PH 618 FINAL TAKE-HOME EXAM

(Due: March 19, 2013, Tuesday by noon at the instructor's mailbox)
(Subject: Time Dependent Quantum Mechanics)

Rule: **You can look up any references but CANNOT communicate with any living person for help, except with the instructor who will only clarify the problems for you but will NOT give you any help in solving them.**

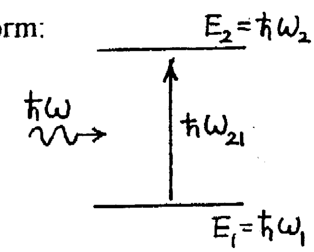
Score: **There are 6 problems altogether. The scores are allocated as follows: Nos. 1, 2, and 6: 40 points each. Nos. 3, 4, 5: 20 points each.**

1. <u>Rotating wave approximation for the 2-level system</u>

For a two-level system being driven by a sinusoidal time-varying field, the time-dependent part of the Hamiltonian of the system can be expressed as:

$$H'(t) = -e\varepsilon z \cos\omega t = V(e^{i\omega t} + e^{-i\omega t}), \qquad (1)$$

with $V = -e\varepsilon z/2$. Consider the TDSE of the system in the following form:



$$\left[H_0 + H'(t)\right]\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}, \qquad (2)$$

where $$\psi(\vec{r},t) = \sum_{n=1}^{2} c_n(t)e^{-i\omega_n t}u_n(\vec{r}). \qquad (3)$$

$H_0 u_n = E_n u_n$

In class, we have established the following <u>exact</u> coupled differential equations for c_1 and c_2:

$$\dot{c}_1 = -\frac{i}{\hbar}V_{12}\left[e^{i(\omega-\omega_{21})t} + e^{-i(\omega+\omega_{21})t}\right]c_2 \qquad (4)$$

$$\dot{c}_2 = -\frac{i}{\hbar}V_{21}\left[e^{i(\omega+\omega_{21})t} + e^{-i(\omega-\omega_{21})t}\right]c_1 \qquad (5)$$

(a) What do we mean by the "rotating wave approximation (RWA)"? (2 pts)

(b) What are the physical arguments which justify the application of the RWA to the above equations (4) and (5)? (5 pts)

(c) Write down the approximate form of (4) and (5) under the RWA in terms of the detuning parameter which is defined by : $\Delta\omega = \omega - \omega_{21}$. (3 pts)

(d) Assuming an initial condition with $c_1(0) = 1$ and $c_2(0) = 0$, show that the equations in part (c) can be solved in the following form:

$$c_1(t) = \left(\cos \omega_r t - \frac{i\Delta\omega}{2\omega_r} \sin \omega_r t \right) e^{i(\Delta\omega)t/2} \tag{6}$$

$$c_2(t) = -\frac{iV_{21}}{\hbar\omega_r} \sin \omega_r t \; e^{-i(\Delta\omega)t/2}, \tag{7}$$

where the Rabi flopping frequency is defined as:

$$\omega_r = \frac{1}{2}\left[\Delta\omega^2 + \left(\frac{2|V_{12}|}{\hbar} \right)^2 \right]^{1/2}. \tag{8}$$

(10 pts)

(e) Comment on the condition for conservation of probability from the results in equations (6) and (7). (5 pts)

(f) For small $\Delta\omega \neq 0$ but $V \ll \hbar\Delta\omega$, show that the transition probability is given by:

$$P_{1\to 2}(t) = |C_{12}(t)|^2 = \left(\frac{2|V_{21}|}{\hbar\Delta\omega} \right)^2 \sin^2\left(\frac{\Delta\omega}{2} t \right). \quad \text{(5 pts)}$$

(g) Show that the result obtained in (f) is the same as that obtained from first order time-dependent perturbation theory by applying Eq. (21.9) in the Lecture Notes. (5 pts)

(h) By including the "counter-rotating" terms, it was stated in the Notes that the result will lead to the so-called "Bloch-Seigert effect" which predicts an intensity-dependent resonance frequency differing from ω_{21} as follows:

$$\omega_r^{BS} = \omega_{21}\left[1 + \frac{1}{4}\left(\frac{\mu\varepsilon}{\hbar\omega_{21}} \right)^2 + \ldots \right],$$

where μ is the electric dipole moment (transition dipole) of the atom and ε is the electric field strength. By making some reasonable numerical estimates [e.g., μ in the order of (electronic charge) x (Bohr radius); $\hbar\omega_{21}$ in the order of eVs;...etc.], show that the Bloch-Seigert effect is generally negligible for ordinary field strengths in the laboratory. (5 pts)

2. **Geometrical description of the two-level system**
(Feynman, Vernon and Hellworth: 1957)

Feynman et al in 1957 pointed out a very important and striking similarity between the TDSE for a two-level system driven by a sinuisoidal electric field [problem (1)], and the dynamics of a nuclear spin in an external RF field in NMR, as described by the Bloch theory.

(a) Refer to Eqs. (4) and (5) in prob.(1). Let us define the "optical Bloch vector ($\vec{\rho}$)" as follows: $\vec{\rho} = (\rho_x, \rho_y, \rho_z)$ where

$$\begin{aligned}
\rho_x &= c_1 c_2^* e^{i\omega_{21}t} + c_2 c_1^* e^{-i\omega_{21}t} = 2\,\mathrm{Re}\left[c_1 c_2^* e^{i\omega_{21}t}\right] \\
\rho_y &= \frac{1}{i}(c_1 c_2^* e^{i\omega_{21}t} - c_2 c_1^* e^{-i\omega_{21}t}) = 2\,\mathrm{Im}\left[c_1 c_2^* e^{i\omega_{21}t}\right] \\
\rho_z &= |c_2|^2 - |c_1|^2
\end{aligned} \tag{9}$$

Show that the time rate of change of (9) is given by the following equations:

$$\begin{aligned}
\frac{d\rho_x}{dt} &= -\omega_{21}\rho_y + \frac{2}{i\hbar}V_-\rho_z \cos\omega t \\
\frac{d\rho_y}{dt} &= \omega_{21}\rho_x - \frac{2}{\hbar}V_+\rho_z \cos\omega t \\
\frac{d\rho_z}{dt} &= -\frac{2}{i\hbar}V_-\rho_x \cos\omega t + \frac{2}{\hbar}V_+\rho_y \cos\omega t
\end{aligned} \tag{10}$$

where $V_+ = V_{12} + V_{21} = 2\,\mathrm{Re}V_{12}$, and $V_- = V_{12} - V_{21} = 2i\,\mathrm{Im}V_{12}$. (30 pts)

(b) By defining an "equivalent external driving field" in the following form: $\vec{F} = (F_x, F_y, F_z)$ with

$$\begin{aligned}
F_x &= \frac{2}{\hbar}V_+ \cos\omega t \\
F_y &= \frac{2}{i\hbar}V_- \cos\omega t \\
F_z &= \omega_{21}
\end{aligned} \tag{11}$$

show that (10) and (11) imply the following "optical Bloch equation" of motion for the Bloch vector:

$$\frac{d\vec{\rho}}{dt} = \vec{F} \times \vec{\rho}\,. \tag{12}$$

Note that (12) is identical in form to the equation of motion for a spin magnetic moment in an external magnetic field. Hence the results obtained in Bloch's theory for NMR can be borrowed directly to the description of the two-level system. This is the origin for the many terminology such as rotating wave approximation, Rabi flopping frequency, counter rotating terms,...etc. (10 pts)

3. **An alternative derivation of Fermi's golden rule**

Let W be the transition rate (i.e. transition probability to the final state 'f' per unit time). Thus according to first order time-dependent perturbation theory, we have:

$$W = \frac{dP_{fi}}{dt} = \frac{d}{dt}\sum_{k\subset f}\left|C_k^{(1)}\right|^2 \rightarrow \frac{d}{dt}\int_{-\infty}^{\infty} dE_{ki}\,\rho_f(E_k)\left|C_k^{(1)}\right|^2$$

where we have summed over "a continuum of final states" $k \subset f$ by introducing the concept of density of states just like we did in class. We have also extended the integration to $(-\infty, \infty)$, taking advantage of the fact that $\left|c_k^{(1)}(t)\right|^2$ behaves almost like a delta function (revealing the condition of "almost exact energy conservation" in the transition process).

(a) Using Eq. (21.9) in the notes, substitute the exact time integral form of $c_k^{(1)}(t)$ and its conjugate into the above expression, so that W is now expressed as a 'triple integral'. Take care of the dummy time variables in the integral expressions! (5 pts)

(b) Assuming the density function is roughly constant and denote it as $\rho(E_f)$, show that, by performing first the integral over $d\omega_{ki} = dE_{ki}/\hbar$, the result in (a) leads back exactly to Fermi's golden rule:

$$W = \frac{2\pi}{\hbar}\left|H'_{fi}\right|^2 \rho(E_f),$$

for constant perturbation H', with $E_f \approx E_i$. [HINT: $\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}dk$] (15 pts)

4. **Principle of detailed balancing**

In class, it was claimed [below eq. (25.14)] that the transition rate for absorption must be equal to that for stimulated emission (for non-degenerate states): $W_{mn} = W_{nm}$. Try to use first order time-dependent perturbation theory to prove this statement. Note that the validity of this principle is very general although here we only demonstrate it using first order perturbation results. Historically, this was first established by Einstein in his1917 theory (his B coefficients: B=B') in which stimulated emission was first introduced. [HINT: starting from Eq. (21.9) in the notes, and making use of the hermiticity of H'(t), show that $c_{nm}^{(1)} = -\left[c_{mn}^{(1)}\right]^*$, and hence the claimed result.] (20 pts)

5. **Estimate of the ratio of stimulated to spontaneous emission**

Referring to Eq. (25.28), we want to estimate the ratio defined as:

$$R = \frac{B'u}{A} = \frac{Bu}{A} = \frac{c^3\pi^2}{\hbar\omega^3}u$$

for an ordinary source as follows. Consider a mercury lamp emitting at a wavelength of 254 nm, with a fractional wavelength spread of 10^{-5}. If the output flux (I) is 1 kWm^{-2}, estimate the ratio R for this light source and show that it is of the order of 10^{-4}. [HINT: $I = (u\Delta\omega)$ x c where $\Delta\omega$ is the spread in angular frequency which can be obtained from the given spread in wavelength.] (20 pts).

6. **Lifetime and intensity of spectroscopic emission from H-atom**

Because of the dipole selection rule $\Delta\ell = 1$, the transitions: $ns \to 1s$ are forbidden in the H-atom. Let us consider the allowed transitions: $np \to 1s$.

(a) The lifetimes (τ) of these np states are essentially given by the inverse of the spontaneous decay rates, i.e. Einstein's A coefficients [eq. (25.31) in the Notes]. Note that ω in (25.31) for the present problem will be simply given by $\frac{[E(np) - E(1s)]}{\hbar} = \frac{\mu e^4}{2\hbar^3}\left(1 - \frac{1}{n^2}\right)$, where μ is the mass of the electron. We want to calculate the lifetime of the 2p state in this problem. So our main job here will be to calculate the following dipole transition matrix element:

$\vec{r}_{mn} = \vec{r}_{2p,1s} = \langle 1s|\vec{r}|2p\rangle = \langle 100|\vec{r}|21m\rangle$, where we have introduced the quantum numbers n, ℓ, m explicitly.

(i) Let us consider only the m = 0 transition, try to derive the following results for the dipole transition matrix element:

$$\langle 100|x|210\rangle = \langle 100|y|210\rangle = 0,$$

$$\langle 100|z|210\rangle = \frac{1}{4\pi\sqrt{2}a^4}\int_0^\infty r^4 e^{-3r/2a}dr \int \cos^2\theta d\Omega = \frac{2^7\sqrt{2}a}{3^5},$$

where $a = \frac{\hbar^2}{\mu e^2}$ is the Bohr radius.

(ii) Using these results into eq. (25.31), show that the Einstein A coefficient is given by the following expression:

$$A = \left(\frac{2}{3}\right)^8 \frac{e^{14}\mu^3 a^2}{\hbar^{10}c^3} = \left(\frac{2}{3}\right)^8 \frac{c}{a}\alpha^4,$$ where $\alpha \equiv \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the so-called fine structure constant. Hence show that the lifetime of this particular 2p state is given by: $\tau \approx 1/A \approx 1.6\times10^{-9}s$.

[NOTE: it can be shown that all the $2p \to 1s$ transition matrix elements are the same whether m= 0, +1, or −1. Hence the lifetime of the 2p state will be really given by the above value after we have averaged over the three transition probabilities from $|210\rangle \to |100\rangle$, from $|211\rangle \to |100\rangle$, and from $|21-1\rangle \to |100\rangle$.] (20 pts)

(b) In the Lyman series of the H-spectrum, the Ly α and the Ly β are the two lines from the $2p \to 1s$ and $3p \to 1s$ transition, respectively. Since the intensity of these emissions $I \propto \hbar\omega \times A$ (why?), where ω is the transition frequency and A the Einstein coefficient, we thus have [from Eq. (25.31)]:

$$\frac{I_\alpha}{I_\beta} = \frac{\omega_\alpha^4}{\omega_\beta^4}\frac{\langle 1s|\vec{r}|2p\rangle^2}{\langle 1s|\vec{r}|3p\rangle^2}.$$

Again, let us look at the $|n10\rangle \to |100\rangle$ transition where n = 2, 3. Similar to the steps in (a) above, show that:

$$\langle 100|x|310\rangle = \langle 100|y|310\rangle = 0,$$

$$\langle 100|z|310\rangle = \frac{1}{\sqrt{2}}\frac{3^3}{2^6}a,$$

and hence obtain: $\frac{I_\alpha}{I_\beta} \approx 3.16$. (20 pts)

[HINT: Given the various eigenfunctions of the H-atom as follows:

$$u_{100} = \frac{1}{\sqrt{\pi}a^{3/2}}e^{-r/a},\quad u_{210} = \frac{1}{4\sqrt{2\pi}}\frac{r}{a^{5/2}}e^{-r/2a}\cos\theta,$$ and

$$u_{310} = \frac{4}{27\sqrt{2\pi}}\frac{1}{a^{3/2}}(1-\frac{r}{6a})\left(\frac{r}{a}\right)\cos\theta e^{-r/3a}.$$

You will also find the following integral useful: $\int_0^\infty x^n e^{-\beta x}dx = \frac{n!}{\beta^{n+1}}$]