Victor Yakovenko, Assistant Professor
Office: Physics 2314
Phone: (301)–405–6151
E-mail: yakovenk@physics.umd.edu

Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of Schwabl.
Equation numbers without period, like (5), refer to the equations of this homework.

Interaction with Electromagnetic Field (Chapter 16)

The absorption and emission of electromagnetic radiation by a quantum system often can be analyzed in the so-called "semiclassical approximation", in which the electromagnetic field is treated classically, whereas the electron is treated quantum-mechanically, via its wave function. In this homework we take this semiclassical point of view.

1. *Adapted from Qualifier, January 1998, August 1991, II-2.*

A charged particle of mass m moves in a one-dimensional attractive potential $U(x) = -\lambda\delta(x)$, where $\delta(x)$ is the Dirac delta-function, and $\lambda > 0$. Initially, the particle is in the ground state of the potential with the energy $E_0 < 0$. Then, a small ac electric field $\mathcal{E}(t) = \mathcal{E}_0 \sin(\omega t)$ of the frequency $\omega > |E_0|/\hbar$ is turned on. The Hamiltonian of the perturbation is

$$V = -2ex\mathcal{E}_0 \sin(\omega t), \tag{1}$$

where e is the electron charge. This perturbation may cause a transition of the particle from the bound state to an unbound state ("ionization" of the "atom").

(a) [**3 points**] Calculate the matrix element of perturbation (1) between the bound ground state and an unbound states excited state. Choose the wave functions of the excited states to have certain parities and use the parity selection rule.

(b) [**5 points**] Using the Fermi golden rule, calculate the ionization rate of the "atom". In other words, calculate the probability of transition of the electron from the ground state to an unbound state per unit time. Make sure the dimensionality of your final result is 1/time.

(c) [**3 points**] Sketch how the ionization rate depends on the frequency ω.

2. *Adapted from Qualifier, Fall 1988, II-2.*

An atom in the ground state is subject to a weak, time-dependent, and uniform in space electric field $\boldsymbol{\mathcal{E}}(t)$. A simplest way to introduce the electric field into the electron Hamiltonian is to select the gauge with the scalar potential $\phi(\mathbf{r}, t) = -\mathbf{r} \cdot \boldsymbol{\mathcal{E}}(t)$ and zero vector potential $\mathbf{A} = 0$. Then, the perturbation of the electron potential energy is

$$\hat{V} = e\phi(\mathbf{r}, t) = -e\mathbf{r} \cdot \boldsymbol{\mathcal{E}}(t). \tag{2}$$

(a) [**5 points**] In the lowest order of the time-dependent perturbation theory, show that the time-dependent expectation value of the electron dipole moment,

$$\mathbf{d}(t) = \langle \psi(t) | e\mathbf{r} | \psi(t) \rangle, \tag{3}$$

depends on the values of the electric field at all previous moments of time:

$$d(t) = \int_0^\infty \alpha(\tau)\mathcal{E}(t-\tau)\, d\tau. \tag{4}$$

In this case, the vectors $\mathbf{d}$ and $\boldsymbol{\mathcal{E}}$ are parallel, but in a more general case the polarizability α would be a tensor. Find an expression for the polarizability $\alpha(\tau)$ in terms of nonvanishing matrix elements of perturbation (2).

(b) [**3 points**] Calculate the frequency-dependent polarizability of the atom, $\alpha(\omega)$, which is a Fourier transform of $\alpha(\tau)$:

$$\alpha(\omega) = \int_0^\infty \alpha(\tau)\, e^{i\omega\tau}\, d\tau. \tag{5}$$

To make integral (5) convergent, assume that the frequency ω has an infinitesimal positive imaginary part ϵ: $\omega = \omega + i\epsilon$. The frequency-dependent polarizability $\alpha(\omega)$ describes response of the atom to a periodic-in-time electric field, such as the electric field of an electromagnetic wave.

(c) [**2 points**] Compare $\alpha(\omega = 0)$ with the expressions for the static polarizability you encountered in previous homework on the time-independent perturbation theory, e.g. Eq. (14.29). Do the two expressions agree?

(d) [**3 points**] Calculate the imaginary part $\alpha''(\omega)$ of $\alpha(\omega)$ **(see Hints)**. Using the Thomas-Reiche-Kuhn sum rule (Problem 16.10), calculate the integral

$$\int_{-\infty}^{+\infty} \omega\alpha''(\omega)\, d\omega \tag{6}$$

and show that it is independent of the nature of the considered system, thus represents a sum rule.

(e) [**3 points**] What is the physical meaning of the real and imaginary parts of the polarizability? Which of them determines

i. velocity of light in hydrogen gas,
ii. absorption of light in hydrogen gas?

Explain why.

(f) [**3 points**] Compare expressions for the frequency-dependent polarizability of a one-dimensional harmonic oscillator and an atom. Contemplate the similarities and differences between the two expressions.

3. *Adapted from Qualifier, Spring 1986, II-2.*

A plane electromagnetic wave specified by the vector potential,

$$\mathbf{A}(\mathbf{r},t) = \mathbf{A}_0(\omega)e^{i(\mathbf{kr}-\omega t)} + \mathbf{A}_0^*(\omega)e^{-i(\mathbf{kr}-\omega t)}, \qquad \phi = 0, \qquad \mathrm{div}\,\mathbf{A} = 0, \tag{7}$$

interacts with an electron that belongs to an atom.

(a) [**3 points**] The energy flux of the electromagnetic wave (7) is defined as the amount of energy crossing a unit area in a unit time:

$$F(\omega) = \frac{c}{4\pi}\langle|\mathbf{E}\times\mathbf{B}|\rangle = \left[\frac{\text{Energy}}{\text{Area}\times\text{Time}}\right], \tag{8}$$

where the angular brackets denote averaging over time.

Show that $F(\omega)$ is given by the following formula in terms of the amplitude $A_0(\omega)$ in Eq. (7):

$$F(\omega) = \frac{\omega^2|A_0(\omega)|^2}{2\pi c}. \tag{9}$$

(b) [**5 points**] Using the Fermi golden rule, derive an expression for the transition rate $R_{i\to f}(\omega)$ per unit time from an electron state $|i\rangle$ to an electron state $|f\rangle$ induced by the field (7) in terms of the wave functions and the energies of the states $|i\rangle$ and $|f\rangle$.

Compare this expression with Eq. (16.85). Do they agree? To answer this question, you need to connect the number of photons n in the quantized theory of electromagnetic radiation with the intensity A_0 in the classical theory.

(c) [**3 points**] The absorption cross section of electromagnetic radiation by the electron, $\sigma_{i\to f}(\omega)$, is defined as the energy absorption rate $\hbar\omega R_{i\to f}(\omega)$ divided by the energy flux $F(\omega)$ (9):

$$\sigma_{i\to f}(\omega) = \frac{\hbar\omega R_{i\to f}(\omega)}{F(\omega)} = \left[\frac{\frac{\text{Energy}}{\text{Time}}}{\frac{\text{Energy}}{\text{Area}\times\text{Time}}}\right] = [\text{Area}]. \tag{10}$$

The advantage of $\sigma_{i\to f}(\omega)$ compared to $R_{i\to f}(\omega)$ is that the former does not contain the external radiation intensity, thus characterizes the atom itself.

Obtain an expression for the absorption cross section $\sigma^{(d)}_{i\to f}(\omega)$ in the long-wavelength approximation (in the dipole approximation). Compare this expression with $\alpha''(\omega)$ found in Problem 2d.

(d) [**3 points**] Let us consider the electron in a ground state $|0\rangle$. The total absorption cross section is the sum of $\sigma_{0\to f}(\omega)$ over all final states: $\sigma(\omega) = \sum_f \sigma_{0\to f}(\omega)$. Using the Thomas-Reiche-Kuhn sum rule (Problem 16.10), prove in the dipole approximation that

$$\int_0^\infty \sigma^{(d)}(\omega)\, d\omega = \frac{2\pi^2 e^2}{mc}, \tag{11}$$

where m is the mass of electron. Note that Eq. (11) is universal in the sense that it does not contain any information about the details of the considered system (the type of the atom). It does not contain even $\hbar$, which means that this result should be valid also classically!

4. [**5 points**] The hydrogen atom in the ground state of the energy $E_0 < 0$ is irradiated by an electromagnetic wave of a frequency $\omega > |E_0|/\hbar$. This perturbation may cause ionization of the atom: an electron transition from the bound state to a unbound state with the wave vector $\mathbf{q}$.

Using the results of Problem 3, calculate the differential cross section $d\sigma$ of the electron excitation to the solid angle $d\Omega$ of the directions of the wave vector $\mathbf{q}$ and the total cross section of ionization, σ.

5. (a) [**5 points**] Let us consider a continuous distribution in the frequency ω of the plane waves of type (7). The energy flux in a small window of frequencies, $\Delta\omega$ can be written as $F(\omega, \Delta\omega) = \int_\omega^{\omega+\Delta\omega} I(\omega)\, d\omega$, where $I(\omega)$ is the spectral density of the energy flux.

Using your solution of Problem 3c and Eq. (10), show that the transition rate $R_{i\to f}$ between two discrete electron states $|i\rangle$ and $|f\rangle$ is proportional the spectral density of the energy flux $I(\omega)$ taken at the frequency of the atomic transition $\hbar\omega = E_f - E_i$:

$$R_{i\to f} = B\, I(\omega), \qquad \text{where} \quad \hbar\omega = E_f - E_i. \tag{12}$$

Find an expression for the coefficient B, which is called the Einstein coefficient B. (Different books have slightly different definitions of B.)

(b) [**3 points**] Compare your expression for B with expression (16.74) for the rate of spontaneous transitions from an excited state $|f\rangle$ to a lower state $|i\rangle$. The spontaneous transition rate (16.74) is called the Einstein coefficient A, by definition. Find a ratio of A to B.

(c) [**3 points**] Substituting the electron wave functions of the hydrogen atom into Eq. (16.74), calculate the lifetime of the 2p state of the hydrogen atom in seconds. Compare your result with the number given in Schwabl on page 305.

This number also determines the excitation rate of the 1s→2p transitions via Eq. (12) and the relation between A and B found in the previous problem.

Hints

2d

$$\mathrm{Im}\frac{1}{x - i\epsilon} = \pi\delta(x), \tag{13}$$

where $\delta(x)$ is Dirac's delta-function. Prove Eq. (13) starting from a finite ϵ and taking the limit $\epsilon \to 0$.