Relaxation behaviour of a biased two-level system, in metals in the weak damping limit

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Abstract. The dynamic properties of a biased two-level system in contact with a dissipative bath are studied in the weak coupling limit using a resolvent expansion method. The theory yields consistent results at low temperatures, a regime in which the widely used dilute bounce gas approximation (DBGA) to an underlying functional integral expression breaks down. The present results are however equivalent to a recently adapted functional integral technique that goes beyond the DBGA. The calculated expressions are relevant for analyzing the neutron scattering data on tunneling of light interstitials, e.g., hydrogen, in metals, at very low temperatures.

1. Introduction

Recently there has been a number of neutron scattering studies of the tunneling motion of hydrogen in a biased (i.e. asymmetric) double-well potential in a metallic system e.g. Nb (Wipf *et al* 1987). The double-well is caused by other immobile interstitial defects (e.g. oxygen or nitrogen) and the bias is due to long range strain interaction between O–H (or N–H) pairs. At very low temperatures ($\sim 10\,\mathrm{K}$) the neutron inelastic scattering shows peaks near the tunneling frequency of the hydrogen with a finite width due to the interaction with the conduction electrons. As the temperature increases there is a cross-over from inelastic to quasi-elastic scattering owing to the destruction of the coherence of tunneling by thermally excited electron–hole pairs. The most striking quantum effect of the metallic electrons is that the width of the quasi-elastic peak decreases with temperature until a minimum is reached around $70\,\mathrm{K}$ when phonon effects set in and enhance the width. In the quasi-elastic regime the experiments require higher defect concentrations in order to distinguish the peak from the background; hence the effect of the bias is very important from this experimental point of view.

In the region of physical interest the pure tunneling motion in a double-well can be adequately described by the Hamiltonian of an effective two-level system (Leggett *et al* 1987):

$$H_S = -\tfrac{1}{2}\hbar\Delta_0\sigma_x + \tfrac{1}{2}\hbar\varepsilon\sigma_z \tag{1}$$

where σ's are the Pauli matrices, Δ_0 is the bare tunneling frequency and ε is the bias.

As is well-known the influence of the low-lying excitations off the Fermi surface of the metallic electrons can be represented by bosons with a specific form of the spectral density (given below in 4)) (Guinea 1984; Chang and Chakravarty 1985). Thus the complete Hamiltonian for the tunneling system, coupled with the conduction electrons, can be written in terms of what is known as the spin-boson Hamiltonian (Leggett *et al* 1987):

$$H = H_S + \sigma_z \sum_j G_j(b_j^+ + b_j) + \sum_j \hbar\omega_j b_j^+ b_j \tag{2}$$

where b_j^+ is the creation operator for the jth boson of frequency ω_j and G_j is the coupling constant. In order that the bosons can effectively describe the fermionic system of metallic electrons the spectral density function $J(\omega)$ has to have a specific form that describes 'Ohmic dissipation'. Thus, $J(\omega)$, defined by

$$J(\omega) \equiv (2/\hbar^2) \sum_j G_j^2 \delta(\omega - \omega_j) \tag{3}$$

is modelled as

$$J(\omega) = K\omega \exp(-\omega/D). \tag{4}$$

In (4) K is a phenomenological dimensionless constant that parameterizes damping, which arises in the model only in the limit of an infinitely large number of bosons, and D is a cut-off frequency of the order of the Fermionic band-width.

The static and dynamic properties of the spin-boson Hamiltonian have been reviewed comprehensively by Leggett *et al* (1987). Much of the theoretical work has relied on the so-called dilute bounce gas approximation (DBGA) to the underlying functional integral expression. Recently, however, it has been demonstrated that a resolvent expansion of the Liouvillian, as is familiar in the literature on relaxation phenomena in chemical physics, yields results that are completely equivalent to those obtained in the DBGA, both in the symmetric ($\varepsilon = 0$) and the biased ($\varepsilon \neq 0$) cases (Dattagupta *et al* 1989). This treatment relies on a unitary transformation that changes the Hamiltonian in (2) to the form:

$$H' = -\tfrac{1}{2}\hbar\Delta_0(B_+\sigma_- + B_-\sigma_+) + \tfrac{1}{2}\hbar\varepsilon\sigma_z + \sum_j \hbar\omega_j b_j^+ b_j \tag{5}$$

where $\sigma_x = \tfrac{1}{2}(\sigma_+ + \sigma_-)$ and where

$$B_\pm \equiv \exp\left(\pm 2\sum_j (G_j/\hbar\omega_j)(b_j - b_j^+)\right). \tag{6}$$

The main point of the transformed Hamiltonian H' is that the interaction term is now given in terms of renormalized coupling strengths $B_\pm$. The DBGA then follows from the 'self-energy' calculated up to second order in a systematic perturbation treatment of the interaction (i.e. the first term in (5)). This fact clarifies the physical meaning and the limitation of the DBGA; though the theory is valid for arbitrary damping (since the original coupling constant G_j now appears in the exponent in $B_\pm$), the tunneling frequency is effectively treated only up to second order— 'interbounce interactions' are neglected.

It is physically plausible that in the limit of either strong damping or high temperatures, coherent tunneling motion would be so impeded that the effective tunneling frequency would be 'small' and the DBGA would be a very good approximation. However it turns out that even for weak damping the DBGA is a systematic approximation at all temperatures, provided $\varepsilon = 0$, since in that case the neglected interbounce interactions can be shown to vanish as K^2 in the limit $K \to 0$. On the other hand, for a biased system ($\varepsilon \neq 0$) and in the limit of weak coupling, the DBGA breaks down at low temperatures, as the interbounce interactions are no longer negligible.

The case of weak damping is especially important for neutron and muon studies of metallic systems at low temperatures as the damping parameter is estimated to be very small, namely $K \approx 0.05$. Motivated by this consideration, Weiss and Wollensak (1989) have recently extended the functional integral technique beyond the DBGA. In this paper we present an alternate treatment, in line with our earlier resolvent expansion approach (Dattagupta *et al* 1989), and show that although the analytic structures of our results are different from those of Weiss and Wollensak, numerically they are hardly distinguishable. Our analysis is based on the simple physical realization that if the damping is weak (i.e. the effect of the second term in (2) is small in some sense) the two terms in H_S (cf. (1)) should be treated on the same footing, and hence it is more meaningful to develop a perturbation theory on the original Hamiltonian in (2) and not the transformed one in (5). The resultant treatment is much more straightforward than the rather formidable functional integral technique and is presented here with the hope that the derived results would be more readily accessible to experimenters interested in neutron scattering of H and muon diffusion in metals at low temperatures.

2. Perturbation treatment in the weak damping limit

2.1 *Preliminaries*

In this and the subsequent sections we follow the same notation as employed in our earlier paper (Dattagupta *et al* 1989). The quantity of interest in the analysis of neutron scattering is the symmetrized correlation function

$$C(t) = \tfrac{1}{2} [\langle \sigma_z(0)\sigma_z(t) \rangle + \langle \sigma_z(t)\sigma_z(0) \rangle] \tag{7}$$

where, for instance,

$$\langle \sigma_z(0)\sigma_z(t) \rangle \equiv \mathrm{Tr}\,(\rho_E \sigma_z(0) \exp{(iHt/\hbar)} \sigma_z(0) \exp{(-iHt/\hbar)}) \tag{8}$$

ρ_E being the density matrix in equilibrium given by

$$\rho_E = \frac{\exp(-\beta H)}{\mathrm{Tr}\,[\exp(-\beta H)]}. \tag{9}$$

In accordance with the objectives spelt out in §1 we would like to treat H_S in (1) exactly. To this end we diagonalize H_S by performing a rotation in the 'spin-space' about the y-axis by an angle $\theta = \mathrm{Arctan}\,(\Delta_0/\varepsilon)$. In the rotated frame the Hamiltonian

in (2) reads

$$\tilde{H} = \frac{1}{2}\hbar\Omega\sigma_z - \frac{1}{\Omega}(\varepsilon\sigma_z + \Delta_0\sigma_x)\sum_j G_j(b_j^+ + b_j) + \sum_j \hbar\omega_j b_j^+ b_j \qquad (10)$$

where

$$\Omega \equiv (\varepsilon^2 + \Delta_0^2)^{\frac{1}{2}}. \qquad (11)$$

Correspondingly,

$$\langle\sigma_z(0)\sigma_z(t)\rangle = \frac{1}{2\Omega^2}\text{Tr}(\tilde{\rho}_E(\varepsilon\sigma_z(0) + \Delta_0\sigma_x(0))(\varepsilon\tilde{\sigma}_z(t) + \Delta_0\tilde{\sigma}_x(t))) \qquad (12)$$

where $\tilde{\rho}_E$ is obtained from (9) upon replacing H by $\tilde{H}$, and

$$\tilde{\sigma}_z(t) \equiv \exp(i\tilde{H}t/\hbar)\sigma_z(0)\exp(-i\tilde{H}t/\hbar). \qquad (13)$$

A similar expression holds for $\tilde{\sigma}_x(t)$.

Our strategy, as set out in §1, is to split $\tilde{H}$ as

$$\tilde{H} = \tilde{H}_S + H_I + H_B \qquad (14)$$

where

$$\tilde{H}_S = \frac{1}{2}\hbar\Omega\sigma_z \qquad (15)$$

$$H_I = -\frac{1}{\Omega}(\varepsilon\sigma_z + \Delta_0\sigma_x)\sum_j G_j(b_j^+ + b_j) \qquad (16)$$

$$H_B = \sum_j \hbar\omega_j b_j^+ b_j. \qquad (17)$$

In the above, we have introduced the subscripts I and B to emphasize that the corresponding terms represent the interaction Hamiltonian and the bath Hamiltonian respectivelty. As we would like to treat H_I perturbatively we make the usual factorization approximation to the density matrix:

$$\tilde{\rho}_E \approx \rho_S \cdot \rho_B \qquad (18)$$

where

$$\rho_S = \frac{1}{2}[1 - \tanh(\frac{1}{2}\hbar\beta\Omega)\sigma_z] \qquad (19)$$

and

$$\rho_B = Z_B^{-1}\exp\left(-\hbar\beta\sum_j \omega_j b_j^+ b_j\right) \qquad (20)$$

Z_B being the partition function associated with the purely bath Hamiltonian H_B.

It is customary to rewrite (13) as

$$\tilde{\sigma}_z(t) = [U(t)\sigma_z(0)] \qquad (21)$$

where $U(t)$ is the so-called time-development operator defined by

$$U(t) \equiv \exp(i\mathscr{L}t) \qquad (22)$$

$\mathscr{L}$ being the Liouvillian associated with $\tilde{H}$. We shall work with the Laplace transform of (22), i.e., the resolvent of the time-development operator given by

$$\hat{U}(z) = 1/(z - i\tilde{\mathscr{L}}).$$ (23)

2.2 *Bath-averaged time-development operator*

Using (7), (12) and (18)–(23), the Laplace transform of the correlation function can be expressed as

$$\hat{C}(z) = \frac{1}{4\Omega^2} \text{Tr}(\rho_B[(\varepsilon\sigma_z(0) + \Delta_0\sigma_x(0)) - \varepsilon\tanh(\tfrac{1}{2}\hbar\beta\Omega)]$$

$$\times [\hat{U}(z)(\varepsilon\sigma_z(0) + \Delta_0\sigma_x(0))]).$$ (24)

We may write out the trace explicitly with the aid of the spin states (denoted by $|\mu\rangle$ with $\mu = \pm 1$) and the occupation number states (denoted by $|n\rangle$), thus

$$\hat{C}(z) = \sum_{nn'}\langle n|\rho_B|n\rangle \sum_{\mu\nu\mu'\nu'} \langle\mu|[\varepsilon\sigma_z(0) + \Delta_0\sigma_x(0) - \varepsilon\tanh(\tfrac{1}{2}\hbar\beta\Omega)]|\nu\rangle$$

$$\langle\nu'|(\varepsilon\sigma_z(0) + \Delta_0\sigma_x(0))|\mu'\rangle(nvn\mu|\hat{U}(z)|n'v'n'\mu').$$ (25)

Introducing then the bath-averaged time-development operator as

$$[U(t)]_{av} \equiv \sum_{nn'}\langle n|\rho_B|n\rangle(nn|U(t)|n'n')$$ (26)

we obtain from (25),

$$\hat{C}(z) = \sum_{\mu\nu\mu'\nu'} \langle\mu|[\varepsilon\sigma_z(0) + \Delta_0\sigma_x(0) - \varepsilon\tanh(\tfrac{1}{2}\hbar\beta\Omega)]|\nu\rangle$$

$$\times \langle\nu'|[\varepsilon\sigma_z(0) + \Delta_0\sigma_x(0)]|\mu'\rangle(\nu\mu|[\hat{U}(z)]_{av}|\nu'\mu').$$ (27)

Recalling from (14) how the Hamiltonian is split, the corresponding Liouvillian operator can be split as

$$\tilde{\mathscr{L}} = \mathscr{L}_S + \mathscr{L}_I + \mathscr{L}_B$$ (28)

Up to second order in $\mathscr{L}_I$ we can then show (Dattagupta 1987)

$$[\hat{U}(z)]_{av} \simeq (z - i\mathscr{L}_S + [\mathscr{L}_I(z - i\mathscr{L}_S - i\mathscr{L}_B)^{-1}\mathscr{L}_I]_{av})^{-1},$$ (29)

where $[\cdots]_{av}$ has been defined in (26).

We need the matrix elements of $[\hat{U}(z)]_{av}$ amongst the spin states (cf. (27)) for calculating $\hat{C}(z)$. Hence it is useful first to enlist the matrix of the *self-energy* in (29). The latter, upon repeated application of the properties of the Liouvillian, can be

written as

$$
\frac{\Delta_0^2}{\Omega^2}
\begin{bmatrix}
\hat{\phi}'(z_-) + \hat{\phi}(z_+) & \hat{\phi}'(z_-) + \hat{\phi}(z_+) & \frac{\varepsilon}{\Delta_0}\{\hat{\phi}(z) + 2\hat{\phi}'(z_-) - \hat{\phi}'(z)\} \\[2mm]
-\hat{\phi}'(z_+) - \hat{\phi}(z_-) & \hat{\phi}'(z_+) + \hat{\phi}(z_-) & \frac{\varepsilon}{\Delta_0}\{\hat{\phi}(z) - 2\hat{\phi}(z_-) + \hat{\phi}'(z)\} \\[2mm]
\frac{\varepsilon}{\Delta_0}\{\hat{\phi}'(z_-) + \hat{\phi}(z_-)\} & -\frac{\varepsilon}{\Delta_0}\{\hat{\phi}'(z_-) + \hat{\phi}(z_-)\} & \hat{\phi}(z) + \hat{\phi}'(z) + 2\frac{\varepsilon^2}{\Delta_0^2}\{\hat{\phi}'(z_-) + \hat{\phi}(z_-)\} \\[2mm]
\frac{\varepsilon}{\Delta_0}\{\hat{\phi}'(z_+) + \hat{\phi}(z_+)\} & -\frac{\varepsilon}{\Delta_0}\{\hat{\phi}'(z_+) + \hat{\phi}(z_+)\} & -\hat{\phi}(z) - \hat{\phi}'(z)
\end{bmatrix}
$$

$$
\begin{bmatrix}
\frac{\varepsilon}{\Delta_0}\{-\hat{\phi}(z) + 2\hat{\phi}(z_+) + \hat{\phi}'(z)\} \\[2mm]
\frac{\varepsilon}{\Delta_0}\{-\hat{\phi}(z) - 2\hat{\phi}'(z_+) + \hat{\phi}'(z)\} \\[2mm]
-\hat{\phi}(z) - \hat{\phi}'(z) \\[2mm]
\hat{\phi}(z) + \hat{\phi}'(z) + 2\frac{\varepsilon^2}{\Delta_0^2}\{\hat{\phi}'(z_+) + \hat{\phi}(z_+)\}
\end{bmatrix}
\tag{30}
$$

where the rows and columns are labelled by $++$, $--$, $+-$ and $-+$ respectively

$$
z_\pm \equiv z \pm i\Omega \tag{31}
$$

$$
\phi(t) \equiv \frac{1}{\hbar^2}\langle X(0)X(t)\rangle_B \tag{32}
$$

and

$$
X(t) \equiv \sum_j G_j(b_j(t) + b_j^+(t)). \tag{33}
$$

In (32) and (33), we have to deal with the statistical mechanical properties of the bath alone. This point has been emphasized by using the subscript B to refer to an average over bath states only, while the time-dependence of the boson operators is governed by just the bath Hamiltonian H_B. The matrix tabulated in (30) has to be combined with the matrix for $z - i\mathscr{L}_S$ and then inverted to obtain the matrix for $[\hat{U}(z)]_{\mathrm{av}}$.

2.3 The bath correlations in the Ohmic case

Uptil now our method has been quite independent of the exact nature of the bath. However, in order to compute $\hat{C}(z)$ we need an explicit structure of the correlation function $\phi(t)$. As the bath consists of an independent set of bosons it is easy to write

$$
\phi(t) = \sum_j G_j^2 [\coth(\tfrac{1}{2}\hbar\beta\omega_j)\cos(\omega_j t) + i\sin(\omega_j t)]. \tag{34}
$$

At this stage we invoke the dissipative character of the bath by going to a continuum

set of bosons, i.e. by replacing the summation over j in (34) by an integral over ω with the aid of an appropriate spectral function (cf. (3)). Choosing for the latter the Ohmic dissipation model (cf. (4)), we find from (34),

$$\phi(t) = \frac{K}{2}\int_0^\infty \omega \exp\left(\frac{-\omega}{D}\right)[\coth(\tfrac{1}{2}\hbar\beta\omega)\cos(\omega t) + i\sin(\omega t)]\,d\omega. \tag{35}$$

The integrals in (35) can be worked out explicitly in terms of Euler's polygamma functions (Abramowitz and Stegun 1965), thus

$$\phi(t) = \frac{K}{2}\frac{1}{(\hbar\beta)^2}\left(\psi'\left(1 + \frac{1}{\hbar\beta D} + \frac{it}{\hbar\beta}\right) + \psi'\left(1 + \frac{1}{\hbar\beta D} - \frac{it}{\hbar\beta}\right)\right.$$
$$\left. + \frac{i}{2}\left(\frac{1}{1+itD}\right)^2 + \frac{i}{2}\left(\frac{1}{1-itD}\right)^2\right) + \frac{iK}{2}\frac{D^3 t}{(1 + D^2 t^2)^2}. \tag{36}$$

Since we are interested in the low temperature dynamics, the limit $\hbar\beta D \gg 1$ applies, which simplifies the result for $\phi(t)$. In this regime the Laplace transform of $\phi(t)$ can be written as

$$\hat{\phi}(z) = \frac{K}{2}zF_1(z) + \frac{K}{2}F_2(z) \tag{37}$$

where

$$F_1(z) = -\psi\left(1 + \frac{z\hbar\beta}{2\pi}\right) - \ln\left(\frac{2\pi}{\hbar\beta}\right) + \frac{\pi}{z\hbar\beta} + \ln(D) - \psi(1) \tag{38}$$

and

$$F_2(z) = i(D - \pi z/2). \tag{39}$$

2.4 Explicit results for the correlation function

As mentioned earlier, we need all the sixteen elements of the matrix for $[\hat{U}(z)]_{av}$ in order to evaluate $\hat{C}(z)$ (cf. (27)). These elements are obtained by inverting a 4×4 matrix as prescribed in (29). Upon employing the algebraic form of $\hat{\phi}(z)$ (cf. (37)), we perform the task of matrix inversion with the use of an algebraic manipulator called REDUCE (Hearn 1985). The following expression emerges for the spin correlation function:

$$\hat{C}(z) = \frac{z^2 + \varepsilon^2 + K[S_1(z) + \tanh(\tfrac{1}{2}\hbar\beta\Omega)S_2(z)] + K^2[Q_1(z) + \tanh(\tfrac{1}{2}\hbar\beta\Omega)Q_2(z)]}{z(z^2 + \Omega^2) + KR_1(z) + K^2 R_2(z)} \tag{40}$$

where

$$S_1(z) \equiv \frac{1}{\Omega^2}(2\varepsilon^2 z_+ z_-(F_1(z_-) + F_1(z_+)) + z\Delta_0^2(z_+ F_1(z_+)$$
$$+ z_- F_1(z_-)) + 2z^2\Delta_0^2 F_1(z)), \tag{41}$$

$$S_2(z) \equiv \frac{1}{z}i(\varepsilon^2\Delta_0^2/\Omega^3)(z_+ F_2(z_-) + z_- F_2(z_+) + 2zF_2(z)), \tag{42}$$

$$R_1(z) \equiv (\varepsilon^2/\Omega^2)z_+ z_-(z_+ F_1(z_-) + z_- F_1(z_+)) + z_+ z_-(z_+ F_1(z_+)$$
$$+ z_- F_1(z_-)) + 2z^3(\Delta_0^2/\Omega^2)F_1(z), \tag{43}$$

$$Q_1(z) \equiv \frac{2}{\Omega^2}(2z_+z_- - \varepsilon^2 F_1(z_-)F_1(z_+) + z\Delta_0^2 F_1(z)(z_+F_1(z_+) + z_-F_1(z_-)))$$

(44)

$$Q_2(z) \equiv \frac{1}{z}i(\varepsilon^2\Delta_0^2/\Omega^3)(z_-F_1(z_-)F_2(z_+) + z_+F_1(z_+)F_2(z_-)$$

$$+ F_2(z)(z_+F_1(z_+) + z_-F_1(z_-)))$$

(45)

$$R_2(z) \equiv \frac{2z}{\Omega^2}(2z_+z_- - \varepsilon^2 F_1(z_-)F_1(z_+) + z\Delta_0^2 F_1(z)(z_+F_1(z_+) + z_-F_1(z_-))).$$

(46)

While this procedure allows us to obtain $\hat{C}(z)$ to all orders in the damping coefficient K, consistency with the present perturbation theory demands that only terms to lowest order in K are retained. Neglecting therefore terms of order K^2 from the numerator and the denominator, (40) is reduced to

$$\hat{C}(z) = \frac{z^2 + \varepsilon^2 + K[S_1(z) + \tanh(\frac{1}{2}\hbar\beta\Omega)S_2(z)]}{z(z^2 + \Omega^2) + KR_1(z)}.$$

(47)

A quantity related to the correlation function $C(t)$, and which allows for a direct comparison with the results of Weiss and Wollensak (1989), is $P(t)$, the time-dependent expectation value $\langle\sigma_z(t)\rangle$, with the specific initial condition that at $t = 0$ the system starts out from one of the two spin-states, say $|+\rangle$. We readily find from (47), for the Laplace transform of $P(t)$,

$$\hat{P}(z) = \frac{z^2 + \varepsilon^2 + K\left[S_1(z) + \frac{\Omega}{\varepsilon}S_2(z)\right]}{z(z^2 + \Omega^2) + KR_1(z)}.$$

(48)

The results given in (47) and (48) describe completely the dynamics of the spin-boson system, in the weak damping limit, down to $T = 0$. Evidently, in the zero damping case ($K = 0$), we have

$$\hat{C}_0(z) = \hat{P}_0(z) = \frac{z^2 + \varepsilon^2}{z(z^2 + \Omega^2)},$$

(49)

a result that can be checked also by a direct calculation of the correlation function for the bare spin-system with the aid of (1) alone.

Finally, one other consistency check on our formalism is to ensure that in the asymptotic ($t \to \infty$) limit the correlation function has its correct equilibrium value. We find from (47), and (36), *before* taking the $\hbar\beta D \gg 1$ limit,

$$\text{Lim}_{t\to\infty} C(t) = \text{Lim}_{z\to 0} z\hat{C}(z) = (\frac{\varepsilon}{\Omega}\tanh(\frac{1}{2}\hbar\beta\Omega))^2.$$

(50)

The right hand side of (50) has the desired form of the square of the expectation value of σ_z in the equilibrium ensemble defined by ρ_s (cf. (19)), as is expected for a thermodynamic system governed by the principle of mixing (Lebowitz and Penrose

1973). This removes an important lacuna of the dilute bounce gas approximation (DBGA) which predicts an incorrect equilibrium value of $C(t)$ (Leggett *et al* 1987; Dattagupta *et al* 1989).

3. Discussion

3.1 *The symmetric case* ($\varepsilon = 0$)

First we concentrate on the symmetric case, the one which has been analyzed in great detail by functional integral and other methods. Setting $\varepsilon = 0$ in (40) we get

$$\hat{C}(z) = \left(z + \frac{\Delta_0^2}{z(1 + 2KF_1(z))} \right)^{-1}. \tag{51}$$

It may be recalled that our expression in (40) was derived by neglecting terms of $O(K^2)$. Interestingly, however, (51) is valid even up to $O(K^2)$, as the corresponding terms cancel out exactly from the numerator and the denominator of (40).

At this stage it is pertinent to compare the result in (51) with that obtained in the DBGA. The latter reads

$$\hat{C}(z) = [z + 2\cos(\pi K)J(z)]^{-1} \tag{52}$$

where $J(z)$ given in terms of certain gamma functions:

$$J(z) = \frac{\Delta_0^2}{2D} \left(\frac{2\pi}{\hbar\beta D} \right)^{2K-1} \frac{\Gamma(1 - 2K)\Gamma(K + z\hbar\beta/2\pi)}{\Gamma(1 - K + z\hbar\beta/2\pi)}. \tag{53}$$

For a meaningful comparison with (51) it is necessary to perform a small K expansion on (52). Doing this, upon which the gamma functions reduce to corresponding digamma functions (Abramowitz and Stegun 1965), (52) can be shown to be identical to (51). Recalling from §1 that the DBGA treats the tunneling term perturbatively the above result implies that for a symmetric system interbounce interactions are negligible, *even* for weak damping. Coupled with the fact that in arriving at (51) we have treated the equilibrium density matrix for the spin system correctly (cf. (19)), we may conclude that the DBGA provides a systematic weak-coupling approximation down to very low temperatures, provided however the asymmetry parameter is zero.

We may finally remark that it is somewhat fortuitous that in the symmetric case and the weak damping limit the DBGA agrees with the present perturbation theory, although in the DBGA the tunneling term is treated perturbatively whereas it has been taken into account exactly in the present work. The mathematical reason behind this is that the tunneling term occurs only as the square of Δ_0 in the symmetric case (cf. (51)) irrespective of how large Δ_0 is. This feature, we believe, is special to the two-level case.

3.2 *The biased case* ($\varepsilon \neq 0$)

The situation now is much more complex, and is described by the full expressions in (47) and (48), in the weak damping limit. These are expected to describe the state of

affairs much more accurately than the DBGA which is known to lead to unphysical results in the weak damping and the low-temperature limit, one of which has been mentioned already in the last paragraph of §2.

Recently, Weiss and Wollensak (1989) have extended the functional integral method and gone beyond DBGA, specifically to treat the low temperature behaviour of the weakly damped system. Their results for $\hat{p}(z)$, obtained after a careful regrouping of all interbounce terms, has a different analytic structure than ours given in (48). We believe, however, that the physical contents of the two results are the same. In order to substantiate this point we plot in figures 1 and 2 $\hat{p}(z)$ obtained from (48) (solid line) and $\hat{p}(z)$ obtained in the modified DBGA (dotted lines). Up to numerical accuracy the two results are practically identical. They, however deviate substantially from the DBGA prediction (the dashed lines).

We compare also numerically the result for the correlation function $\hat{C}(z)$ obtained by us, in the present paper and earlier in the DBGA (Dattagupta *et al* 1989), in figures 3 and 4. While $\hat{C}(z)$ obtained in the present work remains positive, at all temperatures, as it should, the DBGA values become negative at very low temperatures, as can be seen from figure 4.
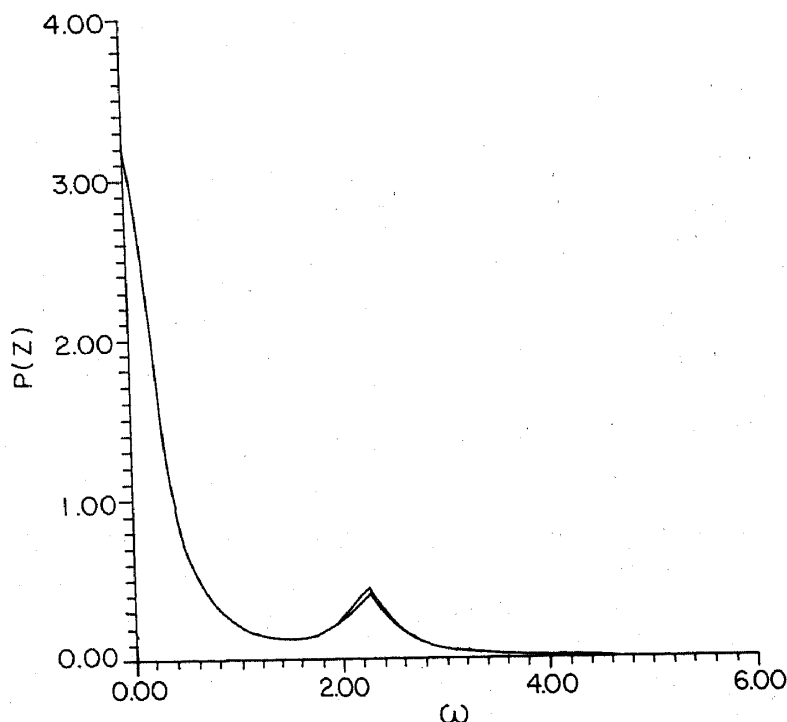
Figure 1. Laplace transformed $P(t)$ based on (48) (solid line), the DBGA result (dashed line) and the result obtained by Weiss and Wollensak (dotted line). The Laplace transform variable is set equal to $i\omega + \Gamma/2$ where Γ has been fixed at 0·5 in order to account for a possible instrumental width in the neutron scattering experiment. The tunneling frequency Δ_0 is fixed at 1, the bias ε at 2, the cutoff D at 100 and the damping coefficient K at 0·001. The temperature $\tau \equiv 1/\hbar\beta$ is 0·01. The solid and the dotted lines overlap with each other.
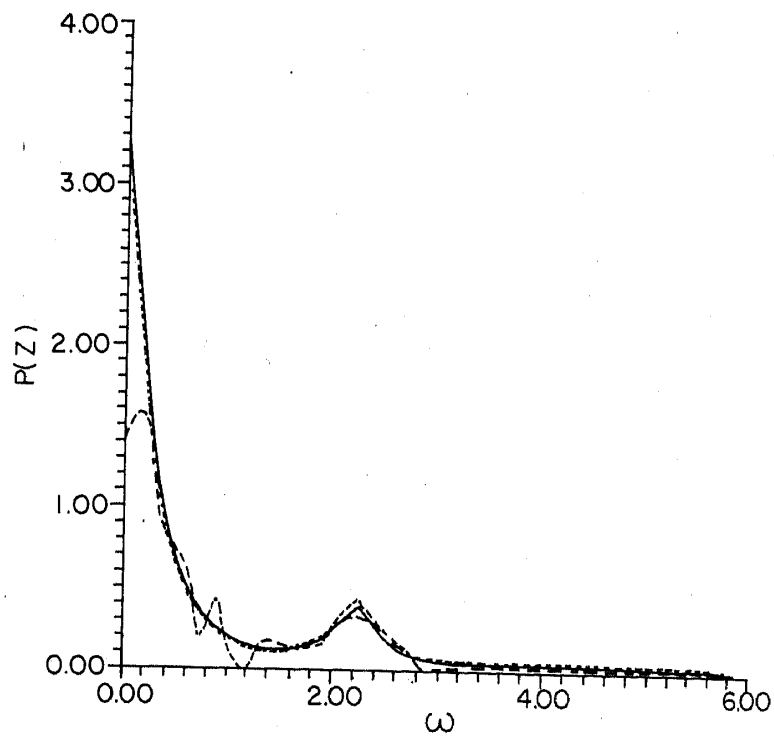
Figure 2. Laplace transformed $P(t)$. All the parameters are the same as in figure 1 except that the temperature τ here is 0.0000001.
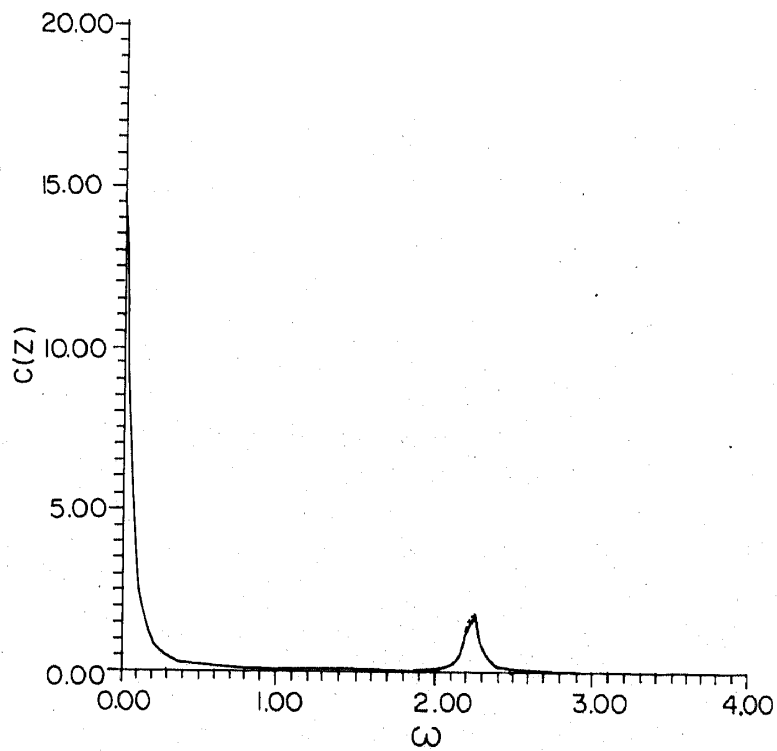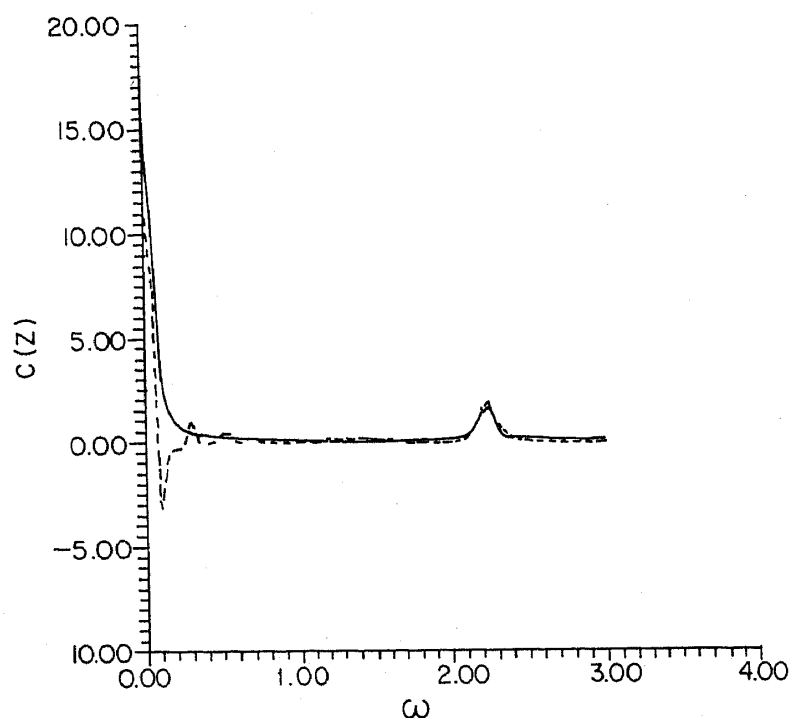

Figure 3. Laplace transformed correlation function $\hat{C}(z)$ based on (47) (solid line) and the DBGA result (dashed line). Γ is fixed at 0.1, Δ_0 at 1, ε at 2, D at 100 and K at 0.001. The temperature τ is 0.001. In this parameter regime our result based on (47) closely matches with the DBGA result.

Figure 4. Laplace transformed correlation function $\hat{C}(z)$. All the parameters are the same as in figure 3 except that τ is 0·0000005. In this regime the DBGA result is totally unphysical as expected. $C(z)$ becomes negative near $\omega = 0$.

4. Conclusions

We have presented a systematic perturbation theory in the weak coupling approximation for a biased two-level dissipative system. The results are expected to be relevant for describing the dynamics of light interstitials e.g. H or μ^+ in metals. Hence they would be of some significance in the analysis of data on neutron scattering and muon spin rotation.

The present work removes also certain unphysical predictions of the widely used DBGA in the weak damping case, especially at low temperatures. On the other hand, the fact that the present and the DBGA results match at high temperatures, even in the weak damping case (cf. figures 1–4), shows that the interbounce interactions become less significant as the temperature increases, a feature which is far from intuitively obvious.

Of course, it should be stressed that the present approach is limited by the fact that the damping is assumed to be weak at the outset. When the damping parameter is not small one has to resort to either the DBGA or its equivalent. However the present work fills in an important gap of the existing theory at low temperatures.

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