Quantum many-body theory of qubit decoherence in a finite-size spin bath. II. Ensemble dynamics

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Decoherence of a center spin or qubit in a spin bath is essentially determined by the many-body bath evolution. The bath dynamics can start either from a pure state or, more generally, from a statistical ensemble. In the preceding article [W. Yang and R. B. Liu, Phys. Rev. B **78**, 085315 (2008)], we developed the cluster-correlation expansion (CCE) theory for the so-called single-sample bath dynamics initiated from a factorizable pure state. Here we present the ensemble CCE theory, which is based on similar ideas of the single-sample CCE. The bath evolution is factorized into the product of all possible cluster correlations, each of which accounts for the authentic (nonfactorizable) collective excitation of a group of bath spins and for the finite-time evolution in the qubit decoherence problem. Convergent results can be obtained by truncating the ensemble CCE by keeping cluster correlations up to a certain size. A difference between the ensemble CCE and single-sample CCE is that the mean-field treatment in the latter formalism of the diagonal part of the spin-spin interaction in the bath is not possible in the former case. The ensemble CCE can be applied to nonfactorizable initial states. The ensemble CCE is checked against the exact solution of an *XY* spin bath model. For small spin baths, it is shown that single-sample dynamics is sensitive to the sampling of the initial state from a thermal ensemble and hence very different from the ensemble average.

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I. INTRODUCTION

The dissipative dynamics of a center spin in a spin bath[1] is an old topic in spin-resonance spectroscopy.[2–5] Recently, this subject is revisited[6–24] mostly due to the decoherence issue in quantum information processing.[25–27] Being a most promising candidate for solid-state qubits, electron spins in quantum dots or impurity centers experience decoherence by coupling to complex solid-state environments. A series of theoretical[9–12] and experimental[6–8] works have identified that the dominating decoherence mechanism for electron-spin qubits at low temperatures (such as below a few kelvins) is the entanglement with nuclear spins of the host lattice.[13–21]

When the qubit flip is suppressed (usually by the large Zeeman energy mismatch between qubit and bath spins in a moderate magnetic field), the Hamiltonian for a qubit-bath system has the general form

$$\hat{H} = |+\rangle\hat{H}^{(+)}\langle+| + |-\rangle\hat{H}^{(-)}\langle-|. \tag{1}$$

The bath dynamics is driven by different Hamiltonians $\hat{H}^{(\pm)}$ depending on the qubit states $|\pm\rangle$. For a given initial bath state $|\mathcal{J}\rangle$ (which could be a random sampling from a thermal ensemble), the qubit coherence at time t is characterized by the "single-sample" propagator $\langle\mathcal{J}|e^{i\hat{H}^{(-)}t}e^{-i\hat{H}^{(+)}t}|\mathcal{J}\rangle$. For a thermal ensemble of bath states characterized by a density matrix $\hat{\rho}$, a further ensemble average should be processed and the qubit coherence is given by the ensemble average $\mathrm{Tr}[\hat{\rho}e^{i\hat{H}^{(-)}t}e^{-i\hat{H}^{(+)}t}]$. In general, the key is to evaluate the ensemble-averaged propagator

$$\mathcal{L} = \mathrm{Tr}(\hat{\rho}e^{i\hat{O}^{(1)}}e^{i\hat{O}^{(2)}}\cdots) \tag{2}$$

for a general density matrix $\hat{\rho}$ and arbitrary bath interaction operators $\{\hat{O}^{(j)}\}$. To address this problem, a variety of quantum many-body theories have been developed, including the density-matrix cluster expansion,[13–17] the pair-correlation approximation,[18–20] and the linked-cluster expansion.[22] The pair-correlation approximation provides a clear physical picture for the bath dynamics by keeping only spin-pair correlations. The linked-cluster expansion accurately takes into account higher-order correlations with a Feynman diagram method, which, however, becomes dramatically tedious with increasing the order of diagrams. The density-matrix cluster expansion simplifies the evaluation of higher-order correlations, but it may not converge to the exact results for relatively small baths.[24]

Very recently, we have developed a cluster-correlation expansion (CCE) theory[24] for the evaluation of the single-sample propagator $L_{\mathcal{J}} \equiv \langle\mathcal{J}|e^{i\hat{O}^{(1)}}e^{i\hat{O}^{(2)}}\cdots|\mathcal{J}\rangle$, which is a special case of the ensemble-averaged propagator in Eq. (2). The CCE method provides a simple and accurate method to systematically take into account the high-order correlations. For a temperature T much higher than the bath interaction strength ($\sim 10^{-9}$ K for nuclear spins in GaAs), the initial thermal ensemble can be well approximated as $\hat{\rho} \approx \exp(-\hat{H}_0/k_BT)$, where $\hat{H}_0$ is the noninteracting Hamiltonian containing only the Zeeman energy. Such an initial ensemble is factorizable and a sampling $|\mathcal{J}\rangle$ from the ensemble can be taken as a product state $|\mathcal{J}\rangle = \otimes_n|j_n\rangle$ of all constituent bath spins, where $|j_n\rangle$ denotes the Zeeman energy eigenstate of the nth bath spin. For a large spin bath, previous study[20] has shown that the qubit decoherence is insensitive to the random sampling of the initial bath state from a thermal ensemble since the statistical fluctuation scales with the number of bath spins N as $1/\sqrt{N}$. Thus the ensemble dynamics can be just identified with the single-sample dynamics with a random choice of the initial state.[20] For a relatively small bath, however, the single-sample dynamics could be sensitive to the sampling of the initial state and the ensemble

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average can be very different from any single sample. More importantly, if the initial state of the bath is entangled, i.e.,

$$\hat{\rho} \neq \sum_{\alpha} P_{\alpha} \bigotimes_{i} \hat{\rho}_{\{i\}}^{(\alpha)}, \tag{3}$$

for any choice of probability distribution $\{P_\alpha\}$ and single spin-density matrices $\{\hat{\rho}_{\{i\}}^{(\alpha)}\}$, the single-sample CCE is not applicable. To extend to general ensemble bath dynamics, one could simply use the Monte Carlo simulation with a sufficiently large random sampling of the initial states from the ensemble. The Monte Carlo simulation is practically cumbersome due to the large number of initial states required for a faithful reproduction of the ensemble dynamics and, more importantly, it cannot be applied to nonfactorizable initial states. In this paper we will develop a CCE formalism suitable for direct evaluation of ensemble-averaged bath evolution.

In Sec. II, we will present the ensemble CCE and compare it to the single-sample CCE. In Sec. III, we check the ensemble CCE against the exact solution of a one-dimensional *XY* mode and compare the single-sample CCE and ensemble CCE. Sec. IV gives the conclusions.

II. ENSEMBLE CLUSTER-CORRELATION EXPANSION

A. Example

Let us consider a bath consisting of N spins and evaluate the bath evolution

$$\mathcal{L} \equiv \mathrm{Tr}(\hat{\rho} e^{i\hat{O}}) \tag{4}$$

averaged over a noninteracting (factorizable) ensemble

$$\hat{\rho} = \hat{\rho}_{\{1\}} \otimes \hat{\rho}_{\{2\}} \otimes \cdots \otimes \hat{\rho}_{\{N\}}, \tag{5}$$

where $\hat{\rho}_{\{i\}} = \Sigma_j p_j |j\rangle\langle j|$ is the noninteracting density matrix for the ith spin $\hat{\mathbf{J}}_i$ and

$$\hat{O} \equiv \sum_{n} \alpha_n \hat{J}_n^z + \sum_{m<n} \beta_{m,n} (\hat{J}_m^+ \hat{J}_n^- + \hat{J}_m^- \hat{J}_n^+) \tag{6}$$

is the dimensionless bath interaction operator. Here $\beta_{m,n}$ is the interaction strength between spins m and n. The coefficients $\{\beta_{m,n}\}$ are treated as small quantities. In the absence of interaction ($\{\beta_{m,n}\}=0$), the propagator assumes a factorized form

$$\mathcal{L}|_{\{\beta_{m,n}\}=0} = \mathcal{L}_{\{1\}} \mathcal{L}_{\{2\}} \cdots \mathcal{L}_{\{N\}},$$

where $\mathcal{L}_{\{n\}} \equiv \tilde{\mathcal{L}}_{\{n\}} \equiv \mathrm{Tr}(\hat{\rho}_{\{n\}} e^{i\hat{O}_{\{n\}}})$ and $\hat{O}_{\{n\}} \equiv \alpha_n \hat{J}_n^z$. For $\{\beta_{m,n}\} \neq 0$, we introduce additional factors (cluster correlations) to account for the interaction corrections. These cluster correlations can be introduced successively as follows.

(1) Two-spin correlations $\{\tilde{\mathcal{L}}_{\{i,j\}}\}$. If the bath consists of only two spins with indices $\{i,j\}$, the propagator would be

$$\mathcal{L}_{\{i,j\}} \equiv \mathrm{Tr}(\hat{\rho}_{\{i,j\}} e^{i\hat{O}_{\{i,j\}}}),$$

with $\hat{\rho}_{\{i,j\}} \equiv \hat{\rho}_{\{i\}} \otimes \hat{\rho}_{\{j\}}$ and

$$\hat{O}_{\{i,j\}} \equiv \alpha_i \hat{J}_i^z + \alpha_j \hat{J}_j^z + \beta_{i,j} (\hat{J}_i^+ \hat{J}_j^- + \hat{J}_i^- \hat{J}_i^+),$$

i.e., $\mathcal{L}_{\{i,j\}}$ is obtained from Eq. (4) by dropping all spins except i and j. Without interaction ($\beta_{i,j}=0$), the propagator is

$$\mathcal{L}_{\{i,j\}}|_{\beta_{i,j}=0} = \mathcal{L}_{\{i\}} \mathcal{L}_{\{j\}} = \tilde{\mathcal{L}}_{\{i\}} \tilde{\mathcal{L}}_{\{j\}}.$$

The interaction correction makes the factorization to be $\mathcal{L}_{\{i,j\}} = \tilde{\mathcal{L}}_{\{i\}} \tilde{\mathcal{L}}_{\{j\}} \tilde{\mathcal{L}}_{\{i,j\}}$. Thus the two-spin correlation is defined as

$$\tilde{\mathcal{L}}_{\{i,j\}} \equiv \frac{\mathcal{L}_{\{i,j\}}}{\tilde{\mathcal{L}}_{\{i\}} \tilde{\mathcal{L}}_{\{j\}}}. \tag{7}$$

Obviously, the Taylor expansion of the pair correlation with respect to the interaction strength is

$$\ln \tilde{\mathcal{L}}_{\{i,j\}} = c_1 \beta_{i,j} + c_2 \beta_{ij}^2 + \cdots = O(\beta), \tag{8}$$

where β denotes the typical magnitude of the interaction strength $\{\beta_{m,n}\}$. Thus $\ln \tilde{\mathcal{L}}_{\{i,j\}}$ is at most a first-order small quantity.

(2) Three-spin correlations $\{\tilde{\mathcal{L}}_{\{i,j,k\}}\}$. For a bath of three spins $\{i,j,k\}$, the propagator is

$$\mathcal{L}_{\{i,j,k\}} \equiv \mathrm{Tr}(\hat{\rho}_{\{i,j,k\}} e^{i\hat{O}_{\{i,j,k\}}}),$$

with $\hat{\rho}_{\{i,j,k\}} \equiv \hat{\rho}_{\{i\}} \otimes \hat{\rho}_{\{j\}} \otimes \hat{\rho}_{\{k\}}$ and

$$\hat{O}_{\{i,j,k\}} \equiv \sum_{n=i,j,k} \alpha_n \hat{J}_n^z + \sum_{m,n=i,j,k}^{m<n} \beta_{m,n} (\hat{J}_m^+ \hat{J}_n^- + \hat{J}_m^- \hat{J}_n^+),$$

i.e., $\mathcal{L}_{\{i,j,k\}}$ is obtained from Eq. (4) by dropping all spins except i, j, and k. Similar to the two-spin case, $\mathcal{L}_{\{i,j,k\}}$ can be factorized as

$$\mathcal{L}_{\{i,j,k\}} = \tilde{\mathcal{L}}_{\{i\}} \tilde{\mathcal{L}}_{\{j\}} \tilde{\mathcal{L}}_{\{k\}} \tilde{\mathcal{L}}_{\{i,j\}} \tilde{\mathcal{L}}_{\{j,k\}} \tilde{\mathcal{L}}_{\{i,k\}} \tilde{\mathcal{L}}_{\{i,j,k\}},$$

where

$$\tilde{\mathcal{L}}_{\{i,j,k\}} \equiv \frac{\mathcal{L}_{\{i,j,k\}}}{\tilde{\mathcal{L}}_{\{i\}} \tilde{\mathcal{L}}_{\{j\}} \tilde{\mathcal{L}}_{\{k\}} \tilde{\mathcal{L}}_{\{i,j\}} \tilde{\mathcal{L}}_{\{j,k\}} \tilde{\mathcal{L}}_{\{i,k\}}} \tag{9}$$

accounts for the nonfactorizable correlation among the three spins. $\ln \tilde{\mathcal{L}}_{\{i,j,k\}}$ would vanish if the interactions in $\hat{O}_{\{i,j,k\}}$ cannot connect the three spins $\{i,j,k\}$ into a linked cluster. For example, if $\beta_{i,j} = \beta_{i,k} = 0$ and $\beta_{j,k} \neq 0$, the three-spin propagator $\mathcal{L}_{\{i,j,k\}}$ would be factorized as

$$\mathcal{L}_{\{i,j,k\}} = \mathcal{L}_{\{i\}} \mathcal{L}_{\{j,k\}},$$

which, together with $\ln \tilde{\mathcal{L}}_{\{i,j\}} = \ln \tilde{\mathcal{L}}_{\{i,k\}} = 0$ [according to Eq. (8)], leads to $\ln \tilde{\mathcal{L}}_{\{i,j,k\}} = 0$ according to Eq. (9). This connectivity property of $\ln \tilde{\mathcal{L}}_{\{i,j,k\}}$ leads to the Taylor expansion

$$\ln \tilde{\mathcal{L}}_{\{i,j,k\}} = c_1 \beta_{i,j} \beta_{i,k} + c_2 \beta_{j,i} \beta_{j,k} + c_3 \beta_{k,i} \beta_{k,j} + O(\beta^3). \tag{10}$$

Thus $\ln \tilde{\mathcal{L}}_{\{i,j,k\}}$ is at most a second-order small quantity.

(3) Cluster correlation $\{\tilde{\mathcal{L}}_C\}$. The above factorization procedure can be carried out for baths consisting of more and

more spins. For a bath of an arbitrary group of spins (denoted as $\mathcal{C}$), the propagator becomes

$$\mathcal{L}_{\mathcal{C}} \equiv \mathrm{Tr}(\hat{\rho}_{\mathcal{C}} e^{i\hat{O}_{\mathcal{C}}}),$$

which is obtained from Eq. (4) by dropping all spins except those belonging to the group $\mathcal{C}$. By introducing the cluster correlation

$$\tilde{\mathcal{L}}_{\mathcal{C}} \equiv \frac{\mathcal{L}_{\mathcal{C}}}{\prod_{\mathcal{C}' \subset \mathcal{C}} \tilde{\mathcal{L}}_{\mathcal{C}'}},$$

the propagator is factorized as

$$\mathcal{L}_{\mathcal{C}} = \prod_{\mathcal{C}' \subseteq \mathcal{C}} \tilde{\mathcal{L}}_{\mathcal{C}'}.$$

By mathematical induction, it can be readily proved that $\ln \tilde{\mathcal{L}}_{\mathcal{C}}$ vanishes if the interactions contained in $\hat{O}_{\mathcal{C}}$ cannot connect all the spins in group $\mathcal{C}$ into a linked cluster. Such connectivity property ensures that in each term of the Taylor expansion of $\ln \tilde{\mathcal{L}}_{\mathcal{C}}$ about the interaction strength, the coefficient $\{\beta_{i,j}\}$'s must appear at least $(|\mathcal{C}|-1)$ times ($|\mathcal{C}|$ being the number of spins in the group). Thus $\ln \tilde{\mathcal{L}}_{\mathcal{C}} = O(\beta^{|\mathcal{C}|-1})$. In particular, the full propagator $\mathcal{L}$ of the whole bath is factorized into the product of all possible cluster correlations as

$$\mathcal{L} = \left(\prod_{i} \tilde{\mathcal{L}}_{\{i\}}\right)\left(\prod_{\{i,j\}} \tilde{\mathcal{L}}_{\{i,j\}}\right) \cdots \tilde{\mathcal{L}}_{\{1,2,\cdots,N\}} = \prod_{\mathcal{C} \subseteq \{1,2,\cdots,N\}} \tilde{\mathcal{L}}_{\mathcal{C}}. \tag{11}$$

An exact evaluation of the ensemble CCE in Eq. (11) is not possible in general, which amounts to exactly solving the many-spin dynamics. In the qubit decoherence problem, it often suffices to truncate the CCE to an appropriate order M (denoted as M-CCE for short) by dropping all cluster correlations with sizes larger than M,

$$\mathcal{L}^{(M)} = \prod_{|\mathcal{C}| \leq M} \tilde{\mathcal{L}}_{\mathcal{C}}. \tag{12}$$

For example, the first-order truncation of the ensemble CCE (the 1-CCE) is

$$\mathcal{L}^{(1)} = \tilde{\mathcal{L}}_{\{1\}} \tilde{\mathcal{L}}_{\{2\}} \cdots \tilde{\mathcal{L}}_{\{N\}} = \prod_{i} \tilde{\mathcal{L}}_{\{i\}}, \tag{13}$$

which is equivalent to Eq. (4) with all interaction terms in $\hat{O}$ dropped. In order to incorporate the interaction effects, the lowest nontrivial order of truncation is the second order (2-CCE)

$$\mathcal{L}^{(2)} = \left(\prod_{i} \tilde{\mathcal{L}}_{\{i\}}\right)\left(\prod_{\{i,j\}} \tilde{\mathcal{L}}_{\{i,j\}}\right), \tag{14}$$

which coincides with the pair-correlation approximation.[18,20]

Since only connected clusters for which $\ln \tilde{\mathcal{L}}_{\mathcal{C}} \neq 0$ contribute to the propagator $\mathcal{L}$, the convergence (and hence the justification for the truncation) of the ensemble CCE can be estimated as follows. First, if each spin interacts, on average, with q spins, then the number of connected size-M clusters is $\sim Nq^{M-1}$, with N the total number of bath spins. Second, for a size-M cluster, $\ln \tilde{\mathcal{L}}_{\mathcal{C}} = O(\beta^{M-1})$. The contribution to $\ln \mathcal{L}$ from all the size-M clusters is $\Sigma_{|\mathcal{C}|=M} \ln \tilde{\mathcal{L}}_{\mathcal{C}} \sim N(q\beta)^{M-1}$. For $q\beta < 1$, the ensemble CCE converges.

B. General theory

The above example can be readily generalized to

$$\mathcal{L} = \mathrm{Tr}(\hat{\rho} e^{i\hat{O}^{(1)}} e^{i\hat{O}^{(2)}} \cdots), \tag{15}$$

with a general ensemble $\hat{\rho}$ and an arbitrary series of time-ordered bath operators $\hat{O}^{(j)}$ $(j=1,2,\cdots)$. The bath interactions need not be purely off diagonal or contain only pairwise interactions and the initial density matrix need not be factorizable. For a thermal ensemble as

$$\hat{\rho} = \exp(-\beta_T \hat{H}), \tag{16}$$

the density matrix itself can be viewed as a propagator with imaginary time $\tau = -i\beta_T$ and the whole propagator can be written as

$$\mathcal{L} = \mathrm{Tr}(\hat{\rho}_0 e^{i(i\beta_T \hat{H})} e^{i\hat{O}^{(1)}} e^{i\hat{O}^{(2)}} \cdots), \tag{17}$$

with $\hat{\rho}_0$ denoting the trivial thermal state at infinite temperature $(\beta_T = 0)$.

In essentially the same way as illustrated in the example above, a hierarchy of cluster correlations $\{\tilde{\mathcal{L}}_{\mathcal{C}}\}$ can be introduced. First, the single-spin correlation is defined as

$$\tilde{\mathcal{L}}_{\{i\}} \equiv \tilde{\mathcal{L}}_{\{i\}},$$

where

$$\mathcal{L}_{\{i\}} \equiv \mathrm{Tr}(\hat{\rho}_{\{i\}} e^{i\hat{O}^{(1)}_{\{i\}}} e^{i\hat{O}^{(2)}_{\{i\}}} \cdots)$$

is obtained from Eq. (15) by dropping all spins except spin i and

$$\hat{\rho}_{\{i\}} \equiv \mathrm{Tr}_{k \neq i}[\hat{\rho}] \tag{18}$$

is the reduced density matrix of the ith spin. Then the cluster correlation for an arbitrary group $\mathcal{C}$ of bath spins is defined as

$$\tilde{\mathcal{L}}_{\mathcal{C}} \equiv \frac{\mathcal{L}_{\mathcal{C}}}{\prod_{\mathcal{C}' \subset \mathcal{C}} \tilde{\mathcal{L}}_{\mathcal{C}'}},$$

where

$$\mathcal{L}_{\mathcal{C}} \equiv \mathrm{Tr}(\hat{\rho}_{\mathcal{C}} e^{i\hat{O}^{(1)}_{\mathcal{C}}} e^{i\hat{O}^{(2)}_{\mathcal{C}}} \cdots)$$

is obtained from Eq. (15) by dropping all bath spins outside group $\mathcal{C}$ and

$$\hat{\rho}_{\mathcal{C}} \equiv \mathrm{Tr}_{k \notin \mathcal{C}}[\hat{\rho}] \tag{19}$$

is the reduced density matrix of the cluster. In particular, the whole bath propagator is factorized into all possible cluster correlations as

$$\mathcal{L} = \prod_{\mathcal{C} \subseteq \{1,2,\cdots,N\}} \tilde{\mathcal{L}}_{\mathcal{C}}, \tag{20}$$

which assumes exactly the same form as Eq. (11).

Now we discuss the convergence property of the ensemble CCE for general bath operators. To focus on the effect of the interaction strength, we consider the case that the initial bath density matrix is factorizable as in Eq. (5). For a factorizable ensemble, it can be readily proved that $\ln \tilde{\mathcal{L}}_{\mathcal{C}}$ vanishes when the interactions contained in operators $\hat{O}_{\mathcal{C}}^{(1)}, \hat{O}_{\mathcal{C}}^{(2)}, \ldots$ cannot connect all the spins in the group $\mathcal{C}$ into a linked cluster. Considering that the operators $\hat{O}^{(j)}$ contains the W-spin interaction such as $\beta_{i_1 i_2 i_3}^{(j)} \hat{J}_{i_1}^x \hat{J}_{i_2}^y \hat{J}_{i_3}^z$ for $W=3$ (in the example of Sec. II A, $W=2$), in the Taylor expansion of $\ln \tilde{\mathcal{L}}_{\mathcal{C}}$ with respect to the dimensionless coupling coefficient β's, the interaction coefficients $\{\beta_{i_1,i_2,\cdots,i_W}^{(j)}\}$ contained in each term must connect all the spins in group $\mathcal{C}$ into a linked cluster. At least $(M-1)/(W-1)$ interaction coefficients are needed to form a size-M linked cluster. As a result,

$$\ln \tilde{\mathcal{L}}_{\mathcal{C}} = O(\beta^{(M-1)/(W-1)}), \tag{21}$$

where β is the typical magnitude of the coupling coefficients. The number of size-M clusters is $\sim N q^{M-1}$. So the total contribution to $\ln \mathcal{L}$ from all size-M clusters is

$$\sum_{|\mathcal{C}|=M} \ln \tilde{\mathcal{L}}_{\mathcal{C}} \sim N(q^{W-1}\beta)^{(M-1)/(W-1)}.$$

Therefore, the ensemble CCE converges for $q^{W-1}\beta < 1$. Interestingly, if the bath has certain initial correlations or entanglement (such as a strongly correlated system at low temperature), the convergence property would be determined by both the inverse temperature β_T and the typical coupling constant β.

C. Comparison to single-sample CCE

The evaluation of the single-sample average

$$\mathcal{L}^{\mathcal{J}} = \langle \mathcal{J} | e^{i\hat{O}^{(1)}} e^{i\hat{O}^{(2)}} \cdots | \mathcal{J} \rangle \tag{22}$$

on a factorizable product state $|\mathcal{J}\rangle = \otimes_n |j_n\rangle$ can be done as a special case of the ensemble CCE by taking $\hat{\rho} = |\mathcal{J}\rangle\langle\mathcal{J}| = \otimes_n \hat{\rho}_{\{n\}}$, with $\hat{\rho}_{\{n\}} \equiv |j_n\rangle\langle j_n|$. This method is slightly different from the previously developed single-sample CCE (Ref. 24) in defining the cluster correlation for a cluster $\mathcal{C}$. Here not only off-diagonal but also diagonal interaction terms involving spins outside cluster $\mathcal{C}$ have been dropped. In contrast, the single-sample CCE in Ref. 24 keeps all the diagonal terms by replacing the spins outside cluster $\mathcal{C}$ with their mean-field values in the initial state $|\mathcal{J}\rangle$. For example, the diagonal interaction $\Sigma_{n\notin\mathcal{C}} \gamma_{i,n} \hat{J}_i^z \hat{J}_n^z$ between a spin $\hat{\mathbf{J}}_{i\in\mathcal{C}}$ inside cluster $\mathcal{C}$ and spins $\{\hat{\mathbf{J}}_{n\notin\mathcal{C}}\}$ outside cluster $\mathcal{C}$ would be replaced with $\hat{J}_i^z \Sigma_{n\notin\mathcal{C}} \gamma_{i,n} \langle \mathcal{J} | \hat{J}_n^z | \mathcal{J} \rangle$, which contributes a *static* local mean field for the ith spin. With such a static mean-field treatment of the diagonal terms, the expansion is carried out with respect to the most essential dynamics of the spin bath, namely, the collective flip-flop of a cluster of spins that is responsible for the *dynamical* local-field fluctuation for the qubit. This procedure, however, is not applicable to the ensemble CCE for each sample state $|\mathcal{J}\rangle$ from the ensemble $\hat{\rho}$ will generate a different static mean field.

With the static local-field fluctuation singled out, the cluster correlation in the single-sample CCE accounts for the collective dynamical local-field fluctuation generated by off-diagonal interactions. As a result, its magnitude in single-sample CCE is determined by the magnitude of off-diagonal interactions, while in ensemble CCE it is determined by the magnitude of all kinds of bath interactions. As an example, consider pairwise interaction such as

$$\hat{O} \equiv \sum_n \alpha_n \hat{J}_n^z + \sum_{m<n} [\beta_{m,n}^{\mathrm{nd}} (\hat{J}_m^+ \hat{J}_n^- + \hat{J}_m^- \hat{J}_n^+) + \beta_{m,n}^{\mathrm{d}} \hat{J}_m^z \hat{J}_n^z].$$

Let $\beta_{\mathrm{nd}}(\beta_{\mathrm{d}})$ be the typical magnitude of the off-diagonal (diagonal) coupling coefficients $\beta_{m,n}^{\mathrm{nd}}(\beta_{m,n}^{\mathrm{d}})$ and β be the greater one of β_{d} and β_{nd}. Then for a size-M cluster, $\ln \tilde{\mathcal{L}}_{\mathcal{C}} = O(\beta^{M-1})$ in the ensemble CCE, while $\ln \tilde{\mathcal{L}}_{\mathcal{C}}^{\mathcal{J}} = O(\beta_{\mathrm{nd}}^{M-1})$ in the single-sample CCE. The single-sample CCE would converge faster than the ensemble CCE. Moreover, the number of clusters in ensemble CCE is greater than that of the single-sample CCE. For example, if a spin $\hat{\mathbf{J}}_i$ in a cluster interacts with others through diagonal interaction only, then it generates no dynamical fluctuations and hence the single-sample cluster correlation vanishes, while the ensemble cluster correlation does not. For a bath with a relatively large number of spins and a factorizable initial state, the ensemble CCE result would be close to the single-sample CCE using a random sampling of the initial bath state. The single-sample CCE is recommended in such cases. For a relatively small bath or a nonfactorizable ensemble, the ensemble CCE is desirable.

III. NUMERICAL CHECK

For a qubit-bath system described by a general pure dephasing Hamiltonian as in Eq. (1), the decoherence of the qubit under the pulse control of the nth-order concatenated dynamical decoupling[17,19,28–30] is characterized by[20]

$$\mathcal{L}_n \equiv \mathrm{Tr}[\hat{\rho} \hat{U}_n^{(-)\dagger} U_n^{(+)}], \tag{23}$$

where $\hat{\rho}$ is the density matrix for the initial bath state and $\hat{U}_n^{(\pm)}$ are recursively defined as

$$\hat{U}_j^{(\pm)} \equiv \hat{U}_{j-1}^{(\mp)} \hat{U}_{j-1}^{(\pm)},$$

with $\hat{U}_0^{(\pm)} \equiv e^{-i\hat{H}^{(\pm)}T}$. For example, free-induction decay, Hahn echo, and Carr-Purcell echo correspond to $n=0$, 1, and 2, respectively.

In this section, we consider an exactly solvable spin bath model (the one-dimensional spin-1/2 XY model) and compare the qubit coherence $\mathcal{L}_n$ from the ensemble CCE to the exact solutions by the Jordan-Wigner transformation.[31–33] The N-spin bath Hamiltonian conditioned on the qubit state $|\pm\rangle$ is

$$\hat{H}^{(\pm)} = \pm \sum_{n=1}^{N} \frac{z_n}{2} \hat{J}_n^z + \sum_{n=1}^{N-1} \left(B_n \pm \frac{b_n}{2} \right) (\hat{J}_{n+1}^+ \hat{J}_n^- + \hat{J}_n^+ \hat{J}_{n+1}^-), \tag{24}$$

where z_n denotes the qubit-bath spin interaction strength (simulating the hyperfine interaction strength for electron-

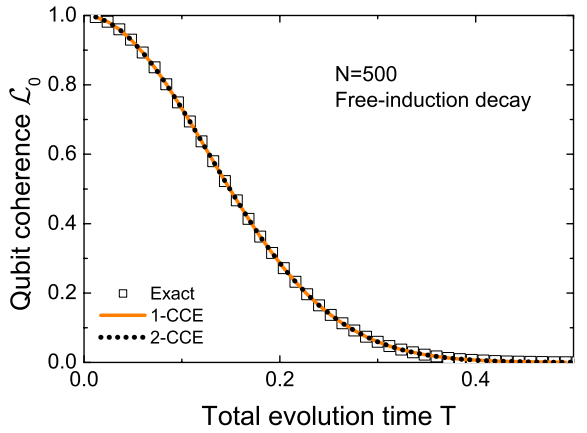

FIG. 1. (Color online) Qubit coherence in free-induction decay for a "sinusoidal" chain with $N=500$ spins: the exact solution (empty squares) vs the results from ensemble CCE truncated to the first order (1-CCE, solid line) and the second order (2-CCE, dotted line).

nuclear spin systems), B_n is the intrinsic bath interaction strength, and b_n is the interaction dependent on the qubit state. The bath is assumed to be in a high-temperature thermal ensemble with $\hat{\rho}\equiv(1/2)^N$. The qubit-bath interaction coefficients $\{z_n\}$ are taken from a sinusoidal distribution $z_n = z_{\max}\sin(n\pi/N)$ (referred to as "sinusoidal" chain) or randomly selected from $[0,z_{\max}]$ (referred to as "random" chain). Hereafter $z_{\max}$ is taken as the unit of energy. The spin-flip interaction strengths $\{B_n\}$ and $\{b_n\}$ are randomly chosen from $[10^{-3},2\times10^{-3}]$, corresponding to typical bath spin flip-flop time $\tau_{\rm sf}\sim10^3$. The convergence of the ensemble CCE then requires B_nT, $b_nT<1$, or equivalently $T<\tau_{\rm sf}$.

First we consider the simplest case, namely, the qubit coherence $\mathcal{L}_0=\mathrm{Tr}[\hat{\rho}e^{i\hat{H}^{(-)}T}e^{-i\hat{H}^{(+)}T}]$ in free-induction decay. The first-order truncation of the ensemble CCE gives

$$\mathcal{L}_0^{(1)}=\prod_i \cos\left(\frac{z_iT}{2}\right), \tag{25}$$

which is indeed the dephasing due to inhomogeneous broadening. In the short-time limit ($z_iT\ll1$), Eq. (25) becomes $\mathcal{L}_0^{(1)}\approx e^{-\Gamma^2T^2/2}$, where

$$\Gamma\equiv\sqrt{\frac{1}{4}\sum_i z_i^2}=\sqrt{\langle(\hat{h}^z)^2\rangle-\langle\hat{h}^z\rangle^2}\sim\sqrt{N}|z_i|$$

is the variance of the "Overhauser" field $\hat{h}^z\equiv\Sigma_n z_n\hat{J}_n^z$ of the spin bath. As evidenced by the good agreement between the 1-CCE and the exact result in Fig. 1, the ensemble free-induction decay is dominated by the inhomogeneous broadening, which leads to rapid decoherence within a time scale much shorter than the inverse qubit-bath interaction strength $z_n^{-1}\sim1$. The corrections due to spin-spin interactions, which could show up on a time scale comparable to the inverse interaction strength $(1/B_n,1/b_n\sim10^3)$ and dominate the single-sample decoherence, are negligible during the ensemble free-induction decay process.

To highlight the role of spin-spin interaction, we consider the qubit coherence $\mathcal{L}_n(n=1,2,\cdots)$ in spin echo or higher-order concatenated control where the inhomogeneous broadening is eliminated and, consequently, the first-order trunca-

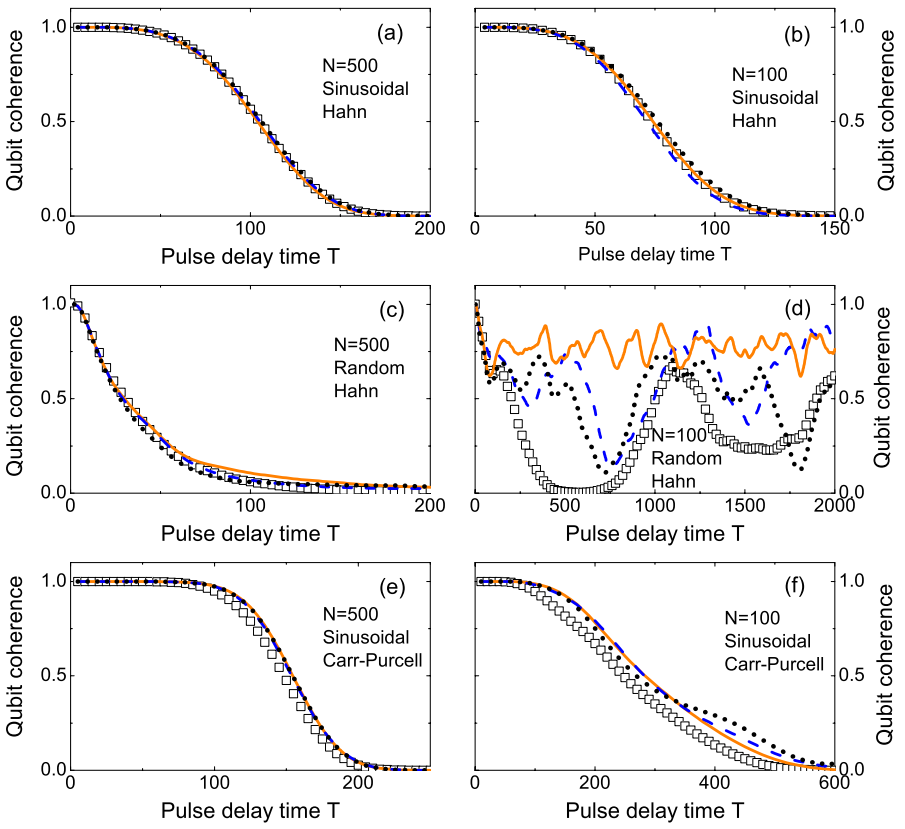

FIG. 2. (Color online) Qubit coherence in Hahn echo ($n=1$) and Carr-Purcell echo ($n=2$) for different baths. The exact ensemble coherence $\mathcal{L}_n$ (empty squares) vs the magnitude $|\mathcal{L}_n^{(\mathcal{J})}|$ of the exact single-sample coherence for three randomly chosen bath states $|\mathcal{J}\rangle$, denoted by the solid, dashed, and dotted lines, respectively.

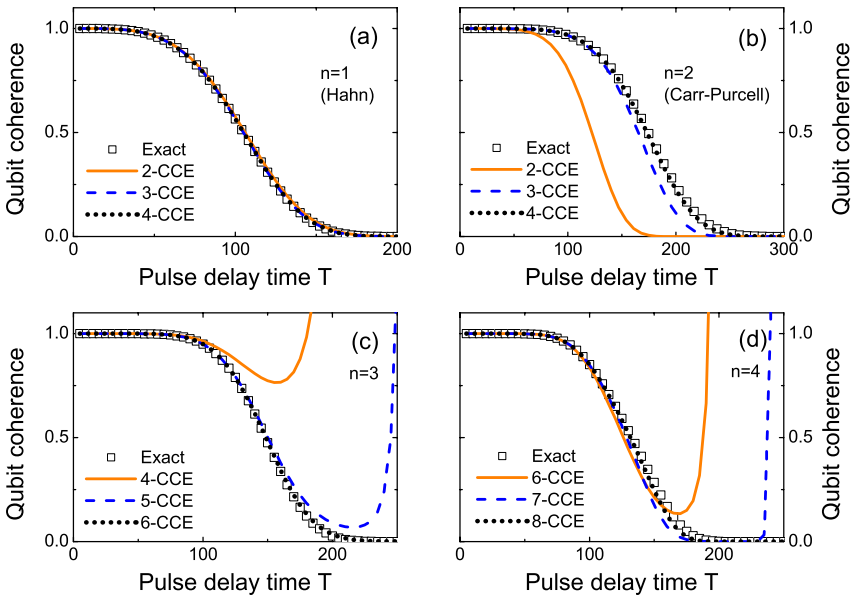

FIG. 3. (Color online) Ensemble qubit coherence in nth-order concatenated dynamical decoupling for a *sinusoidal* chain with $N=500$ spins: the exact ensemble solutions (empty squares) vs the results from the ensemble CCE truncated to different orders.

tion of the ensemble CCE gives no decay: $\mathcal{L}_1^{(1)}=1$. When the random-phase factor leading to the inhomogeneous broadening is eliminated (as in the echo signals), the ensemble-averaged qubit coherence would be close to that averaged on a randomly sampled bath state if the bath is relatively large. This is shown in Figs. 2(a) and 2(b) for a *sinusoidal* chain. The single-sample coherences for three randomly chosen bath states $|\mathcal{J}\rangle$ agree very well with the ensemble coherence.

For a small spin bath, or for a *random* chain where the qubit decoherence is caused by the dynamics of a few small clusters, the qubit decoherence would depend sensitively on the choice of the initial bath state and hence the ensemble average would deviate significantly from the qubit coherence averaged on any specific sample of the initial state. This is clearly seen in Figs. 2(c) and 2(d) for a *random* chain. Even for a relatively large *sinusoidal* chain, the difference between single-sample decoherence and the ensemble average is noticeable when higher-order dynamical decoupling (e.g., Carr-Purcell echo) is applied [see Figs. 2(e) and 2(f)]. This is because that under the higher-order control, the clusters responsible for the qubit decoherence grow larger and larger as the effects of smaller clusters are suppressed and the specificity of the initial state of larger clusters is more important than that of smaller ones.

Figure 3 compares the results from the ensemble CCE to the exact solutions for ensemble coherence under the control of concatenated dynamical decoupling of different orders. For the Hahn echo shown in Fig. 3(a), the second-order truncation of the ensemble CCE already agrees with the exact solution very well, indicating that the decoherence is dominated by spin-pair dynamics. For Carr-Purcell echo in Fig. 3(b), however, the second-order truncation becomes insufficient as the leading order contributing from spin-pair dynamics has been eliminated and the correlated dynamics of larger clusters becomes important.[17] Hence a fourth-order truncation of the ensemble CCE is required to reproduce the exact solution. For concatenated dynamical decoupling of successively higher orders n, the leading contributions from successively larger clusters have been eliminated. As a result, successively higher-order truncations of the ensemble CCE are required to reproduce the exact results: 6-CCE for $n=3$ in Fig. 3(c) and 8-CCE for $n=4$ in Fig. 3(d).

IV. CONCLUSION

The decoherence of a qubit in a spin bath is essentially determined by the many-body bath evolution starting either from a pure or an ensemble state. As an extension of the previously developed single-sample cluster-correlation expansion[24] that addresses the spin bath dynamics starting from a noninteracting pure state, we have developed an ensemble CCE theory to solve the spin bath dynamics starting from an arbitrary ensemble state. In this approach, the ensemble propagator is factorized into the product of all possible cluster correlations, each term accounting for the authentic (nonfactorizable) collective excitation of a group of bath spins. For a finite-time evolution as in the qubit decoherence problem, convergent results can be obtained by truncating the ensemble CCE by keeping cluster correlations up to a certain size, as has been checked using an exactly solvable spin chain model (the one-dimensional spin-1/2 XY model). For the convergence property (for a factorizable initial state), the ensemble CCE is determined by the typical strength of the bath spin interaction, being either diagonal or off-diagonal, while the single-sample CCE is determined only by the off-diagonal interaction coefficients. The ensemble CCE can be applied to baths with nonfactorizable initial state as well.

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