CH651 Assignment 3, Monday, December 1, 2014. Due Monday December 8, 2014

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Q1 Consider the time evolution of a spin state of an electron in a magnetic field. Let the unperturbed hamiltonian be the Zeeman hamiltonian (with static field B_0 taken in the z direction): $H_0 = \gamma B_0 \hat{S}_z$, where γ is the gyromagnetic ratio and $\hat{S}_z$ is the usual spin operator. Let the coupling hamiltonian be a time varying Zeeman interaction in the x direction, $V = \gamma B_1 \hat{S}_x \cos \omega t$, where B_1 is the strength of the perturbing magnetic field and ω is it's frequency.

(i) If the electron is initially in spin state α at $t = 0$, what is the probability of ending up in state in state β as a function of time t? Take $\omega = \gamma B_0$, and use first order perturbation theory.

(ii) How does the answer to part (i) change when second order perturbation theory is used?

(iii) Now lets solve the time-dependent Schrödinger equation exactly for the same problem. To do this, first write down the coupled equations for the coefficients C_α and C_β associated with the states α and β, respectively. Now take the same limit $\omega = \gamma B_0$ in these equations. Carefully consider the time dependence of each term and neglect all terms that vary as $\exp[\pm 2i\omega t]$ in the resulting differential equations. Show that the solutions are the same as those obtained from perturbation theory (taking $\omega = \gamma B_0$) in the limit of small B_1.

Q2 Consider a system of two spin-1/2 particles so that the zero order hamiltonian just contains the kinetic energy due to their spin angular momentum so $\hat{H}_0 = \hat{S}_1^2 + \hat{S}_2^2$. Suppose that in the absence of a magnetic field the two spins interact weakly (small λ) according to a spin vector dot product coupling term $V = \lambda \mathbf{S}_1 \cdot \mathbf{S}_2$ so the total hamiltonian is $H = H_0 + V$. Suppose the coupled system starts out in $|s_1, m_1, s_2, m_2\rangle = |\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\rangle$ at $t = 0$. Use first order time dependent perturbation to compute the probability that the system is in state $|s_1, m_1, s_2, m_2\rangle = |\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\rangle$ at time t. (Hint: compute the vector dot product using angular momentum raising and lowering operators.)

Q3 (i) For classical correlation functions show that $\langle \ddot{A}(t)B(0)\rangle\rangle = -\langle \dot{A}(t)\dot{B}(0)\rangle$ and more generally that $\langle A^{(2n)}(t)B(0)\rangle = (-1)^n \langle A^{(n)}(t)B^{(n)}(0)\rangle$, where $A^{(n)}$ denotes the n-th time derivative.

(ii) For a classical harmonic oscillator whose position and momentum are x and p define the complex amplitude $a(t) = x(t)+(i/(m\omega))p(t)$ so that $x = (1/2)(a+a^*)$ and $p = -(im\omega/2)(a-a^*)$. The classical quantities a and a^* evolve according to $\dot{a} = -i\omega a$ and $\dot{a}^* = i\omega a^*$. Show that for a harmonic oscillator at thermal equilibrium $\langle a^2\rangle = \langle (a^*)^2\rangle = 0$ and $\langle |a|^2\rangle = 2k_bT/(m\omega^2)$.

Use these results to compute classical position correlation function of a harmonic oscillator, $\langle x(t)x(0)\rangle$.

(iii) For the real and imaginary part of the quantum time correlation function

$$C^+_{AB} = C_{AB}(t) + C^*_{AB}(t) = 2\mathrm{Re}C_{AB}(t)$$
$$C^-_{AB} = C_{AB}(t) - C^*_{AB}(t) = 2i\mathrm{Im}C_{AB}(t)$$

Show that $C^+_{AB}(-t) = C^+_{BA}(t)$ and $C^-_{AB}(-t) = -C^-_{BA}(t)$ and that

$$C^+_{AB}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} C^+_{AB}(t) = \tilde{C}_{AB}(\omega) + \tilde{C}_{BA}(-\omega)$$

and $C^-_{AB}(\omega) = \tilde{C}_{AB}(\omega) - \tilde{C}_{BA}(-\omega)$

Q4 (i) The general solutions of the normal mode equations of motion for the harmonic bath are

$$u_j(t) = u_j(0)\cos(\omega_j t) + \omega_j^{-1}\dot{u}_j(0)\sin(\omega_j t)$$
$$\dot{u}_j(t) = -\omega_j u_j(0)\sin(\omega_j t) + \dot{u}_j(0)\cos(\omega_j t)$$

In class we showed that the normal mode positions, u_k, and velocities, $\dot{u}_k$, of a classical thermal harmonic bath satisfy the following thermal equilibrium results $\langle u_k u_{k'}\rangle = (k_B T/\omega_k^2)\delta_{kk'}$ and $\langle \dot{u}_k \dot{u}_{k'}\rangle = k_B T \delta_{kk'}$. (a) Show that these results hold in general at time t and for example $\omega_j^2\langle u_j(t) u_{j'}(t)\rangle = \langle \dot{u}_j(t)\dot{u}_{j'}(t)\rangle = k_B T\delta_{j,j'}$. (b) Using the above results compute the velocity correlation function for classical bath harmonic oscillators, $\langle \dot{u}_j(0)\dot{u}_{j'}(t)\rangle$

(ii) Using harmonic oscillator raising and lowering operators and thermal equilibrium results for quantum harmonic oscillators obtain an expression for the quantum analogue of the result you derived above i.e. $\langle \dot{u}_j(0)\dot{u}_{j'}(t)\rangle_Q$

Q5 (i) For the quantum bath operator $\hat{A} = \sum_j c_j \hat{u}_j$ (where the c_j are constants) use the results obtained in class to express the Fourier transform of the quantum time correlation function $C_{AA}(t)$ *i.e.* $\int_{-\infty}^{\infty} dt e^{i\omega t} C_{AA}(t)$ in terms of the spectral density $J(\omega)$.

(ii) Show that $\int_{-\infty}^{\infty} dt e^{i\omega t} C_{AA}(t) = e^{\beta\hbar\omega}\int_{-\infty}^{\infty} dt e^{i\omega t} C_{AA}(-t) = e^{\beta\hbar\omega}\int_{-\infty}^{\infty} dt e^{-i\omega t} C_{AA}(t)$