

Studies of short-time decoherence for evaluation of quantum computer designs *

Vladimir Privman* and Denis Tolkunov

*Center for Quantum Device Technology, Clarkson University,
Potsdam, NY 13699-5721, USA*

**Corresponding author: privman@clarkson.edu*

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Abstract

We review our recent results on short time approximations, with emphasis on applications for which the system-environment interactions involve a general non-Hermitian system operator Λ , and its conjugate, Λ^\dagger . We evaluate the onset of decoherence at low temperatures in open quantum systems. The developed approach is complementary to Markovian approximations and appropriate for evaluation of quantum computing schemes. Example of a spin system coupled to a bosonic heat bath via $\Lambda \propto \sigma_-$ is discussed.

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1 Introduction

The coupling of a quantum system to environmental degrees of freedom induces decoherence, destroying quantum superposition and reducing pure states to mixed states. Understanding of decoherence is important for quantum control and computing and, generally, for obtaining a description to the evolution of the system's reduced density matrix with the environmental modes traced over. Since this can not be done exactly in most cases, different approximation techniques, which are valid for different time scales,

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were developed. For short times, appropriate for quantum computing gate functions and, generally, for controlled quantum dynamics, approximation schemes for the density matrix have been suggested recently [1–4]. The present survey introduces a new [1] rather general short-time approximation which applies for models with system-bath interactions involving a general system operator. It thus extends the previously known approach [3, 4] developed for couplings involving a single Hermitian system operator.

We assume that the Hamiltonian of an open quantum system is

$$H = H_S + H_B + H_I, \quad (1)$$

where H_S describes the system coupled to a fluctuating dynamical reservoir (the bath). Typically, the bath is modeled by the harmonic modes, as reviewed in [5],

$$H_B = \sum_k \omega_k b_k^\dagger b_k. \quad (2)$$

Here b_k are the annihilation operators of the bath modes, and we use the convention $\hbar = 1$. We assume that the interaction with the bath involves the system operator Λ that couples linearly to the bath modes, as reviewed in [6],

$$H_I = \Lambda \sum_k g_k b_k^\dagger + \Lambda^\dagger \sum_k g_k^* b_k, \quad (3)$$

with the interaction constants g_k .

Let $R(t)$ denote the overall density matrix. It is assumed [3, 7] that at time $t = 0$ the system and bath are not entangled, and the bath modes are thermalized ($\beta \equiv 1/kT$):

$$R(0) = \rho(0) \prod_k \theta_k, \quad (4)$$

$$\theta_k \equiv (1 - e^{-\beta\omega_k}) e^{-\beta\omega_k b_k^\dagger b_k}. \quad (5)$$

We point out that while the quantum system S , described by the reduced density matrix $\rho(t) = \text{Tr}_B R(t)$, is small, typically two-state (qubit) or several-qubit, the bath has many degrees of freedom. The combined effect of the bath modes on the system can be large even if each of them is influenced little by the system. This has been the basis for the arguments for the harmonic approximation for the bath modes and the linearity of the interaction, as well as for the Markovian approximations [6, 7] that assume that the bath modes are “reset” to the thermal state by the “rest of the

universe” on time scales shorter than any dynamical time of the system interacting with the bath.

The frequencies of the oscillators of the bath are usually assumed to be distributed from zero to some cutoff value ω_c . The bath modes with the frequencies close to the energy gaps of the system, $\Delta E_{ij} = E_i - E_j$, contribute to the “resonant” thermalization and decoherence processes. Within the Markovian schemes, the diagonal elements of the reduced density matrix of the system, approach the thermal values $\propto e^{-E_i/kT}$ for large times exponentially, on time scale T_1 . The off-diagonal elements vanish, which represents decoherence, on time scale T_2 , which, for resonant processes, is given by $T_2 \simeq 2T_1$. However, generally decoherence is expected to be faster than thermalization because, in addition to resonant processes, it can involve virtual processes that do not conserve energy. It has been argued that this additional “pure” decoherence is dominated by the bath modes with near-zero frequencies [3, 6, 7]. At low temperatures, this “pure decoherence” is expected [8] to make $T_2 \ll T_1$.

Since the resetting of these low-frequency modes to the thermal state occurs on time scales $\hbar/kT = \beta$, the Markovian approach cannot be used at low temperatures [3, 7]. For quantum computing in semiconductor-heterostructure architectures [8–15], temperatures as low as few tens of mK are needed. This brings the thermal time scale to $\beta \sim 10^{-9}$ sec, which is close to the single-qubit control times 10^{-11} - 10^{-7} sec. Alternatives to the Markovian approximation have been suggested [1–4, 16–21].

2 Short-time approximation

In quantum computing applications, calculations with only a single qubit or few qubits are necessary for evaluation of the local “noise,” to use the criteria for quantum error correction [22–27]. For example, the system Hamiltonian is frequently taken proportional to the Pauli matrix σ_z . The interaction operator Λ can be proportional to σ_x , which is Hermitian. Such cases are covered by the short-time approximation developed earlier [3, 4]. However, one can also consider models with $\Lambda \propto \sigma_-$. Similarly, models with non-Hermitian Λ are encountered in quantum optics [28]. In this Section, we develop our short time approximation scheme. Results for a spin-boson type model are given in the next Section.

We derive a general expression for the time evolution operator of the system (1)–(3) within the short time approximation. The overall density matrix, assuming time-independent Hamiltonian over the quantum-

computation gate function time intervals [8–15], evolves according to

$$R(t) = U(t)R(0)[U(t)]^\dagger, \quad (6)$$

$$U(t) \equiv e^{-i(H_S+H_B+H_I)t}. \quad (7)$$

The general idea of our approach is to break the exponential operator in (7) into products of simpler exponentials. This involves an approximation, but allows us to replace system operators by their eigenvalues, when spectral representations are used, and then calculate the trace of $R(t)$ over the bath modes, obtaining explicit expressions for the elements of the reduced density matrix of the system. For Hermitian coupling operators, $\Lambda^\dagger = \Lambda$, our approach reduces to known results [3, 4].

In order to define “short time,” we consider dimensionless combinations involving the time variable t . There are several time scales in the problem. These include the inverse of the cutoff frequency of the bath modes, $1/\omega_c$, the thermal time $\beta = 1/kT$, and the internal characteristic times of the system $1/\Delta E_{ij}$. Also, there are time scales associated with the system-bath interaction-generated thermalization and decoherence, $T_{1,2}$. The shortest time scale at low temperatures (when β is large) is typically $1/\omega_c$. The most straightforward expansion in t yields a series in powers of $\omega_c t$. The aim of developing more sophisticated short-time approximations [1, 3, 4] has been to preserve unitarity and obtain expressions approximately valid up to intermediate times, of order of the system and interaction-generated time scales. The applicability for intermediate times can only be argued for heuristically in most cases, and checked by model calculations.

We split the exponential evolution operator into terms that do not have any noncommuting system operators in them. This requires an approximation. For short times, we start by using the factorization

$$\begin{aligned} & e^{-i(H_S+H_B+H_I)t+O(t^3)} \\ &= e^{-\frac{i}{2}H_S t} e^{-i(H_I+H_B)t} e^{-\frac{i}{2}H_S t}, \end{aligned} \quad (8)$$

where we have neglected terms of the third and higher orders in t in the exponent. The middle exponential in (8),

$$\Xi \equiv e^{-i(H_B+H_I)t} = e^{-i(H_B+\Lambda G^\dagger+\Lambda^\dagger G)t}, \quad (9)$$

where

$$G \equiv \sum_k g_k^* b_k, \quad (10)$$

still involves noncommuting terms as long as Λ is non-Hermitian. In terms of the Hermitian operators

$$L \equiv \frac{1}{2} (\Lambda + \Lambda^\dagger), \quad (11)$$

$$M \equiv \frac{i}{2} (\Lambda - \Lambda^\dagger), \quad (12)$$

we have

$$\Lambda G^\dagger + \Lambda^\dagger G = L (G + G^\dagger) + iM (G - G^\dagger). \quad (13)$$

We then carry out two additional short-time factorizations within the same quadratic-in- t (in the exponent) order of approximation,

$$\begin{aligned} \Xi &= e^{\frac{1}{2}[M(G-G^\dagger)-iH_B]t} e^{\frac{i}{2}H_B t} \\ &\times e^{-i[H_B+L(G+G^\dagger)]t} e^{\frac{i}{2}H_B t} e^{\frac{1}{2}[M(G-G^\dagger)-iH_B]t}. \end{aligned} \quad (14)$$

This factorization is chosen in such a way that Ξ remains unitary, and for $M = 0$ or $L = 0$ the expression is identical to that used for the Hermitian case [3, 4]. The evolution operator then takes the form

$$U = e^{-\frac{i}{2}H_S t} \Xi e^{-\frac{i}{2}H_S t}, \quad (15)$$

with Ξ from (14), which is an approximation in terms of a product of several unitary operators. The form of the higher-order corrections was considered in [1].

It has been recognized [1, 3, 4] that approximations of this sort, which are not perturbative in powers of H_I , are superior to the straightforward expansion in powers of $\omega_c t$. Specifically, in (8), we notice that H_S is factored out in such a way that H_B , which commutes with H_S , drops out of many commutators that enter the higher-order correction terms. This suggests that a redefinition of the energies of the modes of H_B should have only a limited effect on the corrections and serves as a heuristic argument for the approximation being valid beyond the shortest time scale $1/\omega_c$, up to intermediate time scales.

Our goal is to approximate the reduced density matrix of the system. We consider its energy-basis matrix elements,

$$\rho_{mn}(t) = \text{Tr}_B \langle m | U R(0) U^\dagger | n \rangle, \quad (16)$$

where

$$H_S |n\rangle = E_n |n\rangle. \quad (17)$$

We next use the factorization (8), (14) to systematically replace system operators by c-numbers, by inserting decompositions of the unit operator in the bases defined by H_S , L , and M . First, we collect the expressions (4), (14), (15), (17), and use two energy-basis decompositions of unity to get

$$\begin{aligned} \rho_{mn}(t) &= \sum_{pq} e^{\frac{i}{2}(E_n+E_q-E_m-E_p)t} \rho_{pq}(0) \\ &\times \text{Tr}_B [\langle m | \Xi | p \rangle \prod_k \theta_k \langle q | \Xi^\dagger | n \rangle]. \end{aligned} \quad (18)$$

We define the eigenstates of L and M ,

$$L |\lambda\rangle = \lambda |\lambda\rangle, M |\mu\rangle = \mu |\mu\rangle. \quad (19)$$

The operators Ξ and Ξ^\dagger introduce exponentials in (18) that contain L or M in the power. By appropriately inserting $\sum_\lambda |\lambda\rangle \langle \lambda|$ or $\sum_\mu |\mu\rangle \langle \mu|$ between these exponentials, we can convert all the remaining system operators to c-numbers.

Now the trace in (18) can be evaluated, by using operator identities for bosonic operators [28] and the coherent-states technique. We obtain our final result for the density matrix evolution [1],

$$\begin{aligned} \rho_{mn}(t) &= \sum_{p,q} \sum_{\mu_j \lambda_j} e^{\frac{i}{2}(E_n+E_q-E_m-E_p)t - \mathcal{P}} \rho_{pq}(0) \\ &\times \langle m | \mu_1 \rangle \langle \mu_1 | \lambda_1 \rangle \langle \lambda_1 | \mu_2 \rangle \langle \mu_2 | p \rangle \\ &\times \langle q | \mu_3 \rangle \langle \mu_3 | \lambda_2 \rangle \langle \lambda_2 | \mu_4 \rangle \langle \mu_4 | n \rangle, \end{aligned} \quad (20)$$

where the first sum over p and q is over the energy eigenstates of the system; the second sum is over λ_1, λ_2 and μ_1, \dots, μ_4 , which label the eigenstates of the operators L and M , respectively. The power in the exponential is

$$\begin{aligned} \mathcal{P} &= B^2(t) (\lambda_-^2 + \mu'_- \mu''_-) + B^2(t/2) (\mu''_- - \mu'_-)^2 \\ &- F(t) (\mu''_- - \mu'_-) \lambda_- - iC(t) \lambda_- \lambda_+ - iC(t/2) \\ &\times (\mu'_- \mu'_+ + \mu''_- \mu''_+) + iS(t) (\lambda_- \mu''_+ - \lambda_+ \mu'_-) \\ &- iC_1(t) \mu'_- \mu''_+. \end{aligned} \quad (21)$$

Here we introduced the variables

$$\mu'_\pm = \mu_1 \pm \mu_4, \quad (22)$$

$$\mu''_\pm = \mu_2 \pm \mu_3, \quad (23)$$

and

$$\lambda_{\pm} = \lambda_1 \pm \lambda_2. \quad (24)$$

and the spectral sums over the bath modes,

$$B^2(t) = 2 \sum_k \frac{|g_k|^2}{\omega_k^2} \sin^2 \frac{\omega_k t}{2} \coth \frac{\beta \omega_k}{2}, \quad (25)$$

$$C(t) = \sum_k \frac{|g_k|^2}{\omega_k^2} (\omega_k t - \sin \omega_k t); \quad (26)$$

these functions are well known [29, 30]. The result also involves the new spectral functions

$$S(t) = -2 \sum_k \frac{|g_k|^2}{\omega_k^2} \sin^2 \frac{\omega_k t}{2}, \quad (27)$$

$$F(t) = 4 \sum_k \frac{|g_k|^2}{\omega_k^2} \sin^2 \frac{\omega_k t}{4} \sin \frac{\omega_k t}{2} \coth \frac{\beta \omega_k}{2}. \quad (28)$$

Furthermore, we defined

$$C_1(t) = 2C(t/2) - C(t). \quad (29)$$

3 Discussion and application

In most applications evaluation of decoherence will require short-time expressions for the reduced density matrix of a single qubit. Few- and multi-qubit systems will have to be treated by utilizing additive quantities [31–33], accounting for quantum error correction (requiring measurement), etc. For a two-state system—a qubit—the summation in (20) involves $2^8 = 64$ terms, each of them being a product of several factors calculation of which is straightforward. We carry out the calculation for an illustrative example.

We consider the model [34] defined by

$$H = \mathcal{A} \sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sum_k \left(g_k \sigma_- b_k^\dagger + g_k^* \sigma_+ b_k \right), \quad (30)$$

where $\mathcal{A} \geq 0$ is a constant, $\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm i\sigma_y)$ and σ_z are the Pauli matrices, b_k^\dagger and b_k are the bosonic creation and annihilation operators, and g_k are

the coupling constants. Physically this model may describe, for example, a qubit interacting with a bath of phonons, or a two-level molecule in an electromagnetic field. In the latter case, this is a variant of the multi-mode Jaynes-Cummings model [28, 35]. Certain spectral properties of this model, the field-theoretic counterpart of which is known as the Lee field theory, are known analytically, e.g., [36]. However, the trace over the bosonic modes, to obtain the reduced density matrix for the spin, has not been calculated exactly.

For the model (30) we have $\Lambda = \sigma_-$ and $\Lambda^\dagger = \sigma_+$, so that $L = \sigma_x/2$ and $M = \sigma_y/2$. We have $|\lambda_{1,2}\rangle = (|\uparrow\rangle \pm |\downarrow\rangle)/\sqrt{2}$, with the eigenvalues $\lambda_{1,2} = \pm 1/2$, and $|\mu_{1,2}\rangle = (|\uparrow\rangle \pm i|\downarrow\rangle)/\sqrt{2}$, with the eigenvalues $\mu_{1,2} = \pm 1/2$. For the initial state, let us assume that the spin at $t = 0$ is in the excited state $|\uparrow\rangle\langle\uparrow|$, so that the initial density matrix has the form

$$\rho(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (31)$$

Our calculation yielded the following results for the density matrix elements: $\rho_{12}(t) = 0$ and

$$\begin{aligned} 4\rho_{11}(t) &= 2 + e^{-2B^2(t)} + e^{-4B^2(\frac{t}{2})} \cosh(2F) \\ &+ 2e^{-2B^2(\frac{t}{2})} \sinh(B_1) \cos(S) + 2e^{-B^2(\frac{t}{2})} \\ &\times \cos(C_1) \sin(S) + ie^{-B^2(t)-B^2(\frac{t}{2})} [e^{iC_1} \\ &\times \sinh(-iS + F) + e^{-iC_1} \sinh(-iS - F)], \end{aligned}$$

where C_1 was defined in (29) and

$$B_1(t) = 2B^2(t/2) - B^2(t). \quad (32)$$

Where not explicitly shown, the argument of all the spectral functions entering (32) is t .

In order to obtain irreversible behavior and evaluate a measure of decoherence, we consider the continuum limit of infinite number of bath modes. We introduce the density of the bosonic bath states $\mathcal{D}(\omega)$, incorporating a large-frequency cutoff ω_c , and replace the summations in (25)–(28) by integrations over ω [5, 29, 37, 38]. For instance, (25) takes the form

$$B^2(t) = \int_0^\infty d\omega \frac{\mathcal{D}(\omega) |g(\omega)|^2}{\omega^2} \sin^2 \frac{\omega t}{2} \coth \frac{\beta\omega}{2}. \quad (33)$$

We will use the standard Ohmic-dissipation [5] expression, with an exponential cutoff, for our illustrative calculation,

$$\mathcal{D}(\omega) |g(\omega)|^2 = \Omega \omega e^{-\omega/\omega_c}, \quad (34)$$

where Ω is a constant.

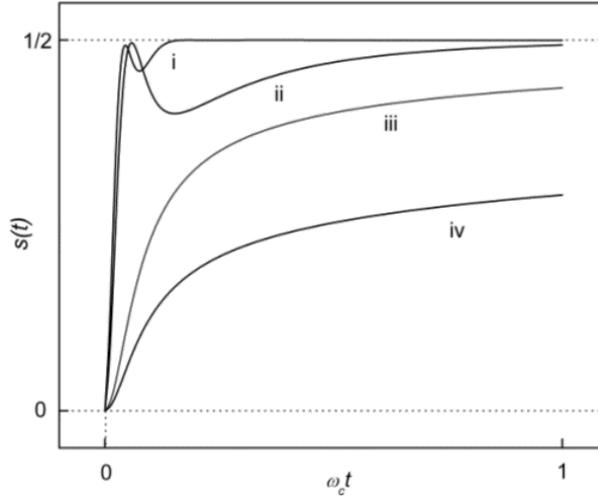


Figure 1: Schematic behavior of $s(t)$ for different values of Ω , decreasing from i to iv.

Our results for the density matrix elements depend on the dimensionless variable $\omega_c t$, as well as on the dimensionless parameters Ω and $\omega_c \beta$ ($= \hbar \omega_c / kT$, where we remind the reader that \hbar , set to 1, must be restored in the final results). Interestingly, the results do not depend explicitly on the energy gap parameter \mathcal{A} , see (30). This illustrates the point that short-time approximations do not capture the “resonant” relaxation processes, but rather only account for “virtual” relaxation/decoherence processes dominated by the low-frequency bath modes. However, the short-time approximations of the type considered here are meaningful only for systems with well-defined separation of the resonant vs. virtual decoherence processes, i.e., for $\hbar/\mathcal{A} \gg 1/\omega_c$. For such systems, $\hbar/\mathcal{A} = 1/\mathcal{A}$ defines one of the “intermediate” time scales beyond which the approximation cannot be trusted.

As an example, we calculated a measure of deviation of a qubit from a pure state in terms of the “linear entropy” [31, 33, 39],

$$s(t) = 1 - \text{Tr} [\rho^2(t)]. \quad (35)$$

Figure 1 schematically illustrates the behavior of $s(t)$ for different Ω values, for the case $\omega_c^{-1} \ll \beta$. The values of $s(t)$ increase from zero, corresponding to a pure state, to $1/2$, corresponding to a completely mixed state, with superimposed oscillations. For Ohmic dissipation, three time regimes can be identified [30]. The shortest time scale is set by $t < O(1/\omega_c)$. The quantum-fluctuation dominated regime corresponds to $O(1/\omega_c) < t < O(1/kT)$. The thermal-fluctuation dominated regime is $t > O(1/kT)$. Our short time approximation yields reasonable results in the first two regimes. For $t > O(1/kT)$ it cannot correctly reproduce the process of thermalization. Instead, it predicts approach to the maximally mixed state.

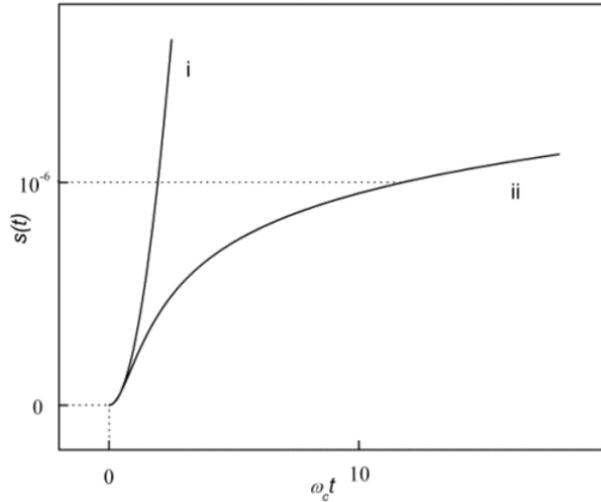


Figure 2: Comparison between the $O(t^2)$ expansion, i, and the short-time approximation, ii.

Figure 2 corresponds to the parameter values typical for low temperatures and appropriate for quantum computing applications, $\omega_c \beta = 10^3$, with $\Omega = 1.5 \cdot 10^{-7}$ chosen to represent weak enough coupling to the bath to have the decoherence measure reach the threshold for fault-tolerance, of order 10^{-6} , for “gate” times well exceeding $1/\omega_c$, here for $\omega_c t$ over 10. The leading-order quadratic expansion in powers of the time variable t , the validity of which is limited to $t < O(1/\omega_c)$, is also shown for comparison.

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