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Generalised master equation: dissipative dynamics of the double-well system

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Abstract. We applied the generalised master equation (GME) to the analysis of the object function, $s(t)$, which describes the motion of the tunnelling particle in a double-well system coupled to a reservoir consisting of independent bosonic-type elementary excitations. First, using the 'unrelaxed' initial condition and a suitable projection operator we give the exact formal solution of the GME. Then, the memory operator in the GME is explicitly calculated in the weak-tunnelling regime and the function $s(t)$ is obtained. An independent derivation is given which enables us to obtain the exact expansion of the function $s(t)$ by means of a purely algebraic method. This expansion forms a basis on which our GME method and the well known functional-integral approach are compared: the GME-weak-tunnelling approximation is shown to be identical to the commonly used non-interacting-blip approximation ensuing from the functional-integral method. A new approximation is analysed which is weaker than the non-interacting-blip one.

1. Introductory remarks: definition of the model

Let us consider the motion of a particle (single degree of freedom) in a double-well potential. The quantum particle has the possibility of tunnelling through the potential barrier to the other well and will do so with a frequency Δ. In addition to that, the particle interacts with a reservoir. As a result of the specific form of the interaction (see below), the motion of the particle is connected to the local changes in the reservoir, i.e. with the motion of the 'cloud' of reservoir excitations. This leads to the destruction of the coherent motion and to a dissipative behaviour. On the whole, the tendency to coherent oscillatory motion competes with that to localisation.

The dynamics of the dissipative double-well system was recently reviewed to be an extremely relevant problem in several areas of physics [1]. Let us mention some of them: dynamics of the protonation in organic compounds [2], spin-phonon relaxation phenomena [3], transitions in chiral molecules [4], the question of observing a quantum coherence effect on a macroscopic level in SQUID rings [5], description of para-electric impurities with phonon coupling [6]. It is believed that the common features of these dynamical problems can be adequately described using the Hamiltonian

$$\frac{1}{\hbar}\mathbf{H} = \Delta \mathbf{N} \otimes \mathbf{1}_R + \mathbf{S} \otimes \mathbf{R} + \mathbf{1}_S \otimes \frac{1}{\hbar}\mathbf{H}_R. \tag{1}$$

Here the pseudospin operator $\mathbf{N} = \frac{1}{2}(|+\rangle\langle -| + |-\rangle\langle +|)$ describes pure oscillatory motion of the particle between two sites $|+\rangle$ (the 'left' well) and $|-\rangle$ (the 'right' well) and Δ is

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the bare tunnelling frequency. The particle-reservoir interaction is linear in the particle-coordinate operator—the continuous coordinate is replaced by the operator $\mathbf{S}=\frac{1}{2}(|+\rangle\langle+|-|-\rangle\langle-|)$ whose spectrum displays only two discrete values $-\frac{1}{2}$, $+\frac{1}{2}$. $\mathbf{H}_R$, $\mathbf{1}_R$ and $\mathbf{R}$ are reservoir operators.

Usually, the above-mentioned situation leads to the assumption that the reservoir can be described by independent bosonic-type elementary excitations. The number of modes, M, is assumed to be very large. Further, the operator $\mathbf{R}$ in (1) is supposed to be linear in the lowering and raising operators of these excitations. Thus we have

$$\frac{1}{\hbar}\mathbf{H}_R=\sum_{i=1}^{M}\omega_i\mathbf{B}_i^{\dagger}\mathbf{B}_i \qquad \mathbf{R}=\sum_{i=1}^{M}\kappa_i(\mathbf{B}_i^{\dagger}+\mathbf{B}_i). \tag{2}$$

For the model to be completely determined, one needs an explicit prescription for the coupling parameters κ_i, $i=1,\ldots,M$ and for the phonon frequencies ω_i, $i=1,\ldots,M$. Instead, one assumes that the number of degrees of freedom of the reservoir tends to infinity and one introduces the strength function [7, 8]

$$\gamma(\omega)=\lim_{M\to\infty}\sum_{i=1}^{M}\kappa_i^2\delta(\omega-\omega_i). \tag{3}$$

The assumption of an infinite reservoir is then implicit in the replacements of sums by integrals. This will be done at an appropriate stage of calculation and we shall use the specific form of the strength function according to the formula (Ohmic coupling, [9, 8])

$$\gamma(\omega)=\gamma\frac{\omega}{\omega_c}\exp\left\{-\frac{\omega}{\omega_c}\right\}. \tag{4}$$

The parameter γ measures the overall strength of the coupling and the cut-off frequency, ω_c, gives the relevant interaction bandwidth.

The primary interest of the dynamical studies connected with Hamiltonian (1) is the calculation of the mean value of the particle coordinate as a function of time. Given the initial condition for the whole particle-plus-reservoir density matrix, $\rho(0)$, one desires to calculate the real function, $s(t)$, the normalised mean value of the particle coordinate

$$s(t)=\frac{(\mathbf{S}\otimes\mathbf{1}_R|\rho(t))}{(\mathbf{S}\otimes\mathbf{1}_R|\rho(0))} \tag{5}$$

with $s(0)=0$ and $s(t)\in\langle-1,+1\rangle$. Here and below, the Hilbert-Schmidt scalar product is used: $(\mathbf{A}|\mathbf{B})=\mathrm{Tr}_{S+R}(\mathbf{A}^{\dagger}\mathbf{B})$.

From the theoretical point of view one is thus faced with the typical open-system dynamics problem. The exact solution of the problem is not known and approximations are inevitable. The theoretical methods used fall into the following main categories: unitary transformation method (i.e. partial diagonalisation of Hamiltonian (1), (2) by means of the polaron transformation [10] or the Fulton-Gouterman transformation [11]), variational approaches [12, 13], instanton methods [14], GME approach [9, 15, 16], path integral methods [1, 17, 18] (usually in connection with the so-called non-interacting-blip approximation).

Apart from this very broad recent discussion, several open problems survive. It turns out that the model is extremely sensitive to possible approximations. It is the question of asymptotic localisation, above all, that does not seem to be convincingly

solved. Other problems are the temperature dependence of the function $s(t)$ and the role of the strength function, describing the particle–reservoir interaction in the infinite reservoir limit. The behaviour of the function $s(t)$ in the asymptotic region was shown to be sensitive to the low-frequency behaviour of the strength function.

In this paper we use the time-convolution GME and our objective is to obtain its solution in the experimentally interesting weak-tunnelling arbitrary coupling case. We shall formulate the technical parts of the calculations at the superoperator (rather than operator) level. The superoperators will be designated by script letters, e.g. $\mathscr{L}$, $\mathscr{M}$, $\mathscr{R}$, $\mathscr{T}$. In § 2, this approach gives us a general structure of the exact solution, equation (16). This is then used in § 3 to obtain a weak-tunnelling expansion of the GME memory operator and, subsequently, the approximative forms of the function $s(t)$. Eventually, in the discussion, the interpretation of these results lead us to a connection between the GME method and the functional-integral approach. As for the numerical calculations, we need the numerical procedure for the inverse Laplace transformation. We have adapted the one from [19, 20] and employed it to the inversion of the basic formulae (26) and (32).

Our problem, we recall, is a typical initial-value dynamical one. It should be noted that we do not deal with the equilibrium state correlations [8]; nor do we study the interesting question whether in the limit $t \to \infty$ the state of the joint system converges to its equilibrium state.

2. The GME and its formal solution

The Liouville equation for the double-well-plus-reservoir density matrix, $\rho(t)$, reads

$$\frac{\mathrm{d}}{\mathrm{d}t}|\rho(t)) = -\mathrm{i}\mathscr{L}|\rho(t)). \tag{6}$$

Here $\mathbf{H}$ is as in (1) and $\mathscr{L} = (1/\hbar)[\mathbf{H}, *]$ is the Liouville superoperator [21]. We shall use the term 'operator' since the distinction between operators and superoperators is given by the symbols used (e.g. $\mathscr{L}$ as opposed to $\mathbf{L}$). Introducing the basis $|1) = ||-\rangle\langle -|)$, $|2) = ||+\rangle\langle +|)$, $|3) = ||-\rangle\langle +|)$, $|4) = ||+\rangle\langle -|)$ in the Liouville space of the particle (notice the ordering of the basis) and using the scalar product $(\mathbf{A}_S|\mathbf{B}_S) = \mathrm{Tr}_S(\mathbf{A}_S^+\mathbf{B}_S)$ the Liouville operator can be expressed in the form of a 4×4 matrix whose elements are operators in the reservoir space. More specifically, one obtains

$$\mathscr{L} \equiv \mathscr{L}_D + \mathscr{L}_N = \mathrm{diag}(\mathscr{L}_R - \mathscr{T}, \mathscr{L}_R + \mathscr{T}, \mathscr{L}_R - \mathscr{R}, \mathscr{L}_R + \mathscr{R}) + \Delta\mathscr{M} \otimes \mathscr{I}_R \tag{7}$$

where $\mathrm{diag}(*, *, *, *)$ is a diagonal matrix. The diagonal term $\mathscr{L}_D$ corresponds to $\mathscr{L}_{SR}$ and $\mathscr{I}_S \otimes \mathscr{L}_R$, i.e. to the second and the third part of (1). We have introduced the assignment $\mathscr{T} = \frac{1}{2}[\mathbf{R}, *]$, $\mathscr{R} = \frac{1}{2}\{\mathbf{R}, *\}$ with $\mathbf{R}$ as in (2) and with $\{\mathbf{X}, \mathbf{Y}\}$ being the anticommutator of the operators $\mathbf{X}$ and $\mathbf{Y}$. The matrix $\mathscr{M}$ in (7) is

$$\mathscr{M} = \frac{1}{2}\begin{pmatrix} 0 & 0 & -1 & +1 \\ 0 & 0 & +1 & -1 \\ -1 & +1 & 0 & 0 \\ +1 & -1 & 0 & 0 \end{pmatrix}. \tag{8}$$

At this point, we must specify the initial condition to be used in connection with (6). We assume that the particle is initialy localised in the 'left' well and the reservoir

is in the equilibrium state up to $t=0$ when the double-well system is joined to it [22]. Thus the variables of the particle and those of the reservoir are initially uncorrelated. The whole initial condition then reads ($\beta \equiv 1/(k_B T)$)

$$\rho(0) = |-\rangle\langle -| \otimes \pi_R \qquad \pi_R = \frac{\exp(-\beta \mathbf{H}_R)}{\mathrm{Tr}_R[\exp(-\beta \mathbf{H}_R)]}. \tag{9}$$

It should be emphasised that (9) is not the equilibrium density matrix of the whole particle-plus-reservoir system $\rho_{EQV} \propto \exp(-\beta \mathbf{H})$ nor is it the state of the localised particle with the boson reservoir relaxed around it [1, 16].

It follows from the above formulation that we are not interested in the complete information carried by the particle-plus-reservoir density matrix $\rho(t)$. The relevant information describes the time evolution of the double-well system *per se* including, of course, all consequences of the interaction with the reservoir. This information is represented by the reduced density matrix $\sigma(t) = \mathrm{Tr}_R[\rho(t)]$. Provided the reduced density matrix $\sigma(t)$ is known, the object function (5) can be expressed as

$$s(t) = \frac{(\mathbf{S}|\sigma(t))}{(\mathbf{S}|\sigma(0))} = (1|\sigma(t)) - (2|\sigma(t)) = 2(1|\sigma(t)) - 1. \tag{10}$$

Here, the symbol $(*|*)$ means the scalar product in the particle Liouvile space.

The above-mentioned reduction of the information is formally peerformed using a suitable projection operator [21, 23]. In view of our choice of the initial condition, equation (9), it is reasonable to employ the projection operator $\mathcal{D}_0 = \mathcal{I}_S \otimes \mathcal{P}_0$ with $\mathcal{P}_0 = |\pi_R)(\mathbf{1}_R|$, where π_R was introduced in (9). The point is that with this projector one gets $\mathcal{D}_0|\rho(0)) = |\rho(0))$ and, consequently, the inhomogenous term in the convolution-type GME [24–26] is equal to zero. For later use it is convenient to introduce also the orthogonal projectors $\mathcal{D}_1 = \mathcal{I}_S \otimes \mathcal{I}_R - \mathcal{D}_0$ and $\mathcal{P}_1 = \mathcal{I}_R - \mathcal{P}_0$.

Applying the projector $\mathcal{D}_0$ and $\mathcal{D}_1$ on both sides of the Liouville equation (6) one acquires a system of coupled equations for $\mathcal{D}_0|\rho(t))$ and $\mathcal{D}_1|\rho(t))$. The solution of this system leads directly to a closed integrodifferential equation for the reduced density matrix $|\sigma(t))$, i.e. to the GME [24–26]

$$\frac{\mathrm{d}}{\mathrm{d}t}|\sigma(t)) = -\mathrm{i}\Delta\mathcal{M}|\sigma(t)) - \int_0^t \mathcal{K}(t-t')|\sigma(t'))\,\mathrm{d}t' \tag{11}$$

where the memory operator, $\mathcal{K}(t)$, is given by the formula

$$\mathcal{K}(t) = (\mathbf{1}_R|\mathcal{D}_0\mathcal{L}\exp(-\mathrm{i}t\mathcal{D}_1\mathcal{L}\mathcal{D}_1)\mathcal{D}_1\mathcal{L}\mathcal{D}_0|\pi_R). \tag{12}$$

In the next step we make use of some simple properties of the operators involved. Utilising the respective definitions one can prove the equalities $\mathcal{L}_R\mathcal{P}_0 = \mathcal{P}_0\mathcal{L}_R = 0$, $\mathcal{D}_0\mathcal{L}_{SR}\mathcal{D}_0 = 0$, $\mathcal{P}_1\mathcal{T} = \mathcal{T}$ and $\mathcal{P}_1\mathcal{L}_R = \mathcal{L}_R$. Then, using these formulae, the memory operator acquires the final form

$$\mathcal{K}(t) = (\mathbf{1}_R|\mathrm{diag}(0, 0, -\mathcal{R}, +\mathcal{R})\exp(-\mathrm{i}t\mathcal{W})\,\mathrm{diag}(-\mathcal{T}, +\mathcal{T}, -\mathcal{R}, +\mathcal{R})|\pi_R) \tag{13}$$

where the operator $\mathcal{W}$ in the exponent is

$$\mathcal{W} \equiv \mathcal{W}_D + \mathcal{W}_N = \mathrm{diag}(\mathcal{L}_R - \mathcal{T}, \mathcal{L}_R + \mathcal{T}, \mathcal{L}_R - \mathcal{P}_1\mathcal{R}, \mathcal{L}_R + \mathcal{P}_1\mathcal{R}) + \Delta\mathcal{M} \otimes \mathcal{I}_R. \tag{14}$$

Let us introduce the notation $k_{ij}(t) = (i|\mathcal{K}(t)|j)$ for the matrix elements of the memory operator; $k_{ij}(t)$ are already c-number functions of time. The elements $k_{1_j}(t)$ and $k_{2_j}(t)$ $j = 1, \ldots, 4$ are clearly seen to be zero. Furthermore, it follows from the obvious properties $(1|\sigma(t)) + (2|\sigma(t)) = 1$, $(3|\sigma(t))^* = (4|\sigma(t))$ that $k_{31}^*(t) = k_{41}(t)$,

$k_{32}^*(t) = k_{42}(t)$, $k_{33}^*(t) = k_{44}(t)$ and $k_{34}^*(t) = k_{43}(t)$. Thus the whole memory operator is determined by the eight real functions of time. It will be useful to take them as

$$\begin{aligned} v_1(t) &= \mathrm{Re}[k_{33}(t) + k_{34}(t)] & w_1(t) &= \mathrm{Re}[k_{31}(t) + k_{32}(t)] \\ v_2(t) &= \mathrm{Re}[k_{33}(t) - k_{34}(t)] & w_2(t) &= \mathrm{Re}[k_{31}(t) - k_{32}(t)] \\ v_3(t) &= \mathrm{Im}[k_{33}(t) + k_{34}(t)] & w_3(t) &= \mathrm{Im}[k_{31}(t) + k_{32}(t)] \\ v_4(t) &= \mathrm{Im}[k_{33}(t) - k_{34}(t)] & w_4(t) &= \mathrm{Im}[k_{31}(t) - k_{32}(t)]. \end{aligned} \tag{15}$$

Before we embark on the calculation of the functions $k_{ij}(t)$ and/or $v_i(t)$, $w_i(t)$, it is useful to employ the known global structure of the matrices $\mathcal{M}$, $\mathcal{K}(t)$ and formally solve the GME. Applying the Laplace transformation on both sides of (11) one acquires a system of four algebraic equations for the functions $(i|\sigma(z))$, $i = 1, \ldots, 4$, i.e. for the Laplace transforms of the functions $(i|\sigma(t))$, $i = 1, \ldots, 4$. This system can be readily solved; leaving out the details of this algebra, we write down the final formula for the Laplace transform of the object function, $s(t)$:

$$s(z) = \frac{1}{z}\left(z + \Delta\frac{(z+v_1)w_3 - v_3 w_1}{(z+v_1)(z+v_2)+v_3 v_4}\right)\left(z + \Delta\frac{(z+v_1)(\Delta - w_4)+v_3 w_2}{(z+v_1)(z+v_2)+v_3 v_4}\right)^{-1}. \tag{16}$$

Here v_i, w_i, $i = 1, \ldots, 4$ are meant as the Laplace transforms of the functions (15).

The formulae (15) and (16) constitute the starting point for the further calculation. They give the Laplace transform of the function $s(t)$ in terms of the matrix elements of the memory operator. In the forthcoming section we shall develop a technique for the explicit evaluation of these matrix elements. Eventually, in the last section, the inverse Laplace transform of the expressions stemming from (16) will be performed and the desired function, $s(t)$, acquired.

3. The weak-tunnelling approximation (WTA)

In dealing with the memory operator (13), the principal difficulty lies in the non-diagonal nature of the operator $\mathcal{W}$ in the exponent. Furthermore, the matrix elements of the operator $\mathcal{W}$, by their own, are non-commuting reservoir operators. These facts hinder the exact treatment of the exponential operator $\exp(-it\mathcal{W})$ in (13). At this point an approximation is unavoidable.

In many cases of physical interest the particle-reservoir coupling cannot be assumed to be weak. On the other hand, the tunnelling parameter, Δ, is small when the potential barrier between the two wells is sufficiently high, i.e. when the overlap between the localised states $|-\rangle$ and $|+\rangle$ is weak. If this is indeed the case we can express the memory operator (13) and (14) as a power series in the tunnelling parameter and, subsequently, take into account just several lower terms.

To this end, we employ the identity which is well known from perturbation theory [26]

$$\exp[-it(\mathcal{W}_D + \mathcal{W}_N)] = \exp[-it\mathcal{W}_D] - i\int_0^t \exp[-i(t-t')\mathcal{W}_D]\mathcal{W}_N \exp[-it'\mathcal{W}_D]\,dt' + \ldots \tag{17}$$

and use it in (13). As a result, we obtain the Δ expansion of the memory operator:

$$\mathcal{K} = \sum_{n=0}^{\infty} \mathcal{K}^{(n)}(t) \qquad \mathcal{K}^{(n)} \propto \Delta^n. \tag{18}$$

The first term of this series is

$$\mathcal{K}^{(0)}(t) = \mathrm{diag}(0, 0, k_{33}^{(0)}(t), k_{44}^{(0)}(t)), \tag{19}$$

$$k_{33}^{(0)}(t) = [k_{44}^{(0)}(t)]^* = (\mathbf{1}_R|\mathcal{R}\ \exp[-\mathrm{i}t(\mathcal{L}_R - \mathcal{P}_1\mathcal{R})]\mathcal{R}|\pi_R). \tag{20}$$

The second term reads

$$\mathcal{K}^{(1)}(t) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ k_{31}^{(1)}(t) & k_{32}^{(1)}(t) & 0 & 0 \\ k_{41}^{(1)}(t) & k_{42}^{(1)}(t) & 0 & 0 \end{pmatrix} \tag{21}$$

with the matrix elements

$$\left.\begin{matrix} k_{31}^{(1)}(t) \\ k_{32}^{(1)}(t) \end{matrix}\right\} = \frac{\mathrm{i}\Delta}{2}\int_0^t (\mathbf{1}_R|\mathcal{R}\ \exp[-\mathrm{i}(t-t')(\mathcal{L}_R - \mathcal{P}_1\mathcal{R})]\ \exp[-\mathrm{i}t'(\mathcal{L}_R \mp \mathcal{T})]\mathcal{T}|\pi_R)\ \mathrm{d}t' \tag{22}$$

and $k_{41}^{(1)}(t) = [k_{31}^{(1)}(t)]^*$, $k_{42}^{(1)}(t) = [k_{32}^{(1)}(t)]^*$.

Now, it turns out under a closer examination of the series (18) that all its even terms $\mathcal{K}^{(2n)}(t)$, $n = 1, 2, \ldots$, have their non-zero matrix elements only in the lower diagonal 2×2 block. On the other hand, all non-zero matrix elements of the odd terms $\mathcal{K}^{(2n+1)}(t)$, $n = 0, 1, \ldots$, fill the bottom-left non-diagonal 2×2 block as in (21). Stating it differently, the Δ expansion of the real combinations $v_i(t)$, $i = 1, \ldots, 4$ contains only even powers of the tunnelling parameter, whereas the functions $w_i(t)$, $i = 1, \ldots, 4$ are odd in the parameter Δ. Eventually, the functions v_i, w_i being substituted into the basic formula (16), the exact function $s(t)$ is clearly seen to be even in the parameter Δ.

After these preliminary considerations we take just the first term (20) of the series (18). For definiteness, let us call the ensuing approximation the weak-tunnelling approximation of zeroth order (the WTA$^{(0)}$). In this approximation, confronting the definitions (15) with the operator (20), one immediately obtains $w_i(t) = 0$, $i = 1, \ldots, 4$. Further, as will be seen below, the function $k_{33}^{(0)}(t)$ is real, i.e. $v_3(t) = v_4(t) = 0$ and $v_1(t) = v_2(t) = k_{33}^{(0)}(t)$. On the whole, it is sufficient to calculate the function $v_1(t)$.

In considering this function, that is the matrix element (20), one should notice that it is the projector $\mathcal{P}_1$ in the exponent which makes a direct evaluation exceedingly cumbersome. One feels, however, that the function $v_1(t)$ should be connected, in a way, with the more simple function

$$p(t) \equiv (\mathbf{1}_R|\ \exp[-\mathrm{i}t(\mathcal{L}_R - \mathcal{R})]|\pi_R). \tag{23}$$

Such a connection actually exists-we deal with it in appendix 2. It follows from the theorem therein that the Laplace transforms of the functions in question fulfil the crucial equality

$$v_1(z) = -z + \frac{1}{p(z)}. \tag{24}$$

Having thus expressed the function $v_1(z)$ through the Laplace transform of the more transparent matrix element, equation (23), we now focus on the evaluation of the function $p(t)$ itself. To this end, the operator in the exponent, $\mathcal{L}_R - \mathcal{R}$, is expressed as a sum of commuting operators $\mathcal{L}_{Ri} - \mathcal{R}_i$, $i = 1, \ldots, M$, each for one individual reservoir mode. Then, the three operators $\mathcal{L}_{Ri}$, $\mathcal{R}_i$ and $\mathcal{S}_i \equiv \frac{1}{2}\kappa_i\{\mathbf{B}_i^+ - \mathbf{B}_i, *\}$ are shown to form the Lie algebra, that is they have closed commutation relations. Using this

observation, it is possible to factorise the operator $\exp[-it(\mathscr{L}_R - \mathscr{R})]$ and, subsequently, perform the averaging in (23). On the whole, this procedure yields (see appendix 1 for some more details)

$$p(t) = \exp[-f_2(t)] \qquad f_2(t) \equiv \sum_{i=1}^{M} \left(\frac{\kappa_i}{\omega_i}\right)^2 (1 - \cos \omega_i t) \coth \frac{\beta \hbar \omega_i}{2}. \tag{25}$$

At this point, we may collect all the above properties of the functions $v_i(t)$, $w_i(t)$, and use them in (16). After this substitution is done, the expression for $s(z)$ simplifies extremely:

$$s(z) = \frac{1}{z + \Delta^2 p(z)}. \tag{26}$$

This is our final result in the WTA$^{(0)}$—the calculation of the object function is reduced to the evaluation of the direct Laplace transform of $p(t)$, equation (25), and subsequent inversion of $s(z)$, equation (26).

We now turn our attention to the weak-tunnelling approximation of the first order (WTA$^{(1)}$) which takes into account both the first and the second term of the series (18). It follows from the above discussion, we recall, that the functions $v_i(t)$, $i = 1, \ldots, 4$ will not be affected in the WTA$^{(1)}$, that is they will have the same form as in the WTA$^{(0)}$. Presently, according to (21), we only have to deal with the functions $k_{31}^{(1)}(t)$ and $k_{32}^{(1)}(t)$. Below, we give merely some basic points of this procedure.

First, we get rid of the projector $\mathscr{P}_1$ in expressions (22). We employ once more the theorem from appendix 2 and we acquire the equalities

$$k_{31}^{(1)}(z) = +\frac{i\Delta}{2} \frac{p(z) - z q_{31}(z)}{p(z)} \qquad k_{32}^{(1)}(z) = -\frac{i\Delta}{2} \frac{p(z) - z q_{32}(z)}{p(z)} \tag{27}$$

where the function $p(t)$ is defined in (25) and

$$\left.\begin{matrix} q_{31}^{(1)}(t) \\ q_{32}^{(1)}(t) \end{matrix}\right\} \equiv \int_0^t (\mathbf{1}_R | \mathscr{B}_-(t - t') \mathscr{A}_{\mp}(t') | \pi_R) \, dt'. \tag{28}$$

In the last formula we have used the notation

$$\mathscr{A}_{\pm}(t) \equiv \exp[-it(\mathscr{L}_R \pm \mathscr{T})] \qquad \mathscr{B}_{\pm}(t) \equiv \exp[-it(\mathscr{L}_R \pm \mathscr{R})]. \tag{29}$$

These reservoir operators will play a fundamental role in the next section.

Second, we evaluate explicitly the matrix elements in (28) (again, one uses the Lie-algebraic factorisation—some hints are given in appendix 1). For example

$$(\mathbf{1}_R | \mathscr{B}_+(t - t') \mathscr{A}_-(t') | \pi_R) = p(t - t') \exp\{i[f_1(t - t') - f_1(t) + f_1(t')]\} \tag{30}$$

where

$$f_1(t) \equiv \sum_{i=1}^{M} \left(\frac{\kappa_i}{\omega_i}\right)^2 \sin \omega_i t. \tag{31}$$

The functions $f_1(t)$, $f_2(t)$ are extremely important as they control, in a sense, the whole physics of the present model. We shall see that it is only through them that the reservoir parameters κ_i, ω_i and the temperature enter the exact solution.

Collecting again all the above results, one gets $s(z)$ from (16) in the fairly compact form

$$s(z)=\frac{1}{z+\Delta^2 z q(z)} \tag{32}$$

where

$$q(t)\equiv\int_0^t p(t')\cos[f_1(t')-f_1(t)+f_1(t-t')]\,\mathrm{d}t'. \tag{33}$$

This concludes the calculation in the WTA$^{(1)}$.

Summarising, in this section the calculation was based on the Δ expansion of the memory operator. Our main results, (26) and (32), correspond to the truncation of the series in question after the first and the second term, respectively. However, while these procedures may well be accepted methodologically, they do not evoke a physical interpretation of the above truncation. A logical question to ask, for instance, is that of physical differences between the WTA$^{(0)}$ and WTA$^{(1)}$. Surprisingly, the search for a physical motivation led us to the connection between the GME method and the functional-integral approach.

4. Discussion of the results

On first glancing at the exact formal solution (16) as well as at the results in the WTA$^{(0)}$, equation (26), and in the WTA$^{(1)}$, equation (32), it becomes evident that the physical limits $\Delta\to 0$ and $\gamma\to 0$ are properly described. Actually, if $\gamma=0$, then $s(t)=\cos\Delta t$ and the particle coherently oscillates between the sites $|-\rangle$ and $|+\rangle$. On the other hand, $\Delta=0$ gives $s(t)=1$, i.e. the particle does not move at all. Using the scaling property of the inverse Laplace transformation the object function, $s(t)$, is seen to depend on the time only through the combination $\tau\equiv t\omega_c$ and, when the scaling parameter ω_c is fixed, the whole dynamics is governed solely by the three dimensionless parameters: $\tilde{\Delta}\equiv\Delta/\omega_c$, $\tilde{\gamma}\equiv\gamma/\omega_c$ and $\tilde{T}\equiv(\beta\hbar\omega_c)^{-1}$. The parameter $\tilde{\Delta}$ measures the tendency to a coherent motion, the parameter $\tilde{\gamma}$ that to a localisation and $\tilde{T}$ is the reduced temperature of the reservoir.

As we have mentioned above, the functional-integral method was shown to be a very efficient tool in connection with the double-well model. Within this technique, one can start with the clear physical picture of a tunnelling object in an (effective) potential which possesses two degenerate minima. Several authors [1, 34, 36] have investigated the circumstances under which the dissipative dynamics in a double-well-shaped potential may be reduced to the present double-state formulation. This discussion connects the parameters of the original problem to the above parameters Δ, γ, T and ω_c. The imaginary-time functional-integral approach was pioneered by Caldeira and Leggett [35]; for a thorough analysis of this thermodynamics method and for the detailed list of references see the recent paper by Görlich and Weiss [30]. In the dynamical studies, one works with the real-time functional-integral scheme which is based on the Feynman-Vernon theory [28]. This formulation has already been applied to the calculation of the double-well [1, 17, 18, 32] and multiwell [31] dynamics. Technically, both approaches are deceptively similar. However, as stressed in [30], one has to test the domains of validity for formally identical approximations separately in both schemes. Thus, e.g., the domain of parameters for which the

non-interacting-blip approximation (see below) is justified was shown [30] to be smaller in the imaginary-time formulation.

The essence of the real-time functional-integral technique consists in the exact calculation of the influence functional [28] and subsequent summation over all possible ways (≡paths) of the time evolution leading from a given initial condition to a final state. As a result, one obtains the Δ expansion of the function $s(t)$ in the form [1, 17, 32]

$$s(t)=1+\sum_{n=1}^{\infty}(-\mathrm{i}\Delta)^{2n}\frac{1}{n_{\mathrm{p}}}\sum_{n\ \mathrm{paths}}\int_0^t \mathrm{d}t_{2n}\int_0^{t_{2n}}\mathrm{d}t_{2n-1}\ldots\int_0^{t_2}\mathrm{d}t_1 s^{(n)}(t_1,\ldots,t_{2n};\mathrm{path}) \tag{34}$$

where n_{p} is the number of paths with $2n$ transitions between the subspace of the diagonal elements $|1)$, $|2)$ and that of the non-diagonal elements $|3)$, $|4)$. The functions $s^{(n)}$ are specific for a given path and will be given below.

We have found an independent derivation of this exact functional-integral expansion which rests solely on the algebraical properties of the reservoir operators $\mathscr{A}_{\pm}(t)$, $\mathscr{B}_{\pm}(t)$ (cf (29) for their definition). For reasons of space we simply sketch the derivation here. Further details and extensions will be given elsewhere.

Let us return to the original Liouville equation (6). We decompose the Liouville operator as $\mathscr{L}=\mathscr{L}_D+\mathscr{L}_N$ where $\mathscr{L}_D\equiv\mathscr{L}_{SR}+\mathscr{I}_S\otimes\mathscr{L}_R$ and $\mathscr{L}_N=\Delta\mathscr{M}\otimes\mathscr{I}_R$. Further, we make use of the perturbation expansion (17) with $\mathscr{L}_D$ instead of $\mathscr{W}_D$ and $\mathscr{L}_N$ instead of $\mathscr{W}_N$. It then takes several simple steps to handle the exact formal solution of the Liouville equation, $|\rho(t))=\exp(-\mathrm{i}t\mathscr{L})|\rho(0))$, and arrive at the expansion (34) with the functions $s^{(n)}$ given as

$$\begin{aligned}&s^{(n)}(t_1,\ldots,t_{2n};\mathrm{path})\\&\quad\equiv s^{(n)}(t_1,\ldots,t_{2n};\alpha_1,\ldots,\alpha_{n-1};\beta_1,\ldots,\beta_n)\\&\quad=(\mathbf{1}_R|\mathscr{A}_-(a_n)\mathscr{B}_{\beta_n}(b_n)\mathscr{A}_{\alpha_{n-1}}(a_{n-1})\ldots\mathscr{A}_{\alpha_1}(a_1)\mathscr{B}_{\beta_1}(b_1)\mathscr{A}_-(a_0)|\pi_R).\end{aligned} \tag{35}$$

In keeping with the terminology from [1], the operator $\mathscr{B}_{\beta_i}(b_i)$ represents the ith blip, $i=1,\ldots,n$, $\mathscr{B}_i=\pm1$ being its sign and $b_i=t_{2i}-t_{2i-1}$ its length. Thus there are n time-ordered blips in the matrix element (35). Similarly, think of the operator $\mathscr{A}_{\alpha_i}(a_i)$ as of the ith sojourn, $i=0,\ldots,n$, where $\alpha_i=\pm1$ is its sign and $a_i=t_{2i+1}-t_{2i}$ is its length. The zeroth and the nth sojourns have the sign $-$.

Now, it suffices to evaluate the matrix element in (35). First, one should note that the whole matrix element can be cast into the form of the product of M matrix elements, each for one individual mode of the reservoir. The calculation of a one-mode matrix element gives an exponential (see below). Hence, in the final product, the summation over the modes occurs in the exponent which is then included in the functions $f_1(t)$ and $f_2(t)$. For a moment, let us confine ourselves to a fixed one-mode matrix element. Its calculation proceeds through the following four steps.

(1) Using the formulae (A1.1) from appendix 1, we can factorise the one-mode exponential operators $\mathscr{A}_{\pm i}(t)$, $\mathscr{B}_{\pm i}(t)$. In other words, we can write them as a product of the two exponentials. The first exponential wil be of the form $\exp(\alpha\mathscr{L}_{Ri})$ and the second will have only the operators $\mathscr{R}_i$, $\mathscr{S}_i$ (for $\mathscr{A}_{\pm i}$) or only the operators $\mathscr{T}_i$, $\mathscr{U}_i$ (for $\mathscr{B}_{\pm i}$) in the exponent.

(2) As $(\mathbf{1}_R|\exp(\alpha\mathscr{L}_{Ri})=(\mathbf{1}_R|$, one wants to get all operators of the form $\exp(\alpha\mathscr{L}_{Ri})$ to the left. This is done using the formulae (A1.2) from appendix 1.

(3) Similarly, as both $(\mathbf{1}_R|\mathscr{T}_i$ and $(\mathbf{1}_R|\mathscr{U}_i$ are equal to zero, one commutes all operators of the form $\exp(\phi\mathscr{T}_i+\psi\mathscr{U}_i)$ to the left. The formula (A1.3) shows how to do it. Loosely speaking, for a given blip, all the previous sojourns have to be commuted

over it (towards $(\mathbf{1}_R|$). This gives the 'interaction' of this blip with the previous soujourns—see the factors $A_1^{(n)}$, $A_2^{(n)}$ in the final formula below.

(4) Eventually, one has only some element of the form $(\mathbf{1}_R|\exp(\delta\mathscr{R}+\varepsilon\mathscr{S})|\pi_R)$. This is evaluated by means of the averaging prescription (A1.4). In this manner, the temperature-dependent factors $B_1^{(n)}$, $B_2^{(n)}$ are generated in the final formula (36). It is only within this last step that the specific structure of the reservoir density matrix enters the calculation.

Leaving out all further details, we now write the final result in a fairly compact form:

$$s^{(n)}(t_1,\ldots,t_{2n};\alpha_1,\ldots,\alpha_{n-1};\beta_1,\ldots,\beta_n)=A_1^{(n)}A_2^{(n)}B_1^{(n)}B_2^{(n)} \tag{36}$$

where

$$A_1^{(n)}=\exp\left(\mathrm{i}\sum_{i=1}^{n}\beta_i\alpha_{i-1}[f_1(t_{2i}-t_{2i-1})-f_1(t_{2i}-t_{2j-2})+f_1(t_{2i-1}-t_{2j-2})]\right) \tag{37}$$

$$A_2^{(n)}=\exp\left(\mathrm{i}\sum_{i=1}^{n}\sum_{j=0}^{i-2}\beta_i\alpha_j[f_1(t_{2i}-t_{2j+1})-f_1(t_{2i}-t_{2j})-f_1(t_{2i-1}-t_{2j+1})+f_1(t_{2i-1}-t_{2j})]\right) \tag{38}$$

$$B_1^{(n)}=\exp\left(-\sum_{j=1}^{n}f_2(t_{2j}-t_{2j-1})\right) \tag{39}$$

$$B_2^{(n)}=\exp\left(\sum_{i,j=1,i>j}^{n}\beta_i\beta_j[f_2(t_{2i}-t_{2j})-f_2(t_{2i}-t_{2j-1})-f_2(t_{2i-1}-t_{2j})+f_2(t_{2i-1}-t_{2j-1})]\right). \tag{40}$$

It is clear from the above sketch that the various factors in (36) can now be regarded as 'interactions' between the blips, and between blips and sojourns. Thus the factor $B_1^{(n)}$ expresses, for an arbitrary given blip (the summation over i in the exponent), the self-interaction of this blip. The factor $B_2^{(n)}$ is an interaction between different blips. For a given pair of the blips (index i and j in the summation), this interaction depends on the relative sign $\beta_i\beta_j$. A given blip interacts only with the previous ones. The factors $A_1^{(n)}$ and $A_2^{(n)}$ represent the interaction of an arbitrary given blip (the summation over i) with all preceding sojourns. For this fixed blip, the former factor describes its interaction with just the neighbouring previous sojourn whereas the latter describes the interaction with all other previous ones.

The aim of the following discussion is to bring out the meaning of our main results (26) and (32) in the light of the above exact expansion as given by (34) and (36)-(40).

First, consider the result of the WTA$^{(0)}$, equation (26). The Laplace transform $s(z)$ can be written as a sum of the infinite Δ series

$$s(z)=\frac{1}{z}+\frac{1}{z}\sum_{n=1}^{\infty}(-\mathrm{i}\Delta)^{2n}\left[\frac{p(z)}{z}\right]^n. \tag{41}$$

Taking the inverse Laplace transform, one readily arrives at the series, which is equivalent to the result (34), (36)-(40) provided one puts $A_1^{(n)}=1$, $A_2^{(n)}=1$ and $B_2^{(n)}=1$, $n=1,\ldots,$ therein. More particularly, one obtains

$$s(t)=1+\sum_{n=1}^{\infty}(-\mathrm{i}\Delta)^{2n}\int_0^t \mathrm{d}t_{2n}\int_0^{t_{2n}}\mathrm{d}t_{2n-1}\ldots\int_0^{t_2}\mathrm{d}t_1 p(b_n)\,p(b_{n-1})\ldots p(b_1) \tag{42}$$

where the one-blip contribution, $p(t)$, is defined in (25) and $b_i=t_{2i}-t_{2i-1}$ as above. Accordingly, in order to get the WTA$^{(0)}$ result from the exact solution, one has to neglect

all interactions between separate blips *and* all interactions between an arbitrary given blip and all sojourns preceding this blip. Thus the WTA$^{(0)}$ is equivalent to the approximation which is commonly referred to as the non-interating-blip approximation, but which would be called, more properly, the isolated-blip approximation.

Next, let us consider the WTA$^{(1)}$. Expanding again the respective result from the preceding section, equation (32), one has

$$s(z)=\frac{1}{z}+\frac{1}{z}\sum_{n=1}^{\infty}(-\mathrm{i}\Delta)^{2n}[q(z)]^n \tag{43}$$

$$s(t)=1+\sum_{n=1}^{\infty}(-\mathrm{i}\Delta)^{2n}\int_0^t \mathrm{d}t_n\int_0^{t_n}\mathrm{d}t_{n-1}\ldots\int_0^{t_2}\mathrm{d}t_1\, q(b_n)q(b_{n-1})\ldots q(b_1). \tag{44}$$

It takes a little effort to devise a tricky substitution and to show that the last formula is equivalent to the expansion (34), (36)-(40) provided we set $A_2^{(n)}=1$ and $B_2^{(n)}=1$, $n=1,\ldots,$ therein. In other words, in the WTA$^{(1)}$, one takes into account not only the independent-blips factor $B_1^{(n)}=1$ (as in the WTA$^{(0)}$), but *also* the interaction of an arbitrary given blip with just the previous sojourn. Thus the WTA$^{(1)}$ could be referred to as the isolated blip-previous-sojourn pairs approximation.

As an example, let us consider the term $n=1$ in the exact expansion (34), (36)-(40). We have only one blip, i.e. the factors $A_2^{(1)}$, $B_2^{(1)}$ are equal to unity by their definition. Further, we have only one blip-preceding-sojourn pair—the first blip and the zeroth sojourn. It follows from the above arguments, as well as from the direct evaluation that, in the WTA$^{(1)}$, one gets the exact form of the term $s^{(1)}$ whereas the WTA$^{(0)}$ already gives this term approximately. For $n=2$ one has two blips and two blip-preceding-sojourn pairs. In this case, both the WTA$^{(0)}$ and WTA$^{(1)}$ yield approximate forms of the contribution $s^{(2)}$. As for the WTA$^{(1)}$, the interaction between the both blips as well as the correlation between the second blip and the zeroth sojourn are not described in this case.

More generally, an important conclusion emerges. Taking the first n terms in the Δ expansion of the memory operator, that is invoking our WTA$^{(n-1)}$, means, in terms of the functional-integral approach, that one takes into account the inner interactions within the k clusters of neighbouring blips and sojourns, where $k=1,\ldots,n$. Furthermore, one feels from this general argument that there could be a qualitative distinction between the WTA$^{(2)}$ results and the WTA$^{(1)}$ ones. In the latter approximation, a given blip feels the preceding one and thus all the blips are, in a way, connected. Intuitively speaking, this observation could affect the conclusions concerning the asymptotic behaviour of the function $s(t)$.

The non-interacting-blips approximation and its range of validity has been thoroughly investigated in [1, 18, 32]. Here, we merely want to comment on the relation between the WTA$^{(0)}$ and WTA$^{(1)}$. It follows from the comparison of the final formulae, (26) and (32), that, in the WTA$^{(0)}$, the isolated blip function $r(z)\equiv p(z)/z$ plays the same role as the isolated-blip-previous-sojourn function $q(z)$ in the WTA$^{(1)}$. Switching into the time domain, one is faced with the comparison of the functions $r(t)$ and $q(t)$ where

$$r(t)=\int_0^t p(t')\,\mathrm{d}t' \tag{45}$$

$$q(t)=\int_0^t p(t')\cos[f_1(t')-f_1(t)+f_1(t-t')]\,\mathrm{d}t'. \tag{46}$$

To compare these two functions let us consider the specific form of the strength function as given by (4). One has $f_1(t) = \tilde{\gamma} \tan^{-1} t$ and the evaluation of the integral corresponding to $f_2(t)$ gives

$$p(t) = \left[\sqrt{1+\tau^2} \frac{|\Gamma(\tilde{T} + i\tau\tilde{T})|^2}{\Gamma^2(\tilde{T})} \right]^{\tilde{\gamma}}. \tag{47}$$

Here $\Gamma(z)$ denotes the Euler gamma function of a complex argument. Some particular cases are:

$$\begin{aligned}
&\tilde{T} = 0 \qquad && p(t) = [\sqrt{1+\tau^2}]^{-\tilde{\gamma}} \\
&\tilde{T} \ll 1 \qquad && p(t) = \left[\frac{\pi\tau\tilde{T}}{\sqrt{1+\tau^2}\sinh(\pi\tau\tilde{T})} \right]^{\tilde{\gamma}} \\
&\tilde{T} = \tfrac{1}{2} \qquad && p(t) = \left[\frac{\sqrt{1+\tau^2}}{\cosh(\pi\tau/2)} \right]^{\tilde{\gamma}} \\
&\tilde{T} = 1 \qquad && p(t) = \left[\frac{\pi\tau\sqrt{1+\tau^2}}{\sinh(\pi\tau)} \right]^{\tilde{\gamma}}
\end{aligned} \tag{48}$$

other cases are given in [15]. In fact, an explicit formula can be given provided $\tilde{T}$ equals an integer or a half-integer. Notice that if $\tilde{T} > 0$, the function $p(t)$ decreases exponentially and this guarantees the convergence of the above integrals $r(t)$, $q(t)$.

Further, it will be useful to designate through $\tilde{r}(t)$ and $\tilde{q}(t)$ the integrals of the functions $r(t')$ and $q(t')$ from zero to t. Eventually, let r_∞ be the asymptotic value $\lim_{t\to\infty} r(t)$. Similar meanings appertain to the symbols q_∞, $\tilde{r}_\infty$ and $\tilde{q}_\infty$.

The inspection of (45) shows that the function $r(t)$ is a monotonically increasing function. So is $q(t)$ provided $\tilde{\gamma} < 1$. If $\tilde{\gamma} \geq 1$ the cos function in (46) changes the sign and the function $q(t)$ acquires a local maximum. This is demonstrated in figure 1 by means of the numerical evaluation of the respective integrals $r(t)$ and $q(t)$. As for the

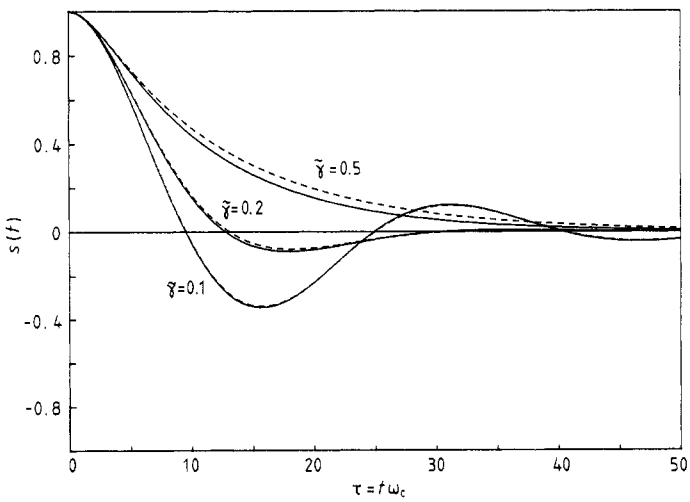

Figure 1. The time dependence of the integrals $r(t)$ (full curves), $q(t)$ (broken curves) for $\tilde{T} = 0$ and $\tilde{\gamma} = 0.5$ (the two topmost curves), $\tilde{\gamma} = 1$ (the central pair of curves) and $\tilde{\gamma} = 2$ (the bottom pair of curves).

asymptotic behaviour of these functions, if $\tilde{T} > 0$, the two numbers r_∞ and q_∞ are finite and generally $r_\infty \neq q_\infty$. If $\tilde{T} = 0$, then r_∞ equals a finite constant for $\tilde{\gamma} > 1$ and $r_\infty = \infty$ for $\tilde{\gamma} \leqslant 1$. On the other hand, for q_∞ and $\tilde{T} = 0$, one gets $q_\infty = \infty$ for $\tilde{\gamma} < 1$, $q_\infty = \pi/2$ for $\tilde{\gamma} = 1$ and $q_\infty = 0$ for $\tilde{\gamma} > 1$ [1]. Thus in the case $\tilde{T} = 0$, $\tilde{\gamma} \geqslant 1$ the asymptotic behaviour of the functions $r(t)$ differs from that of the function $q(t)$.

The numerical inspection of the object function, $s(t)$, is exemplified in figure 2. Here, the inverse Laplace transforms of the functions (26) and (32) are plotted. In principle, these expressions are valid for small $\tilde{\Delta}$. However, provided $\tilde{\gamma} \ll 1$, we have proved them to hold for a general $\tilde{\Delta}$ as well.

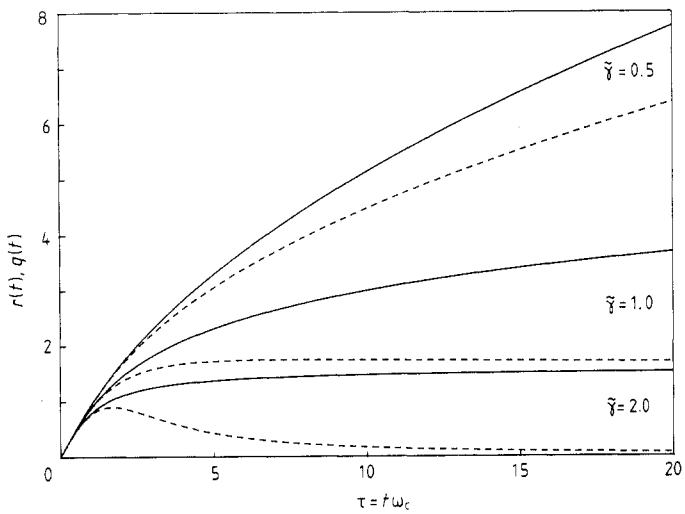

Figure 2. The time dependence of the function $s(t)$. The full curves represent the WTA$^{(0)}$ result (i.e. the calculation is based on (26)) and the broken ones demonstrate the dependence in the WTA$^{(1)}$ (the calculation is based on (32)). The parameters used are: $\tilde{T} = 0.5$, $\tilde{\Delta} = 0.2$ and $\tilde{\gamma}$ is denoted in the picture.

Let us now briefly contrast our WTA$^{(1)}$ against some other approaches going beyond non-interacting-blip approximation. Considering the exact expression for the particle coordinate, $s(t)$, as given by (34), (36)–(40), one has two global strategies for performing the summation in (36). First, analysing the relations between different blips and sojourns, one can approximate the contribution of *every path* in a physically motivated manner so as to take into account just such configurations of the blips and sojourns which are supposed to give a significant contribution to the integrals occurring in (36). This category comprises the WTA$^{(1)}$ which takes into account isolated-blip contributions and blip-preceding-sojourn interactions. However, it is also possible to neglect all blip-soujourn interactions and take into account (besides isolated-blip factor) the neighbouring blips interactions. This possibility was investigated in [17]. In our GME scheme it would correspond to neglecting all terms in the expansion (18) besides $\mathcal{K}^{(0)}(t)$ and $\mathcal{K}^{(2)}(t)$. Second, in a specific domain of parameters, one can pick up *certain relevant set of paths* and treat these paths exactly, i.e. with all possible blip-sojourn and blip-blip interactions. Recent works [30–32] have found the procedure for the physical identification of the 'relavant paths'—it is closely connected with the real-time functional-integral analysis of the original problem. It is then actually possible

(e.g. in the domain $\tilde{\gamma}=1$) to sum up all such defined paths and to obtain analytic formulae which are not accessible within the first strategy.

Eventually, let us comment on a subtle problem of the possible symmetry breaking. The question is whether the asymptotic value of the function $s(t)$, i.e. the number s_∞, is zero or not [9]. Usually, since $\lim_{t\to\infty} s(t) \equiv \lim_{z\to 0} zs(z)$, one investigates the small-z properties of the complex function $s(z)$ with $\mathrm{Re}\, z>0$. These are, in principle, given by the exact expression (16). However, one does not know the functions $v_i(z)$, $w_i(z)$ and so the crucial point is whether the small-z behaviour of $s(z)$ as given by (16) could be affected by performing the WTA$^{(0)}$ or the WTA$^{(1)}$. For example, as follows from the discussion in § 3, the terms v_3w_1, v_3w_2, v_3v_4 equal zero in both the WTA$^{(0)}$ and WTA$^{(1)}$ and it is only in the WTA$^{(2)}$ that they enter the formula (16). Thus, as regards the possibility of the asymptotic localisation, the WTA$^{(0)}$ or WTA$^{(1)}$ conclusions have to be accepted with certain circumspection.

Having this remark in mind, it will not be so surprising that the WTA$^{(0)}$ predicts somewhat different asymptotics as compared with that given by the WTA$^{(1)}$. In the WTA$^{(0)}$, one works with the final expression (26) and this gives

$$s_\infty = \frac{1}{1+\Delta^2 \lim_{z\to 0} r(z)} = \frac{1}{1+\Delta^2 \tilde{r}_\infty}. \tag{49}$$

Since $r(t)$ is for any parameter a non-decreasing function, we have $\tilde{r}_\infty = \infty$, i.e. $s_\infty = 0$: there is no asymptotic localisation in the WTA$^{(0)}$.

Next, let us consider the WTA$^{(1)}$. Formula (32) yields

$$s_\infty = \frac{1}{1+\Delta^2 \lim_{z\to 0} q(z)} = \frac{1}{1+\Delta^2 \tilde{q}_\infty}. \tag{50}$$

Now, for $\tilde{q}_\infty$ to be a finite number, two conditions have to be fulfilled: $q_\infty = 0$ and convergence of $q(t)$ to this final value must be sufficiently fast. Analysing these conditions themselves, one can use the observation that the function $q(t)$ has the same asymptotics as the somewhat simpler function

$$u(t) \equiv \int_0^t p(t') \cos[f_1(t')]\, \mathrm{d}t'. \tag{51}$$

The reason is, roughly speaking, that $f_1(t-t') \simeq f_1(t)$ for large enough t and small enough t' (for which $p(t') \geqslant \varepsilon > 0$ where ε is a sufficiently small number). The conditions for the $\tilde{u}_\infty$ to be finite were found in e.g. [1, 15, 16]: $\tilde{T}=0$ and $\tilde{\gamma}>2$. Thus also our WTA$^{(1)}$ predicts asymptotic localisation in the range $\tilde{T}=0$ and $\tilde{\gamma}>2$. On the other hand, the short-time behaviour of the function $q(t)$ is different from that of the function $u(t)$ and, consequently, the number $\tilde{q}_\infty$ itself is different from the value [9, 15] $\tilde{u}_\infty = [\omega_c^2(\tilde{\gamma}-1)(\tilde{\gamma}-2)]^{-1}$. For instance, the parameters $\tilde{T}=0$, $\tilde{\gamma}=4$ give $\tilde{u}_\infty \simeq 1.667/\omega_c^2$ whereas the numerical calculation of the double integral $\tilde{q}(t)$ shows $\tilde{q}_\infty \simeq 1.002/\omega_c^2$. However, we recall that it could well be that this 'WTA$^{(1)}$ localisation' disappears in the WTA$^{(2)}$. We have given both the physical and formal arguments supporting this hypothesis.

Summarising, the main conclusions of the present work are as follows.

(1) Using the GME technique, we obtained the general form of the exact solution, equation (16).

(2) We have developed the connection between the class of approximations based on the Δ expansion of the memory operator and the functional-integral description of the exact solution.

(3) In particular, our $\text{WTA}^{(0)}$ is equivalent to the commonly used non-interacting-blip approximation. Contrary to this approximation, the $\text{WTA}^{(1)}$ takes into account, at least to some extent, the correlations between the blips and sojourns.

(4) The numerical calculation was given which reveals the differences between the specific approximations used.

In conclusion, our work is yet another example of the power of the GME method in dealing with simple microscopical models of relaxation processes.

Acknowledgments

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Appendix 1

At several places in the main text we deal with the similarity transformations and/or with the factorisation of the exponentials involving the reservoir operators. As a rule, these procedures are performed separately for each index $i = 1, \ldots, M$, i.e. for each individual mode of the reservoir. In this appendix, we restrict ourselves to just one fixed reservoir mode. Hence we drop the index i and we designate $u \equiv \kappa/\omega$.

The procedures mentioned involve just the five reservoir operators (see below) and the essential point is that these operators form the Lie algebra [29]. Table 1 gives their definitions as well as their mutual commutators.

Table 1: The commutators are given in the form [row, column].

	$\mathscr{L}$	$\mathscr{R}$	$\mathscr{S}$	$\mathscr{T}$	$\mathscr{U}$
$\mathscr{L} \equiv [\mathbf{B}^+\mathbf{B}, *]$	0	$\mathscr{S}$	$\mathscr{R}$	$\mathscr{U}$	$\mathscr{T}$
$\mathscr{R} \equiv \frac{1}{2}u\{\mathbf{B}^+ + \mathbf{B}, *\}$	$-\mathscr{S}$	0	0	0	$u^2\mathscr{I}_R$
$\mathscr{S} \equiv \frac{1}{2}u\{\mathbf{B}^+ - \mathbf{B}, *\}$	$-\mathscr{R}$	0	0	$-u^2\mathscr{I}_R$	0
$\mathscr{T} \equiv \frac{1}{2}u[\mathbf{B}^+ + \mathbf{B}, *]$	$-\mathscr{U}$	0	$u^2\mathscr{I}_R$	0	0
$\mathscr{U} \equiv \frac{1}{2}u[\mathbf{B}^+ - \mathbf{B}, *]$	$-\mathscr{T}$	$-u^2\mathscr{I}_R$	0	0	0

This Lie algebra and/or its subalgebras can be treated by the parameter differentiation method. Wilcox's article [29] presents the *modus operandi* at great length. Here we give merely the list of identities needed in the main text.

(1) Let α be an arbitrary complex number. Then the following factorisation take place

$$\begin{aligned} \exp[\alpha(\mathscr{L} \pm \mathscr{T})] &= \exp(\alpha\mathscr{L}) \exp[\pm\mathscr{T} \sinh\alpha \pm \mathscr{U}(1-\cosh\alpha)] \\ \exp[\alpha(\mathscr{L} \pm \mathscr{R})] &= \exp(\alpha\mathscr{L}) \exp[\pm\mathscr{R} \sinh\alpha \pm \mathscr{S}(1-\cosh\alpha)]. \end{aligned} \tag{A1.1}$$

(2) Let α, β be two complex numbers. By means of the following formulae, the left commutation of the operator $\exp(\gamma\mathscr{L})$ can be done:

$$\begin{aligned}\exp(\alpha\mathscr{T}+\beta\mathscr{U})\exp(\gamma\mathscr{L}) &= \exp(\gamma\mathscr{L})\exp[(\alpha\cosh\gamma-\beta\sinh\gamma)\mathscr{T}+(-\alpha\sinh\gamma+\beta\cosh\gamma)\mathscr{U}] \\ \exp(\alpha\mathscr{R}+\beta\mathscr{S})\exp(\gamma\mathscr{L}) &= \exp(\gamma\mathscr{L})\exp[(\alpha\cosh\gamma-\beta\sinh\gamma)\mathscr{R}+(-\alpha\sinh\gamma+\beta\cosh\gamma)\mathscr{S}].\end{aligned} \tag{A1.2}$$

(3) Let α, β, γ and δ be arbitrary complex numbers. Then

$$\exp(\alpha\mathscr{R}+\beta\mathscr{S})\exp(\gamma\mathscr{T}+\delta\mathscr{U}) = \exp(\gamma\mathscr{T}+\delta\mathscr{U})\exp(\alpha\mathscr{R}+\beta\mathscr{S})\exp[u^2(\alpha\delta-\beta\gamma)]. \tag{A1.3}$$

(4) Let μ, ν be arbitrary complex numbers and π_R be a one-mode version of the canonical density matrix in the initial condition (9). Then

$$(\mathbf{1}_R|\exp(\mu\mathscr{R}+\nu\mathscr{S})|\pi_R) = \exp\left[\tfrac{1}{2}u^2(\mu^2-\nu^2)\coth\left(\frac{\hbar\beta\omega}{2}\right)\right]. \tag{A1.4}$$

Appendix 2.

Theorem. Let $\mathscr{G}$ be an operator in the reservoir Liouville space, $|\mathbf{X})$ an element of this space and $\mathscr{P}_1 = \mathscr{I}_R - |\pi_R)(\mathbf{1}_R|$ the projector. Let us define the three functions $a(t)$, $b(t)$ and $c(t)$:

$$a(t) \equiv (\mathbf{1}_R|\exp(-\mathrm{i}t\mathscr{G})|\pi_R) \tag{A2.1}$$

$$b(t) \equiv (\mathbf{1}_R|\mathscr{G}\exp(-\mathrm{i}t\mathscr{G})|\mathbf{X}) \tag{A2.2}$$

$$c(t) \equiv (\mathbf{1}_R|\mathscr{G}\exp(-\mathrm{i}t\mathscr{P}_1\mathscr{G})|\mathbf{X}). \tag{A2.3}$$

Then their Laplace transforms fulfil the equality

$$b(z) = za(z)c(z). \tag{A2.4}$$

Proof. First, we expand the above functions into their Taylor series. We have e.g. $a(t) = \sum_{n=0}^{\infty}(-\mathrm{i}t)^n a_n/n!$ where the moments $a_n \equiv (\mathbf{1}_R|\mathscr{G}^n|\pi_R)$, $n = 0, 1, \ldots$ were introduced. Then using the definition of the projection operator, the moments a_n, b_n, c_n are shown to obey the equalities $b_n = \sum_{k=0}^{n} a_k c_{n-k}$, $n = 0, 1, \ldots$ Eventually, the Laplace transforms of the Taylor series are used and the terms corresponding to the same powers of $1/z$ are compared.

Particular case. If $|\mathbf{X}) = \mathscr{G}|\pi_R)$ then $b(t)$ equals to the negative second derivative from $a(t)$. If, in addition, $(\mathbf{1}_R|\mathscr{G}|\pi_R) = 0$, one has $b(z) = -z^2 a(z) + z$. Therefore, in this particular case, (A2.4) acquires the form $c(z) = -z + 1/a(z)$. This was used in connection with (24) in the main text.

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