epl draft

Spin-boson dynamics: A unified approach from weak to strong coupling

Francesco Nesi[1], Elisabetta Paladino[2], Michael Thorwart[3] and Milena Grifoni[1]

[1] *Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany*
[2] *MATIS INFM-CNR & Dipartimento di Metodologie Fisiche e Chimiche, Università di Catania, 95125 Catania, Italy*
[3] *Institut für Theoretische Physik, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany*

PACS `05.30.-d` – Quantum statistical mechanics
PACS `03.65.Yz` – Decoherence; open systems; quantum statistical methods

Abstract. - We present a novel approximation scheme to describe the influence of a harmonic bath on the dynamics of a two-level particle over almost the whole regime of temperatures and coupling to the environment, for a wide class of bath spectral densities. Starting from the exact path-integral solution for the two-level system density matrix, effective intra-blip correlations are fully included, while inter-blip and blip-sojourn interactions are considered up to first order. In the proper regimes, an excellent agreement with conventional perturbative approaches and ab-initio path-integral results is found.

Introduction. – The problem of a two-level system (TLS) suffering from environmental decohering effects is ubiquitous to many physical and chemical situations [1–3]. Standard examples involve electron and proton transfer reaction in condensed phases [4], defect tunneling in metals [5] or tunneling systems in glasses [6,7]. Recently, several realizations of TLSs have been experimentally demonstrated in superconducting [8] and semiconducting [9] devices as possible unit (quantum bit) for future quantum computers. In these solid state systems, decoherence is a major obstacle towards the realization of a usable quantum computer [10–12]. Hence, a proper understanding of dissipation over a broad parameter regime is of outermost importance.

For a description of the dissipative dynamics the spin-boson model, in which the TLS is bilinearly coupled to a harmonic bath, is very frequently used. It reads [1–3]

$$\hat{H}(t) = \frac{\hbar}{2}[\varepsilon(t)\hat{\sigma}_z - \Delta\hat{\sigma}_x] - \frac{1}{2}\hat{\sigma}_z\hat{X} + \hat{H}_{\rm B}\ . \qquad (1)$$

The basis states $|\mathrm{R}\rangle$ and $|\mathrm{L}\rangle$ are the localized eigenstates of the "position" operator $\hat{\sigma}_z$, Δ describes the coupling between the two-states due to tunneling, and $\varepsilon(t)$ is an external control field. The Hamiltonian $\hat{H}_{\rm B} = \sum_i \hbar\omega_i(\hat{b}_i^\dagger\hat{b}_i + 1/2)$ represents a bath of bosons, and the collective variable $\hat{X} = \sum_i c_i(\hat{b}_i + \hat{b}_i^\dagger)/2$ describes the bath polarization. Despite the huge amounts of works on the subject [1–3], the existing schemes for a portrayal of the time-evolution of the TLS reduced density matrix mostly reduce to two main roads of approximation. On the one hand the so termed noninteracting-blip approximation (NIBA) [1,2], or equivalent projection operator techniques [13] based on an expansion to leading order in the tunneling matrix element Δ, has been proved to be successful in the regimes of high temperatures and/or strong friction. On the other hand the weak coupling and low-temperature regime, where NIBA fails for an asymmetric TLS, is typically tackled within an expansion to lowest order in the TLS-bath coupling. In this latter case path-integral methods [14,15] as well as the Bloch-Redfield formalism are used [16] (the two methods have been demonstrated to yield the same dynamics for weak Ohmic damping [17]), or a Born approximation [18]. To date, only numerical ab-initio calculations [12,19–21] can provide a description of the TLS dynamics smoothly interpolating between a weak and a strong coupling situation.

In this work, we present an interpolating approximation scheme, enabling to describe the weak and strong coupling regimes in a unique scheme. We call it weakly-interacting blip approximation (WIBA), within which the dynamics of the population difference $\langle\hat{\sigma}_z\rangle_t \equiv P(t)$ is

$$\dot{P}(t) = -\int_0^t dt'[K^a(t,t') - W(t,t') + K^s(t,t')P(t')]\ . \quad (2)$$

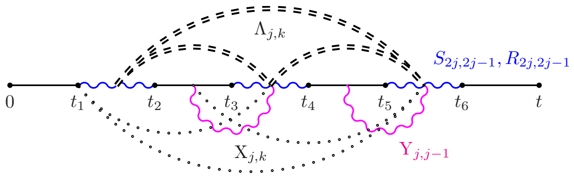

Fig. 1: Generic path with $2n = 6$ transitions at flip times $t_1, t_2, ..t_{2n}$. The system is in an off-diagonal state (blip) of the reduced density matrix in the time intervals $\tau_j \equiv t_{2j} - t_{2j-1}$ and in a diagonal state (sojourn) at times $t_{2j+1} - t_{2j}$. The interactions $S_{2j,2j-1}$, $R_{2j,2j-1}$ and $Y_{j,j-1}$ (intra-dipole and blip-preceeding-sojourn interactions), Eq. (7), are symbolized by the wiggled lines (blue and magenta online, respectively). The double-dashed lines denote the inter-dipole interactions $\Lambda_{j,k}$, while the bold-dotted lines are the remaining blip-sojourn interactions $X_{j,k}$, cf. Eq. (11).

The irreducible kernels $K^{(s/a)}$, W entering this generalized master equation are neither perturbative in the tunneling matrix Δ nor in the TLS-bath coupling, and are given in analytical form in (18), (19) and (20) below. By comparing the predictions of the WIBA with known perturbative results as well as with exact ab-initio calculations, we show that the WIBA well describes the TLS dynamics over the whole regime of temperature and environmental coupling.

In the spin-boson model all the effects of the bath on the TLS are captured by the spectral density $G(\omega) = \pi\hbar^{-2}\sum_i c_i^2 \delta(\omega - \omega_i)$. In the following we shall consider a class of spectral densities with a continuous spectrum:

$$G(\omega) = 2\delta_s \omega_{\rm ph}^{1-s} \omega^s e^{-|\omega|/\omega_c} \,, \tag{3}$$

with δ_s being a dimensionless coupling parameter, $\omega_{\rm ph}$ a characteristic phonon frequency, and ω_c the bath cut-off frequency. Thus, (3) encompasses the commonly considered Ohmic spectrum ($s = 1$) [1–5, 13, 17–19, 21, 22], with $\delta_1 = \alpha$ being the so-called TLS Kondo parameter, and the super-Ohmic case [1, 2, 6, 7, 11]. The applicability of the WIBA to other classes, as e.g. structured baths [4, 12], will be discussed elsewhere.

Exact path-integral formulation. – To start with, we assume a factorized initial condition at time $t = 0$ with the particle having been held at the site $|R\rangle$ ($\sigma_z = +1$) from time $t_0 = -\infty$ till $t = 0$, and with the bath in thermal equilibrium. Then the exact formal solution for $P(t)$ can be expressed in terms of a real time double path integral over forward $\sigma(\tau)$ and backward $\sigma'(\tau)$ spin paths [2, 3] with piecewise constant values ± 1. Upon introducing the linear combinations $\eta(\tau)/\xi(\tau) = [\sigma(\tau) \pm \sigma'(\tau)]/2$, one finds

$$P(t) = \int \mathcal{D}\xi\mathcal{D}\eta\mathcal{A}[\xi, \eta] \exp\{\Phi[\xi, \eta]\} \,, \tag{4}$$

where $\mathcal{A}$ is the path weight in the absence of the bath coupling. A generic double path can now be visualized as a single path over the four-states of the reduced density matrix, characterized by ($\eta(\tau) = \pm 1\,, \xi(\tau) = 0$) and ($\eta(\tau) = 0\,, \xi(\tau) = \pm 1$). The time intervals spent in a diagonal ($\xi(\tau) = 0$) and off-diagonal ($\eta(\tau) = 0$) state are

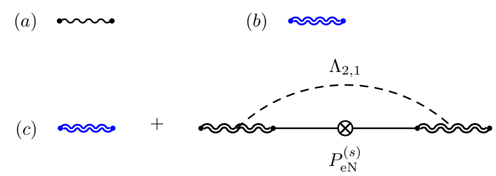

Fig. 2: Irreducible kernel $K^{(s)}(t, t')$ in the NIBA (a), in the *extended*-NIBA (blue online) (b) and in the WIBA (c). The single-dashed lines are the *linearized* blip-blip interactions between the first and last dipole. The inner bubble denotes the infinite sum of *extended*-NIBA diagrams yielding the symmetric part of $P(t)$ within the *extended*-NIBA, denoted $P^{(s)}_{\rm eN}$.

dubbed "sojourns" and "blips", respectively [1]. Due to the initial condition, the path sum runs over all paths with boundary conditions $\xi(0) = \xi(t) = 0$ and $\eta(0) = 1$, $\eta(t) = \pm 1$. Environmental effects are in the functional

$$\Phi[\xi, \eta] \equiv \int_0^t dt_2 \int_0^{t_2} dt_1\, \dot\xi(t_2)\Big[S_{2,1}\dot\xi(t_1) + iR_{2,1}\dot\eta(t_1)\Big], \tag{5}$$

with the bath correlation function $Q = S + iR$ being

$$Q(t) = \int_0^\infty d\omega \frac{G(\omega)}{\omega^2}\Big[\coth\Big(\frac{\hbar\omega}{2k_{\rm B}T}\Big)(1 - \cos\omega t) + i \sin\omega t\Big] \tag{6}$$

and $Q_{j,k} := Q(t_j - t_k)$. For a generic path with $2n$ transitions at times t_j, $j = 1, 2, ..., 2n$, one finds $\dot\xi(\tau) = \sum_{j=1}^{2n} \xi_j \delta(\tau - t_j)$ and $\dot\eta(\tau) = \sum_{j=0}^{2n} \eta_j \delta(\tau - t_j)$. Here is $\eta_0 = 1$ due to the initial preparation and $\xi_j = \pm 1$, $\eta_j = \pm 1$ for $j > 0$. Because $\xi_{2j} = -\xi_{2j-1}$, the influence function in (5) becomes $\Phi^{(n)} = \Phi^{(n)}_{\rm intra,bps} + \Phi^{(n)}_{\rm inter}$ (Fig. 1). The function $\Phi^{(n)}_{\rm intra,bps}$ describes intra-blip and blip-preceeding sojourn correlations, and reads

$$\begin{aligned}\Phi^{(n)}_{\rm intra,bps} &= -\sum_{j=1}^{n}\Big[S_{2j,2j-1} - i\xi_j\eta_{j-1}X_{j,j-1}\Big] \\ &= \Phi^{(n)}_{\rm intra} + \Phi^{(n)}_{\rm bps}\,,\end{aligned} \tag{7}$$

$$\Phi^{(n)}_{\rm intra} = -\sum_{j=1}^{n}\Big[S_{2j,2j-1} - i\xi_j\eta_{j-1}R_{2j,2j-1}\Big]\,, \tag{8}$$

$$\Phi^{(n)}_{\rm bps} = i\sum_{j=1}^{n} \xi_j\eta_{j-1}Y_{j,j-1}\,, \tag{9}$$

where we split $X_{j,j-1} = R_{2j,2j-1} + Y_{j,j-1}$, with

$$Y_{j,j-1} = R_{2j-1,2j-2} - R_{2j,2j-2}\,. \tag{10}$$

Moreover, the functional $\Phi^{(n)}_{\rm inter}$ accounts for inter-blip and blip-sojourns interactions [1, 2]

$$\Phi^{(n)}_{\rm inter} = -\sum_{j=2}^{n}\sum_{k=1}^{j-1}\xi_j\xi_k\Lambda_{j,k} + i\sum_{j=2}^{n}\sum_{k=0}^{j-2}\xi_j\eta_k X_{j,k}\,. \tag{11}$$

The function $\Lambda_{j,k}$ contains the blip-blip interactions between the flip pairs $\{j, k\}$, while the blip-sojourn interaction $X_{j,k}$ yields a phase factor. To be definite, for $k > 0$,

$$\Lambda_{j,k} = S_{2j,2k-1} + S_{2j-1,2k} - S_{2j,2k} - S_{2j-1,2k-1}, \quad (12a)$$

$$X_{j,k} = R_{2j,2k+1} + R_{2j-1,2k} - R_{2j,2k} - R_{2j-1,2k+1}. \quad (12b)$$

The correlations $X_{j,0}$ depend on the initial preparation [2]. The summation over the path histories then reduces to an expansion in the number of tunneling transitions yielding formally exact, but practically untractable, equations for $P(t)$ of the form (2) [14].

Known and novel approximation schemes. – To find appropriate approximation schemes to the TLS dynamics, let us start from the familiar non-interacting-blip approximation (NIBA) [1,2]. Within the NIBA, one sets $\Phi^{(n)}_{\rm inter} = 0$, namely the inter-blip correlations $\Lambda_{j,k}$ and the blip-sojourn interactions $X_{j,k}$ ($k \neq j-1$) are neglected. The blip-preceeding-sojourn interactions $Y_{j,j-1}$ in Eq. (10) are neglected as well. Hence, $X_{j,j-1}$ reduces to $X_{j,j-1} \approx R_{2j,2j-1}$. The influence function (7) then splits into individual influence factors depending only on the dipole length $\tau_j := t_{2j} - t_{2j-1}$. The dynamics is thus described by (2) with NIBA kernels corresponding to the one-dipole irreducible contributions (Fig. 2a),

$$\begin{aligned} K^s_{\rm N}(t,t') &= \Delta^2 \mathcal{C}(t-t') \cos[\zeta(t,t')] \,, \\ K^a_{\rm N}(t,t') &= \Delta^2 \mathcal{S}(t-t') \sin[\zeta(t,t')] \,, \end{aligned} \quad (13)$$

with $\zeta(t,t') = \int_{t'}^t dt'' \varepsilon(t'')$, intra-blip contributions $\mathcal{C}(t) = e^{-S(t)} \cos[R(t)]$, and $\mathcal{S}(t) = e^{-S(t)} \sin[R(t)]$. Here, $W_{\rm N} = 0$. The kernels are of lowest order in the tunneling matrix Δ but are *non*-perturbative in δ_s. Due to the simplicity of the kernels (13), the NIBA has been a very popular approximation so far. For sub-Ohmic damping, $s < 1$, NIBA is expected to be a valid approximation for all temperatures with the TLS exhibiting incoherent dynamics even for very small coupling δ_s. For Ohmic and super-Ohmic damping, NIBA is expected to be a good approximation only at high enough temperature and/or strong damping [2]. However, its limit of validity are *not clearly* defined. The NIBA is known to fail at low temperatures and weak coupling for an asymmetric TLS for Ohmic and super-Ohmic damping, because the dipole-dipole correlations $\Lambda_{j,k}$ contribute already to terms which depend linearly on the spectral density $G(\omega)$. For example, in the case of a TLS with static asymmetry $\varepsilon(t) = \varepsilon_0$, NIBA predicts the unphysical asymptotic limit

$$P^\infty_{\rm N} = -\tanh(\frac{\beta\hbar\varepsilon_0}{2}) \,, \quad (14)$$

implying localization of the TLS ($P^\infty_{\rm N} = -1$) at zero temperature even for infinitesimal asymmetries. In order to overcome the NIBA shortcomings, a weak-coupling approximation (WCA) has been proposed in [2,14,15] with WCA kernels being linear in δ_s and nonperturbative in Δ. Within the WCA, the TLS dynamics shows damped coherent oscillations with a renormalized energy splitting $\hbar\Omega$, with $\Omega^2 = \Delta^2_{\rm eff}[1 - 2{\rm Re}\, u(iE/\hbar)] + \varepsilon_0^2$, towards the equilibrium value

$$P^\infty_{\rm WCA} = -\frac{\hbar\varepsilon_0}{E} \tanh(\frac{\beta E}{2}) \,. \quad (15)$$

Here, the frequency shift is related to the frequency integral $u(z) = \frac{1}{2}\int_0^\infty d\omega \frac{G(\omega)}{\omega^2+z^2}[\coth(\hbar\beta\omega/2) - 1]$. Moreover, $E = \hbar\sqrt{\Delta^2_{\rm eff} + \varepsilon_0^2}$ and the effective bath-renormalized tunneling coupling $\Delta_{\rm eff}$ for the cases $s \geq 1$ reads [2]

$$\begin{aligned} \Delta_{\rm eff} &= \Delta[\Gamma(1-2\alpha)\cos(\pi\alpha)]^{\frac{1}{2(1-\alpha)}} (\Delta/\omega_c)^{\frac{\alpha}{1-\alpha}} \,, \quad s = 1 \,, \\ \Delta_{\rm eff} &= \Delta \exp[\delta_s \Gamma(s-1)(\omega_c/\omega_{\rm ph})^{s-1}], \quad s > 1 \,, \end{aligned} \quad (16)$$

with $\Gamma(z)$ the Gamma function. Finally, the relaxation Γ_r and dephasing Γ_ϕ rates are given by the perturbative (in δ_s) expressions $\Gamma_r = (\pi\hbar^2\Delta^2_{\rm eff}/2E^2)A(E/\hbar)$ and $\Gamma_\phi = \Gamma_r/2 + (\pi\hbar^2\varepsilon_0^2/2E^2)A(0)$, where the spectral function $A(\omega) = G(\omega)\coth(\hbar\omega/2k_{\rm B}T)$ is related to emission and absorption of a single phonon.

To smoothly bridge between the high and low T limits, let us now start to discuss a more refined approximation, which we call *extended*-NIBA (Fig. 2b). As in NIBA, $\Phi_{\rm inter}$ is neglected, while the approximation on the blip-preceeding sojourn interactions $X_{j,j-1}$ is improved, considering also $Y_{j,j-1}$ in an effective way. Specifically, expanding $Y_{j,j-1} = -R_{2j,2j-2} + R_{2j-1,2j-2}$ up to first order in the blip lengths τ_j, we set $X_{j,j-1} \approx R(\tau_j) - \tau_j \dot{R}_{2j-1,2j-2}$. As a result, the *extended*-NIBA kernels $K^{s/a}_{\rm eN}(t,t')$ have the same form as (13) with $\mathcal{C}(t) \to \mathcal{C}'(t) = e^{-S(t)}\cos[\tilde{R}(t)]$. Here is $\tilde{R}(t) \equiv R(t) - t\,\dot{R}(t)$. Moreover, $W_{\rm eN} = K^s_{\rm eN} - K^s_{\rm N}$. A comparison between NIBA and *extended*-NIBA, as well as with other approximation schemes discussed below, is shown in Figs. 3a - 3d. In Figs. 3b - 3d we also show results obtained with the numerical ab-initio path-integral approach QUAPI [20]. The short-time dynamics is always well approximated by the NIBA (*extended*-NIBA). At long times, however, correlations neglected in the NIBA become relevant. In particular, already at intermediate temperatures and damping (Figs. 3c, 3d) the *extended*-NIBA correctly reproduces the QUAPI results while NIBA fails. At low T and small damping, both NIBA and *extended*-NIBA fail to reproduce the correct long time dynamics (Fig. 3a), as predicted e.g. from the WCA.

To bridge between the moderate damping situation well described by the *extended*-NIBA and the extremely underdamped case we observe that, for spectral densities of the form (3), the blip-blip interaction terms $\Lambda_{j,k}$ as well as the blip-sojourn terms $X_{j,k}$ ($k \neq j-1$) are intrinsically small compared to unity. Hence, we propose a novel approximation scheme, which we call the weakly-interacting blip approximation (WIBA). Within the WIBA, the full $\Phi^{(n)}_{\rm intra,bps}$ is retained as in the *extended*-NIBA and one expands the influence functional $\exp\{\Phi^{(n)}_{\rm inter}\}$ up to *linear order* in the blip-blip and blip-preceeding sojourns inter-

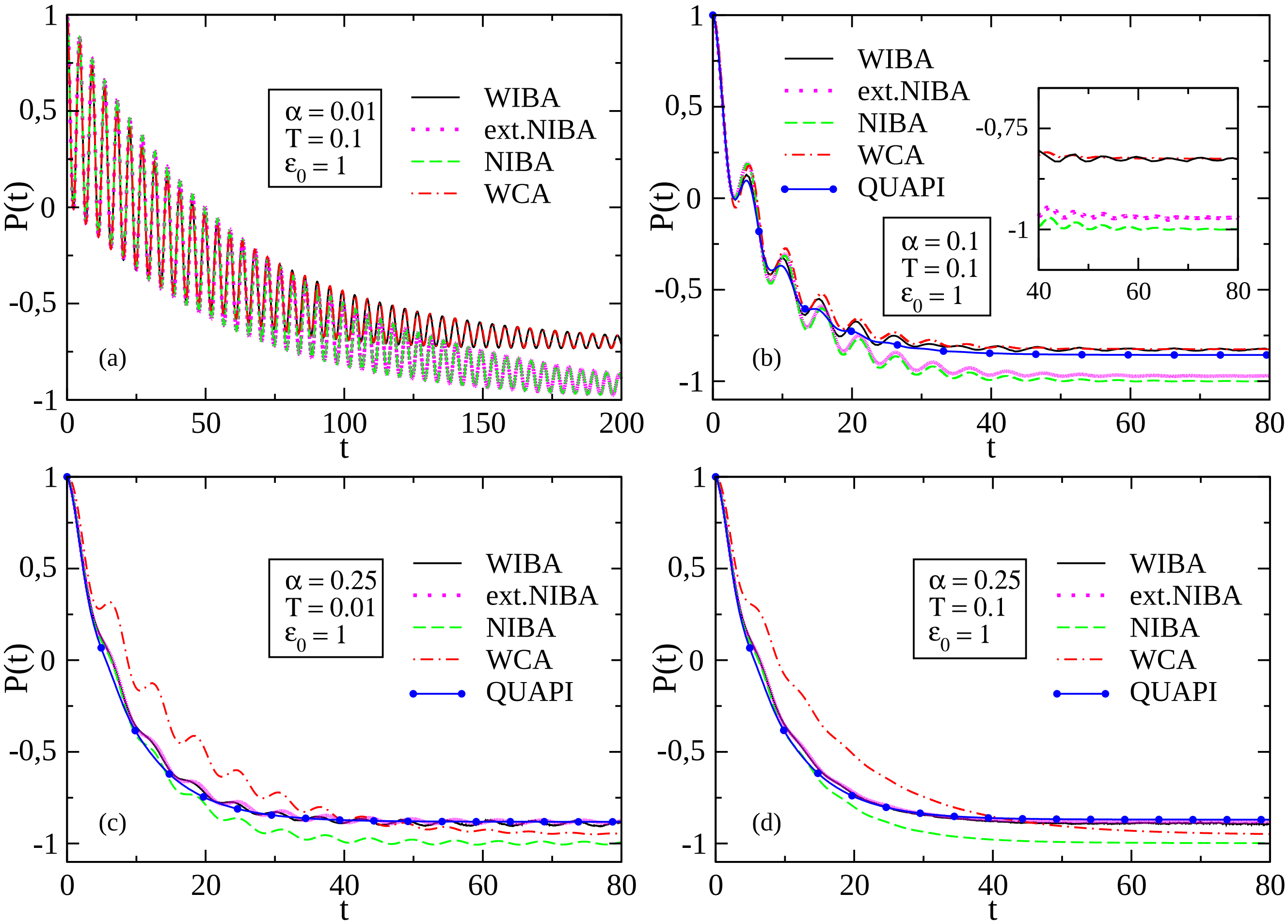

Fig. 3: Time evolution of the expectation value $P(t)$ at low/moderate temperatures $k_{\rm B}T \lesssim E$ for several values of the Ohmic coupling parameter α. Full lines depict the WIBA, dashed lines the NIBA, dotted lines the *extended*-NIBA, the dot-dashed ones are results for the weak-coupling approach (WCA) while the lines with bullets are the ab-initio QUAPI predictions. All quantities are expressed in units of Δ. At low damping and temperatures, Fig. 3a, the TLS exhibits damped coherent oscillations towards the asymptotic value $P^\infty_{\rm WCA}$. As the damping is increased, the oscillations are more strongly damped, see Figs. 3b, 3c, 3d. In the chosen regime of parameters, the equilibrium value P^∞ is neither well described by $P^\infty_{\rm N}$ nor by $P^\infty_{\rm WCA}$.

actions $\Lambda_{j,k}$ and $X_{j,k}$. In other terms,

$$\exp\{\Phi^{(n)}\} \approx \exp\{\Phi^{(n)}_{\rm intra,bps}\}\left(1+\Phi^{(n)}_{\rm inter}\right). \qquad (17)$$

Within an expansion in the number of tunneling transitions, the lowest order self-energy corresponds to the *extended*-NIBA, while higher order terms describe a set of blips in which the first and last blip are interacting, Fig. 2c. Summing up the higher contributions, the WIBA kernels, *neither perturbative in* Δ *nor in* δ_s, read

$$\begin{aligned} K^s_{\rm W}(t_4,t_1) &= K^s_{\rm eN}(t_4,t_1)\\ &- \Delta^4\int_{t_1}^{t_4} dt_3 \int_{t_1}^{t_3} dt_2 \mathcal{C}'(t_4-t_3)\sin[\zeta(t_4,t_3)]P^s_{\rm eN}(t_3-t_2)\\ &\times \Lambda_{2,1}\mathcal{C}'(t_2-t_1)\,\sin[\zeta(t_2,t_1)]\,, \end{aligned} \qquad (18)$$

$$\begin{aligned} K^a_{\rm W}(t_4,t_1) &= K^a_{\rm eN}(t_4,t_1)\\ &- \Delta^4\int_{t_1}^{t_4} dt_3 \int_{t_1}^{t_3} dt_2 \mathcal{C}'(t_4-t_3)\sin[\zeta(t_4,t_3)]P^s_{\rm eN}(t_3-t_2)\\ &\times[-\Lambda_{2,1}\mathcal{S}(t_2-t_1)+X_{2,0}\mathcal{C}(t_2-t_1)]\cos[\zeta(t_2,t_1)]\,. \end{aligned} \qquad (19)$$

Moreover,

$$\begin{aligned} W_{\rm W}(t_4,t_1) &= W_{\rm eN}(t_4,t_1)\\ &- \Delta^4\int_{t_1}^{t_4} dt_3 \int_{t_1}^{t_3} dt_2 \mathcal{C}'(t_4-t_3)\sin[\zeta(t_4,t_3)]P^s_{\rm eN}(t_3-t_2)\\ &\times[\Lambda_{2,1}\delta\mathcal{C}(t_2-t_1)-X_{2,0}\mathcal{S}(t_2-t_1)]\sin[\zeta(t_2,t_1)]\,, \end{aligned} \qquad (20)$$

where $\delta\mathcal{C} \equiv \mathcal{C}'-\mathcal{C}$. Moreover, $P^s_{\rm eN}(t)$ is the symmetric part (in ε_0) of $P_{\rm eN}(t)$ *within* the *extended*-NIBA. Thus, at high temperatures, where the blip-blip interactions are negligible, the WIBA kernels reduce to the *extended*-NIBA ones. By expanding the WIBA kernels to first order in δ_s

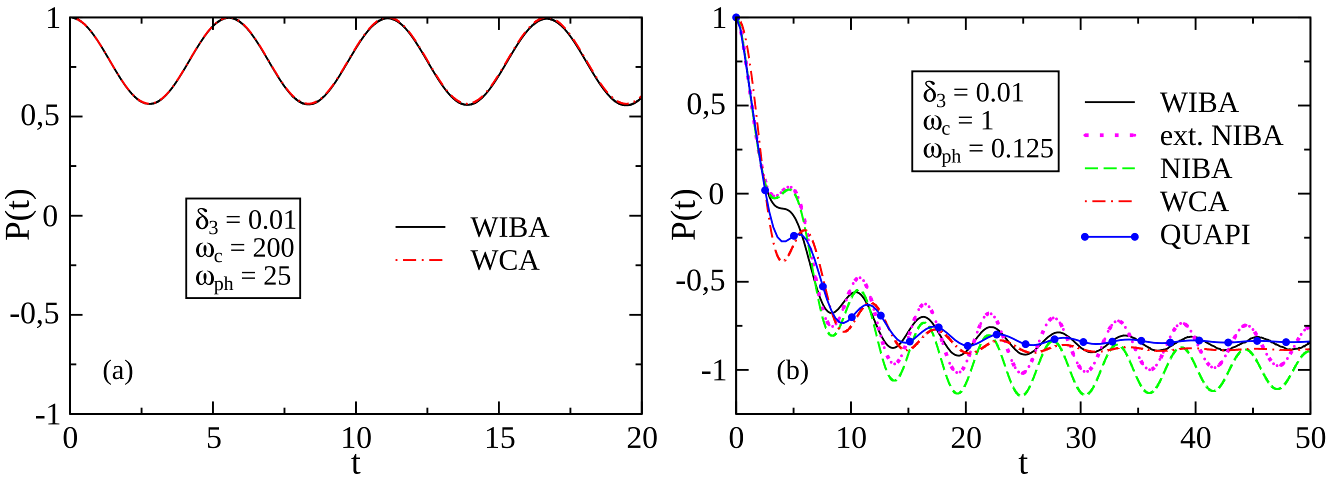

Fig. 4: Time evolution of $P(t)$ for super-Ohmic damping (coupling parameter δ_3). Here the ratio $\omega_c/\omega_{\rm ph} = 8$ is kept constant in both panels and we set $T = 0.1$, $\varepsilon_0 = 1$ (in units of Δ). Full lines are the WIBA predictions, dot-dashed lines are results of the WCA, dashed lines represent the NIBA predictions, dotted lines denote the *extended*-NIBA dynamics and finally bulleted lines are results of QUAPI.

and approximating $X_{j,j-1}$ to $R_{2j-2j-1}$, the weak damping kernels in [2, 14] are recovered.

Ohmic damping. – As a benchmark for the WIBA, we consider the evolution of the population difference $P(t)$ for the important case of Ohmic damping. In Fig. 3, the Ohmic case ($\omega_c = 50\Delta$ and $\varepsilon(t) = \varepsilon_0 = \Delta$) is shown. An excellent agreement is found for weak damping and temperatures (Fig. 3a) between WIBA and WCA, whereas the *extended*-NIBA matches the NIBA and predicts the wrong asymptotic limit $P_{\rm N}^{\infty}$. As the coupling is increased (or by raising the temperature), the WCA is expected to fail. However, as for the NIBA, the limits of validity of the WCA are not clearly defined. Indeed, Figs. 3b to 3d show an intermediate parameter regime where both approximations fail, since dipole-dipole interactions as well as two-phonon processes are relevant. Comparison with results from QUAPI shows that the short time dynamics is well approximated by the NIBA (WIBA). At intermediate and long times, the WIBA reasonably well approaches QUAPI and its asymptotic value. From a comparison with QUAPI, we notice that the higher order dipole correlations neglected in the WIBA yield a larger dephasing rate than predicted from WIBA. In particular, QUAPI predicts a complete suppression of the coherent oscillations already at $\alpha = 0.25, T = 0.01$. An interesting case is shown in Fig. 3b, with a small-to-intermediate value of the coupling strength ($\alpha = 0.1$), where the *extended*-NIBA slightly moves from the NIBA towards the WIBA predictions, reaching an intermediate asymptotic value (see inset).

Super-Ohmic damping. – Let us now consider the predictions of the WIBA in the super-Ohmic case ($s = 3$). Since $S(t \sim \Delta^{-1})$ differs only little from its asymptotic value $S(t \to \infty)$, the interblip interactions are weak and the WCA is expected to be a good approximation in a wide regime of parameters. This also implies that $S(t)$ is *not* effective in suppressing long-blip lenghts and the NIBA might not be justified. Indeed, for small δ_s and large ω_c (see Fig. 4a), no differences among WCA and WIBA occur. Similarly to the Ohmic case, we show in Fig. 4b the parameter regime where the WCA and the NIBA are expected to fail. With respect to Fig. 4a, we keep here the same ratio $\omega_c/\omega_{\rm ph}$ constant, being now $\omega_c \sim \Delta$, i.e. the bath becoming "slow". This case is the most difficult one, since the bath is very coherent and memory effects are to be taken into account, which requires to perform a very good description of the full bath dynamics. One sees that the NIBA completely fails to reproduce the dynamics, even reaching unphysical values. The *extended*-NIBA works better, approaching closer the QUAPI predictions. Nevertheless, too few correlations are taken into account, and it oscillates still too much with respect to the numerical plot of QUAPI. The WIBA shows discrepancies from the QUAPI as well, being still "too" coherent, even though its predictions are more accurate than the *extended*-NIBA. The WCA, despite better than WIBA in this regime, also lies apart from the numerical prediction of QUAPI. In this range of parameters, the multiphonon processes become relevant and the perturbative weak-coupling approximation begins to fail. This agrees with ab-initio simulations for charge qubits interacting with piezoelectric phonons [11]. Hence, further analysis of the complicated super-Ohmic case is to be done, in order to better understand the different dynamical situations which take place by varying the coupling strength δ_s, the cutoff frequency ω_c and the phonon frequency $\omega_{\rm ph}$.

Conclusions. – We have discussed a generalized master equation for the population difference $P(t)$ of a spin-boson system in the whole regime of temperatures and couplings. This equation can be solved using standard iteration schemes [17, 22]. For Ohmic damping the WIBA is able to reproduce known results in various complementary regimes, yielding a good, though not perfect agreement, with *ab-initio* QUAPI calculation in the regime of intermediate temperatures and damping. Hence, it overcomes the limits of validity of the perturbative approaches (NIBA, WCA) which, up to date, was possible only with numerical ab-initio models. For super-Ohmic damping the WIBA works well for large cut-off frequencies and low-to-moderate temperatures. However, disagreement with QUAPI is found in the case of a "slow" bath.

We mention some general contexts for the need of a bridging approach: i) The common experimental situation where bath temperature or TLS asymmetry are varied over a wide range (WCA and NIBA are unreliable at high temperatures and intermediate bias, respectively). ii) Several TLS's interacting with a common heat bath, as e.g. in glasses at low-temperatures [6, 7]. Due to the wide distribution of tunneling parameters and asymmetries, neither the WCA nor the NIBA can describe the dynamics of the whole ensemble consistently.

We must, however, notice that in the case of "slow" environments with cut-off frequency of the order of the tunneling frequency, our model needs some improvements, since neither the WIBA nor other analytical approximation schemes are able to reproduce the correct onset of decoherence which in fact takes place. This situation occurs e.g. in non-adiabatic electron transfer [4] or for charge qubits interacting with piezo-electric phonons [11].

* * *

Acknowledgments. – Discussions with L. Hartmann, D. Bercioux, M. Storcz, A. Donarini and support under the DFG programs GKR638 and SFB631 are acknowledged.

REFERENCES

[1] Leggett A. J., Chakravarty S., Dorsey A. T., Fisher M. P. A., Garg A. and Zwerger W., *Rev. Mod. Phys.*, **59** (1987) 1.
[2] Weiss U., *Quantum Dissipative Systems, 2nd Ed.* (World Scientific, Singapore) 1999.
[3] Grifoni M. and Hänggi P., *Phys. Rep.*, **304** (1998) 229.
[4] Garg A., Onuchic J. N. and Ambegaokar V., *J. Chem. Phys.*, **83** (1985) 4491.
[5] Golding B., Zimmerman N. M. and Coppersmith S. N., *Phys. Rev. Lett.*, **68** (1992) 998.
[6] Stockburger J., Grifoni M., Sassetti M. and Weiss U., *Z. Phys. B*, **94** (1994) 447.
[7] Würger A., *Phys. Rev. B*, **57** (1998) 347.
[8] Nakamura Y., Pashin Yu. A. and Tsai J. S., *Nature*, **398** (1999) 786; Vion D., Aassime A., Cottet A., Joyez P., Pothier H., Urbina C., Esteve D. and Devoret M. H., *Science*, **296** (2002) 886; Chiorescu I., Nakamura Y., Harmans C. and Mooij J. E., *Science*, **299** (2003) 1869.
[9] Hayashi T., Fujisawa T., Cheong H. D., Jeong Y. H. and Hirayama Y., *Phys. Rev. Lett.*, **91** (2003) 226804; Petta J. R., Johnson A. C., Marcus C. M., Hanson M. P. and Gossard A. C., *Phys. Rev. Lett.*, **93** (2004) 186802.
[10] Makhlin Yu., Schön G. and Shnirman A., *Rev. Mod. Phys.*, **73** (2001) 357.
[11] Vorojtsov S., Mucciolo E. R. and Baranger H. U., *Phys. Rev. B*, **71** (2005) 205322; Thorwart M., Eckel J. and Mucciolo E. R., *Phys. Rev. B*, **72** (2005) 235320.
[12] Goorden M. C., Thorwart M. and Grifoni M., *Phys. Rev. Lett.*, **93** (2004) 267005.
[13] Aslangul C., Pottier N. and Saint-James D., *J. Phys. (Paris)*, **47** (1986) 757; Dakhnovskii Yu., *Phys. Rev. B*, **49** (1994) 4649; Goychuk I. A., Petrov E. G. and May V., *Phys. Rev. E*, **52** (1995) 2392.
[14] Grifoni M., Paladino E. and Weiss U., *Eur. Phys. J. B*, **10** (1999) 719.
[15] Görlich R., Sassetti M. and Weiss U., *Europhys. Lett.*, **10** (1989) 507.
[16] Argyres P. N. and Kelley P. L., *Phys. Rev.*, **134** (1964) A98.
[17] Hartmann L., Goychuk I. A., Grifoni M. and Hänggi P., *Phys. Rev. E*, **61** (2000) R4687.
[18] DiVincenzo D. P. and Loss D., *Phys. Rev. B*, **71** (2005) 035318.
[19] Egger R. and Weiss U., *Z. Phys. B*, **89** (1992) 97.
[20] Makarov D. E. and Makri N., *Phys. Rev. E*, **52** (1995) 5863.
[21] Stockburger J. T., *Phys. Rev. E*, **59** (1999) R4709; Stockburger J. T. and Mak C. H., *J. Chem. Phys.*, **105** (1996) 8126.
[22] Thorwart M., Grifoni M. and Hänggi P., *Ann. Phys.*, **293** (2001) 15.