PHYSICAL REVIEW B VOLUME 45, NUMBER 23 15 JUNE 1992-I

# Universality of dissipative two-state systems

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(Received 7 January 1992)

The static properties of a dissipative two-state system are studied by perturbation, mapping to the quantum sine-Gordon model, and a variational approach. We find that its properties at zero temperature depend not only on the spectral density $J(\omega) \sim \sum_l g_l^2 \delta(\omega - \omega_l)$, but also on the explicit form of the coupling strength $g_l \sim \omega_l^\lambda$ ($\omega_l$ is the phonon frequency). For weak coupling ($\lambda \geq 1$), the effect of displacement of the phonon state is dominant; while for strong coupling ($\lambda < 1$), one must take account of both displacement and deformation. Displaced squeezed states are proposed as ground states of the bath under strong coupling, and we show that the localization transition of the Ohmic dissipation occurs at $\alpha_c = 3 - 2\lambda$ instead of $\alpha_c = 1$ as for the weak-coupling case.

Recently, there has been much interest in the dissipative effect of a bath in the quantum tunneling or two-state system (TSS),[1] e.g., in dissipative macroscopic tunneling phenomena[2] and atomic tunneling states in solids.[3,4] This system can be described by a spin-boson Hamiltonian[1]

$$H = -\Delta_0 \sigma_x + \sum_l \omega_l b_l^\dagger b_l + \sigma_z \sum_l g_l (b_l^\dagger + b_l) \quad , \tag{1}$$

where $\sigma_x$, $\sigma_z$ are Pauli matrices, $\Delta_0$ the bare tunneling parameter, while the bath is described by a set of harmonic oscillators with frequencies $\omega_l$ and coupling constants

$$g_l = g_0 (\omega_l/\omega_0)^\lambda \quad , \tag{2}$$

and $\omega_0$ is the upper cutoff.

It has been argued, by using path-integral techniques,[1] that complete information about the effect of the bath is contained in the spectral density

$$J(\omega) \sim \sum_l g_l^2 \delta(\omega - \omega_l) \sim \omega^s \quad , \tag{3}$$

independent of the explicit form of the coupling strength $g_l$. This concept of universality seems to be well accepted by many researchers in the field.[5] The basic assumption of this argument is that the bath degrees of freedom can be integrated out as Gaussian integrals with displaced centers.[6] It is implicitly assumed that the only effect of the tunneling particle on the bath is to displace the centers of harmonic oscillators.

We would like to point out in this paper that this assumption is not always true. In fact, the coupling of the bath to TSS may give rise to two effects: displacement and deformation of the phonon states. In the weak-coupling case when $g_l/\omega_l \ll 1$, the displacement is the dominating effect. However, in the strong-coupling case when $g_l/\omega_l \gg 1$, both effects should be considered.[7] We show in this paper that the physical behavior of TSS depends not only on $J(\omega)$, but also on $g_l$ explicitly if the deformation is taken into account. This means the universality fails in this case. We will focus on the case of Ohmic dissipation $s = 1$, when there exists a sharp localization transition due to the infrared divergences induced by low-frequency bath phonons.[8]

In Hamiltonian (1) we can complete the square to obtain

$$H = -\Delta_0 \sigma_x + \sum_l \omega_l [b_l^\dagger + (g_l/\omega_l)\sigma_z][b_l + (g_l/\omega_l)\sigma_z] - \sum_l (g_l^2/\omega_l) \quad . \tag{4}$$

If we neglect the first term in (4) temporarily, the phonon state is described by a displaced oscillator characterized by $A(\omega_l) = g_l/\omega_l = (g_0/\omega_0)(\omega_l/\omega_0)^{\lambda-1}$. At this stage, we may subdivide the coupling into two different regimes depending on the index $\lambda$. For weak couplings $\lambda > 1$, $A(\omega_l)$ will increase from zero to $g_0/\omega_0$ as $\omega_l$ goes from zero to $\omega_0$; while for the strong-coupling regime $\lambda < 1$, $A(\omega_l)$ will decrease from *infinity* to $g_0/\omega_0$ and hence the corresponding displaced state is *not* a well-defined function for low-frequency phonons. Different physical pictures emerge when we consider the first term in (4). In the weak-coupling regime, the low-frequency phonons ($\omega_l \ll \Delta_0$) nearly decouple from TSS and one can safely integrate out the displaced phonons in the adiabatic approximation. However, the adiabatic approximation does not work in the regime $\lambda < 1$ because of strong coupling of the low-frequency phonons to TSS and so one cannot simply integrate out the bath. To get a full description for the bath, we apply, as usual, the unitary transformation

$$S_1 = \exp\left(\sigma_z \sum_l (g_l/\omega_l)(b_l^\dagger - b_l)\right) \tag{5}$$

to (4). One can see that there are two kinds of influence on the phonon subsystem due to coupling with TSS.[9] The first is the diagonal term containing $\sigma_x$, providing static influence of TSS in its ground state ($\sigma_x = +1$) or in its excited state ($\sigma_x = -1$). The second is the nondiagonal term containing $\sigma_y$, representing dynamic influence of the transition of TSS between its ground and excited states. This case is analogous to the small-polaron problem.[10] Thus, the nondiagonal term will be important only for temperatures $T > \Delta/k_B$ (where $\Delta = \Delta_0\kappa$ is the renormalized tunneling parameter with $\kappa$ as the phonon overlapping integral). At low temperatures, the nondiagonal term may be treated as perturbation and then projecting the transformed Hamiltonian on to the subspace of $\sigma_x = +1$ gives an effective Hamiltonian for the bath. The unperturbed Hamiltonian (neglecing the dynamic effect) is

$$H_{\rm ph}^{(0)} = \sum_l \omega_l b_l^\dagger b_l - \Delta_0 \cosh\left(\sum_l (2g_l/\omega_l)(b_l^\dagger - b_l)\right) \quad , \tag{6}$$

where we have discarded an unimportant constant. $H_{\rm ph}^{(0)}$ represents a phonon system with nonlinear interaction. Normal ordering of phonon operators, needed for calculating the ground-state energy, shows the nonlinear interaction is proportional to the phonon overlapping integral $\kappa$. As we will see later, the leading term of the dynamic effect is proportional to $\kappa^3$ [Eq. (22)]. Therefore $H_{\rm ph}^{(0)}$ is *exact* at the limit $T \to 0$, $\kappa \to 0$, but $k_BT/\Delta_0\kappa \ll 1$. Because of the nonlinear interaction, it is difficult to find an exact solution of $H_{\rm ph}^{(0)}$, and one must look for approximations.

For weak couplings ($\lambda > 1$), the hyperbolic function in (6) may be expanded with respect to $(g_l/\omega_l)$. To zeroth order, the ground states of $H_{\rm ph}^{(0)}$ are vacuum states $\Phi_{\rm vac}$, or displaced states in the original basis

$$\Phi_{1(\pm)} = \exp\left(\mp \sum_l (g_l/\omega_l)(b_l^\dagger - b_l)\right) \Phi_{\rm vac} \quad , \tag{7}$$

where $\pm$ corrrespond to $\sigma_z = \pm 1$. It is easy to calculate the renormalized tunneling parameter

$$\Delta_1 = \Delta_0 \exp\left(-\alpha \int \frac{J(\omega)}{\omega^2} d\omega\right) \tag{8}$$

with

$$\alpha = 2(g_0/\omega_0)^2 \quad , \tag{9}$$

$$J(\omega) = \omega^s/\omega_0^{s-1} \quad , \tag{10}$$

$$s = 2\lambda + n - 1 \quad . \tag{11}$$

Here $n$ is the exponent of the phonon density of states $D(\omega) = \omega^{n-1}/\omega_0^n$.

For strong couplings ($\lambda < 1$), however, the expansion with respect to $(g_l/\omega_l)$ fails because it tends to infinity as $\omega_l \to 0$. Therefore, the displaced-state approximation is no longer valid. In order to make the expansion of the hyperbolic function in (6) available, we apply the second unitary transformation

$$S_2 = \exp\left(\sum_l \gamma_l (b_l b_l - b_l^\dagger b_l^\dagger)\right) \quad , \tag{12}$$

where the parameter $\gamma_l$ will be determined later. $S_2$ represents the simplest kind of deformation of the bath, namely, the rescaling of phonon coordinates.[9] Using the properties of $S_2$, we obtain

$$\begin{aligned} \overline{H}_{\rm ph}^{(0)} &= S_2 H_{\rm ph}^{(0)} S_2^{-1} \\ &= \sum_l \omega_l [b_l^\dagger b_l \cosh 4\gamma_l + \tfrac{1}{2}(b_l^\dagger b_l^\dagger + b_l b_l)\sinh 4\gamma_l] - \Delta_0 \cosh\left(\sum_l (2\overline{g}_l/\omega_l)(b_l^\dagger - b_l)\right) + \sum_l \omega_l (\sinh 2\gamma_l)^2 \quad , \end{aligned} \tag{13}$$

with $\overline{g}_l = g_l e^{-2\gamma_l}$. Then we may expand the hyperbolic function with respect to $\overline{g}_l/\omega_l$. By normal ordering phonon operators and expanding up to $(\overline{g}_l/\omega_l)^2$, we have

$$\begin{aligned} \overline{H}_{\rm ph}^{(0)} = &\sum_l [\omega_l \cosh 4\gamma_l + (4\overline{g}_l^2 \Delta_2/\omega_l^2)] b_l^\dagger b_l \\ &+ \sum_l \tfrac{1}{2}[\omega_l \sinh 4\gamma_l - (4\overline{g}_l^2\Delta_2/\omega_l^2)](b_l^\dagger b_l^\dagger + b_l b_l) + \sum_l \omega_l (\sinh 2\gamma_l)^2 - \Delta_2 \end{aligned} \tag{14}$$

with

$$\Delta_2 = \Delta_0 \exp\left(-2\sum_l (\overline{g}_l/\omega_l)^2\right) \quad . \tag{15}$$

In deriving (14), we have omitted the coupling between different modes. The parameter $\gamma_l$ is now chosen to diagonalize $H_{\rm ph}^{(0)}$ in (14) to yield

$$\overline{H}_{\rm ph}^{(0)} = \sum_l [\omega_l e^{4\gamma_l} b_l^\dagger b_l + \omega_l (\sinh 2\gamma_l)^2] - \Delta_2 \quad , \tag{16}$$

$$\gamma_l = \tfrac{1}{8} \ln[1 + (8g_l^2\Delta_2/\omega_l^3)] \quad . \tag{17}$$

The ground states of (16) are vacuum states [which are different from $\Phi_{\rm vac}$ in (7)], or displaced squeezed states in the original basis

$$\Phi_{2(\pm)} = \exp\left(\mp\sum_l (g_l/\omega_l)(b_l^\dagger - b_l)\right) \times \exp\left(-\sum_l \gamma_l(b_l b_l - b_l^\dagger b_l^\dagger)\right)\overline{\Phi}_{\rm vac} \ . \quad (18)$$

It is easy to prove that the corresponding renormalized tunneling parameter is $\Delta_2$, which can be rewritten as

$$\Delta_2 = \Delta_0 \exp\left(-\alpha\int\frac{\overline{J}(\omega)}{\omega^2}d\omega\right) \ , \quad (19)$$

$$\overline{J}(\omega) = \omega^s/\omega_0^{s-1}(1+8g_0^2\Delta_2\omega_0^{2\lambda}\omega^{2\lambda-3})^{1/2} \ . \quad (20)$$

Before proceeding further, we would like to analyze the range of validity for expansion in $(\overline{g}_l/\omega_l)$. Equation (17) gives $\overline{g}_l/\omega_l \sim \omega^{(2\lambda-1)/4}$ at low-frequency limit. Therefore, the expansion is self-consistent as long as $1 > \lambda \geq \frac{1}{2}$.

As an application of the present theory, we investigate the influence of the deformation on the localization transition for Ohmic dissipation ($s = 1$). Following the iterative treatment of Ref. 1, from (8) we can find the localizaion transition takes place at $\alpha_c = 1$ for the limit $\Delta_0/\omega_0 \ll 1$ if we introduce an infrared cutoff $\omega_m \sim \Delta_1$. Let $\Delta_2 = \Delta_0\kappa$, then (19) becomes

$$\kappa^{(\alpha'-1)/2\alpha'} = B^{1/2} + (B+\kappa)^{1/2} \ , \quad (21)$$

with $B = \omega_0^3/8g_0^2\Delta_0, \alpha' = \alpha/(3-2\lambda)$. For $\Delta_0/\omega_0 \ll 1$, we find $\kappa \neq 0$ for $\alpha' < 1$, $\kappa = 0$ for $\alpha' > 1$, i.e., the localization transition occurs at $\alpha'_c = 1$ or $\alpha_c = 3-2\lambda > 1$ for the strong-coupling regime, instead of $\alpha_c = 1$ for the weak-coupling regime.

To include the dynamic effect of TSS on phonons, we use second-order perturbation with $\sigma_y$ term, which gives

$$\overline{H}_{\rm ph}^{(2)} = \overline{H}_{\rm ph}^{(0)} - \frac{\Delta_0}{2\kappa}\left[\sinh\left(\sum_l(2g_l/\omega_l)(b_l^\dagger - b_l)\right)\right]^2 \ . \quad (22)$$

Following a similar treatment as above, we get the same equation as (21) except $B$ is replaced by $\overline{B} = B(1+\kappa^2)^{-1}$. Therefore, including the dynamic effect does not change the result $\alpha_c = 3-2\lambda$ for $\Delta_0/\omega_0 \ll 1$. Hence we have shown that the localization transition for the Ohmic dissipative system depends explicitly on $\lambda$ in the strong-coupling regime.

A typical strong-coupling case is materialized for the model of a two-state system interacting with one-dimensional acoustic phonons where $\lambda = \frac{1}{2}$. The present theory gives $\alpha'_c = \alpha_c/2 = (g_0/\omega_0)_c^2 = 1$. This result can also be obtained *exactly* in another way. Introducing the following operators

$$\phi(x) = i\sum_l(\omega_0/2\pi\omega_l)^{1/2}(b_l e^{ilx} - b_l^\dagger e^{-ilx}) \ , \quad (23)$$

$$\pi(x) = \sum_l(\omega_0\omega_l/2\pi)^{1/2}(b_l e^{ilx} + b_l^\dagger e^{-ilx}) \ , \quad (24)$$

which obey the canonical commutation relation

$$[\phi(x), \pi(x')] = i\delta(x-x') \ , \quad (25)$$

we can rewrite $H_{\rm ph}$ as

$$H_{\rm ph} = \int dx\left(\tfrac{1}{2}\{\pi^2(x) + [\nabla\phi(x)]^2\} - \delta(x)\frac{A}{B^2}\cos[B\phi(x)]\right) \ , \quad (26)$$

where $A/B^2 = \Delta_0$, $B = 2^{3/2}\pi^{1/2}(g_0/\omega_0)$. Then $H_{\rm ph}$ maps on to the quantum sine-Gordon model which has a well-known phase transition at $B_c^2 = 8\pi$,[11-13] and it gives $(g_0/\omega_0)_c^2 = 1$,[14] thus confirming our result in the special case $\lambda = \frac{1}{2}$.

The above results can also be derived from a variational treatment for $\Delta_0/\omega_0 \ll 1$. It has been proved[15] that the variational displaced state

$$\Phi_1 = \exp\left(-\sigma_z\sum_l \lambda_l(b_l^\dagger - b_l)\right)\Phi_{\rm vac} \quad (27)$$

gives localization transition at $\alpha_c = 1$. In (27), $\Phi_{\rm vac}$ denotes both the vacuum state for phonons and the symmetric state for the two-state system ($\sigma_x\Phi_{\rm vac} = \Phi_{\rm vac}$). The energy of state $\Phi_1$ is

$$E_1 = -\Delta_0\kappa_1(1-\alpha) \ , \quad (28)$$

with $\kappa_1 = (2e\Delta_0/\omega_0)^{\alpha/(1-\alpha)}$. The variational displaced squeezed state has the form[16]

$$\Phi_2 = \exp\left(-\sigma_z\sum_l(g_l/\omega_l)(b_l^\dagger - b_l)\right) \times \exp\left(-\sum_l\gamma_l(b_l b_l - b_l^\dagger b_l^\dagger)\right)\Phi_{\rm vac} \ , \quad (29)$$

where $\gamma_l$ is determined by minimising the energy $E_2$ of $\Phi_2$. We get the same condition for $\gamma_l$ as in (17). Then $\Phi_2$ gives the same localization transition condition as that by perturbation. Inserting $\gamma_l$ into $E_2$ leads to

$$E_2 = -\Delta_0\kappa_2(1-\alpha') \ , \quad (30)$$

with $\kappa_2 = (2\Delta_0 g_0^2/\omega_0^3)^{\alpha'/(1-\alpha')}$. $E_1$ and $E_2$ depend on $\lambda$ via the relation $\alpha' = \alpha/(3-2\lambda)$. It can be proved[16] that $E_1 < E_2$ for $\lambda \geq 1$ and $0 < \alpha < 1$, while $E_1 > E_2$ for $\lambda < 1$ and $0 < \alpha < 3-2\lambda$. Therefore, the displaced squeezed state is preferable for the strong-coupling regime at least in view of the ground-state energy.

Before making conclusions, we would like to discuss the possible origin of the discrepancy between the present theory and the previous studies. We want to point out, on the one hand, the present results are valid in the limit $T \to 0$ and $\Delta \to 0$, but $k_B T/\Delta \ll 1$. On the other hand, we emphasize that the correct order of taking the limit is important and one should be very careful. There may be, for example, two different ways of taking the limit $T \to 0$ in the path-integral approach: before or after the Gaussian integrals about displaced coordinates

$x_l' = x_l(1+\delta)$ with the relative displacement

$$\delta \sim \omega_l^{\lambda+1}/(\omega_l^2+\omega_m^2) \quad , \tag{31}$$

where $\omega_m \sim T$ is the Matsubara frequency.[6] If the $T \to 0$ limit is taken after integration, $\omega_m$ acts as a low-frequency cutoff and there is no infrared divergence. If, however, the limit $\omega_m \to 0$ is taken first, the behavior of $\delta$ as $\omega_l \to 0$ depends on the index $\lambda$: $\delta \to 0$ for $\lambda > 1$; $\delta \to \infty$ for $\lambda < 1$ and the corresponding Gaussian integrals are not well defined. Therefore, these two different limits are *not interchangeable* for strong couplings $\lambda < 1$. We believe the discrepancy may stem from different treatments of the low-frequency modes of the bath: we have considered the infrared divergence properly while previous studies have not. In fact, previous results are recovered if we assume that the low-frequency modes are not important. In this case, the dissipative effect of the bath mainly comes from the high-frequency modes and the parameter $\gamma_l$ may be written as

$$\gamma_l = \frac{1}{8}\ln\left(1+4\alpha\frac{\Delta_0}{\omega_0}\right) \tag{32}$$

in the high-frequency approximation. Then the critical value $\alpha_c$ is determined by

$$\alpha_c[1+4\alpha_c(\Delta_0/\omega_0)]^{-1/2} = 1 \quad . \tag{33}$$

In the limit $\Delta_0/\omega_0 \ll 1$, it gives $\alpha_c = 1+2(\Delta_0/\omega_0)$ which is precisely the same as that of previous studies.[8,17,18]

In conclusion, by considering carefully the effects due to coupling with a two-state system on the phonon states of a bath, we have shown the static properties of a dissipative two-state system at zero temperature depend, not only on the spectral density, but also on the explicit form of the coupling strength. Our results, contrary to the previous studies, indicate *there is no universality in dissipative two-state systems at zero temperature.* The effects of strong coupling on dynamical properties are under consideration now.

One of the authors (H.C.) is grateful to Professor X. Wu, Dr. G. M. Zhang, Professor U. Weiss, and Professor G. Schön for interesting discussions. H.C. would like to thank Professor Abdus Salam, the International Atomic Energy Agency, for hospitality at the International Centre for Theoretical Physics, Trieste, Italy, where this work was completed.

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