PHY662, Spring 2004, Apr. 20, 2004

22nd April 2004

1 Miscellaneous

1. Today, we will work on the transition rates for stimulated absorption and the photoelectric effect.
2. Homework will be due on Thursday, April 29. If you want to get started, it includes Shankar 18.5.1 and Shankar 18.5.2(1) [not part (2) of problem 18.5.2.]
3. Comments on HWK #11.
   (a) Please work out your own solution, for comprehension.
   (b) Approaches using $\frac{\partial \mathcal{H}}{\partial p}$ were classical approaches.
   (c) $[\pi_i, \pi_m \pi_m] \neq 0$.
4. The final exam is on Monday, May 3. It is currently scheduled for 7:15 PM (yes, 7:15 PM).
5. What should we cover next week? 2nd quantization & spontaneous emission (Casimir effect?)? Scattering theory & Born approximation? Superconductivity? EPR and Bell inequality or Berry's phase?

2 Electromagnetic waves

2.1 Electromagnetic modes

We can simply express solutions to the wave equation for $\vec{A}$ using plane waves in a box of volume V as

$$\vec{A}(\vec{r}, t) = \sum_{k\vec{\lambda}} \frac{1}{\sqrt{V}} \left[A_{k\vec{\lambda}} \vec{\lambda}(\vec{k}) e^{i(\vec{k}\cdot\vec{r}-\omega t)} + A^*_{k\lambda} \vec{\lambda}^*(\vec{k}) e^{-i(\vec{k}\cdot\vec{r}-\omega t)} \right] ,$$

where the second term is the c.c. of the first to ensure that $\vec{A}$ is real (which it must be, in order for particle conservation to hold and for $\vec{B}$ to be real) and the $V^{-1/2}$ factor is a convenient normalization. The Coulomb gauge condition $\vec{\nabla} \cdot \vec{A} = 0$ is satisfied iff $\vec{k} \cdot \vec{\lambda} = 0$. The polarization vectors $\vec{\lambda}$ can be complex, but one often chooses two plane polarizations, with $\vec{\lambda}_{1,2} \perp \vec{k}$, $\vec{\lambda}_1 \perp \vec{\lambda}_2$. The scalar $A_{\vec{k}\lambda}$ gives the amplitude and phase of the wave.

The total electromagnetic energy in the volume V is

$$E = \sum_{\vec{k}\vec{\lambda}} \frac{\omega^2}{2\pi c^2} |A_{\vec{k}\lambda}|^2 .$$

3 Calculating electromagnetic transition rates

So let's imagine a single-electron atom in its ground state and bathed in incoherent radiation, such as from a typical black body or vapor lamp. How long does the atom spend in the ground state $|0\rangle$ before it is excited to a given state $|n\rangle$ of higher energy?

Applying Fermi's golden rule gives

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar} |\langle n| \left(\frac{-e}{mc}\right) \vec{A} \cdot \vec{p}|0\rangle|^2 \delta(E_n - E_0 - \hbar\omega) ,$$

where the interaction term that is proportional to A^2 in the interaction Hamiltonian has been dropped, taking the intensity of the incident radiation small compared to the electric field due to the nucleus of the atom and we are working in the Coulumb gauge, $\vec{A} \cdot \vec{p} = \vec{p} \cdot \vec{A}$.

For light atoms, transitions involve photons with wavelengths of the order of 100's of nm, much larger than the atomic size of order $0.1\,\mathrm{nm}$, so it is fair to write $A_{\vec{k}\vec{\lambda}} e^{-i\vec{k}\cdot\vec{r}}$ just as $A_{\vec{k}\vec{\lambda}}$ (in a moment we will see why this is referred to as the electric dipole approximation).

Writing this as a sum over incoherent positive-frequency modes (since absorption) gives

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar} \sum_{\vec{k},\vec{\lambda}} V^{-1} |A_{\vec{k}\vec{\lambda}}|^2 |\langle n| \left(\frac{-e}{mc}\right) \vec{\lambda} \cdot \vec{p}|0\rangle|^2 \delta(E_n - E_0 - \hbar\omega) .$$

Now consider the matrix element $\langle n|\vec{p}|0\rangle$. Using $\vec{p}/m = (i\hbar)^{-1}[\vec{r}, H_0]$,

$$\begin{aligned}\langle n|\vec{p}|0\rangle &= \frac{m}{i\hbar} \langle n|(\vec{r}H_0 - H_0\vec{r})|0\rangle \\ &= \frac{m}{i\hbar} (E_0 - E_n) \langle n|\vec{r}|0\rangle .\end{aligned}$$

Using $(E_n - E_0) = \hbar\omega$, we can now write

$$\Gamma_{0\to n} = \frac{2\pi e^2}{\hbar c^2} \sum_{\vec{k},\vec{\lambda}} \omega^2 V^{-1} |A_{\vec{k}\vec{\lambda}}|^2 |\vec{\lambda} \cdot \langle n|\vec{r}|0\rangle|^2 \delta(E_n - E_0 - \hbar\omega) .$$

To carry out the calculation further, we need to work with the sum $\sum_{\vec{k},\vec{\lambda}}$, to convert it into an integral over energy. As the dispersion relation for light is rather simple, $\omega = ck$,

$$\sum_{\vec{k}} \to \left(\frac{L}{2\pi}\right)^3 \int d^3k = V \int \frac{k^2 dk d\Omega}{(2\pi)^3} = V \int \frac{\omega^2 d\omega d\Omega}{(2\pi c)^3},$$

we get

$$\begin{aligned} \Gamma_{0\to n} &= \frac{2\pi e^2}{\hbar c^2 (2\pi c)^3} \int d\omega d\Omega\, \omega^4 |A_{\vec{k}\vec{\lambda}}|^2 |\vec{\lambda} \cdot \langle n|\vec{r}|0\rangle|^2 \delta(E_n - E_0 - \hbar\omega) \\ &= \frac{2\pi e^2 \omega^4}{\hbar^2 c^2 (2\pi c)^3} \int d\Omega\, |A_{|\vec{k}|=\omega/c,\vec{\lambda}}|^2 |\vec{\lambda} \cdot \langle n|\vec{r}|0\rangle|^2 . \end{aligned}$$

The $\langle n|\vec{r}|0\rangle$ is an off-diagonal dipole matrix element and we are considering electric dipole transitions (the operator $e\vec{r}$ is the electric dipole operator). Consider radiation incident upon the atom from an incoherent polarized source with an intensity measured in energy per unit solid angle per frequency interval, $I(\omega)$. It turns out that

$$I(\omega) = \frac{d\Omega \omega^4 |A_{k\lambda}|^2}{(2\pi c)^4} .$$

Substituting this in gives

$$\Gamma_{0\to n} = \frac{2\pi e^2 \omega^4}{\hbar c^2 (2\pi c)^3} (2\pi c)^4 \omega^{-4} I(\omega) |\lambda \cdot \langle n|\vec{r}|0\rangle|^2 .$$

What can we infer from this form of the rate? We can also work with total position operator $\sum r = R$. Here we are considering these operators in an interchangable fashion.

If l, m are good quantum numbers, we can use $[L_z, R_z] = 0$, $[L_z, R_x] = i\hbar R_y$, $[L_z, R_y] = -i\hbar R_x$ to get selection rules for m', m. We can also get $l' = l \pm 1$, using $[L^2, [L^2, R]] = 2\hbar^2(\vec{R}L^2 + L^2\vec{R})$.]

3.1 Photoelectric effect

This previous type of calculation is described in Baym. Shankar considers the photoelectric effect, where the final state is a plane wave state. There, you also have to be careful in the initial state - to do this calculation in lowest order consistently, the initial state should be an s-state. For $\hbar k/p \ll 1$, where k is the wavevector of the incident light and p is the momentum of the bound electron, we can neglect spin interactions and make the dipole approximation ($e^{ikr} \sim 1$). Let's take the ground state of a Hydrogen atom. Shankar uses $\cos(kr + \omega t)$ instead of $e^{ikr - i\omega t}$, so there is a factor of 2 ($\frac{e}{2mc}$, not $\frac{e}{mc}$). Shankar goes directly to the large volume limit. In this case, the matrix element H_{fi} is found using integration by parts is

$$\left(\frac{e}{2mc}\right)\left(\frac{1}{2\pi\hbar}\right)^{3/2} (\pi a_0^3)^{-1/2} \int d^3\vec{r}\, e^{-i\vec{p}_f \cdot \vec{r}/\hbar} \vec{A}_0 \cdot (-i\hbar\nabla) e^{-r/a_0} \quad = \quad N\vec{A}_0 \cdot \vec{p}_f \int d^3\vec{r}\, e^{-i\vec{p}_f \cdot \vec{r} - r/a_0}$$

$$= \quad \frac{N(\vec{A}_0 \cdot \vec{p}_f)(8\pi/a_0)}{[(1/a_0)^2 + (p_f/\hbar)^2]^2}$$

and inserting into the golden rule gives

$$\Gamma = \frac{2\pi}{\hbar} N^2 (\vec{A}_0 \cdot \vec{p}_f)^2 \frac{64\pi^2 a_0^6}{[1 + (p_f a_0/\hbar)^2]^4} \delta(E_f - E_i - \hbar\omega)\,.$$

Given incident light of frequency $\omega = (E_f - E_i)/\hbar$, the transition rate into the angle $d\Omega$ is found by converting $\delta(\frac{p_f^2}{2m} - E_i - \hbar\omega)$ into $\frac{m}{p_f}\delta[p_f - (2m)^{1/2}(E_i + \hbar\omega)^{1/2}]$, so that integrating over the magntiude of the final state momentum gives, using $d^3p_f = d\Omega p_f^2 dp_f$,

$$\Gamma_{i \to d\Omega} = \frac{4a_0^3 e^2 p_f |\vec{A}_0 \cdot \vec{p}_f|^2}{m\pi\hbar^4 c^2 [1 + (p_f a_0/\hbar)^2]^4} d\Omega\,.$$

This is the transition rate for the photoelectric effect.

Which way does the electron like to go?

Integrating over $d\Omega = d\phi d(\cos\theta)$ gives

$$\Gamma = \frac{16 a_0^3 e^2 p_f^3 |A_0|^2}{3m\hbar^4 c^2 \left[1 + (p_f a_0/\hbar)^2\right]^4}$$