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Dynamics of an impurity spin coupled to a spin-boson dissipative system

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Abstract. We study the dynamics of an impurity spin coupled to a spin-boson dissipative system. We calculate the transverse correlation function of the impurity spin and compare the result with that obtained from an equivalent stochastic model. A phenomenological rate parameter in the stochastic model is represented in terms of microscopically obtained quantities. We also calculate the NMR lineshapes for various temperatures which are relevant in the context of a particular physical realization of the model. Motional narrowing of lines is observed at high temperatures.

1. Introduction

The topic of the dynamics of an impurity spin coupled to conduction electrons in metals is important in contemporary condensed matter physics. Starting with the problem of a magnetic impurity in a metal giving rise to the Kondo effect, recent years have witnessed much effort towards the understanding of the motion of defects, such as positive muons or hydrogen in metals. These effects are usually significant at very low temperatures when the phonon contributions are suppressed. For a comprehensive review of the subject of defects in metals we refer the reader to a recent article by Kondo [1].

A defect tunnelling between two trap sites in a metal is an example of a quantum two-state system in contact with a thermal bath. Although the latter is made up of fermions, the low-temperature behaviour is dominated by low-lying excitations off the Fermi surface which are approximately described by bosons. This has motivated the introduction of the spin-boson Hamiltonian that has been the focus of much attention in recent years [2]. The Hamiltonian, written as

$$\mathcal{H} = -\tfrac{1}{2}\hbar\Delta_0\sigma_x + \sigma_z \sum_j G_j(b_j + b_j^+) + \sum_j \hbar\omega_j b_j^+ b_j \tag{1.1}$$

accompanied by the spectral function

$$J(\omega) \equiv \frac{2}{\hbar^2}\sum_j G_j^2\delta(\omega - \omega_j) = K\omega \exp\left(\frac{-\omega}{D}\right) \tag{1.2}$$

provide a mapping of the two-state system in a fermion bath to a two-state system in contact with a bosonic bath. In the above equations the σ are Pauli spin operators representing the two-state system, Δ_0 is the tunnelling frequency, b_j and b_j^+ are the annihilation and creation operators, respectively, for the jth boson of frequency ω_j and

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G_j is the coupling constant. The assumed form of the spectral density given by the last term in (1.2) describes what is known as ohmic dissipation parametrized by the dimensionless constant K and the high-frequency cut-off D.

The object of the present investigation is *not* tunnelling states in metals but the spin dynamics of an impurity spin I coupled to a spin-boson Hamiltonian. What we study is therefore a variant of the problem posed in (1.2) in that the σ now represent a real spin-$\frac{1}{2}$ entity which in turn interacts with another spin I. The chosen Hamiltonian is written as

$$\mathcal{H} = \tfrac{1}{2} a I_z \sigma_z + \sigma_x \sum_j G_j (b_j + b_j^+) + \sum_j \hbar\omega_j b_j^+ b_j + \sum_j \frac{G_j^2}{\hbar\omega_j} \tag{1.3}$$

where a is a coupling parameter and the last term is a counter term that disappears upon a unitary transformation on $\mathcal{H}$ (see below). We are interested in what should be the influence of the dissipative dynamics of the σ on the spin dynamics of I. In particular, we are interested in calculating the transverse correlation function

$$C_{xx}(t) = \langle I_x(0) I_x(t) \rangle \tag{1.4}$$

where $\langle \ldots \rangle$ denotes statistical average.

A motivating factor behind formulating the Hamiltonian in (1.3) is in fact the original Kondo problem in the context of which σ represents the electronic spin of the impurity atom and I represents the nuclear spin of the impurity atom. The first term in (1.3) may therefore be viewed as decribing a uniaxial hyperfine interaction with coupling constant a whereas the spin-boson part is taken to model the interaction between the localized spin σ and the conduction electrons, as is appropriate for a highly anisotropic Kondo system [2]. A quantity such as $C_{xx}(t)$ would be relevant in interpreting resonance experiments (e.g. NMR) [3]. A related quantity is also useful for analysing hyperfine lineshapes as can be measured by the Mössbauer and angular correlation techniques [3].

One other motivation for studying (1.3) arises from the interest in examining the interplay of quantum and dissipative effects, as in the case of the original spin-boson problem. A detailed analysis is also expected to throw light on the underlying basis of certain equivalent Hamiltonians which are often introduced from purely stochastic considerations. Such considerations are derived from the observation that the Hamiltonian in (1.3), in the interaction picture, may be written as

$$\mathcal{H}(t) = \tfrac{1}{2} a I_z \sigma_z(t). \tag{1.5}$$

Hence, in order to simulate dissipative effects it makes sense to replace $\mathcal{H}(t)$ by an effective stochastic Hamiltonian

$$\mathcal{H}(t) = \tfrac{1}{2} a I_z \hbar(t). \tag{1.6}$$

In view of the fact that σ_z can take values $+1$ or -1 it is appropriate to regard $\hbar(t)$ as a two-level jump process in which $\hbar(t)$ is taken to jump at random between two values $+1$ and -1 [4]. The underlying stochastic process, assumed to be Markovian, is specified completely in terms of the rate λ at which the field jumps from $+1$ to -1 and vice versa†. The stochastic model given by (1.6) allows us to make a rather straightforward calculation

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† The assumption that the rate of jump from $+1$ to -1 is the same as that from -1 to $+1$ breaks down, of course, if there is a symmetry-breaking transition in which one of the two states $\sigma_z = \pm 1$ is preferred [2]. Such a transition, however, does not occur in a fermionic system in which K is restricted to be less than or equal to one half [5].

of $C_{xx}(t)$. The resultant expression can then be compared with that obtained from the more detailed quantum mechanical analysis of the dynamics of $\mathcal{H}$ given in (1.3). Such a comparison lends a microscopic meaning to the phenomenological parameter λ that appears in the stochastic model. The connection between models based on stochastic as opposed to dynamic considerations has been the topic of some recent studies of optical processes [6] and our work is a further step in this direction.

The plan of the paper is as follows. In section 2 we set up the method of calculating $C_{xx}(t)$ based on the Hamiltonian given in (1.3). The method, which goes under the name of 'relaxation theory', is only briefly sketched here as most of the details have already been given in our earlier paper on the structure factor calculation for the spin-boson model [7]. As shown in [7], our approach is entirely equivalent to the dilute bounce gas approximation within a functional integral formulation of the problem [2, 7]. In section 3 we present the stochastic theory result of $C_{xx}(t)$ and make a comparison with the result derived in section 2. Our principal conclusions are summarized in section 4.

2. The transverse correlation function

2.1. *The preliminaries*

We have argued earlier [7] that a convenient perturbative treatment of the spin–bath coupling (i.e. the second term in (1.3)) ensues upon making a unitary transformation of the Hamiltonian:

$$\tilde{\mathcal{H}} = S\mathcal{H}S^{-1} \tag{2.1}$$

where S is a unitary operator defined by

$$S \equiv \exp\left(-\sigma_x \sum_j \frac{G_j}{\hbar\omega_j}(b_j - b_j^+)\right). \tag{2.2}$$

We obtain

$$\tilde{\mathcal{H}} = \tfrac{1}{2}aI_z(B_+\sigma_- + B_-\sigma_+) + \sum_j \hbar\omega_j b_j^+ b_j \tag{2.3}$$

where $\sigma_\pm = \sigma_x \pm \mathrm{i}\sigma_y$ and where

$$B_\pm = \exp\left(\pm 2\sum\nolimits_j \frac{G_j}{\hbar\omega_j}(b_j - b_j^+)\right). \tag{2.4}$$

In terms of $\tilde{\mathcal{H}}$ the transverse correlation function in (1.4) may be written as

$$C_{xx}(t) = \mathrm{Tr}[\tilde{\rho} I_x(0)\tilde{I}_x(t)] \tag{2.5}$$

where

$$\tilde{\rho} = \exp(-\beta\tilde{\mathcal{H}})/\mathrm{Tr}[\exp(-\beta\tilde{\mathcal{H}})] \tag{2.6}$$

and

$$\tilde{I}_x(t) = \exp(\mathrm{i}\tilde{\mathcal{H}}t)\, I_x(0)\exp(-\mathrm{i}\tilde{\mathcal{H}}t). \tag{2.7}$$

We may further write

$$\tilde{I}_x(t) = U(t)I_x(0) \tag{2.8}$$

where

$$U(t) \equiv \exp(\mathrm{i}\tilde{L}t) \tag{2.9}$$

$\tilde{L}$ being the Liouvillian associated with $\tilde{\mathcal{H}}$ (the notation used here is the same as in [7]).

Making the customary factorization approximation the density matrix $\tilde{\rho}$ can be expressed as

$$\tilde{\boldsymbol{\rho}} \simeq [1/2(2I+1)]\boldsymbol{\rho}_{\mathrm{B}} \tag{2.10}$$

where $\boldsymbol{\rho}_{\mathrm{B}}$ is the density matrix for the bath, the Hamiltonian of which is given by the second term in (2.3), and I is the value of the spin I. This approximation is very good if $a \ll K_{\mathrm{B}}T$ as is often the case for the hyperfine interaction in metals. With this the Laplace transform of $C_{xx}(t)$ is given by

$$\tilde{C}_{xx}(z) = [1/2(2I+1)]\,\mathrm{Tr}_{\mathrm{s}}\{I_x\,\mathrm{Tr}_{\mathrm{B}}[\boldsymbol{\rho}_{\mathrm{B}}\hat{U}(z)]\,I_x\} \tag{2.11}$$

where

$$\hat{U}(z) = 1/(z - \mathrm{i}\hat{L}) \tag{2.12}$$

and Tr_{s} and Tr_{B} represent the traces over the quantum states of the coupled spin system (of I and σ) and the bath, respectively. Denoting the states of I by the indices m_0 and m_1 and those of σ by the indices μ and ν, (2.11) may be re-expressed as

$$\tilde{C}_{xx}(z) = \frac{1}{2(2I+1)} \sum_{m_0 m_1} |\langle m_1|I_x|m_0\rangle|^2 \times \sum_{\nu} (m_0\nu, m_1\nu|\mathrm{Tr}_{\mathrm{B}}[\boldsymbol{\rho}_{\mathrm{B}}\hat{U}(z)]|m_0\nu', m_1\nu').$$

In writing (2.13) we have used the fact that $\mathcal{H}_1$ is diagonal amongst the states of I.

2.2. Resolvant expansion

Our strategy is first to evaluate the trace over the bath states. Formally,

$$\mathrm{Tr}_{\mathrm{B}}[\boldsymbol{\rho}_{\mathrm{B}}\hat{U}(z)] \equiv [\hat{U}(z)]_{\mathrm{av}} = \sum_{n,n'} \langle n|\boldsymbol{\rho}_{\mathrm{B}}|n\rangle\,(nn|\hat{U}(z)|n'n') \tag{2.14}$$

where $|n\rangle$ denotes the occupation number states for the boson operators and $|nn)$ the 'states' for the corresponding Liouvillian (see [7]). Developing the interaction term, i.e. the term associated with the first term in (2.3), as a perturbation and suitably rearranging terms up to the second order, we have

$$[\hat{U}(z)] = 1/\{z + [L_1(z - iL_{\mathrm{B}})^{-1}L_1]_{\mathrm{av}}\} \tag{2.15}$$

where L_1 is the Liouvillian associated with the interaction Hamiltonian

$$\mathcal{H}_1 = \tfrac{1}{2}aI_z(B_+\sigma_- + B_-\sigma_+) \tag{2.16}$$

and L_{B} is the Liouvillian associated with the bath Hamiltonian

$$\mathcal{H}_{\mathrm{B}} = \sum_j \hbar\omega_j b_j^+ b_j. \tag{2.17}$$

As we need the matrix elements of $[\hat{U}(z)]_{\mathrm{av}}$ amongst the combined spin states of I and σ it is convenient first to tabulate the matrix elements of the self-energy in (2.15). Applying the properties of the Liouvillian, we find that

$$(m_0\mu, m_1\nu|[L_1(z - \mathrm{i}L_{\mathrm{B}})^{-1}L_1]_{\mathrm{av}}|m_0\mu', m_1\nu') = \frac{1}{\hbar^2}\sum_{n,n'} \langle n|\boldsymbol{\rho}_{\mathrm{B}}|n\rangle \left(\sum_{\eta} \frac{m_0\mu n|\mathcal{H}_1|m_0\eta n'\rangle\langle m_0\eta n'|\mathcal{H}_1|m_0\mu' n\rangle}{z - (\mathrm{i}/\hbar)(E_{n'} - E_n)}\,\delta_{\nu\nu'}\right.$$

$$
\begin{aligned}
&+\sum_{\eta}\frac{\langle m_1\nu' n|\mathcal{H}_{\mathrm{I}}|m_1\eta n'\rangle\langle m_1\eta n'|\mathcal{H}_{\mathrm{I}}|m_1\nu n\rangle}{z-(\mathrm{i}/\hbar)(E_n-E_{n'})}\,\delta_{\mu\mu'}\\
&-\frac{\langle m_0\mu n|\mathcal{H}_{\mathrm{I}}|m_0\mu' n'\rangle\langle m_1\nu' n'|\mathcal{H}_{\mathrm{I}}|m_1\nu n\rangle}{z-(\mathrm{i}/\hbar)(E_{n'}-E_n)}\\
&-\frac{\langle m_0\mu n|\mathcal{H}_{\mathrm{I}}|m_0\mu' n'\rangle\langle m_1\nu' n'|\mathcal{H}_{\mathrm{I}}|m_1\nu n\rangle}{z-(\mathrm{i}/\hbar)(E_n-E_{n'})}\Bigg)
\end{aligned}
\tag{2.18}
$$

where E_n is the eigenvalue of the bath Hamiltonian $\mathcal{H}_{\mathrm{B}}$. The next step is to plug in the explicit form of $\mathcal{H}_{\mathrm{I}}$ (cf (2.16)), rewrite the denominators back in the form of integrals over t and express the sum over the bath states (n, n', etc) as correlation functions for bath operators. We find for the matrix of $[L_{\mathrm{I}}(z-\mathrm{i}L_{\mathrm{B}})^{-1}L_{\mathrm{I}}]_{\mathrm{av}}$, for a fixed set of m_0 and m_1 and within the subspace of σ, the elements:

$$
\begin{bmatrix}
a_0^2m_0^2\hat{\Phi}_{-+}(z)+a_1^2m_1^2\hat{\Phi}'_{-+}(z) & -a_0a_1m_0m_1[\hat{\Phi}_{-+}(z)+\hat{\Phi}'_{-+}(z)] & 0 & 0\\
-a_0a_1m_0m_1[\hat{\Phi}_{+-}(z)+\hat{\Phi}'_{+-}(z)] & a_0^2m_0^2\hat{\Phi}_{+-}(z)+a_1^2m_1^2\hat{\Phi}'_{+-}(z) & 0 & 0\\
0 & 0 & a_0^2m_0^2\hat{\Phi}_{-+}(z)+a_1^2m_1^2\hat{\Phi}'_{+-}(z) & -a_0a_1m_0m_1[\hat{\Phi}_{--}(z)+\hat{\Phi}'_{--}(z)]\\
0 & 0 & -a_0a_1m_0m_1[\hat{\Phi}_{++}(z)+\hat{\Phi}'_{++}(z)] & a_0^2m_0^2\hat{\Phi}_{+-}(z)+a_1^2m_1^2\hat{\Phi}'_{-+}(z)
\end{bmatrix}
\tag{2.19}
$$

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

$$
\Phi_{\pm\pm}(t)=(1/4\hbar^2)\langle B_\pm(0)B_\pm(t)\rangle.
\tag{2.20}
$$

Further, all primed quantities are obtained by replacing the argument t by $-t$, and the hat denotes the Laplace transform. It may be stressed that the angular brackets in (2.20) denote thermal averages governed by ρ_{B} and the time development of $B_\pm(t)$ is dictated by $\mathcal{H}_{\mathrm{B}}$ alone. It may also be noted that in writing the elements in (2.19) we have kept in mind the possibility that the hyperfine constant takes two distinct values a_0 and a_1 depending on whether the state is m_0 or m_1. This is particularly relevant in an experiment involving the Mössbauer effect wherein the states m_0 and m_1 refer to the ground and excited states of the nucleus. On the other hand, in the case of magnetic resonance or angular correlation experiments, $a_0=a_1=a$ [3].

The matrix (2.19) has to be added to z and then inverted. However, as is evident from (2.13), we need to focus only on the upper left block in (2.19), and thus we find (displaying only the upper left block) for the matrix of $[\tilde{U}(z)]_{\mathrm{av}}$

$$
\frac{1}{\det(m_0,m_1)}
\begin{bmatrix}
z+a_0^2m_0^2\hat{\Phi}_{+-}(z)+a_1^2m_1^2\hat{\Phi}'_{+-}(z) & m_0m_1a_0a_1[\hat{\Phi}_{-+}(z)+\hat{\Phi}'_{-+}(z)]\\
m_0m_1a_0a_1[\hat{\Phi}_{+-}(z)+\hat{\Phi}'_{+-}(z)] & z+a_0^2m_0^2\hat{\Phi}_{-+}(z)+a_1^2m_1^2\hat{\Phi}'_{-+}(z)
\end{bmatrix}
\tag{2.21}
$$

where $\det(m_0,m_1)$ is given by

$$
\begin{aligned}
\det(m_0,m_1)\equiv z^2&+z\{(a_0m_0)^2[\hat{\Phi}_{+-}(z)+\hat{\Phi}_{-+}(z)]\\
&+(a_1m_1)^2[\hat{\Phi}'_{+-}(z)+\hat{\Phi}'_{-+}(z)]\}+(a_0^2m_0^2-a_1^2m_1^2)\\
&\times[(a_0m_0)^2\hat{\Phi}_{+-}(z)\hat{\Phi}_{-+}(z)-(a_1m_1)^2\hat{\Phi}'_{+-}(z)\hat{\Phi}'_{-+}(z)].
\end{aligned}
\tag{2.22}
$$

Using the correlation function for the bath variables within the ohmic dissipation model we have shown earlier that [7]

$$\begin{aligned}\hat{\Phi}_{+-}(z) = \hat{\Phi}_{-+}(z) \equiv \hat{\Phi}(z) = F(z)\ \exp(\mathrm{i}\pi K)\\ \hat{\Phi}'_{+-}(z) = \hat{\Phi}'_{-+}(z) \equiv \hat{\Phi}'(z) = F(z)\exp(-\mathrm{i}\pi K)\end{aligned} \qquad (2.23)$$

where

$$F(z) = (1/4D\hbar^2)(2\pi/\hbar\beta D)^{2K-1}[\Gamma(1-2K)\Gamma(K + z\hbar\beta/2\pi)/\Gamma(1-K+z\hbar\beta/2\pi)]. \qquad (2.24)$$

2.3. Result for the correlation function

It is evident from (2.13) that the quantity of central importance are the matrix elements of the averaged time-development operator that may be denoted as

$$G_{m_0 m_1}(z) \equiv \sum_{\nu\nu'} (m_0\nu, m_1\nu|(\mathrm{Tr}_{\mathrm{B}}[\rho_{\mathrm{B}}\hat{U}(z)])|m_0\nu', m_1\nu'). \qquad (2.25)$$

A knowledge of $G_{m_0m_1}(z)$ is adequate for evaluating the lineshapes for different kinds of hyperfine spectra [7]. After some algebra we obtain

$$G_{m_0m_1}(z) = \{z + F(z)[(a_0m_0 - a_1m_1)^2\cos(\pi K) + \mathrm{i}(a_0^2m_0^2 - a_1^2m_1^2)\sin(\pi K)]\}^{-1}. \qquad (2.26)$$

Specializing here to NMR, and also for simplicity considering the case $I = \frac{1}{2}$, we find that

$$\tilde{C}_{xx}(z) = 1/[z + a^2F(z)\cos(\pi K)]. \qquad (2.27)$$

Equation (2.26) forms the basis for comparison with the stochastic model results given next in section 3.

3. Stochastic theory

The physical ideas behind the stochastic considerations have already been expounded in section 1. The stochastic Hamiltonian, given in (1.6), affords a drastic simplification to the theory in that a quantum many-body problem is replaced by an effective classical one in which the field $\hbar(t)$ is viewed as a two-level jump process [3]. The extent to which this simplified picture is valid and its limitations are the subject of this section.

In terms of λ, the rate at which the field jumps from +1 to −1 and vice versa, the Laplace transform of the averaged time-development operator is given as [3]

$$[\hat{U}(z)]_{\mathrm{av}} = \{z + (1/\hbar^2)[(aI_z^x)^2/(z+\lambda)]\}^{-1} \qquad (3.1)$$

where I_z^x is the Liouvillian associated with I_z. Needless to say, $[\ldots]_{\mathrm{av}}$ now represents the average over the underlying stochastic process in contrast with the previous case in which the averaging involves the quantum states of the heat bath. Consequently (cf (2.26)),

$$G_{m_0m_1}(z) = \{z + (1/\hbar^2)[(a_0m_0 - a_1m_1)^2/(z+\lambda)]\}^{-1}. \qquad (3.2)$$

In the NMR case for $I = \frac{1}{2}$, we have

$$G_{m_0m_1}(z) = [z + (a/2\hbar)^2/(z+\lambda)]^{-1}. \qquad (3.3)$$

When we contrast (3.2) to the result given in (2.26) which is obtained from a more detailed analysis, it is evident that the latter is much richer in structure. First of all, the relaxation parameters in (2.26) described by the second term inside the braces depend strongly on the frequency z. Such non-Markovian features are expected, of course, when the heat bath is a quantum system. Second, these parameters depend also on the hyperfine constants (a_0 and a_1), indicating the importance of the 'feedback' of the subsystem into the heat bath.

The comparison with the stochastic model is clearer in the case of NMR and also for $I = \frac{1}{2}$. From (2.27) and (3.3) we see that the term which plays the role of $z + \lambda$ *is* $\gamma(K, z)$ where

$$\gamma(K,z) \equiv D(\hbar\beta D/2\pi)^{2K-1}[\Gamma(1-K+z\hbar\beta/2\pi)/\Gamma(1-2K)\Gamma(K+z\hbar\beta/2\pi)]\sec(\pi K). \tag{3.4}$$

Making a 'weak-coupling' expansion we may write

$$\gamma(K,z) = \gamma(0,z) + K[\partial\gamma(K,z)/\partial K]|_{k=0} + \ldots \simeq z + K[\partial\gamma(K,z)/\partial K]|_{k=0}. \tag{3.5}$$

Thus the 'relaxation rate' is described by the second term in (3.5) which is still frequency dependent.

Another special situation which allows for an explicit comparison with the stochastic theory results is the 'motional narrowing' limit in which λ is so large that $z + \lambda$ may be replaced by λ in the second term in (3.3), yielding

$$G_{m_0 m_1}(z) = [z + (a/2\hbar)^2/\lambda]^{-1}. \tag{3.6}$$

Therefore, in this limit, λ turns out to be same as $\gamma(K, z = 0)$ where

$$\gamma(K,0) \equiv D(\hbar\beta D/2\pi)^{2K-1}[\Gamma(1-K)/\Gamma(1-2K)\Gamma(K)]\sec(\pi K). \tag{3.7}$$

The motional narrowing limit is relevant when the temperature is high, i.e. β is small so that the term $z\hbar\beta$ in the argument of the gamma functions in (3.4) may be ignored. This is also in conformity with the result given in (3.7) which shows that the rate of relaxation increases with increasing temperature (for $K < \frac{1}{2}$). However, the significant point is that this increase is governed by a 'power law' of the form T^{1-2K} which is entirely a non-classical feature.

4. Concluding analysis

We have studied a system of interacting spins coupled to a heat bath, using a fully quantum mechanical analysis. The relaxation behaviour of such a system depends on the nature of the correlation functions of the bath. Various studies have been made earlier on similar systems where the system–heat bath coupling is treated perturbatively [6]. Explicit analysis is possible only in the following two limiting cases. In the first, the heat bath coupling viewed as noise is assumed to vary so slowly that the system—the spin system in the present context—has time to maintain its quantum coherence and to evolve quantum mechanically. In the second, the noise is assumed to vary so quickly that the quantum coherence is completely lost and the Brownian picture (that obtained in the 'motionaly narrowed' regime) is what one expects to see.

For most systems, however, the correlation time of the noise is somewhere between the two extremes and this is where an explicit dynamical study of the bath becomes important. In our analysis of the model we have probed a wide regime of the noise

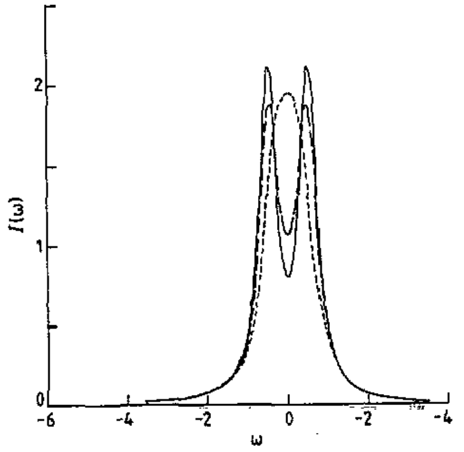

Figure 1. NMR lineshape based on (2.27). For convenience, we have introduced the dimensionless variables $\tau = 2\pi/a\beta$, $\omega_D = \hbar D/a$ and $s = \hbar z/a$. The Laplace transform variable s is set equal to $i\omega + \Gamma/2$ where Γ has been fixed at 0.5 in order to account for the possible instrumental width. The temperature τ is fixed at 10 and the dimensionless cut-off ω_D at 100. We plot the dimensionless lineshape $I(\omega) = (a/\hbar)\hat{C}(z)$: ——, $K = 0$; – – –, $K = 0.05$; · · · · ·, $K = 0.2$.

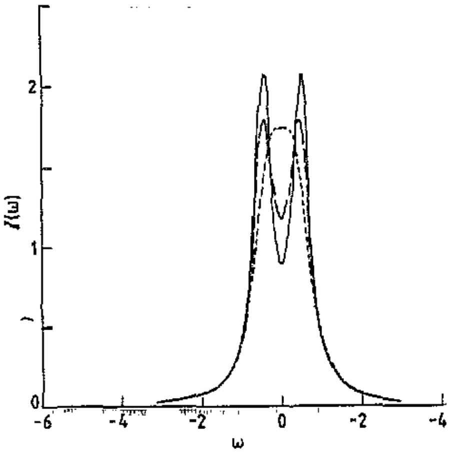

Figure 2. NMR lineshape for $K = 0.01$, $\omega_D = 100$ and $\Gamma = 0.5$ for various values of the temperature τ: ——, $\tau = 1$; – – –, $\tau = 15$; · · · · ·, $\tau = 50$.

correlation time. The two extreme cases are easily recoverable as shown in section 3 and also in NMR plots (figure 1). These plots are based on our general result given in (2.27). For weak coupling, quantum coherence manifests itself in two narrow peaks. For strong coupling, the two lines collapse into a single 'motionally narrowed' line centred at $\omega = 0$.

In a real experiment the quantity which can be manipulated is the temperature; so we also look at the NMR lineshapes for various temperatures and constant coupling strength (figure 2). Again we see that the two peaks at low temperatures collapse into a single peak as the temperature is increased. Thus the study explicitly brings out the interplay of quantum and dissipative effects which was one of the motivations behind the present work.

The results obtained by us are valid for a wide range of temperatures and coupling strengths. They can, however, be improved for very small values of K at very low temperatures.

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