Quantum Physics III (8.06) — Spring 2016

Assignment 4

Readings

- Griffiths Chapter 10 on the adiabatic approximation

Problem Set 4

1. **Vibrational Modes of Carbon Dioxide (30 points)**

   This problem will consider the absorption of infrared radiation by CO_2. Carbon dioxide is a (nearly) linear molecule, and we will treat it as a collection of three point masses (at positions x_1, x_2, x_3) connected by springs each with spring constant k. We will make a somewhat less justifiable approximation as well by supposing that each atom has the same mass m. (This approximation simplifies the calculations while leaving the physics still qualitatively valid.)

spring constant		k		k	
	O	═══	C	═══	O
position	x_1		x_2		x_3
mass	m		m		m

   Thus the Hamiltonian is

   $$H_0 = \frac{{p_1}^2}{2m} + \frac{{p_2}^2}{2m} + \frac{{p_3}^2}{2m} + \frac{k}{2}(x_1 - x_2)^2 + \frac{k}{2}(x_2 - x_3)^2 \tag{1}$$

   We can also write $H_0 = T + V$, where

   $$T = \frac{{p_1}^2}{2m} + \frac{{p_2}^2}{2m} + \frac{{p_3}^2}{2m} \qquad \text{and} \qquad V = \frac{k}{2}(x_1 - x_2)^2 + \frac{k}{2}(x_2 - x_3)^2 \tag{2}$$

   Here all motion is in the $\hat{x}$ direction and p_1, p_2, p_3 and x_1, x_2, x_3 refer to the momenta and positions respectively of the three different atoms.

   (a) We can rewrite V in terms of a matrix K as

   $$V = \vec{x}^T K \vec{x} = \begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} K \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \quad \text{where} \quad K = \frac{k}{2} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

Diagonalize K. That is, find a diagonal matrix Λ (with $\Lambda_{11} \geq \Lambda_{22} \geq \Lambda_{33}$) and a rotation matrix R (i.e. $R^T R = I$) such that $K = R\Lambda R^T$. You may find it convenient to use a computer for this step; however, your answers should be exact (e.g. write $1/\sqrt{2}$ instead of $0.70711\ldots$). The columns of R are the eigenvectors of K, and are also called the normal modes. One of the eigenvalues of K is zero (so by our convention $\Lambda_{33} = 0$). What is the physical significance of this?

(b) Define normal mode displacement operators $\vec{y} = R^T \vec{x}$ (i.e. $y_i = \sum_{j=1}^{3} R_{ji} x_j$ for $i = 1, 2, 3$). Write V in terms of $\vec{y}$.

(c) Define normal mode momentum operators $\vec{\pi} = R^T \vec{p}$ (i.e. $\pi_i = \sum_{j=1}^{3} R_{ji} p_j$). Show that

$$[y_i, \pi_j] = i\hbar\delta_{i,j}.$$

Write T in terms of $\vec{\pi}$. [Hint: You may find it helpful to use the fact that $(R^T R)_{ij} = (RR^T)_{ij} = \delta_{ij}$.]

(d) You should now find that H_0 breaks up into three pieces that depend separately on π_1, y_1, on π_2, y_2, and on π_3. Show that the first two of these pieces are equivalent to harmonic oscillators and the third corresponds to a free particle. That is, find frequencies ω_1, ω_2 (in terms of k and m) and operators a_1, a_2 (in terms of $\vec{y}$, $\vec{\pi}$ and the other parameters) such that

$$H_0 = \hbar\omega_1 \left(a_1^\dagger a_1 + \frac{1}{2} \right) + \hbar\omega_2 \left(a_2^\dagger a_2 + \frac{1}{2} \right) + \frac{\pi_3^2}{2m}$$

and a_1, a_2 satisfy the commutation relations

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad \text{and} \qquad [a_1, a_2] = [a_1^\dagger, a_2^\dagger] = 0.$$

For the rest of the problem, we will work in the energy eigenbasis of H_0. This basis can be written $|n_1, n_2, \pi_3\rangle = |n_1\rangle \otimes |n_2\rangle \otimes |\pi_3\rangle$, where n_1, n_2, π_3 label eigenstates of $a_1^\dagger a_1$, $a_2^\dagger a_2, \pi_3$ respectively.

(e) We are now ready to add radiation. Unlike the most common gases in the atmosphere (N_2, O_2, Ar), CO_2 has covalent bounds that are weakly polar. This is because the oxygen atoms attract electrons more strongly than the carbon atom (i.e. have higher electronegativity). We model this by assuming that the oxygen atoms each have charge $-q$ and the carbon atom has charge $2q$. (The Coulomb interaction is effectively already included in (1) so there is no need to modify H_0.) Thus the dipole moment $\vec{d}$ is

$$\vec{d} = (-qx_1 + 2qx_2 - qx_3)\hat{x}.$$

Write $\vec{d}$ in terms of the $a_i, a_i^\dagger$ operators. If an oscillating electric field is applied, which mode, if any, will contribute to the absorption of light?

2. **Decay of the Three Dimensional Harmonic Oscillator (25 points)**

The object of this problem is to calculate the lifetime of a charged particle (charge q, mass m) in the first excited states of the three-dimensional harmonic oscillator (frequency ω). By analogy with the hydrogen atom, we refer to the states $|1,0,0\rangle, |0,1,0\rangle, |0,0,1\rangle$ as the $2p$ states, and we call the ground state $|0,0,0\rangle$ the $1s$ state. An alternate basis for the $2p$ states is given by eigenstates of L_z.

$$|m_\ell = 1\rangle = \frac{|1,0,0\rangle - i|0,1,0\rangle}{\sqrt{2}}$$
$$|m_\ell = 0\rangle = |0,0,1\rangle$$
$$|m_\ell = -1\rangle = \frac{|1,0,0\rangle + i|0,1,0\rangle}{\sqrt{2}}$$

a) Write down an expression for the transition rate per unit time, $\Gamma(2p \to 1s)$, for the particle to *spontaneously* emit electromagnetic radiation and make a transition to the ground state. Γ should depend on the frequency of the emitted light and on the matrix element of the operator $q\vec{r}$. *[Hint: Use the relation (from class and/or Griffiths) between the spontaneous emission rate and the absorption rate, for the appropriate frequency of radiation.]*

b) Show that the transition rate *is independent of* m_ℓ.

c) Finally, give a formula for $\Gamma(2p \to 1s)$ in terms of m, ω, q, and fundamental constants.

d) What is the relationship between the transition rate per unit time and the "lifetime" of the $2p$ state?

3. **Adiabatic Spin Rotation (20 points)**

Consider a spin one-half particle at rest, with its spin free to rotate in response to a time-dependent magnetic field. The Hamiltonian of the system is

$$H = -\frac{2\mu_0}{\hbar}\vec{S}\cdot\vec{B}(t)\ .$$

Assume $\mu_0 > 0$. We will start (at time $t = -T$) with a large magnetic field mostly in the $-\hat{z}$ direction which we will slowly decrease to zero and then increase in the opposite direction until time $t = T$. At the same time, we will assume that there is a constant small field in the $\hat{x}$-$\hat{y}$ plane. The magnetic field is then

$$\vec{B}(t) = (B_x, B_y, \gamma t) \qquad \text{for } -T \le t \le T.$$

Assume that $\gamma > 0$ and $\gamma T \gg \sqrt{B_x^2 + B_y^2}$; i.e. that for $t = \pm T$, the field is mostly in the $\pm\hat{z}$ direction. Denote the ground state at time t by $|\psi_+(t)\rangle$ and the excited state at time t by $|\psi_-(t)\rangle$. These correspond to spins that are either aligned or anti-aligned with the magnetic field. Suppose that at time $t = -T$, the spin is in state $|\psi_+(-T)\rangle$.

(a) Use the adiabatic theorem to show that the particle initially in the state $|\psi_+(-T)\rangle$ finishes in the state $|\psi_+(T)\rangle$ (up to an overall phase) with nearly unit probability, as long as B_x, B_y, γ are consistent with the adiabatic condition. What is the condition on the parameters of the problem for the adiabatic theorem to apply?

(b) Give conditions on B_x, B_y, γ such that $|\psi_+(-T)\rangle \approx |-\rangle$ and $|\psi_+(T)\rangle \approx |+\rangle$. In this case we will adiabatically convert the state from $\approx |-\rangle$ to $\approx |+\rangle$, assuming the adiabatic theorem applies. Explain why the condition here is compatible with the adiabatic condition you found in part (a).

(c) Now, instead of a time-varying magnetic field, consider a *spatially* varying magnetic field. We can use the adiabatic theorem to understand the magnetic traps used by MIT atomic physicists to trap very cold gases of *spin-polarized* atoms. Classically, the force on a dipole $\vec{\mu}$ from a magnetic field gradient is

$$\vec{F} = (\vec{\mu} \cdot \vec{\nabla})\vec{B}(x). \tag{3}$$

One can design magnetic field gradients such that an atom which has its spin antiparallel to the local magnetic field $\vec{B}(x)$ experiences a force toward the center of the trap. Those atoms with spins parallel to $\vec{B}(x)$ feel a force which expels them from the trap. This way, one can trap only atoms of one polarization state. But this raises a question: since $\vec{B}(x)$ varies in space, how can we ensure that the thermal movements of the atoms within the trap preserve the property that their spins are always anti-aligned with the local magnetic field? Assume that the atoms have mass m and temperature T, and state an inequality in terms of $m, k_B T, \mu_0, \vec{B}$ that must be satisfied for the adiabatic condition to be valid.

(d) Since it is magnetic *gradients* which exert the trapping forces, you might think that there would be no problem if at one point in the trap, $\vec{B} = 0$. In fact, this *does* cause problems, and the traps are designed to have $\vec{B} \neq 0$ everywhere. Explain why.

4. **Engineering Adiabatic Transitions (25 points)**

This problem is similar to the last one, except that now the particle has spin one, and therefore has three eigenstates $|+\rangle$, $|0\rangle$, and $|-\rangle$.

The Hamiltonian is given by

$$H = -\frac{2\mu_0}{\hbar}\vec{S} \cdot \vec{B}(t) - \frac{\Lambda}{\hbar^2}S_z^2 \ .$$

In the last term, $\Lambda > 0$, so that it favors the states $|\pm\rangle$ over the state $|0\rangle$.

(a) Write the operators S_x, S_y, and S_z for a spin-1 field in the $|+\rangle$, $|0\rangle$, and $|-\rangle$ basis. (You may write them from memory or your notes, or you can derive them.) Check that your matrices obey the correct angular momentum commutation relations.

(b) Suppose that the magnetic field has a small constant field in the x-direction and a large time-dependent field in the z-direction:

$$\vec{B}(t) = (B_x, 0, B_0 - \beta t) \ .$$

Assume the following hierarchy of energies:

$$\mu_0 B_0 \gg \Lambda \gg \mu_0 B_x \gg \hbar\beta/B_x \ .$$

Sketch the energy levels of this system as a function of time.

(c) Suppose the system starts out in the state $|-\rangle$ at $t = 0$. Show that upon assuming the hierarchy of energies above, this state evolves to a state that is approximately equal to $|0\rangle$ and then evolves to $|+\rangle$. Explain how you would alter the time dependence of $\vec{B}(t)$ in order that the initial state transforms into $|0\rangle$ at late times.

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