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A note on localized transition in the spin-boson model by variational calculation*

Chen Zhi-De(陈芝得)† and Hou Zhi-Lan(侯志兰)

Department of Physics, Jinan University, Guangzhou 510632, *China*

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We present mathematical analyses of the evolution of solutions of the self-consistent equation derived from variational calculations based on the displaced-oscillator-state and the displaced-squeezed-state in spin-boson model at a zero temperature and a finite temperature. It is shown that, for a given spectral function defined as $J(\omega) = \pi \sum_k c_k^2 = \frac{\pi}{2}\alpha\omega^s\omega_c^{1-s}$, there exists a universal s_c for both kinds of variational schemes, the localized transition happens only for $s \leq s_c$, moreover, the localized transition is discontinuous for $s < s_c$ while a continuous transition always occurs when $s = s_c$. At $T = 0$, we have $s_c = 1$, while for $T \neq 0$, $s_c = 2$ which indicates that the localized transition in super-Ohmic case still exists, manifesting that the result is in discrepancy with the existing result.

Keywords: spin-boson model, localized transition, variational calculation
PACC: 7335C, 7215R, 0570F

1. Introduction

The spin-boson model is an important toy model in dissipative quantum systems. The influence of environmental dissipation on the coherence of a two-state-system has been an important subject in condensed matter physics.[1,2] Although the Hamiltonian of the model looks simple, it is now known that even the solution for a single mode case cannot be found analytically. One important issue in this model is the phonon-induced localization(also called the localized transition), a topic which has been studied by using various methods over decades.[1−17] Such a localized transition due to the dissipation in spin-boson model is considered as a special class of quantum phase transition called boundary phase transition,[18] and it also has a classical correspondence, i.e. an Ising model with a long-range interaction.[6,10] However, recently it has been shown that such a quantum-classical mapping fails for a sub-Ohmic bath with $s < 1/2$,[13] where s is the bath parameter given in the spectral function(see the definition given below). Variational calculation is an important tool in dealing with the localized transition in spin-boson model. Recently variational calculation at a finite temperature has raised a lot of interest. The localized transition at a finite temperature shows a more complicated behaviour than that at a zero-temperature.[5,14,16,17] Variational calculation at $T = 0$ shows that the Ohmic bath with $s = 1$ is the boundary of the transition, i.e. the localized transition is discontinuous for a sub-Ohmic bath with $0 < s < 1$ and no transition for a super-Ohmic bath with $s > 1$.[1,2,4,14] Variational calculation at a finite temperature predicts a discontinuous transition for an Ohmic bath,[16] showing that $s = 1$ is not the boundary at $T \neq 0$. It is not yet clear whether there is a boundary of transition in variational calculation at $T \neq 0$, while it is known that, by mapping spin-boson model to a long-range Ising model, there appears no transition for the super-Ohmic bath with $s > 1$.[1,2,6,10] In the present paper, we present mathematical analyses of the self-consistent equation derived from variational schemes, separately, at $T = 0$ and $T \neq 0$ to see how the transition behaviour depends on the bath parameter s. There are mainly two kinds of variational schemes for spin-boson model, one is based on the displaced-oscillator-state (DOS)[4,5,12,14,17] and the other is based on the displaced-squeezed state (DSS).[7−9] The later one is specially suitable for the so-called strong coupling regime and the solution in this case was found to be dependent on the density of states of the bath as well, leading to a question on the universality.[9] It has been known that the transition points are different for two kinds of variational

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†Corresponding author. E-mail: tzhidech@jnu.edu.cn

calculations.[4,9] In the present paper, it will be shown that a universal s_c exists for both kinds of variational calculations, the localized transition predicted by the variational calculation is discontinuous for $s < s_c$, no transition is found for $s > s_c$ and a continuous transition always occurs at $s = s_c$. It turns out that $s_c = 1$ at $T = 0$ and $s_c = 2$ at $T \neq 0$. The rest of the present paper is organized as follows. The model and the derivation of the self-consistent equation by variational calculation are presented in Section 2. In Section 3 we present the mathematical analysis of the evolution of the solutions of the self-consistent equation to show how the localized transition depends on the bath parameter s. Conclusions and discussion are given in the final section.

2. The model and the self-consistent equation

The Hamiltonian of the spin-boson model is given by (setting $\hbar = 1$)[1,2]

$$\hat{H} = -\frac{\Delta_0}{2}\hat{\sigma}_x + \sum_k \hat{b}_k^\dagger \hat{b}_k \omega_k + \hat{\sigma}_z \sum_k c_k(\hat{b}_k^\dagger + \hat{b}_k), \quad (1)$$

where $\hat{\sigma}_i (i = x, y, z)$ is the Pauli matrix, $\hat{b}_k(\hat{b}_k^\dagger)$ is the annihilation(creation) operator of the kth phonon mode with energy ω_k, and c_k is the coupling parameter. The bath spectral function(density) is defined as[1,2]

$$\begin{aligned} J(\omega) =& \pi \sum_k c_k^2 \delta(\omega - \omega_k) \\ =& \frac{\pi}{2}\alpha\omega^s/\omega_c^{s-1}, \qquad 0 < \omega \leq \omega_c, \end{aligned} \quad (2)$$

where ω_c is the cut-off frequency and α is a dimensionless coupling strength which characterizes the dissipation strength. Parameter s is the bath parameter that specifies the property of the bath: $s = 1$ represents the Ohmic bath, $0 < s < 1$ and $s > 1$ are for the sub-Ohmic both and the super-Ohmic bath respectively.

The variational calculation starts from the trial ground state, for the variational scheme based on the DOS, the trial ground state is[4]

$$|\Phi_v\rangle = \frac{1}{\sqrt{2}}(|\phi_+\rangle|\uparrow\rangle + |\phi_-\rangle|\downarrow\rangle), \quad (3)$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of $\hat{\sigma}_z$ and

$$|\phi_\pm\rangle = \exp\{\mp \sum_k g_k\ (\hat{b}_k - \hat{b}_k^\dagger)\}|0\rangle \quad (4)$$

are the DOS of the bath with g_k as a variational parameter. On the other hand, trial ground state for the variational scheme based on the DSS is[7]

$$|\Psi_v\rangle = \frac{1}{\sqrt{2}}(|\psi_+\rangle|\uparrow\rangle + |\psi_-\rangle|\downarrow\rangle), \quad (5)$$

where

$$\begin{aligned} |\psi_\pm\rangle =& \exp\Big\{ \mp \sum_k \frac{c_k}{\omega_k}\ (\hat{b}_k - \hat{b}_k^\dagger)\Big\} \\ & \times \exp\Big\{ -\sum_k \gamma_k(\hat{b}_k^2 - \hat{b}_k^{\dagger 2})\Big\}|0\rangle \end{aligned} \quad (6)$$

are the DSS of the bath and γ_k is the variational parameter. Using the trial ground states given above, on the one hand, at $T = 0$ one can find out the ground state energy $E_0 = \langle\Phi_v|\hat{H}|\Phi_v\rangle$ (or $E_0 = \langle\Psi_v|\hat{H}|\Psi_v\rangle$), then the variational parameter is determined by the variational condition[4,12,17]

$$\frac{\delta E_0}{\delta g_k} = 0, \quad \text{or} \quad \frac{\delta E_0}{\delta \gamma_k} = 0. \quad (7)$$

On the other hand, at $T \neq 0$ the upper bound on free energy of the system can be found by using the Bogoliubov's theorem,[5,14] and the variational parameters are determined by minimizing the upper bound on free energy A_B, i.e.

$$\frac{\delta A_B}{\delta g_k} = 0, \quad \text{or} \quad \frac{\delta A_B}{\delta \gamma_k} = 0. \quad (8)$$

Usually the variational condition (7) or (8) can lead to a self-consistent equation of the dressing factor K defined as

$$K = \frac{\Delta}{\Delta_0}, \quad (9)$$

where Δ is the tunnelling splitting in the presence of dissipation. The self-consistent equation has the form

$$\begin{aligned} K &= f(K, T, \alpha, s) \\ &= \exp\Big\{ -\alpha \int_0^{\omega_c} \omega^s \omega_c^{1-s} G(K, T, \omega)\mathrm{d}\omega \Big\}, \end{aligned} \quad (10)$$

where $G(K, T, \omega)$ is variational-scheme-dependent, for the variational scheme based on DOS, it is found that[14]

$$\begin{aligned} & G_1(K, T, \omega) \\ &= \frac{\coth(\beta\omega/2)}{[\omega + K\Delta_0 \coth(\beta\omega/2)\tanh(\beta K\Delta_0/2)]^2}, \end{aligned} \quad (11)$$

which reduces to the well-known result at $T = 0$, viz $G_1(K, T = 0, \omega) = (\omega + K\Delta_0)^{-2}$, while for variational scheme based on DSS, we have

$$G_2(K, T, \omega)$$

$$= \frac{\coth(\beta\omega/2)}{\sqrt{\omega^4 + K\Delta_0 \coth(\beta\omega/2)\tanh(\beta K\Delta_0/2)g(\omega)}}, \quad (12)$$

where $g(\omega) = 2\omega^{s-n+2}\omega_c^{n+1-s}$, n comes from the density of states of the bath, defined by $\rho(\omega) = \omega^{n-1}/\omega_c^n$, and n can be considered as a dimension degree of the bath in the long-wavelength approximation.[9] For both kinds of variational schemes, it can be found that

$$\lim_{K\to\infty} f(K,T,\alpha,s) \to 1, \quad (13)$$

and

$$\frac{\partial f(K,T,\alpha,s)}{\partial K} > 0, \quad \text{for} \quad K > 0 \quad (14)$$

indicating that $f(K,T,\alpha,s)$ is a monotonically ascending and bounded function of K for $K \in [0,\infty)$.

Variational calculations determine the localized transition by examining the evolution of solutions of the self-consistent equation(10).[17] The trivial solution $K = 0$ and non-zero solution $K \neq 0$ represent respectively the localized phase and the delocalized phase. Usually the self-consistent equation has both trivial and non-zero solutions when α is small (see the detail given below), and when α increases to some critical value α_c, the only solution is a trivial solution when $\alpha > \alpha_c$, accordingly the localized transition happens at $\alpha = \alpha_c$. It should be noted that, for a discontinuous transition, the evolution of the solutions can be more complicated as can be seen from Ref.[17].

3. Mathematical analysis on the self-consistent equation

In the following, we shall present mathematical analysis on the self-consistent equation to see how the localized transition depends on the parameter s. If the localized transition exists, the self-consistent equation must have trivial and non-zero solutions, which is the essential condition for a localized transition. For a given set of parameters (T_0, α_0, s_0), geometrically the solutions of the self-consistent equation are the cross-points of curve $y = F(x) \equiv f(x, T_0, \alpha_0, s_0)$ and a line $y = x$, consequently the essential condition for the self-consistent equation having a trivial solution is

$$f(K = 0, T, \alpha, s) = 0. \quad (15)$$

On the other hand, since $f(K,T,\alpha,s)$ is a bounded function of K and $y = x$ is unbounded for $x \to \infty$, the essential condition for the existence of non-zero solution is

$$f(K,T,\alpha,s) > K, \quad \text{for some} \quad K \in (0,1]. \quad (16)$$

It can be seen that $f(K,T,\alpha,s)$ is a continuous function of both α and K and we have $\lim_{\alpha\to 0} f(K,T,\alpha,s) \to 1$, which implies that condition (16) can always be satisfied for $\alpha \ll 1$ and $K \ll 1$. On the other hand, condition (15) means that the integral in the exponent given in Eq.(10) should be divergent as $K \to 0$. It is well known that the integrand has an infrared divergence, i.e. as $\omega \to 0$,[1)]

$$\lim_{\omega\to 0}\lim_{K\to 0} \omega^s G_{1,2}(K,T,\omega) \propto \begin{cases} \omega^{s-3}, & T \neq 0, \\ \omega^{s-2}, & T = 0, \end{cases} \quad (17)$$

from which one can see that condition (15) leads to

$$s \leq s_c, \qquad s_c = \begin{cases} 2, & T \neq 0, \\ 1, & T = 0. \end{cases} \quad (18)$$

This result indicates that, at $T = 0$, variational calculation predicts the localized transition for both Ohmic bath and sub-Ohmic bath, however, at $T \neq 0$, we have the localized transition for sub-Ohmic bath, Ohmic bath, and super-Ohmic bath as well. Numerical solution of self-consistent equation (10) confirms the above conclusion.

Now we turn to see the influence of s on the nature of the localized transition by variational calculation. The conclusion is that a continuous transition can be found only when $s = s_c$ and all the predicted transitions are discontinuous for $0 < s < s_c$. The order parameter of the localized transition is K, when the value of α approaches the critical point α_c, if the non-zero solution decreases continuously to zero, the transition is continuous, on the other hand, if the non-zero solution disappears suddenly, the transition is discontinuous.[17] In the following, we shall show that the transition behaviour depends on f' defined as

$$f' \equiv \lim_{K\to 0} \frac{\partial f(K,T,\alpha,s)}{\partial K}\bigg|_{\alpha<\alpha_c}, \quad (19)$$

for $f' > 1$, the transition is continuous, while for $f' < 1$, the transition is discontinuous. The different transition behaviours come from the fact that the number of non-zero solutions of the self-consistent equation is even in the case of $f' < 1$ but odd in the case of $f' > 1$. As shown in Fig.1(a), starting from the trivial solution, the curve $y = F(x)$ lies

[1)] For finding the limitation of $G_2(K,T,\omega)$, we have employed the condition for variational calculation based on DSS,[9] $1 \leq s - n + 1 < 2$.

below the line $y = x$ at the beginning in the case of $f' < 1$. Since we have non-zero cross-points for $\alpha < \alpha_c$, $F'(x) = dF(x)/dx$ must be larger than 1 for some $x > 0$ to have a cross-point K_1. After the cross-point K_1, however, the curve will bend down since $F(x)$ is a bounded function, which leads to the second cross-point K_2. As a result, the non-zero solutions in this case are paired. On the other hand, in the case of $f' > 1$, as shown in Fig.1(b), the curve $y = F(x)$ lies above the line $y = x$ at the beginning, as x increases, the curve will bend down to have a cross-point K_0 since $y = F(x)$ is a bounded function. Starting from K_0, if there are more cross-points, the situation is just like the case of $f' < 1$ with moving the origin to $x = K_0$, hence more cross-points are paired, which leads the total number of non-zero solutions to be odd. Numerical analysis shows that, for $K \in (0, 1]$, the number of non-zero solutions is always 2 in the case of $f' < 1$, while in the case of $f' > 1$, only one non-zero solution can be found.

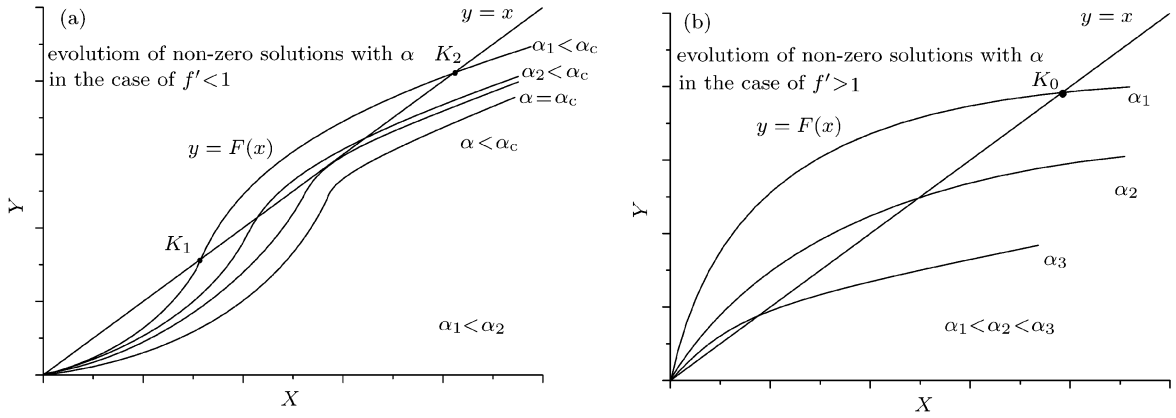


Fig.1. Typical evolution of the solutions of the self-consistent equation with the increase of coupling strength α for $f' < 1$ (a) and $f' > 1$ (b).

It is easy to see that $f(K, T, \alpha, s)$ is a monotonically descending function of α, i.e.

$$\frac{\partial f(K, T, \alpha, s)}{\partial \alpha} < 0, \quad \text{for } \alpha > 0, \tag{20}$$

which implies that

$$f(K, T, \alpha_1, s) > f(K, T, \alpha_2, s), \quad \text{for} \quad \alpha_1 < \alpha_2.$$

Consequently, as shown in Fig.1(a), in the case of $f' < 1$, the non-zero solutions K_1 increases while K_2 decreases as α increases, leading to a result that the non-zero solution cannot decreases to zero continuously as $\alpha \to \alpha_c$. The transition in the case of $f' < 1$ is discontinuous since the non-zero solution disappears suddenly when $\alpha = \alpha_c$, where two non-zero solutions K_1 and K_2 merge to one solution. On the other hand, in the case of $f' > 1$, the non-zero solution can decrease to zero when $\alpha \to \alpha_c$ as shown in Fig.1(b), and the transition is continuous in this case. It is interesting to note that the two non-zero solutions for a discontinuous transition is in accord with Landau theory for a first order transition.[17]

The above analysis shows that the transition behaviour depends on f' defined in Eq.(19), and we shall show that

$$\lim_{K \to 0} \frac{\partial f(K, T, \alpha, s)}{\partial K} \to 0, \qquad \text{for} \quad s < s_c, \tag{21}$$

and

$$\lim_{K \to 0} \left. \frac{\partial f(K, T, \alpha, s)}{\partial K} \right|_{\alpha < \alpha_c} \to \infty, \qquad \text{for} \quad s = s_c. \tag{22}$$

In the following, the arguments of the functions $f(K, T, \alpha, s)$ and $G(K, T, \omega)$ are omitted if necessary to save the space. Using Eq.(10), one can find that

$$\frac{\partial f}{\partial K} = \alpha \omega_c^{1-s} f(K, T, \alpha, s) \times \int_0^{\omega_c} \omega^s \left(-\frac{\partial G(K, T, \omega)}{\partial K} \right) d\omega, \tag{23}$$

it can be seen that the integral in the above equation has an infrared divergence in the limit $K \to 0$, and the leading terms can be found

$$\lim_{\omega_0\to 0}\lim_{K\to 0}\int_{\omega_0}^{\omega_c}\omega^s\left(-\frac{\partial G_1}{\partial K}\right)\mathrm{d}\omega\propto\begin{cases}1/\omega_0^{4-s}, & T\neq 0,\\ 1/\omega_0^{2-s}, & T=0,\end{cases}\tag{24}$$

$$\lim_{\omega_0\to 0}\lim_{K\to 0}\int_{\omega_0}^{\omega_c}\omega^s\left(-\frac{\partial G_2}{\partial K}\right)\mathrm{d}\omega\propto\begin{cases}1/\omega_0^{5+n-2s}, & T\neq 0,\\ 1/\omega_0^{3+n-2s}, & T=0,\end{cases}\tag{25}$$

together with the following result in the case of $s<s_c$

$$\lim_{\omega_0\to 0}\lim_{K\to 0} f\propto\begin{cases}\exp\{-\omega_0^{s-2}\}, & T\neq 0,\\ \exp\{-\omega_0^{s-1}\}, & T=0.\end{cases}\tag{26}$$

One can find the conclusion given in Eq.(21). On the other hand, in the case of $s=s_c$, the leading term of the function $f(K,T,\alpha,s)$ changes into

$$\lim_{\omega_0\to 0}\lim_{K\to 0} f(K,T,\alpha,s)\propto\exp\{\alpha\ln\omega_0\}=\omega_0^{\alpha},\tag{27}$$

yielding the result given in Eq.(22).[2)] As a conclusion, the transition is discontinuous in the case of $s<s_c$ but continuous in the case of $s=s_c$.

As shown in Fig.1(b), geometrically the transition point in the case of $s=s_c$ can be found from

$$\lim_{K\to 0}\frac{\partial f(K,T,\alpha_c,s_c)}{\partial K}=1,\tag{28}$$

at $T=0$, the variational calculations show $\alpha_c=1$ for the DOS case and $\alpha_c=1+n$ for the DSS case,[3)] in agreement with the existing result.[4,9] The value of α_c in this case can be easily derived from the leading terms given in Eqs.(24)–(27). In fact, such a condition has been used to determine the transition point in the Ohmic case at $T=0$.[12]

4. Conclusion and discussion

We have presented mathematical analyses on the evolution of solutions of the self-consistent equation derived from variational calculation based on the DOS and the DSS separately. It is found that the localized transition happens only for $s\leq s_c$, where s is the parameter characterizing the property of the bath defined in the spectral function $J(\omega)$. For variational calculation based on the DSS, it has been known that the solution depends on the spectral function as well as the density of states of the bath, however, it turns out that s_c is the same for both kinds of variational calculations at $T=0$ and $T\neq 0$. This result is interesting and unexpected since it is well known that different variational schemes predict different transition points. The conclusion that $s_c=2$ at $T\neq 0$ looks unusual since it is in discrepancy with the existing result that the spin-boson model with a super-Ohmic bath has localized transition.[1,2,6,10] As one can see from Eqs.(10)–(12), the difference between $s_c(T=0)$ and $s_c(T\neq 0)$ comes from the factor, $\tanh(\beta\omega/2)$, in the integrand. The result that $\lim_{\omega\to 0}J(\omega)\tanh(\beta\omega/2)\propto\omega^{s-1}$ indicates that the appearance of $\tanh(\beta\omega/2)$ in the integrand increases the weight of low frequency mode by effectively changing the spectral function from $\propto\omega^s$ to $\propto\omega^{s-1}$ as $\omega\to 0$, and hence extends the boundary to $s_c=2$. As is known, the variational calculation based on the DOS predicts the results in agreement with those obtained by using other methods.[5,14] Such a discrepancy could be an artifact of variational calculation.[19,20] In the present paper, the main interest is the localized transition controlled by the dissipation strength α. In the case of $T\neq 0$, there is another kind of localized transition controlled by temperature, namely, the transition can happen, with the value of α fixed but temperature raised. Such a situation can be analysed in the way presented in this paper and a similar conclusion can be obtained.

[2)] At $T=0$ and $s=s_c$, we have $\alpha_c=1$ and $\alpha_c=2$ for variational calculation based on DOS and DSS respectively (see, for example, Ref.[4,9]). It is found that $\alpha_c(T\neq 0)<\alpha_c(T=0)$ for both kinds of variational calculation.

[3)] Using the notation of Ref.[9], the result is $\alpha_c=3-2\lambda$. From Eq.(11) in this reference, it is found that $s=2\lambda+n-1$, for $s=1$, we have $2\lambda=2-n$, this leads to $3-2\lambda=n+1$.

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