22.51 Quantum Theory of Radiation Interactions

Final Exam - Solutions
Tuesday December 15, 2009

Problem 1 Harmonic oscillator *20 points*

Consider an harmonic oscillator described by the Hamiltonian $\mathcal{H} = \hbar\omega(\hat{N} + \frac{1}{2})$. Calculate the evolution of the expectation value of the position of the harmonic oscillator $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$ in the following cases:

a) The harmonic oscillator is initially prepared in a superposition of *number* states:

$$|\psi(t = 0)\rangle = c_a|2\rangle + c_b|3\rangle$$

where c_a, c_b are coefficients such that the state is normalized (here for example take $c_a = \cos(\vartheta/2)$ and $c_b = e^{i\varphi}\sin(\vartheta/2)$)
We can use the Schrödinger picture to find the evolution of the state:

$$|\psi(t)\rangle = \cos(\vartheta/2)e^{-i2\omega t}|2\rangle + e^{i\varphi}\sin(\vartheta/2)e^{-i3\omega t}|3\rangle$$

(Notice that I've already eliminated the common phase factor $e^{-i\frac{1}{2}\omega t}$). Then we can calculate the expectation value of x:

$$\langle x(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\cos(\vartheta/2)e^{i2\omega t}\langle 2| + e^{-i\varphi}\sin(\vartheta/2)e^{i3\omega t}\langle 3|\right)(a + a^\dagger)\left(\cos(\vartheta/2)e^{-i2\omega t}|2\rangle + e^{i\varphi}\sin(\vartheta/2)e^{-i3\omega t}|3\rangle\right)$$

Only the terms $\langle 2|a|3\rangle = \sqrt{3}$ and $\langle 3|a^\dagger|2\rangle = \sqrt{3}$ survive, yielding

$$\langle x(t)\rangle = \sqrt{\frac{3\hbar}{2m\omega}}\sin(\vartheta)\cos(\omega t - \varphi)$$

It could have been maybe simpler to use the Heiseberg picture, remembering that $a(t) = a(0)e^{-i\omega t}$. Then:

$$\langle x(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\cos(\vartheta/2)\langle 2| + e^{-i\varphi}\sin(\vartheta/2)\langle 3|\right)(ae^{-i\omega t} + a^\dagger e^{i\omega t})\left(\cos(\vartheta/2)|2\rangle + e^{i\varphi}\sin(\vartheta/2)|3\rangle\right)$$

and the same result as above is directly obtained.

b) The initial state of the harmonic oscillator is a superposition of *coherent* states:

$$|\psi(t = 0)\rangle = c_a|\alpha\rangle + c_b|\beta\rangle$$

where c_a, c_b are coefficients such that the state is normalized.
In this case it is convenient to use the Heisenberg picture:

$$\langle x(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}(c_a^*\langle\alpha| + c_b^*\langle\beta|)(ae^{-i\omega t} + a^\dagger e^{i\omega t})(c_a|\alpha\rangle + c_b|\beta\rangle)$$

The important point here was to remember that although the coherent states are normalized, they are not orthogonal, thus $\langle\alpha|\beta\rangle \neq 0$, but

$$\langle\alpha|\beta\rangle = O_{\alpha,\beta} = e^{-(|\alpha|^2+|\beta|^2-2\alpha^*\beta)/2}$$

We then have

$$\langle x(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(|c_a|^2(\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}) + |c_b|^2(\beta e^{-i\omega t} + \beta^* e^{i\omega t}) + c_a^* c_b(\alpha^* e^{i\omega t} + \beta e^{-i\omega t})O_{\alpha,\beta} + c_a c_b^*(\alpha e^{-i\omega t} + \beta^* e^{i\omega t})O_{\alpha,\beta}^*\right)$$

c) Would the choice $c_a = \cos(\vartheta/2)$ and $c_b = e^{i\varphi}\sin(\vartheta/2)$ normalize the above state?
With the above choice

$$\langle\psi|\psi\rangle = \cos(\vartheta/2)^2 + \sin(\vartheta/2)^2 + \sin(\vartheta/2)\cos(\vartheta/2)\left(O_{\alpha,\beta}e^{i\varphi} + O_{\alpha,\beta}^* e^{-i\varphi}\right) = 1 + \sin(\vartheta)e^{-(|\alpha|^2+|\beta|^2)/2}Re[e^{\alpha^*\beta}e^{i\varphi}] \neq 1$$

Problem 2 Coupling of a spin to an harmonic oscillator *20 points*

Consider the system in figure 1. A cantilever with a magnetic tip is positioned closed to a spin-$\frac{1}{2}$ (of gyromagnetic ratio γ) in a strong external magnetic field B along the z-direction. The magnetic tip creates a magnetic gradient G_z such that the field felt by the spin depends on the position of the tip itself, $B_{tot} = B + G_z z$. In the limit of small displacements, the cantilever can be modeled as an harmonic oscillator of mass m, oscillating along the z direction at its natural frequency ω_c.

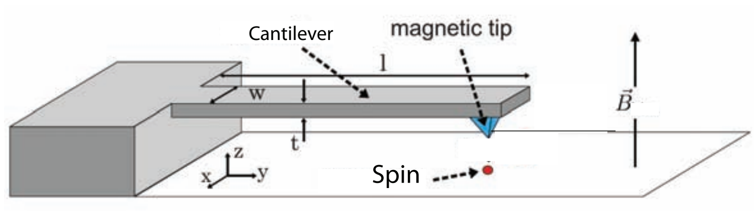

Figure 1: A cantilever coupled to a spin. Adapted from P. Rabl, P. Cappellaro, M.V. Gurudev Dutt, L. Jiang, J.R. Maze, and M.D. Lukin, "Strong magnetic coupling between an electronic spin qubit and a mechanical resonator", Phys. Rev. B 79, 041302 R 02 (2009)

a) What is the total Hamiltonian of the system (spin+harmonic oscillator)?

$$\mathcal{H}_{spin} = \hbar\gamma B S_z = \frac{1}{2}\hbar\gamma B\sigma_z = \frac{1}{2}\hbar\omega\sigma_z$$

$$\mathcal{H}_{h.o.} = \hbar\omega_c(\hat{n} + \frac{1}{2})$$

The coupling between the cantilever and the spin is given by the extra field $G_z z(t)$ acting on the spin:

$$V = \hbar\gamma G_z z S_z = \hbar\gamma G_z \frac{\sigma_z}{2}\sqrt{\frac{\hbar}{2m\omega_c}}(a + a^\dagger) = \hbar\frac{\lambda}{2}\sigma_z(a + a^\dagger)$$

with $\lambda = \gamma G_z\sqrt{\frac{\hbar^3}{2m\omega_c}}$. The total Hamiltonian is thus

$$\mathcal{H}_{tot} = \mathcal{H}_0 + V = \frac{1}{2}\hbar\omega\sigma_z + \hbar\omega_c(\hat{n} + \frac{1}{2}) + \hbar\frac{\lambda}{2}\sigma_z(a + a^\dagger)$$

b) The magnetic gradient is usually small, thus the coupling term between the spin and the harmonic oscillator can be considered a small perturbation. Use perturbation theory to calculate the energy and eigenstates to the lowest non-vanishing order.

The eigenstatates of $\mathcal{H}_0$ are eigenstates of the σ_z and $\hat{n}$ operators:

$$|\psi_{0,n}^{(0)}\rangle = |0\rangle|n\rangle, \quad |\psi_{1,n}^{(0)}\rangle = |1\rangle|n\rangle$$

with energies:

$$E_{0,n}^{(0)} = -\frac{1}{2}\hbar\omega + \hbar\omega_c(n + \frac{1}{2}), \quad E_{1,n}^{(0)} = \frac{1}{2}\hbar\omega + \hbar\omega_c(n + \frac{1}{2})$$

The first order correction is calculated as $\Delta^{(1)} = \langle\psi_k^0|V|\psi_k^0\rangle$. Here:

$$\Delta_{0,n}^{(1)} = \hbar\frac{\lambda}{2}\langle 0|\langle n|[\sigma_z(a + a^\dagger)]|0\rangle|n\rangle = 0$$

and $\Delta_{1,n}^{(1)} = 0$ as well. Thus we need to calculate the second order energy shift. First we calculate the first order eigenstates.

$$|\psi_{0,n}^{(1)}\rangle = \sum_{m\neq n}\frac{\langle 0,m|V|0,n\rangle|0,m\rangle}{E_{0,n}^{(0)} - E_{0,m}^{(0)}} + \sum_m \frac{\langle 1,m|V|0,n\rangle|1,m\rangle}{E_{0,n}^{(0)} - E_{1,m}^{(0)}}$$

$$= \sum_{m\neq n}\frac{\lambda\langle 0|\sigma_z|0\rangle\langle m|(a + a^\dagger)|n\rangle}{2\omega_c(n-m)}|0,m\rangle + \sum_m \frac{\lambda\langle 1|\sigma_z/2|0\rangle\langle m|(a + a^\dagger)|n\rangle}{E_{0,n}^{(0)} - E_{1,m}^{(0)}}|1,m\rangle$$

finally,

$$|\psi_{0,n}^{(1)}\rangle = \frac{\lambda}{\omega_c}\left(\sqrt{n}|0,n-1\rangle - \sqrt{n+1}|0,n+1\rangle\right)$$

Similarly, we obtain

$$|\psi_{1,n}^{(1)}\rangle = -\frac{\lambda}{\omega_c}\left(\sqrt{n}|1,n-1\rangle - \sqrt{n+1}|1,n+1\rangle\right)$$

The second order energy shift can be calculated from $\Delta^2 = \langle\psi_k^0|V|\psi_k^1\rangle$:

$$\Delta_{0,n}^2 = \frac{\lambda^2}{2\omega}[n-(n+1)] = -\frac{\lambda^2}{2\omega}$$

Problem 3 Time-dependent perturbation theory: harmonic perturbation *35 points*

Use time-dependent perturbation theory to derive the transition rate for a perturbation Hamiltonian $V(t) = V_0\cos(\omega t)$. You can use the following steps:

a) The unperturbed Hamiltonian is $\mathcal{H}_0$, with eigenvectors and eigenvalues: $\mathcal{H}_0|k\rangle = \hbar\omega_k|k\rangle$. In the interaction picture defined by $\mathcal{H}_0$, the state evolves under the propagator $U_I(t)$: $|\psi(t)\rangle_I = U_I(t)|\psi(0)\rangle$). What is the differential equation describing the evolution of $U_I(t)$?

$$i\hbar\frac{dU_I}{dt} = V_I(t)U_I(t)$$

with $V_I(t) = e^{i\mathcal{H}_0 t}V(t)e^{-i\mathcal{H}_0 t}$.

b) Write an expansion for $U_I(t)$ to first order (Dyson series) .
Integrating the equation above:

$$U_I(t) = \mathbb{1} - \frac{i}{\hbar}\int_0^t dt' V_I(t')$$

c) Calculate the transition amplitude $c_{ki}(t) = \langle k|U_I(t)|i\rangle$ from the initial state $|i\rangle$ to the eigenstate $|k\rangle$ to first order, as a function of $\omega_{ki} = \omega_k - \omega_i$, $V_{ki} = \langle k|V_0|i\rangle$ and ω. Hint: the following integral might be useful:

$$\int_0^t dt' e^{i\omega_1 t'}e^{\pm i\omega_2 t'} = 2e^{i(\omega_1\pm\omega_2)t/2}\frac{\sin\left((\omega_1\pm\omega_2)t/2\right)}{\omega_1\pm\omega_2}$$

From the expression in b) and the definition of V_I:

$$c_{ki}(t) = \langle k|U_I(t)|i\rangle = \delta_{ik} - \frac{i}{\hbar}\int_0^t dt'\langle k|V_I(t')|i\rangle = \delta_{ik} - \frac{i}{\hbar}\int_0^t dt'\langle k|V(t')|i\rangle e^{i(\omega_k-\omega_i)}$$

Taking $k = i$ we have:

$$c_{ki}(t) = -\frac{i}{\hbar}\int_0^t dt'\langle k|V_I(t')|i\rangle = -\frac{i}{\hbar}\langle k|V_0|i\rangle\int_0^t dt'\cos(\omega t)e^{-i(\omega_i-\omega_k)}$$

Setting $\omega_{ki} = \omega_k - \omega_i$ and using the given formula, we have:

$$c_{ki}(t) = -\frac{iV_{ki}}{\hbar}\left[e^{i(\omega_{ki}+\omega)t/2}\frac{\sin\left((\omega_{ki}+\omega)t/2\right)}{\omega_{ki}+\omega} + e^{i(\omega_{ki}-\omega)t/2}\frac{\sin\left((\omega_{ki}-\omega)t/2\right)}{\omega_{ki}-\omega}\right]$$

d) Calculate the probability of transition $p_{ki}(t) = |c_{ki}(t)|^2$ in the long time limit, with the following approximations:

$$\lim_{t\to\infty}\frac{\sin^2(\Omega t/2)}{\Omega^2} = \frac{\pi}{2}t\delta(\Omega)$$

and

$$\lim_{t\to\infty}\frac{\sin(\Omega_1 t/2)\sin(\Omega_2 t/2)}{\Omega_1\Omega_2} = 0$$

(for $\Omega_1 = \Omega_2$)
The probability $p_{ki}(t) = |c_{ki}(t)|^2$ will have contributions from terms like

$$\left| e^{i(\omega_{ki}+\omega)t/2} \frac{\sin((\omega_{ki}+\omega)t/2)}{\omega_{ki}+\omega} \right|^2$$

and

$$\left(e^{i(\omega_{ki}+\omega)t/2} \frac{\sin((\omega_{ki}+\omega)t/2)}{\omega_{ki}+\omega} \right) \left(e^{i(\omega_{ki}-\omega)t/2} \frac{\sin((\omega_{ki}-\omega)t/2)}{\omega_{ki}-\omega} \right)^*$$

This last term goes to zero by the second relationship provided, while the first terms give:

$$p_{ik} = \frac{\pi |V_{ik}|^2}{2\hbar^2} t \left[\delta(\omega_{ki}+\omega) + \delta(\omega_{ki}-\omega) \right]$$

e) Finally, you should write down the transition rate $W_{ik} = \frac{dp_{ik}}{dt}$. The transition rate is just the probability per time:

$$W_{ik} = \frac{\pi |V_{ik}|^2}{2\hbar^2} \left[\delta(\omega_{ki}+\omega) + \delta(\omega_{ki}-\omega) \right]$$

Problem 4 Rayleigh light scattering *35 points*

Consider the elastic scattering of light from a molecule in the atmosphere. We want to calculate the frequency dependence of the cross-section, to understand why the sky is blue and the sunset is red.
The system of interest is described by a molecule, with eigenstates $|m_k\rangle$ and energies $\mathcal{E}_k$ and two modes of the radiation field, k and k' with energies $\hbar\omega_k$ and $\hbar\omega'_k$ and polarizations λ and λ'. For convenience the system is enclosed in a cavity of volume $V = L^3$. The interaction between the radiation field and the molecule is describe by the hamiltonian $\mathcal{V} = -\vec{d} \cdot \vec{E}$ in the dipole approximation, where

$$\vec{E} = \sum_{h,\xi} \sqrt{\frac{2\pi\hbar\omega_h}{V}} \left(a_{h\xi} e^{i\vec{h}\cdot\vec{R}} + a^\dagger_{h\xi} e^{-i\vec{h}\cdot\vec{R}} \right) \vec{\epsilon}_{h\xi}$$

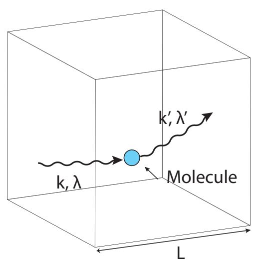

Figure 2: Rayleigh scattering, showing the incoming and outgoing photon into the volume of interest.

with R is the position of the center of mass of the molecule.
You can use the following steps to calculate the scattering cross section $d\sigma = \frac{W_{fi}}{\Phi_{inc}}$, with $W_{fi} = \frac{2\pi}{\hbar} |\langle f|T|i\rangle|^2 \rho(E_f)$, where T is the transition matrix and $\rho(E_f)$ the final density of states.

a) Write a formal expression for the transition matrix element $\langle f|T|i\rangle$, to the lowest non-zero order in the perturbation $\mathcal{V}$.

$$\langle f|T|i\rangle = \langle f|\mathcal{V}|i\rangle + \sum_l \frac{\langle f|\mathcal{V}|l\rangle\langle l|\mathcal{V}|i\rangle}{E_i - E_l} + \dots$$

As $\mathcal{V}$ does not allow transitions involving two photons, the first order term is zero and we have:

$$\langle f|T|i\rangle = \sum_l \frac{\langle f|\mathcal{V}|l\rangle\langle l|\mathcal{V}|i\rangle}{E_i - E_l}$$

b) What are the possible intermediate (virtual) states that we need to consider in this scattering process? Use them to simplify the expression in a). The initial state is $|m_i, 1_{k,l\lambda}, 0_{k',\lambda'}\rangle$ and final state $|m_i, 0_{k,l\lambda}, 1_{k',\lambda'}\rangle$. Intermediate states are such that there is only 1-photon transition, either $|m_l, 0_{k,l\lambda}, 0_{k',\lambda'}\rangle$ or $|m_l, 1_{k,l\lambda}, 1_{k',\lambda'}\rangle$. Thus:

$$\langle f|T|i\rangle = \sum_l \frac{\langle m_f, 0_{k,l\lambda}, 1_{k',\lambda'}|\mathcal{V}|m_l, 0_{k,l\lambda}, 0_{k',\lambda'}\rangle\langle m_l, 0_{k,l\lambda}, 0_{k',\lambda'}|\mathcal{V}|m_i, 1_{k,l\lambda}, 0_{k',\lambda'}\rangle}{(\mathcal{E}_i + \hbar\omega_k) - \mathcal{E}_l}$$

$$+ \sum_l \frac{\langle m_f, 0_{k,l\lambda}, 1_{k',\lambda'}|\mathcal{V}|m_l, 1_{k,l\lambda}, 1_{k',\lambda'}\rangle\langle m_l, 1_{k,l\lambda}, 1_{k',\lambda'}|\mathcal{V}|m_i, 1_{k,l\lambda}, 0_{k',\lambda'}\rangle}{(\mathcal{E}_i + \hbar\omega_k) - (\mathcal{E}_l + \hbar\omega_k + \hbar\omega'_k)}$$

Using the explicit expression for $\mathcal{V}$, we have:

$$\langle f|T|i\rangle = \frac{2\pi\hbar}{V}\sqrt{\omega_k\omega_k'}e^{i(k-k)\cdot R}\sum_l \left(\frac{(\vec{\epsilon}_k'\cdot\vec{d}_{fl})(\vec{\epsilon}_k\cdot\vec{d}_{li})}{\mathcal{E}_i-\mathcal{E}_l+\hbar\omega_k}+\frac{(\vec{\epsilon}_k\cdot\vec{d}_{fl})(\vec{\epsilon}_k'\cdot\vec{d}_{li})}{\mathcal{E}_i-\mathcal{E}_l-\hbar\omega_k'}\right)$$

c) What is the flux of incoming photons and the density of states of the outgoing photons?

$$\Phi_{inc} = c/L^3$$

and

$$\rho(E_f) = \left(\frac{L}{2\pi}\right)^3\frac{\omega_k^2}{\hbar c^3}d\Omega$$

d) Find an expression for the differential cross section $\frac{d\sigma}{d\Omega}$ (where $d\Omega$ is the solid angle into which the photon is scattered)
From $d\sigma = \frac{W_{fi}}{\Phi_{inc}} = \frac{2\pi}{\hbar}\frac{|\langle f|T|i\rangle|^2}{\Phi_i nc}\rho(E_f)$ we find:

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar}\frac{L^3}{c}\left(\frac{L}{2\pi}\right)^3\frac{\omega_k^2}{\hbar c^3}\frac{4\pi^2\hbar^2}{L^6}(\omega_k\omega_{k'})\left|\frac{(\vec{\epsilon}_{k'}\cdot\vec{d}_{fl})(\vec{\epsilon}_k\cdot\vec{d}_{li})}{\mathcal{E}_i-\mathcal{E}_l+\hbar\omega_k}+\frac{(\vec{\epsilon}_k\cdot\vec{d}_{fl})(\vec{\epsilon}_{k'}\cdot\vec{d}_{li})}{\mathcal{E}_i-\mathcal{E}_l-\hbar\omega_{k'}}\right|^2$$

simplifying the expression:

$$\frac{d\sigma}{d\Omega} = \frac{\omega_k^3\omega_{k'}}{c^4}\left|\frac{(\vec{\epsilon}_{k'}\cdot\vec{d}_{fl})(\vec{\epsilon}_k\cdot\vec{d}_{li})}{\mathcal{E}_i-\mathcal{E}_l+\hbar\omega_k}+\frac{(\vec{\epsilon}_k\cdot\vec{d}_{fl})(\vec{\epsilon}_{k'}\cdot\vec{d}_{li})}{\mathcal{E}_i-\mathcal{E}_l-\hbar\omega_{k'}}\right|^2$$

e) In the case of elastic scattering $|m_f\rangle = |m_i\rangle$ and $\omega_k = \omega_k'$. What is the scattering cross-section dependence on the photon frequency ω_k? How does that help explaining why the sky is blue and the sunset red?
We can further simplify the cross section to

$$\frac{d\sigma}{d\Omega} = \frac{\omega_k^4}{c^4}\left|\frac{2(\vec{\epsilon}_{k'}\cdot\vec{d}_{il})(\vec{\epsilon}_k\cdot\vec{d}_{li})(\mathcal{E}_i-\mathcal{E}_l)}{(\mathcal{E}_i-\mathcal{E}_l)^2-(\hbar\omega_k)^2}\right|^2$$

As $(\mathcal{E}_i-\mathcal{E}_l)\gg\hbar\omega_k$, the cross section depends on the frequency as ω_k^4, thus blue light is scattered more than red light, giving the color of the sky.

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