfrac{1}{2}i\theta\right)^k}{k!} = \mathbf{I}\cos(\theta/2) + i\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\sigma}}\sin(\theta/2)\,.$$

[3]A common mistake made by students is to neglect the fact that $\hat{\boldsymbol{n}}$ appearing in eq. (11) must be a *unit vector*. Note that $\hat{\boldsymbol{n}}$ in eq. (12) is properly normalized so that $\hat{\boldsymbol{n}}\boldsymbol{\cdot}\hat{\boldsymbol{n}} = 1$.

In light of eq. (6), it follows that the relevant initial conditions are

$$c_1(0) = c_1'(0) = 1 \quad \text{and} \quad c_2(0) = c_2'(0) = 0\,,$$

and

$$\begin{aligned}
|c_1(t)|^2 &= |c_1'(t)|^2 = |\cos(\theta/2) + i n_z \sin(\theta/2)|^2 = \cos^2(\theta/2) + n_z^2 \sin^2(\theta/2)\,, \\
|c_2(t)|^2 &= |c_2'(t)|^2 = n_x^2 \sin^2(\theta/2)\,.
\end{aligned}$$

An important check of the above result is:

$$|c_1(t)|^2 + |c_2(t)|^2 = \cos^2(\theta/2) + (n_x^2 + n_z^2)\sin^2(\theta/2) = 1\,,$$

where we have used the fact that $n_x^2 + n_z^2 = n_x^2 + n_y^2 + n_z^2 = 1$, keeping in mind that $n_y = 0$ and $\hat{\boldsymbol{n}}$ is a unit vector. Using the explicit forms of n_x, n_z and θ given in eqs. (13) and (14) we arrive at:

$$\boxed{|c_2(t)|^2 = \frac{4\gamma^2}{4\gamma^2 + \hbar^2(\omega - \omega_{21})^2} \sin^2\left(\left[\tfrac{\gamma^2}{\hbar^2} + \tfrac{1}{4}(\omega - \omega_{21})^2\right]^{1/2} t\right)\,, \qquad |c_1(t)|^2 = 1 - |c_2(t)|^2} \tag{15}$$

Note that the initial conditions $c_1(0) = 1$ and $c_2(0) = 0$ are indeed satisfied.

<u>ALTERNATIVE DERIVATION:</u>

Starting from eq. (5), it immediately follows that

$$i\hbar \frac{d}{dt}\left(\frac{i\hbar}{\gamma} e^{it(\omega-\omega_{21})} \frac{dc_2}{dt}\right) = \gamma e^{it(\omega-\omega_{21})}\, c_2\,.$$

After evaluating the derivative on the left-hand side of the above equation, the exponential factors cancel out, resulting in

$$\frac{d^2 c_2}{dt^2} + i(\omega - \omega_{21})\frac{dc_2}{dt} + \frac{\gamma^2 c_2}{\hbar^2} = 0\,.$$

The solution is obtained by solving the auxiliary equation:

$$x^2 + i(\omega - \omega_{21})x + \frac{\gamma^2}{\hbar^2} = 0 \quad \Rightarrow \quad x = -i\left[\tfrac{1}{2}(\omega - \omega_{21}) \pm \Delta\right]\,.$$

where

$$\Delta \equiv \sqrt{\tfrac{\gamma^2}{\hbar^2} + \tfrac{1}{4}(\omega - \omega_{21})^2}\,. \tag{16}$$

It follows that:

$$c_2(t) = A\left[\exp\left\{-it\left[\tfrac{1}{2}(\omega - \omega_{21}) + \Delta\right]\right\} - \exp\left\{-it\left[\tfrac{1}{2}(\omega - \omega_{21}) - \Delta\right]\right\}\right]\,, \tag{17}$$

after imposing the initial condition $c_2(0) = 0$. To determine the overall coefficient, we make use of eqs. (5) and (17) to obtain:

$$\frac{\gamma}{i\hbar} e^{-it(\omega-\omega_{21})} c_1 = \frac{dc_2}{dt} = -iA\left[\tfrac{1}{2}(\omega-\omega_{21})+\Delta\right]\exp\left\{-it\left[\tfrac{1}{2}(\omega-\omega_{21})+\Delta\right]\right\}$$
$$+iA\left[\tfrac{1}{2}(\omega-\omega_{21})-\Delta\right]\exp\left\{-it\left[\tfrac{1}{2}(\omega-\omega_{21})-\Delta\right]\right\}. \quad (18)$$

Setting $t = 0$ and using $c_1(0) = 1$, one obtains:

$$A = \frac{\gamma}{2\hbar\Delta}. \quad (19)$$

Thus, eqs. (17) and (9) yield:

$$\begin{aligned}
|c_2(t)|^2 &= \frac{\gamma^2}{4\hbar^2\Delta^2}\left[2 - 2\,\mathrm{Re}\Big(\exp\left\{-it\left[\tfrac{1}{2}(\omega-\omega_{21})+\Delta\right]\right\}\exp\left\{it\left[\tfrac{1}{2}(\omega-\omega_{21})-\Delta\right]\right\}\Big)\right] \\
&= \frac{\gamma^2}{4\hbar^2\Delta^2}\left[2 - 2\,\mathrm{Re}\big(e^{-2it\Delta}\big)\right] \\
&= \frac{\gamma^2}{2\hbar^2\Delta^2}\left[1 - \cos(2t\Delta)\right] \\
&= \frac{\gamma^2}{\hbar^2\Delta^2}\sin^2(t\Delta).
\end{aligned}$$

Finally, we take the absolute square of eq. (18), which yields:

$$\begin{aligned}
\frac{\gamma^2}{\hbar^2}|c_1(t)|^2 &= A^2\left[\tfrac{1}{2}(\omega-\omega_{21})+\Delta\right]^2 + A^2\left[\tfrac{1}{2}(\omega-\omega_{21})-\Delta\right]^2 - 2A^2\left[\tfrac{1}{4}(\omega-\omega_{21})^2-\Delta^2\right]\mathrm{Re}(e^{-2it\Delta}) \\
&= 2A^2\left[\tfrac{1}{4}(\omega-\omega_{21})^2+\Delta^2\right] - 2A^2\left[\tfrac{1}{4}(\omega-\omega_{21})^2-\Delta^2\right]\cos(2t\Delta) \\
&= A^2(\omega-\omega_{21})^2\sin^2(t\Delta) + 4A^2\Delta^2\cos^2(t\Delta) \\
&= 4A^2\left(\Delta^2 - \frac{\gamma^2}{\hbar^2}\right)\sin^2(t\Delta) + 4A^2\Delta^2\cos^2(t\Delta) \\
&= 4A^2\left[\Delta^2 - \frac{\gamma^2}{\hbar^2}\sin^2(t\Delta)\right],
\end{aligned}$$

where in the penultimate step we used $(\omega-\omega_{21})^2 = 4(\Delta^2 - \gamma^2/\hbar^2)$, which follows from the definition of Δ [cf. eq. (16)]. Noting that $4A^2 = \gamma^2/(\hbar^2\Delta^2)$ [cf. eq. (19)], we end up with

$$|c_1(t)|^2 = 1 - \frac{\gamma^2}{\hbar^2\Delta^2}\sin^2(t\Delta) = 1 - |c_2(t)|^2.$$

Thus, we have correctly reproduced the results of eq. (15).

(b) Do the same problem using time-dependent perturbation theory to lowest nonvanishing order. Compare the two approaches for small values of γ. Treat the following two cases separately: (i) ω very different from ω_{21}, and (ii) ω close to ω_{21}.

Using the results of time-dependent perturbation theory, we identify $c_n(t)$ of part (a) as:

$$c_n(t) = \langle n|U_I(t,0)|i\rangle \,,$$

where $U_I(t,0)$ is the time-evolution operator in the interaction representation. The first-order perturbation theory expression for $c_n(t)$ obtained in class is:

$$c_n(t) = \delta_{ni} - \frac{i}{\hbar}\int_0^t e^{i\omega_{ni}t'}\, V_{ni}(t')\, dt' \,.$$

Thus, to first order in perturbation theory, $c_1(t) \simeq 1$ and

$$c_2(t) = -\frac{i}{\hbar}\int_0^t e^{i\omega_{21}t'}\,\gamma e^{-i\omega t'}\, dt' = \frac{\gamma\left[1 - e^{i(\omega_{21}-\omega)t}\right]}{\hbar(\omega_{21}-\omega)} \,.$$

Hence,

$$|c_2(t)|^2 = \frac{2\gamma^2\left[1-\cos(\omega_{21}-\omega)t\right]}{\hbar^2(\omega_{21}-\omega)^2} = \frac{4\gamma^2}{\hbar^2(\omega_{21}-\omega)^2}\sin^2\!\left(\tfrac{1}{2}(\omega_{21}-\omega)t\right) . \tag{20}$$

We observe that eq. (20) agrees with the exact formula obtained in eq. (15) in the limit of $\gamma \ll \frac{1}{2}\hbar|\omega_{21}-\omega|$. Note that the latter inequality is never satisfied near resonance when $\omega \simeq \omega_{21}$. However, if $\omega \simeq \omega_{21}$ then the exact formula, eq. (15), reduces to

$$|c_2(t)|^2 = \sin^2(\gamma t/\hbar) \,, \qquad \text{for } \ \omega = \omega_{21} \,.$$

In contrast, the corresponding first-order perturbative result exhibited in eq. (20) is:

$$|c_2(t)|^2 \simeq \frac{\gamma^2 t^2}{\hbar^2} \,, \qquad \text{for } \ \omega = \omega_{21} \,.$$

Thus, near the resonance, the exact result for $|c_2(t)|^2$ agrees with the first-order perturbative result in the limit of $t \ll \hbar/\gamma$.

To summarize, the first-order perturbative result is a good approximation to the exact result in the limit of a weak perturbation (which corresponds to small γ). Away from the resonance, small γ means $\gamma \ll \frac{1}{2}\hbar|\omega_{21}-\omega|$, whereas near the resonance (where $\omega \simeq \omega_{21}$) small γ means $\gamma \ll \hbar/t$. For a fixed value of γ, the latter can be satisfied only at early times t.

2. This problem provides a crude model for the photoelectric effect. Consider the hydrogen atom in its ground state (you may neglect the spins of the electron and proton). At time $t = 0$, the atom is placed in a high frequency uniform electric field that points in the z-direction,

$$\vec{\boldsymbol{\mathcal{E}}}(t) = \mathcal{E}_0 \hat{\boldsymbol{z}} \sin\omega t \,.$$

We wish to compute the transition probability per unit time that an electron is ejected into a solid angle lying between Ω and $\Omega + d\Omega$.

(a) Determine the minimum frequency, ω_0, of the field necessary to ionize the atom.

The minimum frequency, ω_0, of the field necessary to ionize the atom is equal to the ionization energy divided by $\hbar$. The ionization energy of the ground state of hydrogen is equal to the negative of the bound state energy, and is given by 1 Ry = 13.6 eV. That is,

$$\omega_0 = \frac{me^4}{2\hbar^3} \,. \tag{21}$$

(b) Using Fermi's golden rule for the transition rate at first-order in time-dependent perturbation theory, obtain an expression for the transition rate per unit solid angle as a function of the polar angle θ of the ejected electron (measured with respect to the direction of the electric field).

The perturbing Hamiltonian is given by:

$$H^{(1)}(t) = ez\mathcal{E}_0 \sin\omega t = \frac{ez\mathcal{E}_0}{2i}\left(e^{i\omega t} - e^{-i\omega t}\right) \,. \tag{22}$$

Fermi's golden rule for the transition rate for the absorption of energy due to the harmonic perturbation given in eq. (22) is given by:

$$\Gamma_{a\to b}(t) = \frac{2\pi}{\hbar}\left|\left\langle b^{(0)}\right| \tfrac{1}{2}ez\mathcal{E}_0 \left|a^{(0)}\right\rangle\right|^2 \rho(E_b^{(0)}) \,, \tag{23}$$

where $\rho(E_b^{(0)})$ is the density of states of the ionized electron. The state $\left|a^{(0)}\right\rangle$ is the unperturbed wave function for the ground state of hydrogen,

$$\left|a^{(0)}\right\rangle = \Psi_{100}(r) = \frac{1}{(\pi a_0^3)^{1/2}}\, e^{-r/a_0} \,, \qquad\qquad a_0 \equiv \frac{\hbar^2}{me^2} \,.$$

The state $\left|b^{(0)}\right\rangle$ is the unperturbed wave function for the ionized wave function. This wave function is actually quite complicated, since one cannot really neglect the effects of the long-range Coulomb potential. Nevertheless, we shall simplify the computation by assuming the wave function of the ejected electron is a free-particle plane wave, with wave number vector $\vec{\boldsymbol{k}}$, where the direction of $\vec{\boldsymbol{k}}$ corresponds to that of the ejected electron. That is, $\left|b^{(0)}\right\rangle = e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}/\sqrt{V}$. Taking the hermitian conjugate yields,

$$\left\langle b^{(0)}\right| = \frac{1}{\sqrt{V}}\, e^{-i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}\,.$$

Note that we have normalized the free-particle plane wave by placing the system in a very large box of volume V. Imposing periodic boundary conditions, the possible values of $\vec{\boldsymbol{k}}$ are quantized as discussed in class. This will be convenient since we can later use the expression derived in class for the free-particle density of states.

We are now ready to compute the matrix element, $\left\langle b^{(0)}\right| \tfrac{1}{2}ez\mathcal{E}_0 \left|a^{(0)}\right\rangle$. Employing spherical coordinates, $z = r\cos\theta$ and

$$\left\langle b^{(0)}\right| \tfrac{1}{2}ez\mathcal{E}_0 \left|a^{(0)}\right\rangle = \frac{e\mathcal{E}_0}{2(V\pi a_0^3)^{1/2}} \int_0^\infty dr'\, r'^3 e^{-r'/a_0} \int d\Omega' e^{-i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}'} \cos\theta'\,. \tag{24}$$

In order to perform this integral, we make use of the expansion of the exponential in terms of spherical harmonics:

$$e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}'} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell j_\ell(kr')[Y_\ell^m(\theta',\phi')]^* Y_\ell^m(\theta,\phi)\,, \tag{25}$$

where the vector $\vec{\boldsymbol{x}}'$ points in a direction with polar and azimuthal angles θ', ϕ' with respect to a fixed z-axis, and the vector $\vec{\boldsymbol{k}}$ points in a direction with polar and azimuthal angles θ, ϕ with respect to a fixed z-axis. Taking the complex conjugate of eq. (25) and inserting the result into eq. (24) yields:

$$\left\langle b^{(0)}\right| \tfrac{1}{2}ez\mathcal{E}_0 \left|a^{(0)}\right\rangle = \frac{4\pi e\mathcal{E}_0}{2(V\pi a_0^3)^{1/2}} \sum_{\ell=0}^{\infty} i^\ell \int_0^\infty dr'\, r'^3 e^{-r'/a_0} j_\ell(kr') \sum_{m=-\ell}^{\ell} [Y_\ell^m(\theta,\phi)]^* \int d\Omega' \cos\theta'\, Y_\ell^m(\theta',\phi')\,. \tag{26}$$

Noting that we can write:

$$\cos\theta' = \left(\frac{4\pi}{3}\right)^{1/2} [Y_1^0(\theta',\phi')]^*\,,$$

the integration over solid angles in eq. (26) can be immediately performed:

$$\int d\Omega'\, \cos\theta'\, Y_\ell^m(\theta',\phi') = \left(\frac{4\pi}{3}\right)^{1/2} \int d\Omega'\, \cos\theta'\, Y_\ell^m(\theta',\phi')[Y_1^0(\theta',\phi')]^* = \left(\frac{4\pi}{3}\right)^{1/2} \delta_{\ell 1}\delta_{m0}\,, \tag{27}$$

where we have used the orthogonality relations of the spherical harmonics,

$$\int d\Omega\, Y_\ell^m(\Omega)\, [Y_{\ell'}^{m'}(\Omega)]^* = \delta_{\ell\ell'}\delta_{mm'}\,. \tag{28}$$

Inserting eq. (27) back into eq. (26) collapses both the sums over m and ℓ, respectively. Only the $\ell = 1$, $m = 0$ term of the sums survives. Thus, using $Y_1^0(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$, eq. (27) reduces to:

$$\left\langle b^{(0)}\right| \tfrac{1}{2}ez\mathcal{E}_0 \left|a^{(0)}\right\rangle = \frac{2\pi i e\mathcal{E}_0\cos\theta}{(V\pi a_0^3)^{1/2}} \int_0^\infty dr\, r^3 e^{-r/a_0} \left(\frac{\sin kr}{k^2r^2} - \frac{\cos kr}{kr}\right)\,,$$

where we have used $j_1(y) = (\sin y - y\cos y)/y^2$. (For notational convenience, I have now dropped the primes on the integration variable r.) My integral tables provide the following results:[4]

$$\int_0^\infty r\, e^{-r/a_0} \sin kr\, dr = \frac{2ka_0^3}{(1+k^2a_0^2)^2}\,,$$

$$\int_0^\infty r^2\, e^{-r/a_0} \cos kr\, dr = \frac{2a_0^3(1-3k^2a_0^2)}{(1+k^2a_0^2)^3}\,.$$

Thus,

$$\int_0^\infty dr\, r^3 e^{-r/a_0}\left(\frac{\sin kr}{k^2r^2} - \frac{\cos kr}{kr}\right) = \frac{8ka_0^5}{(1+k^2a_0^2)^3}\,.$$

Hence, it follows that:

$$\left\langle b^{(0)}\right| \tfrac{1}{2}ez\mathcal{E}_0 \left|a^{(0)}\right\rangle = 16ie\mathcal{E}_0\cos\theta\left(\frac{\pi a_0^5}{V}\right)^{1/2}\frac{ka_0}{(1+k^2a_0^2)^3}\,.$$

We are now ready to compute the transition rate. Using the density of states derived in class,

$$\rho(E) = \frac{Vm\hbar k}{(2\pi\hbar)^3}\, d\Omega\,,$$

the transition rate [see eq. (23)] is given by:

$$\Gamma_{a\to b} = \frac{2\pi}{\hbar}\,\frac{Vm\hbar k}{(2\pi\hbar)^3}\, d\Omega\left(\frac{256\pi e^2\mathcal{E}_0^2 a_0^5\cos^2\theta}{V}\right)\frac{(ka_0)^2}{(1+k^2a_0^2)^6}\,.$$

Simplifying the above result, and noting that $me^2/\hbar^2 = 1/a_0$, we end up with:

$$\boxed{\frac{d\Gamma_{a\to b}}{d\Omega} = \frac{64\mathcal{E}_0^2 a_0^3\cos^2\theta}{\pi\hbar}\,\frac{(ka_0)^3}{(1+k^2a_0^2)^6}}$$

The factors of the volume V have canceled out, which indicates that the transition rate for ionization is a physical quantity.

Fermi's golden rule also imposes energy conservation. The initial energy is the ground state energy of hydrogen, which is given by $E_a^{(0)} = -\hbar\omega_0$, as noted in part (a). The final state energy is $E_b^{(0)} = \hbar^2k^2/(2m)$. Since this is an absorption process, a quantum of energy $\hbar\omega$ from the harmonic perturbation must account for the energy difference between the final and initial state energies. Therefore,

$$\hbar\omega = \frac{\hbar k^2}{2m} + \hbar\omega_0\,.$$

[4] For simple integrals, my reference table of choice is H.B. Dwight, *Table of Integrals and other Mathematical Data* (Macmillan Publishing Co., Inc., New York, 1961).

Solving for k^2, we can write:

$$k^2 a_0^2 = \frac{2ma_0^2}{\hbar}(\omega - \omega_0) = \frac{2\hbar^3}{me^4}(\omega - \omega_0) = \frac{\omega - \omega_0}{\omega_0}\,,$$

where we have used the definition of the Bohr radius, $a_0 \equiv \hbar^2/(me^2)$, and the results of part (a). Thus, we can rewrite the differential transition rate for ionization as:

$$\boxed{\frac{d\Gamma_{a\to b}}{d\Omega} = \frac{64\mathcal{E}_0^2 a_0^3}{\pi\hbar}\left(\frac{\omega_0}{\omega}\right)^6\left(\frac{\omega}{\omega_0} - 1\right)^{3/2}\cos^2\theta}$$

Note that as ω_0 is the minimum frequency of the field necessary to ionize the hydrogen atom, it follows that $\omega \geq \omega_0$.

(c) Integrate the result of part (b) over all solid angles to obtain the total ionization rate as a function of the frequency of the field. Determine the value of ω [in terms of ω_0 obtained in part (a)] for which the total ionization rate is maximal.

Integrating over solid angles [using $\int d\Omega\cos^2\theta = 4\pi/3$], we find that the total ionization rate is given by:

$$\boxed{\Gamma_{a\to b} = \frac{256\mathcal{E}_0^2 a_0^3}{3\hbar}\left(\frac{\omega_0}{\omega}\right)^6\left(\frac{\omega}{\omega_0} - 1\right)^{3/2}}$$

Note that the ionization rate approaches zero both in the limit of $\omega \to \omega_0$ and in the limit of $\omega \to \infty$. Moreover, the ionization rate (which is a physical observable) must be non-negative for $\omega_0 \leq \omega < \infty$. Thus, there must be some value of ω in the range $\omega_0 \leq \omega < \infty$ for which the ionization rate is maximal. To find this value of ω, take the derivative of the expression above with respect to ω and set it to zero. Thus, we solve:

$$-\frac{6}{\omega^7}\left(\frac{\omega}{\omega_0} - 1\right)^{3/2} + \frac{3}{2\omega^6\omega_0}\left(\frac{\omega}{\omega_0} - 1\right)^{1/2} = 0\,.$$

This can be easily simplified, and one finds that the the above equation is satisfied for only one value, $\omega = \frac{4}{3}\omega_0$. We conclude that at this frequency, the ionization rate must be maximal.[5]

[5] Of course, one can also verify this by computing the sign of the second derivative.

3. Consider the spontaneous emission of an $E1$ photon by an excited atom. The magnetic quantum numbers (m and m') of the initial and final atomic state are measured with respect to a fixed z-axis. Suppose the magnetic quantum number of the atom decreases by one unit.

(a) Compute the angular distribution of the emitted photon.

The transition rate for spontaneous E1 emission is given by:

$$\frac{d\Gamma_{if}}{d\Omega} = \frac{e^2\omega^3}{2\pi\hbar c^3}\sum_\lambda |\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{\epsilon}}_\lambda^{\,*}|^2\,, \qquad \text{where}\;\; \vec{\boldsymbol{d}}_{if} = \langle f|\vec{\boldsymbol{x}}|i\rangle\,.$$

The sum over polarizations can be performed by computing:

$$\begin{aligned}\sum_\lambda |\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{\epsilon}}_\lambda^{\,*}|^2 &= (d_{if})_i(d^*_{if})_j\sum_\lambda(\epsilon^*_\lambda)_i(\epsilon_\lambda)_j = (d_{if})_i(d^*_{if})_j\left(\delta_{ij}-\frac{k_ik_j}{k^2}\right)\\ &= \vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{d}}^{\,*}_{if} - \frac{(\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{k}})(\vec{\boldsymbol{d}}^{\,*}_{if}\cdot\vec{\boldsymbol{k}})}{k^2}\,, \end{aligned} \tag{29}$$

where there is an implicit sum over the repeated indices i and j above. Thus,

$$\frac{d\Gamma_{if}}{d\Omega} = \frac{e^2\omega^3}{2\pi\hbar c^3}\left(\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{d}}^{\,*}_{if} - \frac{(\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{k}})(\vec{\boldsymbol{d}}^{\,*}_{if}\cdot\vec{\boldsymbol{k}})}{k^2}\right)\,. \tag{30}$$

We shall denote the initial state by $|i\rangle = |j\,m\rangle$ and $|f\rangle = |j'\,m-1\rangle$. The z-axis in this problem is the quantization axis which is used to define the magnetic quantum numbers of the atomic states. (Other attributes of the atomic states are suppressed.)

We can evaluate he non-zero components of $\vec{\boldsymbol{d}}_{if}$ with the help of the Wigner-Eckart theorem, which states that the matrix elements of a spherical tensor $T^{(k)}_q$ with respect to definite angular momentum states must satisfy[6]

$$\langle j'\,m'|T^{(k)}_q|j\,m\rangle = 0 \qquad \text{if}\;\; m'\neq q+m\,. \tag{31}$$

One can apply this result to the matrix elements of $\vec{\boldsymbol{x}}$ by recognizing the latter as a spherical tensor of rank-one. That is, certain linear combinations of the components of $\vec{\boldsymbol{x}} \equiv (x,y,z) = r(\sin\theta'\cos\phi', \sin\theta'\sin\phi', \cos\theta')$ are proportional to the components of the rank-one spherical tensor $rY_{1M}(\theta',\phi')$, for $M=+1,0,-1$. In particular,

$$rY_{10}(\theta',\phi') = \sqrt{\frac{3}{4\pi}}\,z\,, \qquad rY_{1,\pm1}(\theta',\phi') = \mp\sqrt{\frac{3}{8\pi}}(x\pm iy)\,. \tag{32}$$

[6]Eq. (31) can be interpreted as saying that the the spherical tensor $T^{(k)}_q$ imparts angular momentum when acting on a state. Conservation of the z-component of angular momentum then requires that $m' = q+m$. If this is not satisfied, then the states $|j'\,m'\rangle$ and $T^{(k)}_q\,|j\,m\rangle$ are orthogonal states, in which case the matrix element given in eq. (31) vanishes.

Eq. (31) implies that if $m' = m - 1$, then $\langle j'\,m-1|T^{(1)}_q|j\,m\rangle = 0$ if $q = 0, +1$. Using eq. (32), we therefore conclude that:

$$(d_{if})_z = 0\,, \qquad\qquad (d_{if})_x + i(d_{if})_y = 0\,. \tag{33}$$

Hence, it follows that $\vec{\boldsymbol{d}}_{if}$ must have the following form:

$$\boxed{\vec{\boldsymbol{d}}_{if} = d(1\,,\,i\,,\,0)} \tag{34}$$

where d is some (complex) constant. Writing $\vec{\boldsymbol{k}} = k(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, where the polar angle θ and the azimuthal angle ϕ measure the direction of the emitted photon with respect to the z-axis, it follows that

$$\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{k}} = ke^{i\phi}\sin\theta\,. \tag{35}$$

Inserting eqs. (34) and (35) into eq. (30) then yields:[7]

$$\boxed{\frac{d\Gamma_{if}}{d\Omega} = \frac{e^2\omega^3|d|^2}{2\pi\hbar c^3}(1+\cos^2\theta)}$$

That is, the angular distribution of the emitted photon is proportional to $1+\cos^2\theta$.

ADDED NOTE: The derivation of eq. (34) given above is very simple, as it follows immediately from eq. (31). If one ignores spin, then one can also derive eq. (34) by explicitly evaluating

$$\vec{\boldsymbol{d}}_{if} = \langle \ell'\,, m-1|\,\vec{\boldsymbol{x}}\,|\ell\,m\rangle = \int \vec{\boldsymbol{x}}\,Y^*_{\ell'\,m-1}(\Omega)\,Y_{\ell m}(\Omega)\,d\Omega\,.$$

It is convenient to express $\vec{\boldsymbol{x}}$ as a rank-one spherical tensor, $rY_{1M}(\Omega)$, as in eq. (32). Then, one must compute:

$$\int Y^*_{\ell'\,m-1}(\Omega)\,Y_{\ell m}(\Omega)\,Y_{1M}(\Omega)\,d\Omega = \sqrt{\frac{3(2\ell+1)}{4\pi(2\ell'+1)}}\,\langle \ell\,m;1\,M|\ell'\,m-1\rangle\langle \ell\,0;1\,0|\ell'\,0\rangle\,,$$

where we have used eq. (17-36) on p. 365 of Baym and the orthogonality relation of the spherical harmonics [cf. eq. (28)]. We immediately notice that conservation of L_z yields:

$$\langle \ell\,m;1\,M|\ell'\,m-1\rangle = 0\,, \qquad \text{if} \quad M = 0, +1\,,$$

which implies that only the $M = -1$ component of $\vec{\boldsymbol{d}}_{if}$ (when expressed as a spherical rank-one tensor) is non-vanishing. This result immediately implies eq. (33) and it then follows that $\vec{\boldsymbol{d}}_{if} = d(1\,,\,i\,,\,0)$. In this calculation, we can explicitly evaluate the constant d in terms of non-vanishing Clebsch-Gordon coefficients:

$$d = \sqrt{\frac{2(2\ell+1)}{(2\ell'+1)}}\langle \ell\,m;1\,,-1|\ell'\,m-1\rangle\langle \ell\,0;1\,0|\ell'\,0\rangle\,\langle f|r|i\rangle\,,$$

[7] Using eqs. (34) and (35), $\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{d}}^*_{if} - (\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{k}})(\vec{\boldsymbol{d}}^*_{if}\cdot\vec{\boldsymbol{k}})/k^2 = |d|^2(2-\sin^2\theta) = |d|^2(1+\cos^2\theta)$.

where $\langle f|r|i\rangle$ is the remaining radial integral (which is independent of the angular momentum quantum numbers m and m' of the initial and final atomic state). Note that $\langle \ell\, 0; 1\, 0|\ell'\, 0\rangle = 0$ if $|\ell - \ell'| \neq 1$, so that one must only consider the two cases where $\ell' = \ell \pm 1$.[8] To make further progress, one would have to know the details of the atomic wave functions in order to evaluate $\langle f|r|i\rangle$. However, it is not necessary to evaluate the constant d to answer any of the questions posed in this problem.

(b) Determine the polarization of the photon emitted in the z-direction.

Define the following (complex) orthonormal set of vectors: $\{\hat{\boldsymbol{e}}_{\mathbf{1}}, \hat{\boldsymbol{e}}_{\mathbf{2}}, \hat{\boldsymbol{e}}_{\mathbf{3}}\}$, where $\hat{\boldsymbol{e}}_{\mathbf{3}} \equiv \hat{\boldsymbol{k}}$. Any complex three-vector can be expanded in terms of this orthonormal set. In particular,

$$\vec{\boldsymbol{d}}_{if} = (d_{if})_1\hat{\boldsymbol{e}}_{\mathbf{1}} + (d_{if})_2\hat{\boldsymbol{e}}_{\mathbf{2}} + (d_{if})_3\hat{\boldsymbol{e}}_{\mathbf{3}}\,.$$

Since $\hat{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_\lambda = 0$, it follows that:

$$\vec{\boldsymbol{d}}_{if}\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_\lambda = \left[(d_{if})_1\hat{\boldsymbol{e}}_{\mathbf{1}} + (d_{if})_2\hat{\boldsymbol{e}}_{\mathbf{2}}\right]\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_\lambda \equiv (\vec{\boldsymbol{d}}_{if})_\perp\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_\lambda\,,$$

where $(\vec{\boldsymbol{d}}_{if})_\perp$ is the component of $\vec{\boldsymbol{d}}_{if}$ that is perpendicular to $\vec{\boldsymbol{k}}$. It then follows that $\vec{\boldsymbol{\epsilon}}_\lambda$ *is proportional to* $(\vec{\boldsymbol{d}}_{if})_\perp$.

Applying this result to the present problem, we note that if $\vec{\boldsymbol{k}} = k\hat{\boldsymbol{z}}$, then eq. (34) yields: $(\vec{\boldsymbol{d}}_{if})_\perp = \vec{\boldsymbol{d}}_{if} = d(1\,,\,i\,,\,0)$. Hence, the polarization vector of the outgoing photon is:

$$\vec{\boldsymbol{\epsilon}} \propto (\vec{\boldsymbol{d}}_{if})_\perp = \frac{-1}{\sqrt{2}}(1\,,\,i\,,\,0) = \vec{\boldsymbol{\epsilon}}_L\,.$$

That is, the photon emitted in the $\hat{\boldsymbol{z}}$-direction is *left-circularly polarized* (in the optics convention). It is easy to check that a right circularly polarized photon, $\vec{\boldsymbol{\epsilon}}_R = \frac{1}{\sqrt{2}}(1\,,\,-i\,,\,0)$ does not contribute, since $\vec{\boldsymbol{d}}_{if}\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_R = 0$.

(c) Verify that the result of part (b) is consistent with angular momentum conservation for the whole (atom plus photon) system.

In the optic convention adopted in part (b), a left-circularly polarized photon traveling in the $\hat{\boldsymbol{z}}$-direction carries away orbital angular momentum $L_z = +\hbar$, whereas a right-circularly polarized photon traveling in the $\hat{\boldsymbol{z}}$-direction carries away orbital angular momentum $L_z = -\hbar$. We have shown in parts (a) and (b) that if the initial atomic state has $L_z = m\hbar$ and the final atomic state has $L_z = (m-1)\hbar$, then the photon emitted in the $\hat{\boldsymbol{z}}$-direction is left-circularly polarized. Thus, we see that L_z is conserved, since $m\hbar = (m-1)\hbar + \hbar$, i.e. the photon emitted in the z-direction carries away orbital angular momentum $L_z = +\hbar$.

[8]The fact that $\vec{\boldsymbol{d}}_{if} = 0$ if $\ell' = \ell$ also follows from parity considerations, since $\vec{\boldsymbol{x}}$ is a parity-odd operator, whereas the state $|\ell\, m\rangle$ is an eigenstate of parity with eigenvalue $(-1)^\ell$.

4. Consider the elastic scattering of photons off electrons in atoms, assuming that the incident photon energies are large compared to the atomic binding energies. However, you should assume that the photon wavelength is still substantially larger than a typical atomic radius.

(a) Using the quantum theory of radiation, argue that the $\vec{\boldsymbol{A}}$ field operator must occur at least twice in the matrix element in order that there be a non-zero contribution in perturbation theory.

The quantized electromagnetic vector potential is given by:

$$\vec{\boldsymbol{A}}(\vec{\boldsymbol{x}},t) = \left(\frac{2\pi\hbar c^2}{V}\right)^{1/2} \sum_{\vec{\boldsymbol{k}},\lambda} \frac{1}{\sqrt{\omega_k}} \left[\vec{\boldsymbol{\epsilon}}_\lambda\, e^{i\vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}-i\omega t}\, a_{\vec{\boldsymbol{k}},\lambda} + \vec{\boldsymbol{\epsilon}}^{\,*}_\lambda\, e^{-i\vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}+i\omega t}\, a^\dagger_{\vec{\boldsymbol{k}},\lambda}\right] , \tag{36}$$

where $a^\dagger_{\vec{\boldsymbol{k}},\lambda}$ creates one photon in the mode $(\vec{\boldsymbol{k}},\lambda)$ and $a_{\vec{\boldsymbol{k}},\lambda}$ annihilates one photon in the mode $(\vec{\boldsymbol{k}},\lambda)$. The process of interest for this problem is the elastic scattering:

$$\gamma(\vec{\boldsymbol{k}},\lambda) + e^- \longrightarrow \gamma(\vec{\boldsymbol{k}}^{\,\prime},\lambda') + e^- , \tag{37}$$

where $|\vec{\boldsymbol{k}}| = |\vec{\boldsymbol{k}}^{\,\prime}| \equiv k$. The latter implies that $\omega_k = \omega_{k'} = kc$. Since eq. (37) implies that one photon in the mode $(\vec{\boldsymbol{k}},\lambda)$ is annihilated and one photon in the mode $(\vec{\boldsymbol{k}}^{\,\prime},\lambda')$ is created, the $\vec{\boldsymbol{A}}$-field operator must appear at least twice in the matrix element that is evaluated using Fermi's Golden Rule (one time is not enough). To see why this is true, note that the relevant matrix element is of the form

$$\langle f\,;1_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}\,,\,0_{\vec{\boldsymbol{k}},\lambda}|H_{\rm int}|i\,;\,0_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}\,,\,1_{\vec{\boldsymbol{k}},\lambda}\rangle\,, \tag{38}$$

where $|i\rangle$ is the initial state of the electron and $|f\rangle$ is the final state of the electron. Note that we have specified explicitly the photon occupation numbers for the modes $(\vec{\boldsymbol{k}},\lambda)$ and $(\vec{\boldsymbol{k}}^{\,\prime},\lambda')$. All other photon modes [which are suppressed in eq. (38)] are absent and thus their photon occupation numbers are zero. Thus, the only way for the matrix element exhibited in eq. (38) to be non-zero is if $H_{\rm int}$ contains the terms $a^\dagger_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}a_{\vec{\boldsymbol{k}},\lambda}$ and/or $a_{\vec{\boldsymbol{k}},\lambda}a^\dagger_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}$. That is,[9]

$$\langle 1_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}\,,\,0_{\vec{\boldsymbol{k}},\lambda}|a^\dagger_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}a_{\vec{\boldsymbol{k}},\lambda}|0_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}\,,\,1_{\vec{\boldsymbol{k}},\lambda}\rangle = 1\,, \tag{39}$$

$$\langle 1_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}\,,\,0_{\vec{\boldsymbol{k}},\lambda}|a_{\vec{\boldsymbol{k}},\lambda}a^\dagger_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}|0_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}\,,\,1_{\vec{\boldsymbol{k}},\lambda}\rangle = 1\,, \tag{40}$$

while all other matrix elements vanish if the operators that appear consist of other combinations of a and $a^\dagger$ taken either singly or in pairs. We conclude that $H_{\rm int}$ must contain $\vec{\boldsymbol{A}}$ exactly twice.

[9]Recall that the commutation relations for the creation and annihilation operators are:

$$[a_{\vec{\boldsymbol{k}},\lambda}\,,\,a^\dagger_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}] = \delta_{\vec{\boldsymbol{k}}\,\vec{\boldsymbol{k}}^{\,\prime}}\delta_{\lambda\,\lambda'}\,.$$

Thus, for $\vec{\boldsymbol{k}} \neq \vec{\boldsymbol{k}}^{\,\prime}$, it follows that $a_{\vec{\boldsymbol{k}},\lambda}a^\dagger_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'} = a^\dagger_{\vec{\boldsymbol{k}}^{\,\prime},\lambda'}a_{\vec{\boldsymbol{k}},\lambda}$.

(b) Treating the quadratic $\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}$ term in the interaction Hamiltonian to *first order* in perturbation theory, compute the differential cross-section in the dipole approximation. Show that:

$$\frac{d\sigma}{d\Omega} = r_0^2|\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_{\lambda'}|^2\,,$$

where $r_0 \equiv e^2/(mc^2)$ is the classical radius of the electron.

The interaction Hamiltonian is given by

$$H_{\rm int} = -\frac{e}{c}\int d^3r\,\vec{\boldsymbol{j}}(\vec{\boldsymbol{r}})\boldsymbol{\cdot}\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}},t) + \frac{e^2}{2mc^2}\int d^3r\,\rho(\vec{\boldsymbol{r}})\,\vec{\boldsymbol{A}}^2(\vec{\boldsymbol{r}},t)\,,$$

where

$$\rho(\vec{\boldsymbol{r}}) = \delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{x}})\,,\qquad\qquad \vec{\boldsymbol{j}}(\vec{\boldsymbol{r}}) = \frac{1}{2m}\left[\vec{\boldsymbol{p}}\,\delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{x}}) + \delta^3(\vec{\boldsymbol{r}}-\vec{\boldsymbol{x}})\,\vec{\boldsymbol{p}}\right]\,.$$

To first order in perturbation theory, only the $\vec{\boldsymbol{A}}^2$ term of the interaction Hamiltonian contributes a non-zero result to the matrix element given by eq. (38). Using Fermi's Golden rule, it follows that

$$\Gamma^{(1)}_{if} = \frac{2\pi}{\hbar}|\langle f|H_{\rm int}|i\rangle|^2\delta(E_f-E_i)\,,$$

where the superscript (1) indicates that this is a first-order perturbation theory result. The initial and final energies are given by:

$$E_i = E_e + \hbar\omega\,,\qquad\qquad E_f = E_e + \hbar\omega'\,,$$

where E_e is the electron energy[10] and $\hbar\omega$ and $\hbar\omega'$ are the initial and final state photon energies. Thus,

$$\Gamma^{(1)}_{if} = \frac{2\pi}{\hbar}\left(\frac{e^2}{2mc^2}\right)^2\left|\langle e^-_f\,,\,1_{\vec{\boldsymbol{k}}',\lambda'}\,,\,0_{\vec{\boldsymbol{k}},\lambda}|\vec{\boldsymbol{A}}^2(\vec{\boldsymbol{x}},t)|e^-_i\,,\,0_{\vec{\boldsymbol{k}}',\lambda'}\,,\,1_{\vec{\boldsymbol{k}},\lambda}\rangle\right|^2\delta(\hbar\omega'-\hbar\omega)\,. \qquad (41)$$

As noted in part (a), only the $a^\dagger_{\vec{\boldsymbol{k}}',\lambda'}a_{\vec{\boldsymbol{k}},\lambda}$ and the $a_{\vec{\boldsymbol{k}},\lambda}a^\dagger_{\vec{\boldsymbol{k}}',\lambda'}$ cross-terms arising from $\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{A}}$ contribute to the matrix element above. In detail, inserting the expansion for the quantized vector potential [cf. eq. (36)] yields only one non-zero term:

$$\begin{aligned}\langle 1_{\vec{\boldsymbol{k}}',\lambda'}\,,\,0_{\vec{\boldsymbol{k}},\lambda}|\vec{\boldsymbol{A}}^2(\vec{\boldsymbol{x}},t)|0_{\vec{\boldsymbol{k}}',\lambda'}\,,\,1_{\vec{\boldsymbol{k}},\lambda}\rangle &= 2\cdot\frac{2\pi\hbar c^2}{V\sqrt{\omega\omega'}}\,\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}_{\lambda'}\,\langle 1_{\vec{\boldsymbol{k}}',\lambda'}\,,\,0_{\vec{\boldsymbol{k}},\lambda}|a^\dagger_{\vec{\boldsymbol{k}}',\lambda'}a_{\vec{\boldsymbol{k}},\lambda}|0_{\vec{\boldsymbol{k}}',\lambda'}\,,\,1_{\vec{\boldsymbol{k}},\lambda}\rangle \\ &\qquad\times\langle e^-_f|e^{i(\vec{\boldsymbol{k}}-\vec{\boldsymbol{k}}')\boldsymbol{\cdot}\vec{\boldsymbol{x}}}\,e^{-i(\omega-\omega')t}|e^-_i\rangle \\ &= \frac{4\pi\hbar c^2}{\omega V}\,\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}_{\lambda'}\langle e^-_f|e^{i(\vec{\boldsymbol{k}}-\vec{\boldsymbol{k}}')\boldsymbol{\cdot}\vec{\boldsymbol{x}}}|e^-_i\rangle\,, \end{aligned} \qquad (42)$$

where we have used the fact that the energy-conserving delta function in eq. (41) sets $\omega' = \omega$. Note that an overall factor of 2 in eq. (42) has been included since the matrix

[10] In the case of *elastic scattering*, the initial and final state electron energies are the same. That is, the photon scatters elastically off the electron without altering the atomic state.

elements of $a^\dagger_{\vec{\boldsymbol{k}}',\lambda'}a_{\vec{\boldsymbol{k}},\lambda}$ and $a_{\vec{\boldsymbol{k}},\lambda}a^\dagger_{\vec{\boldsymbol{k}}',\lambda'}$ yield the same result if $\vec{\boldsymbol{k}} \neq \vec{\boldsymbol{k}}'$ [as shown in eqs. (39) and (40)]. Therefore, eq. (41) yields:

$$\Gamma^{(1)}_{if} = \frac{2\pi}{\hbar^2}\left(\frac{e^2}{2mc^2}\right)^2\left(\frac{4\pi\hbar c^2}{\omega V}\right)^2 |\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}_{\lambda'}|^2\,|\langle e^-_f|e^{i(\vec{\boldsymbol{k}}-\vec{\boldsymbol{k}}')\boldsymbol{\cdot}\vec{\boldsymbol{x}}}|e^-_i\rangle|^2\,\delta(\omega'-\omega)\,,$$

after noting that $\delta(\hbar\omega'-\hbar\omega) = \hbar^{-1}\delta(\omega'-\omega)$.

The problem states that we may assume that the photon wavelength is substantially larger than a typical atomic radius. This means that we can work in the dipole approximation, in which case

$$e^{i(\vec{\boldsymbol{k}}-\vec{\boldsymbol{k}}')\boldsymbol{\cdot}\vec{\boldsymbol{x}}} \simeq 1\,.$$

Since $|i\rangle$ and $|f\rangle$ represent the *same* normalized atomic states (since the electron energy is unchanged in the elastic scattering), it follows that $\langle f|i\rangle = 1$. Hence,

$$\Gamma^{(1)}_{if} = \frac{2\pi}{\hbar^2}\left(\frac{e^2}{2mc^2}\right)^2\left(\frac{4\pi\hbar c^2}{\omega V}\right)^2 |\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}_{\lambda'}|^2\;\delta(\omega'-\omega)\,. \tag{43}$$

We are now in position to compute the cross section,

$$\sigma_{if} = \frac{\displaystyle\sum_f \Gamma_{if}}{\text{incident flux}}\,. \tag{44}$$

Since the incident photon has velocity c, the incident flux is given by c/V. The sum over final states f is a sum over the outgoing photon momenta $\vec{\boldsymbol{k}}'$. Taking the infinite volume limit, we may take

$$\sum_{\vec{\boldsymbol{k}}'} \longrightarrow \frac{V}{(2\pi)^3}\int k'^2 dk' d\Omega = \frac{V}{(2\pi c)^3}\int \omega'^2 d\omega'\, d\Omega\,,$$

where we have used $\omega' = k'c$. Inserting eq. (43) into eq. (44) and taking the infinite volume limit,

$$\sigma_{\lambda\lambda'} = \frac{2\pi}{\hbar^2}\left(\frac{e^2}{2mc^2}\right)^2\left(\frac{4\pi\hbar c^2}{\omega V}\right)^2\left(\frac{V}{c}\right)\,|\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}_{\lambda'}|^2\,\frac{V}{(2\pi c)^3}\int \omega'^2\, d\omega' d\Omega\,\delta(\omega'-\omega)\,.$$

As expected, the volume factors cancel out. The integral over ω' is trivial (it just enforces energy conservation). Hence, we end up with:

$$\frac{d\sigma_{\lambda\lambda'}}{d\Omega} = \left(\frac{e^2}{mc^2}\right)^2\,|\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}_{\lambda'}|^2\,.$$

Denoting the classical radius of the electron by $r_0 \equiv e^2/(mc^2)$, the differential cross-section can be written as:

$$\boxed{\frac{d\sigma}{d\Omega} = r_0^2|\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_{\lambda'}|^2} \tag{45}$$

BONUS MATERIAL:

Proof that the second order perturbative contribution to the transition rate is negligible compared to the first-order transition rate

At second order in perturbation theory, the $\vec{\boldsymbol{j}}\cdot\vec{\boldsymbol{A}}$ term of the interaction Hamiltonian also yields a non-zero contribution to the transition rate. However, if the energy of the incident photon is large compared to the electron energy, then the $\vec{\boldsymbol{A}}\cdot\vec{\boldsymbol{A}}$ term of the interaction Hamiltonian, taken at first order in the perturbation expansion, will dominate the second order contribution due to the $\vec{\boldsymbol{j}}\cdot\vec{\boldsymbol{A}}$ term.

To verify this assertion, consider the second-order version of Fermi's Golden Rule. The the transition rate at second order in perturbation theory is given by:

$$\Gamma_{if}^{(2)} = \frac{2\pi}{\hbar}\left|\sum_k \frac{\langle f|H_{\rm int}|k\rangle\langle k|H_{\rm int}|i\rangle}{E_i - E_k + i\epsilon}\right|^2 \delta(E_f - E_i)\,.$$

Thus, it follows that:

$$\Gamma_{if}^{(2)} = \frac{2\pi}{m^2\hbar}\left|\sum_k \frac{\langle e_f^-\,,\,1_{\vec{\boldsymbol{k}}\,',\lambda'}\,,\,0_{\vec{\boldsymbol{k}},\lambda}|\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}(\vec{\boldsymbol{x}},t)|k\rangle\langle k|\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{A}}(\vec{\boldsymbol{x}},t)|e_i^-\,,\,0_{\vec{\boldsymbol{k}}\,',\lambda'}\,,\,1_{\vec{\boldsymbol{k}},\lambda}\rangle}{E_e + \hbar\omega - E_k + i\epsilon}\right|^2 .$$

We can compare the magnitudes of the first-order and second-order contributions to the transition rates by employing the following estimates. In light of eq. (36), we shall replace $\vec{\boldsymbol{A}}$ with

$$\frac{2m\hbar c^2}{(\omega V)^{1/2}}\,\vec{\boldsymbol{\epsilon}}_\lambda\,.$$

Hence, the first-order transition rate behaves as,

$$\Gamma^{(1)} \sim \frac{2\pi}{\hbar}\left(\frac{e^2}{2mc^2}\right)^2\left(\frac{2\pi\hbar c^2}{\omega V}\right)^2 |\vec{\boldsymbol{\epsilon}}_\lambda\cdot\vec{\boldsymbol{\epsilon}}^{\,*}_{\lambda'}|^2\delta(E_f - E_i)\,,$$

To estimate the second-order transition rate, we approximate $E_e + \hbar\omega - E_k + i\epsilon \simeq \hbar\omega$, since the photon energy is by assumption much larger than the electron energy. The sum over intermediate states can now be performed using completeness. Thus, we estimate:

$$\Gamma^{(2)} \sim \frac{2\pi}{m^2\hbar}\left(\frac{e^2}{2mc^2}\right)^2\left(\frac{2\pi\hbar c^2}{\omega V}\right)^2 \frac{|(\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{\epsilon}}_\lambda)(\vec{\boldsymbol{p}}\cdot\vec{\boldsymbol{\epsilon}}^{\,*}_{\lambda'})|^2}{\hbar^2\omega^2}\delta(E_f - E_i)\,.$$

Thus, roughly we have:

$$\frac{\Gamma^{(2)}}{\Gamma^{(1)}} \sim \frac{E_e}{E_\gamma} \ll 1\,,$$

in terms of the electron energy $E_e = \vec{\boldsymbol{p}}\,^2/(2m)$ and the photon energy $E_\gamma = \hbar\omega$. By assumption, the former is much smaller than the latter. Therefore in this limit, we expect the first-order perturbative contribution to the transition rate to be the dominant one.

(c) Compute the total cross-section, assuming that the initial photon beam is unpolarized and the polarization of the final state photon is not measured.

Assuming that the initial and final photons are unpolarized, we average over the initial polarizations and sum over the final polarizations. Thus

$$\frac{d\sigma_{\rm unpol}}{d\Omega} = \tfrac{1}{2}\sum_{\lambda\,\lambda'} \frac{d\sigma_{\lambda\,\lambda'}}{d\Omega}\,. \tag{46}$$

Using the polarization sum formula,

$$\sum_\lambda [\epsilon^*_\lambda(\vec{\boldsymbol{k}})]_i [\epsilon_\lambda(\vec{\boldsymbol{k}})]_j = \delta_{ij} - \frac{k_i k_j}{k^2}\,,$$

it follows that

$$\tfrac{1}{2}\sum_{\lambda\,\lambda'} |\vec{\boldsymbol{\epsilon}}_\lambda\boldsymbol{\cdot}\vec{\boldsymbol{\epsilon}}^{\,*}_{\lambda'}|^2 = \frac{1}{2}\left(\delta_{ij} - \frac{k_i k_j}{k^2}\right)\left(\delta_{ij} - \frac{k'_i k'_j}{k'^2}\right) = \frac{1}{2}\left[1 + \frac{(\vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{k}}')^2}{k^2 k'^2}\right] = \tfrac{1}{2}(1+\cos^2\theta)\,, \tag{47}$$

where θ is the angle between $\vec{\boldsymbol{k}}$ and $\vec{\boldsymbol{k}}'$. In deriving eq. (47), we noted for example that: $\delta_{ij}\delta_{ij} = \delta_{ii} = 3$ (where there is an implicit sum over repeated indices, which run over the values 1,2,3), $\delta_{ij}k_i k_j = k^2$, and $\delta_{ij}k_i k'_j = \vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{k}}' = kk'\cos\theta$. Hence, eqs. (45) and (46) yield:

$$\frac{d\sigma_{\rm unpol}}{d\Omega} = \tfrac{1}{2} r_0^2 (1+\cos^2\theta)\,.$$

Integrating over solid angles,

$$\int d\Omega\,(1+\cos^2\theta) = 2\pi \int_{-1}^{1} d\cos\theta\,(1+\cos^2\theta) = \frac{16\pi}{3}\,.$$

Hence, the total unpolarized cross-section is given by:

$$\boxed{\sigma_{\rm unpol} = \frac{8\pi r_0^2}{3}}$$

This is called the *Thomson cross-section.* Although the energies of the atomic electrons were taken to be negligible as compared with the photon energies, we still assumed that the photon wavelength was long compared to typical atomic scales. Thus, the Thomson cross-section is a long-wavelength limit of photon scattering.

5. Consider a non-interacting gas of N fermions that occupies a cubical box of volume V. Assume that V and N are macroscopically large. Let $\Psi_s(\vec{\boldsymbol{x}})$ be the field operator that annihilates a fermion of spin orientation s at position $\vec{\boldsymbol{x}}$. The particle number density operator is given by

$$n(\vec{\boldsymbol{x}}) = \sum_s \Psi_s^\dagger(\vec{\boldsymbol{x}})\Psi_s(\vec{\boldsymbol{x}})\,, \tag{48}$$

and the total number operator is $N = \int d^3x\, n(\vec{\boldsymbol{x}})$. The Fourier transform of the number density operator is defined by

$$n_{\vec{\boldsymbol{q}}} = \int d^3x\, n(\vec{\boldsymbol{x}})\, e^{-i\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{x}}}\,.$$

(a) Show that $n_{\vec{\boldsymbol{q}}}$ can be expressed in terms of fermion creation and annihilation operators as follows:

$$n_{\vec{\boldsymbol{q}}} = \sum_{\vec{\boldsymbol{k}}}\sum_s a^\dagger_{\vec{\boldsymbol{k}},s}\, a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},\,s}\,.$$

The field operators $\Psi_s(\vec{\boldsymbol{x}})$ and $\Psi_s^\dagger(\vec{\boldsymbol{x}})$ are given by

$$\Psi_s(\vec{\boldsymbol{x}}) = \sum_{\vec{\boldsymbol{k}}} \frac{e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}}{\sqrt{V}}\, a_{\vec{\boldsymbol{k}},s}\,, \qquad \Psi_s^\dagger(\vec{\boldsymbol{x}}) = \sum_{\vec{\boldsymbol{k}}} \frac{e^{-i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}}{\sqrt{V}}\, a^\dagger_{\vec{\boldsymbol{k}},s}\,.$$

We have taken space to be a cubical box of length $L \equiv V^{1/3}$ and volume V and imposed periodic boundary conditions, so that the possible discrete value of $\vec{\boldsymbol{k}}$ are given by

$$\vec{\boldsymbol{k}} = \frac{2\pi\vec{\boldsymbol{n}}}{V^{1/3}}\,,$$

where $\vec{\boldsymbol{n}} = (n_x, n_y, n_z)$ is a vector of integer values. The creation and annihilation operators satisfy anticommutation relations,

$$\{a_{\vec{\boldsymbol{k}},s}\,,\, a^\dagger_{\vec{\boldsymbol{k}}\,',s'}\} = \delta_{\vec{\boldsymbol{k}}\vec{\boldsymbol{k}}\,'}\,\delta_{ss'}\,. \tag{49}$$

The density operator defined in eq. (48) is therefore given by

$$n(\vec{\boldsymbol{x}}) = \sum_{\vec{\boldsymbol{k}}}\sum_{\vec{\boldsymbol{k}}\,'}\sum_s \frac{e^{i\vec{\boldsymbol{x}}\cdot(\vec{\boldsymbol{k}}-\vec{\boldsymbol{k}}\,')}}{V}\, a^\dagger_{\vec{\boldsymbol{k}}\,',s}\, a_{\vec{\boldsymbol{k}},s}\,. \tag{50}$$

The Fourier transform of $n(\vec{\boldsymbol{x}})$ is given by

$$n_{\vec{\boldsymbol{q}}} = \int d^3x\, n(\vec{\boldsymbol{x}}) e^{-i\vec{\boldsymbol{q}}\cdot\vec{\boldsymbol{x}}}\,. \tag{51}$$

Plugging in for $n(\vec{\boldsymbol{x}})$ above using eq. (50) then yields

$$n_{\vec{\boldsymbol{q}}} = \frac{1}{V}\sum_{\vec{\boldsymbol{k}}}\sum_{\vec{\boldsymbol{k}}\,'}\sum_s a^\dagger_{\vec{\boldsymbol{k}}\,',s}\, a_{\vec{\boldsymbol{k}},s}\int d^3x\, e^{i\vec{\boldsymbol{x}}\cdot(\vec{\boldsymbol{k}}-\vec{\boldsymbol{k}}\,'-\vec{\boldsymbol{q}})}\,.$$

The above integral is easily evaluated using

$$\int d^3x\, e^{i\vec{\boldsymbol{x}}\cdot(\vec{\boldsymbol{k}}-\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}})} = \delta_{\vec{\boldsymbol{k}},\,\vec{\boldsymbol{k}}'+\vec{\boldsymbol{q}}}\,,$$

and we end up with

$$n_{\vec{\boldsymbol{q}}} = \sum_{\vec{\boldsymbol{k}}}\sum_{s} a^\dagger_{\vec{\boldsymbol{k}},s}\, a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},\,s}\,, \tag{52}$$

as required.

(b) The *static structure function* for non-interacting fermions is defined as:

$$S_0(\vec{\boldsymbol{q}}) \equiv \frac{1}{N}\langle\Phi_0|\, n_{\vec{\boldsymbol{q}}}\, n_{-\vec{\boldsymbol{q}}}\, |\Phi_0\rangle\,, \tag{53}$$

where $|\Phi_0\rangle$ is the N-particle ground state of the fermion gas (cf. Baym pp. 424–425). Evaluate $S_0(\vec{\boldsymbol{q}})$ explicitly in the continuum limit.

We consider separately the cases $\vec{\boldsymbol{q}} = 0$ and $\vec{\boldsymbol{q}} \neq 0$. First, in the case of $\vec{\boldsymbol{q}} = 0$ we note that eqs. (51) and (52) yield

$$n_{\vec{\boldsymbol{q}}=0} = \int d^3x\, n(\vec{\boldsymbol{x}}) = \sum_{\vec{\boldsymbol{k}}}\sum_{s} a^\dagger_{\vec{\boldsymbol{k}},s}\, a_{\vec{\boldsymbol{k}},s} = \sum_{\vec{\boldsymbol{k}}}\sum_{s} N_{\vec{\boldsymbol{k}},s} = \mathcal{N}\,, \tag{54}$$

where $\mathcal{N}$ is the *total* number operator. Moreover, $|\Phi_0\rangle$ is an eigenstate of $\mathcal{N}$ whose eigenvalue is equal to the number of fermions in the ground state, N. That is,

$$\mathcal{N}\,|\Phi_0\rangle = N\,|\Phi_0\rangle\,. \tag{55}$$

Since $|\Phi_0\rangle$ is a normalized state, i.e. $\langle\Phi_0|\Phi_0\rangle = 1$, it immediately follows from eqs. (53)–(55) that

$$S_0(\vec{\boldsymbol{q}}=0) = \frac{1}{N}\langle\Phi_0|\mathcal{N}^2\,|\Phi_0\rangle = N\,. \tag{56}$$

Next, we consider the case of $\vec{\boldsymbol{q}} \neq 0$. Using eq. (52),

$$S_0(\vec{\boldsymbol{q}}) = \frac{1}{N}\sum_{\vec{\boldsymbol{k}}}\sum_{s}\sum_{\vec{\boldsymbol{k}}'}\sum_{s'} \langle\Phi_0|\, a^\dagger_{\vec{\boldsymbol{k}},s}\, a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},\,s}\, a^\dagger_{\vec{\boldsymbol{k}}',s'}\, a_{\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}},\,s'}\, |\Phi_0\rangle\,.$$

Note that $a^\dagger_{\vec{\boldsymbol{k}}',s'}\, a_{\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}},\,s'}\,|\Phi_0\rangle$ is a state where one fermion with wave number $\vec{\boldsymbol{k}}' - \vec{\boldsymbol{q}}$ and spin s' is removed from the ground state of the N-fermion system and one fermion with wave number $\vec{\boldsymbol{k}}'$ and spin s' is added. If $\langle\Phi_0|\, a^\dagger_{\vec{\boldsymbol{k}},s}\, a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},\,s}\, a^\dagger_{\vec{\boldsymbol{k}}',s'}\, a_{\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}},\,s'}\,|\Phi_0\rangle \neq 0$, then the state $a^\dagger_{\vec{\boldsymbol{k}}',s}\, a_{\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}},\,s'}\,|\Phi_0\rangle$ must not be orthogonal to the state $a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},\,s}\, a_{\vec{\boldsymbol{k}},s}\,|\Phi_0\rangle$, which corresponds to a state with one fermion with wave number $\vec{\boldsymbol{k}}$ and spin s removed and one fermion with wave number $\vec{\boldsymbol{k}} + \vec{\boldsymbol{q}}$ and spin s added.

However, the states $a^\dagger_{\vec{\boldsymbol{k}}',s'} a_{\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}},s'} |\Phi_0\rangle$ and $a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a_{\vec{\boldsymbol{k}},s} |\Phi_0\rangle$ are orthogonal unless the following three conditions are satisfied:

$$\text{(i)}\quad \vec{\boldsymbol{k}} = \vec{\boldsymbol{k}}' - \vec{\boldsymbol{q}}\,, \qquad \text{(ii)}\quad \vec{\boldsymbol{k}} + \vec{\boldsymbol{q}} = \vec{\boldsymbol{k}}'\,, \qquad \text{(iii)}\quad s = s'\,.$$

Note that conditions (i) and (ii) are consistent. We conclude that

$$\langle\Phi_0|\, a^\dagger_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a^\dagger_{\vec{\boldsymbol{k}}',s'} a_{\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}},s'} |\Phi_0\rangle = \delta_{\vec{\boldsymbol{k}},\vec{\boldsymbol{k}}'-\vec{\boldsymbol{q}}}\,\delta_{ss'}\ \langle\Phi_0|\, a^\dagger_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a_{\vec{\boldsymbol{k}},s} |\Phi_0\rangle\,. \tag{57}$$

To simplify eq. (57), we shall employ the anticommutation relations given in eq. (49). Since $\vec{\boldsymbol{q}} \neq 0$ by assumption, it follows that $\vec{\boldsymbol{k}} \neq \vec{\boldsymbol{k}} + \vec{\boldsymbol{q}}$. Hence,

$$\begin{aligned} a^\dagger_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a_{\vec{\boldsymbol{k}},s} &= -a^\dagger_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a_{\vec{\boldsymbol{k}},s} a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} = +a^\dagger_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} \\ &= a^\dagger_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}},s}\left[1 - a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s}\right] = N_{\vec{\boldsymbol{k}},s}\left(1 - N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s}\right)\,, \end{aligned} \tag{58}$$

where we have introduced the number operators at the last step,

$$N_{\vec{\boldsymbol{k}},s} \equiv a^\dagger_{\vec{\boldsymbol{k}},s} a_{\vec{\boldsymbol{k}},s}\,, \qquad\qquad N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} \equiv a^\dagger_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s} a_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s}\,.$$

Using eqs. (57) and (58), it follows that

$$S_0(\vec{\boldsymbol{q}}) = \frac{1}{N}\sum_{\vec{\boldsymbol{k}}}\sum_s \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s}\big(1 - N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s}\big)\,|\Phi_0\rangle\,. \tag{59}$$

In light of eqs. (54) and (55),

$$\sum_{\vec{\boldsymbol{k}},s} \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s}\,|\Phi_0\rangle = \langle\Phi_0|\,\mathcal{N}\,|\Phi_0\rangle = N\,.$$

Hence, we can rewrite eq. (59) as

$$S_0(\vec{\boldsymbol{q}}) = 1 - \frac{1}{N}\sum_{\vec{\boldsymbol{k}},s} \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s} N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},s}\,|\Phi_0\rangle\,. \tag{60}$$

In order to evaluate the matrix element given in eq. (60), recall that the Fermi momentum k_f is defined such that

$$n_{\vec{\boldsymbol{k}},s} \equiv \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s}\,|\Phi_0\rangle = \Theta(k_f - k) = \begin{cases} 1\,, & \text{if } k < k_f\,, \\ 0\,, & \text{if } k > k_f\,, \end{cases} \tag{61}$$

where $k \equiv |\vec{\boldsymbol{k}}|$, and $\Theta(k_f - k)$ is the step function. Applying eqs. (54) and (55), we sum eq. (61) over all modes to obtain,

$$N = \langle\Phi_0|\,\mathcal{N}\,|\Phi_0\rangle = \sum_{\vec{\boldsymbol{k}}}\sum_s \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s}\,|\Phi_0\rangle = \sum_{\vec{\boldsymbol{k}}}\sum_s \Theta(k_f - k)\,. \tag{62}$$

We shall evaluate sums over the discrete modes $\{\vec{\boldsymbol{k}}, s\}$ by taking the continuum limit,

$$\sum_{\vec{\boldsymbol{k}},s} \longrightarrow 2\,\frac{V}{(2\pi)^3}\int d^3k\,, \tag{63}$$

where the factor of 2 above corresponds to the two possible spin orientations, $s = \pm\frac{1}{2}$. Applying the continuum limit in eq. (62), it follows that

$$N = 2\,\frac{V}{(2\pi)^3}\int \Theta(k_f - k)\, d^3k = 2\,\frac{V}{(2\pi)^3}\cdot 4\pi \int_0^{k_f} k_f^2 dk_f = \frac{Vk_f^3}{3\pi^2}\,, \tag{64}$$

where the integral has been evaluated using spherical coordinates. Note that eq. (64) yields

$$k_f = \left(\frac{3\pi^2 N}{V}\right)^{1/3}\,. \tag{65}$$

Similarly, employing eqs. (63) and (61), it follows that

$$\sum_{\vec{\boldsymbol{k}}}\sum_{s} \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s} N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}},\,s}\,|\Phi_0\rangle = 2\,\frac{V}{(2\pi)^3}\int \Theta(k_f - k)\,\Theta(k_f - |\vec{\boldsymbol{k}} + \vec{\boldsymbol{q}}|)\, d^3k\,. \tag{66}$$

Thus, to evaluate eq. (60), we focus on the integral,

$$\mathcal{I}(k_f, q) \equiv \int \Theta(k_f - k)\,\Theta(k_f - |\vec{\boldsymbol{k}} + \vec{\boldsymbol{q}}|)\, d^3k\,. \tag{67}$$

The integral $\mathcal{I}(k_f, q)$ can be interpreted geometrically as the volume of the overlapping region of two spheres of radius k_f, one centered at the origin and the other centered at $-\vec{\boldsymbol{q}}$. In particular, one must determine the range of integration in which the two step functions are simultaneously non-zero. A direct evaluation of $\mathcal{I}(k_f, q)$ can be found in the Appendix. Here, we shall employ an alternative technique that makes use of the relation between the step function and the delta function,

$$\frac{d}{dk_f}\,\Theta(k_f - k) = \delta(k_f - k)\,. \tag{68}$$

We can use eq. (68) to evaluate the derivative of $\mathcal{I}(k_f, q)$ with respect to k_f,

$$\frac{\partial}{\partial k_f}\mathcal{I}(k_f, q) \equiv \int \delta(k_f - k)\,\Theta(k_f - |\vec{\boldsymbol{k}} + \vec{\boldsymbol{q}}|)\, d^3k + \int \Theta(k_f - k)\,\delta(k_f - |\vec{\boldsymbol{k}} + \vec{\boldsymbol{q}}|)\, d^3k\,.$$

In the second integral above, we can change the integration variable to $\vec{\boldsymbol{k}}^{\,\prime} = \vec{\boldsymbol{k}} + \vec{\boldsymbol{q}}$. The second integral above then becomes

$$\int \delta(k_f - k')\,\Theta(k_f - |\vec{\boldsymbol{k}}^{\,\prime} - \vec{\boldsymbol{q}}|)\, d^3k'$$

Since $\vec{\boldsymbol{k}}'$ is an integration variable, we can simply rename it $\vec{\boldsymbol{k}}$, in which case it follows that

$$\frac{\partial}{\partial k_f}\mathcal{I}(k_f,q) = \int \delta(k_f-k)\,\left[\Theta(k_f-|\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}}|)+\Theta(k_f-|\vec{\boldsymbol{k}}-\vec{\boldsymbol{q}}|)\right]\,d^3k\,.$$

We can evaluate the above integral in spherical coordinates. We choose a coordinate system such that $\vec{\boldsymbol{k}}\boldsymbol{\cdot}\vec{\boldsymbol{q}} = kq\cos\theta$. Then after performing the free integral over the azimuthal angle,

$$\frac{\partial}{\partial k_f}\mathcal{I}(k_f,q) = 2\pi\int_{-1}^{1} d\cos\theta\int_0^\infty k^2\,dk\,\delta(k_f-k)$$
$$\times\left[\Theta\biggl(k_f-\sqrt{k^2+q^2+2qk\cos\theta}\biggr)+\Theta\biggl(k_f-\sqrt{k^2+q^2-2qk\cos\theta}\biggr)\right]\,.$$

In fact, the two step functions contribute equally, since one can simply redefine the integration variable $\cos\theta\to-\cos\theta$ in the second term above. Hence,

$$\frac{\partial}{\partial k_f}\mathcal{I}(k_f,q) = 4\pi\int_{-1}^{1} d\cos\theta\int_0^\infty k^2\,dk\,\delta(k_f-k)\,\Theta\biggl(k_f-\sqrt{k_f^2+q^2-2qk_f\cos\theta}\biggr)\,. \tag{69}$$

Note that we have set $k=k_f$ inside the square root factor in eq. (69) due to the presence of the delta function. The integration over k is now trivial due to the presence of the delta function, and we are left with

$$\frac{\partial}{\partial k_f}\mathcal{I}(k_f,q) = 4\pi k_f^2\int_{-1}^{1} d\cos\theta\;\Theta\biggl(k_f-\sqrt{k_f^2+q^2-2qk_f\cos\theta}\biggr)\,. \tag{70}$$

The step function above is zero unless the argument is positive. This condition implies that $k_f^2 > k_f^2+q^2-2qk_f\cos\theta$ or equivalently,

$$\cos\theta > \frac{q}{2k_f}\,.$$

Hence, eq. (70) yields

$$\frac{\partial}{\partial k_f}\mathcal{I}(k_f,q) = 4\pi k_f^2\,\Theta(2k_f-q)\int_{q/(2k_f)}^{1} d\cos\theta\,.$$

where the factor of $\Theta(2k_f-q)$ above arises since for values of $q>2k_f$, the argument of the step function in eq. (70) is always negative which implies that it vanishes. The final integration is now trivial, and we end up with

$$\frac{\partial}{\partial k_f}\mathcal{I}(k_f,q) = 4\pi k_f^2\left(1-\frac{q}{2k_f}\right)\,\Theta(2k_f-q)\,. \tag{71}$$

We can now determine $\mathcal{I}(k_f,q)$ by performing an indefinite integration over k_f. Note that $\mathcal{I}(k_f,q)=0$ for $q>2k_f$, and $\mathcal{I}(k_f,q)$ must be a continuous function of k_f at $k_f=\frac{1}{2}q$. Integrating eq. (71) for $q<2k_f$ yields

$$\mathcal{I}(k_f,q) = 4\pi\left(\frac{k_f^3}{3}-\frac{qk_f^2}{4}\right)+C(q)\,,\qquad \text{for } 0<q<2k_f\,,$$

where $C(q)$ is the integration "constant," which can depend on q. However, $C(q)$ is determined by the continuity condition, $\mathcal{I}(k_f = \frac{1}{2}q) = 0$. It follows that $C = \pi q^3/12$. Hence,

$$\mathcal{I}(k_f, q) = \frac{\pi}{12}\left[16k_f^3 - 12qk_f^2 + q^3\right]\,\Theta(2k_f - q)\,. \tag{72}$$

Plugging in this result for the integral in eq. (66), it follows that

$$\sum_{\vec{\boldsymbol{k}}}\sum_s \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s}N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}}\,,\,s}\,|\Phi_0\rangle = \frac{V}{48\pi^2}\left[16k_f^3 - 12qk_f^2 + q^3\right]\,\Theta(2k_f - q) \qquad \text{for } \vec{\boldsymbol{q}} \neq 0\,. \tag{73}$$

It is convenient to introduce the dimensionless variable,

$$x \equiv \frac{q}{2k_f}\,, \tag{74}$$

and rewrite eq. (73) as:

$$\sum_{\vec{\boldsymbol{k}}}\sum_s \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s}N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}}\,,\,s}\,|\Phi_0\rangle = \frac{Vk_f^3}{6\pi^2}(1-x)^2(2+x)\,\Theta(1-x)\,, \qquad \text{for } x > 0\,.$$

Employing eq. (65) for the Fermi momentum then yields

$$\sum_{\vec{\boldsymbol{k}}}\sum_s \langle\Phi_0|\, N_{\vec{\boldsymbol{k}},s}N_{\vec{\boldsymbol{k}}+\vec{\boldsymbol{q}}\,,\,s}\,|\Phi_0\rangle = \tfrac{1}{2}N(1-x)^2(2+x)\,\Theta(1-x)\,, \qquad \text{for } x > 0\,. \tag{75}$$

Hence, using eq. (60),

$$S_0(\vec{\boldsymbol{q}}) = 1 - \tfrac{1}{2}(1-x)^2(2+x)\,\Theta(1-x)\,, \qquad \text{for } \vec{\boldsymbol{q}} \neq 0\,. \tag{76}$$

The derivation of eq. (76) was based on the assumption that $\vec{\boldsymbol{q}} \neq 0$ (or equivalently $x \neq 0$), since this latter assumption was invoked following eq. (57). However, we have already determined $S_0(\vec{\boldsymbol{q}} = 0)$ in eq. (56). Hence, after substituting for x using eq. (74) the final answer takes the following form:

$$S_0(\vec{\boldsymbol{q}}) = \begin{cases} N\,, & \text{for } \vec{\boldsymbol{q}} = 0\,, \\[6pt] \dfrac{q}{4k_f}\left(3 - \dfrac{q^2}{4k_f^2}\right), & \text{for } 0 < q < 2k_f\,, \\[6pt] 1\,, & \text{for } q \geq 2k_f\,, \end{cases}$$

where $q \equiv |\vec{\boldsymbol{q}}|$. For all values of $\vec{\boldsymbol{q}} \neq 0$, $S_0(\vec{\boldsymbol{q}})$ expresses the correlation of the Fourier modes of $n(\vec{\boldsymbol{x}})$ for two *different* values of $\vec{\boldsymbol{q}}$, namely $\vec{\boldsymbol{q}}$ and $-\vec{\boldsymbol{q}}$. Clearly, $\vec{\boldsymbol{q}} = 0$ is a special point since for this case alone, $\vec{\boldsymbol{q}} = -\vec{\boldsymbol{q}}$. Consequently, it is not surprising that $S_0(\vec{\boldsymbol{q}})$ is not continuous at $\vec{\boldsymbol{q}} = 0$, i.e. $S(\vec{\boldsymbol{q}} = 0) \neq \lim_{q\to 0} S_0(\vec{\boldsymbol{q}})$.[11]

[11] Indeed, $\lim_{q\to 0} S_0(\vec{\boldsymbol{q}}) = 0$ is a consequence of the Pauli exclusion principle!

The static structure function $S_0(\vec{q})$ arises in the study of correlations of fermi systems. It can also be defined for an interacting systems of fermions and can be measured in scattering processes. For further details, you may wish to consult Chapter 2.4 of David Pines and Philippe Nozières, *The Theory of Quantum Liquids*, Volumes I (Westview Press, Boulder, CO, 1994). In this section, the authors show how to evaluate the integral $\mathcal{I}(k_f, q)$ using an elegant geometric anlaysis that directly computes the overlapping volume of the two spheres of radius k_f [cf. eq. (67) and the text that follows].

In an advanced course on the quantum theory of many-particle systems (often called "many-body theory"), you will learn how to compute $S_0(\vec{q})$ for a system of interacting fermions using perturbative techniques. In general, an exact analytic expression for $S_0(\vec{q})$ cannot be obtained in an interacting theory.

APPENDIX: A direct evaluation of $\mathcal{I}(k_f, q)$

We computed $\mathcal{I}(k_f, q)$ [defined in eq. (67)] by first evaluating the derivative of $\mathcal{I}(k_f, q)$ and then computing an indefinite integral of the result (using the appropriate boundary condition to fix the constant of integration). In this Appendix, we will compute $\mathcal{I}(k_f, q)$ directly by carefully examining the effect of the delta functions on the limits of integration.

By definition,

$$\mathcal{I}(k_f, q) \equiv \int \Theta(k_f - k)\, \Theta(k_f - |\vec{k} + \vec{q}\,|)\, d^3k\,. \tag{77}$$

Geometrically, $\mathcal{I}(k_f, q)$ is the volume of the overlapping region of two spheres of radius k_f whose centers are separated by a distance $q \equiv |\vec{q}|$. Employing spherical coordinates,

$$\begin{aligned} \mathcal{I}(k_f, q) &= \int_0^\infty k^2 dk \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi \int \Theta(k_f - k)\, \Theta(k_f - |\vec{k} + \vec{q}\,|) \\ &= 2\pi \int_0^{k_f} k^2 dk \int_{-1}^{1} d\cos\theta\ \Theta\big(k_f - \sqrt{k^2 + q^2 + 2qk\cos\theta}\big)\,, \end{aligned} \tag{78}$$

where we have invoked the $\Theta(k_f - k)$ function to restrict the integration range of k. The remaining step function will constrain the integration regions of k and $\cos\theta$. Note that $\Theta\big(k_f - \sqrt{k^2 + q^2 + 2qk\cos\theta}\big) = 0$ unless

$$k_f^2 \geq k^2 + q^2 + 2qk\cos\theta\,,$$

which is equivalent to the condition that

$$\cos\theta \leq \frac{k_f^2 - k^2 - q^2}{2kq}\,. \tag{79}$$

Since q is a variable, we shall consider three separate cases.

Case 1: If $0 < q < k_f$, then

$$\begin{aligned} &\int_0^{k_f} k^2 dk \int_{-1}^{1} d\cos\theta\ \Theta\big(k_f - \sqrt{k^2 + q^2 + 2qk\cos\theta}\big) \\ &\qquad = \int_0^{k_f - q} k^2 dk \int_{-1}^{1} d\cos\theta + \int_{k_f - q}^{k_f} k^2 dk \int_{-1}^{(k_f^2 - k^2 - q^2)/(2kq)} d\cos\theta\,. \end{aligned} \tag{80}$$

The upper limit of the $\cos\theta$ integration in the second integral on the right hand side of eq. (80) is a consequence of the condition derived in eq. (79). One can check that for Case 1, if $k_f - q \leq k \leq k_f$ then $-1 \leq (k_f^2 - k^2 - q^2)/(2kq) \leq 1$, whereas if $0 \leq k \leq k_f - q$, then $|\cos\theta| \leq 1$ is consistent with the inequality given in eq. (79). The integrations in eq. (80) are straightforward, and the end result is:

$$\begin{aligned}\int_0^{k_f} k^2 dk \int_{-1}^{1} d\cos\theta\; \Theta\big(k_f - \sqrt{k^2+q^2+2qk\cos\theta}\big) &= \tfrac{2}{3}(k_f-q)^3 + \tfrac{17}{24}q^3 - 2k_f q^2 + \tfrac{3}{2}k_f^2 q \\ &= \tfrac{1}{24}\left(q^3 - 12qk_f^2 + 16k_f^3\right) . \qquad (81)\end{aligned}$$

Case 2: If $k_f < q < 2k_f$, then

$$\int_0^{k_f} k^2 dk \int_{-1}^{1} d\cos\theta\; \Theta\big(k_f - \sqrt{k^2+q^2+2qk\cos\theta}\big) = \int_{q-k_f}^{k_f} k^2 dk \int_{-1}^{(k_f^2-k^2-q^2)/(2kq)} d\cos\theta\,. \qquad (82)$$

One can check that for Case 2, if $q-k_f \leq k \leq k_f$ then $-1 \leq (k_f^2-k^2-q^2)/(2kq) \leq 1$, whereas if $0 \leq k \leq q - k_f$, then $|\cos\theta| \leq 1$ is *inconsistent* with the inequality given in eq. (79). In particular, for $0 \leq k \leq q - k_f$ (with $q > k_f$) it follows that $(k_f^2 - k^2 - q^2)/(2kq) < -1$, in which case eq. (79) cannot be satisfied in the region where $|\cos\theta| \leq 1$. Thus, there is only one integral to perform in eq. (82) and we obtain

$$\int_0^{k_f} k^2 dk \int_{-1}^{1} d\cos\theta\; \Theta\big(k_f - \sqrt{k^2+q^2+2qk\cos\theta}\big) = \tfrac{1}{24}\left(q^3 - 12qk_f^2 + 16k_f^3\right) . \qquad (83)$$

Remarkably the result for the integral in Cases 1 and 2 coincide!

Case 3: If $q > 2k_f$, then[12]

$$\int_0^{k_f} k^2 dk \int_{-1}^{1} d\cos\theta\; \Theta\big(k_f - \sqrt{k^2+q^2+2qk\cos\theta}\big) = 0\,, \qquad (84)$$

since for Case 3, if $0 \leq k \leq k_f$ (with $q > 2k_f$) it follows that $(k_f^2 - k^2 - q^2)/(2kq) < -1$, in which case eq. (79) cannot be satisfied in the region where $|\cos\theta| \leq 1$. This is easily checked by observing that

$$\frac{k_f^2 - k^2 - q^2}{2kq} \geq 1 \quad \Longrightarrow \quad k_f^2 \geq (q-k)^2\,,$$

Since $0 \leq k \leq k_f$ and $q \geq 2k_f$, it follows that $k_f \geq q - k$, or equivalently $k \geq q - k_f$. But this last condition is not compatible with $0 \leq k \leq k_f$ and $q \geq 2k_f$. Hence, the condition $(k_f^2 - k^2 - q^2)/(2kq) \geq -1$ cannot be satisfied. In light of eq. (79), this means that the step function in eq. (84) is always equal to zero.

Combining the results of eqs. (80), (82) and (84), it follows that

$$\mathcal{I}(k_f, q) = \frac{\pi}{12}\left[q^3 - 12qk_f^2 + 16k_f^3\right]\Theta(2k_f - q)\,,$$

which confirms the result obtained in eq. (72).

[12]Geometrically, eq. (84) is the statement that two spheres of radius k_f whose centers are separated by a distance larger than $2k_f$ do not overlap (and hence the volume of the overlapping region is zero).