

Low frequency, low temperature properties of the spin-boson problem^{*}

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Received 7 July 2000 and Received in final form 8 August 2000

Abstract. Low temperature and low frequency properties of a spin-boson model are investigated within a super operator and Liouville space formulation. The leading contributions are identified with the help of projection operators projecting onto the equilibrium state. The quantities of interest are expressed in terms of weighted bath propagators and static linear and nonlinear susceptibilities. In particular the generalized Shiba relation and Wilson ratio are recovered.

PACS. 05.30.-d Quantum statistical mechanics – 66.35.+a Quantum tunneling of defects

1 Introduction

The spin-boson model is one of the simplest models to study the interplay of quantum mechanics and dissipation due to the interaction with an environment. It consists in a quantum mechanical spin $\frac{1}{2}$ weakly coupled to a macroscopic heat bath made up of harmonic oscillators. This and similar models of dissipative quantum systems have been widely studied in the literature [1–3].

The total system including the bath is described by a Hermitean Hamiltonian and the corresponding Schrödinger or Heisenberg equation. The goal is, however, to obtain an effective description of the dynamics of the subsystem having averaged over the bath degrees of freedom. An example is the dynamics of a spin $\frac{1}{2}$ ruled by Bloch equations.

Especially for low frequencies and low temperatures one expects that an effective description might exist which is of the same structure as perturbation theory but with renormalized parameters. This is expected in analogy to the Landau-Fermi-liquid theory where effective masses and interactions can be obtained from static expectation values or experiments.

For the spin-boson model results of this kind are known. For instance the ratio of the specific heat at low temperature and the static transverse susceptibility is determined by a bath propagator weighted with the spin-bath interaction. This has been found by Sasseti and Weiss [4] as generalization of the corresponding ratio for the Kondo problem, known as Wilson ratio. Perturbation theory yields the same result but with the transverse susceptibility replaced by its free value. Another example is

the Shiba relation for the Anderson model [5] generalized again to the spin-boson model [4]. It states that the long time behavior of the transverse correlation function at zero temperature is again given by the static transverse susceptibility and the long time property of a weighted bath propagator. Again this result agrees with perturbation theory provided the susceptibility is replaced by its free value.

The present paper deals with the low frequency and low temperature properties of a spin-boson system. In particular a setup is investigated which allows to express the low frequency and low temperature properties in terms of bath propagators and static linear and nonlinear susceptibilities. This setup is based on a Liouville space formulation [6, 7]. The first Section gives a brief survey of this formalism. The spin-boson model is introduced in Section 2 and the weighted bath propagators are discussed. Section 3 deals with the long time behavior of transverse and longitudinal correlation and response functions. This includes the Shiba relation and fluctuation dissipation theorems. The specific heat at low temperature and the Wilson ratio are discussed in Section 4. As mentioned above the present analysis is based on the existence of certain static linear and nonlinear susceptibilities. The question under which conditions they do exist or do not exist [3], for instance because of localization, is not addressed. Furthermore the susceptibilities may depend on the high frequency cutoff of the bath oscillators resulting in non universal prefactors.

2 Liouville space and super operators

A convenient starting point is a formulation in Liouville space [6, 7]. This is the linear space spanned by quantum mechanical Hermitean operators and each operator \hat{A}

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is considered as a vector $|A\rangle$ in this space. Super operators \mathcal{O} are introduced as mappings of the quantum mechanical operators onto themselves. An example is the von Neumann equation for the statistical operator $\hat{\rho}(t)$

$$\frac{d}{dt}\hat{\rho}(t) = -i[\hat{H}(t), \hat{\rho}(t)] \Leftrightarrow \mathcal{L}(t)|\rho(t) \quad (2.1)$$

defining the Liouville super operator $\mathcal{L}(t)$. Here and in the following $\hbar = 1$ is assumed.

There are several possibilities to define a scalar product. In the following

$$(A|B) = \text{Tr } \hat{A}\hat{B} \quad (2.2)$$

is used.

The temporal evolution is described by the super operator $\mathcal{U}(t, t')$ which obeys

$$\frac{d}{dt}\mathcal{U}(t, t') = \mathcal{L}(t)\mathcal{U}(t, t') \quad (2.3)$$

with initial condition $\mathcal{U}(t, t) = \mathbf{I}$ and $\mathbf{I}|A\rangle = |A\rangle$.

The measurement of an observable \hat{A} can also be represented as the action of a super operator \mathcal{A} with

$$\mathcal{A}|X\rangle \Leftrightarrow \frac{1}{2}\{\hat{A}\hat{X} + \hat{X}\hat{A}\} \quad (2.4)$$

where the identity vector $|1\rangle$ obeys $\mathcal{A}|1\rangle = |A\rangle$. This allows to write the equilibrium correlation functions for time independent \mathcal{L} and $t > t'$ as

$$C_{AB}(t, t') = (1|\mathcal{A}\mathcal{U}(t, t')\mathcal{B}|\bar{\rho}). \quad (2.5)$$

The equilibrium statistical operator obeys $\mathcal{L}|\bar{\rho}\rangle = 0$.

Adding external fields to the Hamiltonian $\hat{H}(t) \rightarrow \hat{H} - h_B(t)\hat{B}$ response functions are defined as

$$G_{AB}(t, t') = \frac{\delta \langle \hat{A}(t) \rangle}{\delta h_B(t')} = (1|\mathcal{A}\mathcal{U}(t, t')\tilde{\mathcal{B}}|\bar{\rho}) \quad (2.6)$$

with

$$\tilde{\mathcal{B}}|X\rangle \Leftrightarrow i[\hat{B}, \hat{X}]. \quad (2.7)$$

For spin $\frac{1}{2}$ a complete set of quantum mechanical operators is formed by the identity and the Pauli matrices. They can be used as basis vectors of the corresponding Liouville space:

$$\begin{aligned} |1\rangle &\Leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & |x\rangle &\Leftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ |y\rangle &\Leftrightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} & |z\rangle &\Leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \quad (2.8)$$

This results in a 4-dimensional representation

$$\begin{aligned} |1\rangle &\Leftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} & |x\rangle &\Leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\ |y\rangle &\Leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} & |z\rangle &\Leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \end{aligned} \quad (2.9)$$

Super operators are then 4×4 matrices, for instance

$$\begin{aligned} \sigma_x &\Leftrightarrow \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} & \tilde{\sigma}_x &\Leftrightarrow 2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \\ \sigma_z &\Leftrightarrow \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} & \tilde{\sigma}_z &\Leftrightarrow 2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \end{aligned} \quad (2.10)$$

For particles, especially the bath oscillators, the Wigner representation is used. The corresponding Liouville space is spanned by functions $|X\rangle \Leftrightarrow X(p, x)$ of the coordinates x and momenta p . The scalar product is

$$(Y|X) = \int dp dx Y(p, x) X(p, x). \quad (2.11)$$

The super operators for the measurement of position and momentum and the corresponding response operators are

$$\begin{aligned} \mathbf{x} &\Leftrightarrow x & \tilde{\mathbf{x}} &\Leftrightarrow -\frac{\partial}{\partial p} \\ \mathbf{p} &\Leftrightarrow p & \tilde{\mathbf{p}} &\Leftrightarrow \frac{\partial}{\partial x}. \end{aligned} \quad (2.12)$$

A general super operator \mathcal{O} in Wigner representation is a function of four variables $\mathcal{O}(x, p, x', p')$.

The Liouville space of the combined system and bath oscillators is the direct product of the individual spaces, for instance the four dimensional space of a spin $\frac{1}{2}$ and a Wigner representation for each bath oscillator.

3 Spin-boson problem

The Hamiltonian of a tunneling center or a spin $\frac{1}{2}$ interacting with a thermal bath of N harmonic oscillators is

$$\begin{aligned} \hat{H} &= -\frac{1}{2}\Delta\hat{\sigma}_x - \frac{1}{2}\varepsilon\hat{\sigma}_z - \frac{1}{\sqrt{N}}\sum_k \Lambda_k \hat{x}_k \hat{\sigma}_z \\ &+ \frac{1}{2}\sum_k \{\hat{p}_k^2 + \omega_k^2 \hat{x}_k^2\} \end{aligned} \quad (3.1)$$

where Δ is the bare tunneling splitting and ε a bias or anisotropy. Eventually the limit $N \rightarrow \infty$ is considered and the $1/\sqrt{N}$ scaling of the spin-bath coupling constants is explicitly written down. In the following the isotropic case $\varepsilon = 0$ is considered primarily, but generalizations to the general case are possible.

The resulting Liouville operator (2.1) is

$$\begin{aligned} \mathcal{L} = & \frac{1}{2}\Delta\tilde{\sigma}_x + \frac{1}{2}\varepsilon\tilde{\sigma}_z + \frac{1}{\sqrt{N}} \sum_k A_k \left\{ \sigma_z \tilde{x}_k + x_k \tilde{\sigma}_z \right\} \\ & - \sum_k \left\{ p_k \tilde{p}_k + \omega_k^2 x_k \tilde{x}_k \right\}. \end{aligned} \quad (3.2)$$

The bath is characterized by its density of states

$$J(\omega) = \frac{1}{N} \sum_k \frac{A_k^2}{\omega_k} \delta(\omega - \omega_k) = \alpha \Theta^{1-s} \omega^s e^{-\omega/\Theta} \quad (3.3)$$

where the special case of a power law dependence is of interest. The case $s = 1$ is usually referred to as Ohmic case. A tunneling center in a crystal or glass requires a super Ohmic spectrum with $s = 3$. There is a high frequency cutoff Θ representing the Debye frequency and the same frequency is used to define the dimensionless coupling constant α for $s \neq 1$.

Because of the $1/\sqrt{N}$ dependence of the couplings the correlation and response functions of the bath oscillators are unperturbed. For an oscillator with frequency ω_k the x_k - x_k -response function for $t > 0$ is

$$F_k(t) = \frac{1}{\omega_k} \sin \omega_k t \quad (3.4)$$

and the corresponding correlation function at temperature $T = 1/\beta$ is

$$D_k(t) = \frac{n(\omega_k)}{\omega_k} \cos \omega_k t \quad (3.5)$$

with

$$n(\omega) = \frac{1}{2} \coth \frac{1}{2} \beta \omega. \quad (3.6)$$

The action of the bath on the spin involves the weighted bath propagators

$$F(t) = \frac{1}{N} \sum_k A_k^2 F_k(t) \quad (3.7)$$

and

$$D(t) = \frac{1}{N} \sum_k A_k^2 D_k(t). \quad (3.8)$$

Introducing the Fourier transforms

$$\hat{F}(\omega) = \int_0^\infty dt e^{i\omega t} F(t) \quad (3.9)$$

and

$$\hat{D}(\omega) = \int_{-\infty}^\infty dt e^{i\omega t} D(t) \quad (3.10)$$

one finds for the imaginary part of $\hat{F}(\omega)$

$$\Im \hat{F}(\omega) = \frac{\pi}{2} \text{sign}(\omega) J(|\omega|) \quad (3.11)$$

and for $\hat{D}(\omega)$

$$\hat{D}(\omega) = \pi n(|\omega|) J(|\omega|) = 2n(\omega) \Im \hat{F}(\omega). \quad (3.12)$$

This last expression is a special case of the quantum mechanical fluctuation dissipation theorem (FDT) [6, 7]

$$\hat{C}_{AB}(\omega) = 2n(\omega) \Im \hat{G}_{AB}(\omega) \quad (3.13)$$

which holds for any pair of operators A and B having the same parity with respect to time reversal.

For the power law density of states (3.3) one finds

$$\begin{aligned} F(t) = & \alpha \Theta^2 \Gamma(s+1) \sin \left((s+1) \arctan(\Theta t) \right) \\ & \times \left(1 + (\Theta t)^2 \right)^{-(s+1)/2} \end{aligned} \quad (3.14)$$

and for $T = 0$

$$\begin{aligned} D_0(t) = & \frac{1}{2} \alpha \Theta^2 \Gamma(s+1) \cos \left((s+1) \arctan(\Theta t) \right) \\ & \times \left(1 + (\Theta t)^2 \right)^{-(s+1)/2}. \end{aligned} \quad (3.15)$$

The leading correction for finite temperature is $\delta D(t) = D(t) - D_0(t)$ with

$$\begin{aligned} \delta D(t) = & \int_0^\infty d\bar{\omega} \frac{J(\bar{\omega})}{e^{\beta\bar{\omega}} - 1} \cos \bar{\omega} t \\ = & \alpha T^2 (\Theta/T)^{1-s} d(Tt) \end{aligned} \quad (3.16)$$

and

$$\begin{aligned} d(\tau) = & \int_0^\infty dx \frac{x^s}{e^x - 1} \cos x\tau \\ = & \sum_{\ell=1}^\infty \Gamma(s+1) \cos \left((s+1) \arctan(\tau/\ell) \right) \\ & \times \left(\ell^2 + \tau^2 \right)^{-(s+1)/2} \\ \xrightarrow{\tau \rightarrow 0} & \Gamma(s+1) \zeta(s+1) - \frac{1}{2} \Gamma(s+3) \zeta(s+3) \tau^2 \\ \xrightarrow{\tau \rightarrow \infty} & \Gamma(s) \cos(s\pi/2) \tau^{-s} + \frac{1}{2} \Gamma(s+1) \\ & \times \sin(s\pi/2) \tau^{-s-1}. \end{aligned} \quad (3.17)$$

A formal perturbation theory for expressions like (2.5) or (2.6) can be set up by writing

$$\mathbf{u}(t, t') = \mathbf{T} \left[\exp \int_{t'}^t ds \mathcal{L}(s) \right] \quad (3.18)$$

operator $|\bar{\rho}\rangle = \mathbf{u}(t', -\infty)|i\rangle$ is used. The initial state is not relevant assuming that the system has equilibrated at time t' . As a next step the exponential is expanded in a sum of products of free evolution operators in spin space and bath operators. Finally all bath operators have to be contracted in pairs to bath response functions $F(t)$ or correlation functions $D(t)$.

4 Long time behavior

The following analysis of the long time behavior is based on two arguments:

- 1) The system tends towards equilibrium

$$\mathbf{U}(t) \xrightarrow[t \rightarrow \infty]{} |\bar{\rho}\rangle(1) \quad (4.1)$$

2) The long time properties are ruled by the long time properties of the averaged bath response function $F(t)$, (3.14), and the bath correlation function $D(t)$, (3.15) and (3.16).

In order to isolate the leading contributions at long time a set of projection operators is introduced

$$\begin{aligned} \mathcal{P}_0 &= |\bar{\rho}\rangle(1) \\ \mathcal{P}_1 &= \sum_k \left\{ \tilde{\mathbf{x}}_k |\bar{\rho}\rangle(1) \mathbf{p}_k - \tilde{\mathbf{p}}_k |\bar{\rho}\rangle(1) \mathbf{x}_k \right\} \\ \mathcal{P}_\ell &= \frac{1}{\ell!} : \left[\sum_k \left\{ \tilde{\mathbf{x}}_k \mathbf{p}_k - \tilde{\mathbf{p}}_k \mathbf{x}_k \right\} \right]^\ell |\bar{\rho}\rangle(1) : \end{aligned} \quad (4.2)$$

where the normal product $:\dots:$ means that all bath response operators $\tilde{\mathbf{x}}_k$ and $\tilde{\mathbf{p}}_k$ have to be arranged to the left of $|\bar{\rho}\rangle(1)$ and the operators \mathbf{x}_k and \mathbf{p}_k to the right. Furthermore for $\ell > 1$ each value of k may appear only once.

Assume a projector \mathcal{P}_ℓ is inserted into the time evolution $\mathbf{U}(t, t')$ at some time $t > t_0 > t'$

$$\mathbf{U}(t, t') \rightarrow \mathbf{U}(t, t_0) \mathcal{P}_\ell \mathbf{U}(t_0, t'). \quad (4.3)$$

If the contraction of pairs of bath operators to bath propagators is performed, as outlined at the end of the previous section, exactly ℓ such propagators reach from some time $> t_0$ to some time $< t_0$. The proposal is that the leading contribution for long time is given by the lowest order projector which can be inserted.

Let me start with the investigation of the response function

$$\begin{aligned} G_{zz}(t) &= (1 | \sigma_z \mathbf{U}(t, 0) \tilde{\sigma}_z | \bar{\rho}) \\ &= (1 | \sigma_z \mathbf{U}(t, 0) \tilde{\sigma}_z \mathbf{U}(0, -\infty) | i). \end{aligned} \quad (4.4)$$

Trying to insert \mathcal{P}_0 at some time $t > t_0 > 0$ results in vanishing contributions because $(1 | \mathbf{U}(t_0, 0) = (1 |$ and $(1 | \tilde{\sigma}_z = 0$.

Next \mathcal{P}_1 is inserted. This yields

$$\begin{aligned} &(1 | \sigma_z \mathbf{U}(t, t_0) \mathcal{P}_1 \mathbf{U}(t_0, 0) \tilde{\sigma}_z \mathbf{U}(0, -\infty) | i) \\ &= \int_{t_0}^t ds \int_0^{t_0} ds' (1 | \sigma_z \mathbf{U}(t, t_0) \tilde{\sigma}_z | \bar{\rho}) F(s - s') \\ &\quad \times (1 | \sigma_z \mathbf{U}(t_0, 0) \tilde{\sigma}_z | \bar{\rho}) \\ &= \int_{t_0}^t ds \int_0^{t_0} ds' G_{zz}(t - s) F(s - s') G_{zz}(s'). \end{aligned} \quad (4.5)$$

It is proposed that (4.5) yields the leading contribution to $G_{zz}(t)$ for $t \rightarrow \infty$ and choosing for instance $t_0 = t/2$ the

s - and s' -integration can be performed replacing $F(s - s')$ by $F(t)$. This results in

$$\begin{aligned} G_{zz}(t) &\xrightarrow[t \rightarrow \infty]{} \bar{\chi}_{zz}^2 F(t) \\ &\xrightarrow[t \rightarrow \infty]{} \alpha \Theta^{1-s} \Gamma(s + 1) \cos(\frac{1}{2} s \pi) \bar{\chi}_{zz}^2 t^{-1-s} \end{aligned} \quad (4.6)$$

where

$$\bar{\chi}_{zz} = 2 \frac{\partial \langle \sigma_z \rangle}{\partial \varepsilon} = \int_0^\infty dt G_{zz}(t) \quad (4.7)$$

is static susceptibility which is assumed to be finite. This means that the asymptotic behavior of the time dependent transverse response function is determined by the static susceptibility and the averaged bath propagator. The bare parameters Δ , ε and temperature enter only implicitly *via* $\bar{\chi}_{zz}$. For the Ohmic case $s = 1$ the first line of (4.6) is still valid but in the second line $F(t) \rightarrow 2\alpha \Theta^{-1} t^{-3}$ has to be inserted.

There are several points which have to be checked: In the integrals of (4.5) we have replaced $F(s - s')$ by $F(t)$ assuming that the main contribution comes from $t - s \ll t$ and $s' \ll t$. This is actually the case for a bath spectrum with $s > 0$. If the asymptotic contribution (4.6) is inserted for $G_{zz}(t - s)$ or $G_{zz}(s')$ in (4.5) corrections $\sim t^{-1-2s}$ are obtained.

Instead of \mathcal{P}_1 some other projector \mathcal{P}_ℓ could have been inserted. For a symmetric system with $\varepsilon = 0$ the next nonvanishing contribution is obtained from $\ell = 3$. A corresponding evaluation yields a contribution $\frac{1}{2} \bar{\chi}_{zzzz}^2 F(t) D^2(t)$ where $\bar{\chi}_{zzzz} = 8 \partial^3 \langle \sigma_z \rangle / \partial \varepsilon^3$ is a static nonlinear susceptibility. This contribution vanishes $\sim t^{-3(1+s)}$ for $t \ll \beta$ or $\sim T^2 t^{-1-3s}$ for $t \gg \beta$. For $\varepsilon \neq 0$ corrections $\sim t^{-2(1+s)}$ or $\sim T t^{-1-2s}$ result from insertion of \mathcal{P}_2 . In any case (4.6) yields the leading contribution.

Further contributions arise from insertion of $\mathcal{Q} = \mathbf{I} - \sum_\ell \mathcal{P}_\ell$. They are determined by the decay towards equilibrium. Within perturbation theory or NIBA [1–3] this decay is exponential and as a result the leading contribution (4.6) is indeed due to the first nonvanishing insertion of the projector \mathcal{P}_ℓ with lowest $\ell = 1$. The above analysis yields the restriction $s > 0$. In addition the existence of the static susceptibility (4.7) has been assumed which may impose further restrictions [10] on s or α .

The Fourier transform

$$\hat{G}_{zz}(\omega) = \int_0^\infty dt e^{i\omega t} G_{zz}(t) \quad (4.8)$$

can be written as

$$\begin{aligned} \hat{G}_{zz}(\omega) &= \frac{1}{\bar{\chi}_{zz}^{-1} - \hat{\Sigma}_{zz}(\omega)} \\ &\xrightarrow[\omega \rightarrow 0]{} \bar{\chi}_{zz} + \bar{\chi}_{zz} \Sigma_{zz}(\omega) \bar{\chi}_{zz} \end{aligned} \quad (4.9)$$

with a self energy $\Sigma_{zz}(\omega)$ vanishing for $\omega \rightarrow 0$. With (3.9) and (4.6)

$$\hat{\Sigma}_{zz}(\omega) \xrightarrow[\omega \rightarrow 0]{} \hat{F}(\omega) - \hat{F}(0) \sim \omega^s. \quad (4.11)$$

The analysis of the correlation function $C_{zz}(t)$ follows similar lines. The Fourier transform

$$\hat{C}_{zz}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} C_{zz}(t) \quad (4.12)$$

may be written as

$$\hat{C}_{zz}(\omega) = \hat{G}_{zz}(\omega) \hat{\Gamma}_{zz}(\omega) \hat{C}_{zz}(-\omega) \quad (4.13)$$

defining the self energy $\Gamma_{zz}(t)$. Again the leading contribution at low frequencies or long time is due to an insertion of \mathcal{P}_1 . Depending on whether a bath response function F or a bath correlation function D crosses the insertion point at t_0 several contributions are found. In analogy to (4.5)

$$C_{zz}(t) = \int_{t_0}^t ds \int_{-\infty}^{t_0} ds' G_{zz}(t-s) F(s-s') C_{zz}(s') \quad (4.14)$$

$$+ \int_{t_0}^t ds \int_{-\infty}^0 ds' G_{zz}(t-s) D(s-s') G_{zz}(-s').$$

The second term is identified as due to the long time or low frequency part of $\Gamma_{zz}(t)$ and therefore

$$\hat{\Gamma}_{zz}(\omega) \xrightarrow{\omega \rightarrow 0} \hat{D}(\omega). \quad (4.15)$$

The bath propagators fulfill an FDT (3.13) and therefore the same holds for the self energy $\Sigma_{zz}(\omega)$ and $\Gamma_{zz}(\omega)$. As a consequence the correlation- and response functions C_{zz} and G_{zz} also fulfill the FDT. This is not surprising. It shows the consistency of the above analysis.

The leading time dependence for $t \rightarrow \infty$ is in analogy to (4.6)

$$C_{zz}(t) \xrightarrow{t \rightarrow \infty} \hat{\chi}_{zz}^2 D(t) \quad (4.16)$$

and with (3.15) $C_{zz}(t) \sim t^{-s-1}$ for $t \rightarrow \infty$ and $t \ll \beta$. In the opposite limit $t \rightarrow \infty$ and $t \gg \beta$ an asymptotic decay $\sim T t^{-s}$ is found from (3.16).

The above result is a generalization of the Shiba relation originally proposed for the Kondo problem [5] and generalized to the spin boson problem by Sasseti and Weiss [4] and others [8,9] for $T = 0$. Note that their definition of $\hat{\chi}_{zz}$ differs by a factor 4 from the present one.

The analysis of the long time properties of the longitudinal response function

$$G_{xx}(t) = (1 | \sigma_x \mathbf{U}(t) \tilde{\sigma}_x | \bar{\rho}) \quad (4.17)$$

follows similar lines. The lowest order projector which can be inserted is \mathcal{P}_2 resulting in

$$G_{xx}(t) \approx \int_{t_0}^t ds \int_{t_0}^t dr \int_0^{t_0} ds' \int_{-\infty}^0 dr' \langle \sigma_x(t) \tilde{\sigma}_z(s) \tilde{\sigma}_z(r) \rangle$$

$$\times \left[F(s-s') D(r-r') \langle \sigma_z(s') \tilde{\sigma}_x(0) \tilde{\sigma}_z(r') \rangle \right.$$

$$\left. + F(s-s') F(r-r') \langle \sigma_z(s') \tilde{\sigma}_x(0) \sigma_z(r') \rangle \right] \quad (4.18)$$

where $\langle \dots \rangle$ are correlation-response functions of higher order. Investigating the contribution of the first term, $F(s-s') D(r-r')$ is replaced by $F(t) D(t)$ resulting in

$$G_{xx}(t) \xrightarrow{t \rightarrow \infty} \bar{\chi}_{xxx}^2 F(t) D(t) \quad (4.19)$$

where

$$\bar{\chi}_{xxx} = 4 \frac{\partial^2 \langle \sigma_x \rangle}{\partial \varepsilon^2} = 4 \frac{\partial^2 \langle \sigma_z \rangle}{\partial \Delta \partial \varepsilon} \quad (4.20)$$

is a static nonlinear susceptibility. The second term in (4.18) can be shown to be subdominant for $t \rightarrow \infty$. As a result again the leading contribution at long time has been expressed in terms of nonlinear susceptibilities and weighted bath propagators.

The longitudinal correlation function is obtained by applying fluctuation dissipation theorems. The resulting asymptotic expression is

$$C_{xx}(t) - \langle \sigma_x \rangle^2 \xrightarrow{t \rightarrow \infty} \frac{1}{2} \bar{\chi}_{xxx}^2 D(t)^2 \quad (4.21)$$

decaying $\sim t^{-2-2s}$ for $t \ll \beta$ and $\sim T^2 t^{-2s}$ for $t \gg \beta$. The same asymptotic behavior for $T = 0$ has been obtained by Guinea [11] for $s=1$. The result obtained by Lang *et al.* [12] can not be compared since it refers to the longitudinal correlation function involving polaron dressed operators whereas (4.21) involves the bare operator σ_z .

5 Specific heat

In this section it is shown that thermal properties at low temperature can also be expressed in terms of static susceptibilities and bath propagators. The free energy of the system at temperature $T = 1/\beta$ is

$$F_T = -\frac{1}{\beta} \left\{ \ln \text{Tr} e^{-\beta H} - \ln \text{Tr} e^{-\beta H_B} \right\} \quad (5.1)$$

where H is given by (3.1) and H_B is the Hamiltonian of the bath without coupling to the spin.

Let me investigate the derivative

$$\frac{\partial F_T}{\partial A_k} = -\frac{1}{\sqrt{N}} \langle x_k \sigma_z \rangle$$

$$= -\frac{1}{N} \int_0^\infty dt A_k \left\langle \sigma_z(t) \left\{ D_k(t) \tilde{\sigma}_z(0) + F_k(t) \sigma_z(0) \right\} \right\rangle$$

$$= -\frac{1}{N} \int_0^\infty dt A_k \left\{ D_k(t) G_{zz}(t) + F_k(t) C_{zz}(t) \right\}. \quad (5.2)$$

Because of the $1/\sqrt{N}$ dependence of the spin-bath couplings the functions $G_{zz}(t)$ and $C_{zz}(t)$ can be treated as independent on A_k for $N \rightarrow \infty$. This means that F is a linear functional of $A_k^2 D_k(t)$ and $A_k^2 F_k(t)$ respectively.

The free energy F_T depends on temperature only *via* $D_k(t)$. In order to evaluate $\delta F_T = F_T - F_0$ the excess

$$\delta D_k(t) = D_k(t; T) - D_k(t; 0)$$

$$= \frac{1}{\omega_k} \frac{1}{e^{\beta \omega_k} - 1} \cos \omega_k t \quad (5.3)$$

is introduced. At low temperature the leading contribution is linear in $\delta D_k(t)$ and

$$\begin{aligned} \delta F_T \xrightarrow{T \rightarrow 0} & -\frac{1}{2N} \sum_k A_k^2 \int_0^\infty dt \delta D_k(t) G_{zz}(t) \quad (5.4) \\ & = -\frac{1}{2} \int_0^\infty dt \delta D(t) G_{zz}(t) \end{aligned}$$

with $\delta D(t)$ given by (3.16). For $T \rightarrow 0$ the integral in (5.4) can be evaluated by using $\delta D(0)$ instead of $\delta D(t)$ because this function actually varies on a time scale $\beta = 1/T \rightarrow \infty$. This results in

$$\begin{aligned} \delta F_T \xrightarrow{T \rightarrow 0} & -\frac{1}{2} \bar{\chi}_{zz} \delta D(0) \quad (5.5) \\ & = -\frac{1}{2} \bar{\chi}_{zz} \alpha T^2 (\Theta/T)^{1-s} \Gamma(s+1) \zeta(s+1). \end{aligned}$$

The specific heat is obtained from

$$C = -T \frac{\partial^2 \delta F_T}{\partial T^2} \quad (5.6)$$

resulting in

$$C = \frac{1}{2} \bar{\chi}_{zz} \alpha T^s \Theta^{1-s} s(s+1) \Gamma(s+1) \zeta(s+1). \quad (5.7)$$

which is a generalization of the Wilson ratio [4]. Note again the difference in the definition of the transverse static susceptibility.

It is a pleasure to thank Reimer Kühn and Andreas Mielke for stimulating discussions. Support within the EPS program SPHINX is also acknowledged.

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