Initial Decoherence of Open Quantum Systems

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We present a new short-time approximation scheme for evaluation of decoherence. At low temperatures, the approximation is argued to apply at intermediate times as well. It then provides a tractable approach complementary to Markovian-type approximations, and appropriate for evaluation of deviations from pure states in quantum computing models.

1. INTRODUCTION

Consider a microscopic quantum system with the Hamiltonian H_S. We will refer to the quantum-computing single quantum bit (qubit) or multi-qubit paradigm to help define the questions and set up the challenges, in describing how the system, S, interacts with the surrounding macroscopic world. However, in principle S can be any quantum system.

Interactions with the surroundings can be quite different depending on the setting. For example, in quantum measurement, which for orthodox quantum theory is not fully understood, the wavefunction of the system is probed, so part of the process would involve a strong interaction with the measuring device, such that the system's own Hamiltonian plays no role in the process. However, in most applications, the external interactions are actually quite weak. Furthermore, the aim is to minimize their effect, especially in quantum computing.

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Traditionally, interactions with the surrounding world have been modeled by the modes of a bath, B, with each mode described by its Hamiltonian M_K, so that the bath of modes is represented by

$$H_B = \sum_K M_K. \tag{1.1}$$

The interaction, I, of the bath modes with the system S, will be modeled by

$$H_I = \Lambda_S P_B = \Lambda_S \sum_K J_K, \tag{1.2}$$

where Λ_S is some Hermitean operator of S, coupled to the operator P_B of the bath.

The bath, or "heat bath," can be a collection of modes, such as photons, phonons, spins, excitons, etc. For a bosonic bath of oscillators,[1–6] which we use for derivation of specific results, we take

$$M_K = \omega_K a_K^\dagger a_K, \tag{1.3}$$

$$J_K = g_K^* a_K + g_K a_K^\dagger. \tag{1.4}$$

Here we have assumed that the energy of the ground state is shifted to zero for each oscillator, and we work in units such that $\hbar = 1$.

The total Hamiltonian of the system and bath is

$$H = H_S + H_B + H_I. \tag{1.5}$$

More generally, the interaction, (1.2), can involve several system operators, each coupling differently to the bath modes, or even to different baths. The bath modes, in turn, can be coupled to specified external objects, such as impurities.

Let $\rho(t)$ represent the reduced density matrix of the system at time $t \geq 0$, after the bath modes have been traced over. For large times, the effect of the environment on a quantum system that is not otherwise externally controlled, is expected to be thermalization: the density matrix should approach

$$\rho(t \to \infty) = \frac{\exp(-\beta H_S)}{\mathrm{Tr}_S[\exp(-\beta H_S)]}, \tag{1.6}$$

where $\beta \equiv 1/kT$. At all times, we can consider the degree to which the system has departed from coherent pure-quantum-state evolution. This departure is due to the interactions and entanglement with the bath. We also expect that the temperature, T, and other external parameters that

might be needed to characterize the system's density matrix, are determined by the properties of the bath, which in turn might interact with the rest of the universe.

Let us introduce the eigenstates of H_S,

$$H_S |n\rangle = E_n |n\rangle, \tag{1.7}$$

and have ΔE denote the characteristic energy gap values of S. We also consider the matrix elements of $\rho(t)$,

$$\rho_{mn}(t) = \langle m| \rho(t) |n\rangle. \tag{1.8}$$

For large times, we expect the diagonal elements ρ_{nn} to approach values proportional to $e^{-\beta E_n}$, while the off-diagonal elements, $\rho_{m \neq n}$, to vanish. These properties can be referred to as thermalization and decoherence in the energy basis, though "thermalization" in the strong sense of (1.6) implies decoherence.

To establish these thermalization and decoherence properties, several assumptions are made regarding the system and bath dynamics.[1–11] At time $t = 0$, it is usually assumed that the bath modes, K, are thermalized, i.e., have density matrices

$$\theta_K = e^{-\beta M_K} / \operatorname{Tr}_K(e^{-\beta M_K}). \tag{1.9}$$

The density matrix R of the system plus bath at time $t = 0$ is assumed to be the direct product

$$R(0) = \rho(0) \prod_K \theta_K, \tag{1.10}$$

and the system and bath modes are not entangled with each other.

Now, a series of assumptions are made, e.g., the Markovian and secular approximations. The most important is the Markovian approximation, which, even though it can be stated and introduced in various ways, essentially assumes that the density matrices of the bath modes are reset externally to the thermal ones, on time scales shorter than any dynamical times of the system interacting with the bath, and the product form of the full density matrix is maintained. This is a natural assumption, because each bath mode is coupled only weakly to the system, whereas it is "monitored" by the rest of the universe and kept at temperature T. In its straightforward version, this amounts to using (1.10) for times $t > 0$. Ultimately, such approaches aim at master equations for the evolution of $\rho_{mn}(t)$ at large times, consistent with the Golden Rule and with the expected thermalization and decoherence properties.

In variants of these formalisms, several time scales are identified. One is the inverse of the upper cutoff, Debye frequency of the bath modes, $1/\omega_D$. Another is the thermal time $\hbar/kT = \beta$ (in units of $\hbar = 1$). The system S has its own characteristic time, $1/\Delta E$, as well as the system-bath dynamical times of thermalization and decoherence, etc., $T_{1, 2,...}$, corresponding to the "intrinsic" NMR/ESR times T_1, T_2, etc. Heuristically, bath modes of frequencies ω comparable to ΔE are needed to drive thermalization and decoherence. Initial decoherence can be also mediated by the modes near $\omega = 0$. At low temperatures, we can assume that $1/\omega_D < 1/\Delta E < \beta$.

There is evidence[7, 11, 12] that at low temperatures, the Markovian-type and other approximations used in the derivation of equations for thermalization and decoherence, are only valid for times larger than the thermal time scale β. For quantum computing applications, in solid-state semiconductor-heterostructure architectures,[13–19] we expect temperatures of several tens of μK. The thermal time scale then becomes dangerously close to the external single-qubit control, Rabi-flip time even for slower qubits, those based on nuclear spins. We emphasize that not all the approximation schemes have this problem.[11]

In Section 2, we offer additional comments on decoherence and quantum computing. Then, in Section 3, we develop a short-time-decoherence approximation. In a discussion at the end of Section 3, we offer arguments that, at low temperatures, our approximation is actually valid for intermediate times, larger than $1/\omega_D$, hopefully up to times comparable or larger than $1/\Delta E$. Specific results for the bosonic heat bath are presented in Section 4. Section 5 comments on the case of adiabatic decoherence, when the short-time approximation becomes exact.

2. DECOHERENCE AND QUANTUM COMPUTING

Quantum computing architectures usually emphasize systems, both the qubits and the modes that couple them (and at the same time act as a bath mediating unwanted coupling to the rest of the universe), that have large spectral gaps. It is believed that, especially at low temperatures, spectral gaps slow down relaxation processes. Therefore, quantum computing architectures usually assume[13–19] qubits in quantum dots, or in atoms, or subject to large magnetic fields, and coupled by highly nondissipative quantum media.[14, 19]

The spectral gaps are expected to slow down exponentially, by the Boltzmann factor, the processes of thermalization, involving energy exchange. Off-shell virtual exchanges, will be also slowed down, but less profoundly. The latter processes contribute to decoherence. Therefore, at low temperatures, we might expect separation of time scales of the initial

decoherence vs. later-stage thermalization and further decoherence. The latter two processes are described by the traditional NMR/ESR intrinsic T_1 and T_2, respectively.

Since only thermalization is clearly associated with the energy eigenbasis, one can also ask whether the energy basis is the appropriate one to describe decoherence for short and intermediate times, before the thermalizing processes, that also further drive decoherence, take over. The issue of the appropriate basis for studying decoherence, has also come up in models of quantum measurement. It has been argued[20-24] that the eigenbasis of the interaction operator, Λ_S, may be more appropriate for intermediate times than the energy eigenbasis.

Yet another aspect of decoherence in quantum computing, involves the observation that we really want to retain a *pure state* in the quantum computation process.[25-30] Decay of off-diagonal matrix elements, in whatever basis, might not be the best measure of deviations from the pure-state density matrix, where by pure states we mean those with density matrices that are projection operators $|\psi\rangle\langle\psi|$. For instance, the deviation of $\text{Tr}_S[\rho^2(t)]$ from 1, may be more appropriate, and is easer to calculate than other measures, specifically those motivated by the "entropic" expressions proportional to $\text{Tr}_S[\rho \ln(\rho)]$. Therefore, it is desirable to have basis-independent expressions for the reduced density operator $\rho(t)$.

Recently, several groups have reported[12, 19, 24, 31-41] results for spin decoherence in solid state systems appropriate for quantum computing architectures. Some of these works have not invoked the full battery of the traditional approximations, Markovian and secular, etc., or have utilized the spectral gap of the bath modes, to achieve better reliability of the short-time results. In ref. 41, interaction of the spin-exciton bath modes with impurities was accounted for, as the main mechanism of decoherence. In the present work, we limit ourselves to the bath modes only interacting with the system. Experimental efforts are picking up momentum, with the first limited results available[42, 43] by traditional NMR/ESR techniques, with the quantum-computing emphasis.

An approach, termed adiabatic decoherence, has been developed by us,[24] expanding the earlier works,[12, 31-33] with the goal of avoiding the ambiguity of the basis selection and achieving exact solvability. The price paid was the assumption that H_S is conserved (a particular version of the quantum nondemolition processes), which is equivalent to requiring that

$$[H_S, H] = [H_S, \Lambda_S] = 0 \qquad \text{(adiabatic case).} \qquad (2.1)$$

This makes the eigenbasis of H_S and Λ_S the same, but precludes energy relaxation, thus artificially leaving only energy-conserving relaxation

pathways that contribute to decoherence. We will comment on the results of this approach in Section 5.

Most of the results referred to earlier, have involved approximations of one sort or another. The most popular and widely used approximation has been the second-order perturbative expansion in the interaction strength, H_I, though some nonperturbative results have also been reported. In Section 3, we describe a novel approximation scheme[44] that is valid for short times. It has several advantages, such as becoming exact in the adiabatic case, allowing derivation of several explicit results, and, at least in principle, permitting derivation of higher-order approximations. Certain models of quantum measurement evaluate decoherence by effectively setting $H_S = 0$. Our approximation then becomes exact, and our results are consistent with these studies.[45, 46]

Our formulation in Section 3, will be quite general, and we will not use the specific bath or thermalization assumptions. However, we do utilize the factorization property (1.10) at time $t = 0$. Thus, we do have to assume that, at least initially, the system and the bath modes are not entangled. In fact, the present formulation also relies on that the Hamiltonians at hand are all time-independent. Therefore, we have excluded the possibility of controlled dynamics, in the quantum computing sense, when gate functions are accomplished by external couplings to individual qubits and by external control of their pairwise interactions. Our formulation, therefore, applies to "idling" qubits or systems of (possibly interacting) qubits. It is reasonable to assume that a lower limit on decoherence rate can be evaluated in such an idling state, even though for quantum error correction, qubits otherwise idling, might be frequently probed (measured) and entangled with ancillary qubits.[25–30]

The $t = 0$ factorization assumption (1.10), shared by all the recent spin-decoherence studies, then represents the expectation that external control by short-duration but large externally applied potentials, measurement, etc., will "reset" the qubits, disentangling them from the environment modes to which the affected qubits are only weakly coupled. Thus, we assert that it is the qubit system that gets approximately reset and disentangled from the bath towards time $t = 0$, instead of the bath being thermalized by the rest of the universe, as assumed in Markovian approximation schemes.

3. SHORT-TIME DECOHERENCE

In addition to the energy basis, (1.7), we also define the eigenstates of the interaction operator Λ_S, by

$$\Lambda_S |\gamma\rangle = \lambda_\gamma |\gamma\rangle, \tag{3.1}$$

where the Greek index labels the eigenstates of Λ_S, with eigenvalues λ_γ, while the Roman indices will be used for the energy basis, and, when capitalized, for the bath modes, (1.2)–(1.4).

The time dependence of the density matrix $R(t)$ of the system and bath, is formally given by

$$R(t) = e^{-i(H_S + H_B + H_I)t} R(0) e^{i(H_S + H_B + H_I)t}. \tag{3.2}$$

We will utilize the following approximate relation for the exponential factors, as our short-time approximation,

$$e^{i(H_S + H_B + H_I)t + O(t^3)} = e^{iH_S t/2} e^{i(H_B + H_I)t} e^{iH_S t/2}. \tag{3.3}$$

This relation has the following appealing properties. It becomes exact for the adiabatic case, (2.1). Furthermore, if we use the right-hand side and its inverse to replace $e^{\pm iHt}$, then we are imposing three time-evolution-type transformations on $R(0)$. Therefore, the approximate expression for $R(t)$ will have all the desired properties of a density operator. Finally, extensions to higher-order approximations in powers of t are possible, by using relations derived in ref. 47, where various expressions valid to $O(t^4)$ and $O(t^5)$ were considered.

Our goal is to evaluate the resulting approximation to the matrix element,

$$\rho_{mn}(t) = \text{Tr}_B \langle m | e^{-iH_S t/2} e^{-i(H_B + H_I)t} e^{-iH_S t/2} R(0) e^{iH_S t/2} e^{i(H_B + H_I)t} e^{iH_S t/2} | n \rangle. \tag{3.4}$$

First, we apply the operators H_S in the outer exponentials, acting to the left on $\langle m|$, and to the right on $|n\rangle$, replacing H_S by, respectively, E_m and E_n. We then note that the second exponential operator in (3.4) contains Λ_S, see (1.2). Therefore, we insert the decomposition of the unit operator in the system space, in terms of the eigenbasis of Λ_S, before the second exponential, and one in terms of the eigenbasis of H_S after it. This allows us to apply Λ_S in the second exponential and also H_S in the third exponential. The same substitution is carried out on the other side of $R(0)$, with the result

$$\rho_{mn}(t) = \sum_{\gamma p q \delta} \text{Tr}_B \left[e^{-iE_m t/2} \langle m | \gamma \rangle \langle \gamma | p \rangle e^{-i(H_B + \lambda_\gamma P_B)t} e^{-iE_p t/2} \rho_{pq}(0) \right.$$
$$\left. \times \left(\prod_K \theta_K \right) e^{iE_q t/2} e^{i(H_B + \lambda_\delta P_B)t} \langle q | \delta \rangle \langle \delta | n \rangle e^{iE_n t/2} \right]. \tag{3.5}$$

The next step is to collect all the terms, and also identify that the trace over the bath can be now carried out for each mode separately. We use (1.1) and (1.2) to write

$$\rho_{mn}(t) = \sum_{\gamma p q \delta} \left\{ e^{i(E_q + E_n - E_p - E_m)\,t/2} \langle m \,|\, \gamma \rangle \langle \gamma \,|\, p \rangle \, \rho_{pq}(0) \, \langle q \,|\, \delta \rangle \langle \delta \,|\, n \rangle \right.$$
$$\left. \times \prod_K \mathrm{Tr}_K \left[e^{-i(M_K + \lambda_\gamma J_K)\,t} \theta_K \, e^{i(M_K + \lambda_\delta J_K)\,t} \right] \right\}. \tag{3.6}$$

While this expression looks formidable, it actually allows rather straightforward calculations in some cases. Specifically, the simplest quantum-computing applications involve two-state systems. Then the sums in (3.6) are over two terms each. The calculations involving the overlap Dirac brackets between the eigenstates of H_S (labeled by m, n, p and q) and of Λ_S (labeled by γ and δ), as well as the energy-basis matrix elements of $\rho(0)$, cf. (1.8), involve at most diagonalization of two-by-two Hermitean matrices. Of course, the approximation (3.6) can be used for evaluation of short-time density matrices for systems more general than two-state.

The challenging part of the calculation involves the trace over each mode of the bath. Since these modes have identical structure, e.g., (1.3) and (1.4) for the bosonic bath case, but with K-dependent coupling constants, the calculation needs only be done once, in the space of *one mode*. Furthermore, results for the bath models ordinarily used, such as the bosonic and spin baths, are either already available in the literature or can be calculated without much difficulty. For the thermalized initial bath-mode density matrix θ_K, we give the exact bosonic-model expression in the next section.

In the remainder of this section, we first further analyze the trace over one bath mode entering (3.6). We then comment on the limits of validity of the present approximation.

In an obvious shorthand notation, we write the single-mode trace in (3.6) as

$$\mathrm{Tr}[e^{-i(M+\gamma J)\,t} \theta \, e^{i(M+\delta J)\,t}] = \mathrm{Tr}[\theta \, e^{i(M+\delta J)\,t} \, e^{-i(M+\gamma J)\,t}]. \tag{3.7}$$

Now, to the same order of approximation as used in (3.3), we can write

$$e^{i(M+\delta J)\,t + O(t^3)} = e^{iMt/2} \, e^{i\delta Jt} \, e^{iMt/2}. \tag{3.8}$$

The resulting approximation for the trace (3.7) reads

$$\mathrm{Tr}[(e^{-iMt/2} \theta \, e^{iMt/2}) \, e^{i(\delta - \gamma)\,Jt}], \tag{3.9}$$

which illustrates that, within this approximation, the product of traces in (3.6) is a function of the difference $\lambda_\gamma - \lambda_\delta$. In fact, this product is exactly 1 for $\lambda_\gamma = \lambda_\delta$ and, in most applications, the following form is likely to emerge,

$$\prod_K \mathrm{Tr}_K[\,\cdots\,] = e^{-\mathrm{const}(\lambda_\gamma - \lambda_\delta)^2\, t^2 + O(t^3)}, \tag{3.10}$$

though we caution the reader that (3.10) is somewhat speculative and suggested by the exact result for the bosonic heat bath, reported in the next section.

Finally, we point out that in most cases of interest, the initial single-mode density matrix θ will commute with the bath-mode energy operator M. In fact, the thermalized θ is a function of M. Therefore, (3.9) can be further simplified to

$$\mathrm{Tr}[\theta e^{i(\delta - \gamma)\, Jt}]. \tag{3.11}$$

However, let us emphasize that the approximate relations (3.9)–(3.11) are likely of value only as far as they help to derive basis-independent (operator) approximations to $\rho(t)$, by a technique illustrated in the next section. Indeed, for most bath models it is advisable to calculate the single-mode trace exactly first, according to (3.6), and then attempt various approximations.

The latter statement reflects our expectation that the approximation developed here is valid, for low temperatures, not only for short times, defined by $t < 1/\omega_D$, but also for intermediate times, exceeding $1/\omega_D$. This is suggested by the result of an illustrative calculation in the next section, but mainly by the fact that (3.11) only includes the bath-mode energy scales via θ, and, therefore, at low temperatures, is dominated by the lowest bath-mode excitations, and is not sensitive to frequencies of order ω_D. Thus, we expect our approximation to be applicable complementary to the Markovian-type approximations and definitely break down in the regime of fully developed thermalization, for $t \geqslant O(\beta)$. Additional supporting observations are offered in Section 5, when we consider the adiabatic case (2.1).

4. THE BOSONIC HEAT BATH

In this section, we consider the bosonic heat bath,[6] see (1.3) and (1.4), in the initially thermalized state,

$$\theta_K = e^{-\beta M_K} / \mathrm{Tr}_K(e^{-\beta M_K}) = (1 - e^{-\beta \omega_K})\, e^{-\beta \omega_K a_K^\dagger a_K}. \tag{4.1}$$

The product of the single-mode traces in (3.6), is then available in the literature,[12, 24, 31]

$$\rho_{mn}(t) = \sum_{\gamma p q \delta} \left\{ e^{i(E_q + E_n - E_p - E_m)t/2} \langle m \mid \gamma \rangle \langle \gamma \mid p \rangle \langle q \mid \delta \rangle \langle \delta \mid n \rangle \rho_{pq}(0) \right.$$
$$\times \exp\left(-\sum_K \frac{|g_K|^2}{\omega_K^2} \left[2(\lambda_\gamma - \lambda_\delta)^2 \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta \omega_K}{2} \right.\right.$$
$$\left.\left.\left. + i(\lambda_\gamma^2 - \lambda_\delta^2)(\sin \omega_K t - \omega_K t) \right] \right) \right\}. \tag{4.2}$$

The last term in the exponent, linear in t, is usually viewed as "renormalization" of the system energy levels due to its interaction with the bath modes. It can be removed by adding the term,

$$H_R = \Lambda_S^2 \sum_K |g_K|^2 / \omega_K, \tag{4.3}$$

to the total Hamiltonian. However, the usefulness of this identification for short times is not clear, and we will not use it. One can check that, *unmodified*, (4.2) is consistent with the expectation (3.10).

Let us now define two non-negative real spectral sums, $B(t)$ and $C(t)$, over the bath modes,

$$B^2(t) = 8 \sum_K \frac{|g_K|^2}{\omega_K^2} \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta \omega_K}{2}, \tag{4.4}$$

$$C(t) = \sum_K \frac{|g_K|^2}{\omega_K^2} (\omega_K t - \sin \omega_K t). \tag{4.5}$$

When converted to integrals over the bath mode frequencies, with the cutoff at ω_D, these sums have been discussed extensively in the literature,[6, 12, 31] for several choices of the bath mode density of states and coupling strength g as functions of the mode frequency.

The final expression is,

$$\rho_{mn}(t) = \sum_{\gamma p q \delta} \left\{ e^{i(E_q + E_n - E_p - E_m)t/2} \langle m \mid \gamma \rangle \langle \gamma \mid p \rangle \langle q \mid \delta \rangle \langle \delta \mid n \rangle \rho_{pq}(0) \right.$$
$$\left. \times \exp\left[-\tfrac{1}{4} B^2(t)(\lambda_\gamma - \lambda_\delta)^2 - iC(t)(\lambda_\gamma^2 - \lambda_\delta^2) \right] \right\}. \tag{4.6}$$

When the spectral functions are expanded in powers of t, this result confirms all the conclusions and conjectures discussed in Section 3, in connection with relations (3.9)–(3.11).

Let us now turn to the derivation of the basis-independent representation for $\rho(t)$, by utilizing the integral identity

$$\sqrt{\pi} \exp[-B^2(\Delta\lambda)^2/4] = \int_{-\infty}^{\infty} dy\, e^{-y^2} \exp[iyB(\Delta\lambda)]. \qquad (4.7)$$

Exponential factors in (4.6) can then be reproduced by applying operators on the wavefunctions entering the overlap Dirac brackets, with the result

$$\sqrt{\pi}\, \rho(t) = \int dy\, e^{-y^2} e^{-iH_S t/2}\, e^{i[yB(t)\,\Lambda_S - C(t)\,\Lambda_S^2]}\, e^{-iH_S t/2}\, \rho(0)$$

$$\times\, e^{iH_S t/2}\, e^{-i[yB(t)\,\Lambda_S - C(t)\,\Lambda_S^2]}\, e^{iH_S t/2}. \qquad (4.8)$$

Within the $O(t^2)$ approximation (3.3), given that B and C are of order linear or higher in t, we can combine the exponential operators to get an alternative approximation,

$$\sqrt{\pi}\, \rho(t) = \int dy\, e^{-y^2} e^{-i[tH_S - yB(t)\,\Lambda_S + C(t)\,\Lambda_S^2]}\, \rho(0)\, e^{i[tH_S - yB(t)\,\Lambda_S + C(t)\,\Lambda_S^2]}, \qquad (4.9)$$

though (4.6) and (4.8) are in fact easier to handle in actual calculations.

As an application, let us consider the case of H_S proportional to the Pauli matrix σ_z, e.g., a spin-1/2 particle in magnetic field, and $\Lambda_S = \sigma_x$, with the proportionality constant in the latter relation absorbed in the definition of the coupling constants g_K in (1.4). Let us study the deviation of the state of a spin-1/2 qubit, initially in the energy eigenstate $|\uparrow\rangle$ or $|\downarrow\rangle$, from pure state, by calculating $\mathrm{Tr}_S[\rho^2(t)]$ according to (4.8). We note that for a two-by-two density matrix, this trace can vary from 1 for pure quantum states to the lowest value of $1/2$ for maximally mixed states.

A straightforward calculation with $\rho(0) = |\uparrow\rangle\langle\uparrow|$ or $|\downarrow\rangle\langle\downarrow|$, yields

$$\mathrm{Tr}_S[\rho^2(t)] = \tfrac{1}{2}[1 + e^{-2B^2(t)}]. \qquad (4.10)$$

As the time increases, the function $B^2(t)$ grows monotonically from zero.[6, 12, 24, 31] Specifically, for Ohmic dissipation, $B^2(t)$ increases quadratically for short times $t < O(1/\omega_D)$, then logarithmically for $O(1/\omega_D) < t < O(\hbar/kT)$, and linearly for $t > O(\hbar/kT)$. For other bath models, it need not diverge to infinity at large times.

Both approximations, (4.8) and (4.9), make the deviation from a pure state $\rho(0) = |\psi_0\rangle\langle\psi_0|$ apparent: $\rho(t > 0)$ is obviously a *mixture* (integral

over y) of pure-state projectors $|\psi(y,t)\rangle\langle\psi(y,t)|$, where, for instance for (4.9),

$$\psi(y,t) = e^{-i[tH_S - yB(t)\Lambda_S + C(t)\Lambda_S^2]}\psi_0, \tag{4.11}$$

with a somewhat different expression for (4.8).

5. THE ADIABATIC CASE

Relation (2.1) corresponds to the system's energy conservation. Therefore, energy flow in and out of the system is not possible, and normal thermalization mechanisms are blocked. This "adiabatic decoherence" limit thus corresponds to "pure dephasing;" see ref. 48.

The fact that our approximation becomes exact in this case, provides support to the expectation that, at low temperatures, it is generally valid beyond the cutoff time scale $1/\omega_D$, providing a reasonable evaluation of decoherence and deviation from a pure state, as exemplified by the calculation yielding (4.10), in Section 4.

With (2.1), we can select a common eigenbasis for H_S and Λ_S. Then the distinction between the lower-case Roman and Greek indices in (3.6) becomes irrelevant, and the sums can all be evaluated to yield

$$\rho_{mn}(t) = e^{i(E_n - E_m)t}\rho_{mn}(0)\prod_K \text{Tr}_K[e^{-i(M_K + \lambda_m J_K)t}\theta_K e^{i(M_K + \lambda_n J_K)t}]. \tag{5.1}$$

This expression was discussed in detail in our work on adiabatic decoherence.[24] Specifically, for the initially thermalized bosonic heat bath case, we have, for the absolute values of the density matrix elements,

$$|\rho_{mn}(t)| = |\rho_{mn}(0)|\, e^{-B^2(t)(\lambda_m - \lambda_n)^2/4}. \tag{5.2}$$

The decay of the off-diagonal matrix elements thus depends of the properties of the spectral function $B^2(t)$ as the time increases. Such explicit results[12, 24, 31–33] illustrate that for irreversibile behavior, the number of bath modes must be infinite, with the spectral function evaluated in the continuum limit.

In summary, we have derived short-time approximations for the density matrix and its energy-basis matrix elements. Our expressions are quite easy to work with, because for few-qubit systems they only involve manipulation of finite-dimensional matrices, and they will be useful in estimating decoherence and deviation from pure states in quantum computing models, including results for low temperatures.

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