Quantum theory of condensed matter II

Mesoscopic physics (Quantum transport)

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S	neet 8		

1. Relaxation and dephasing times of the spin boson model

Consider now the spin boson model as a specific example of the generic system-bath model introduced in the previous exercise sheet:

$$\hat{H}_{S} = \epsilon_{g}|g\rangle\langle g| + \epsilon_{e}|e\rangle\langle e| \tag{1}$$

$$\hat{H}_{B} = \sum_{i} \hbar\omega_{i} \left(\frac{1}{2} + \hat{b}_{i}^{\dagger}\hat{b}_{i}\right)$$

$$\hat{H}_{S-B} = \gamma \sum_{i} \left(|g\rangle\langle e| + |e\rangle\langle g|\right) \left(\hat{b}_{i}^{\dagger} + \hat{b}_{i}\right)$$

where $|g\rangle$ ($|e\rangle$) is the vector of the ground (excited) state of a two level system. The latter is coupled to a bosonic bath generated by the set of operators $\{\hat{b}_i^{\dagger}\}$.

1. By following the same steps described in the previous exercise sheet, derive the equation of motion for the reduced density matrix of the two level system to lowest non vanishing perturbative order in the coupling constant γ . Take as initial condition for the bosonic bath the thermal distribution $\hat{\rho}_{\rm B}(0) = \exp(-\beta \hat{H}_{\rm B})/\mathcal{Z}$, where $\beta = (k_{\rm B}T)^{-1}$ is the inverse temperature and $\mathcal{Z} = \text{Tr}_{\rm B} \{\exp(-\beta \hat{H}_{\rm B})\}$ is the canonical partition function for the bath. Prove that the equation of motion for the reduced density operator written in the Schrödinger picture, can be recast into the form:

$$\dot{\hat{\rho}}_{\rm red}(t) = -\frac{i}{\hbar} [\hat{H}_{\rm S}, \hat{\rho}_{\rm red}(t)] + \int_0^t \mathrm{d}t' \mathcal{K}(t-t') [\hat{\rho}_{\rm red}(t')], \qquad (2)$$

where the propagation kernel \mathcal{K} reads:

$$\mathcal{K}(t-t')[\hat{\rho}_{\rm red}(t')] = -\frac{1}{\hbar^2} \operatorname{Tr}_{\rm B}\left\{ \left[\hat{H}_{\rm S-B,I}(t'-t), \hat{U}_{\rm S}^{\dagger}(t'-t)\hat{\rho}_{\rm red}(t')\hat{U}_{\rm S}(t'-t)\otimes\hat{\rho}_{\rm B}(0) \right] \right\}$$
(3)

and $\hat{U}_{\mathrm{S}}(t) := e^{-\frac{i}{\hbar}\hat{H}_{\mathrm{S}}t}$. (2 Points))

2. Prove the following relation:

$$\operatorname{Tr}_{B}\left\{\hat{H}_{S-B}\hat{H}_{S-B,I}(t'-t)\hat{O}_{S}\otimes\hat{\rho}_{B}(0)\right\} = \gamma^{2}\left\{|g\rangle\!\langle g|\hat{O}_{S}e^{-\frac{i}{\hbar}\Delta(t-t')} + |e\rangle\!\langle e|\hat{O}_{S}(t')e^{+\frac{i}{\hbar}\Delta(t-t')}\right\}C(t-t')$$

$$\tag{4}$$

where $\hat{O}_{\rm S}$ is a generic system operator, $\Delta = \epsilon_{\rm e} - \epsilon_{\rm g}$ is the Bohr frequency and the correlator C(t - t') reads:

$$C(t - t') = \sum_{j} \left[n_{\rm B}(\omega_j) e^{-i\omega_j(t - t')} + (1 + n_{\rm B}(\omega_j)) e^{i\omega_j(t - t')} \right]$$

with $n_{\rm B}(\omega) := (e^{\beta \hbar \omega} - 1)^{-1}$ being the Bose function.

(2 Points)

3. Prove that in the limit $\Gamma = \frac{2\pi}{\hbar}\gamma^2 D \ll (\hbar\beta)^{-1}$, where $D = J(\Delta)$ is the bosonic density of states calculated at the Bohr frequency $\Delta = \epsilon_e - \epsilon_g$, the generalized master equation (GME) given in Eq. (2) can be approximated by:

$$\dot{\hat{\rho}}_{\rm red}(t) = -\frac{i}{\hbar} [\hat{H}_{\rm S}, \hat{\rho}_{\rm red}(t)] + \int_0^\infty \mathrm{d}t' \mathcal{K}(t') [\hat{\rho}_{\rm red}(t)], \tag{5}$$

known as the Markov approximation of the GME.

Hint: Start by proving the decaying behaviour of the propagation kernel \mathcal{K} on the time scale $\hbar\beta$. Assume for definiteness a density of states $J(\omega) = \alpha \omega$ and a cut-off frequency ω_c .

4. Calculate explicitly the equation of motion of for the matrix elements of the reduced density matrix. Neglect for simplicity the imaginary components of the propagation kernel \mathcal{K} . You should obtain:

$$\dot{\rho}_{\rm gg} = -\dot{\rho}_{\rm ee} = -\Gamma n_{\rm B}(\Delta)\rho_{\rm gg} + \Gamma [1 + n_{\rm B}(\Delta)]\rho_{\rm ee}, \qquad (6)$$
$$\dot{\rho}_{\rm eg} = \dot{\rho}_{\rm ge}^* = -i\frac{\Delta}{\hbar}\rho_{\rm eg} - \frac{\Gamma}{2}[2n_{\rm B}(\Delta) + 1](\rho_{\rm eg} - \rho_{\rm ge}).$$

(2 Points)

where $n_{\rm B}(\Delta) = (e^{\beta\Delta} - 1)^{-1}$ is the Bose function calculated at the system Bohr frequency. (4 Points)

- 5. Calculate the stationary solution $\hat{\rho}_{\text{red}}^{\infty}$ for the reduced density operator. In particular prove that the coherences vanish, when $\hat{\rho}_{\text{red}}^{\infty}$ is written in the energy eigenbasis for the system. Prove moreover that $\rho_{\text{ee}}^{\infty}/\rho_{\text{gg}}^{\infty} = e^{-\beta\Delta}$. Comment on this result.
- 6. Prove that the populations of $\hat{\rho}_{red}$ written in the energy eigenbasis approach the stationary solution according to:

$$\rho_{\rm ii}(t) = \rho_{\rm ii}(0)e^{-t/\tau_{\rm rel}} + \rho_{\rm ii}^{\infty}(1 - e^{-t/\tau_{\rm rel}}) \qquad {\rm i = g, e}$$

where $\tau_{\rm rel} = [\Gamma \coth(\beta \frac{\Delta}{2})]^{-1}$

7. Prove that if $\Delta/\hbar > \frac{1}{2\tau_{\rm rel}}$ the coherences oscillate and decay exponentially on the time scale $\tau_{\rm deph} = 2\tau_{\rm rel}$. How does the coherences dynamics changes if $\Delta/\hbar > \frac{1}{2\tau_{\rm rel}}$? (2 Points)

Frohes Schaffen!