Decoherence by a nonlinear environment: canonical vs. microcanonical case

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Abstract

We compare decoherence induced in a simple quantum system (qubit) for two different initial states of the environment: canonical (fixed temperature) and microcanonical (fixed energy), for the general case of a fully interacting oscillator environment. We find that even a relatively compact oscillator bath (with the effective number of degrees of freedom of order 10), initially in a microcanonical state, will typically cause decoherence almost indistinguishable from that by a macroscopic, thermal environment, except possibly at singularities of the environment’s specific heat (critical points). In the latter case, the precise magnitude of the difference between the canonical and microcanonical results depends on the critical behavior of the dissipative coefficient, characterizing the interaction of the qubit with the environment.
I. INTRODUCTION

Recent years have seen significant experimental advances in manipulation of quantum states in a variety of physical systems \[1\textbf{--}5\]. In addition to the intrinsic interest that these experiments have with regard to the fundamentals of quantum mechanics, they suggest that a high degree of control and coherence in simple quantum systems can be achieved, perhaps eventually sufficient to implement a useful quantum computation \[6\] in an assembly of such individual units (qubits).

Unlike a classical computer, in which the only source of errors is uncontrolled transitions between the states, a quantum computation is sensitive also to random changes in phases of the basis states. Such changes occur due to interaction of the qubit with the environment. They are referred to as decoherence, and the time scale over which the phase will drift by an amount of order one is referred to as decoherence time \(t_d\). It is advantageous to make \(t_d\) or, more precisely, the ratio \(t_d/t_s\), where \(t_s\) is the switching time, as large as possible.

In many cases, the basic operations on qubits (quantum gates) can be approximated as evolution of certain two-level systems under an external influence (a pulse of voltage, current, etc.). In this paper, we concentrate on cases when the environment is comprised by interacting oscillators, described for brevity by a single real scalar field \(\phi\), and the interaction of the two-level system with the environment is linear, with the Hamiltonian of the form \(\[1\]

\[H_J(t) = -\int d^3x J(x, t) \phi(x, t) \] .

In addition to \(H_J\), the Hamiltonian of the environment contains the free Hamiltonian \(H_0\) and a Hamiltonian \(H_{\text{int}}\), the latter describing nonlinear interactions among the oscillators themselves. Our method is sufficiently general to include fully interacting oscillator environments, i.e. any reasonable form of \(H_{\text{int}}\). One motivation for doing so is the possibility to consider environments that are near phase transitions (or the vestiges of such in finite systems).

The “current” \(J(x, t)\) depends on the state of the two-level system and represents its switching history.\[2\] This current, of course, does not have to be the usual electric current, although it may coincide with it in some specific cases of interactions. For example, in a persistent current qubit \[7\], where the basis states differ by the value of the electric current, \(J\) can indeed be interpreted as the current density, and \(\phi\) as a component of the electromagnetic field.

An important example, where \([1]\) applies but \(J\) is unrelated to electric current, is the swap gate based on two coupled quantum dots \[8\]. Key features of this gate are as follows. There is an electronic spin \(1/2\) associated with each dot. These spins are coupled to each other through an exchange interaction, and the interaction Hamiltonian is given by the

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1Bilinear and higher-order couplings in \(\phi\) can be studied in a similar way.

2We use word “switching” to denote a controlled transition between states of a qubit, and not a switching on and off the interaction with the bath. The latter interaction in general cannot be switched off at will; see, however, remarks on the swap gate in the next paragraph.
energy of the singlet-triplet splitting. The exchange interaction can be switched on and off by varying the potential barrier between the dots; the latter is controlled by gate voltage \( v \), which can be viewed as a sum of some average voltage \( \bar{v} \) and a fluctuation \( \delta v \). Then, the singlet-triplet splitting energy can be written as

\[
E_{T-S}(v) \approx E_{T-S}(\bar{v}) + \frac{\partial E_{T-S}}{\partial v} \delta v.
\]  

(2)

The first term contributes to the Hamiltonian of the qubit, while the second term describes the interaction of the qubit with the environment. We see that this second term is precisely of the form \( (\square) \), with \( -\partial E_{T-S}/\partial v \) playing the role of the “current”, and \( \delta v \) the role of the environment. For the case when fluctuations of \( v \) are the usual thermal (Nyquist) fluctuations, decoherence induced by \( \delta v \) was considered previously in ref. \([9]\).

The splitting energy \( E_{T-S} \) is substantial only during a pulse of voltage that temporarily lowers the potential barrier. Thus, the duration of the pulse is the switching time of the gate. From \( (\square) \), we see that in this particular case the duration of the pulse also determines the duration of the interaction between the qubit and the environment.

Whenever \( (\square) \) applies, the evolution of the field \( \phi \) from a known initial state is completely determined by the current \( J(x,t) \), i.e. the switching history. In other words, the gate in this case works as an antenna, producing a definite “radiation” state of \( \phi \). (Again, this “radiation” does not have to be an electromagnetic wave, but can be any kind of propagating excitation.) Decoherence can be associated with the probability to emit or absorb a nonzero number of quanta of \( \phi \).

Typically, the initial state of \( \phi \) is taken to be a thermal state, with probabilities of different energy levels given by the canonical distribution at some temperature \( T \). In this paper, we want to deviate from this practice and consider a microcanonical initial state, in which the oscillators are constrained to have their total energy equal to some \( E \). There are several reasons why we think that this problem is interesting and potentially important for analysis of various qubit designs.

First, in thermodynamics we are accustomed to canonical and microcanonical ensembles being essentially equivalent in the macroscopic limit. It is interesting to see if, and to what accuracy, the same applies to calculations of quantum coherence, which is an intrinsically time-dependent quantity.

Second, some of the environments important for current qubit designs are in fact comprised by relatively few degrees of freedom. Consider, for example, the swap gate described by eq. \( (\square) \), and suppose that the pulse of voltage is delivered to the gate via a transmission line. Suppose further that the line is open at one end (where it attaches to the gate) and closed at the other (and the pulse is obtained, say, through inductive coupling of the line to some control circuit). For a line of length \( L \), the number of modes significantly populated at temperature \( T \) is of order

\[ 3 \]

The current \( J \) will be set to zero at the initial moment, which can always be done by a time-independent redefinition of \( \phi \). This makes choosing a microcanonical initial state for the bath equivalent to choosing it for the entire qubit+bath system.
For $L = 1\,\text{m}$ and $T = 0.1\,\text{K}$, we obtain $N_{\text{eff}} \sim 10$. At this point, it is actually not obvious that this $N_{\text{eff}}$, i.e. the number of populated modes, is what controls the transition to the thermodynamic limit. However, later in the paper we show that this is indeed the case.

Now, although an ensemble of identical oscillators baths contained in identical experimental apparatus may be well described by a thermal density matrix, in each individual experiment the bath initially has nearly fixed energy, with some broadening due to the initial state’s preparation. If the broadening is larger than the level spacing of the bath but smaller than the typical energy fluctuation in a thermal state, the microcanonical initial state is a better approximation than the canonical one. Because the level spacing decreases exponentially with the size of the bath, while relative thermal fluctuations only go as inverse square root of $N_{\text{eff}}$, we expect that such a situation will in fact be typical for relatively small, “mesoscopic” environments. In this case, one may wonder how much the microcanonical decoherence, induced by the interaction of the qubit with the bath, differs from the thermal (canonical) result. In particular, one of the main goals of our project was to see if such a small environment can cause any significant decoherence at all.

Finally, because decoherence is associated with the response of the environment to changes in the system, one may expect that anomalously large deviations from the thermal result will occur when fluctuations in the environment are large and the relaxation is slow, e.g. near a critical point. Our calculation lends some support to this idea.

Our main results are as follows. (i) If, for a microcanonical state of energy $E$, we formally define temperature $T$ by the usual thermodynamic formula, then the expansion parameter that controls the difference between the canonical and microcanonical results for decoherence is $1/N_{\text{eff}}$, where by definition $N_{\text{eff}} = E/k_B T$. For a one-dimensional transmission line, this is of the same order as eq. (3). (ii) We consider an expansion of microcanonical decoherence in powers of $1/N_{\text{eff}}$ and find that the leading difference between the canonical and microcanonical results is formally of order $1/N_{\text{eff}}$. We present both a general formula for this correction, applicable for any nonlinear environment, and an explicit formula for an environment with Ohmic dissipation. In particular, for the case of a transmission line we find that already for $N_{\text{eff}} \sim 10$ the environment causes significant decoherence, which is practically indistinguishable from the thermal result. (iii) The $1/N_{\text{eff}}$ correction contains a term proportional to the derivative of the heat capacity of the environment with respect to the temperature, $\partial C_V/\partial T$, which becomes singular near a critical point. Although in a finite system there can be no “true” critical singularity, a finite enhancement of $\partial C_V/\partial T$ remains. It is significant in this respect that our results apply to the general case of a fully nonlinear environment, rather than to a collection of harmonic oscillators, for which no critical phenomena are expected. A simple application of finite-size scaling shows that the critical singularity of $\partial C_V/\partial T$ alone cannot completely cancel the $1/N_{\text{eff}}$ suppression factor (although it can reduce the suppression considerably). However, the correction also depends on the dissipative coefficient, characterizing the interactions of the qubit with the environment, and it is ultimately the critical behavior of this coefficient that determines both the size and the sign of the correction at a critical point.

In summary, while our results are somewhat inconclusive on the critical behavior of decoherence (due to the lack of understanding of the critical behavior of the dissipative coeffi-
cient), we obtain a clear demonstration that away from criticality even a relatively compact, “mesoscopic” bath of oscillators, initially in a microcanonical state, induces decoherence of practically the same magnitude as a truly macroscopic, thermal environment.

In the course of the evolution, the qubit and the bath exchange energy, as described by the interaction Hamiltonian (I). Moreover, because the qubit itself is controlled by some external means, even the compound qubit+bath system is not strictly isolated (except at times before and after the switching). We assume, however, that there is no additional, “direct” interaction of the bath with the outside world. This seems to us a reasonable assumption, since in most cases one will want to isolate the qubit and its immediate surroundings from the larger room-temperature environment.

Our work, then, has some elements in common with the earlier work of Jensen and Shankar [10] on a strictly isolated small system. These authors have observed statistical behavior in a numerical solution of the Schrödinger equation for seven interacting spins. In particular, they have found that the distribution of probabilities for one spin in their system closely resembles the canonical distribution expected if the full spin chain were in a microcanonical state. In the present context, the selected spin plays the role of the qubit (albeit not subject to any external control), while the remaining spins play the role of the bath.

Apart from the question of perfect versus imperfect isolation of the compound qubit+bath system, the main difference between the work of ref. [10] and ours is that [10] compares results for a pure initial state to those for a microcanonical ensemble, for a compound system, while we are interested in comparing results between canonical and microcanonical initial states for such a system. As we will see, that latter comparison can be done, for a rather general case, without a recourse to numerical integrations. Instead, our calculation makes use of a steepest-descent evaluation of an integral relating the canonical and microcanonical averages, the accuracy of this procedure being again controlled by $1/N_{\text{eff}}$.

The paper is organized as follows. In Sect. 2 we present the definition of coherence as a functional of the switching history, the latter being represented by the current in (I). We discuss a suitable form of the current. Although our main results are not based on a perturbative expansion of coherence, we pause in Sect. 3 to describe a convenient way to perform such an expansion, based on the coherent-state formalism. In Sect. 4, we compute coherence, as defined in Sect. 2, for a thermal initial state and recover some familiar expressions. In Sect. 5, we construct the density matrix for a microcanonical initial state. In Sect. 6, we compute microcanonical decoherence. Sect. 7 is a conclusion.

In what follows we use the system of units with $\hbar = 1$ and $k_B = 1$.

II. DEFINITION OF COHERENCE

If we know that at some initial time $t = 0$, the environment started out in a definite quantum state $|\Psi(0)\rangle$, we can define coherence remaining in the qubit at arbitrary time $t$ in the following way. Find the final state of the environment using the evolution operator $U_J(t, 0)$, where the “current” $J$ represents the switching history of the qubit. Coherence equals the overlap of that final with the state that would obtain if no switching took place:
\[ C(t) = \langle \Psi(0)|U^\dagger_J(t,0)U_J(t,0)|\Psi(0) \rangle . \] (4)

A decrease of the overlap with time (decoherence) is due to the divergence of the evolution histories of the environment corresponding to different histories of the qubit. It therefore reflects the measuring influence that the environment had on the qubit.

An obvious extension of this definition to the case when the state at \( t = 0 \) is a mixed state with a density matrix \( \rho(0) \) is

\[ C(t) = \text{Tr} \left[ U_J(t,0)\rho(0)U^\dagger_J(t,0) \right] . \] (5)

It is convenient to incorporate the moments of time 0 and \( t \) in the definition of the current. To save notation, we describe the environment by a single real scalar \( \phi(x, t) \) with real-valued oscillator modes \( \psi_n \):

\[ \phi(x, t) = \sum_n \phi_n(t)\psi_n(x) \] (6)

(generalizations are of course possible). We assume that each mode couples to some smooth \( J_n(\tau) \), which is zero at \( \tau < 0 \), switches on at \( \tau \approx 0 \), stays on a plateau until \( \tau \approx t \), and then switches off, see Fig. 1. Thus, the Lagrangian of the field is

\[ L = \sum_n \left\{ \frac{1}{2}\dot{\phi}_n^2 - \frac{1}{2}\omega_n^2\phi_n^2 + J_n\phi_n \right\} + L_{\text{int}}[\phi] , \] (7)

where \( L_{\text{int}} \) describes a self-interaction.

![FIG. 1. Profile of the current \( J_n \) representing the switching history of the qubit.](image)

The above form of the current can describe either of the following two experimental setups. For the swap gate described by the Hamiltonian (2), the profile shown in Fig. 1 represents a single gate operation: both the initial and final states of the qubit correspond to \( J_n = 0 \). So, the switching time of the qubit is the entire time \( t \). On the other hand, if one basis state of the qubit corresponds to \( J_n = 0 \), and another to the plateau value \( J_n = A_n \), then the current of Fig. 1 represents two switching operations: from the first state to the second and back. In this case, the switching time is the ramp time of the current, \( \tau_r \).  

\[ ^4 \text{And coherence defined by (5) coincides in this case with what is perhaps a more familiar definition: the value at time } t \text{ of the off-diagonal element of the qubit’s density matrix, relative to its value at } t = 0; \omega_r = 2\pi/\tau_r \text{ acts as a frequency cutoff.} \]
For this form of the current, we can relate \( \rho(0) \) to the density matrix at some \( T_i < 0 \) in the distant past as

\[
\rho(0) = U_J(0, T_i) \rho(T_i) U_J^\dagger(0, T_i)
\]

(since at \( t < 0 \) \( U_J \) and \( U_0 \) coincide) and also extend \( t \) in (5) to some \( T_f \) in the distant future. In this way, we obtain coherence as a functional of \( J_n(\tau) \):

\[
C[J] = \text{Tr} \left[ U_J(T_f, T_i) \rho(T_i) U_J^\dagger(T_f, T_i) \right].
\]

Further, using the environment’s \( S \)-matrix

\[
S_J = e^{iH_{\text{free}} T_f} U_J(T_f, T_i) e^{-iH_{\text{free}} T_i},
\]

where \( H_{\text{free}} \) is the Hamiltonian in the absence of self-interactions (and interaction with the system), we can rewrite (8) as

\[
C[J] = \text{Tr} \left[ S_J \rho_i S_0^\dagger \right],
\]

where

\[
\rho_i = e^{iH_{\text{free}} T_i} \rho(T_i) e^{-iH_{\text{free}} T_i}.
\]

Under the usual assumption of adiabatic switching on of the interaction in the distant past, \( \rho_i \) is independent of \( T_i \). Thus, specifying it is a convenient way to impose initial conditions.

Eq. (11) is the definition of coherence that we use in what follows. We observe that coherence defined in this way coincides with the generating functional of the Green functions corresponding to the state \( \rho_i \). In perturbation theory, it can be computed order by order with the help of the Schwinger-Keldysh diagram technique.

If we are to have small decoherence, it is natural to assume that the currents \( J_n \) are weak. Then, provided that the field \( \phi \) does not have a nontrivial expectation value, the leading term in \( Q[J] = -\ln C[J] \) is bilinear in \( J \):

\[
Q[J] = -\frac{i}{2} \sum_{mn} \int dt dt' J_m(t) \Delta_{mn}(t, t') J_n(t') + O(J^3),
\]

where \( \Delta_{mn} \) is the full (connected) Green function of \( \phi \) in the state \( \rho_i \):

\[
\Delta_{mn}(t, t') = i \text{Tr} \left\{ S_0^\dagger T_0 [\phi_I^\dagger_m(t) \phi_I^n(t') S_0(x, y)] \rho_i(x, y) \right\};
\]

\( \phi_I^\dagger \) is the field operator in the interaction representation. The real part of \( Q \), related to the imaginary part of \( \Delta \), determines the exponential suppression of coherence due to switching and can be called the decoherence exponent.

For specific calculations, we will use the following expression for the Fourier transform of the current:

\[
\tilde{J}_n(\Omega) = \frac{A_n}{i\Omega} \left( e^{i\Omega t} - 1 \right) \exp(-|\Omega|/2\omega_r),
\]

where \( \omega_r = 2\pi/\tau_r \), and \( A_n \) are real constants. In the limit \( \omega_r \to \infty \), eq. (15) becomes the Fourier transform of a rectangular pulse: \( J_n(\tau) = A_n \) for \( 0 < \tau < t \) and zero otherwise.
III. PERTURBATIVE EXPANSION

Although our main results are not based on a perturbative expansion, we pause here to outline a convenient way to carry it out.

As we have seen, coherence naturally acquires an exponential form. So, it is convenient to compute (11) in a representation in which the trace reduces to a saddle-point integral: such integrals produce exponentials automatically. A good choice is the coherent-state (holomorphic) representation [11,12], which we now review. (For a scattering problem with a large but not macroscopic number of particles and microcanonical initial conditions, the coherent state representation was used in ref. [13].)

Any state of the environment can be represented by an anti-analytical function $\psi(a^*)$ of the complex variable $a$ labeling the coherent states. Action of an arbitrary operator $\hat{A}$ is represented by an integral of the form

$$ (\hat{A}\psi)(b^*) = \int \frac{da^* da}{2\pi i} e^{-a^* a} A(b^*, a) \psi(a^*) , $$

(16)

where $A(b^*, a)$ is the kernel of the operator $\hat{A}$ defined by

$$ A(b^*, a) = \langle b | \hat{A} | a \rangle . $$

(17)

A product of two operators is represented by the convolution of their kernels:

$$ (\hat{A}_1 \hat{A}_2)(b^*, b) = \int \frac{da^* da}{2\pi i} e^{-a^* a} A_1(b^*, a) A_2(a^*, b) . $$

(18)

The $S$-matrix is given by [11–13]

$$ S_J(b^*, a) = \langle b | S_J | a \rangle = \int d\phi_id\phi_f D\phi e^{B_i+B_f+i\int L dt} , $$

(19)

which contains a functional integral over the field $\phi$ as well as ordinary integrals over the field’s boundary values $\phi_{i,n}$ and $\phi_{f,n}$. The boundary terms $B_i$ and $B_f$ read

$$ B_i = \sum_n \left[ -\frac{1}{2}a_n^2 e^{-2i\omega_n T_i} - \frac{1}{2}\omega_n \phi_{i,n}^2 + \sqrt{2\omega_n} a_n \phi_{i,n} e^{-i\omega_n T_i} \right] , $$

(20)

$$ B_f = \sum_n \left[ -\frac{1}{2}(b_n^*)^2 e^{2i\omega_n T_f} - \frac{1}{2}\omega_n \phi_{f,n}^2 + \sqrt{2\omega_n} b_n^* \phi_{f,n} e^{i\omega_n T_i} \right] . $$

(21)

The perturbation expansion for $S_J$ is generated in the usual way via the relation (see e.g. ref. [12])

$$ S_J = \exp[i \int L_{int}(\delta / i\delta J) dt] S'_{J} , $$

(22)

where

$$ S'_{J} = \int d\phi_id\phi_f D\phi e^{B_i+B_f+i\int (L_{free}+J\phi) dt} , $$

(23)

and $L_{free}$ is the Lagrangian of free oscillators.
The integrals in (23) are Gaussian and can be evaluated exactly at the corresponding saddle points. The saddle-point equation for $\phi_n(t)$ is simply the equation of motion
\begin{equation}
\dddot{\phi}_n + \omega_n^2 \phi_n = J_n(t),
\end{equation}
while the saddle-point equations for $\phi_i$ and $\phi_f$ supply the boundary conditions
\begin{align}
\omega_n \phi_{i,n} + i \dot{\phi}_{i,n} &= \sqrt{2\omega_n} e^{-i\omega_n T_i} \alpha_n, \\
\omega_n \phi_{f,n} - i \dot{\phi}_{f,n} &= \sqrt{2\omega_n} e^{i\omega_n T_f} \beta_n. 
\end{align}
The solution to (24) with these boundary conditions is
\begin{equation}
\phi_n(t) = \frac{1}{\sqrt{2\omega_n}} [a_n e^{-i\omega_n t} + b_n^* e^{i\omega_n t}] + \int dt' G_n(t, t') J_n(t')
\end{equation}
where $G_n$ is the free causal Green function
\begin{equation}
G_n(t, t') = \frac{i}{2\omega_n} e^{-i\omega_n |t-t'|}.
\end{equation}
Substituting the saddle-point solution (27) into (19), we obtain (cf. ref. [12])
\begin{align}
S'_{J}(b^*, a) &= \exp \sum_n \left\{ a_n b_n^* + \frac{i}{\sqrt{2\omega_n}} \int dt J_n(t) [a_n e^{-i\omega_n t} + b_n^* e^{i\omega_n t}] \\
&+ \frac{i}{2} \int dt dt' J_n(t) G_n(t, t') J_n(t') \right\}.
\end{align}
This can be conveniently rewritten in terms of Fourier transforms of $J_n$ and $G_n$, defined as
\begin{align}
\tilde{J}_n(\Omega) &= \int_{-\infty}^{\infty} J_n(\tau) e^{i\Omega \tau} d\tau, \\
\tilde{G}_n(\Omega) &= \int_{-\infty}^{\infty} G_n(\tau) e^{i\Omega \tau} d\tau.
\end{align}
We obtain
\begin{align}
S'_{J}(b^*, a) &= \exp \sum_n \left\{ a_n b_n^* + \frac{i}{\sqrt{2\omega_n}} [\tilde{J}_n^*(\omega_n) a_n + \tilde{J}_n(\omega_n) b_n^*] + \frac{i}{2} \int \frac{d\Omega}{2\pi} \tilde{G}_n(\Omega) |\tilde{J}_n(\Omega)|^2 \right\}.
\end{align}
This can be used in eq. (22) to produce a perturbative expansion for the $S$-matrix.

IV. THERMAL DECOHERENCE

Returning to our definition of coherence, eq. (11), we see that in the absence of self-interaction we would have $S_0 = 1$ and $S_J = S'_J$, so that
\begin{equation}
C[J] = \text{Tr} [S'_J \rho_i] = \int \frac{da^* da db^* db}{2\pi i} e^{-a^* a - b^* b} \rho_i(a^*, b) S'_J(b^*, a).
\end{equation}
In particular, for a thermal initial state with inverse temperature $\beta$,
\begin{equation}
\rho_i(a^*, b) = \prod_n \left( 1 - e^{-\beta \omega_n} \right) \exp \left( a_n^* b_n e^{-\beta \omega_n} \right) .
\end{equation}

In this case, the integrals in (33) are Gaussian and can be evaluated explicitly. We obtain
\begin{equation}
C[J] = \exp(-Q[J])
\end{equation}
with
\begin{equation}
Q[J] = \sum_n \left\{ \frac{|\tilde{J}_n(\omega_n)|^2}{4\omega_n} [2n_B(\omega_n) + 1] - \frac{i}{2} \int d\Omega \frac{|\tilde{J}_n(\Omega)|^2}{2\pi} \text{Re} \tilde{G}_n(\Omega) \right\} ,
\end{equation}
where \( n_B(\omega) = [\exp(\beta \omega) - 1]^{-1} \) is the Bose distribution. Eq. (35) is the noninteracting limit of the more general eq. (13).

For an interacting environment, (34) is still the correct initial condition for a thermal state, because the interaction is assumed absent in the distant past (and the interacting state is obtained by an adiabatic switching on of the interaction, while maintaining the fixed temperature \( 1/\beta \)). In the limit of small \( J \), we now use eq. (13), according to which the real and imaginary parts of \( Q \) are determined, respectively, by the anti-Hermitean and Hermitean parts of \( \Delta_{mn}(\Omega) \) (the Fourier transform of \( \Delta_{mn} \)). The anti-Hermitean part (which itself is an Hermitean matrix)
\begin{equation}
\Delta''_{mn}(\Omega) = \frac{1}{2i} \left[ \tilde{\Delta}_{mn}(\Omega) - \tilde{\Delta}_{nm}^*(\Omega) \right]
\end{equation}
can be expressed through the spectral density of the environment \( D_{mn} \) in the corresponding channel: at \( \omega > 0 \),
\begin{equation}
\Delta''_{mn}(\omega) = \Delta''_{mn}(-\omega) = \frac{\pi}{2\omega} D_{mn}(\omega) \coth(\beta \omega/2) .
\end{equation}
\( D_{mn} \) includes effects of the self-interaction.

The real part of \( Q \) (the decoherence exponent) becomes
\begin{equation}
Q_R[J] = \sum_{mn} \int_0^\infty d\omega \frac{\omega}{4\omega} J_m^*(\omega) D_{mn}(\omega) J_n(\omega) \coth(\beta \omega/2) .
\end{equation}
The imaginary part is given by
\begin{equation}
Q_I[J] = -\frac{1}{2} \sum_{mn} \int_{-\infty}^\infty \frac{d\Omega}{2\pi} \tilde{J}_m^*(\Omega) \Delta'_{mn}(\Omega) J_n(\Omega) ,
\end{equation}
where the Hermitean part \( \Delta'_{mn}(\Omega) \) can be expressed through the spectral density \( D_{mn} \) via a dispersion relation:
\begin{equation}
\Delta'_{mn}(\Omega) = P \int_0^\infty \frac{d\omega}{2\omega} \left[ \frac{D_{mn}(\omega)}{\omega - \Omega} + \frac{D_{nm}(\omega)}{\omega + \Omega} \right] ;
\end{equation}
\( P \) denotes the principal value.

For a current of the form (14), we can introduce also another kind of spectral density, which takes into account the interaction of \( \phi \) with the current:
\begin{equation}
F(\omega) = \frac{\pi}{2\omega} \sum_{mn} A_mA_n D_{mn}(\omega) .
\end{equation}
We can now rewrite the decoherence exponent as

$$Q_R(t) = \frac{1}{\pi} \int_{0}^{\infty} \frac{d\omega}{\omega^2} F(\omega)[1 - \cos \omega t] e^{-\omega/\omega_r} \coth(\beta \omega/2).$$

This is, of course, a familiar expression for thermal decoherence, although it is usually discussed for an environment comprised by harmonic oscillators. Here, we obtain it for the fully nonlinear case.

For Ohmic dissipation, when

$$F(\omega) = \eta \omega,$$

the integral in (42) coincides with an integral computed by Chakravarty and Leggett [14], so we can use their result to obtain an explicit functional form of $Q_R(t)$:

$$Q_R(t) = \frac{\eta}{2\pi} \ln(1 + \omega_r^2 t^2) + \frac{\eta}{\pi} \ln \left[ \frac{\beta}{\pi t} \sinh \left( \frac{\pi t}{\beta} \right) \right].$$

One should keep in mind, though, that despite this formal similarity, the macroscopic quantum coherence (MQC) problem, considered in ref. [14], is different from ours. In the MQC case, transitions between basis states occur spontaneously, while in a quantum gate they are externally induced. In particular, the cutoff frequency $\omega_r$ in our case in general depends on the switching method. We also reiterate that in our treatment, the Ohmic form (43) refers to a fully interacting environment, rather than to a collection of harmonic oscillators. So, for example, the dissipative coefficient $\eta$ can now depend on temperature.

**V. MICROCANONICAL DENSITY MATRIX**

In the operator language, the microcanonical density matrix for energy $E$ can be written as (cf. ref. [13])

$$\hat{\rho} = \mathcal{N}^{-1} \delta(\hat{H} - E) = \frac{\mathcal{N}^{-1}}{2\pi} \int_{C} d\xi \exp[i\xi(\hat{H} - E)],$$

where $\hat{H}$ is the Hamiltonian of $\phi$, and $\mathcal{N}$ is a normalization factor. The contour $C$ runs just above the real axis (as shown in Fig. 2 by a dashed line): a small positive imaginary part of $\xi$ regulates the contribution of states with large eigenvalues of $\hat{H}$.
FIG. 2. The original contour $C$ (dashed line), used in the definition (45) of the microcanonical density matrix, and the deformed contour (solid line), passing through saddle points (circles). Locations of the four saddle points correspond to an environment with an acoustic dispersion law in three spatial dimensions, see eq. (53).

In this section, we calculate $\mathcal{N}$, starting from the normalization condition

$$\text{Tr} \hat{\rho} = \frac{\mathcal{N}^{-1}}{2\pi} \int_{C} d\xi e^{-iE\xi} Z(-i\xi) = 1. \quad (46)$$

Here $Z(-i\xi) = \text{Tr} \exp(i\xi \hat{H})$ is the thermal partition sum analytically continued to a complex inverse temperature $-i\xi$.

The integrand in (46) has a saddle point at $\xi = i\beta$, where $\beta$ is determined by

$$E = -\frac{\partial}{\partial \beta} \ln Z(\beta). \quad (47)$$

Hence, $\beta$ is the inverse temperature related to energy $E$ in the usual thermodynamic fashion. The integration contour can be deformed to pass through the saddle point. Note that it is essential that the contour was originally defined to run above the real axis, as the point $\xi = 0$ is typically an essential singularity of the integrand in (46). Calculation by steepest descent in the vicinity of $\xi = i\beta$ gives

$$\mathcal{N} = \beta (2\pi/C_V)^{1/2} \exp[E\beta + \ln Z(\beta)], \quad (48)$$

where $C_V$ is the field’s heat capacity.$^5$

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$^5$Note that using steepest descent near $\xi = i\beta$ implies $C_V > 0$, the usual condition of thermodynamic stability. It is curious that we have in effect derived this condition without ever referring directly to the second law of thermodynamics, the usual source of such inequalities.
\[ C_V(\beta) = \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z(\beta). \] (49)

For (48) to be a good approximation, two conditions must be satisfied. First, to use the steepest descent, we must have

\[ E\beta \gg 1, \] (50)

and, second, no other saddle point should give a contribution larger than (48). The left-hand side of (50) is our definition of the effective number of degrees of freedom, \( N_{\text{eff}} \). (Recall for comparison that, for a collection of noninteracting classical oscillators at temperature \( T \), \( E/T \) is precisely the number of oscillators). So, (50) is the condition that the environment is relatively macroscopic.

As for the role of other saddle points, it has, strictly speaking, to be checked case by case, i.e. for each specific model of the environment. As an illustration, we include here results for two simple cases: noninteracting (linear) environments with an acoustic dispersion law,

\[ \omega_n = v_s k_n, \] (51)

in three and one spatial dimensions. The first case can correspond for example to phonons, while the second to electromagnetic waves in a one-dimensional transmission line (then, \( v_s \sim c \)).

For linear environments,

\[ \ln Z(-i\xi) = -\sum_n \ln(1 - e^{i\omega_n \xi}). \] (52)

So, in the first case

\[ \ln Z(-i\xi) = -\text{const} \times \frac{iV}{\xi^3} + O(L^2), \] (53)

where the volume of the tree-dimensional region is denoted by \( V \), and its characteristic linear size by \( L \). In the second case,

\[ \ln Z(-i\xi) = \text{const} \times \frac{iL}{\xi} + O(\ln L), \] (54)

where \( L \) is the length of the one-dimensional region. In both (53) and (54), the constants are positive. Note that in the case of a transmission line, the field \( \phi \) is the “prepotential”, related to fluctuations of voltage along the line, \( \delta v(x,t) \), via

\[ \delta v = \frac{1}{\sqrt{C}} \frac{\partial \phi}{\partial t}, \] (55)

where \( C \) is the line capacitance per unit length. So, the correlator of \( \delta v \) at coincident \( x \) will be Ohmic, with the “dissipative coefficient” proportional to the \((\mathcal{L}/C)^{1/2}\) impedance of the line.

We assume that in both cases the environment is relatively macroscopic, so that the finite-size corrections indicated in (53), (54) are negligible. Then, in the case of eq. (53), the integrand of (10) has four saddle-points—at \( \xi = \beta, -\beta, i\beta, \) and \( -i\beta \). The integration contour can be deformed to pass through the first three of these, as shown in Fig. 2, and we find that under condition (50) the main contribution to the integral indeed comes from the vicinity of \( \xi = i\beta \). In the case of eq. (54), there are only two saddle points, at \( \xi = \pm i\beta \), and only the upper one contributes to the integral after deformation of the contour.
VI. MICROCANONICAL DECOHERENCE

Using the definition (11) with \( \rho_i \) given by eq. (45), we obtain microcanonical decoherence in the form

\[
C[J] = N^{-1} \int_C \frac{d\xi}{2\pi} \exp \left\{ -i\xi E + \ln Z(-i\xi) - Q[\xi, J] \right\},
\]

(56)

where \( Q[\xi, J] \) is the thermal decoherence analytically continued to a complex inverse temperature equal to \(-i\xi\). In the limit of small \( J_n \) (weak decoherence), the real and imaginary parts of the thermal \( Q \) are given by (38), (39).

Let us compare the magnitudes of different terms in the exponent of (56) on the saddle point \( \xi = i\beta \) with \( \beta \) determined from (47). The first two terms are macroscopically enhanced: they are proportional to the effective number of degrees of freedom \( N_{\text{eff}} = E\beta \).

(57)

The third term, \(-Q[\xi, J]\), although a sum over \( n, m \), in most cases does not have any macroscopic enhancement, because the couplings \( J_n \) scale as \( 1/\sqrt{N_{\text{eff}}} \), and, while the diagonal entries of \( D_{mn} \) are \( O(1) \), most of the off-diagonal entries are \( O(1/N_{\text{eff}}) \). As a result, to the leading order in \( N_{\text{eff}} \), the microcanonical decoherence coincides with thermal decoherence at inverse temperature \( \beta \), while corrections are formally \( O(1/N_{\text{eff}}) \).

Even though \( Q[i\beta, J] \) is not enhanced by \( N_{\text{eff}} \), in some cases (e.g. for Ohmic dissipation, cf. (44)) it grows with \( t \) (the time for which \( J_n \) is on) and at large \( t \) can in principle become a large correction. However, for applications to qubits, we are interested only in cases when \( Q_R[i\beta, J] \), i.e. decoherence accumulated during time \( t \), is much smaller than one. In these cases, corrections to the thermal result remain formally suppressed by \( 1/N_{\text{eff}} \).

Let us calculate the first of these corrections. The exponent of eq. (58) can be written as

\[
f[\xi, J] = -iE\xi + \ln Z(-i\xi) - Q[\xi, J] \equiv f_0(\xi) - Q[\xi, J].
\]

Here, \( f_0(\xi) = f[\xi, 0] \) has a saddle point at \( \xi = i\beta \), found in the previous section. The corresponding saddle point of the full \( f[\xi, J] \) is shifted to

\[
\xi = i\beta + \delta,
\]

(59)

with a small \( \delta \). Treating \( Q[\xi, J] \) in (58) as a perturbation, we find

\[
\delta = \frac{Q[i\beta, J]}{f_0'(i\beta)},
\]

(60)

where primes denote derivatives with respect to \( \xi \) (so that \( \delta \) is in general complex). Note that \( f_0''(i\beta) = -C_V/\beta^2 \), where \( C_V \propto N_{\text{eff}} \) is the heat capacity given by (49). Therefore, \( \delta = O(1/N_{\text{eff}}) \).

The saddle-point calculation that led to eq. (48) in the previous section is now modified in two ways. First, both the extra term in (58) and the shift of the saddle point contribute to the saddle-point exponent. Second, they also modify the second derivative of \( f \), which determines the preexponent. As a result, to the leading order in \( 1/C_V \), we obtain
\[ C(t) = \left\{ 1 + \frac{1}{2} \frac{\partial}{\partial \beta} \left( \frac{Q_{\beta}}{f_{0,\beta}} \right) \right\} \exp \left\{ -Q[i\beta, J] - \frac{1}{2} \frac{Q_{\beta}^2}{f_{0,\beta}} \right\}, \tag{61} \]

where subscripts following commas are used to denote derivatives with respect to \( \beta \). The correction to the exponent is always negative, since \( f_{0,\beta} = C_V/\beta^2 > 0 \). Note, however, that although the corrections to both the exponent and preexponent are of the same order in \( 1/C_V \), the first is also \( O(Q^2) \), while the second is \( O(Q) \). Thus, in the most interesting to us limit of weak decoherence, the correction to the preexponent is more important.

In fact, for an interacting environment, we are not really allowed to keep the correction in the exponent, since the higher-order terms in \( Q \), due to the self-interaction, can give rise to corrections of the same order, cf. eq. (13). We nevertheless retain this correction in (61) (and in (63) below) because of the traditional interest in linear environments, for which it is the main \( O(Q^2) \) correction.

As an example, let us take a look at eq. (61) for the case of Ohmic dissipation. We specialize further to the large-\( t \) limit, \( t \gg \beta \), so we can use for \( Q_R[i\beta, J] \) the large-\( t \) limit of the thermal expression (44):

\[ Q_R[i\beta, J] = \frac{\eta t}{\beta}, \tag{62} \]

while \( Q_I \), which is not Bose-enhanced, can be neglected. We find

\[ C(t) = \left\{ 1 + \frac{t}{2\beta^2} \frac{\partial}{\partial T} \left( \frac{\eta}{C_V} \right) \right\} \exp \left\{ -\frac{\eta t}{\beta} - \frac{\eta^2 t^2}{2\beta^2 C_V} \right\}, \tag{63} \]

where \( T = 1/\beta \) is the temperature. The correction to the preexponent, which is the main correction in the limit

\[ 1 \ll t/\beta \ll 1/\eta \tag{64} \]

is negative whenever \( C_V/\eta \) is a growing function of \( T \). That is the case, for example, for linear environments with acoustic dispersion laws, such as those considered in the previous section. However, as we discuss in the conclusion, there are interesting cases when \( \partial C_V/\partial T < 0 \), and it is in principle possible to have a positive correction to coherence.

For the transmission line considered in the previous section, \( E \propto T^2 \), so that \( C_V = 2N_{\text{eff}} \propto T \), while \( \eta \) is \( T \)-independent. Then, the preexponent in (63) is equal to \( 1 - \eta t/4\beta N_{\text{eff}} \), which should be compared to \( 1 - \eta t/\beta \), the expansion of the exponent in the limit (64). We see that already for \( N_{\text{eff}} = 10 \), the correction to the thermal result is only 2.5%.

\[ \text{VII. CONCLUSION} \]

Our main result is the calculation of a correction to the thermal result for decoherence, for a system interacting with a nonlinear environment that is initially in a microcanonical (rather than canonical) state. We expect this result to apply when a qubit interacts mainly with a relatively compact, “mesoscopic” environment, whose initial spread in energy is smaller that the typical size of \( 1/\sqrt{N_{\text{eff}}} \) relative fluctuations characteristic of a canonical ensemble.
The correction is given by eq. (61) for the general case, and by eq. (63) for an Ohmic environment. We see that the correction is in general of order $1/N_{\text{eff}}$ and so is typically small already for $N_{\text{eff}} \sim 10$, but it may be enhanced where $\partial C_V/\partial T$ diverges, i.e. in a proximity of a critical point.

Mathematically, the correction to the exponent in (61), (63) results from the shift in the saddle-point value of $\xi$. According to (59), such a shift can be interpreted as a change in the effective temperature of the environment, due to its interaction with the system. In view of its relation (88) to the anti-Hermitean part of the full Green function, the decoherence exponent $Q_R$ (when it is small) can be interpreted as the probability for the system to emit or absorb an excitation quantum, as a result of the current switching from $J_n = 0$ to $J_n = A_n$. Since in a thermal state the emission is more probable than the absorption, it is easy to imagine that the change in the effective temperature will be positive, leading to an increase in decoherence. (The emission probability is proportional to $(n_B + 1)$, and the absorption probability to $n_B$; combined, the two make the $\coth(\beta \omega/2)$ factor in (88).) For example, for Ohmic dissipation in the $t \gg \beta$ limit, we have

$$
\delta = -i \eta t / C_V, \tag{65}
$$

which indeed corresponds to an increase in the effective temperature. We recall, however, that the corresponding increase in decoherence is an $O(Q^2)$ effect, subleading in the limit of weak decoherence.

The correction to the preexponent, which is the leading correction in the weak-decoherence limit, represents a different phenomenon, namely, a change in the typical size of fluctuations in the environment as it interacts with the system. The enhancement of the correction near a critical point reflects the presence of large fluctuations at $T = T_c$. Given that, as a condition of thermodynamic stability, $C_V > 0$, and that it peaks at $T = T_c$, we notice that $\partial C_V / \partial T < 0$ whenever $T$ is sufficiently close to $T_c$ from above. From (61), we see that in this case the term containing $\partial C_V / \partial T$ is positive, i.e. it tends to suppress decoherence.

For an environment of a finite size, the singularity of $C_V$ at $T = T_c$ appears through $C_V^{-1} \partial C_V / \partial T$ scaling as some positive power of the total volume. An application of the standard finite-size scaling techniques [15], together with hyperscaling, gives $C_V \propto L^{d+\alpha/\nu} = L^{2/\nu}$ and

$$
\left. \frac{1}{C_V^2} \frac{\partial C_V}{\partial T} \right|_{T=T_c} \propto L^{-1/\nu}, \tag{66}
$$

where $L$ is the linear size of the volume, $d$ is the number of dimensions, $\alpha$ is the specific-heat exponent, and $\nu$ is the correlation-length one. Since $\nu > 0$, (66) shows that the critical singularity of $\partial C_V / \partial T$ cannot completely overcome the macroscopic suppression (but can reduce it significantly: for comparison, away from the critical point, the left-hand side of (60) scales as $L^{-d}$). However, according to eq. (61), the part of the correction that is proportional to $\partial C_V / \partial T$ is also proportional to the relevant dissipative coefficient, such as $\eta$ in eq. (83). In addition, there is a part of the correction containing the derivative of $\eta$. Thus, it is the scaling of the dissipative coefficient that ultimately determines whether the correction to the thermal result can be large enough to be experimentally observable.
We note that the critical behavior of the dissipative coefficient determines also the leading, thermal part of decoherence near a critical point. As far as we can tell, however, specific results regarding that behavior are not readily obtainable. In particular, these dissipative coefficients are distinct from the usual kinetic coefficients introduced in the dynamical theory \[16\], since they involve a summation over the modes of the environment, cf. eq. \[II\]. Our results, then, can be taken to underscore the importance of a study of these quantities for different types of interacting environments.

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REFERENCES

[1] Y. Nakamura, Yu. A. Pashkin, and J. S. Tsai, Nature 398, 786 (1999).
[2] J. R. Friedman et al., Nature 406, 43 (2000).
[3] C. H. van der Wal et al., Science 290, 773 (2000).
[4] H. Jeong, A. M. Chang, and M. R. Melloch, Science 293, 2221 (2001).
[5] L. M. K. Vandersypen et al., Nature 414, 883 (2001).
[6] D. Deutsch, Proc. R. Soc. Lond. A 400, 97 (1985).
[7] T. P. Orlando et al., Phys. Rev. B 60, 15398 (1999).
[8] D. Loss and D. P. DiVincenzo, Phys. Rev. A 57, 120 (1998).
[9] X. Hu and S. Das Sarma, Phys. Rev. A 61, 062301 (2000).
[10] R. V. Jensen and R. Shankar, Phys. Rev. Lett. 54, 1879 (1985).
[11] F. A. Berezin, The Method of Second Quantization (Nauka, Moscow, 1987) [in Russian]; (Academic Press, New York, 1966).
[12] L. D. Faddeev and A. A. Slavnov, Gauge Fields, Introduction to Quantum Theory (Benjamin/Cummings, Reading, Mass., 1980).
[13] S. Khlebnikov, V. Rubakov, and P. Tinyakov, Nucl. Phys. B367, 334 (1991).
[14] S. Chakravarty and A. J. Leggett, Phys. Rev. Lett. 52, 5 (1984).
[15] Finite Size Scaling and Numerical Simulation of Statistical Systems, edited by V. Privman (World Scientific, Singapore, 1990).
[16] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. 49, 435 (1977).