HOMEWORK II

QM B[illegible] Sol [illegible]-5.10

- Problem 1

The potential we are asked to consider is

$$H = H^0 + H' = \hbar\omega(a^\dagger a + \tfrac{1}{2}) + (\lambda t/\tau)X$$

If we define $X = \sqrt{\hbar/2m\omega}\,(a + a^\dagger) \equiv \beta(a + a^\dagger)$

we can write

$$H^0 = \hbar\omega(a^\dagger a + \tfrac{1}{2}) \quad H' = (\lambda\beta t/\tau)(a + a^\dagger)$$

The general operator relationship ~~between~~ for the interaction picture is given by, for any operator Ω,

$$\Omega_I = (U_S^0)^\dagger \Omega_S U_S^0 = e^{iH^0 t/\hbar}\,\Omega_S\, e^{-iH^0 t/\hbar}$$

where H^0 is, in this case, the pure HO hamiltonian. So for example, for $\Omega_S = a$, we have

$$a_I = e^{iH^0 t/\hbar}\, a\, e^{-iH^0 t/\hbar}$$

Applying this to the arbitrary HO eigenstate n, we find

$$a_S|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$e^{iH^0 t/\hbar}\, a\, e^{-iH^0 t/\hbar}|n\rangle = e^{(-i\omega t)(n+\frac{1}{2})}\, e^{iH^0 t/\hbar}\, a|n\rangle =$$

$$\sqrt{n}\, e^{-i\omega t \hbar (n+\frac{1}{2})} e^{iH_0 t/\hbar} |n-1\rangle = \sqrt{n}\, e^{-i\omega t(n+\frac{1}{2})} e^{i\omega t/\hbar\,(n-\frac{1}{2})} |n-1\rangle$$

$$= \sqrt{n}\, e^{-i\omega t} |n-1\rangle$$

Since this is true for arbitrary $|n\rangle$, or any linear combination thereof, we see that $a_I(t) = e^{-i\omega t} a$. It's easy to see that $a_I^+(t) = e^{i\omega t} a^+$, and so

$$\boxed{a_I^{(+)}(t) = e^{\pm i\omega t} a}$$

Where "+" $\Leftrightarrow a^+$ and "−" $\Leftrightarrow a$. Thus, in the interaction picture, we find

$$\boxed{X_I = \beta(a_I + a_I^+) = \beta(a e^{-i\omega t} + a^+ e^{i\omega t})}$$

Now, at leading order, the interaction picture propagator is given by

$$U_I(t,0) = I - \frac{i}{\hbar}\int_0^t H_I'(t')\,dt'$$

$$= I - \frac{i}{\hbar}\int_0^t \frac{\lambda\beta t'}{\tau}\left[a e^{-i\omega t'} + a^+ e^{i\omega t'}\right] dt'$$

$$= I - i\frac{\lambda\beta}{\hbar\tau}\left[\int_0^t t' e^{-i\omega t'} a\, dt' + \int_0^t t' e^{i\omega t'} a^+\, dt'\right]$$

Thus we require the integral

$$\int_0^t t' e^{\pm i\omega t'} dt' = \text{by parts} = \pm\frac{1}{i\omega}\Big[t' e^{\pm i\omega t'}\Big]_0^t \mp \left[\frac{\pm 1}{i\omega}\int_0^t e^{\pm i\omega t'} dt'\right]$$

$$= \pm\frac{t}{i\omega} e^{\pm i\omega t} - \left[-\frac{1}{\omega^2}\Big[e^{\pm i\omega t'}\Big]_0^t\right]$$

$$= \pm\frac{t}{i\omega} e^{\pm i\omega t} + \frac{1}{\omega^2}\Big[e^{\pm i\omega t} - 1\Big]$$

whence we seem to find

$$\boxed{U_I(\tau,0) \simeq I - i\frac{\lambda p}{\hbar\tau}\left\{\left[-\frac{t}{i\omega}e^{-i\omega t} + \frac{1}{\omega^2}\left(e^{-i\omega t} - 1\right)\right]a + \left[\frac{t}{i\omega}e^{i\omega t} + \frac{1}{\omega^2}\left(e^{i\omega t} - 1\right)\right]a^{+}\right\}}$$

Next, we want the leading-order probability that the particle makes a transition from the ground to the first excited state. For this, clearly only the a^{+} term is relevant. ~~In the sudden~~ Setting $t = \tau$, and using the sudden approximation $\omega\tau \ll 1$, the a^{+} term becomes

$$\frac{t}{i\omega}e^{i\omega t} + \frac{1}{\omega^2}\left(e^{i\omega t} - 1\right) \longrightarrow$$ setting $t = \tau$ + using $t\tau << 1$

$$\cong \frac{\tau}{i\omega}\left[1 + i\omega\tau\right] + \frac{1}{\omega^2}\left[1 + i\omega\tau - \frac{\omega^2\tau^2}{2} - 1\right]$$

$$= \frac{\tau}{i\omega} + \tau^2 + i\frac{\tau}{\omega} - \frac{\tau^2}{2} = \frac{\tau^2}{2}$$

to leading order in τ. ~~Now, in the int. picture~~ ~~$|n_I\rangle = e^{i\omega_n t}|n\rangle$~~ This yields, for the a^+ piece of $U_I(\tau,0)$

$$U_I^{(1)}(\tau,0) \cong I - \frac{i\lambda\beta}{\hbar\tau}\frac{\tau^2}{2}a^+ = I - \frac{i}{2\hbar}\lambda\beta\tau a^+ \quad \text{with} \quad \beta = \sqrt{\frac{\hbar}{2m\omega}}$$

Now, in the interaction picture, $|n_I\rangle = e^{i\omega_n t}|n\rangle$, and the transition amplitude is given by

$$A(\tau) = \langle 1_I|U_I(\tau,0)|0_I\rangle = e^{-i\omega_1 t}\langle 1|I - \frac{i}{2\hbar}\lambda\beta\tau a^+|0\rangle$$

$$= -\frac{ie^{-i\omega_1 t}}{2\hbar}\lambda\beta\tau$$

The transition probability is the square of this:

$$P(\tau) = \frac{\lambda^2\beta^2\tau^2}{4\hbar^2} = \boxed{\frac{\lambda^2\tau^2}{8m\omega\hbar}}$$

Problem 2 (Bohm-Aharonov effect)

For this it will be helpful to recall that, in cylindrical coordinates (ρ, θ, z)

$$\vec{\nabla} = \frac{\partial}{\partial \rho}\hat{\rho} + \frac{1}{\rho}\frac{\partial}{\partial \theta}\hat{\theta} + \frac{\partial}{\partial z}\hat{z}$$

$$\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}$$

(a) We evaluate

$$\vec{\nabla}\chi = \vec{\nabla}\left(\frac{\Phi}{2\pi}\theta\right) = \frac{\Phi}{2\pi\rho}\hat{\theta}$$

Then, $\vec{\nabla}\cdot(\vec{\nabla}\chi) = \frac{1}{\rho}\frac{\partial}{\partial\theta}\left(\frac{\Phi}{2\pi\rho}\hat{\theta}\right) = 0$ so the Coulomb condition applies

Stokes' theorem tells us that

$$\int(\vec{\nabla}\times\vec{A})\cdot d\vec{a} = \oint \vec{A}\cdot d\vec{l}$$

The lhs gives $\int(\vec{\nabla}\times\vec{A})\cdot d\vec{a} = \int \vec{B}\cdot d\vec{a} = \Phi$

The rhs gives $\oint \frac{\Phi}{2\pi\rho}d\theta \overset{\text{since } \rho = R}{=} \oint \frac{\Phi}{2\pi R}d\theta = \frac{\Phi}{2\pi R}\cdot 2\pi R = \Phi$

So all is good.

(b) To include the effect of the EM field, we make the substitution

$$\vec{p} \rightarrow \vec{p} - \frac{q}{c}\vec{A}$$

which gives us the ~~SE~~ time-independent SE

$$\left[\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)\cdot\left(\vec{p} - \frac{q}{c}\vec{A}\right)\right]\psi = E\psi$$

In terms of operators, this gives

$$\left[\left(-i\hbar\vec{\nabla} - \frac{q}{c}\vec{\nabla}\chi\right)\cdot\left(-i\hbar\vec{\nabla} - \frac{q}{c}\vec{\nabla}\chi\right)\right]\psi = 2mE\psi$$

Multiplying this out, we find that

$$\left[-\hbar^2\nabla^2 + \frac{i\hbar q}{c}\left(\underbrace{\cancel{\vec{\nabla}\cdot\vec{\nabla}\chi}}_{0 \text{ by Coulomb condition}} + \vec{\nabla}\chi\cdot\vec{\nabla}\right) + \frac{q^2}{c^2}\vec{\nabla}\chi\cdot\vec{\nabla}\chi\right]\psi = 2mE\psi$$

Now, $\vec{\nabla}\chi = \frac{\Phi}{2\pi R}\hat{\theta}$, which leads us to, once we recall that all ρ and z derivatives of the wavefunction are 0,

$$\left[\frac{-\hbar^2}{R^2}\frac{d^2}{d\theta^2} + \frac{i\hbar q\Phi}{2\pi Rc}\frac{1}{R}\frac{d}{d\theta} + \frac{q^2}{c^2}\frac{\Phi^2}{4\pi^2R^2}\right]\psi(\theta) = 2mE\psi(\theta)$$

or ...

$$\left[-\hbar^2\frac{d^2}{d\theta^2} + \frac{i\hbar q\Phi}{2\pi c}\frac{d}{d\theta} + \frac{q^2\Phi^2}{4\pi^2c^2}\right]\psi(\theta) = 2mR^2E\,\psi(\theta)$$

(c) This looks to be a bit of a mess to solve, but in fact it's not, because there is no θ-dependence in the operator that acts on ψ. Let's call this operator H_{eff}, ie.,

$$H_{eff} = -\hbar^2\frac{d^2}{d\theta^2} + \frac{i\hbar q\Phi}{2\pi c}\frac{d}{d\theta} + \frac{q^2\Phi^2}{4\pi^2c^2}$$

We then note that, easily, $H_{eff}\frac{d}{d\theta} = \frac{d}{d\theta}H_{eff}$, or.

$$\left[H_{eff}, \frac{d}{d\theta}\right] = 0$$

Thus, H_{eff} and $d/d\theta$ will have simultaneous eigenstates. But the eigenstates of $d/d\theta$ satisfy

$$\frac{d}{d\theta}\psi(\theta) = a\,\psi(\theta)$$

which, when we put in the periodic boundary conditions, yields

$$\psi_n(\theta) = \exp\left[i\frac{n\theta}{2\pi}\right] \quad \text{for } n \text{ integer.}$$

These should be the energy eigenstates, which we verify by plugging into H_{eff}

$$H_{se}\,\psi_n(\theta) = \left[+\frac{\hbar^2 n^2}{4\pi^2} - \frac{n\hbar q\Phi}{4\pi^2 c} + \frac{q^2\Phi^2}{4\pi^2 c^2} \right] \psi_n(\theta) = 2mR^2 E_n \psi_n(\theta)$$

so indeed the $\psi_n(\theta)$ are energy eigenfunctions. We find

$$\cancel{E_n = \frac{1}{8\pi^2 mR^2}\left[\frac{q^2\Phi^2}{c^2} - n^2 - n\hbar \right.}$$

$$E_n = \frac{1}{8\pi^2 mR^2}\left[\hbar^2 n^2 - \frac{n\hbar q\Phi}{c} + \frac{q^2\Phi^2}{c^2} \right]$$

and indeed, the energy eigenvalues depend upon Φ!

Homework Problem 3

For shorthand, write the unperturbed eigenstates as

$$\begin{pmatrix}1\\0\end{pmatrix} = |1\rangle \qquad \begin{pmatrix}0\\1\end{pmatrix} = |2\rangle$$

In the interaction picture we expand an arbitrary state $|\psi(t)\rangle$ in terms of the unperturbed eigenstates with time-dependent coefficients given by $|\psi_I(t)\rangle = [U_I^0(t)]^\dagger |\psi_S(t)\rangle$, with $U_I^0(t) = \exp[-iH^0 t/\hbar]$; in other words

$$|\psi_I(t)\rangle = C_1(t)e^{i\omega_1 t}|1\rangle + C_2(t)e^{i\omega_2 t}|2\rangle$$

with $\omega_i = E_i/\hbar$ and initial conditions $C_1(0) = 1$ $C_2(0) = 0$. Now, to leading order in TDPT,

$$|\psi_I(t)\rangle = |\phi\rangle + \frac{1}{i\hbar}\int_0^t dt' \, V_I(t')|\phi\rangle$$

where we have used that $|\psi_I(0)\rangle = |\psi_S(0)\rangle = |\phi\rangle$

Now, $V_I(t') = e^{iH_0 t'/\hbar} V(t') e^{-iH_0 t'/\hbar}$, whence

$$|\psi_I(t)\rangle = |\phi\rangle + \frac{1}{i\hbar}\int_0^t dt' e^{iH_0 t'/\hbar} V(t') e^{-i\omega_1 t'} |1\rangle =$$ using the provided form of $V(t)$

$$= |1\rangle + \frac{1}{i\hbar}\int_0^t dt' e^{iH_0 t'/\hbar}\left[\lambda \cos(\omega t')\right] e^{-i\omega_1 t'} |2\rangle =$$

$$= |1\rangle + \frac{\lambda}{i\hbar}\int_0^t dt'\, e^{i(w_2-w_1)t'/\hbar} \cos(wt')\, |2\rangle$$

$$= |1\rangle + \frac{\lambda}{2i\hbar}\int_0^t dt'\, e^{iw_{21}t'} \left[e^{iwt'} + e^{-iwt'}\right]|2\rangle$$

where we have defined $w_{21} = (E_2 - E_1)/\hbar$. Thus,

$$|\psi_I(t)\rangle = |1\rangle + \frac{\lambda}{2i\hbar}\int_0^t dt' \left[\exp\left(i[w_{21}+w]t'\right) + \exp\left(i[w_{21}-w]t'\right)\right]|2\rangle =$$

-other little calculus

$$= |1\rangle - \frac{i\lambda}{\hbar}\left[\frac{e^{i(w_{21}+w)t/2}\sin\left[(w_{21}+w)t/2\right]}{w_{21}+w} + \frac{e^{i(w_{21}-w)t/2}\sin\left[(w_{21}-w)t/2\right]}{w_{21}-w}\right]|2\rangle$$

The transition amplitude is given by

$A(t) = \langle 2_I | \psi_I(t)\rangle$ where $|2_I\rangle = e^{+iw_2 t}|2\rangle$, so

$$A(t) = -\frac{i\lambda}{\hbar}\left[\frac{e^{i(w_{21}+w)t/2}\sin\left[(w_{21}+w)t/2\right]}{w_{21}+w} + \frac{e^{i(w_{21}-w)t/2}\sin\left[(w_{21}-w)t/2\right]}{w_{21}-w}\right]$$

Finally, the transition probability

$$P(t) = |A(t)|^2 = \frac{\lambda^2}{\hbar^2}\left[\frac{\sin^2[(\omega_{21}+\omega)t/2]}{(\omega_{21}+\omega)^2} + \frac{\sin^2[(\omega_{21}-\omega)t/2]}{(\omega_{21}-\omega)^2} + \frac{(\cos\omega t - \cos\omega_{21} t)}{(\omega_{21}^2-\omega^2)}\right]$$

This is a resonance-like behavior, with the transition probability growing as $\omega \to \omega_{21}$, so in the statement of the problem, $\omega_p = \omega_{21}$. The approach clearly breaks down in this limit since this expression becomes greater than 1. The definition of "too close for this approach" is roughly

$$|\omega_{21}-\omega| \lesssim \frac{\lambda}{\hbar}$$

Problem 4

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,

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

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, $|b^{(0)}\rangle = e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}}/\sqrt{V}$. Taking the hermitian conjugate yields,

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

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, $\langle b^{(0)}|\,\tfrac{1}{2}ez\mathcal{E}_0\,|a^{(0)}\rangle$. Employing spherical coordinates, $z = r\cos\theta$ and

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

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:

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

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:

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

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:

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

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.

Problem 5

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:

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

$$= \vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{d}}^{\,*}_{if} - \frac{(\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{k}})(\vec{\boldsymbol{d}}^{\,*}_{if}\cdot\vec{\boldsymbol{k}})}{k^2}, \tag{29}$$

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 $\langle j'\, m-1|T_q^{(1)}|j\, m\rangle = 0$ if $q = 0, +1$. Using eq. (32), we therefore conclude that:

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

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

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

where d is some (complex) constant. Writing $\vec{k} = k(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, 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

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

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 $1+\cos^2\theta$.

<u>*ADDED NOTE*</u>: 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

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

It is convenient to express $\vec{x}$ 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 $\vec{d}_{if}$ (when expressed as a spherical rank-one tensor) is non-vanishing. This result immediately implies eq. (33) and it then follows that $\vec{d}_{if} = d(1\,,\,i\,,\,0)$. 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), $\vec{d}_{if}\cdot\vec{d}^{\,*}_{if} - (\vec{d}_{if}\cdot\vec{k})(\vec{d}^{\,*}_{if}\cdot\vec{k})/k^2 = |d|^2(2-\sin^2\theta) = |d|^2(1+\cos^2\theta)$.

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: $\{\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_2, \hat{\boldsymbol{e}}_3\}$, where $\hat{\boldsymbol{e}}_3 \equiv \hat{\boldsymbol{k}}$. Any complex three-vector can be expanded in terms of this orthonormal set. In particular,

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

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

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

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 $\vec{\boldsymbol{d}}_{if}\cdot\vec{\boldsymbol{\epsilon}}_R^{\,*} = 0$.

(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 $(-1)^\ell$.