Short-Time Decoherence and Deviation from Pure Quantum States

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Abstract: In systems considered for quantum computing, i.e., for control of quantum dynamics with the goal of processing information coherently, decoherence and deviation from pure quantum states, are the main obstacles to error correction. At low temperatures, usually assumed in quantum computing designs, some of the accepted approaches to evaluation of relaxation mechanisms break down. We develop a new formalism for estimation of decoherence at short times, appropriate for evaluation of quantum computing architectures.
Consider a microscopic quantum system described by the Hamiltonian $H_S$. This system, $S$, can be a quantum bit (qubit), or several qubits, controlled externally individually and by switching on and off pairwise qubit interactions. This qubit paradigm helps to define the questions in describing how $S$ interacts with the surrounding macroscopic world. Interactions with the surroundings depend on the setting. For example, in quantum measurement, the wavefunction of the system is probed, and part of the process involves a strong interaction with the measuring device. However, in most applications, the external interactions are quite weak. In quantum computing, the aim is to minimize their effect.

Traditionally, interactions with the surroundings have been modelled by the modes of a “bath” $B$, with the mode Hamiltonians $M_K$,

$$H_B = \sum_K M_K .$$  \hspace{1cm} (1)

The interaction of the bath modes with $S$, will be modelled by

$$H_I = \Lambda_{SP_B} = \Lambda_S \sum_K J_K ,$$  \hspace{1cm} (2)

where $\Lambda_S$ is a Hermitean operator of $S$, coupled to the operator $P_B$ of $B$. For a bosonic bath [1,2], which we use as a prototype,

$$M_K = \omega_K a_K^\dagger a_K , \quad J_K = g_K^* a_K + g_K a_K^\dagger ,$$  \hspace{1cm} (3)

where the ground state is shifted to zero, and we work in units $\hbar = 1$. The total Hamiltonian is then $H = H_S + H_B + H_I$.

Let $\rho(t)$ represent the reduced density matrix of $S$, after $B$ has been traced over. For large times, the effect of the environment on an “idle” quantum system, i.e., one that is not otherwise externally controlled, is expected to be thermalization: this density matrix should approach $\exp(-\beta H_S)/\text{Tr}_S[\exp(-\beta H_S)]$, where $\beta \equiv 1/kT$. For times $t \geq 0$, we can consider the degree to which the system has departed from coherent pure-quantum-state evolution, due to the interactions and entanglement with the bath. The temperature and other external parameters needed to characterize $\rho(t)$, are determined by the properties of $B$, which in turn might interact with “the rest of the universe.”

In the eigenbasis of $H_S$, we consider the matrix elements of $\rho(t)$,

$$H_S|n\rangle = E_n|n\rangle , \quad \rho_{mn}(t) = \langle m|\rho(t)|n\rangle .$$  \hspace{1cm} (4)
For large times, we expect the diagonal $\rho_{nn}$ to approach values $\propto e^{-\beta E_n}$, while the off-diagonal elements $\rho_{m \neq n} \to 0$, corresponding to thermalization and decoherence in the energy basis. To establish this, several assumptions are traditionally made [1-5]. At time $t = 0$, it is assumed that the bath is thermalized, i.e., its modes, $K$, have density matrices $\theta_K = e^{-\beta M_K} / \text{Tr}_K (e^{-\beta M_K})$. The overall density matrix $R$ is then unentangled,

$$\left[ R(t) = \rho(t) \prod_K \theta_K \right]_{t=0}. \tag{5}$$

Now, a series of assumptions are made, e.g., the Markovian and secular approximations. The Markovian approximation essentially assumes that the density matrices of the bath modes are reset to the thermal ones, on time scales shorter than any dynamical times of the system interacting with the bath. This amounts to using (5) for times $t > 0$ and 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 $T$. Such approaches aim at master equations for $\rho_{mn}$ at large times, consistent with the Golden Rule, thermalization and decoherence. In variants of these formalisms, two external (to $S$) times scales are identified. One is the inverse of the upper cutoff frequency of the bath modes, $1/\omega_D$. Another is the “thermal” time $\hbar/kT = \beta$.

There is evidence [3,5,6] that the Markovian-type approximations are only valid for times large than both these time scales. This is hardly a limitation at room temperatures. However, for quantum computing, in semiconductor-heterostructure architectures [7-10], $T \approx 10 - 100 \mu K$. The thermal time then becomes dangerously close to the single-qubit control time even for slower qubits, based on nuclear spins. We emphasize that not all the approximation schemes have this problem [5]. We also point out that quantum computing architectures utilize [7-10] qubits and modes that couple them, that have large spectral gaps. It is believed that, especially at low temperatures, spectral gaps slow down relaxation processes. Thus, qubit levels are considered in quantum dots, in atoms, in large magnetic fields, and coupled by highly nondissipative “quantum” media [8,10], e.g., the quantum-Hall two-dimensional electron gas.

At low temperatures, spectral gaps lead to separation of time scales of the initial decoherence vs. later-stage thermalization and further decoherence driven by energy-conserving processes. One can then question whether the energy basis is the best to describe decoherence for times before the thermalizing processes take over. The issue of the basis has also
come up in models of quantum measurement [11,12], where the eigenbasis of the interaction, $\Lambda_S$, may be more appropriate. In fact, in quantum computing applications we really want to retain a pure quantum state [12,13]. The value of $1 - \text{Tr}_S[\rho^2(t)]$, of other measure, may be more indicative than off-diagonal matrix elements. Therefore, it is desirable to have basis-independent expressions for the reduced density operator $\rho(t)$.

Recently, several groups have reported [6,10,12,14-16] results for spin decoherence in quantum computing systems. Some have not invoked all 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. Experimental efforts are picking up momentum, with the first limited results available [17] by NMR/ESR techniques. An approach, termed adiabatic decoherence, has been developed [12] to avoid the ambiguity of the basis selection and achieve exact solvability [6,12,14,15]. The price paid was the assumption that $H_S$ is conserved (a version of the quantum nondemolition assumption), i.e., $[H_S, H] = [H_S, \Lambda_S] = 0$. This makes the eigenbasis of $H_S$ and $\Lambda_S$ the same, but precludes energy exchange, leaving only relaxation pathways that contribute to decoherence. Generally, $\Lambda_S|\gamma\rangle = \lambda_\gamma|\gamma\rangle$, where the Greek index labels the eigenstates of $\Lambda_S$; the Roman indices will be used for the energy, (4), and, capitalized, for the bath modes, (2,3).

The most widely used approximation has been the second-order perturbative expansion in the interaction, $H_I$. In the present work, we report a different scheme, valid for short times. It has several advantages, such as becoming exact in the adiabatic case, yielding several explicit results, and permitting derivation of higher-order approximations. We do assume that at $t = 0$ the system and bath modes are not entangled. Our formulation also relies on that the Hamiltonians are all time-independent, and, therefore, applies to “idling” (possibly interacting) qubits. It is reasonable to assume that a lower limit on decoherence rate can be evaluated in such an idling state. The $t = 0$ factorization assumption, shared by all the recent spin-decoherence studies, represents the expectation that control by short-duration but large externally applied potentials, will “reset” the qubits, disentangling them from the environment to which they are only weakly coupled. Thus, it is the qubit system that gets approximately reset and disentangled from the bath at $t = 0$, rather than the bath is thermalized by the “rest of the universe,” as assumed in Markovian approximation schemes.

The overall density matrix is $R(t) = e^{-i(H_S+H_B+H_I)t} R(0) e^{i(H_S+H_B+H_I)t}$. The fol-
lowing relation for the exponential factors will be used as our short-time approximation,
\[ e^{i(H_S+H_B+H_I)t+O(t^3)} = e^{iH_S t/2} e^{i(H_B+H_I)t} e^{iH_S t/2}. \] (6)

It becomes exact for the adiabatic-decoherence case. Furthermore, \( e^{\pm iHt} \) are replaced by three consecutive time-evolution-type transformations on \( R(0) \). Therefore, the approximate expression for \( R(t) \) will have all the desired positivity properties. Extensions to higher-orders in powers of \( t \) are possible: see [18] for various expressions valid to \( O(t^4) \) and \( O(t^5) \) in our nomenclature. In the resulting approximation to the matrix element,

\[ \rho_{mn}(t) = \text{Tr}_B \langle m | e^{-iH_S t/2} e^{-i(H_B+H_I)t} e^{-iH_S t/2} R(0) e^{iH_S t/2} e^{i(H_B+H_I)t} e^{iH_S t/2} | n \rangle, \] (7)

we insert the decomposition of the unit operator in the \( S \) space in terms of the eigenbasis of \( \Lambda_S \) before the second exponential, and in terms of the eigenbasis of \( H_S \) after it, etc.,

\[
\rho_{mn}(t) = \sum_{\gamma \, p \, q \, \delta} \text{Tr}_B \left\{ e^{-iE_m t/2} \langle m | \gamma \rangle \langle \gamma | p \rangle e^{-i(H_B+\lambda_\gamma P_B)t} e^{-iE_p t/2} \rho_{pq}(0) \right.
\]
\[
\times \left( \prod_K \theta_K \right) e^{iE_q t/2} e^{i(H_B+\lambda_\delta P_B)t} \langle q | \delta \rangle \langle \delta | n \rangle e^{iE_n t/2} \right\}. \] (8)

We use (1,2) to write

\[
\rho_{mn}(t) = \sum_{\gamma \, p \, q \, \delta} \left\{ e^{i(E_q+E_n-E_p-E_m)t/2} \langle m | \gamma \rangle \langle \gamma | p \rangle \langle q | \delta \rangle \langle \delta | n \rangle \rho_{pq}(0) \right.
\]
\[
\times \left( \prod_K \text{Tr} \left[ e^{-i(M_K+\lambda_\gamma J_K)t} \theta_K e^{i(M_K+\lambda_\delta J_K)t} \right] \right). \] (9)

This expression actually allows rather straightforward calculations in typical quantum-computing applications which involve single or few two-state systems. The overlap brackets are between the eigenstates of \( H_S \) (labeled by \( m, n, p \) and \( q \)) and of \( \Lambda_S \) (labeled by \( \gamma \) and \( \delta \)). The traces are over the modes of \( B \). Since these modes have identical structure, with \( K \)-dependent coupling constants, the calculation needs only be done once, in the space of one mode.

For the bosonic bath [2], see (3), with the thermal initial \( \theta_K = (1 - e^{-\beta \omega_K}) e^{-\beta \omega_K a_K^\dagger a_K} \), the product of traces in (9) is known [6,12,14],

\[
\rho_{mn}(t) = \sum_{\gamma \, p \, q \, \delta} \left\{ e^{i(E_q+E_n-E_p-E_m)t/2} \langle m | \gamma \rangle \langle \gamma | p \rangle \langle q | \delta \rangle \langle \delta | n \rangle \rho_{pq}(0) \right.
\]
\[
\times \left( \prod_K \text{Tr} \left[ e^{-i(M_K+\lambda_\gamma J_K)t} \theta_K e^{i(M_K+\lambda_\delta J_K)t} \right] \right). \] (9)
\[
\times \exp \left( - \sum_{K} \frac{|g_K|^2}{\omega_K^2} \left[ 2 (\lambda_\gamma - \lambda_\delta)^2 \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta \omega_K}{2} + i (\lambda_\gamma^2 - \lambda_\delta^2) (\sin \omega_K t - \omega_K t) \right] \right) \right). \tag{10}
\]

The last term in the exponent, linear in \(t\), is the “renormalization” of the system energy levels due to its interaction with the bath modes. It could be removed by adding the term \(H_R = \Lambda^2_S \sum_{K} |g_K|^2 / \omega_K\) to the total Hamiltonian. The non-negative real spectral sums, \(B(t)\) and \(C(t)\),

\[
B^2(t) = 8 \sum_K \frac{|g_K|^2}{\omega_K^2} \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta \omega_K}{2}, \tag{11}
\]

\[
C(t) = \sum_K \frac{|g_K|^2}{\omega_K^2} (\omega_K t - \sin \omega_K t), \tag{12}
\]

when converted to integrals over the bath mode frequencies, with the cutoff at \(\omega_D\), have been discussed extensively in the literature [2,6,14], for several choices of the bath mode density of states and coupling strength \(g\) as functions of the mode frequency. In summary, we get the approximation

\[
\rho_{mn}(t) = \sum_{\gamma p q \delta} \left\{ e^{i(E_q + E_n - E_p - E_m)t/2} \langle m|\gamma\rangle\langle\gamma|p\rangle\langle q|\delta\rangle\langle\delta|n\rangle \rho_{pq}(0) \right. \]

\[
\times \exp \left[ - \frac{1}{4} B^2(t) (\lambda_\gamma - \lambda_\delta)^2 + iC(t) (\lambda_\gamma^2 - \lambda_\delta^2) \right] \right\}, \tag{13}
\]

which is exact for all times in the adiabatic case [6,12,14,15,19], and has the properties of a density operator.

A basis-independent representation for \(\rho(t)\) is obtained by using \(\sqrt{\pi} \exp[-B^2(\Delta \lambda)^2/4] = \int_{-\infty}^{\infty} dy e^{-y^2} \exp[iyB(\Delta \lambda)]\). Exponential factors in (13) can then be reproduced by applying operators on the wavefunctions, and the sums carried out,

\[
\sqrt{\pi} \rho = \int dy e^{-y^2} e^{-iH_S t/2} e^{i[yB(t)\Lambda_S + C(t)\Lambda_S^2] - iH_S t/2} \rho(0) e^{iH_S t/2} e^{-i[yB(t)\Lambda_S + C(t)\Lambda_S^2] - iH_S t/2}. \tag{14}
\]

Decoherence is explicit in (14): if \(\rho(0)\) is a projection operator \(|\psi_0\rangle\langle\psi_0|\) (a pure state), then \(\rho(t > 0)\) is obviously a mixture (integral over \(y\)) of projectors \(|\psi(y, t)\rangle\langle\psi(y, t)|\), where

\[
\psi(y, t) = e^{-iH_S t/2} e^{i[yB(t)\Lambda_S + C(t)\Lambda_S^2] - iH_S t/2} \psi_0.
\]

As an application, let us consider the case of \(H_S\) proportional to the Pauli matrix \(\sigma_z\), e.g., spin-1/2 in magnetic field, and \(\Lambda_S = \sigma_x\), with the proportionality constant absorbed.
in the couplings $g_K$ in (3). We 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 $\text{Tr}_S[\rho^2(t)]$. For a two-by-two density matrix, this trace can vary from 1 for pure quantum states to $1/2$ for maximally mixed states. With $\rho(0) = |\uparrow\rangle\langle\uparrow|$ or $|\downarrow\rangle\langle\downarrow|$, 

$$\text{Tr}_S[\rho^2(t)] = \frac{1}{2} \left[1 + e^{-2B^2(t)}\right]. \quad (15)$$

As the time increases, the function $B^2(t)$ grows monotonically from zero [2,6,12,14]. For Ohmic dissipation, $B^2(t)$ increases quadratically for short times $t < O(1/\omega_D)$, then logarithmically for $O(1/\omega_D) < t < O(h/kT)$, and linearly for $t > O(h/kT)$. (For other bath models, it need not diverge to infinity at large times.) This calculation illustrates that the present approximation can yield reasonable results for short and even intermediate times.

In summary, we have derived short-time approximations, (13,14), for the density matrix or its energy-basis matrix elements, for the case of the bosonic heat bath with initially fully thermalized modes. Other baths can be studied by using (9).

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