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Anti-resonance approach to soft tunnelling centres

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Abstract. In recent years various theoretical methods have been used to handle the fundamental decay problem of the archetypal Hamiltonian in quantum diffusion. In our study we determine the fundamental Green function (GF), which governs the decay, by an anti-resonance *ansatz* and a factorisation procedure beyond Hartree–Fock. The resulting GF is able to satisfy rigorous frame requirements (high-temperature expansions, sum rules, low-temperature laws derived from *ab initio* calculations). The spectral and temporal decay behaviour according to this GF is discussed for various coupling laws. In the case of 'Ohmic dissipation' (linear power-law coupling) we find a cross-over temperature, depending on the coupling strength, above which coherence disappears, the diffusion constant displaying a $T^{+2\alpha-1}$ behaviour in the intermediate temperature region.

1. Introduction

Tunnelling centres coupled to a 'soft' surrounding of elementary excitations (phonons, electronic excitations, etc.) have experienced much theoretical attention during the last 20 years. In the first stages of these studies para-electric (para-elastic) centres were the central physical object of interest [1–4]. Later additional motivation for the study grew up in the context of glasses [5]. On the other hand these centres have always been considered as a prototype for discussing quantum diffusion in solids [2], and there has been much recent activity in this particular field [6–10].

In almost all theoretical approaches a two-site Hamiltonian of the form

$$H = \Delta\sigma_z + \tfrac{1}{2}\sum_k \Omega_k(P_k^2 + Q_k^2) + \sum_k \Omega_k D_k Q_k \sigma_x \tag{1}$$

has been employed, where the pseudo-spin operators are projectors in the 'left–right' space of the tunnelling particle,

$$\sigma_x = (1/2)(|l\rangle\langle l| - |r\rangle\langle r|) \tag{2a}$$

$$\sigma_y = (1/2\mathrm{i})(|l\rangle\langle r| - |r\rangle\langle l|) \tag{2b}$$

$$\sigma_z = -(1/2)(|l\rangle\langle r| + |r\rangle\langle l|) \tag{2c}$$

and Q_k, P_k are the coordinates of the modes of the surrounding medium. These operators satisfy the commutation rules $[Q_k, P_{k'}]_- = \mathrm{i}\delta_{kk'}$ and $[\sigma_x, \sigma_y]_- = \mathrm{i}\sigma_z$ etc. In most papers a coupling of the form

$$\rho(\Omega)D^2(\Omega)\Omega^2 = 4\alpha\Omega_D(\Omega/\Omega_D)^m \qquad 0 \leqslant \Omega \leqslant \Omega_D \tag{3}$$

has been adopted, where $\rho(\Omega)$ is the frequency density and Ω_D is the Debye (= cut-off) frequency of the bath modes. For phonons normally $m = 3$ has been taken [11], whereas in those cases where electronic excitations play the role of the bath, $m = 1$ ('Ohmic dissipation') is considered adequate [7].

Many different theoretical techniques have been invoked to handle both the dynamics and thermodynamics of these centres (golden rule, Green functions (GFs), Mori formalism, path integrals, etc.). A particular difficulty of the GF method in this context is the inadequacy of the Hartree–Fock (HF) type of factorisation procedure, which in many other examples of coupled systems has proved successful.

The aim of the present paper is to find an appropriate way of by-passing the HF factorisation and overcoming its main faults.

2. Zubarev Green functions

We employ Green functions of the Zubarev type [12] defined by

$$\langle\langle A(t)\,|\,B(t')\rangle\rangle^{(r_1 a)} \equiv \mp\, \mathrm{i}\theta(\pm(t-t'))\langle[A(t), B(t')]_-\rangle_T^H = \int_{-\infty}^{+\infty} \langle\langle A\,|\,B\rangle\rangle_E\, \mathrm{e}^{-\mathrm{i}\omega(t-t')}\, \mathrm{d}\omega. \tag{4}$$

The general equation of motion for the Fourier-transformed Zubarev GF $\langle\langle A\,|\,B\rangle\rangle_E$ ($E = \omega \pm \mathrm{i}\varepsilon$, $\varepsilon = 0_+$) reads

$$E\langle\langle A\,|\,B\rangle\rangle_E = (1/2\pi)\langle[A, B]_-\rangle_T^H + \langle\langle[A, H]_-\,|\,B\rangle\rangle_E \tag{5a}$$

or alternatively

$$E\langle\langle A\,|\,B\rangle\rangle_E = (1/2\pi)\langle[A, B]_-\rangle_T^H - \langle\langle A\,|\,[B, H]_-\rangle\rangle_E. \tag{5b}$$

As shown later, the whole dynamics and thermodynamics of soft tunnelling centres may be traced back to the GF $\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_E$. Employing (5*a*) we get the hierarchy

$$E\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_E = -\mathrm{i}\Delta\langle\langle\sigma_y\,|\,\sigma_x\rangle\rangle_E \tag{6}$$

$$E\langle\langle\sigma_y\,|\,\sigma_x\rangle\rangle_E = -(\mathrm{i}/2\pi)\langle\sigma_z\rangle_T^H + \mathrm{i}\Delta\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_E - \mathrm{i}\sum_k \Omega_k D_k \langle\langle\sigma_z Q_k\,|\,\sigma_x\rangle\rangle_E. \tag{7}$$

We now apply (5*b*) to get

$$E\langle\langle\sigma_z Q_k\,|\,\sigma_x\rangle\rangle_E = (\mathrm{i}/2\pi)\langle\sigma_y Q_k\rangle_T^H + \mathrm{i}\Delta\langle\langle\sigma_z Q_k\,|\,\sigma_y\rangle\rangle_E \tag{8}$$

$$E\langle\langle\sigma_z Q_k\,|\,\sigma_y\rangle\rangle_E = -(\mathrm{i}/2\pi)\langle\sigma_x Q_k\rangle_T^H - \mathrm{i}\Delta\langle\langle\sigma_z Q_k\,|\,\sigma_x\rangle\rangle_E + \mathrm{i}\sum_{k'} \Omega_{k'} D_{k'} \langle\langle\sigma_z Q_k\,|\,\sigma_z Q_{k'}\rangle\rangle_E. \tag{9}$$

Inserting (7) in (6) and (9) in (8) we have

$$(E^2 - \Delta^2)\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_E = -\,\Delta\langle\sigma_z\rangle/2\pi - \Delta\sum_k \Omega_k D_k \langle\langle\sigma_z Q_k\,|\,\sigma_x\rangle\rangle_E \tag{10}$$

$$(E^2 - \Delta^2)\langle\langle\sigma_z Q_k\,|\,\sigma_x\rangle\rangle_E = (1/2\pi)(\mathrm{i}E\langle\sigma_y Q_k\rangle_T^H + \Delta\langle\sigma_x Q_k\rangle_T^H) - \Delta\sum_{k'} \Omega_{k'} D_{k'} \langle\langle\sigma_z Q_k\,|\,\sigma_z Q_{k'}\rangle\rangle_E. \tag{11}$$

At this stage we use the identity $\langle [A, H]_- \rangle_T^H = 0$, which yields

$$\langle \sigma_y Q_k \rangle_T^H = 0. \tag{12}$$

Then from (10), (11) and (12) we finally are left with

$$(E^2 - \Delta^2)\langle\langle \sigma_x | \sigma_x \rangle\rangle_E = \frac{\Delta\langle -\sigma_z \rangle}{2\pi} + \frac{\Delta^2}{E^2 - \Delta^2} \times \left(\frac{-1}{2\pi} \sum_k \Omega_k D_k \langle \sigma_x Q_k \rangle_T^H + \sum_k \sum_{k'} D_k \Omega_k D_{k'} \Omega_{k'} \langle\langle \sigma_z Q_k | \sigma_z Q_{k'} \rangle\rangle_E \right) \tag{13}$$

which is the crucial equation for our further discussion. By virtue of the existence of the bath we may assume that $\langle\langle \sigma_x | \sigma_x \rangle\rangle_E$ has no pole for $E \to \pm\Delta$. Hence the LHS of (13) disappears for $E \to \pm\Delta$. Since the first term of the RHS is a constant we therefore must conclude that the expression in parentheses must be proportional to $(E^2 - \Delta^2)$ in the neighbourhood of $E \to \pm\Delta$, whence we may write it in the form

$$\left(\sum_k \sum_k D_k \Omega_k D_{k'} \Omega_{k'} \langle\langle \sigma_z Q_k | \sigma_z Q_{k'} \rangle\rangle_E - \frac{1}{2\pi} \sum_k D_k \Omega_k \langle \sigma_x Q_k \rangle_T^H \right) = \frac{2\pi\Delta}{\langle -\sigma_z \rangle} \frac{E^2 - \Delta^2}{\Delta^2} \langle\langle \sigma_x | \sigma_x \rangle\rangle_E G_1(E). \tag{14}$$

This is a beautiful manifestation of the anti-resonance behaviour of certain bath GFs as first discovered by Fano [13]. However, $G_1(E)$ is still an unknown function. We know, however, that it is finite at $E = \pm\Delta$ and has the limiting value

$$\lim_{E \to \pm\Delta} G_1(E) = -\frac{\langle -\sigma_z \rangle^2}{(2\pi)^2} \left(\lim_{E \to \pm\Delta} \langle\langle \sigma_x | \sigma_x \rangle\rangle_E \right)^{-1}. \tag{15}$$

Inserting (14) in the anti-resonance equation (13) we have

$$\langle\langle \sigma_x | \sigma_x \rangle\rangle_E = \frac{\Delta\langle -\sigma_z \rangle}{2\pi} \left(E^2 - \Delta^2 - \frac{2\pi\Delta}{\langle -\sigma_z \rangle} G_1(E) \right)^{-1}. \tag{16}$$

A stringent prerequisite for the evaluation of the unknown function $G_1(E)$ is the requirement that the GF $\langle\langle \sigma_x | \sigma_x \rangle\rangle_E$ must satisfy the Kramers–Kronig relation. Generally we define the spectral function $I_{AB}(\omega)$ of a Green function $\langle\langle A | B \rangle\rangle_E$ as

$$I_{AB}(\omega) = \frac{\mathrm{i}}{\mathrm{e}^{\beta\omega} - 1} \lim_{\varepsilon \to 0^+} [\langle\langle A | B \rangle\rangle_{\omega + \mathrm{i}\varepsilon} - \langle\langle A | B \rangle\rangle_{\omega - \mathrm{i}\varepsilon}]. \tag{17}$$

Then, since $A = A^+ = \sigma_x = B$, $I_{\sigma_x\sigma_x}(\omega)$ must be a real function for which the fluctuation–dissipation theorem assumes the form

$$\mathrm{Im}\langle\langle \sigma_x | \sigma_x \rangle\rangle_{\omega + \mathrm{i}\varepsilon} = -\tfrac{1}{2}(\mathrm{e}^{\beta\omega} - 1) I_{\sigma_x\sigma_x}(\omega). \tag{18}$$

The Kramers–Kronig relation then reads

$$\mathrm{Re}\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_{\omega+\mathrm{i}\varepsilon} = -\frac{1}{\pi}\,\mathrm{P}\int_{-\infty}^{+\infty}\frac{1}{\omega-\omega'}\,\mathrm{Im}\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_{\omega'+\mathrm{i}\varepsilon}\,\mathrm{d}\omega'$$

$$= \frac{1}{2\pi}\,\mathrm{P}\int_{-\infty}^{+\infty}(\mathrm{e}^{\beta\omega'}-1)\frac{I_{\sigma_x\sigma_x}(\omega')}{\omega-\omega'}\,\mathrm{d}\omega'. \tag{19}$$

A very flexible form which is shown below to satisfy (19) is established by the *ansatz*

$$G_1(E) = A_0 + \sum_r B_r^2/(E^2-\Lambda_r^2) \tag{20}$$

where A_0, B_r, Λ_r are real constants. Inserting (20) in (16), $\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_E$ transmutes into

$$\langle\langle\sigma_x\,|\,\sigma_x\rangle\rangle_E = \frac{\Delta\langle-\sigma_z\rangle}{\Lambda_s}\frac{\Lambda_s}{2\pi}\frac{1}{E^2-\Lambda_s^2-\Sigma_r\Lambda_s\Lambda_r V_r^2/(E^2-\Lambda_r^2)} \tag{21}$$

where

$$\Lambda_s^2 = \Delta^2 + (2\pi\Delta/\langle-\sigma_z\rangle)A_0 \tag{22a}$$

$$\Lambda_s\Lambda_r V_r^2 = B_r^2 2\pi\Delta/\langle-\sigma_z\rangle. \tag{22b}$$

In the next section we will show that the structural form (21) is just the same as the one that also appears in the oscillator–bath problem. In this manner it automatically guarantees the validity of the Kramers–Kronig relations and of the fluctuation–dissipation theorem. The oscillator–bath problem is one of the few exactly solvable multimode problems [14–16]. In particular it permits a simple calculation of the lower sum rules. In this manner the sum rules can be adopted as a means to determine the yet unknown parameters A_0, Λ_r, B_r.

3. Exactly solvable sister problem (oscillator–bath)

The oscillator–bath problem is characterised by the Hamiltonian

$$H_{\mathrm{ob}} = \tfrac{1}{2}\Lambda_s(p_s^2+q_s^2) + \tfrac{1}{2}\sum_r\Lambda_r(p_r^2+q_r^2) + \sum_r V_r q_r q_s. \tag{23}$$

The decay problem $\langle q_s(0)q_s(t)\rangle$ pertinent to this Hamiltonian is one of the very few exactly solvable models in statistical physics and has been handled by Ullersma [14], by Louisell and Walker [15], and more recently by one of us [16]. The GF $\langle\langle q_s\,|\,q_s\rangle\rangle_E$ can be obtained from the hierarchy of equations of motion

$$E\langle\langle q_s\,|\,q_s\rangle\rangle_E = \mathrm{i}\Lambda_s\langle\langle p_s\,|\,q_s\rangle\rangle_E \tag{24}$$

$$E\langle\langle p_s\,|\,q_s\rangle\rangle_E = -(\mathrm{i}/2\pi) - \mathrm{i}\Lambda_s\langle\langle q_s\,|\,q_s\rangle\rangle_E - \mathrm{i}\sum_r V_r\langle\langle q_r\,|\,q_s\rangle\rangle_E \tag{25}$$

$$E\langle\langle q_r\,|\,q_s\rangle\rangle_E = \mathrm{i}\Lambda_r\langle\langle p_r\,|\,q_s\rangle\rangle_E \tag{26}$$

$$E\langle\langle p_r | q_s \rangle\rangle_E = -\mathrm{i}\Lambda_r \langle\langle q_r | q_s \rangle\rangle_E - \mathrm{i}V_r \langle\langle q_s | q_s \rangle\rangle_E. \tag{27}$$

From (24)–(27) $\langle\langle q_s | q_s \rangle\rangle_E$ reads

$$\langle\langle q_s | q_s \rangle\rangle_E = \frac{\Lambda_s}{2\pi} \frac{1}{E^2 - \Lambda_s^2 - \Sigma_r \Lambda_r \Lambda_s V_r^2/(E^2 - \Lambda_r^2)} \tag{28}$$

and thus is seen to be just of the form found for $\langle\langle \sigma_x | \sigma_x \rangle\rangle_E$ (see expression (21))

$$\langle\langle \sigma_x | \sigma_x \rangle\rangle_E = (\Delta\langle -\sigma_z \rangle / \Lambda_s) \langle\langle q_s | q_s \rangle\rangle_E \tag{29}$$

if we keep to the identifications (22*a*, *b*). In this manner we have traced back the tunnelling problem to the exactly solvable oscillator–bath problem. We have to bear in mind, however, that the effective quantities $\{\Lambda_r, V_r\}$ must not be identified either in size or in number with the set of quantities $\{\Omega_k, D_k\}$ of the original bath attached to the tunnelling problem. Additionally, the quantities $\{\Lambda_r, V_r\}$ may depend on temperature.

4. Sum rules

In our context the great efficacy of the return to the oscillator–bath problem lies in the fact that the odd sum rules for $I_{q_s q_s}(\omega)$ are of a particularly simple nature. The spectral function $I_{AB}(\omega)$ of the Zubarev GF $\langle\langle A | B \rangle\rangle_E$ is the Fourier transform of the correlation function $\langle B(0)A(t)\rangle_T^H$:

$$\langle B(0)A(t)\rangle_T^H = \int_{-\infty}^{+\infty} I_{AB}(\omega)\, \mathrm{e}^{-\mathrm{i}\omega t}\, \mathrm{d}\omega. \tag{30}$$

From (30) we can derive the moments $M_{AB}^{(n)}$ for $I_{AB}(\omega)$, if we invoke the Heisenberg equation and choose $t = 0$:

$$M_{AB}^{(0)} \equiv \int_{-\infty}^{+\infty} I_{AB}(\omega)\, \mathrm{d}\omega = \langle B \cdot A \rangle_T^H \tag{31a}$$

$$M_{AB}^{(1)} \equiv \int_{-\infty}^{+\infty} I_{AB}(\omega)\omega\, \mathrm{d}\omega = \langle B \cdot [A, H]\rangle_T^H = \langle [H, B] \cdot A \rangle_T^H \tag{31b}$$

$$\begin{aligned} M_{AB}^{(2)} \equiv \int_{-\infty}^{+\infty} I_{AB}(\omega)\omega^2\, \mathrm{d}\omega &= \langle B \cdot [[A, H], H]\rangle_T^H = \langle [H, [H, B]] \cdot A \rangle_T^H \\ &= \langle [H, B] \cdot [A, H]\rangle_T^H. \end{aligned} \tag{31c}$$

Specifically for the spectral function $I_{\sigma_x\sigma_x}(\omega)$ of the tunnelling problem we have from (31):

$$M_{\sigma_x\sigma_x}^{(0)} = 1/4 \tag{32a}$$

$$M_{\sigma_x\sigma_x}^{(1)} = (\Delta/2)\langle \sigma_z \rangle \tag{32b}$$

$$M_{\sigma_x\sigma_x}^{(2)} = \Delta^2/4 \tag{32c}$$

$$M_{\sigma_x\sigma_x}^{(3)} = \frac{\Delta}{2}\left(\Delta^2\langle\sigma_z\rangle + \Delta \sum_k \Omega_k D_k \langle \sigma_x Q_k \rangle\right) \tag{32d}$$

$$M_{\sigma_x\sigma_x}^{(4)} = \frac{\Delta^2}{4}\left(\Delta^2 + \sum_k \sum_{k'} D_k \Omega_k D_{k'} \Omega_{k'} \langle Q_k Q_{k'} \rangle\right) \tag{32e}$$

$$M^{(5)}_{\sigma_x\sigma_x} = \frac{\Delta^5}{2}\langle\sigma_z\rangle + \frac{\Delta^4}{2}\sum_k D_k\Omega_k\langle\sigma_x Q_k\rangle + \frac{\Delta^3}{2}\left\langle\sigma_z\left(\sum_k D_k\Omega_k Q_k\right)^2\right\rangle$$
$$+\frac{\Delta^2}{2}\sum_k D_k\Omega_k^3\langle\sigma_x Q_k\rangle + \frac{\Delta^2}{2}\left\langle\sigma_x\left(\sum_k D_k\Omega_k Q_k\right)^3\right\rangle. \tag{32f}$$

Similarly we write down the oscillator–bath sum rules:

$$M^{(0)}_{q_sq_s} = \langle q_s^2\rangle \tag{33a}$$

$$M^{(1)}_{q_sq_s} = (1/2)(\langle[H, q_s]\cdot q_s\rangle + \langle q_s\cdot[q_s, H]\rangle) = \mathrm{i}(\Lambda_s/2)(\langle q_s\cdot p_s\rangle - \langle p_s\cdot q_s\rangle)$$
$$= -\Lambda_s/2 \tag{33b}$$

$$M^{(2)}_{q_sq_s} = \langle[H, q_s]\cdot[q_s, H]\rangle = \Lambda_s^2\langle p_s^2\rangle \tag{33c}$$

$$M^{(3)}_{q_sq_s} = (1/2)(\langle[H, q_s]\cdot[[q_s, H], H]\rangle + \langle[H,[H, q_s]]\cdot[q_s, H]\rangle)$$
$$= \mathrm{i}(\Lambda_s^3/2)\langle q_sp_s - p_sq_s\rangle = -\Lambda_s^3/2 \tag{33d}$$

$$M^{(4)}_{q_sq_s} = \langle[H,[H, q_s]]\cdot[[q_s, H], H]\rangle = \langle(\Lambda_s^2 q_s + \sum_r \times \Lambda_s V_r q_r)^2\rangle \tag{33e}$$

$$M^{(5)}_{q_sq_s} = (1/2)(\langle[H,[H,[H, q_s]]]\cdot[[q_s, H], H]\rangle + \langle[H,[H, q_s]]\cdot[[[q_s, H], H], H]\rangle)$$
$$= \frac{-\Lambda_s}{2}\left(\Lambda_s^4 + \sum_r V_r^2\Lambda_s\Lambda_r\right). \tag{33f}$$

Up to this stage both the sum rule formulae for the spin–bath as well as for the oscillator–bath problems have been exact. We now return to our original motivation for introducing the oscillator–bath problem, which has been the *ansatz* (20). Via this *ansatz* the spin GF $\langle\langle\sigma_x|\sigma_x\rangle\rangle$ has been traced back to an effective oscillator–bath problem characterised by the parameters $\{\Lambda_s, \Lambda_r, V_r\}$. Since in the formulae above we have derived the exact moments both for the spin–bath and the oscillator–bath problems, we may employ the identification (29) to determine the effective quantities $\{\Lambda_s, \Lambda_r, V_r\}$. Translated to the moments, (29) reads

$$M^{(m)}_{\sigma_x\sigma_x} = \frac{\Delta\langle-\sigma_z\rangle}{\Lambda_s}M^{(m)}_{q_sq_s}. \tag{34}$$

Employing (32) and (33) we get from (34) for the odd moments

$$M^{(1)}: \quad \frac{\Delta}{2}\langle\sigma_z\rangle = \frac{\Delta\langle-\sigma_z\rangle}{\Lambda_s}\left(-\frac{\Lambda_s}{2}\right) \tag{35a}$$

$$M^{(3)}: \quad \frac{\Delta}{2}\left(\Delta^2\langle\sigma_z\rangle + \Delta\sum_k \Omega_k D_k\langle\sigma_x Q_k\rangle\right) = \frac{\Delta\langle-\sigma_z\rangle}{\Lambda_s}\left(-\frac{\Lambda_s^3}{2}\right) \tag{35b}$$

$$M^{(5)}: \quad \frac{\Delta^5}{2}\langle\sigma_z\rangle + \frac{\Delta^4}{2}\sum_k D_k\Omega_k\langle\sigma_x Q_k\rangle + \frac{\Delta^3}{2}\left\langle\sigma_z\left(\sum_k D_k\Omega_k Q_k\right)^2\right\rangle$$
$$+\frac{\Delta^2}{2}\left[\sum_k D_k\Omega_k^3\langle\sigma_x Q_k\rangle + \left\langle\sigma_x\left(\sum_k D_k\Omega_k Q_k\right)^3\right\rangle\right]$$
$$= \frac{\Delta\langle-\sigma_z\rangle}{\Lambda_s}\frac{(-\Lambda_s)}{2}\left(\Lambda_s^4 + \sum_r V_r^2\Lambda_r\Lambda_s\right). \tag{35c}$$

Obviously, the first of these equations is automatically satisfied. From (35*b*) we find

$$\Lambda_s^2 = \Delta^2 + (\Delta/\langle\sigma_z\rangle)\sum_k \Omega_k D_k \langle\sigma_x Q_k\rangle. \tag{36}$$

The fifth moment could be employed to determine the sum $\Sigma_r V_r^2 \Lambda_r$, etc. In this manner the unknown quantities $\{\Lambda_s, \Lambda_r, V_r\}$ are expressed by means of thermal expectation values of the spin–bath problem, such as $\langle\sigma_z\rangle$, $\Sigma_k D_k \Omega_k \langle\sigma_x Q_k\rangle$, etc. Naturally these expectation values are not known up to now, but we also have not yet used the even sum rules of the sets of equations (32) and (33). If we confine ourselves to be correct up to the third moment inclusive, the odd sum rules leave undetermined the quantities $\{\Lambda_r, V_r\}$ and $\langle\sigma_z\rangle$, $\Sigma_k D_k \Omega_k \langle\sigma_x Q_k\rangle$. These quantities are interconnected by the requirement that the zeroth and second moments must be satisfied. This still leaves open a great flexibility for the choice of $\{\Lambda_r, V_r\}$. But in the next section we will present a simple way to fix these parameters.

5. Factorisation beyond Hartree–Fock

We return to equation (10) of § 2:

$$(E^2 - \Delta^2)\langle\langle\sigma_x | \sigma_x\rangle\rangle_E = -(\Delta\langle\sigma_z\rangle/2\pi) - \Delta\sum_k \Omega_k D_k \langle\langle\sigma_z Q_k | \sigma_x\rangle\rangle_E.$$

The most simple way to close the hierarchy of equations of motion piling up in the continuation of this equation would be a kind of HF factorisation:

$$\langle\langle\sigma_z Q_k | \sigma_x\rangle\rangle_E = \langle\sigma_z\rangle_T^H \langle\langle Q_k | \sigma_x\rangle\rangle_E. \tag{37}$$

This type of factorisation has proved fruitful in many other systems and it has also been used in an earlier approach to the tunnelling problem [10]. However, in the mode-assisted tunnelling system, it turns out that this factorisation violates even the lowest sum rules. In order to find an appropriate factorisation we have to keep track at least to the lowest moments of the spectral function pertaining to the GF $\langle\langle\sigma_z Q_k | \sigma_x\rangle\rangle_E$,

$$M^{(0)}_{\sigma_z Q_k;\sigma_x} = \langle\sigma_x \cdot \sigma_z Q_k\rangle_T^H = -(\mathrm{i}/2)\langle\sigma_y Q_k\rangle_T^H = 0 \tag{38a}$$

$$M^{(1)}_{\sigma_z Q_k;\sigma_x} = \langle[H, \sigma_x] \cdot \sigma_z Q_k\rangle_T^H = \mathrm{i}\Delta\langle\sigma_y \sigma_z Q_k\rangle = -(\Delta/2)\langle\sigma_x Q_k\rangle \neq 0 \tag{38b}$$

etc

where (12) has been used. On the other hand the moments of the spectral function of the GF $\langle\langle Q_k | \sigma_x\rangle\rangle_E$ are

$$M^{(0)}_{Q_k;\sigma_x} = \langle\sigma_x Q_k\rangle_T^H \neq 0 \tag{39a}$$

$$M^{(1)}_{Q_k;\sigma_x} = \langle[H, \sigma_x] \cdot Q_k\rangle_T^H = \mathrm{i}\Delta\langle\sigma_y Q_k\rangle_T^H = 0. \tag{39b}$$

Since $M^{(0)}_{Q_k;\sigma_x}\langle\sigma_z\rangle \neq 0$, already the lowest sum rule of the HF factorisation (37) is violated. We therefore have to search for an improved factorisation. A first option in this direction would be to try to correct the shortcoming of the HF approximation (37) by an addition of the basic GF $\langle\langle\sigma_x|\sigma_x\rangle\rangle_E$ itself

$$\langle\langle\sigma_z Q_k|\sigma_x\rangle\rangle_E = \eta\langle\langle Q_k|\sigma_x\rangle\rangle_E + \zeta\langle\langle\sigma_x|\sigma_x\rangle\rangle_E \tag{40}$$

where the two real parameters η and ζ are determined by the requirement that the lowest two sum rules of (40) be preserved. This then yields

$$M_0: \qquad 0 = \eta\langle\sigma_x Q_k\rangle_T^H + \zeta(1/4) \tag{41}$$

$$M_1: \qquad -(\Delta/2)\langle\sigma_x Q_k\rangle_T^H = \eta\cdot 0 + \zeta(\Delta/2)\langle\sigma_z\rangle. \tag{42}$$

So we finally reach a factorisation of the form

$$\langle\langle\sigma_z Q_z|\sigma_x\rangle\rangle_E = \frac{1}{4\langle\sigma_z\rangle}\langle\langle Q_k|\sigma_x\rangle\rangle_E + \frac{\langle\sigma_x Q_k\rangle}{\langle-\sigma_z\rangle}\langle\langle\sigma_x|\sigma_x\rangle\rangle_E. \tag{43}$$

The most striking feature of this formula is the fact that $\langle\sigma_z\rangle_T^H$ appears in the denominator, which is the inverse behaviour as in the Hartree–Fock factorisation (37). Consequently, the thermal behaviour of physical properties such as the damping or the tunnelling frequency of the diffusion process is quite different, not to say opposite, to the results based on (37).

Equation (43) permits us to continue the hierarchy of equations of motion:

$$E\langle\langle Q_k|\sigma_x\rangle\rangle_E = \mathrm{i}\Omega_k\langle\langle P_k|\sigma_x\rangle\rangle_E \tag{44}$$

$$E\langle\langle P_k|\sigma_x\rangle\rangle_E = -\mathrm{i}\Omega_k\langle\langle Q_k|\sigma_x\rangle\rangle_E - \mathrm{i}D_k\Omega_k\langle\langle\sigma_x|\sigma_x\rangle\rangle_E. \tag{45}$$

Combining (44), (45) and (43) we have

$$\langle\langle Q_k|\sigma_x\rangle\rangle_E = \frac{D_k\Omega_k^2}{E^2-\Omega_k^2}\langle\langle\sigma_x|\sigma_x\rangle\rangle_E \tag{46}$$

$$\langle\langle\sigma_z Q_k|\sigma_x\rangle\rangle_E = \frac{1}{\langle-\sigma_z\rangle}\left(-\frac{1}{4}\frac{D_k\Omega_k^2}{E^2-\Omega_k^2} + \langle\sigma_x Q_k\rangle\right)\langle\langle\sigma_x|\sigma_x\rangle\rangle_E \tag{47}$$

which inserted in (10) yields

$$\langle\langle\sigma_x|\sigma_x\rangle\rangle_E = \frac{\Delta\langle-\sigma_z\rangle}{2\pi}\left\{E^2 - \left[\Delta^2 + (\Delta/\langle\sigma_z\rangle)\sum_k D_k Q_k\langle\sigma_x Q_k\rangle\right] - (\Delta/4\langle-\sigma_z\rangle)\sum_k D_k^2\Omega_k^3/(E^2-\Omega_k^2)\right\}^{-1}. \tag{48}$$

This result has just the form of (21) if we identify the set of parameters $\{\Lambda_r\}$ with $\{\Omega_k\}$ and further

$$\Lambda_s^2 = \Delta^2 + \frac{\Delta}{\langle\sigma_z\rangle}\sum_k D_k\Omega_k\langle\sigma_x Q_k\rangle \tag{49}$$

$$V_k^2 = \frac{\Delta}{4\langle-\sigma_z\rangle}\frac{1}{\Lambda_s}D_k^2\Omega_k^2. \tag{50}$$

This establishes the connection with the results of the preceding section; we observe that Λ_s as given by (49) coincides with the one found in the last section (see (36)) in a completely different manner. Additionally we have achieved our aim of fixing the parameters, which have remained free in the last section. In this manner we have closed our formalism: the only two unknown quantities $\langle\sigma_z\rangle$ and $\Sigma_k D_k \Omega_k \langle\sigma_x Q_k\rangle$ are found by self-consistency.

In closing we add that in a next step a further suitable term could be added to the *ansatz* (40), which would establish the flexibility of satisfying still higher sum rules.

6. Self-consistency procedure

We return to the zeroth and second moments of the spectral function $I_{\sigma_x\sigma_x}(\omega)$, which is obtained from (48) via definition (17):

$$I_{\sigma_x\sigma_x}(\omega) = \frac{\Delta\langle-\sigma_z\rangle}{\pi} \frac{\Gamma(\omega)}{\{\omega^2 - [\Delta^2 + (\Delta/\langle\sigma_z\rangle)\Sigma_k D_k \Omega_k \langle\sigma_x Q_k\rangle] - \Pi(\omega)\}^2 + \Gamma^2(\omega)} \times \frac{1}{\mathrm{e}^{\beta\omega} - 1} \tag{51}$$

where

$$\Gamma(\omega) = \frac{\pi}{2} \frac{\Delta}{4\langle-\sigma_z\rangle} \sum_k D_k^2 \Omega_k^2 [\delta(\omega - \Omega_k) - \delta(\omega + \Omega_k)]$$

$$= \frac{\pi}{2} \frac{\Delta}{4\langle-\sigma_z\rangle} D^2(|\omega|)\omega^2 \rho(|\omega|) \frac{\omega}{|\omega|} \tag{52a}$$

$$\Pi(\omega) = \frac{\Delta}{4\langle-\sigma_z\rangle} \sum_k \mathrm{P} \frac{D_k^2 \Omega_k^3}{\omega^2 - \Omega_k^2} = \frac{\Delta}{4\langle-\sigma_z\rangle} \mathrm{P} \int_0^{\Omega_\mathrm{D}} \frac{D^2(\Omega)\Omega^3 \rho(\Omega)}{\omega^2 - \Omega^2} \mathrm{d}\Omega. \tag{52b}$$

Here we have replaced $\Sigma_k \ldots$ by an integral, where $\rho(\Omega)$ is the frequency density and Ω_D the Debye frequency of the bath in (1). Then for the moments of $I_{\sigma_x\sigma_x}(\omega)$ we find

$$M^{(2n+1)}_{\sigma_x\sigma_x} = -\Delta\langle-\sigma_z\rangle \int_0^{\Omega_\mathrm{D}} S(\omega)\omega^{2n+1}\, \mathrm{d}\omega \tag{53}$$

$$M^{(2n)}_{\sigma_x\sigma_x} = \Delta\langle-\sigma_z\rangle \int_0^{\Omega_\mathrm{D}} S(\omega)\omega^{2n} \coth(\beta\omega/2)\, \mathrm{d}\omega \tag{54}$$

with

$$S(\omega) = \frac{1}{\pi} \frac{\Gamma(\omega)}{\{\omega^2 - [\Delta^2 + (\Delta/\langle\sigma_z\rangle)\Sigma_k D_k \Omega_k \langle\sigma_x Q_k\rangle] - \Pi(\omega)\}^2 + \Gamma^2(\omega)}. \tag{55}$$

Inserting the exact values of the zeroth and second moments of $I_{\sigma_x\sigma_x}(\omega)$, $M^{(0)}_{\sigma_x\sigma_x} = 1/4$ and $M^{(2)}_{\sigma_x\sigma_x} = \Delta^2/4$ (see equations (32)) on the LHS of (54), we get two self-consistency conditions for the determination of the unknown thermal expectation values $\langle\sigma_z\rangle$ and $\Sigma_k D_k \Omega_k \langle Q_k \sigma_x\rangle$:

$$\Delta\langle-\sigma_z\rangle \int_0^{\Omega_D} S(\omega)\coth(\beta\omega/2)\,d\omega = 1/4 \tag{56}$$

$$\Delta\langle-\sigma_z\rangle \int_0^{\Omega_D} S(\omega)\omega^2\coth(\beta\omega/2)\,d\omega = \Delta^2/4. \tag{57}$$

In the limit $\Delta \to 0$ we have $\langle\sigma_x Q_k\rangle_T^H \to -D_k/4$ and hence

$$\sum_k D_k\Omega_k\langle\sigma_x Q_k\rangle_T^H \to -\tfrac{1}{4}\sum_k \Omega_k D_k^2 = -\tfrac{1}{4}\int_0^{\Omega_D} \rho(\Omega)D^2(\Omega)\Omega\,d\Omega$$
$$= -\alpha\Omega_D/m \tag{58}$$

where we have used the coupling law (3). So it proves useful to introduce a quantity B by means of the definition

$$\sum_k \Omega_k D_k\langle\sigma_x Q_k\rangle_T^H = -(\alpha\Omega_D/m)(1-B). \tag{59}$$

B will turn out to be a small quantity ($B \ll 1$) for all cases of practical interest. We now consider again the power-law coupling set-ups of (3) and further introduce the abbreviations

$$x_s = \Delta/\Omega_D \qquad x = \omega/\Omega_D \qquad \xi = \alpha/\langle-\sigma_z\rangle. \tag{60}$$

Then the self-consistency equations (56)–(57) for $\langle\sigma_z\rangle$ and B read ($m = 1$ or 3)

$$\langle-\sigma_z\rangle \int_0^1 \left[\xi x_s^2 x^m \coth\left(\frac{\beta\Omega_D}{2}x\right)\right]\Big/\Xi\,dx = \tfrac{1}{2} \tag{61}$$

$$\langle-\sigma_z\rangle \int_0^1 \left[\xi x^{m+2} \coth\left(\frac{\beta\Omega_D}{2}x\right)\right]\Big/\Xi\,dx = \tfrac{1}{2} \tag{62}$$

where

$$\Xi = \left[x^2\left(1 + x_s\xi\frac{m-1}{2}\right) - x_s^2\left(1 - \frac{B\xi}{mx_s}\right) - \frac{x_s\xi}{2}x^m \ln\left|\frac{1+x}{1-x}\right|\right]^2 + \left(\frac{\pi}{2}x_s\xi x^m\right)^2.$$

So for any given values of the coupling strength α and of the temperature the corresponding values of $\langle-\sigma_z\rangle$ and B can be calculated numerically. The result for $\langle-\sigma_z\rangle$ is illustrated in figure 1 for $m = 1$ (Ohmic dissipation). The broken curve indicates the cross-over from coherent to non-coherent behaviour. This will be explained in § 8 in more detail. For $m = 3$ the qualitative behaviour is similar, but there is no cross-over line.

7. Additional counter-check by Goldberger–Adams expansions

Beyond the virtue that our spectral function $I_{\sigma_x\sigma_x}(\omega)$ satisfies the lowest four sum rules and—as can be seen by inserting Λ_s and $\{\Lambda_r, V_r\}_r$ in (35c)—also the fifth moment, if (Δ, α, T) are not too large, we have the additional option of counter-checking the self-consistency requirements (61) and (62) themselves by exact series expansions. Applying

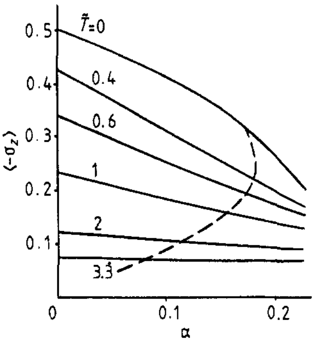

Figure 1. $\langle -\sigma_z \rangle_T^H$ as a function of temperature and coupling strength for Ohmic dissipation, i.e. $m = 1$ ($\tilde{T} = k_B T/\Delta$; $x_s = \Delta/\Omega_D = 0.1$). The broken curve is the cross-over line.

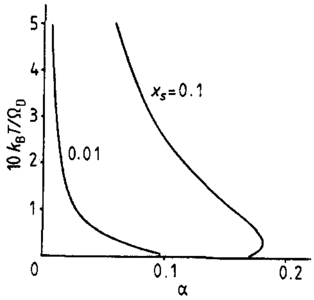

Figure 2. Cross-over temperature as a function of the coupling strength α for Ohmic dissipation, i.e. $m = 1$ ($x_s = \Delta/\Omega_D$).

the Goldberger–Adams theorem [17] we can derive such expansions for all thermodynamic properties of Hamiltonian (1) in the whole temperature range. The details of this calculation are given elsewhere. Specifically it can be shown that for small α the internal energy $U = \langle H \rangle_T^H$ and the specific heat $C = \partial U/\partial T$ of this Goldberger–Adams (GA) expansion are in exact agreement up to the leading coupling term with the corresponding quantities deduced from our GF $\langle\langle \sigma_x | \sigma_x \rangle\rangle_E$ or $I_{\sigma_x\sigma_x}(\omega)$ respectively. Furthermore the thermal expectation value $\langle \sigma_z \rangle_T^H$ and the quantity B of the GA and GF calculation are the same in the whole temperature region; in the intermediate temperature regime $\Delta \ll k_B T \ll \Omega_D$ one gets for instance

$$\langle \sigma_z \rangle = \begin{cases} -\beta \dfrac{\Delta}{4}\left[1 - 2\alpha\left(\ln \dfrac{\beta\Omega_D}{2} + \dfrac{2}{\beta\Omega_D} - \dfrac{2}{3}\right)\right] + O(\alpha^2) & \text{for } m = 1 \quad (63a) \\ -\dfrac{\beta\Delta}{4}\left[1 - 2\alpha\left(\dfrac{1}{2} - \dfrac{2}{\beta\Omega_D}\right)\right] + O(\alpha^2) & \text{for } m = 3 \quad (63b) \end{cases}$$

and

$$B = \begin{cases} \dfrac{x_s\beta\Delta}{2}\left(\ln \dfrac{\beta\Omega_D}{2} + \dfrac{2}{\beta\Omega_D} - \dfrac{2}{3}\right) + O(\alpha) & \text{for } m = 1 \quad (64a) \\ \dfrac{3x_s\beta\Delta}{4}\left(1 - \dfrac{4}{\beta\Omega_D} + \dfrac{80}{9}\dfrac{1}{(\beta\Omega_D)^2}\right) + O(\alpha) & \text{for } m = 3. \quad (64b) \end{cases}$$

8. Temporal and spectral behaviour

We now want to apply the GF $\langle\langle \sigma_x | \sigma_x \rangle\rangle_E$ of (48) or the corresponding spectral function $I_{\sigma_x\sigma_x}$ to the diffusion problem attached to Hamiltonian (1). According to (2a) σ_x describes the occupation difference between 'left' and 'right'. The diffusion process can be characterised by the relaxation behaviour of $\langle \sigma_x \rangle(t)$ after a non-equilibrium occupation $\langle \sigma_x \rangle(t =$

0) $\neq 0$ has been established via adiabatic symmetry breaking. This situation is described by an additional Hamiltonian term $H_1(t)$,

$$H_1(t) = -\Lambda\sigma_x\, e^{\varepsilon t}\theta(-t) \qquad (\theta \text{ is the step function, } \varepsilon = 0_+) \tag{65}$$

which yields the Kubo time evolution

$$\langle\sigma_x\rangle(t) = -\Lambda \int_{-\infty}^{+\infty} \frac{\langle\langle\sigma_x|\sigma_x\rangle\rangle_{\omega+i\varepsilon} - \langle\langle\sigma_x|\sigma_x\rangle\rangle_{\omega-i\varepsilon}}{i\omega+\varepsilon}\, e^{-i\omega t}\, d\omega \qquad \text{for } t \geqslant 0. \tag{66}$$

Hence all the details of the decay are incorporated in our GF $\langle\langle\sigma_x|\sigma_x\rangle\rangle_E$. The quantity

$$R(\omega) \equiv -\frac{\langle\langle\sigma_x|\sigma_x\rangle\rangle_{\omega+i\varepsilon} - \langle\langle\sigma_x|\sigma_x\rangle\rangle_{\omega-i\varepsilon}}{i\omega+\varepsilon} \tag{67}$$

can be considered as the Fourier transform of $\langle\sigma_x\rangle(t)$. Via (17), the function $R(\omega)$ is directly related to the spectral function $I_{\sigma_x\sigma_x}(\omega)$ via

$$I_{\sigma_x\sigma_x}(\omega) = \frac{\omega}{e^{\beta\omega}-1} R(\omega) \tag{68}$$

and from (51) and (55) we have

$$I_{\sigma_x\sigma_x}(\omega) = \frac{\Delta\langle-\sigma_z\rangle}{e^{\beta\omega}-1} S(\omega). \tag{69}$$

Adopting the power-law coupling of (3) again, we are left with ($m = 1$ or 3)

$$I_{\sigma_x\sigma_x}(\omega) = \begin{cases} \dfrac{x_s^2\alpha}{2\Omega_D}\dfrac{1}{e^{\beta\Omega_D x}-1}\dfrac{x^m}{\Xi} & \text{for } |x| < 1 \\ 0 & \text{for } |x| > 1 \end{cases} \tag{70}$$

where $x = \omega/\Omega_D$ and Ξ is defined below (62). To derive simple analytic expressions we simplify the denominator of $I_{\sigma_x\sigma_x}$ by means of the argument that the tunnelling frequency Δ (i.e. $x_s = \Delta/\Omega_D$) will be a very small quantity, whence we may expect the region far below the cut-off frequency Ω_D to play the dominant role. We therefore write

$$\ln|(1+x)/(1-x)| \simeq 2x \tag{71}$$

whence for Ohmic dissipation ($m = 1$) we are left with

$$I_{\sigma_x\sigma_x}(\omega) = \frac{x_s^2\alpha}{2\Omega_D}\frac{1}{e^{\beta\Omega_D x}-1}\frac{1}{(1-x_s\xi)^2}\frac{x}{[x^2-(a^2-b^2/2)]^2+b^2(a^2-b^2/4)} \tag{72}$$

where

$$a^2 = \frac{x_s(x_s - B\xi)}{1-x_s\xi} \qquad b = \frac{\pi}{2}\frac{x_s\xi}{1-x_s\xi}. \tag{73}$$

The relaxation behaviour of $\langle\sigma_x\rangle(t)$ is determined by the poles of $R(\omega)$ or $I_{\sigma_x\sigma_x}(\omega)$ respectively. From (72) we learn that for $a^2 < b^2/4$ the poles of $I_{\sigma_x\sigma_x}(\omega)$ are purely

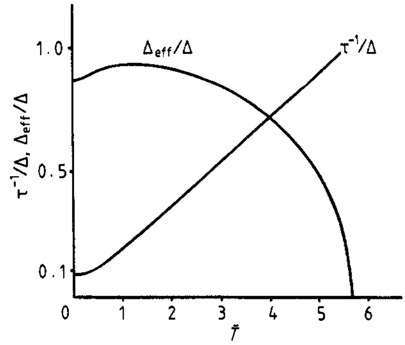

Figure 3. Tunnelling frequency Δ_{eff} and damping τ^{-1} as functions of temperature for $\alpha = 0.05$ and Ohmic dissipation, i.e. $m = 1$ ($x_s = \Delta/\Omega_D = 0.1$; $\tilde{T} = k_BT/\Delta$).

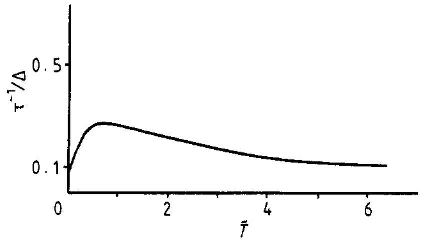

Figure 4. Damping or inverse relaxation time τ^{-1} as a function of temperature for $\alpha = 0.2$ and Ohmic dissipation, i.e. $m = 1$ ($x_s = \Delta/\Omega_D = 0.1$, $\tilde{T} = k_BT/\Delta$).

imaginary ones which produce a non-oscillating, exponentially damped decay behaviour. On the other hand, $a^2 > b^2/4$ yields complex poles which correspond to an oscillating relaxation of $\langle\sigma_x\rangle(t)$. For $a^2 = b^2/4$, which is equivalent to

$$B = \frac{x_s}{\xi}\left(1 - \frac{\pi^2}{16}\frac{\xi^2}{1 - x_s\xi}\right) \tag{74}$$

we have a cross-over from oscillating to non-oscillating relaxation. Inserting (74) in the self-consistency equations (61)–(62) we obtain the $T_c(\alpha)$ lines illustrated in figure 2. In the high-temperature limit the cross-over line follows the analytic relation

$$\alpha \simeq \frac{\Delta}{\pi k_B T_c}\left(1 - \frac{\Delta}{6\pi k_B T_c}\right). \tag{75}$$

In the oscillation regime, i.e. for small α and temperatures below $T_c(\alpha)$, the relaxation reads

$$\langle\sigma_x\rangle(t) = \frac{\Lambda}{\Omega_D}\frac{\alpha x_s^2}{(1 - x_s\xi)^2}\frac{\pi}{4uv(u^2 + v^2)}[u\cos(u\Omega_D t) + v\sin(u\Omega_D t)]\,e^{-v\Omega_D t} \tag{76}$$

with

$$u = (|a^2 - b^2/4|)^{1/2} \qquad v = b/2 \tag{77}$$

where $(\pm u \pm iv)\Omega_D$ are the poles of $I_{\sigma_x\sigma_x}(\omega)$. The temperature behaviour of the tunnelling frequency $\Delta_{eff} = u\Omega_D$ and the damping $\tau^{-1} = v\Omega_D$ is given in figure 3. The damping shows an almost linear increase, whereas the tunnelling frequency decreases and turns to zero at the cross-over point.

In the non-oscillation region the poles are $\pm i(v + u)\Omega_D$, $\pm i(v - u)\Omega_D$, whence we are left with

$$\langle\sigma_x\rangle(t) = \frac{\Lambda}{\Omega_D}\frac{\alpha x_s^2}{(1 - x_s\xi)^2}\frac{1}{8uv}\frac{e^{-(v-u)\Omega_D t}}{v - u}\left(1 - \frac{v - u}{v + u}e^{-2u\Omega_D t}\right). \tag{78}$$

Hence the dominant relaxation time τ is given by

$$\tau^{-1} = (v - u)\Omega_D. \tag{79}$$

This is illustrated in figure 4 for $\alpha = 0.2$; we note that the damping τ^{-1} decreases for $\tilde{T} > 1$.

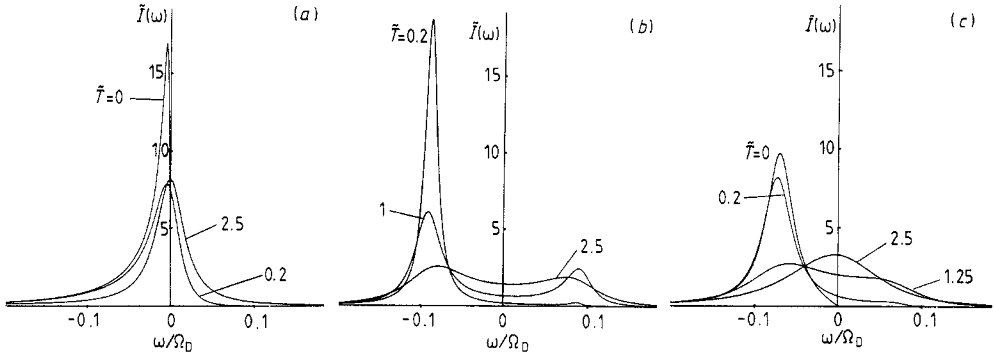

Figure 5. Spectral function $\tilde{I}_{\sigma x\sigma x}(\omega) = 2\Omega_D I_{\sigma x\sigma x}(\omega)$ for different couplings and temperatures (Ohmic dissipation $m = 1$; $x_s = \Delta/\Omega_D = 0.1$; $\tilde{T} = k_B T/\Delta$): (*a*) $\alpha = 0.2$, (*b*) $\alpha = 0.05$, (*c*) $\alpha = 0.1$.

The qualitative relaxation behaviour can also be seen from the spectral function $I_{\sigma_x\sigma_x}(\omega)$. In figure 5 these lines are given for different values of α and temperature. Figure 5(*a*) for instance shows the 'central peak', which is typical for a non-oscillating decay. Figure 5(*b*) reveals the oscillating behaviour of a small α value, whereas in figure 5(*c*) the transition from oscillation at low temperature to a central peak non-oscillating behaviour at high temperature (i.e. the cross-over) can be observed.

To evaluate analytical expressions for the relaxation time, we should know $\langle\sigma_z\rangle$ and B as functions of the coupling strength and temperature. In the intermediate temperature regime $\Delta \ll k_B T \ll \Omega_D$ these quantities are given by (63*a*, *b*) and (64*a*, *b*). In the Appendix we show that (for $\Delta \ll k_B T \ll \Omega_D$) the damping is given by

$$\tau^{-1} = \alpha\pi \frac{1}{1 - \frac{7}{3}\alpha} k_B T \sim T \qquad \text{in the oscillatory regime} \tag{80}$$

and

$$\tau^{-1} = \frac{\Delta x_s}{\pi\alpha} e^{-\alpha} \left(\frac{2k_B T}{\Omega_D}\right)^{2\alpha - 1} \qquad \text{in the non-oscillatory region.} \tag{81}$$

Let us now consider the coupling case $m = 3$, where, neglecting the ln term (which is of order x^4), we arrive at

$$I_{\sigma_x\sigma_x}(\omega) = \frac{x_s^2\alpha}{2\Omega_D} \frac{1}{e^{\beta\Omega_D x} - 1}$$

$$\times \frac{1}{(x_s\xi\pi/2)^2 x^6 + x^4(1 + x_s\xi)^2 - 2(1 + x_s\xi)x_s(x_s - B\xi/3)x^2 + x_s^2(x_s - B\xi/3)^2}. \tag{82}$$

The denominator is then a polynomial of third degree in x^2, whose zeros can be found exactly by means of the Cardini formulae. A straightforward calculation yields that there

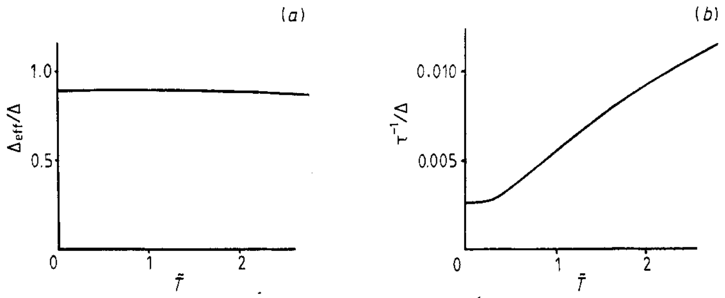

Figure 6. Tunnelling frequency $\Delta_{\rm eff}$ and damping τ^{-1} as functions of temperature for $\alpha = 0.2$ and $m = 3$ coupling ($x_s = \Delta/\Omega_{\rm D} = 0.1$; $\tilde{T} = k_{\rm B}T/\Delta$).

is no cross-over temperature as in the case $m = 1$ and that the relaxation behaviour of $\langle\sigma_x\rangle(t)$ is always an oscillating one:

$$\langle\sigma_x\rangle(t) = \frac{\Lambda}{2\Omega_{\rm D}} \frac{\alpha x_s^2}{(1 + x_s\xi)^2} \frac{\pi}{2\tilde{u}\tilde{v}} [\tilde{u}\cos(\tilde{u}\Omega_{\rm D}t) - \tilde{v}\sin(\tilde{u}\Omega_{\rm D}t)]\, {\rm e}^{-(\tilde{v}\Omega_{\rm D}t)} \tag{83}$$

where the tunnelling frequency $\Delta_{\rm eff}$ and the damping, i.e. the inverse relaxation time τ^{-1}, are

$$\Delta_{\rm eff} = \tilde{u}\Omega_{\rm D} = \Delta\left(\frac{1 - B\xi/3x_s}{1 + x_s\xi}\right)^{1/2} \qquad \tau^{-1} = \tilde{v}\Omega_{\rm D} = \Delta\frac{1 - B\xi/3x_s}{1 + x_s\xi}\frac{\pi}{4}\frac{x_s^2\xi}{1 + x_s\xi}. \tag{84}$$

The temperature dependence of $\Delta_{\rm eff}$ and τ^{-1} for $\alpha = 0.2$ due to (84) is illustrated in figure 6 (the values of B and ξ for given temperature have been calculated from (61)–(62) by self-consistency). We recognise that $\Delta_{\rm eff}$ is almost independent of T, whereas the damping obviously shows an almost linear increase. In the intermediate temperature region $\Delta \ll k_{\rm B}T \ll \Omega_{\rm D}$ the damping τ^{-1} is given by (85) (see Appendix), if α is not too large:

$$\tau^{-1} \simeq \pi x_s^2 \alpha (k_{\rm B}T)\left[1 - 8\alpha\frac{k_{\rm B}T}{\Omega_{\rm D}}\left(1 + \frac{10}{9}\frac{k_{\rm B}T}{\Omega_{\rm D}}\right)\right]. \tag{85}$$

9. Summary and discussion

In this paper we have presented a Green function approach to handle the fundamental decay problem attached to the archetypal Hamiltonian (1), which has been studied by many workers during the past 30 years. We have given a procedure for how to trace back the fundamental GF $\langle\!\langle\sigma_x|\sigma_x\rangle\!\rangle_E$, which governs the diffusive process to the GF of an exactly solvable oscillator–bath problem with temperature-dependent constants. These parameters in principle could be determined in such a way that the sum rules of the spectral function $I_{\sigma_x\sigma_x}(\omega)$ up to a desired order be preserved. If we confine ourselves to the lowest four moments of $I_{\sigma_x\sigma_x}$, the corresponding Green function $\langle\!\langle\sigma_x|\sigma_x\rangle\!\rangle_E$ can be obtained by a factorisation beyond Hartree–Fock. In addition to subject our *ansatz* the frame provided by the sum rules we have counter-checked our calculation by comparison with Goldberger–Adams expansions.

In the second part of our paper we investigate the decay process by a Kubo response formalism based on our GF $\langle\!\langle\sigma_x|\sigma_x\rangle\!\rangle_E$. In the case of Ohmic dissipation coupling we find that for weak coupling the decay is an exponentially damped oscillating one below some critical temperature T_c. If Δ is small enough such that $\Delta \ll k_B T \ll k_B T_c$ the diffusion constant follows a T^1 law. Above this cross-over temperature (or, if the coupling α is strong enough, in the whole temperature range) the relaxation process is a non-oscillating one. In this case the diffusion decreases according to a $T^{2\alpha-1}$ law in the intermediate temperature region $\Delta \ll k_B T \ll \Omega_D$. For $m = 3$ coupling we find no cross-over temperature and a damped oscillatory decay in the whole α/T range.

Since the presented tunnelling model for the Ohmic dissipation coupling set-up presently experiences prominent research activity, the result of a $T^{2\alpha-1}$ behaviour of the diffusion constant has been found in many different ways [3, 18, 19] in succession to the Kondo derivation [7]. This result also seems to be justified by experiments [20–24]. However, up to the present, a Green function approach, which for many other decay problems has proven successful, has failed to display its power for the tunnelling problem. Therefore the motivation for our work has been to find a key to apply the Green function technique also here. We have found that the archetypal model of mode-assisted tunnelling satisfies a rigorous anti-resonance condition between the spin and bath Green functions, which provides, in combination with sum rules, a possible key.

Appendix. Analytical expressions for the relaxation time

We first turn to the case $m = 1$, where in the oscillation region (for weak coupling) the damping is given by

$$\tau^{-1} = v\Omega_D = \Omega_D \frac{\pi}{4} \frac{x_s \xi}{1 - x_s \xi} = \frac{\Delta}{4} \pi \frac{\alpha}{\langle -\sigma_z \rangle - x_s \alpha}. \tag{A1}$$

Inserting $\langle -\sigma_z \rangle$ according to (63a) we get in the intermediate temperature region $\Delta \ll k_B T \ll \Omega_D$

$$\tau^{-1} = \frac{\alpha\pi}{\beta} \left[1 - 2\alpha \left(\ln \frac{\beta\Omega_D}{2} + \frac{4}{\beta\Omega_D} - \frac{2}{3} \right) \right]^{-1}. \tag{A2}$$

For $2 \leqslant \beta\Omega_D \leqslant 10$ the term in parentheses is nearly a constant, the value of which is about $\frac{7}{6}$; so the inverse relaxation time is given by

$$\tau^{-1} \simeq \alpha\pi \frac{1}{1 - \frac{7}{3}\alpha} k_B T. \tag{A3}$$

In the non-oscillation region the damping is given by (79); because $a^2/b^2 \ll 1$ we can approximate

$$u = \left(\frac{b^2}{4} - a^2 \right)^{1/2} \simeq \frac{b}{2} \left(1 - \frac{2a^2}{b^2} \right) \qquad (v - u) = \frac{b}{2} - u \simeq \frac{a^2}{b}. \tag{A4}$$

With (63a) and (64a) we arrive at

$$\tau^{-1} = \Omega_D \frac{x_s - B\xi}{(\pi/2)\xi} = \frac{\langle -\sigma_z \rangle x_s - B\alpha}{(\pi/2)\alpha} \Omega_D = \Delta \frac{\beta\Delta/2}{\pi\alpha} \left\{ 1 - 2\alpha \ln\left(\frac{\beta\Omega_D}{2} \right) - 2\alpha \left[\ln\left(\frac{\beta\Omega_D}{2} \right) + \frac{4}{\beta\Omega_D} - \frac{4}{3} \right] \right\}. \tag{A5}$$

By the same argument we have just used above, this expression can be simplified to

$$\tau^{-1} = \Delta \frac{\beta\Delta/2}{\pi\alpha}\left(1 - 2\alpha \ln \frac{\beta\Omega_{\mathrm{D}}}{2} - \alpha\right) = \frac{\Delta x_s}{\pi\alpha} \mathrm{e}^{-\alpha}\left(\frac{\beta\Omega_{\mathrm{D}}}{2}\right)^{1-2\alpha}. \tag{A6}$$

For $m = 3$ we have from (63*b*), (64*b*) and (84)

$$\tau^{-1} = \pi x_s^2 \alpha(k_{\mathrm{B}}T) \frac{1 + \alpha[8k_{\mathrm{B}}T/\Omega_{\mathrm{D}} - 2 - \frac{80}{9}(k_{\mathrm{B}}T/\Omega_{\mathrm{D}})^2]}{[1 + \alpha(8k_{\mathrm{B}}T/\Omega_{\mathrm{D}} - 1)]^2} \tag{A7}$$

which for small α can be simplified to

$$\tau^{-1} \simeq \pi x_s^2 \alpha(k_{\mathrm{B}}T)\left[1 - 8\alpha \frac{k_{\mathrm{B}}T}{\Omega_{\mathrm{D}}}\left(1 + \frac{10}{9}\frac{k_{\mathrm{B}}T}{\Omega_{\mathrm{D}}}\right)\right]. \tag{A8}$$

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