Variational Approach to the Spin-boson Model With a Sub-Ohmic Bath

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The influence of dissipation on quantum tunneling in the spin-boson model with a sub-Ohmic bath is studied by a variational calculation. By examining the evolution of solutions of the variational equation with the coupling strength near the phase boundary, we are able to present a scenario of discontinuous transition in sub-Ohmic dissipation case in accord with Ginzburg-Landau theory. Based on the constructed picture, it is shown that the critical point found in the general way is not thermodynamically the critical point, but the point where the second energy minimum begins to develop. The true cross-over point is calculated and the obtained phase diagram is in agreement with the result of numerical renormalization group calculation. 

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I. INTRODUCTION

The spin-boson model is an important toy model for investigating the influence of dissipation on quantum tunneling and has a wide range of applications.\[1, 2\] Over decades the model has been studied by various methods.\[1, 2\] like path integral,\[3\] renormalization group calculation,\[4, 5\] variational calculation,\[6, 7, 8, 9, 10\] and the numerical renormalization group (NRG) calculation,\[11\] etc. One important issue is to study the cross-over from the delocalized to localized phases as the dissipation increases. Most of the studies are concentrated on the Ohmic dissipation case which is considered as corresponding to real physical systems and the cross-over picture is well understood. On the other hand, the situation for the sub-Ohmic dissipation, which is of less physics interest but still important for a well understanding of the spin-boson model, has some confusions. Renormalization group calculation shown that quantum tunneling is totally suppressed by dissipation for any non-zero sub-Ohmic coupling at $T=0$.\[1, 4\] while different conclusion was found by mapped the spin-boson model to an Ising model\[12\] and using the well-known result for Ising model.\[13\] The sub-Ohmic case was also studied by using infinitesimal unitary transformation and the cross-over was found to be discontinuous.\[14\] Recently, the NRG calculation, which is considered as a powerful tool for investigation of the Kondo model and its generalizations, confirmed the delocalized to localized phase cross-over in sub-Ohmic dissipation case and the cross-over is identified as continuous.\[13\] Variational calculation has been used to study the spin-boson model with a Ohmic bath and the result of cross-over boundary is in good agreement with the renormalization group calculation.\[8, 9, 10, 11\] The variational calculation for non-zero temperature\[4\] was generalized to sub-Ohmic case recently and the discontinuous cross-over behavior was found to exist at non-zero-temperature.\[12\] Up to now, the description for this discontinuous cross-over is just limited to the discontinuous change of the tunneling splitting at the cross-over point, while a scenario for such a discontinuous cross-over is still lacking. According to Ginzburg-Landau theory,\[17, 18\] the evolution of the free energy around the critical point for the first order (discontinuous) phase transition is rather complicated and merely a discontinuous change of order parameter at the cross-over point is certainly no enough for a complete description of this discontinuous transition. In this paper, we present further analysis on this discontinuous cross-over by examining the evolution of the solutions of the self-consistent equation derived from the variational calculation. It is found that the evolution of the solutions near the phase boundary is consistent with the general picture of the first order phase transition. Basing on the constructed picture, it is shown that the critical points determined in the general way are not thermodynamically critical points and the true critical point is calculated. The arrangement of the paper is as follows. In the next section, the model and a brief explanation on variational calculation are presented. In section III we present analysis on the discontinuous phase transition by comparing the evolution of the solutions of the self-consistent equation for Ohmic and sub-Ohmic dissipation cases near the critical point. Conclusions and discussion are given in the last section.

II. THE MODEL AND VARIATIONAL CALCULATION

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

$$H = \frac{\epsilon}{2} \sigma_z + \frac{\Delta}{2} \sigma_x + \sum_k b_k^\dagger b_k \omega_k + \sigma_z \sum_k c_k (b_k^\dagger + b_k),$$ \hspace{1cm} (1)

where $\sigma_i (i=x, y, z)$ is the Pauli matrix, $b_k (b_k^\dagger)$ is the annihilation (creation) operator of the $k$th phonon mode with energy $\omega_k$ and $c_k$ is the coupling parameter. The main interest of the present paper will be the zero temperature so we set the bias $\epsilon=0$ in the following. It is known that the solution of this model is determined by the so-called the bath spectral function (density) defined
Generally $J(\omega)$ is characterized by a cut-off frequency $\omega_c$ and has a power-law form, i.e.,

$$J(\omega) = \frac{\pi}{2} \alpha \omega^s / \omega_c^{s-1}, \quad 0 < \omega \leq \omega_c,$$

where $\alpha$ is a dimensionless coupling strength which characterizes the dissipation strength. Parameter $s$ specifies the property of the bath, $s = 1$ is the case of Ohmic dissipation and $0 \leq s < 1$ the sub-Ohmic dissipation case. It should be noted that $J(\omega)$ can take some different forms, but leaving the parameter $g_k$ to be determined from the condition that the ground state energy of the whole system is a minimum with respect to $g_k$. Substituting the above equation to Eq.(4), the ground state energy of the whole system is found to be

$$E[g_k] = \sum_k (\omega_k g_k^2 - 2c_k g_k) - \frac{1}{2} \Delta \exp\{-2 \sum_k g_k^2\},$$

which is a functional of $g_k$, then $\frac{\partial E}{\partial g_k} = 0$ leads to

$$g_k = \frac{c_k}{\omega_k + \Delta \exp\{-2 \sum_k g_k^2\}},$$

the tunneling splitting, by Eq.(5), is given by

$$\Delta' = K \Delta, \quad K = F[g_k] \equiv \exp\{-2 \sum_k g_k^2\}.$$
FIG. 1: Phase boundary determined by $\alpha_c$ for various $\Delta/\omega_c$. The inset shows the comparison with the result by using different spectral function $J_1(\omega)$ and $J_2(\omega)$ (see the text) in the case of $\Delta/\omega_c = 0.01$.

III. THE DISCONTINUOUS CROSS-OVER IN SUB-OHMIC CASE

Now we turn to present a scenario for such a discontinuous cross-over from the delocalized to localized phases in sub-Ohmic case. The key point is to examine the evolution of the solutions of the self-consistent equation with the coupling strength $\alpha$ near the phase boundary. For clarity, we first see what happens in the Ohmic case. Fig. 2 shows the evolution of the solutions of Eq. (10) with the increase of $\alpha$ in Ohmic dissipation case. When $\alpha > \alpha_c$, we have the trivial solution only, while a non-zero solution ($K_1 \neq 0$) appears for $\alpha < \alpha_c$. As one can see from the figure, the non-zero solution $K_1$ continuously tends to 0 as $\alpha$ approaches $\alpha_c$. This is consistent with the picture of a continuous (second order) transition: above the critical point ($\alpha > \alpha_c$), there is only one stable phase (one energy minimum located at some $g_{k0}$ satisfying $F[g_{k0}] = 0$ in the present case), below the critical point, this stable phase becomes unstable ($E[g_{k0}]$ becomes the maximum of the energy) and a second stable phase appears ($E[g_{k1}]$ is the new energy minimum, where $F[g_{k1}] = K_1 > 0$), the cross-over behavior is continuous.

The situation for the sub-Ohmic dissipation case is qualitatively different. As shown in Fig. 3, when $\alpha < \alpha_c$, there are two non-zero solutions of Eq. (10) ($K_2 > K_1)$ in additional to the trivial solution. As the coupling strength $\alpha$ increases, $K_2$ decreases while $K_1$ increases and tends to meet $K_2$ as $\alpha$ approaches $\alpha_c$. At $\alpha = \alpha_c$, we have $K_1 = K_2 = K_0 \neq 0$ and at this point $K_0$ is the point of tangency for the line $y = x$ and curve $y = f(x)$. At $\alpha = \alpha_c + 0$, the solution $K_0$ disappears suddenly and only the trivial solution is found. The $\alpha$-dependence of the non-zero solutions of Eq. (10) for Ohmic and sub-Ohmic dissipation cases are shown in Fig. 4 where one can see

FIG. 2: Evolution of the solutions of Eq. (10) with the increase of coupling strength $\alpha$ for $\Delta/\omega_c = 0.1$ in the case of Ohmic dissipation $s = 1$.

FIG. 3: Evolution of the solutions of Eq. (10) with the increase of coupling strength $\alpha$ for $\Delta/\omega_c = 0.1$ in the case of sub-Ohmic dissipation $s = 0.3$.

FIG. 4: The $\alpha$-dependence of the non-zero solution of Eq. (10) for $s = 1$ (left) and $s = 0.3$ (right). As $\alpha/\alpha_c \rightarrow 1$, the non-zero solution of $s = 1$ approaches 0 continuously, while for $s = 0.3$, the non-zero solution jumps from $K_0 \neq 0$ to 0.
the tunneling splitting should decrease with \( \alpha \), continuously at the point \( \alpha = \alpha_c \) strength \( \alpha \). Energy \( E \) with coupling strength \( Eq.(10) \) and thus the tunneling splitting \( \Delta \) cross-over is discontinuous since the non-zero solution of sub-Ohmic dissipation case clearly shows that the second minimum begins to develop. The non-zero solution. As one can see from Fig.4(right), solutions when \( \alpha < \alpha_c \) are just the point where the non-zero solution

\[ E(K_1) > E(0) \] and at the point \( \alpha = \alpha_c \), these two energy extrema merge into a point of inflection at \( F[g_k] = K_0 \), then only one energy minimum \( E[g_k] \) survives when \( \alpha > \alpha_c \). Based on the picture for the discontinuous phase transition, it is now clear that \( \alpha_c \) is not the critical point for the cross-over to happen, but just the point where the second energy minimum begins to develop. \( \alpha_c \) can be considered as the limit of metastability for superheating, i.e., the limit of metastability for increasing the dissipation strength in the present case. Thermodynamically the critical point, as shown in Fig.6, should be \( \alpha_1 \) where we have

\[ E(K_1) = E(0), \] (11)
from this, $\alpha_1$ can be determined by Eqs.(7), (8) and (10). Comparison between the phase boundary determined by $\alpha_c$ and $\alpha_1$ is shown in Fig.7. It is easy to see that $\alpha_1 < \alpha_c$ while the difference between $\alpha_c$ and $\alpha_1$ decreases as $s$ increases and tends to zero as $s \rightarrow 1$ where the transition becomes continuous. We also find that the difference between $\alpha_c$ and $\alpha_1$ decreases with $\Delta/\omega_c$. The phase boundary deduced in this way is shown in Fig.8 which is similar to that shown in Fig.1 but with all the critical points lower. It is found that the phase boundary determined by $\alpha_1$ is in good agreement with that obtained by NRG calculation when $\Delta/\omega_c \leq 0.01$.

IV. CONCLUSIONS AND DISCUSSION

In conclusion, we have study the cross-over behavior from localized to delocalized phases of a spin-boson model with a sub-Ohmic bath by variational method. By examining the evolution of the solutions of self-consistent equation (10) with the coupling strength, we are able to present the scenario of the discontinuous transition in sub-Ohmic dissipation case. Based on the constructed picture, it is shown that the $\alpha_c$, at which the self-consistent equation begins to have non-zero solutions, is not thermodynamically the critical point, but just the point where the second energy minimum begins to develop. The true critical point is determined according to Ginzburg-Landau theory for the first order phase transition and the obtained phase boundary is in agreement with the NRG calculation. Our analysis shows that the cross-over behavior in spin-boson model is directly related to the evolution of solutions of the self-consistent equation derived from the variational calculation. The evolution behavior of solutions for a continuous cross-over (in Ohmic dissipation case) is qualitatively different from that of a discontinuous cross-over (in sub-Ohmic dissipation case). The present work, on one hand, provides convincing evidence for a discontinuous cross-over in sub-Ohmic case and on the other hand, demonstrates the new way to deal with the cross-over behavior in spin-boson model by the variational method.

According to the definition of stable and unstable fixed points for renormalization group, geometrically one can see from Fig.3 that, both $K = 0$ and $K_2$ are stable fixed points while $K_1$ is unstable fixed point as $\alpha < \alpha_c$ in sub-Ohmic case. On the other hand, we only have one stable fixed point (i.e., $K_1$) and one unstable fixed point as $\alpha < \alpha_c$ in Ohmic case. This result is in agreement with the NRG calculation, where 3 fixed points (2 stable and 1 unstable) were found in sub-Ohmic case while the third unstable fixed point disappeared in Ohmic case. However, the cross-over behavior in sub-Ohmic case was identified as continuous in NRG calculation, this implies further analysis is needed for seeking a deeper relation. Although the work by Kehrein and Mielke is not based on the variational calculation, the cross-over behavior was studied by a self-consistent equation and the discontinuous behavior was judged by the discontinuous change of the tunneling splitting at the critical point $\alpha_c$, where the self-consistent equation begins to have non-zero solutions. Some results, like the $\Delta/\omega_c$ dependence of critical coupling $\alpha_c$ and the $s$-dependence of tunneling splitting at the critical point also show quantitative agreement with our work determined from Eq.(10) at $\alpha = \alpha_c$. This may lead to a conclusion the the critical point determined in ref. is just $\alpha_c$ given in the present work, i.e., not thermodynamically the critical point.

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