22.51 Quantum Theory of Radiation Interactions

Problem set # 6

Issued on Tuesday Nov 27, 2012. Due on Friday Dec. 7, 2012

Problem 1: The dipolar approximation

We have seen in class that the Hamiltonian for the interaction of atoms and radiation fields is given by

$$\mathcal{H} = \frac{p^2}{2m} + \frac{e^2}{2mc^2}A^2 - \frac{e}{mc}\vec{A}\cdot\vec{p}$$

in the Coulomb gauge. To first order in in e/c, the interaction term is then given by $V = -\frac{e}{mc}\vec{A}\cdot\vec{p}$. From the quantization in the Lorentz gauge we instead obtained an interaction term arising from the electric dipole of the atom interacting with the electric field

$$V_L = \vec{d}\cdot\vec{E} = -e\vec{r}\cdot\vec{E}.$$

In this problem, we want to analyze a regime where the two descriptions are equivalent.
Reminder: In the Coulomb gauge, the vector potential is

$$\vec{A} = \sum_{k,\lambda}\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}(a_{\vec{k},\lambda}e^{i\vec{k}\cdot\vec{r}} + a^\dagger_{\vec{k},\lambda}e^{-i\vec{k}\cdot\vec{r}})\vec{\epsilon}_{\vec{k},\lambda}$$

and in the Lorentz gauge, the electric field is

$$\vec{E} = \sum_{k,\lambda}\sqrt{\frac{2\pi\hbar\omega_k}{V}}(a_{\vec{k},\lambda}e^{i\vec{k}\cdot\vec{r}} + a^\dagger_{\vec{k},\lambda}e^{-i\vec{k}\cdot\vec{r}})\vec{\epsilon}_{\vec{k},\lambda}$$

where $\vec{r}$ is the atom's position.

a) Consider the case of optical light interacting with an atom. Then the wavelength is much longer than the atom's size, thus we can replace $\vec{k}\cdot\vec{r}$ with $\vec{k}\cdot\vec{R}$, where R is the nucleus position. Write a matrix element $\langle n_{k,\lambda}, a_n|\, V\, |m_{k',\lambda'}, a_m\rangle$ of the operator $V = -\frac{e}{mc}\vec{A}\cdot\vec{p}$, separating the contributions from the field and atom operators (here $|n_{k,\lambda}\rangle$ are number states of the field and $|a_n\rangle$ are eigenstates of the atom's Hamiltonian $\mathcal{H}_a = \frac{p^2}{2m}$)

b) Evaluate the term $\langle a_n|\, \vec{\epsilon}_{k,\lambda}\cdot\vec{p}\,|a_m\rangle$ that you should have found in part a). Show also that $\langle a_n|\, \vec{\epsilon}_{k,\lambda}\cdot\vec{p}\,|a_n\rangle = 0$.
[Hint: express $\vec{p}$ in terms of the commutator of the atom's kinetic energy $\mathcal{H}_a$ and its position]

c) Show that under resonance between the atom's transitions and the photon frequency (that is, by setting $E_n - E_m = \hbar\omega_k$, where E_n's are the eigenvalues of the eigenstates $|a_n\rangle$) we can obtain the equivalence between the pseudo-momentum Hamiltonian $V = -\frac{e}{mc}\vec{A}\cdot\vec{p}$ and the dipolar Hamiltonian $V_L = -e\vec{r}\cdot\vec{E}$.
Notice that in the process we have also shown that the interaction has no diagonal elements.

Problem 2: Perturbation theory for Harmonic Oscillator

a) A particle of mass m and charge q oscillates in a one-dimensional harmonic potential (so that $\omega = \sqrt{k/m}$) and is subject to an electric field E. Calculate the energy shift caused by the electric field (on the oscillator energy) to the lowest non-vanishing order.

b) Consider now an harmonic oscillator with frequency $\omega = \sqrt{k/m}$ (where m is the mass of the oscillator). A small perturbing potential $V^{(1)} = \frac{1}{2}\delta kx^2$ is added to the main potential $V^0 = \frac{1}{2}kx^2$. Calculate the first and second order perturbations to the energy and compare the result with the exact result (which is trivial!)

Problem 3: Neutron scattering

A thermal neutron beam is scattered by a single, resting free nucleus of mass M. Derive an expression for the double-differential cross section by answering the following steps:

a) Write a formal expression for the *rate* of scattering and an explicit expression for the first non-zero order approximation.

b) What is the density of final states for the neutrons? What is the incoming flux? [Hint: Assume as usual a square cavity geometry]

c) Although the nuclear potential is complex and very strong, in the Fermi's approximation it can be written as $V(r) = \frac{2\pi\hbar^2}{m_n} b\,\delta(r)$. Explain briefly what is b and the validity of this approximation.

d) Using the result above, write an expression for the double-differential scattering cross section and express it in terms ofthe dynamic structure factor $S(Q,\omega)$, (where $Q = k_f - k_i$).

Problem 4: Incoherence in thermal neutron scattering

Consider first thermal neutrons scattering off hydrogen atoms. The bound coherence scattering length depends on the total spin of the system hydrogen+neutron. If the spins are aligned, $S = I + \frac{1}{2}$ we have the bound scattering length b^+ and b^- for $S = I - \frac{1}{2}$ instead.

a) Taking into account the multiplicity of spin states (the number of m_z states for a given total spin), calculate the average and second moment ($\langle b \rangle, \langle b^2 \rangle$) of the scattering length. What is the coherent and incoherent scattering length?

b) Consider isotope incoherence in thermal neutron scattering from a sample containing a variety of isotopic species of the same element. Each isotope has a different bound scattering length b_l and a fractional abundance c_l. What are the coherent and incoherent scattering lengths?

c) Consider now neutron scattering from a mixture of heavy and light water (H_2O and D_2O). Given the following values for the aligned and anti-aligned scattering lengths:

	$b_+(10^{-12}cm)$	$b_-(10^{-12}$ cm)
^{1}H	1.08	-4.74
^{2}D	0.95	0.10
^{16}O	0.5804	

what is the percentage (fractional abundance) of D_2O such that the coherent scattering cross section is zero?

Problem 5: Neutron scattering from molecular hydrogen

This problem is taken from Chen-Kotlarchyk (Interaction of photons and neutrons with matter). The objective of this problem is to calculate the total cross-section for the scattering of cold neutrons from molecular hydrogen in the gas phase under the assumption that intermolecular correlations can be neglected. Follow the steps below:

a) Define the scattering-length operator to be $b = A + B\vec{S}\cdot\vec{I}$, where $S = \frac{1}{2}$ and I denote spin operators for the neutron and a target nucleus, respectively. A and B are constants to be determined. Now introduce the total neutron-nucleus spin operator $\vec{J} = \vec{S} + \vec{I}$ (we indicate by lower cases their eigenvalues, e.g. the eigenvalue of I^2 is $i(i+1)$). Find an expression for the eigenvalues of $S \cdot I$ in terms of the eigenvalues of $\vec{J}$, $\vec{S}$ and $\vec{I}$.

b) By demanding that operator b has eigenvalue b_+ when $j = i + \frac{1}{2}$ and eigenvalue b_- when $j = i - \frac{1}{2}$, obtain the following values for the two constants:

$$A = \frac{i+1}{2i+1}b_+ + \frac{i}{2i+1}b_-, \qquad \text{and} \qquad B = \frac{2}{2i+1}(b_+ - b_-)$$

c) The differential cross-section for neutron scattering from molecular hydrogen, between an initial spin-state $|i\rangle$, and a final spin-state $|f\rangle$ of the molecule-neutron system, is

$$\left.\frac{d\,\sigma}{d\,\Omega}\right|_{i,f} = \frac{k'}{k}\left|\langle f|\sum_n b_n e^{i\vec{Q}\cdot\vec{r}_n}\,|i\rangle\right|^2$$

where the index $n = 1, 2$ runs over the two protons of the molecule. However, if one is interested in the scattering of cold neutrons (energy - 3 meV) , the wavelength (~ 5 Å) is large compared to the inter-proton separation of 0.74 Å in the hydrogen molecule, and one is justified in neglecting spatial interference effects due to the separation of the two protons. This means that the exponential factor appearing in the matrix element can simply be set to unity, $e^{i\vec{Q}\cdot\vec{r}_n} \approx 1$. Then, for a given initial state $|i\rangle$, the measured cross section is obtained by summing over the final states $|f\rangle$, and we can write

$$\left.\frac{d\,\sigma}{d\,\Omega}\right|_{i} = \frac{k'}{k}\,\langle i|\,(b_1+b_2)^\dagger(b_1+b_2)\,|i\rangle$$

The relevant initial state of the molecule-neutron system is $|i\rangle = |I, m_I\rangle\,|s, m_s\rangle$ where the first ket represents the total spin-state of the hydrogen molecule, $\vec{I} = \vec{I}_1 + \vec{I}_2$, which is the sum of the spin operators for the two protons. Show that

$$(b_1+b_2)^\dagger(b_1+b_2) = (2A + B\vec{s}\cdot\vec{I})^2 = 4A^2 + \left(4AB - \frac{B^2}{2}\right)\vec{s}\cdot\vec{I} + \frac{B^2}{4}I^2$$

[Hint: show first that $(\vec{s}\cdot\vec{I})^2 = \frac{I^2}{4} - \frac{1}{2}\vec{s}\cdot\vec{I}$]

d) For an unpolarized incident neutron beam, show that

$$\left.\frac{d\,\sigma}{d\,\Omega}\right|_{unpol} = \frac{k'}{k}\left[4A^2 + \frac{B^2}{4}I(I+1)\right]$$

e) There are two types of molecular hydrogen: When the two proton spins are parallel ($I = 1$), one has orthohydrogen; when the spins are anti-parallel ($I = 0$), one has parahydrogen. Show that

$$\left.\frac{d\,\sigma}{d\,\Omega}\right|_{ortho} = \frac{k'}{k}\left[\frac{1}{4}(3b_+ + b_-)^2 + \frac{1}{2}(b_+ - b_-)^2\right]$$

and

$$\left.\frac{d\,\sigma}{d\,\Omega}\right|_{para} = \frac{k'}{k}\left[\frac{1}{4}(3b_+ + b_-)^2\right]$$

f) Show that the total scattering cross-sections for the two types of molecular hydrogen are given by:

$$\sigma_{ortho} = \frac{4\pi}{9}\left[(3b_+ + b_-)^2 + 2(b_+ - b_-)^2\right]$$

$$\sigma_{para} = \frac{4\pi}{9}\left[(3b_+ + b_-)^2\right]$$

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