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Thermodynamics of dissipative two-level system: A perturbation approach based on unitary transformation

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Abstract

The thermodynamics of a dissipative two-level system is studied by means of the perturbation approach based on a unitary transformation. Both the Ohmic and non-Ohmic dissipative heat-bath are treated. Analytical results for entropy, specific heat, and static susceptibility are obtained for the scaling limit $\Delta/\omega_c \ll 1$ as well as the general $0 < \Delta/\omega_c < 1$ case. For the sub-Ohmic bath the transition between the delocalized and localized phase is discussed. Our approach is quite simple and yet it gives correct thermodynamics for the lower-temperature region and weak coupling case.

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1. Introduction

During the past two decades the low-temperature properties of a two-level system coupled to a heat-bath (spin–boson model, SBM) have attracted considerable attention, since it provides a universal model for numerous physical and chemical processes [1,2], such as defect-tunnelling in solids [3], the exciton excitation coupled to phonons in quantum dots [4], and the macroscopic quantum coherence experiment in SQUID's [5]. The Hamiltonian of SBM is

$$H = -\frac{1}{2}\Delta\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \frac{1}{2}\sum_k g_k\left(b_k^\dagger + b_k\right)\sigma_z, \tag{1}$$

here $b_k^\dagger$ (b_k) is the creation (annihilation) operator of boson mode with frequency ω_k, σ_x and σ_z are Pauli matrices to describe the two-level system. Δ is the bare tunnelling amplitude and g_k the coupling constant. The heat-bath is characterized by its spectral density [1,2]

$$\sum_k g_k^2 \delta(\omega - \omega_k) = 2\alpha_s \omega_c^{1-s} \omega^s \theta(\omega_c - \omega), \tag{2}$$

where α_s is the dimensionless coupling constant and $\theta(x)$ is the usual step function. In this Letter we consider in general $s > 0$ spectra. Usually, $s = 1$ is called Ohmic bath, $s > 1$ the super-Ohmic one, while $0 < s < 1$ the sub-Ohmic one.

The Hamiltonian (1) seems quite simple. However, it cannot be solved exactly and various approximate analytical and numerical methods have been used [1–20]. The dynamics of SBM as a function of the coupling α_s has been the subject of extensive studies and the main theoretical interest is to understand how the environment influences the dynamics of the two-level system and, in particular, how dissipation destroys quantum coherence. Although the thermodynamical properties of SBM should be also of interests, as far as we know, previous detailed studies of the thermodynamics of SBM are not so much. The path integral method was used by Goerlich and Weiss [21] to calculate the partition function of the dissipative two-state system for both Ohmic and non-Ohmic dissipation. But, generally speaking the results from path integral method are restricted

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to small tunnelling $\Delta/\omega_c \ll 1$. The numerical renormalization group with a fermionic bath was used by Costi [22] to study SBM with Ohmic dissipation. The Bethe-ansatz method was used by Costi and Zarand [23] to determine the entropy, the specific heat and the static susceptibility as functions of the temperature. This method is valid only for $s = 1$, since it depends on the mapping between Kondo model and SBM. Besides, since the bosonization technique is used to map Kondo model to SBM [23], the equivalence between SBM and Kondo model is rigorous only in the limit where the momentum cutoff $1/a$ goes to infinity. This is equivalent to $\omega_c \to \infty$ in this work. This is to say that, away from the scaling limit and when $0 < \Delta < \omega_c$, the equivalence between SBM and Kondo model is approximately and one can expect some deviation of the properties of SBM from those of Kondo model. Very recently, the numerical renormalization group for a bosonic bath was used by Bulla et al. to study SBM with Ohmic as well as non-Ohmic spectra [18].

If the tunnelling term in (1), $-\frac{1}{2}\Delta\sigma_x$, is substituted by $-\frac{1}{2}\epsilon\sigma_z$, the model becomes the two-level (with level difference ϵ) independent boson model [24] which can be solved exactly. The physical difference between the two models is the following: The spin–boson coupling in SBM (the third term in (1)) describes a transition between two eigen-states of $-\frac{1}{2}\Delta\sigma_x$ (the first term in (1)), but in independent boson model the fermion–boson interaction is on the level.

In this Letter we study the thermodynamics of dissipative SBM with a $s > 0$ spectral density. We present a new analytical approach [20] based on the unitary transformation method and the perturbation theory for calculating the thermodynamic quantities of SBM. Usually, people believe that perturbation approach is not good for dissipative SBM because of the infrared divergence in calculating the renormalized tunnelling frequency and other physical quantities by perturbation expansion. Here we try to get rid of the divergence by using a unitary transformation. This approach works well for the low-temperature region and weak coupling case with $0 < \Delta < \omega_c$. Throughout this Letter we set $\hbar = 1$ and $k_B = 1$.

2. Unitary transformation

Here we present a treatment using a unitary transformation. The transformation, which is defined as $H' = \exp(S)H \times \exp(-S)$, is applied to H and its aim is to take into account the correlation between the spin and bosons. We propose the following form for the generator:

$$S = \sum_k \frac{g_k}{2\omega_k}\xi_k\left(b_k^\dagger - b_k\right)\sigma_z. \tag{3}$$

Here, we introduce in S a k-dependent function ξ_k and its form will be determined later. Performing the transformation one gets the result

$$H' = H_0' + H_1' + H_2', \tag{4}$$

$$H_0' = -\frac{1}{2}\eta\Delta\sigma_x + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k}\xi_k(2-\xi_k), \tag{5}$$

$$\begin{aligned} H_1' = {} & \frac{1}{2}\sum_k g_k(1-\xi_k)\left(b_k^\dagger + b_k\right)\sigma_z \\ & - \frac{1}{2}\eta\Delta i\sigma_y \sum_k \frac{g_k}{\omega_k}\xi_k\left(b_k^\dagger - b_k\right), \end{aligned} \tag{6}$$

$$\begin{aligned} H_2' = {} & -\frac{1}{2}\Delta\sigma_x\left(\cosh\left\{\sum_k \frac{g_k}{\omega_k}\xi_k\left(b_k^\dagger - b_k\right)\right\} - \eta\right) \\ & - \frac{1}{2}\Delta i\sigma_y\left(\sinh\left\{\sum_k \frac{g_k}{\omega_k}\xi_k\left(b_k^\dagger - b_k\right)\right\}\right. \\ & \left. - \eta\sum_k \frac{g_k}{\omega_k}\xi_k\left(b_k^\dagger - b_k\right)\right), \end{aligned} \tag{7}$$

where the renormalization of the tunnelling term is

$$\eta = \exp\left[-\sum_k \frac{g_k^2}{2\omega_k^2}\xi_k^2 \coth\left(\frac{\omega_k}{2T}\right)\right]. \tag{8}$$

H_0' is now the unperturbed part of H' and, obviously it can be solved exactly since the spin and bosons are decoupled. The eigenstate of H_0' is a direct product: $|s\rangle|\{n_k\}\rangle$, where $|s\rangle$ is the eigenstate of σ_x: $|s_1\rangle = \frac{1}{\sqrt{2}}\binom{1}{1}$ or $|s_2\rangle = \frac{1}{\sqrt{2}}\binom{1}{-1}$, and $|\{n_k\}\rangle$ is the eigenstate of bosons with n_k bosons for mode k. In particular, $|\{0_k\}\rangle$ is the vacuum state in which $n_k = 0$ for every k. The ground state of H_0' is

$$|g_0\rangle = |s_1\rangle\left|\{0_k\}\right\rangle. \tag{9}$$

H_1' and H_2' are treated as a perturbation and they should be as small as possible. For this purpose ξ_k is determined as

$$\xi_k = \frac{\omega_k}{\omega_k + \eta_0\Delta}, \tag{10}$$

where $\eta_0 = \eta(T=0)$. Note that $0 \leqslant \xi_k \leqslant 1$ measures the intensity of the spin–boson coupling: $\xi_k \sim 1$ if the boson frequency ω_k is larger than the renormalized tunnelling $\eta_0\Delta$; but $\xi_k \ll 1$ for $\omega_k \ll \eta_0\Delta$. Since the transformation generated by S is a displacement one, physically, one can see that high-frequency bosons ($\omega_k > \eta_0\Delta$) follow the tunnelling particle adiabatically because the displacement is $g_k\xi_k/\omega_k \sim g_k/\omega_k$. However, bosons of low-frequency modes $\omega_k < \eta_0\Delta$ in general are not always in equilibrium with the tunnelling particle, and hence the particle moves in a retarded potential arising due to the low-frequency modes. When the non-adiabatic effect dominates, $\omega_k \ll \eta_0\Delta$, the displacement $\xi_k \ll 1$. Because of this definition for ξ_k we have

$$H_1' = \frac{1}{2}\eta_0\Delta\sum_k \frac{g_k}{\omega_k}\xi_k\left[b_k^\dagger(\sigma_z - i\sigma_y) + b_k(\sigma_z + i\sigma_y)\right], \tag{11}$$

when $T = 0$, and $H_1'|g_0\rangle = 0$. This is essential in our approach. By choosing the form of ξ_k (Eq. (10)) and η (Eq. (8)) it is possible to treat H_1' and H_2' as perturbation because of the following reason. If we treat the coupling term in the original Hamiltonian H as the perturbation, the dimensionless expanding parameter is g_k^2/ω_k^2. For Ohmic bath $s = 1$ it is $2\alpha_1/\omega$ which is logarithmic divergent in the infrared limit. But for the coupling in transformed Hamiltonian, H_1', the expanding parameter is