Quasi-Hamiltonian Method for Computation of Decoherence Rates

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We present a general formalism for the dissipative dynamics of an arbitrary quantum system in the presence of a classical stochastic process. It is applicable to a wide range of physical situations, and in particular it can be used for qubit arrays in the presence of classical two-level systems (TLS). In this formalism, all decoherence rates appear as eigenvalues of an evolution matrix. Thus the method is linear, and the close analogy to Hamiltonian systems opens up a toolbox of well-developed methods such as perturbation theory and mean-field theory. We apply the method to the problem of a single qubit in the presence of TLS that give rise to pure dephasing 1/f noise and solve this problem exactly. The exact solution gives an experimentally observable improvement over the popular Gaussian approximation.

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I. INTRODUCTION

With researchers motivated by the prospect of quantum computing, qubit dephasing has been a topic of intense research over the past decade. Various models of this venerable phenomenon have been investigated. The most popular have been the spin-boson or spin bath models. Another important version has been that of an electron spin coupling to nuclei. In recent studies of superconducting qubits, however, it has been found that 1/f-type noise is the chief source of dephasing with a wide spectrum of switching rates. The sources of this noise are two-level systems (TLS) with a wide spectrum of switching rates. It is likely to be important in virtually any solid-state system that serves as a host for qubits, as TLS are ubiquitous in bulk materials. This noise is usually modeled as classical noise.

Our aim in this paper will be to present a formalism that solves for the dissipative dynamics of an arbitrary quantum system in the presence of a classical stochastic process. This is a very general model of classical noise. The formalism depends on a combination of the ”Liouvillian” approach to the evolution of the density matrix with methods from the classical theory of stochastic processes. In particular, the formalism applies to an ensemble of TLS with any distribution of switching rates and couplings to the quantum system. It has the great advantage of reducing to a linear system of equations, and in fact there is a close analogy to the usual Hamiltonian formulation of quantum mechanics. It is exact, making no approximation as to the strength of the coupling relative to the inverse of the time scales of the noise.

This method has been derived for a specific example in previous work. As an illustrative case, we use the new method to solve the problem of a single qubit in the presence of TLS that give rise to pure dephasing 1/f noise. Other solutions of this problem have been found by previous authors, there have been numerical studies, and the subject has recently been comprehensively reviewed, so this problem is a good testbed for our method. It also allows us to exhibit the Hamiltonian analogy, which is in this case to a spin 1/2 system. The illustrative case points the way to other interesting models that are not exactly solvable, but to which the method also applies.

This paper is concerned with mathematical methods. Application to specific physical systems will be given in future work. The particular case of superconducting qubits has recently been treated. The main new results of a general nature are found in Eqs. and the physical interpretation following Eq. New results for strong-coupling (1/f and similar) noise are found in Eqs. and The most convenient starting point for future calculations of the effects of 1/f and other broad-spectrum noise is found in Eq.
II. GENERAL METHOD

We consider the general problem of a quantum system in the presence of classical noise. The quantum system is an $N_q$-state system, so its Hilbert space is $N_q$-dimensional. The classical system has $N_c$ states labeled by the index $a$. The initial state of the composite system is given by the Hermitian $N_q \times N_q$ density matrix $\rho(t=0)$ and the classical probability distribution $P_a(t=0)$. $0 \leq P_a \leq 1$. $\rho$ and $P$ satisfy

$$\text{Tr}\, \rho(t) = 1 \quad \text{and} \quad \sum_{a=1}^{N_c} P_a(t) = 1$$

(1)

at all times $t$. The classical environment passes through a sequence $S$ of discrete states during the course of the time evolution. The probability distribution of these states evolves according to the master equation

$$\frac{dP_a(t)}{dt} = \sum_{b=1}^{N_c} V_{ab} P_b(t).$$

(2)

$V$ is a real matrix of transition probabilities. It satisfies $\sum_a V_{ab} = 0$. The Hamiltonian for the quantum system is $H$: it is a function of the sequence of states of the classical environment, and is therefore time-dependent. For a fixed sequence $S$ the density matrix evolves according to the Von Neumann equation

$$\frac{d\rho_S}{dt} = -i [H(S), \rho_S]$$

(3)

in units with $\hbar = 1$. However, we are interested in the density matrix averaged over all sequences. We shall denote averages over $S$ by an overbar, so the actual density matrix is $\rho = \overline{\rho_S}$. We shall treat both the quantum system and the classical environment as finite-dimensional.

Since $a$ is a classical random variable, this is a classical noise model. The model applies when the noise sources are more strongly coupled to an external bath than to the qubit, so that back action of the qubit on the noise sources is negligible. The Hamiltonian $H$ is a function of $a$, the state of the classical system, but $V_{ab}$ is independent of $\rho$. This implies that quantum information that leaves the qubit leaves forever. The conditions under which such a model is appropriate have been considered in more detail by Galperin et al. [19].

A. Transfer Matrix for a Fixed Noise Sequence

We wish to compute the qubit density matrix $\rho_S(t)$, given $\rho_S(0)$, for a fixed sequence $S$. Our first step is to rewrite this in terms of the evolution of a generalized Bloch vector $n_i(t)$:

$$\rho_S(t) = \frac{1}{N_q} \left[ I + \sum_{i=1}^{N_q^2-1} n_i(S, t) \lambda_i \right],$$

(4)

where $n_i$ is a set of $N_q^2-1$ real numbers, $I$ is the $N_q \times N_q$ unit matrix and $\lambda_i$ are the generators of $SU(N)$. The $\lambda_i$ are time-independent $N_q \times N_q$ matrices and they are chosen to satisfy

$$\text{Tr}\, \lambda_i = 0, \quad \lambda_i^\dagger = \lambda_i, \quad \text{and} \quad \frac{1}{2} \text{Tr}\, \lambda_i \lambda_j = \delta_{ij}. \quad (5)$$

The $\lambda_i$ form an orthonormal basis for the quantum state space of density matrices under the inner product $(\rho_1, \rho_2) = \frac{1}{2} \text{Tr}\, (\rho_1 \rho_2)$. The fact that the $\lambda_i$ are traceless, together with Eq. [4], immediately implies the conservation of probability: $\text{Tr}\, \rho = 1$.

Consider a short time interval $\Delta t$ in which $H$ is constant and the environment is in a fixed state $a$. The formal solution to Eq. [3] is

$$\rho_S(a, \Delta t) = U(a, \Delta t) \rho(0) U(a, \Delta t)^\dagger.$$ 

(6)

with $U(a, t) = \exp [-itH(a)]$. In terms of the $\lambda_i$, Eq. [4] is

$$\frac{1}{2} I_{\alpha\beta} + \frac{1}{2} n_i(a, \Delta t) \lambda_{1\alpha\beta} = U_{\alpha\gamma}(a, \Delta t) U_{\beta\delta}^\dagger (a, \Delta t) \left[ \frac{1}{2} I_{\gamma\delta} + \frac{1}{2} n_i(0) \lambda_{1\gamma\delta} \right].$$
where we have temporarily included Greek subscripts for clarity. These indices denote components in the Hilbert space of the quantum system. They take on the values $\alpha = 1, 2, \ldots, N_q$. The Roman subscripts take on the values $i = 1, 2, \ldots, N_q^2 - 1$. Both are subject to a summation convention. The identity matrix term cancels out ($I_{\alpha\beta}$ has no dynamics) and we have

$$n_i(a, \Delta t) \lambda_{i,\alpha\beta} = U_{\alpha\gamma}(a, \Delta t) U_{\beta\delta}^\dagger(a, \Delta t) n_i(0) \lambda_{i,\gamma\delta}.$$  

We may extract the components of $n$ by multiplying this equation by the $i$-th generator and taking the trace over the Greek indices. Using the trace identity from Eq. 5 we find

$$n_i(a, \Delta t) = \frac{1}{2} U_{\alpha\gamma}(a, \Delta t) U_{\beta\delta}^\dagger(a, \Delta t) n_j(0) \lambda_{j,\gamma\delta} \lambda_{i,\beta\alpha}.$$  

This is conveniently written as

$$n_i(a, \Delta t) = T_{ij}(a, \Delta t) n_j(0),$$

where

$$T_{ij}(a, \Delta t) = \frac{1}{2} \text{Tr} \left[ \lambda_i U(a, \Delta t) \lambda_j U^\dagger(a, \Delta t) \right].$$  

(7)

$T_{ij}(a, \Delta t)$ is the quantum dynamical map (sometimes referred to as the Liouvillian) for the interval $\Delta t$ in an environment in state $a$ (Some properties of $T$ are given in App. A). From now on the Greek indices will be suppressed; operations in the quantum Hilbert space of operators are indicated by matrix multiplication and the trace.

Thus for the whole sequence $S$,

$$n_S(t) = T(a_N) \cdots T(a_2) T(a_1) n(0),$$

where $t = N\Delta t$ and $a_k$ labels the state of the classical environment in the time interval $k\Delta t$.

### B. Averaging over All Noise Sequences

We are interested in the generalized Bloch vector averaged over all possible sequences, i.e. $n(t) = \overline{n_S(t)} = \overline{T(t)} n(0)$.

To compute $T(t)$, we note each noise sequence $S = \{a_1, a_2, \ldots, a_N\}$ is associated with probability $W_{a_0,a_1}W_{a_1,a_2}\cdots W_{a_N-1,a_N}$, where $W_{a_k,a_{k+1}}$ is the transition probability of the classical system going from state $a_k$ to $a_{k+1}$ at the end of the $k$’th time interval, see Fig. 3 and the infinitesimal expansion of $W(\Delta t)$ is given by

$$W(\Delta t) = I_c + V \Delta t$$

where $I_c$ is the $N_c \times N_c$ unit matrix. $W_{a_0,a_1}$ is put in by hand for later on convenience. As $N \to \infty$ it will not introduce any errors.

Let us defined a $[N_c(N^2 - 1)] \times [N_c(N^2 - 1)]$ tensor $\Gamma$ whose element is

$$\Gamma(a_r,a_{r-1}) = W_{a_r,a_{r-1}} \otimes T(a_r).$$

(10)

The averaged Bloch vector is thus given by

$$n(t) = \sum_{a_1,a_2,\ldots,a_N} P_{a_1}(0) \Gamma(a_N,a_{N-1}) \cdots \Gamma(a_1,a_0) n(0)$$

(11)

Equivalently, we can utilize the tensor nature of $\Gamma$ and write

$$n(t) = \langle x_f | \Gamma^N | i_f \rangle n(0)$$

(12)

where $\langle x_f \rangle = [1, 1, \ldots, 1]$ and $| i_f \rangle = | p_1(0), p_2(0), \ldots, p_{N_c}(0) \rangle$ act on the classical environment. This contraction amounts to averaging over all the $N_c \times N_c$ blocks of $\Gamma^N$, each of which corresponds to the family of time evolutions caused by noise sequences that start from $a_1$ and end with $a_N$. In this formalism, it is possible to put the classical environment into an arbitrarily initial state $| i_f \rangle$. However, in almost all cases of physical interest, both the initial and final states of the environment will be the stationary distribution $| p_\nu \rangle$: the right eigenvector of $V$ corresponding to the eigenvalue zero [17].
This repeated matrix multiplication structure is the key to the formalism. Expand the matrix $\Gamma$ as

$$\Gamma(\Delta t) \approx I - iH_q \Delta t$$

so that in the limit $\Delta t \to 0$ with $t = N\Delta t$ held fixed we have

$$\Gamma^N(t) = (I - iH_q \Delta t)^N = \exp(-iH_q t),$$

and

$$n(t) = T(t)n(0) = \langle x_f | e^{-iH_q t} | i_f \rangle n(0).$$

$H_q$ is the time-independent "quasi-Hamiltonian" given by

$$H_q = i \lim_{\Delta t \to 0} \frac{\Gamma(\Delta t) - I}{\Delta t} = i \frac{d}{dt} \Gamma(t = 0).$$

It completely characterizes the evolution of the open quantum system. $H_q$ is pure imaginary and non-Hermitian. The idea of a non-Hermitian Hamiltonian to characterize dissipation or absorption in quantum systems is not new, going back at least to the optical model of the nucleus [28]. However, the implementation has historically been phenomenological; the results here are exact.

We write the eigendecomposition of $H_q$ as

$$H_q = \sum_{\psi} |\psi\rangle \omega_\psi \langle \psi|,$$

with $|\psi\rangle$ and $\langle \psi|$ being the right and left eigenvectors of $H_q$. Note that since $H_q$ is not Hermitian, $|\psi\rangle$ and $\langle \psi|$ are not dual to each other as in ordinary quantum mechanics.

Note $|\psi\rangle$ is a state of the combined environment-qubit system and the total evolution is given by

$$e^{-iH_q t} = \sum_{\psi} |\psi\rangle e^{-i\omega_\psi t} \langle \psi|,$$

so that Re($\omega_\psi$) gives the oscillation frequencies and $-\text{Im}(\omega_\psi)$ gives the decay rates of the combined system. $\psi = 1, 2, ..., [N_c (N_q^2 - 1)]$. Included in this list of $-\text{Im}(\omega_\psi)$’s are the rates for the environment.
This formalism provides a means of calculating the dissipative evolution of any quantum system evolving in the presence of a classical stochastic process. Furthermore it is completely linear, which means that all of the powerful techniques of linear algebra can be brought to bear, including well-controlled perturbation theory. In favorable cases such as the one to be considered next, the quasi-Hamiltonian is similar to Hamiltonians familiar from other problems in classical or quantum mechanics. The arsenal of methods developed for these situations can then be brought to bear.

We note that the derivation of the quasi-Hamiltonian is similar to the time-slice derivation of the path integral approach to open quantum systems, which leads to the Feynman-Vernon formulas for the influence functional [29]. The difference in starting points is that the environment here is taken as classical. The difference in end results is quite startling, since a non-Hermitian Hamiltonian does not seem to emerge naturally from the Feynman-Vernon approach in any obvious limit.

We note finally that the present formalism is also ideal for the investigation of quantum control schemes such as pulsing a qubit. We only need to sandwich the pulsing operators between the evolution operators. Let the pulsing operators be a unitary operator \( R \) that acts at the time \( t_p \) with \( 0 < t_p < t \). Its action on the generalized Bloch vector is given by the \((N_q^2-1) \times (N_q^2-1)\) matrix

\[
R_{ij} = \frac{1}{2} \text{Tr} \lambda_i R \lambda_j R^\dagger
\]

and writing \( U_p = I_c \otimes R \), we have

\[
n(t) = \langle x_f | e^{-iH_q (t-t_p)} U_p e^{-iH_q t_p} | i_f \rangle \ n(0).
\]

The generalization to more complicated pulsing schemes is immediate.

### III. QUBIT DEPHASING BY TWO LEVEL SYSTEMS

#### A. Quasi-Hamiltonian

We now proceed to solve exactly the problem of the evolution of the density matrix of a qubit in the presence of an environment of \( M \) independently fluctuating TLS that dephase the qubit. Even this simple case of \( N_q = 2 \) and \( N_e = 2^M \) is of great experimental interest. From the exact formulas we will derive qualitative information by extracting and analyzing asymptotic expressions in various limits.

For \( M \) statistically independent TLS we can describe the state of the environment by variables \( s_n(t) = \pm 1 \) that switch at random intervals at an average rate \( \gamma_n \). \( n = 1, 2, ..., M \). The most general expression for the flipping probability matrix is \( W = W_1 \otimes \cdots \otimes W_M \) with

\[
W_n = \begin{pmatrix}
1 - p_n - \delta_n & p_n - \delta_n \\
p_n + \delta_n & 1 - p_n + \delta_n
\end{pmatrix},
\]

or, in index notation \((W_n)_{+1,+1} = 1 - p_n - \delta_n\), etc. This states that the probability of starting and finishing the interval in the +1 state is \( 1 - p_n - \delta_n \), the probability of starting in the +1 state and ending in the −1 state is \( p + \delta \), etc. We can then write \( W_n = 1 - p_n + p_n \tau_{nx} - \delta \tau_{nz} - i \delta \tau_{ny} \), where \( \tau_{ni} \) are the Pauli matrices that act in the state space of fluctuator \( n \). The switching rate is \( \gamma_n = p_n / \Delta t \), while \( \delta_n \) controls the average occupation of the states. We shall focus on the case \( \delta_n = 0 \), the unbiased fluctuators, when we have

\[
W_n = (1 - p_n) I + p_n \tau_{nx}.
\]

and the stationary state is \(|p_n) = [1, 1, ..., 1]/2^M\), which is the unbiased fluctuator.

Here \( N_q = 2 \) and the generators of \( SU(2) \) are the Pauli matrices \( \sigma_x, \sigma_y, \) and \( \sigma_z \). The Hamiltonian of the quantum system is

\[
H(t) = -\frac{1}{2} B_0 \sigma_z - \frac{1}{2} \sum_{n=1}^{M} s_n(t) \ g_n \ \sigma_z.
\]

This is the case of pure dephasing noise. The more general case \( H = -B_0 \sigma_z / 2 - \sum_n s_n(t) \bar{g} \cdot \vec{\sigma} / 2 \) can also be treated
by the same method \cite{18}. Using Eq. \ref{eq:22} we have the $3 \times 3$ matrix

$$T_{ij} \left( \{s_n\}, \Delta t \right) = \frac{1}{2} \text{Tr} \left[ \sigma_i e^{i (B_0 + \sum s_n g_n) \sigma_z} e^{-i (B_0 + \sum s_n g_n) \sigma_z / \Delta t} \right]$$

$$= \left\{ \exp \left[ iL_z \left( B_0 + \sum_n s_n g_n \right) \Delta t \right] \right\}_{ij},$$

\tag{22}$$

where $L_z$ is the usual angular momentum matrix: $(L_z)_{xy} = -i$, $(L_z)_{yx} = i$, and all other $(L_z)_{ij} = 0$. Eq. \ref{eq:22} can be derived by direct calculation or by noting that $\exp \left( i\sigma_z \theta / 2 \right)$ is a rotation by $\theta$ about the $z$-axis in spin space. Substituting Eqs. \ref{eq:20} and \ref{eq:22} into Eqs. \ref{eq:11} and then using Eq. \ref{eq:16} we have the quasi-Hamiltonian for this problem:

$$H_q = \sum_{n=1}^{M} (-i\gamma_n + i\gamma_n \tau_{nx} - g_n \tau_{nz} L_z) - B_0 L_z.$$  

\tag{23}

Note $s_n$ in Eq. \ref{eq:22} are replaced by $\tau_{nz}$ due to the first order expansion.

B. Single Fluctuator

We first consider the case of a single TLS, so that $M = 1$ and $N_c = 2$. This simple case illustrates all the essential mathematical features of the method and the generalization to many independent TLS is almost immediate. We now have

$$H_q = -i\gamma + i\gamma \tau_x - g\tau_z L_z - B_0 L_z.$$  

The problem of qubit evolution has been reduced to the diagonalization of the $6 \times 6$ matrix $H_q$. This is much simplified by the fact that $[L_z, H_q] = 0$ so the problem reduces to a set of 3 smaller problems for $L_z = 0, \pm 1$. In these smaller problems no manipulations more complicated than diagonalizing a $2 \times 2$ matrix are required. We treat the smaller blocks in turn.

1. $L_z = 0$. The $2 \times 2$ block of the quasi-Hamiltonian $H_q$ is

$$H_q (L_z = 0) = (-i\gamma + i\gamma \tau_z)$$

There are 2 eigenvalues and right eigenfunctions that satisfy

$$H_q (L_z = 0) |\Psi_{L_z=0}\rangle = \omega_{L_z=0} |\Psi_{L_z=0}\rangle.$$  

We label them by $s = \pm 1$. The right eigenfunctions and eigenvalues are

$$|\Psi_{L_z=0} (s)\rangle = \left( 1 \over 2 \right) \left( \begin{array}{c} 0 \\ 1 \\ 1 \\ 0 \end{array} \right) \otimes \left( \begin{array}{c} 1 \\ \bar{s} \end{array} \right)$$

$$\omega_{L_z=0} (s) = -i\gamma + is\gamma$$

2. $L_z = +1$. The $2 \times 2$ block is

$$H_q (L_z = 1) = -i\gamma + i\gamma \tau_x - g\tau_z - B_0$$

\tag{24}

The right eigenfunctions and eigenvalues for $s = \pm 1$ are

$$|\Psi_{L_z=1} (s)\rangle = C \left( \begin{array}{c} \sqrt{2} \\ \sqrt{2} \\ 0 \\ 0 \end{array} \right) \otimes \left( \begin{array}{c} i\gamma \\ g + s\sqrt{g^2 - \gamma^2} \end{array} \right);$$

$$\omega_{L_z=1} (s) = -i\gamma - B_0 + s\sqrt{g^2 - \gamma^2}.$$  

Here $C^{-2} = 2s\sqrt{g^2 - \gamma^2} \left( g + s\sqrt{g^2 - \gamma^2} \right)$. The corresponding left eigenvectors $\langle \Psi_{L_z=1} |$ is simply the transpose of $|\Psi_{L_z=1} (s)\rangle$ and $\langle \Psi_{L_z=1} (s) |\Psi_{L_z=1} (s')\rangle = \delta_{s,s'}$. 
3. \( L_z = -1 \).

\[
H_q (L_z = 1) = -i \gamma + i \gamma \tau_x + g \tau_z + B_0
\]

Comparison to Eq. 24 shows that the eigenvalues and eigenvectors for \( L_z = -1 \) are obtained from the \( L_z = 1 \) case by the substitutions \((1/\sqrt{2}, i/\sqrt{2}, 0) \rightarrow (1/\sqrt{2}, -i/\sqrt{2}, 0)\), \( g_n \rightarrow -g_n \), and \( B_0 \rightarrow -B_0 \).

We now perform the analysis over initial states and sum over final states. We assume that \( P_s (t = 0) \) has its steady state values \( P_1 = P_{-1} = 1/2 \), or \(|i_f\rangle = [1, 1]/2\). However, the average and sum are more conveniently performed by taking a partial inner product with the state \(|\sqrt{p_s}\rangle\) of the classical system

\[
|\sqrt{p_s}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix},
\]

which projects onto the quantum subspace. The final \(3 \times 3\) evolution matrix in this subspace is:

\[
\mathcal{T} (t) = \langle \sqrt{p_s} | e^{-iH_q t} | \sqrt{p_s} \rangle.
\]

Note this equivalence between \( \langle \sqrt{p_s} | \cdot | \sqrt{p_s} \rangle\) and \( \langle x_f | \cdot | i_f \rangle\) can only be established if the initial states are uniformly distributed.

Using the eigendecomposition of \( H_q \) we have

\[
\mathcal{T} (t) = \sum_{s, L_z} \langle \sqrt{p_s} | \Psi_{L_z} (s) \rangle e^{-i \omega (L_z, s) t} \langle \Psi_{L_z} (s) | \sqrt{p_s} \rangle,
\]

so we need to do a sum of 6 terms for each member of the matrix. We now compute each member of \( \mathcal{T}_{ij} (t) \) in turn.

For\( \mathcal{T}_{zz} (t) \) only the \( L_z = 0 \), \( s = 1 \) term contributes and we find

\[
\mathcal{T}_{zz} (t) = \exp [-i \omega_{L_z = 0} (s = 1) t] = 1,
\]

This is simply the obvious statement that for pure dephasing noise, \( n_z \) does not decay. In terms of the standard relaxation times, this says that \( T_1 = \infty \).

\[
\mathcal{T}_{xx} (t) = \mathcal{T}_{yy} (t) = \mathcal{T}_{yz} (t) = \mathcal{T}_{zy} (t) = 0.
\]

For \( \mathcal{T}_{xx} (t) \) and \( \mathcal{T}_{yy} (t) \) only the \( L_z = \pm 1 \) blocks contribute. After a straightforward calculation one finds

\[
\mathcal{T}_{xx} (t) = \mathcal{T}_{yy} (t) = \exp (-\gamma t) \cos B_0 t \left[ \cos \left( \sqrt{g^2 - \gamma^2} t \right) + \frac{\gamma}{\sqrt{g^2 - \gamma^2}} \sin \left( \sqrt{g^2 - \gamma^2} t \right) \right],
\]

and finally

\[
\mathcal{T}_{xy} (t) = -\mathcal{T}_{yx} (t) = \exp (-\gamma t) \sin B_0 t \left[ \cos \left( \sqrt{g^2 - \gamma^2} t \right) + \frac{\gamma}{\sqrt{g^2 - \gamma^2}} \sin \left( \sqrt{g^2 - \gamma^2} t \right) \right].
\]

So, for example, if \( \mathbf{n} (t = 0) = (1, 0, 0) \), then we have

\[
\mathbf{n} (t) = (\cos B_0 t, \sin B_0 t, 0) \exp (-\gamma t) \left[ \cos \left( \sqrt{g^2 - \gamma^2} t \right) + \frac{\gamma}{\sqrt{g^2 - \gamma^2}} \sin \left( \sqrt{g^2 - \gamma^2} t \right) \right].
\]

The first factor is the uniform precession, and the rest of the expression gives the decay and non-uniform precession due to the TLS.

In the analysis below, it will be convenient to deal with the relaxation function \( \Gamma (t) \) defined by

\[
\mathcal{T}_{xx} (t) = \cos B_0 t \exp [-\Gamma (t)],
\]

so

\[
\Gamma (t) = \gamma t - \ln \left[ \cos \left( \sqrt{g^2 - \gamma^2} t \right) + \frac{\gamma}{\sqrt{g^2 - \gamma^2}} \sin \left( \sqrt{g^2 - \gamma^2} t \right) \right].
\]
1. Weak Coupling

This is the case \( \gamma > g \). Note that weak coupling (small \( g \)) is the same thing as fast switching (large \( \gamma \)). The arguments of the trigonometric functions are imaginary and \( \Gamma(t) \) is better written in terms of hyperbolic functions:

\[
T_{xx}(t) = \exp \left( -\gamma t \right) \cos B_0 t \left[ \cosh \left( \sqrt{\gamma^2 - g^2} t \right) + \frac{\gamma}{\sqrt{\gamma^2 - g^2}} \sinh \left( \sqrt{\gamma^2 - g^2} t \right) \right]
\]

and the behavior at long times \( t \gg 1/\gamma \) is given by

\[
T_{xx}(t) \approx \frac{1}{2} \left( 1 + \frac{\gamma}{\sqrt{\gamma^2 - g^2}} \right) \exp \left[ \left( -\gamma + \sqrt{\gamma^2 - g^2} \right) t \right].
\]  
(30)

Thus the dephasing rate is

\[
\frac{1}{T_2} = \gamma - \sqrt{\gamma^2 - g^2}.
\]  
(31)

For the extreme weak coupling case \( \gamma \gg g \) we find

\[
\frac{1}{T_2} = \frac{g^2}{2\gamma},
\]  
(32)

which is the standard result from perturbation (Redfield) theory.

In the short time limit \( t \ll 1/\sqrt{\gamma^2 - g^2} \) we have

\[
\Gamma(t) = \frac{1}{2} \frac{g^2 t^2}{6} - \frac{1}{6} \gamma g^2 t^3 + O(t^4).
\]  
(33)

This result is interesting: it shows that the envelope function initially decays quadratically even for a single fluctuator. We shall see below that this behavior is completely generic.

2. Strong Coupling

When \( \gamma < g \), one has

\[
T_{xx} = \exp (-\gamma t) \cos B_0 t \left[ \cos \left( \sqrt{g^2 - \gamma^2} t \right) + \frac{\gamma}{\sqrt{g^2 - \gamma^2}} \sin \left( \sqrt{g^2 - \gamma^2} t \right) \right]
\]  
(34)

and at short times \( t \ll 1/\sqrt{g^2 - \gamma^2} \) we have

\[
T_{xx} = \cos B_0 t \left[ 1 - \frac{1}{2} g^2 t^2 + \frac{1}{3} \gamma g^2 t^3 + O(t^4) \right],
\]  
(35)

and

\[
\Gamma(t) = \frac{1}{2} g^2 t^2 - \frac{1}{3} \gamma g^2 t^3 + O(t^4).
\]  
(36)

Note that when the coupling constant \( g \) is increased past \( \gamma \) the relaxation rate saturates at \( \gamma \). At the same point the oscillation frequency bifurcates into the two frequencies \( B_0 \pm g/\sqrt{g^2 - \gamma^2} \).

We stress that Eq. 34 gives a result that is exact at strong coupling.

C. Many Fluctuators

The quasi-Hamiltonian is given by Eq. 23. Again we have \( [L_z, H_q] = 0 \). The quasi-Hamiltonian for each value of \( L_z \) is a sum of operators acting on the individual fluctuators, which is a sign of the fact that they are statistically
independent: they do not "interact" with one another. Thus the generalization from the single fluctuator case is almost immediate. We have

\[ T_{zz}(t) = 1, \]

which is a sign of pure dephasing, and

\[ T_{xx}(t) = T_{yy}(t) = \exp \left( -\sum_{n=1}^{M} \gamma_n t \right) \cos \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right) + \frac{\gamma_n}{\sqrt{\gamma_n^2 - g_n^2}} \sin \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right), \]

(37)

\[ T_{xy}(t) = -T_{yx}(t) = \exp \left( -\sum_{n=1}^{M} \gamma_n t \right) \sin \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right) + \frac{\gamma_n}{\sqrt{\gamma_n^2 - g_n^2}} \sin \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right), \]

(38)

1. Weak Coupling

If \( g_n < \gamma_n \) for all \( n \), then

\[ \Gamma(t) = \sum_{n=1}^{M} \gamma_n t - \sum_{n=1}^{M} \ln \left[ \cosh \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right) + \frac{\gamma_n}{\sqrt{\gamma_n^2 - g_n^2}} \sin \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right) \right], \]

If \( t \gg \frac{1}{\min_n (\gamma_n)} \), then we have

\[ \Gamma(t) \approx \sum_{n=1}^{M} \left( \gamma_n - \sqrt{\gamma_n^2 - g_n^2} \right) t, \]

so that the decay is exponential at long times. For extreme weak coupling \( g_n \ll \gamma_n \) for all \( n \) then the Redfield result holds:

\[ \frac{1}{T_2} = \frac{1}{2} \sum_{n=1}^{M} \frac{g_n^2}{\gamma_n}. \]

(39)

At short times \( t \ll \frac{1}{\max_n (\gamma_n)} \)

\[ \Gamma(t) = \frac{1}{2} \sum_{n=1}^{M} g_n^2 t^2 - \frac{1}{6} \sum_{n=1}^{M} \gamma_n g_n^2 t^3. \]

(40)

We get deviations from the quadratic behavior at times of order

\[ t \sim \frac{\sum_{n=1}^{M} g_n^2}{\sum_{n=1}^{M} \gamma_n g_n^2}. \]

(41)

Thus the dephasing behavior is essentially exponential rather than quadratic in the weak coupling region.

2. Strong Coupling

If \( g_n > \gamma_n \) for all \( n \), then we find

\[ \Gamma(t) = \sum_{n=1}^{M} \gamma_n t - \sum_{n=1}^{M} \ln \left[ \cos \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right) + \frac{\gamma_n}{\sqrt{\gamma_n^2 - g_n^2}} \sin \left( \sqrt{\frac{g_n^2 - \gamma_n^2}{\gamma_n^2}} t \right) \right]. \]

(42)

This equation is exact and represents a new result for many strong-coupling fluctuators.

At short times \( t \ll \frac{1}{\max_n \sqrt{g_n^2 - \gamma_n^2}} \)

\[ \Gamma(t) \approx \frac{1}{2} \sum_{n=1}^{M} g_n^2 t^2 - \frac{1}{3} \sum_{n=1}^{M} g_n^2 \gamma_n t^3. \]

(43)
We get deviations from the initial quadratic behavior at times of order
\[ t \sim t_s = \frac{\sum_{n=1}^{M} g_n^2}{\sum_{n=1}^{M} \gamma_n g_n^2}. \] (44)

When \( t > t_s \) the behavior is more complicated. We write
\[ \Gamma(t) = \sum_{n=1}^{M} \gamma_n t - \ln \prod_{n=1}^{M} \left[ \frac{1}{2} \left( e^{i\lambda_n t} + e^{-i\lambda_n t} \right) + \frac{\gamma_n}{2i\lambda_n} (e^{i\lambda_n t} - e^{-i\lambda_n t}) \right] \] (45)
where \( \lambda_n = \sqrt{g_n^2 - \gamma_n^2} \) and we need to evaluate the expression
\[ U(t) = \left( \frac{1}{2} \right) \prod_{n=1}^{M} |r_n| \prod_{n=1}^{M} \left[ e^{i(\lambda_n t + \theta_n)} + e^{-i(\lambda_n t + \theta_n)} \right], \] (46)
with \( r_n = 1 - i\gamma_n/\lambda_n = |r_n| \exp(i\theta_n) \); \( |r_n| = (1 + \gamma_n^2/\lambda_n^2)^{1/2} \) and \( \theta_n = \tan^{-1}(-\gamma_n/\lambda_n) \).

To this end we note that \( \sum_{n=1}^{M} s_n (\lambda_n t + \theta_n) \) is the result of a random walk with a large number of steps \( M \). In the long-time limit \( t \gg t_l = 1/\min_n g_n \) the central limit theorem gives
\[ U(t) = \prod_{n=1}^{M} (1 + \gamma_n^2/\lambda_n^2) \exp \left( -\frac{t^2}{2} \sum_{n=1}^{M} g_n^2 \right) \] (47)
\[ = \exp \left\{ -\sum_{n=1}^{M} \left[ \frac{g_n^2 t^2}{2} - \frac{g_n^2}{\lambda_n^2} \right] \right\}. \] (48)
This expression of course neglects any Poincaré recurrences that can occur whenever \( M \) is finite. In terms of \( \Gamma \) we have
\[ \Gamma(t) = t \sum_{n=1}^{M} \gamma_n + \frac{t^2}{2} \sum_{n=1}^{M} g_n^2, \] (49)
so that there is a regime of Gaussian decay at long times when the coupling is strong.

### D. Broad-spectrum Noise

Finally we consider the case when the noise does not satisfy either of the inequalities \( g_n \gtrless \gamma_n \) for all \( n \). The fluctuators can still be divided into \( M_f \) fast (weak coupling, \( g_n < \gamma_n \)) fluctuators and \( M_s \) slow (strong coupling, \( g_n > \gamma_n \)) fluctuators. As we have seen, this is not a qualitative distinction - rather it corresponds to a change in the analytic behavior of the eigenvalues. This does not spoil the solvability of the model. We have
\[ \Gamma(t) = \sum_{n=1}^{M_f} \gamma_n t - \sum_{n=1}^{M_f} \ln \left[ \cosh \left( \sqrt{\gamma_n^2 - g_n^2} t \right) + \frac{\gamma_n}{\sqrt{\gamma_n^2 - g_n^2}} \sinh \left( \sqrt{\gamma_n^2 - g_n^2} t \right) \right] \]
\[ + \sum_{m=1}^{M_s} \gamma_m t - \sum_{m=1}^{M_s} \ln \left[ \cos \left( \sqrt{g_m^2 - \gamma_m^2} t \right) + \frac{\gamma_m}{\sqrt{g_m^2 - \gamma_m^2}} \sin \left( \sqrt{g_m^2 - \gamma_m^2} t \right) \right], \] (50)
and in the short time limit \( t \ll t_s \):
\[ \Gamma(t) \approx \frac{t^2}{2} \left[ \sum_{n=1}^{M_f} g_n^2 + \sum_{m=1}^{M_s} g_m^2 \right], \] (51)
while in the long time limit \( t \gg t_l \):
\[ \Gamma(t) \approx t \sum_{n=1}^{M_f} \left( \gamma_n - \sqrt{\gamma_n^2 - g_n^2} \right) + \frac{t^2}{2} \sum_{m=1}^{M_s} g_m^2, \] (52)
and the slow fluctuators will dominate at long times. This result is consistent with those obtained in Refs. [20] and [19] in more specific models.
IV. COMPARISON TO APPROXIMATE SOLUTIONS

The most usual way to characterize noise is by its power spectrum. Since our noise sources satisfy Poisson statistics and are independent of each other, we have
\[ s_m(t)s_n(t') = \delta_{mn} \exp(-2\gamma_n |t - t'|), \tag{53} \]
and the time auto-correlation function of the noise is
\[ \sum_{mn} b_{mz}(t)b_{nz}(t') = \sum_{mn} g^2 s_m(t)s_n(t') = g^2 \sum_n \exp(-2\gamma_n |t - t'|). \tag{54} \]

The power spectrum is obtained by taking the Fourier transform:
\[ S(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \frac{b_+(t)b_-(0)}{e^{-i\omega t}}. \tag{55} \]

For our case this is
\[ S_{cl}(\omega) = \frac{1}{\pi} \sum_{n=1}^{M} g_n^2 \frac{2\gamma_n}{4\gamma_n^2 + \omega^2}; \tag{56} \]
each individual fluctuator follows Poisson statistics and has a Lorentzian power spectrum. \( S_{cl}(\omega) \) is an even function of frequency; this is probably the main limitation of our classical model, as quantum noise is asymmetric in frequency at low temperatures [20]. In the continuum limit, we find
\[ S_{cl}(\omega) = \frac{1}{\pi} \int_{0}^{\infty} dg \int_{0}^{\infty} d\gamma \ p(g,\gamma) \frac{2g^2\gamma}{4\gamma^2 + \omega^2}, \tag{57} \]
where \( p(g,\gamma) \) is the distribution of couplings and rates, defined as
\[ p(g,\gamma) = \sum_{n=1}^{M} \delta(g - g_n) \ \delta(\gamma - \gamma_n). \tag{58} \]

When many fluctuators are superposed, we can obtain an arbitrary power spectrum by the proper choice of \( p(g,\gamma) \). Indeed, even choosing \( g_n = g_0 \) independent of \( n \) we have
\[ S_{cl}(\omega) = \frac{1}{\pi} g_0^2 \int_{0}^{\infty} d\gamma \ p(\gamma) \frac{2\gamma}{4\gamma^2 + \omega^2} \int_{0}^{\infty} d\tau \cos \omega \tau \int_{0}^{\infty} d\gamma \ p(\gamma) e^{-2\gamma t}. \tag{59} \]

Defining \( p(\gamma) \) by \( p(g,\gamma) = \delta(g - g_0) p(\gamma) \), this equation shows that to obtain \( p(\gamma) \) given \( S_{cl}(\omega) \), we first invert a Fourier cosine transform to obtain the original time auto-correlation function and then \( p(\gamma) \) is proportional to the the inverse Laplace transform of that. We conclude that as long as the only characterization of the noise is its power spectrum, then the results given above provide an exact solution for any \( S(\omega) \).

We have already commented on the relation of the present solution to perturbation (Redfield) theory. The exact solution agrees with the perturbative results when \( g_n \ll \gamma_n \) for all \( n \) and \( t \gg 1/\min_n \gamma_n \).

A more interesting approximation is the Gaussian approximation:
\[ \Gamma_G(t) = \frac{t^2}{2} \int_{-\infty}^{\infty} S_{cl}(\omega) \frac{\sin^2(\omega t/2)}{(\omega t/2)^2} d\omega. \tag{61} \]

See, e.g., Ref. [22] for a derivation. This approximation is valid when noise cumulants of third and higher order vanish. For RTNs, this is not the case - there are cumulants of all orders. For a calculation of some of these cumulants, see Ref. [21]. Cumulants of order \( n \) for a single noise source are proportional to \( g^n \), so we expect that the Gaussian approximation will break down for large \( g \). Qualitatively, the behavior of \( \Gamma_G(t) \) may be obtained by observing that the function \( \sin^2(\omega t/2)/(\omega t/2)^2 \) acts largely as a filter function that passes frequencies \( \omega < 1/t \), so
\[ \Gamma_G(t) \approx t^2 \int_{0}^{1/t} S_{cl}(\omega) d\omega. \tag{62} \]
FIG. 2: (Color online) Envelope of the free induction decay signal $\exp[-\Gamma(t)]$ for weak coupling: $g=0.01, \gamma = 0.2$. The exact result is given by the blue solid line, Gaussian approximation by the green dashed line and the Redfield approximation by the red dashed line. The inset gives the short-time behavior.

Furthermore, the total noise power is proportional to $\int_{-\infty}^{\infty} S_{cl}(\omega) \, d\omega$. For this integral to converge (pathological cases apart) there must be an upper ($\omega_{uv}$) cutoff frequency for $S_{cl}(\omega)$ and a lower ($\omega_{ir}$) frequency at which $S_{cl}(\omega)$ rolls over and becomes a constant $S_{cl}(0)$. Hence the asymptotic behaviors of $\Gamma_{G}(t)$ are

$$\Gamma_{G}(t) \approx \begin{cases} t^2 \int_{0}^{\omega_{uv}} S_{cl}(\omega) \, d\omega, & t \ll 1/\omega_{uv} \\ t S_{cl}(0), & t \gg 1/\omega_{ir}. \end{cases}$$

(63)

There is an initial quadratic decrease of the signal and pure exponential behavior at very long times.

It is now of interest to compare $\Gamma_{G}(t)$ with the exact $\Gamma(t)$ for some interesting distributions $p(g, \gamma)$. For a single fluctuator, we have

$$S_{cl}(\omega) = \frac{2}{\pi} \frac{g^2}{4\gamma^2 + \omega^2}$$

(64)

so that the Gaussian approximation is

$$\Gamma_{G}(t) = \frac{2g^2t^2}{2\pi} \int_{-\infty}^{\infty} \frac{\gamma \sin^2 \omega t/2}{4\gamma^2 + \omega^2 (\omega t/2)^2} \, d\omega$$

$$= \frac{g^2}{4\gamma^4} \left( e^{-2\gamma t} + 2\gamma t - 1 \right).$$

(65)

(66)

Our results may now be compared with Redfield theory and the Gaussian approximation (Eqs. 29). We give the decay function $\exp[-\Gamma(t)]$ in Fig. 2 and 3. For weak coupling $g < \gamma$ [Fig. 2] Redfield theory works except at short times $t \ll 1/\gamma$, while the Gaussian approximation is excellent at all times. For strong coupling $g > \gamma$ the situation is more complicated [Fig. 3]. The exact solution develops oscillations that are not present in the approximate solution. Again, Redfield theory is poor at short times, while the Gaussian approximation is very good at these times, as already noted by other authors [22]. At longer times both approximate solutions have little resemblance to the exact solution. We summarize the situation in Fig. 4. The areas of agreement (to within 1%) are given by the white regions. Notice
FIG. 3: (Color online) Envelope of the free induction decay signal $\exp[-\Gamma(t)]$ for strong coupling: $g=0.01, \gamma = 0.002$. The exact result is given by the blue solid line, Gaussian approximation by the green dashed line and the Redfield approximation by the red dashed line. The inset gives the short-time behavior.

that the normalization is relative to the initial value of the signal. At long times, the ratio of the exact results and the Gaussian approximation can be much different from unity; however, the absolute value of the signal is small and may be difficult to observe. It is interesting to note that the discrepancy between the approximate theory and exact theory is oscillatory and is not well characterized as a "plateau". This phenomenon is more closely analyzed in Ref. [23].

V. CONCLUSIONS

We have given a general formalism for the dissipative dynamics of an arbitrary quantum system in the presence of a classical stochastic process. It is applicable to a very wide range of physical systems. This method has several virtues. It is linear, and the close analogy to Hamiltonian systems opens up a toolbox of well-developed methods such as perturbation theory and mean-field theory. We applied the method to the problem of a single qubit in the presence of TLS that give rise to pure dephasing $1/f$ noise and solved this problem exactly. This has been done before by the method of stochastic differential equations [18]. However, that method depends on a non-linear parameterization of the density matrix that is difficult to generalize. We anticipate that the method can be applied to other quantum systems, such as an array of qubits, and also other kinds of noise.

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FIG. 4: (Color online) Region of validity for Redfield and Gaussian approximations. Envelope function exp[−Γ(t)] calculated from Gaussian and Redfield approximates are compared with the exact envelope. For this figure, we set γ = 1. In the green and yellow region, the error of Gaussian approximation is smaller than 0.01. In the red and yellow region, the error of Redfield approximation is smaller than 0.01. The blue solid line is where the exact envelope dies off (smaller than 0.01). The green and yellow islands are due to the fact that both approximations die off much faster than the exact solution and the exact solution crosses zero many times, as seen in Fig. 3. Note in Fig. 3, there will be 4 islands for Gaussian approximation and 5 islands for Redfield approximation. The red spike in the middle is due to the fact that the envelope calculated from Gaussian approximation crosses the exact envelope. The yellow island on top is due to the fact that both approximations die off much faster than the exact solution and the exact solution crosses zero multiple times, as seen in Fig. 3. Note in Fig. 3, there will be 4 islands for Gaussian approximation and 5 islands for Redfield approximation. The blue boundary has zigzag shape in the strong coupling region. This is due to the oscillations of the exact envelope in the strong coupling region.

APPENDIX A: PROPERTIES OF $T$ AND $\overline{T}$

In this appendix we derive two properties of $T_{ij}$.

1. $T$ is a real matrix. This is shown as follows.

$$T_{ij}^* = \frac{1}{2} \text{Tr} \sigma_i^* U^* \sigma_j^* (U^\dagger)^*$$

$$= \frac{1}{2} \text{Tr} \sigma_i^T (U^{-1})^T \sigma_j^T U^T$$

$$= \frac{1}{2} \text{Tr} U \sigma_j U^{-1} \sigma_i$$

$$= \frac{1}{2} \text{Tr} \sigma_i U \sigma_j U^\dagger$$

$$= T_{ij}$$

2. $T$ is an orthogonal matrix. This is proved most simply by noting that the set of $2 \times 2$ Hermitian traceless matrices $A_i$ form a 3-dimensional real Hilbert space with inner product $\langle A_i, A_j \rangle = \frac{1}{2} \text{Tr}(A_i A_j)$. The $\sigma_i$ are a complete
orthonormal basis for this space. Here is the proof.

\[ T_{ij}T_{kj} = \frac{1}{4} \text{Tr} \left( \sigma_i U \sigma_j U^\dagger \right) \text{Tr} \left( \sigma_k U \sigma_j U^\dagger \right) \]

\[ = \frac{1}{2} \text{Tr} \left( U^\dagger \sigma_i U \sigma_j \right) \times \frac{1}{2} \text{Tr} \left( U^\dagger \sigma_k U \sigma_j \right) \]

\[ = \left( U^\dagger \sigma_i U, \sigma_j \right) \left( U^\dagger \sigma_k U, \sigma_j \right) \]

\[ = \frac{1}{2} \text{Tr} \left( U^\dagger \sigma_i U U^\dagger \sigma_k U \right) \]

\[ = \frac{1}{2} \text{Tr} \left( \sigma_i \sigma_k \right) \]

\[ = \delta_{ik}. \]

The averaged quantity \( \overline{T_{ij}}(t) \) is real since the averaging is over real weights, but \( \overline{T_{ij}}(t) \) is orthogonal only in trivial cases.

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