Quantum Physics III (8.06) — Spring 2018

Assignment 5

Posted:Friday, March 9, 2018

Readings and Announcements

- Time-dependent perturbation theory: Griffiths, Chapter 9.
- Cohen-Tannoudji, Chapter 13 and/or Shankar, Chapter 18.
- This week we have the library sessions of Wed. Mar. 14 and Thurs. Mar. 15 at 7pm.
- Read the term paper information to make sure you know what to expect. Start thinking about topics to work on.

1. Tunneling and the Stark Effect (15 points)

The Stark effect concerns the physics of an atom in an electric field. In this problem, you will explore the possibility that in an electric field the electron in an atomic bound state can tunnel out making the state unstable. We consider this effect in a simpler one-dimensional analog problem.

Suppose an electron is trapped in a one-dimensional square well of depth V_0 and width d:

$$V(x) = \begin{cases} -V_0 & \text{for } |x| < d/2 \\ 0 & \text{for } |x| \geq d/2 \end{cases} .$$

Suppose a weak constant electric field in the x-direction with strength $\mathcal{E}$ is turned on. That means the potential is changed as

$$V(x) \to V(x) - e\mathcal{E}x\,.$$

Assume throughout this problem that $e\mathcal{E}d \ll \hbar^2/2md^2 \ll V_0$.

(a) Set $\mathcal{E} = 0$ in this part of the problem. Estimate the ground state energy (i.e. the amount by which the ground state energy is above the bottom of the potential well) by pretending that the well is infinitely deep. (Because $\hbar^2/2md^2 \ll V_0$, this is a good approximation.) Use this estimate of the ground state energy in subsequent parts of the problem. Note that the true ground state energy is lower than what you've estimated, why?

(b) Sketch the potential with $\mathcal{E} \neq 0$ and explain why the ground state of the $\mathcal{E} = 0$ potential is no longer stable when $\mathcal{E} \neq 0$.

(c) Use the semiclassical approximation to calculate the barrier penetration factor for the ground state. [You should use the fact that $e\mathcal{E}d \ll \hbar^2/2md^2$ to simplify this part of the problem.]

(d) Use classical arguments to convert the barrier penetration factor into an estimate of the lifetime of the bound state.

(e) Now, let's put in numbers that are characteristic of an atomic system. Calculate the lifetime for $V_0 = 20$ eV, $d = 2 \times 10^{-8}$ cm and an electric field of 7×10^4 V/cm. Compare the lifetime you estimate to the age of the universe.

(f) Show that the lifetime goes like $\exp(1/\mathcal{E})$, and explain why this result means that this "instability" could not be obtained in any finite order of perturbation theory, treating $\mathcal{E}$ as a perturbation to the Hamiltonian.

2. **A Time-Dependent Two-State System (15 points)**

Consider a two-state system with Hamiltonian

$$H(t) = \begin{pmatrix} +E & v(t) \\ v(t) & -E \end{pmatrix}$$

where $v(t)$ is real and $\int_{-\infty}^{\infty} |v(t)|$ is finite. We will label the states as

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1}$$

(a) Suppose that at $t = -\infty$ the system is in the state $|2\rangle$. Use time-dependent perturbation theory to determine the probability that at $t = +\infty$ the system is in the state $|1\rangle$, to lowest order in v.

(b) If $E = 0$, the eigenstates of $H(t)$ can be chosen to be independent of t. Use this fact to calculate the probability of a transition from $|2\rangle$ to $|1\rangle$ *exactly*, in this case. What is the result obtained from time-dependent perturbation theory in this case? What is the condition that the perturbative result is a good approximation to the exact result?

In both parts, your answers can be left in terms of integrals involving $v(t)$.

3. **Atom and photon (15 points)** Model an atom as a two-level system with ground state $|g\rangle$ and excited state $|e\rangle$ and energy splitting $\hbar\omega_a$. Suppose it interacts with an electromagnetic field of frequency ω_p, which we model as a harmonic oscillator. Without interactions the Hamiltonian would be

$$\begin{aligned} H_0 &= \frac{\hbar\omega_a}{2} \left(|e\rangle\langle e| - |g\rangle\langle g| \right) \otimes I + \hbar\omega_p \, I \otimes \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \\ &= \frac{\hbar\omega_a}{2} \, \sigma_z \otimes I + \hbar\omega_p \, I \otimes \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \end{aligned}$$

Since the electric field strength is proportional to $\hat{a}+\hat{a}^\dagger$, we can model an atom-photon interaction by

$$\delta H = \alpha\left(|g\rangle\langle e| + |e\rangle\langle g|\right) \otimes \left(\hat{a}+\hat{a}^\dagger\right)$$

for some constant α.

(a) In the rotating frame, we have $\widetilde{\delta H}(t) = e^{iH_0 t/\hbar}\,\delta H\, e^{-iH_0 t/\hbar}$. Compute $\widetilde{\delta H}(t)$.

(b) Set $\omega_a = \omega_p \equiv \omega$. Compute $\int_0^t dt' \widetilde{\delta H}(t')$. If $t \gg 1/\omega$, then which terms can we neglect? [Hint: You should be left with one term that can be interpreted as absorption and another that can be interpreted as spontaneous/stimulated emission.]

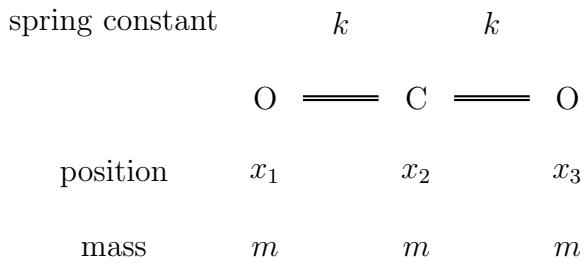
4. **Gaussian pulse (10 points)** Let H_0 be a Hamiltonian with spectrum and energies given by $H_0|n\rangle = E_n|n\rangle$ for $n = 0, 1, 2, \ldots$. Suppose we apply a perturbation

$$\delta H(t) = \frac{\exp\left(-\frac{t^2}{2\tau^2}\right)}{\sqrt{2\pi\tau^2}}\,\hat{V}$$

where $\hat{V}$ is an arbitrary time-independent Hermitian operator and $\tau > 0$ is a constant with units of time. If our system starts in state $|0\rangle$ at time $-\infty$, using first-order time-dependent perturbation theory, what is the probability that our system is in state $|n\rangle$ at time ∞? What happens in the limits $\tau \to 0$ and $\tau \to \infty$? You should express your answers in terms of the matrix elements $V_{mn} \equiv \langle m|\hat{V}|n\rangle$.

5. **Vibrational Modes of Carbon Dioxide (25 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.)



Thus the Hamiltonian is

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

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

$$T = \frac{{p_1}^2}{2m} + \frac{{p_2}^2}{2m} + \frac{{p_3}^2}{2m} \qquad \text{and} \qquad V = \frac{k}{2}(x_1 - x_2)^2 + \frac{k}{2}(x_2 - x_3)^2 \tag{3}$$

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 $a_1^\dagger a_1$, $a_2^\dagger a_2$, π_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 (2) 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?

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