Universität Regensburg Wintersemester 10-11

Density Matrix Theory

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Sheet 9

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1. Real time dynamics of a q-bit coupled to an external bath

Consider the spin boson Hamiltonian:

$$H = H_{\rm S} + H_{\rm S-B} + H_{\rm B} \tag{1}$$

where

$$\begin{aligned} H_{\rm S} &= -\frac{\hbar}{2}(\epsilon\sigma_z + \Delta\sigma_x), \\ H_{\rm S-B} &= \frac{1}{2}\sigma_z \sum_\alpha \hbar\nu_\alpha(b_\alpha^\dagger + b_\alpha) + \Delta V, \\ H_{\rm B} &= \sum_\alpha \hbar\omega_\alpha b_\alpha^\dagger b_\alpha. \end{aligned}$$

The stochastic properties of H are characterized by the spectral density $G(\omega) \equiv \sum_\alpha \nu_\alpha^2 \delta(\omega - \omega_\alpha)$.

1. Prove that the transformation to the energy eigenbasis of $H_{\rm S}$ can be written as a rotation

$$\begin{aligned} |1\rangle &= \cos\frac{\theta}{2}|\uparrow\rangle - \sin\frac{\theta}{2}|\downarrow\rangle \\ |2\rangle &= \sin\frac{\theta}{2}|\uparrow\rangle + \cos\frac{\theta}{2}|\downarrow\rangle \end{aligned}$$

   where $|1\rangle$, $|2\rangle$ are the energy eigenstates. Determine θ as a function of ϵ and Δ.

2. Prove that the Hamiltonian (1), in the basis that diagonalizes $H_{\rm S}$ reads:

$$H = -\frac{\hbar}{2}\Delta_b\sigma_z' + \frac{1}{2}\Big(\frac{\epsilon}{\Delta_b}\sigma_z' - \frac{\Delta}{\Delta_b}\sigma_x'\Big)\sum_\alpha \hbar\nu_\alpha(b_\alpha^\dagger + d_\alpha) + \Delta V + H_{\rm B}$$

   where $\Delta_b = \sqrt{\epsilon^2 + \Delta^2}$.

3. Using the general expression for the time evolution of the two level system coupled to a bath derived in the lecture prove that (neglecting the Lamb shift):

$$\begin{aligned} \rho_{\uparrow\uparrow}(t) = \cos\theta\Big[e^{-\Gamma_{rel}t}(\rho_{11}(0) - \rho_{11}(\infty)) + \rho_{11}(\infty)\Big] + \sin^2\frac{\theta}{2} \\ + \sin\theta e^{-\Gamma_\phi t}\Big[{\rm Re}\Big(\rho_{12}(0)\Big)\cos(\Delta_b t) + {\rm Im}\Big(\rho_{12}(0)\Big)\sin(\Delta_b t)\Big] \end{aligned}$$

   where $\rho_{11}(\infty) = e^{-\beta E_1}/Z$ represent the thermodynamic limit and the relaxation and dephasing rates Γ_{rel} and Γ_ϕ read respectively

$$\begin{aligned} \Gamma_{rel} &= \frac{\pi}{2}\frac{\Delta^2}{\Delta_b^2}[G(-\Delta_b)N(-\Delta_b) + G(\Delta_b)N(\Delta_b)] \\ \Gamma_\phi &= \frac{\Gamma_{rel}}{2} + \frac{\epsilon^2}{\Delta_b^2}\pi\lim_{\omega\to 0} G(\omega)\coth\Big(\frac{\beta\hbar\omega}{2}\Big) \end{aligned}$$

   where $N(\omega) = \coth\left(\frac{\beta\hbar\omega}{2}\right) + 1$.

4. The system-bath coupling is proportional to σ_z. The expectation value of the generalized dimensionless system coordinates reads correspondingly $\langle\tilde{Q}\rangle = \rho_{\uparrow\uparrow} - \rho_{\downarrow\downarrow}$. Calculate the time evolution of $\langle\tilde{Q}\rangle$ for the initial condition $\hat{\rho}(0) = |\uparrow\rangle\langle\uparrow|$. Prove that the result is:

$$\langle\tilde{Q}\rangle(t) = \left[\frac{\epsilon^2}{\Delta_b^2} - \langle\tilde{Q}\rangle(\infty)\right] e^{-\Gamma_{rel} t} + \langle\tilde{Q}\rangle(\infty) + \frac{\Delta^2}{\Delta_b^2} e^{-\Gamma_\phi t} \cos(\Delta_b t)$$

where $\langle\tilde{Q}\rangle(\infty)$ is the expectation value of $\tilde{Q}$ at equilibrium and can be obtained from the thermodynamic limit $\rho_{ii} = \frac{e^{-\beta E_i}}{Z}$ where $i = 1, 2$ label the energy eigenvalues of the system Hamiltonian.

2. Free propagator and classical action

Consider the propagator $K(x_f t, x_i t_0)$ defined as by the relation:

$$K(x_f t, x_i t_0) \equiv \langle x_f | U(t, t_0) | x_i \rangle$$

as the matrix representation in space of the time evolutor $U(tt_0)$ associated to the Schrödinger equation.

1. Prove that the propagator for the free particle can be written in the form:

$$K(x_f t, x_i t_0) = \sqrt{\frac{m}{2\pi\hbar i(t - t_0)}} \exp\left(\frac{i}{\hbar} \frac{m(x_f - x_i)^2}{2(t - t_0)}\right)$$

Hint: Use the fact that the Hamiltonian H for the free particle is time independent to get a simple expression of the propagator in terms of H. Simplify the expression of the propagator by making use of the completeness relation $\mathbf{1} = \sum_n |\phi_n\rangle\langle\phi_n|$ where $|\phi_n\rangle$ is a set of complete eigenstates of the Hamiltonian.

2. Prove that the quantum propagator introduced in the previous point can be written also in terms of the classical action:

$$K(x_f t, x_i t_0) = \sqrt{\frac{m}{2\pi\hbar i(t - t_0)}} \exp\left(\frac{i}{\hbar} S_{\text{cl}}\right)$$

where S_{cl} is the action functional of the classical path x_{cl}.

Hint: Start by proving that the classical path for a free particle can be parametrized with time as:

$$x_{\text{cl}}(s) = x_i + \frac{x_f - x_i}{t - t_0}(s - t_0)$$

and remember the definition of action S of the path x

$$S[x] = \int_{t_0}^{t} \mathrm{d}s \left(\frac{m\dot{x}^2}{2} - V(x)\right)$$

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Frohes Schaffen!