Consistent perturbative treatment of the subohmic spin-boson model yielding arbitrarily small $T_2/T_1$ decoherence time ratios

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We present a perturbative treatment of the subohmic spin-boson model which remedies a crucial flaw in previous treatments. The problem is traced back to the incorrect application of a Markov type approximation to specific terms in the temporal evolution of the reduced density matrix. The modified solution is consistent both with numerical simulations and the exact solution obtained when the bath coupling spin space direction is parallel to the qubit energy basis spin. We therefore demonstrate that the subohmic spin-boson model is capable of describing arbitrarily small ratios of the $T_2$ and $T_1$ decoherence times, associated to the decay of the off-diagonal and diagonal reduced density-matrix elements, respectively. An analytical formula for $T_2/T_1$ at the absolute zero of temperature is provided in the limit of an extremely subohmic bath with vanishing spectral power law exponent. Small ratios closely mimic the experimental results for solid state (flux) qubits, which are subject predominantly to low-frequency electromagnetic noise, and we suggest a re-analysis of the corresponding experimental data in terms of a nonanalytic decay of off-diagonal coherence.

Since the advent of quantum information technology, the problem of two-state systems aka qubits, immersed in environmental (bath) degrees of freedom has increasingly gained importance, cf., e.g.[13]. The spin-boson model, succinctly describing such a physical situation, namely an open two-state quantum system interacting with a bath, accounts for two-state energy relaxation and dephasing, and therefore has been studied extensively[4,5]. It was, for example, used to describe physical contexts diverse as flux qubits implemented within SQUID environments[6-10], electron transfer in biomolecules[11], and phonon coupling in atomic tunneling[12].

The spin-boson model introduces a continuum of independent simple harmonic oscillators with a given spectral weight distribution as the environment, assuming them to couple with the qubit linearly. The Hamiltonian of the entire (closed) system therefore reads (setting $\hbar = 1$)

$$H = H_0 + V, \quad \text{where } H_0 = \frac{1}{2} \omega_s \sigma_z + \sum \omega_k \hat{b}_k^\dagger \hat{b}_k,$$

$$V = \vec{n} \cdot \vec{\sigma} \otimes \sum \lambda_k (\hat{b}_k + \hat{b}_k^\dagger). \quad (1)$$

Here, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the usual Pauli matrices and $\hat{b}_k^\dagger, \hat{b}_k$ are creation and annihilation operators of harmonic oscillators in the (infinitely extended) bath, labelled by the quantum number(s) $k$, which can stand, e.g., for the momentum of the bath excitations. The coupling direction $\vec{n}$ is parametrized by two angles $\theta, \phi$ as $\vec{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$.

The bath is conventionally characterized by the quantity $J(\omega) \equiv \sum \omega_k^2 \delta(\omega - \omega_k)$, which determines the dynamics of the spin-boson model. This spectral density of the bath is effectively a density of states summation weighted by the coupling strength $\lambda_k$, hence the name. Usually it is assumed that $J(\omega)$ is of a power law form up to a cutoff, $J(\omega) = \eta \omega^{1-n} e^{-\omega_0 / \omega}$, where $\omega_c$ is the (physical) cutoff frequency of the bath, assumed to be much larger than the system frequency spacing $\omega_s$. The strength of coupling is parametrized by the dimensionless $\eta$. Baths having $n < 1, n = 1$, and $n > 1$ are called subohmic, ohmic, and superohmic, respectively, where a subohmic bath is dominated by low-frequency oscillators.

The Rabi model, which is a ($\theta = \pi/2$) variant of the spin-boson model with a single-mode “bath” (e.g. a two-level atom in a cavity), is integrable[12]. In principle, an exact solution of the spin-boson model in the same perpendicular coupling case $\theta = \pi/2$ was also obtained[12], which however does not lend itself to a description of the effective qubit dynamics because tracing out the bath is still highly nontrivial. Furthermore, in the simple case that the coupling direction and the energy basis direction of the system commute ($\theta = 0$), the spin-boson model is also exactly solvable[13-15].

Away from the limiting cases of parallel and perpendicular coupling, $\theta = 0, \pi/2$, perturbative approaches have been employed[16,18]. However, as pointed out in [16], the previous perturbative approaches show a pathological behavior for the subohmic heat bath by predicting the instantaneous loss of phase coherence for any finite coupling $\eta$. In addition, in the low temperature limit, the perturbative solution does not agree even qualitatively with the exact solution for $\theta = 0$. Previous perturbative approaches thus cannot be self-consistent. We aim at remedying this situation, by developing a consistent perturbative approach to the subohmic spin-boson model which both agrees with the exactly solvable case $\theta = 0$ and is free of the aforementioned pathological behavior.

The time evolution of the density matrix of the closed system in the interaction picture, $\tilde{\rho}_I(t)$, is determined by the following von Neumann equation

$$\frac{d\tilde{\rho}_I(t)}{dt} = -i [V_I(t), \tilde{\rho}_I(t)], \quad (2)$$

where Schrödinger and interaction picture operators are related by $A_I(t) \equiv U_{t,0}(t)AU_{t,0}^\dagger(t)$. We define the reduced density matrix by tracing out the bath, $\rho_I(t) \equiv \text{Tr}_B \tilde{\rho}_I(t)$, and employ the following three conditions[14]
\{1\} The Born approximation which treats Eq. (2) perturbatively to second order accuracy in \(V_I(t)\).

\{2\} The initial product state assumption \(\hat{\rho}(0) = \rho(0) \otimes \rho_B(0)\) where \(\rho_B(0)\) is the canonical density matrix at temperature \(T\) (or \(\hat{\rho}_I(0) = \rho_I(0) \otimes \rho_B(0)\)).

\{3\} \(\text{Tr}_B[V_I(t), \rho_B(0)] = 0\), due to \(V_I\) having odd and \(\rho_B(0)\) having even spatial parity.

The equation (2) can then be transformed into the perturbative expression (see Eqs. 8.1–8.15 in Ref. 11)

\[
\frac{d\rho_I(t)}{dt} = -\int_0^t ds \text{Tr}_B[V_I(t), [V_I(s), \rho_I(t) \otimes \rho_B(0)]]].
\] (3)

For the purpose of our derivation to follow, we note that in the literature, one encounters rather widely differing notions of what is called “Born” (i.e., weak coupling) and “Markov” (i.e., short-time memory) approximations, which are not necessarily equivalent. For example, Ref. 13 derives Eq. (3) by assuming a product state for arbitrary times \(\hat{\rho}_I(t) = \rho_I(t) \otimes \rho_B(0)\) (instead of only initially as in \{2\}), and terms this “Born” approximation, and then imposes the “Markov” approximation that \(\rho_I(s)\) is replaced by \(\rho_I(t)\) in the integrand to arrive at \{3\}. On the other hand, 12, 14–18 derives Eq. (3) by using the above stated requirements \{1\}–\{3\}, with only the Born approximation in the form of \{1\}, which can be justified rigorously. 12 No (variety of) Markov approximation is employed in deriving \{3\}. In addition, the Markov type approximation \{4\} which we will use and explain in detail below is distinct from that used in, e.g., 12, 14–18.

Employing the spin-boson Hamiltonian \{1\} in the Born-approximation master equation \{3\}, one obtains

\[
\frac{d\rho_I(t)}{dt} = -\int_0^t ds \text{Tr}_B[V_I(s), [\{\nabla \cdot \nabla(s), \rho_I(t)\}]]
\]

\[
\times \left\{ \text{coth} \left[ \frac{\beta\omega}{2} \right] \cos (\omega(t-s)) [\nabla \cdot \nabla(t), [\nabla \cdot \nabla(s), \rho_I(t)]]
\]

\[-i \sin (\omega(t-s)) [\nabla \cdot \nabla(t), [\nabla \cdot \nabla(s), \rho_I(t)]] \right\}.
\] (4)

Here, the \(t\) dependence of the operators \(\nabla \cdot \nabla(t)\) is determined by the spin part of the Hamiltonian, i.e., by \(H^{(s)}_0 = \frac{1}{2} \omega_s \sigma_z\). Previous studies on the spin-boson model \{12–18\} deduced a solution for the evolution of the reduced density matrix \(\rho_I(t)\) of Eq. (4), which, when written in the presently employed notation, reads

\[
\rho_I^{(q)}(t) = \rho_I^{(q)}(1 - \exp\left[\frac{t}{T_1}\right]) + \rho_I^{(i)}(0) \exp\left[\frac{t}{T_1}\right], \quad i = \{1, 2\},
\]

\[
\rho_I^{(1,2)}(t) = \rho_I^{(1,2)}(0) \exp\left[-\frac{t}{T_2}\right] \exp\left[-i \frac{t}{T_3}\right],
\]

\[
\rho_I^{(2,1)}(t) = \rho_I^{(2,1)}(0) \exp\left[-i \frac{t}{T_2}\right] \exp\left[i \frac{t}{T_3}\right],
\] (5)

where the indices refer to qubit space, and \(\rho_I^{(q)}(t) = (1 + \exp[\beta\omega_I])^{-1}\) and \(\rho_I^{(i)}(t) = (1 + \exp[\beta\omega_I])^{-1}\) are canonical equilibrium distributions at the inverse temperature \(\beta\). Finally, the various rates in \{5\} satisfy

\[
\frac{1}{T_1} = 2\pi \sin^2 \theta J(\omega) \text{ coth} \left[ \frac{\beta\omega_I}{2} \right],
\] (6)

\[
\frac{1}{T_2} = \frac{1}{2T_1} + \frac{1}{T_3}, \quad \frac{1}{T_3} = 4\pi k_B T \cos^2 \theta \left( J(x) \right)_{x \to 0}
\] (7)

\[
\frac{1}{T_3} = 2 \sin^2 \theta \int_0^\infty ds d\omega J(\omega), \text{ coth} \left[ \frac{\beta\omega_I}{2} \right] \text{ cos}(\omega s) \sin(\omega s)
\] (8)

where \(T_1\) and \(T_2\) are called (energy) relaxation and dephasing time, respectively. The coupling angle \(\varphi\) does not occur in the above: The two expressions containing \(\varphi\), \((\nabla \cdot \nabla(s)) = \sin \theta e^{-i\varphi}\) and \((\nabla \cdot \nabla(s))_1 = \sin \theta e^{i\varphi}\) enter as absolute squares.

We observe that \(1/T_\alpha\) in Eq. (7) diverges for the subohmic case \(\alpha < 1\) at any finite \(T\) as \(x^{n-1} \to n\); also note that at absolute zero, \(T_2\) cannot be determined from the formula at all. Accordingly, if Eq. (7) is valid for the subohmic regime, this indicates that the dephasing time \(T_2\) should always vanish. This appears to be unphysical, because it implies that phase coherence is destroyed instantaneously as soon as the system comes into contact with a subohmic heat bath, at any value of the coupling strength \(\eta\). We therefore suspect that Eqs. (5)–(8) do not represent a proper perturbative solution of \{4\}.

Furthermore, we now argue that Eqs. (5)–(8) are in contradiction with the exact solution for the commuting case \(\theta = 0\), i.e., when \(\nabla \cdot \nabla = 0\). Using a unitary transformation \{12\}, the exact full density matrix can be found from \{4\} given the initial product state assumption \{2\}. The solution for the reduced density matrix, at any coupling strength \(\eta\), is then

\[
\rho_{1,11}(t) = \rho_{1,11}(0), \quad \rho_{1,22}(t) = \rho_{1,22}(0),
\]

\[
\rho_{1,i,j}(t) = \rho_{1,i,j}(0) \exp[-4\pi \eta k_B T t] \quad i \neq j
\] (9)

To see the inconsistency between Eq. (5)–(8) (with \(\theta = 0\)) and Eq. (9) in a manifest manner, we make them concrete for an ohmic heat bath \((n = 1)\):

\[
\rho_{1,11}(t) = \rho_{1,11}(0), \quad \rho_{1,22}(t) = \rho_{1,22}(0),
\]

\[
\rho_{1,i,j}(t) = \rho_{1,i,j}(0) \exp[-4\pi \eta k_B T t] \quad i \neq j\] (10)

In the high temperature limit \((k_B T \gg \omega_c\)) using the approximation \(\text{coth} \left[ \frac{\beta\omega_I}{2} \right] \approx 2 k_B T \omega\) for \(\omega\) below the cutoff energy, \(Q(t)\) is approximated as \(4\pi \eta k_B T\); hence Eq. (10) and Eq. (9) for large \(T\) give the same results and are consistent with each other. However, at the absolute zero of temperature, Eq. (9) yields the following solution which obviously does not agree with Eqs. (5)–(8), i.e., by setting \(\text{coth} \left[ \frac{\beta\omega_I}{2} \right] = 1 \forall \omega\), we get

\[
\rho_{1,11}(t) = \rho_{1,11}(0), \quad \rho_{1,22}(t) = \rho_{1,22}(0),
\]

\[
\rho_{1,i,j}(t) = \rho_{1,i,j}(0) (1 + (\omega t)^2)^{-2\eta} \quad i \neq j.
\] (11)

Eq. (10) exhibits an exponential decay of the off-diagonal elements of the reduced density matrix, and the decay
We proceed to demonstrate that the approximation {4} to \(I_1, I_2, I_3\), using \(I_1(\infty, \omega_s) = \frac{\pi}{2} J(\omega_s) \coth(\frac{\omega_s}{2})\), \(I_3(\infty, \omega_s) = \frac{\pi}{2} J(\omega_s)\) and noting the definitions for \(T_1, T_2, T_3\) in Eqs. (6)–(8), we derive the following differential equations for the reduced density matrix from Eq. (4),

\[
\begin{align*}
\partial_t \rho_{i,11}(t) &= -\pi \sin^2 \theta J(\omega_s) \left( \coth \left( \frac{\beta \omega_s}{2} \right) + 1 \right) \rho_{i,11}(t) + \pi \sin^2 \theta J(\omega_s) \left( \coth \left( \frac{\beta s}{2} \right) - 1 \right) \rho_{i,22}(t), \\
\partial_t \rho_{i,12}(t) &= -\left( \frac{1}{2T_1} + \frac{i}{T_3} + 4 \cos^2 \theta \theta J(t) \right) \rho_{i,12}(t), \\
\partial_t \rho_{i,21}(t) &= -\left( \frac{1}{2T_1} - \frac{i}{T_3} + 4 \cos^2 \theta \theta J(t) \right) \rho_{i,21}(t), \\
\partial_t \rho_{i,22}(t) &= -\partial_t \rho_{i,11}(t).
\end{align*}
\]

(13)

The first and last line can be rewritten in a compactified notation, using that \(\rho_{i,11}(t) + \rho_{i,22}(t) = 1\), \(\partial_t \rho_{i,11}(t) = -\frac{1}{T_0} (\rho_{i,11}(t) - \rho_{i,11}^{eq})\), \(i = (1, 2)\). The linear first-order differential equations (13) are then readily solved by

\[
\begin{align*}
\rho_{i,11}(t) &= \rho_{i,11}^{eq} \left( 1 - \exp \left[ \frac{t}{T_1} \right] \right) + \rho_{i,11}(0) \exp \left[ -\frac{t}{T_1} \right], \\
\rho_{i,12}(t) &= \rho_{i,12}(0) \exp \left[ -\frac{t}{2T_1} \right] \exp \left[ -i \frac{t}{T_3} \right] \exp[-K(t)], \\
\rho_{i,21}(t) &= \rho_{i,21}(0) \exp \left[ -\frac{t}{2T_1} \right] \exp \left[ i \frac{t}{T_3} \right] \exp[-K(t)], \\
\rho_{i,22}(t) &= \rho_{i,22}^{eq} \left( 1 - \exp \left[ \frac{t}{T_1} \right] \right) + \rho_{i,22}(0) \exp \left[ -\frac{t}{T_1} \right],
\end{align*}
\]

(14)

defining a function \(K(t) = \cos^2 \theta \int_0^t ds I_4(s)\), which replaces \(1/T_0\) in {7},

\[
K(t) = 4 \cos^2 \theta \int_0^\infty ds J(\omega) \coth \left( \frac{\beta \omega}{2} \right) \frac{1 - \cos(\omega t)}{\omega^2}.
\]

(15)

Eq. (14) represents an improved perturbative solution for Eq. (4) in that it does not display any of the unphysical pathology exhibited in Eq. (7), and it is reduced to the exact solution displayed in Eq. (9) if we set \(\theta = 0\). It thus demonstrates perfect consistency with the exact solution for the commuting case. Note that with \(\theta = 0\), \(K(t)\) becomes \(Q(t)\) in (7), and the rates \(\frac{1}{T_1}, \frac{1}{T_3}\) vanish.

At the absolute zero of temperature, by setting \(\coth(\frac{\beta \omega}{2}) = 1\) for all \(\omega\), \(K(t)\) can be calculated for our assumed spectral density of the form \(J(\omega) = \eta \omega_s^{1-n} \omega^{n-1} e^{-\frac{\omega}{\omega_s}}\). For the subohmic case (0 ≤ \(n < 1\)), \(K(t)\) does not diverge even if there is no cutoff energy \(\omega_s\). In this regime, we may thus let \(\omega_s \rightarrow \infty\). Then, \(K(t)\) is given by \(K(t) = 2\pi \eta \cos^2 \theta (\omega_s t)\), for \(n = 0\) and \(K(t) = 4\pi \cos^2 \theta \sin(\frac{\pi n}{2}) \left( \frac{\pi n}{2} \right)^{1-n} \omega_s^{1-n} (\omega_s t)^{1-n}\) for \(0 < n < 1\). For the ohmic and superohmic cases (\(n ≥ 1\)), on the other hand, \(K(t)\) converges only if there is a finite cutoff energy \(\omega_s\). For example, \(K(t) = 2\pi \eta \cos^2 \theta \ln(1 + (\omega_s t)^2)\) for \(n = 1\) and \(K(t) = 4\pi \eta \cos^2 \theta \frac{\omega_s^2}{(\omega_s t)^2} \frac{1}{1 + (\omega_s t)^2}\) for \(n = 2\). The effect of
Combining this with Eq. (6) the ratio $T$ with the numerical solution of (4) for the extremely sub-

ohmic case ($n = 0$) as a function of coupling angle $\theta$. The analytical result (Eq. (16)) is shown by the red line and the numerical results by solving Eq. (4) are indicated by dots. The parameters $\eta$ and $\omega_c$ are the same as in Fig. 1.

for these experimentally realized systems. (16) that the perturbatively treated (extremely) sub-

K(t) is generally strongly cutoff frequency dependent in the superohmic case ($n > 1$, not shown in Fig. 1), and increasingly so with spectral power $n$. The superohmic case thus needs a more elaborate treatment, which we do not pursue here.

The functions $K(t)$ corresponding to different powers $n$ can be numerically compared with each other, see Fig. 1 for the ohmic and subohmic cases. In particular, when we approach the zero of temperature, for the “extremely subohmic” bath ($n = 0$), we obtain an off-diagonal decay which is exactly exponential because then $K(t)$ is linear in $t$, which becomes comparable to $\exp[-t/2T_1]$ (which dominates for the ohmic regime), cf. Eq. (14).

As a result of exponential decay, we can define in this limit of $n \to 0$ the dephasing time $T_2$ properly. Combining Eq. (14) and $K(t) = 2\pi \eta \cos^2 \theta (\omega_c t)$ ($n = 0$ and $T = 0$), the dephasing rate $1/T_2 = \frac{1}{2T_1} + 2\pi \eta \omega_c \cos^2 \theta$. Combining this with Eq. (5) the ratio $T_2/T_1$ can be obtained analytically at the absolute zero of temperature for an extremely subohmic bath, $n \to 0$,

$$\frac{T_2}{T_1} = \frac{2\sin^2 \theta}{2 - \sin^2 \theta}. \quad (16)$$

Hence, contrary to the ohmic case where the ratio $T_2/T_1 = 2$ regardless of the coupling angle $\theta$, the decoherence time ratio can have any value between 0 and 2 depending on the coupling angle $\theta$. This is of particular relevance for the interpretation of studies on flux qubits created using SQUIDs, see for example Refs. [61-63], which are typically dominated by low-frequency electromagnetic (1/f) noise. The experiments report a wide range of decoherence time ratios $T_2/T_1 \sim 0.01 \cdots 2$ rather than this ratio being always identical to two. Thus we conclude from (16) that the perturbatively treated (extremely) subohmic heat bath furnishes a realistic physical description for these experimentally realized systems.

We have validated Eq. (16) by checking its consistency with the numerical solution of (4) for the extremely sub-
currence of a phase transition, the perturbative approach can be applied for the short-time dynamics,\cite{31,32} which in view of the limited coherence times of, in particular, flux qubits will generally suffice. This research was supported by the NRF Korea, Grant No. 2014R1A2A2A01006535.

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