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LETTER TO THE EDITOR

The localisation transition in a dissipative two-state system: a squeezed state approach

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Abstract. A displaced squeezed state is used as the variational ground state of a spin-boson Hamiltonian describing the interaction of a two-state system with a phonon bath. The phase diagram for localisation in the ohmic dissipation is obtained by a method based on the self-consistent calculation of the effective tunnelling splitting. A comparison with the results of the usual displaced state approximation and the renormalisation group theory is also given.

The spin-boson Hamiltonian

$$\mathcal{H} = -\Delta_0\sigma_x + \sum_k \omega_k b_k^+ b_k + \sigma_z \sum_k g_k(b_k^+ + b_k) + \sum_k (g_k^2/\omega_k) \tag{1}$$

has been used to simulate many physical situations with various backgrounds, e.g., dissipative macroscopic tunnelling in a SQUID [1] and atomic tunnelling states in solids [2–4]. Abundant physics can be exhibited from the Hamiltonian (1), ranging from damped oscillation up to localisation. Apparently the low frequency modes of the bath play a crucial role and may modify the motion of the two-state system. The conventional weak coupling picture is then driven into a rather limited region of validity. On the other hand, the adiabatic approximation exaggerates this point and overestimates the occurrence of infrared divergence. In fact, using the renormalisation-group procedure, Chakravarty [5], and Bray and Moore [6] have shown that for the ohmic dissipation and at zero temperature, increasing the dissipation strength triggers a sharp localisation transition. It is believed that such a transition is the result of the infrared divergence induced by the low frequency modes of the bath. Therefore it is important to find a correct description of the ground state of the bath, especially for the low frequency part. Unfortunately, we know little as yet about the ground state of the bath under coupling with a two-state system. The adiabatic approximation ascribes the displaced oscillator of the Glauber coherent state as the ground state, leading invariably to localisation for the ohmic case and completely suppressing the occurrence of the transition.

It is clear that the coupling with a two-state system has two different effects on the ground state of the bath: displacement and deformation. The failure of the Glauber coherent state description arises from the fact that it only takes account of the former and omits the latter [7]. In [8] we have proposed a displaced squeezed state

$$\varphi = \exp\Big(-\sigma_z \sum_k (g_k/\omega_k)(b_k^+ - b_k)\Big) \exp\Big(-\sum_k \gamma_k(b_k b_k - b_k^+ b_k^+)\Big)\varphi_{\rm vac} \qquad (2)$$

as a variational ground state of the Hamiltonian (1), where $\varphi_{\rm vac}$ denotes the vacuum state for the bath and the symmetric state for the two-state system ($\sigma_x\varphi_{\rm vac} = \varphi_{\rm vac}$). This displaced squeezed state includes both displacement and deformation effects induced by coupling with a two-state system. It is easy to verify that the whole system is more stable in the displaced squeezed state than in the Glauber coherent state. The intention of the present letter is to explore the influence of this new ground state on the condition necessary for the occurrence of localisation transitions.

Minimising the ground state energy of the whole system

$$E_g = \langle\varphi|H|\varphi\rangle = -\Delta_0 \exp\Big(-\sum_k (2g_k^2/\omega_k^2)\,{\rm e}^{-4\gamma_k}\Big) + \sum_k (\sinh 2\gamma_k)^2\omega_k \qquad (3)$$

leads to the equation for γ_k:

$$e^{8\gamma_k} = 1 + 8\Delta_0 g_k^2 K/\omega_k^3 \qquad (4)$$

where the phonon overlapping integral K satisfies

$$-\ln K = \sum_k (2g_k^2/\omega_k^2)\,{\rm e}^{-4\gamma_k} = \sum_k (2g_k^2/\omega_k^2)(1 + 8\Delta_0 g_k^2 K/\omega_k^3)^{-1/2}. \qquad (5)$$

The effective tunnelling frequency is $\Delta_{\rm eff} = \Delta_0 K$; therefore the localisation occurs as K vanishes. We see that γ_k tends to infinity as $k \to 0$ for non-zero K. Its effect is just to alleviate the infrared divergency appearing in the Glauber coherent state through the second factor in the right hand side of (5), and to drive the occurrence of the localisation into the appropriate region in the parameter space. For mathematical simplicity, we adopt the power law for both coupling strength g_k and frequency ω_k up to the cut-off value in momentum space:

$$g_k = g_0 k^\lambda \qquad \omega_k = \omega_0 k^\nu \qquad (6)$$

where k is reduced against the cut-off momentum; hence $0 < k < 1$. In the d-dimensional space these reduce (5) to [9]

$$\begin{aligned} -\ln K &= \frac{g_0^2}{\omega_0^2}\frac{2}{3\nu - 2\lambda}\int_0^1 [t^{(\lambda-\nu/2+d)/(3\nu-2\lambda)-1}/(t + A^{-1}K)^{1/2}\,{\rm d}t \\ &= \frac{g_0^2}{\omega_0^2}\frac{2}{\lambda - \nu/2 + d}\left(\frac{A}{K}\right)^{1/2} F\left(\frac{1}{2}, \frac{\lambda - \nu/2 + d}{3\nu - 2\lambda}, \frac{\lambda - \nu/2 + d}{3\nu - 2\lambda} + 1, -\frac{A}{K}\right) \end{aligned} \qquad (7)$$

where $A = \omega_0^3/8\Delta_0 g_0^2$ and $F(a, b, c; z)$ is the hypergeometric function. We assume $2\lambda < 3\nu$ to ensure γ_k tends to zero at a high frequency limit (high frequency modes are harmless to the adiabatic picture). The asymptotic behaviour of $F(a, b, c; z)$ for large z depends crucially on the value of $b(= (\lambda - \nu/2 + d)/(3\nu - 2\lambda))$ [9]:

$$(A/K)^{1/2}F \sim C_1 + C_2(K/A)^{b-1/2}. \qquad (8)$$

Hence there is always a non-zero K when $b > \frac{1}{2}$, and for $b < \frac{1}{2}$, $K = 0$ is the only solution of (7) except when A is unusually small. For the current notation

$$\sum_k g_k^2 \sim \int \omega^s\,{\rm d}\omega$$

we notice $s = (d + 2\lambda)/\nu - 1$. Then $b = (d + \nu)/[d + (2 - s)\nu] - \frac{1}{2}$ is an increasing

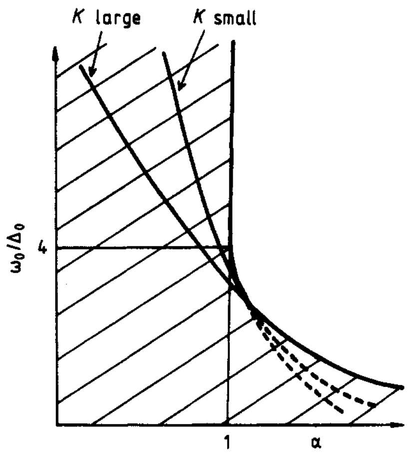

Figure 1. The phase diagram for the localisation–delocalisation transition. The shaded area represents the delocalisation phase and the unshaded area the localisation phase. The full curves represent the stable points with constant K and the broken curves are associated with the saddle points.

function of s. The parameter b larger (or less) than $\frac{1}{2}$ corresponds to s larger (or less) than 1. In the literature these two situations are referred to as superohmic and subohmic respectively [1].

The marginal ohmic case $b = \frac{1}{2}$ ($s = 1$) is the most fascinating, as the integral in (7) then becomes elementary:

$$-\ln K = (g_0^2/4\omega_0^2)[\ln(1 + \sqrt{1 + A^{-1}K}) - \ln\sqrt{A^{-1}K}]. \tag{9}$$

In obtaining (9) we have chosen the boson bath as a three-dimensional acoustic phonon bath, namely with $d = 3$, $\nu = 1$. Introducing the dimensionless dissipation strength $\alpha = \alpha'/4$, with

$$2\sum_k g_k^2 = \alpha' \int_0^{\omega_0} \omega \, \mathrm{d}\omega \tag{10}$$

equation (9) can be rewritten as

$$K^{(\alpha-1)/2\alpha} = A^{1/2} + (A + K)^{1/2} \tag{11}$$

with $A = \omega_0/16\Delta_0\alpha$. For $\alpha < 1$, equation (11) always possesses a solution $K > 0$. The situation is somewhat complicated for $\alpha > 1$: when $A > \frac{1}{4}$, $K = 0$ is the only solution, while for $A < \frac{1}{4}$, two non-zero K-values arise. Detailed analysis of the stability shows that the larger K corresponds to the energy minimum, while the smaller K corresponds to a saddle point. It is convenient to represent these results in the (ω_0/Δ_0)–α plane. In figure 1, the shaded area possesses a stable non-zero K, while the unshaded area corresponds to localisation with $K = 0$ the only solution. The boundary describing the localisation–delocalisation transition consists of two parts: one is the line $\alpha = 1$ from $\omega_0/\Delta_0 = 4$ upwards; the other, for $\alpha > 1$, is the envelope of the family of curves with a constant value of K in (11), i.e.

$$\omega_0/\Delta_0 = 16\alpha(\alpha - 1)^{\alpha-1}/(\alpha + 1)^{\alpha+1}. \tag{12}$$

In the literature the cut-off frequency ω_0 is usually considered to be very large [1], and all the results referred to are in the lowest order of Δ_0/ω_0; thus the transition occurs at $\alpha = 1$, corresponding to the straight line in figure 1. From the spin-boson Hamiltonian one sees that in the strong coupling or small tunnelling limit, the ground state becomes degenerate suggesting the localisation of the spin in one of the spin states (up or down); therefore large α and small Δ_0 (scaled against the cut-off ω_0) favours localisation. In other words, for smaller ω_0/Δ_0, the transition should occur at somewhat larger α. To our knowledge, until now there has been no operative scheme appropriate to the small cut-off limit ($\Delta_0/\omega_0 > 1$) of the present problem. A related problem of a particle in a periodic potential with quasiparticle dissipation has been studied by Guinea and Schön [10]. In many cases, this problem is equivalent to the ohmic dissipative two-level system considered in the present paper. For the small cut-off limit (ω_0/Δ_0 tends to zero), they found that the critical coupling approaches infinity—it is easy to see that (12) has the same asymptotic behaviour. They indicated that the critical coupling depends linearly on Δ_0/ω_0 for the large cut-off limit ($\omega_0/\Delta_0 > 1$). Our critical line follows a similar behaviour, although it smoothly approaches the point $\alpha = 1$, $\omega_0/\Delta_0 = 4$ from below and then becomes a vertical line. When $\Delta_0/\omega_0 < \frac{1}{4}$, our results coincide with those of others [1]: with effective tunnelling $\Delta_{\text{eff}} = \Delta_0(4\alpha\Delta_0/\omega_0)^{\alpha/(1-\alpha)}$ for $\alpha < 1$ and $\Delta_{\text{eff}} = 0$ for $\alpha > 1$, except that α should be replaced by α' defined in (10).

We want to emphasise that our theory shows that the localisation will take place at larger critical coupling where $\alpha' = 4$ instead of $\alpha' = 1$ as in the previous studies. This is the crucial point of the present study. In the following, we would like to deliberate a little more over the possible origin of the difference between α and α'. Leggett *et al* have suggested [11] that the localisation transition condition given by the renormalisation-group procedure can be obtained from an iterative process on the basis of the Glauber coherent state. Alternatively, Hewson and News [12], and Zwerger [13] used a variational ground state

$$\varphi' = \exp\left(-\sigma_z \sum_k C_k(b_k^+ - b_k)\right)\varphi_{\text{vac}} \tag{13}$$

to minimise the energy

$$E_g' = -\Delta_0 K' + \sum_k (\omega_k C_k - 2g_k)C_k + \sum_k g_k^2/\omega_k \tag{14}$$

with

$$C_k = g_k/(\omega_k + 2\Delta_0 K') \tag{15}$$

$$K' = \exp\left(-2\sum_k C_k^2\right) = \left[\frac{2\Delta_0 K'}{\omega_0 + 2\Delta_0 K'}\exp\left(\frac{\omega_0}{\omega_0 + 2\Delta_0 K'}\right)\right]^{\alpha'}. \tag{16}$$

They thus got precisely the same phase diagram for localisation in the ohmic case as they did by using the renormalisation-group procedure for $\Delta_0/\omega_0 \ll 1$, namely $K' = (2e\Delta_0/\omega_0)^{\alpha'/(1-\alpha')}$ for $\alpha' < 1$ and $K' = 0$ for $\alpha' > 1$. It is interesting to compare the energies of these two different approaches. Combining (4), (6) and (15), (3) and (14) ($\Delta_0/\omega_0 \ll 1$) we obtain

$$E_g = -\Delta_0 K(1-\alpha) \qquad E_g' = -\Delta_0 K'(1-\alpha'). \tag{17}$$

It can be shown from (17) that there exists a characteristic value α_c' with $0 < \alpha_c \ll 1$, leading to $E_g' \leqslant E_g$ for $\alpha' < \alpha_c'$; $E_g' > E_g$ for $4 > \alpha' > \alpha_c'$. In order to get a quantitative feeling for α_c', we choose $\Delta_0/\omega_0 = 0.1$ which gives $\alpha_c' = 0.04$, and $E_g'/E_g = 1.004$ for $\alpha' = 0.01$; $E_g'/E_g = 0.04$ for $\alpha' = 0.8$. This means that our displaced squeezed trial state is more stable in the regime $4 > \alpha' > \alpha_c'$. We believe that our description of the transition is preferable at least in the view of the ground state energy. In fact, the ratio α'/α reflects the difference between two kinds of infrared divergence in the neighbourhood of the transition points, namely

$$\frac{\alpha'}{\alpha} = \lim_{K\to 0}\left\{\left(\sum_k \frac{2g_k^2}{(\omega_k + 2\Delta_0 K)^2}\right)\Big/\left[\sum_k \frac{2g_k^2}{\omega_k^2}\left(\frac{1 + 8\Delta_0 g_k^2 K}{\omega_k^3}\right)^{1/2}\right]\right\} = 4 \qquad (18)$$

leading to different Frank–Condon factors. It is worthwhile noticing that the known results for the renormalisation-group procedure are obtained mainly on the assumption of a dilute instanton gas or dilute flip gas. Recently, in the study of dissipative tunnelling out of a metastable state, Zwerger pointed out the possibility that condensation of an instanton gas may cause the breakdown of the dilute gas approximation [14].

In conclusion, we have developed a non-renormalisation-group theory to investigate the localisation transition in a dissipative two-state system. The main feature of the theory is the introduction of a displaced squeezed state as the ground state of the spin-boson model, which is more stable than the Glauber coherent state. The influence of this new ground state on the localisation transition has been studied in detail for the ohmic dissipation case. We find that the transition depends on ω_0/Δ_0 and on the coupling. For coupling smaller than a critical value, the system is in the delocalisation phase and is independent of ω_0/Δ_0. However, when the coupling becomes larger than the critical value, the system can be either in the localisation phase or in the delocalisation phase, depending on the value of ω_0/Δ_0. The important difference between this and previous work is that our critical line for a large ω_0/Δ_0 limit is located at a larger coupling strength.

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