Stochastic averaging of the time-evolution operator for quantum systems driven by Ornstein-Uhlenbeck colored noise: A nonperturbative cluster cumulant method

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We have developed in this paper a nonperturbative cluster-expansion strategy for generating the stochastically averaged time-evolution operator for quantum systems driven by Ornstein-Uhlenbeck (OU) colored noise. The method induces a boson mapping of the (real or complex) stochastic variable f, and interprets the stochastic average of a pair of variables f at two different times as the expectation value of the time-ordered product of the associated bosons with respect to the boson vacuum $|0_B\rangle$. The stochastic evolution is thus mapped onto a deterministic evolution in an expanded Fock space. The evolution of the system from the groups of state of interest is monitored using our recently developed nonperturbative time-dependent multireference coupled-cluster (TDMRCC) method. In this, the evolution operator U is written in a factorized form $U_{ex}U_M$, where U_M evolves in the space of the starting functions (model space) and U_{ex} brings in the virtual functions. U_{ex} and U_M are both written as normal ordered exponentials involving cluster operators. In the present context, the TDMRCC method translates into one for generating the evolution operator U_B for the Hamiltonian containing the additional boson variables, and the stochastic averaging of U_B is realized as the expectation value $\langle 0_B|U_B|0_B\rangle$. We call the TDMRCC method involving the expanded Fock space a cluster cumulant method. We have analyzed the relation of the cluster cumulant approach with the Fox-Kubo operator cumulant expansion and the method of marginal averages involving the Fokker-Planck operator of the OU process. It has been shown that an order by order expansion of our equations in the power of stochastic coupling generates the perturbative cumulant results of Fox and Kubo. It is also demonstrated that the traditional Fokker-Planck method of marginal averages uses a Kubo-Schrödinger operator which is related to our boson mapped Hamiltonian by a transformation which converts the Fokker-Planck operator Γ to a manifestly Hermitian form. However, the method of marginal averages involves a linear expansion of U_B in terms of eigenfunctions of Γ, while the cluster cumulant method uses a cluster expansion, which is nonlinear in the expansion parameters. The former is thus analogous to a configuration-interaction expansion, while the latter is analogous to a coupled-cluster strategy. The method is illustrated by applying it to a simple yet nontrivial problem, viz., a harmonic oscillator linearly perturbed by a (real or complex) stochastic variable. Survivalities of both the ground and the first excited states have been considered for a wide range of coupling strengths and noise correlation times. Our method provides exact results in this case; these have been used as benchmarks for assessing performance of the second- and fourth-order cumulant results.

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I. INTRODUCTION

Stochastic phenomena are ubiquitous in many branches of physics and chemistry. A large class of such processes is generically describable by the time evolution of a quantum system under an external perturbation involving a multiplicative classical stochastic parameter. The relevant quantities of physical interest are then the stochastic averages of the associated operators. Stochastic averaging is routinely encountered, for example, in quantum optics [1] and in relaxation theories [2], where δ-correlated or white noise is taken as the stochastic influence. With the emergence of probes for ultrafast processes, attention has been focused on stochastic processes with *finite correlation times,* i.e., colored noise, in particular of the Ornstein-Uhlenbeck (OU) variety [3]. Quantum systems driven by colored noise lead to rich and nontrivial evolution patterns due to interference between processes taking place within the correlation time of the noise and the characteristic time scale of the system. Monitoring the dynamics of the stochastically averaged observables for the OU colored noise is thus of paramount interest.

There are two established methods for obtaining approximate stochastic averages in quantum dynamics. One of them uses the time-ordered operator cumulant expansion introduced by Kubo [4], and strongly advocated recently by Fox [5], for computing the stochastically averaged time-evolution operator U. Another method invokes the Fokker-Planck formalism [6,7] and generates the marginal average of the time-evolution operator of the associated Kubo-Schrödinger or Kubo-Liouvillian dynamics [1,7]. The Fox-Kubo operator cumulant expansion has been widely successful for white-noise processes and in the weak-coupling limits [7], and forms a cornerstone for many statistical-mechanical models—

particularly the models based on master equations [8]. For strongly coupled systems, and in the colored-noise regime, however, the cumulant expansion is slowly convergent. The advent of recently developed strongly coupled picosecond probes demands that one should develop viable alternatives to an order by order expansion of Kubo and Fox. Some progress has been made in this direction in recent years, involving partial resummation of a set of important terms [9]. In the Fokker-Planck approach, the original Hamiltonian is replaced by a modified Hamiltonian involving the relevant Fokker-Planck operator, and the marginal average of the evolution operator is computed either in a perturbative manner using a continued-fraction approach [1,4,7] or in a nonperturbative manner using a truncated eigenfunction expansion of the Fokker-Planck operator [6]. In both the above approaches, it is difficult to discern a systematic scheme for improvement. Very recently, there has emerged another methodology for stochastic averaging of general noise using the path-integral formalism [10,11]. Although the method shows promise of an alternative nonperturbative approach to stochastic processes, its implementation is rather involved and is yet to be tested on realistic models.

In this paper, we shall develop an easy nonperturbative access to systematic computation of stochastic averages of the evolution operator U for quantum systems, driven by real and complex Ornstein-Uhlenbeck (OU) colored noise. The method induces a *boson mapping* of the stochastic variable, and maps the stochastic averaging to an *expectation value* with respect to the boson vacuum $|0_B\rangle$. The evolution of the mapped operator U_B, written in a factorized cluster expansion, is governed by a deterministic Hamiltonian H_B defined in an *expanded Fock space.* The nonperturbative treatment of the deterministic evolution is done using the time-dependent multireference coupled-cluster formalism [1,14] developed by us recently [12], which offers a systematic cluster-expansion method for solving quantum dynamics. We call our present development a *cluster cumulant approach* and describe the basic formalism in Sec. II. We shall indicate in Sec. III the relationship of our method with the more established ones, such as the cumulant expansion [4–7] and the Fokker-Planck-based approaches [4,6,7]. Numerical applications on simple yet nontrivial problems will be presented in Sec. IV to illustrate the formalism. For the problems treated by us, the cluster cumulant method provides exact results. We have used them to assess the performance of the corresponding second- and fourth-order perturbative cumulant results beyond the perturbative regime of the coupling.

II. CLUSTER CUMULANT APPROACH: THE FORMALISM

A. Boson mapping of the stochastic variable

Let us consider a generic quantum Hamiltonian H_0 perturbed by an operator involving a multiplicative OU stochastic parameter f of the stationary Gaussian distribution [3,7]:

$$H=H_0+g[f(t)V+f^*(t)V^\dagger] , \tag{2.1}$$

where g is the coupling constant. For a real noise, $f(t)$ is real and satisfies

$$\langle\langle f(t)\rangle\rangle=0 , \tag{2.2a}$$

$$\langle\langle f(t_1)f(t_2)\rangle\rangle=\frac{\lambda}{2}e^{-\lambda|t_1-t_2|} , \tag{2.2b}$$

$$\langle\langle f(t_1)\cdots f(t_{2n})\rangle\rangle=\sum_{\text{all pairs}}\prod\langle\langle f(t_i)f(t_j)\rangle\rangle , \tag{2.2c}$$

$$\langle\langle f(t_1)\cdots f(t_{2n+1})\rangle\rangle=0 , \tag{2.2d}$$

where $\langle\langle\ \rangle\rangle$ denotes the stochastic averaging. For complex Gaussian processes, Eqs. (2.2) are modified in the sense that the pair averages are nonzero only when they involve one f and one f^*. The noise correlation time τ_c is of the order of $1/\lambda$, and the pair average is normalized such that its integrated area over all $|t_1-t_2|$ is unity.

The evolution operator U satisfies

$$i\frac{\partial U}{\partial t}=\{H_0+g[f(t)V+f^*(t)V^\dagger]\}U , \tag{2.3}$$

and we are interested in determining the so-called *relaxation operator* [4,5] $R(t)=\langle\langle U(t)\rangle\rangle$.

The starting point in our formalism is the observation that we can induce a *boson image* for $f(t)$, such that the pair-average relation, Eq. (2.2b), can be realized as an *expectation value over the boson vacuum.* Thus, for the real Gaussian process, we introduce the mappings

$$f(t)\rightarrow F^I(t)=(\lambda/2)^{1/2}[be^{-\lambda t}+b^\dagger e^{\lambda t}] , \tag{2.4}$$

$$\langle\langle f(t_1)f(t_2)\rangle\rangle\rightarrow\langle 0_B|T[F^I(t_1)F^I(t_2)]|0_B\rangle , \tag{2.5}$$

where $|0_B\rangle$ is the vacuum for the boson operator b, and T is the time-ordering operator. Similarly, for the complex Gaussian process, we introduce

$$f(t)\rightarrow F^I(t)=(\lambda/2)^{1/2}[be^{-\lambda t}+c^\dagger e^{\lambda t}] , \tag{2.6a}$$

$$f^*(t)\rightarrow\tilde{F}^I(t)=(\lambda/2)^{1/2}[b^\dagger e^{\lambda t}+ce^{-\lambda t}] , \tag{2.6b}$$

where $(b,b^\dagger)$ and $(c,c^\dagger)$ are two independent sets of boson variables. The pair average has the same interpretation as in Eq. (2.5), with $|0_B\rangle$ as the simultaneous vacuum for both b and c. Let us note that, owing to the generalized Wick's theorem, Eqs. (2.2c) and (2.2d) are also *automatically satisfied* by our mapping.

The mapped evolution operator U_B^I satisfies

$$i\frac{\partial U_B^I}{\partial t}=\{H_0+g[F^I(t)V+G^I(t)V^\dagger]\}U_B^I , \tag{2.7}$$

where G^I denotes F^I for real and $\tilde{F}^I$ for complex noise. Equation (2.7) may be interpreted as a deterministic evolution equation *in an expanded Fock space,* in an "interactionlike representation" for the new boson variables. The underlying free-boson Hamiltonian h_B must be non-Hermitian, since $F^I(t)$ involves $e^{\pm\lambda t}$ rather than $e^{\pm i\lambda t}$. Reverting to the associated "Schrödinger-like representation" via

$$U_B=\exp(-ih_Bt)U_B^I\exp(ih_Bt) , \tag{2.8}$$

where

$$h_B = -i\lambda b^\dagger b \quad \text{(real noise)}, \tag{2.9a}$$

$$h_B = -i\lambda[b^\dagger b + c^\dagger c] \quad \text{(complex noise)}, \tag{2.9b}$$

we find that

$$i\frac{\partial U_B}{\partial t} = \{H_0 + g(FV + F^\dagger V^\dagger) + h_B\} U_B , \tag{2.10}$$

with

$$F = (\lambda/2)^{1/2}[b + b^\dagger] \quad \text{(real noise)} \tag{2.11a}$$

$$F = (\lambda/2)^{1/2}[b + c^\dagger] \quad \text{(complex noise)} . \tag{2.11b}$$

The operator $R(t)$ is generated as the expectation value $\langle 0_B | U(t) | 0_B \rangle$.

Let us note that, for any specific problem involving stochastic averaging, one often starts from certain initial states $\{\phi_i\}$, and the relevant quantities of interest are the matrix elements of $R(t)$ between the starting functions. It suffices then to concentrate on determining the *restricted operator UP*, with the projector P characterizing the functions $\{\phi_i\}$, rather than on the global U itself. As it turns out, the time-dependent multireference coupled-cluster (TDMRCC) method developed by us recently [13,14], designed to generate *UP* characterizing the evolution from a group of unperturbed states, is ideally suited for computing the required stochastic averages.

B. The time-dependent multireference coupled-cluster approach: A summary

As mentioned above, the time-dependent multireference coupled-cluster (TDMRCC) approach is most useful when one wishes to monitor the time evolution of a group of initial states describable by a set of "reference functions" $\{\phi_i\}$ characterized by a projector P. The quantity of interest is *UP*, rather than the full U. The TDMRCC method may be viewed as a time-dependent generalization of the stationary multireference coupled-cluster approach [15]. The coupled-cluster representation of *UP* provides a nonperturbative computational strategy, involving an *effective Hamiltonian* H_{eff}, acting on the model space spanned by P. Since our major interest is the computation of $R(t) = \langle 0_B | U(t) | 0_B \rangle$, or more specifically, the survivality amplitudes $A_{ij} = \langle \phi_i 0_B | U(t) | \phi_j 0_B \rangle$, the TDMRCC approach should prove to be quite efficacious, if we take the direct-product states $\{\phi_i\} \otimes |0_B\rangle$ as the model space.

We now give a summary of the TDMRCC formalism. Since we have discussed the TDMRCC method in detail elsewhere [13,14], only a succinct summary will be presented. We shall elaborate only on those aspects that pertain to the adaptation of the TDMRCC approach to the stochastic problem involving Eq. (2.10). Let us assume that the general time-dependent Hamiltonian H can be written in the form

$$H(t) = \sum_i h_i(t) e_i . \tag{2.12}$$

Here e_i's are products of Bose-Fermi creation and/or annihilation operators and form the elements of a unitary group algebra, and h_i's are the time-dependent coefficients. In case the elements $\{e_i\}$ do not satisfy a closed Lie algebra, we may formally assume that the sum in Eq. (2.12) runs also over all the elements needed for the completion of the algebra even when they are countably infinite, with the corresponding null coefficients. A representation of *UP* involving a finite number of cluster operators in the latter case is then necessarily approximate, and would correspond to a truncated representation of *UP*.

For our developments, it is necessary to define a suitable vacuum state $|0\rangle$ for the annihilation operators, wherefrom the model functions $\{\phi_i\}$ are constructed via the action of suitable products of creation operators. *UP* is sought to be represented in the TDMRCC approach in a compact factorized cluster-expansion ansatz, written in terms of *normal ordered exponentials* with respect to $|0\rangle$.

In close analogy with the stationary multireference coupled-cluster (CC) theory [15], we classify all the operators in $\{e_i\}$ into two distinct categories: (a) a closed operator, denoted by the subscript "cl," is one whose action on any model space function produces another model space function; (b) an external operator, denoted by the subscript "ex," is one for which there is *at least one* model space function such that its action thereon produces a virtual function in the space $\mathbb{Q}$, orthogonal to the model space. *UP* in the TDMRCC formalism is written as

$$UP = U_{\text{ex}} U_M P , \tag{2.13}$$

where U_{ex} is written as a normal ordered exponential involving an *external operator S:*

$$U_{\text{ex}} = \{\exp(S)\} , \tag{2.14}$$

and U_M is likewise a normal ordered exponential of a closed operator X:

$$U_M = \{\exp(X)\} . \tag{2.15}$$

The curly braces denote normal ordering.

With the ansatz, Eq. (2.13), for *UP*, we intend to dissect the evolution from P into evolution outside the model space and evolution within the model space. We shall call S and X as cluster operators. Owing to the normal ordering, only the operators giving nonvanishing contributions on $\{\phi_i\}$ should be retained in S and X. Thus *UP* has a simpler structure as compared to that of full U. For a finite Lie algebra we can, however, always choose a suitable "minimal" model space $\{\phi_i\}$, such that S and X just exhaust all the elements of the unitary group algebra, and we shall in that case get even the full U in the factorized form $U_{\text{ex}} U_M$.

In analogy with the stationary case [15], we define an effective Hamiltonian H_{eff} that would govern the evolution of U_M:

$$i\frac{\partial U_M}{\partial t} = H_{\text{eff}} U_M . \tag{2.16}$$

Substituting Eq. (2.13) into the Heisenberg equation of motion, and using Eq. (2.16), we have

$$i\frac{\partial U_{\text{ex}}}{\partial t} = H U_{\text{ex}} - U_{\text{ex}} H_{\text{eff}} . \tag{2.17}$$

Taking the closed part of Eq. (2.17), we find that

$$H_{\text{eff}}=(U_{\text{ex}})_{\text{cl}}^{-1}\left[(HU_{\text{ex}})_{\text{cl}}-i\frac{\partial}{\partial t}(U_{\text{ex}})_{\text{cl}}\right], \tag{2.18}$$

which shows that H_{eff} is defined entirely by H, U_{ex}, and U_M. $[U_{\text{ex}}]_{\text{cl}}$ is arbitrary and we would choose it suitably, viz., in a way that guarantees the connectedness or size extensivity [13–15] of S. Owing to the normal ordering in U_{ex} and U_M, their time derivatives take on rather simple forms. By writing the right sides of Eqs. (2.17) and (2.16) in normal order, we get

$$\left\{i\frac{\partial S}{\partial t}U_{\text{ex}}\right\}=\{\overline{H\exp(S)}U_{\text{ex}}\}-\{U_{\text{ex}}\overline{\exp(S)H_{\text{eff}}}\}, \tag{2.19}$$

$$\left\{i\frac{\partial X}{\partial t}U_M\right\}=\{\overline{H_{\text{eff}}\exp(X)}U_M\}, \tag{2.20}$$

where the composites like $\{\overline{A\exp(B)}\}$ are connected operators in the series

$$\{\overline{A\exp(B)}\}=\{A\}+\{\overline{AB}\}+\frac{1}{2!}\{\overline{\overline{AB}B}\}+\cdots, \tag{2.21}$$

where contractions are always among the creation and/or annihilation operators in A and those in B's, omitting contractions among the operators in A and B themselves. Since the various powers of S and X in, respectively, U_{ex} and U_M are linearly independent, it follows that [13,14]

$$i\frac{\partial S}{\partial t}=\{\overline{H\exp(S)}\}_{\text{ex}}-\{\overline{\exp(S)H_{\text{eff}}}\}_{\text{ex}}, \tag{2.22}$$

$$i\frac{\partial X}{\partial t}=\{\overline{H_{\text{eff}}\exp(X)}\}_{\text{cl}}, \tag{2.23}$$

which may be viewed as the TDMRCC equations for S and X. It is clear that S and X are connected operators, so that all extensive quantities computed from even an approximate *UP* will be size extensive [13,14].

If the functions appearing in the model space are such that they involve only a few creation operators (up to a power n, for example), then S need involve only up to n destruction operators. Moreover, owing to the normal ordering, all the destruction operators in powers of S in U_{ex} remain *uncontracted* and hence active in the TDMRCC equations. If we write S as

$$S=\sum_{k=0}^{n}S^{(k)}, \tag{2.24}$$

where $S^{(k)}$ involves explicitly k destruction operators, then it may be verified easily from Eq. (2.22) that only $S^{(m)}$, with $m\leq k$, can contribute to the equation for $S^{(k)}$:

$$i\frac{\partial S^{(k)}}{\partial t}=\{\overline{H\exp(S^{[k]})}\}_{\text{ex}}-\{\overline{\exp(S^{[k]})H_{\text{eff}}^{[k]}}\}_{\text{ex}}, \tag{2.25}$$

where

$$S^{[k]}=\sum_{m=0}^{k}S^{(m)}. \tag{2.26}$$

Similarly, for $X^{(k)}$, we have

$$i\frac{\partial X^{(k)}}{\partial t}=\{\overline{H_{\text{eff}}^{[k]}\exp(X^{[k]})}\}_{\text{cl}}. \tag{2.27}$$

From now on, we shall refer to $S^{(k)}$ and $X^{(k)}$ as having *valence rank* k [13–15]. Equations (2.25) and (2.27) show two very useful features of the normal ordered representation of *UP*: (i) there is *hierarchical decoupling* of the $S^{(k)}$ and $X^{(k)}$ for various k; starting with $k=0$ upwards, the lower valence $S^{(m)}$'s and $X^{(m)}$'s appear as time-dependent *known parameters* in the equations for $S^{(k)}$ and $X^{(k)}$; (ii) in the equations for $S^{(k)}$ and $X^{(k)}$, the highest possible power of S or X can be k, signifying *finite and terminating expansions* in the powers of S and X in Eqs. (2.25) and (2.27). We shall now use the time-dependent coupled-cluster (TDCC) equations, introduced above, in our present problem of evaluating $R(t)$.

C. The cluster-cumulant methodology

The cluster-cumulant formalism is a direct transcription of the time-dependent coupled-cluster method described above to the dynamics involving the mapped Hamiltonian H_B in an expanded Fock space. For our present problem of computing R, we have in mind a group of states of the system $\{\phi_i\}$, from which we are interested to monitor the evolution. The model space P is taken to consist of the *direct-product states* $[\{\phi_i\}\otimes|0_B\rangle]$. The external operator S_B will involve not only the system boson or fermion variables, but also the stochastic boson operators representing the stochastic coupling. The normal ordering in U_{ex} and U_M is to be taken with respect to the direct-product vacuum $|0\rangle=|0_S\rangle\otimes|0_B\rangle$, where $|0_S\rangle$ is the vacuum for the system Bose and Fermi operators. Owing to the normal ordering in U_{ex}, *only the creation operators of the mapped boson variables need to be included* in S_B, since $R(t)$ ultimately involves expectation values over $|0_B\rangle$. Likewise, the corresponding closed operator X_B cannot involve any mapped boson operators at all—U_M also, being in normal order, ultimately acting on P involving $|0_B\rangle$. We shall henceforth refer to the operators S_B and X_B as external and closed *cluster cumulants*, to distinguish them from ordinary (nonstochastic) cluster operators S and X in the TDMRCC theory sketched in Sec. II B. In our cluster-cumulant formalism, S_B and X_B are governed by Eqs. (2.22) and (2.23), with H_B and H_{eff}^B replacing H and H_{eff}. The cluster-cumulant operators S_B and X_B are *connected*, justifying our terminology, and lead to a size-extensive formulation of the time-dependent effective Hamiltonian H_{eff}^B.

Having solved for S_B and X_B, $R(t)$ is obtained from the relation

$$R=\langle 0_B|\{\exp(S_B)\}\{\exp(X_B)\}|0_B\rangle. \tag{2.28}$$

Owing to the normal ordering in U_{ex} and U_M, only the operators without the stochastic variables can give non-vanishing contributions. Calling these subsets of S_B and X_B as S_B^0 and X_B^0, we have the simplification

$$R=\langle 0_B|\{\exp(S_B^0)\}\{\exp(X_B^0)\}|0_B\rangle. \tag{2.29}$$

In the cluster-cumulant method, it is straightforward

to discern whether or not an exact solution for $R(t)$ is possible. If the Lie algebra for H_B is closed, then exact $U_{\rm ex}$ and U_M are obtainable with a finite number of cluster operators [12–14]. Otherwise, we have to invoke approximation schemes, truncating S_B and X_B after some (reasonably large) particle ranks. While describing the particle rank of an operator, we should distinguish between the rank of the physical Bose-Fermi operators and that of the stochastic boson variables. We emphasize again that the cluster-cumulant equations involve *finite* power series in the variables S_B and X_B, since $U_{\rm ex}$ and U_M are in normal order. Also, since there is the *hierarchical decoupling* [12–14] of the TDCC equations, there is an analogous decoupling of the cluster-cumulant equations, which is very advantageous computationally.

Except for the single reference case when the model space involves just the unperturbed ground state of H_0, S_B will involve both excitations and deexcitations of the Bose-Fermi variables. Due to the stochastic coupling, S_B will involve operators inducing both the growth and the decay of the model space functions as functions of time. If the associated time scales for the processes are markedly different, this may lead to "stiffness" of the cluster-cumulant equations, with attendant instabilities of the solutions. We have found that we can always bypass this difficulty of resorting to an *inverse Riccati transformation* [21], inspired by the analogous strategy developed in our laboratory for handling the instability of the solutions for the time-independent multireference coupled-cluster (CC) formalism [16]. The resulting transcription of the cluster-cumulant equations by the inverse Riccati transformation is described in the Appendix.

III. RELATION OF THE CLUSTER-CUMULANT APPROACH TO OTHER METHODS

A. Relationship with the Fox-Kubo operator-cumulant-expansion method

In order to expound the relationship of our cluster-cumulant method with that of the operator-cumulant perturbative expansion of Fox and Kubo [4,5], it is necessary to rewrite our equations in the *simultaneous interaction representation* for H_0 and h_B. Introducing the transformation

$$U = U_0 U_I = U_0 U^I_{\rm ex} U^I_{\rm cl} \ , \tag{3.1}$$

with

$$U_0 = e^{-i(H_0+h_B)t} \ , \tag{3.2}$$

we have, from Eq. (2.7), the relation

$$\begin{aligned} i\frac{\partial U_I}{\partial t} &= g[F^I(t)V_I + G^I(t)V_I^\dagger]U_I \\ &\equiv J_I U_I \ , \end{aligned} \tag{3.3}$$

where

$$V_I = e^{iH_0 t} V e^{-iH_0 t} \ . \tag{3.4}$$

Since h_B is not Hermitian, this interaction representation is merely a similarity transformation, and not a unitary one. The corresponding cluster-cumulant equations, which are completely equivalent to Eqs. (2.22) and (2.23) in untruncated forms, read as

$$i\frac{\partial S^I_B}{\partial t} = \{\overline{J_I \exp(S^I_B)}\}_{\rm ex} - \{\exp(\overline{S^I_B})\, V^I_{\rm eff}\}_{\rm ex} \ , \tag{3.5}$$

$$\{\exp(\overline{S^I_B})\, V^I_{\rm eff}\}_{\rm cl} = \{\overline{J_I \exp(S^I_B)}\}_{\rm cl} \ , \tag{3.6}$$

$$i\frac{\partial X^I_B}{\partial t} = \{V^I_{\rm eff}\} + \{\overline{V^I_{\rm eff} X^I_B}\} \ . \tag{3.7}$$

Instead of directly solving Eqs. (3.5)–(3.7), we may attempt an iterative solution in order of perturbation in V_I and $V_I^\dagger$. Thus, up to the first order in V_I and $V_I^\dagger$, we have for first order S^I_B, ${}^1S^I_B$, the equation

$$i\frac{\partial({}^1S^I_B)}{\partial t} = J_I \ , \tag{3.8}$$

whose solution provides us with ${}^1S^I_B$. Substituting in Eq. (3.7) leads to equations for ${}^1X^I_B$ and ${}^2X^I_B$:

$$i\frac{\partial({}^1X^I_B)}{\partial t} = \{J_I\}_{\rm cl} \ , \tag{3.9}$$

$$i\frac{\partial({}^2X^I_B)}{\partial t} = \{\overline{J_I\, {}^1S^I_B}\}_{\rm cl} + \{\overline{(J_I\, {}^1S^I_B)\, {}^2X^I_B}\} \ . \tag{3.10}$$

This process may be repeated indefinitely to higher order, using at each order the expression for $V^I_{\rm eff}$ from Eq. (3.6). Thus, at order n,

$$\begin{aligned} {}^nV^I_{\rm eff} &= {}^n\{\overline{J_I \exp(S^I_B)}\}_{\rm cl} \\ &\quad - \sum_{m=1}^{n-2} {}^{(n-m)}\{\{\exp(\overline{S^I_B})\}\, {}^mV_{\rm eff}\}_{\rm cl} \ . \end{aligned} \tag{3.11}$$

Having found ${}^mX_B$ from Eq. (3.7) for $m=1,n$, we may compute R correct up to order n, $R^{[n]}$ in terms of ${}^{[n]}S^I_B$ and ${}^{[n]}X^I_B$:

$$\begin{aligned} R^{[n]} &= \langle 0_B | U^I_{\rm ex} U^I_{\rm cl} | 0_B \rangle \\ &= \langle 0_B | \{\exp({}^{[n]}S^I_B)\}\{\exp({}^{[n]}X^I_B)\} | 0_B \rangle \ , \end{aligned} \tag{3.12}$$

where

$${}^{[n]}A = \sum_{m=1}^{n} {}^mA \ . \tag{3.13}$$

In the Fox-Kubo method, one attempts a similar perturbative expansion for U of the original dynamics, viz., Eq. (2.3). In the interaction picture, we have, from Eq. (2.3),

$$i\frac{\partial U_I}{\partial t} = g(f(t)V_I + f^*(t)V_I^\dagger)U_I = W_I U_I \ , \tag{3.14}$$

leading to

$$U_I(t) = T\exp\left[-i\int_0^t dt' g[f(t')V_I(t') + f^*(t')V_I^\dagger(t')]\right] . \tag{3.15}$$

R is then given by

$$R=\langle\langle U_I(t)\rangle\rangle$$
$$=\left\langle\left\langle T\exp\left[-i\int_0^t dt' g[f(t')V_I(t') + f^*(t')V_I^\dagger(t')]\right]\right\rangle\right\rangle , \quad (3.16)$$

which is written as

$$R=\exp(K) . \quad (3.17)$$

The perturbative expressions for K can then be obtained by comparing Eqs. (3.16) and (3.17) at each power of V_I.

A closer look at the structure of Eq. (3.12) indicates that $R^{[n]}$ can receive contributions only from ${}^{[n]}S_B^I$ and ${}^{[n]}X_B^I$, having no stochastic boson operators at all: in our notation, ${}^{[n]}S_B^{0I}$ and ${}^{[n]}X_B^{0I}$. The stochastic averaging is almost trivial in this case. Equation (3.12) separates S_B^{0I} and X_B^{0I}, i.e., those inducing scattering from the model to complementary space and those keeping transitions within the model space. In contrast, K has both external and closed operators in the exponent of R. This is because, in the conventional Fox-Kubo method, one usually does not invoke the apparatus of the effective-Hamiltonian formalism. There is thus only a *correspondence* with the perturbative solution of the cluster-cumulant method, Eq. (3.12) and Eq. (3.17), *but not a direct equivalence.* Moreover, the traditional cumulant expansion is usually written in terms of a memory kernel, which is *time-retarded.* In contrast, the cluster-cumulant approach generates the operator $R(t)$ in terms of an *instantaneous* effective interaction involving S_B^I and X_B^I.

We may, however, think of an alternative strategy where the Fox-Kubo method is applied on $U_I P$ rather than the global U_I, in Eq. (3.14). Since there is no boson mapping in the Fox-Kubo method, P is taken to span just $\{\phi_i\}$ rather than $\{\phi_i\}\otimes|0_B\rangle$, in contrast to our cluster-cumulant method. Writing $U_I P$ as

$$U_I P=\bar{U}_{\rm ex}^I \bar{U}_{\rm cl}^I P , \quad (3.18)$$

and introducing external and closed cluster operators S_I and X_I, we have

$$i\frac{\partial S_I}{\partial t}=\{\overline{W_I\exp(S_I)}\}_{\rm ex}-\{\overline{\exp(S_I)\,V_{\rm eff}^I}\}_{\rm ex} , \quad (3.19)$$

$$\{\overline{\exp(S_I)\,V_{\rm eff}}\}_{\rm cl}=\{\overline{W_I\exp(S_I)}\}_{\rm cl} , \quad (3.20)$$

$$i\frac{\partial X_I}{\partial t}=\{\overline{W_I\exp(S_I)}\}_{\rm cl}+\{\{\overline{W_I\exp(S_I)}\}_{\rm cl}X_I\} . \quad (3.21)$$

In contrast to what we have in the cluster-cumulant method, Eq. (3.14) has no stochastic boson variables, just the variables f. The external and closed operators S_I and X_I thus have only system variables and f's. A perturbative solution for S_I can be affected in orders of W_I, which is exactly analogous to the perturbative solution of the cluster-cumulant method for S_B^I in powers of J_I. One can next solve X_I perturbatively. The resultant R is then given by

$$R=\langle\langle\{\exp(S_I)\}\{\exp(X_I)\}\rangle\rangle$$
$$\equiv\{\exp(K_{\rm ex})\}\{\exp(K_{\rm cl})\} . \quad (3.22)$$

$K_{\rm ex}$ and $K_{\rm cl}$ can be obtained from a comparison of the external and closed operators in powers of W_I. This corresponds now exactly to the perturbative procedure of the cluster-cumulant method. Unlike the traditional Fox-Kubo method, our modified treatment does lead to both a clean separation of the external and closed operators and to an instantaneous effective interaction. We shall explicitly demonstrate, in Sec. IV, that our perturbative results provide the same Fox-Kubo expressions provided the functions $\{\phi_i\}$ in both cases remain the same.

B. Relationship with the Fokker-Planck dynamics involving marginal averages

In this section, we shall demonstrate that there is a deep connection between the cluster-cumulant method and the method of marginal averages [1,3,4,6,7] in the framework of Fokker-Planck dynamics. To show this, we quickly review essentials of the Fokker-Planck (FP) dynamics, taking as an illustration the real Gaussian Ornstein-Uhlenbeck (OU) process. The case for the complex noise may be derived by a straightforward extension. We shall discuss only those pertinent aspects which make the connection with the cluster-cumulant method particularly transparent.

For the real stationary OU process, the probability distribution $P(Z,0)$ for f at the initial time ($t=0$) is a normalized Gaussian of the form $N\exp(-Z^2/\lambda\sigma^2)$, where $\lambda\sigma^2$ is a measure of the width of the distribution. Since $P(Z,0)$ is symmetric around $Z=0$, we have

$$\langle\langle f(t)\rangle\rangle\equiv\langle\langle f(0)\rangle\rangle=\int ZP(Z,0)dZ=0 , \quad (3.23)$$

where the first equality is a consequence of the stationarity of f. The pair average $\langle\langle f(t_1)f(t_2)\rangle\rangle$ is governed by the joint-probability distribution function P_2:

$$\langle\langle f(t_1)f(t_2)\rangle\rangle\equiv\int Z_1P_2(Z_2,t_2|Z_1,t_1)Z_2dZ_1dZ_2$$
$$=\int Z_1P_2(Z_2,Z_1,t)dZ_1dZ_2 , \quad (3.24)$$

where $t=|t_1-t_2|$. The last equality is again due to the assumed stationarity of the OU process. Let us introduce the conditional probability distribution ω_2 as

$$\omega_2(Z_2,Z_1,t)=P_2(Z_2,Z_1,t)/P(Z_2,0) . \quad (3.25)$$

ω is governed by the Fokker-Planck equation [7], involving the Fokker-Planck operator Γ:

$$\frac{\partial\omega_2}{\partial t}=\Gamma(Z_1)\omega_2 . \quad (3.26)$$

For the pair average, we have

$$\langle\langle f(t_1)f(t_2)\rangle\rangle\equiv\langle\langle f(t)f(0)\rangle\rangle$$
$$=\int Ze^{\Gamma t}ZP(Z,0)dZ . \quad (3.27)$$

For the stationary OU process, $\Gamma(Z)$ is given by [7]

$$\Gamma(Z)=\lambda\frac{\partial}{\partial Z}\left[Z+\sigma^2\lambda\frac{\partial}{\partial Z}\right] . \quad (3.28)$$

Introducing the scaled variable y as $Z/\sigma\lambda^{1/2}$, we have

$$\Gamma=\lambda\frac{\partial}{\partial y}\left[y+\frac{\partial}{\partial y}\right] . \tag{3.29}$$

It is straightforward to demonstrate [6,7] that the modified, transformed operator $\bar{\Gamma}$, given by

$$\bar{\Gamma}=\exp(y^2/2)\Gamma\exp(-y^2/2) , \tag{3.30}$$

is Hermitian and is related to a harmonic-oscillator Hamiltonian:

$$\bar{\Gamma}=-\lambda\left[\frac{1}{2}\frac{\partial^2}{\partial y^2}+\frac{1}{2}y^2-\frac{1}{2}\right] . \tag{3.31}$$

Its eigenfunctions are the harmonic-oscillator eigenfunctions h_n:

$$\bar{\Gamma}|h_n\rangle=\lambda_n|h_n\rangle , \tag{3.32a}$$

$$\langle h_n|\bar{\Gamma}=\langle h_n|\lambda_n . \tag{3.32b}$$

The eigenvalues λ_n are $-n\lambda$, $n=0,1,\ldots$.

The right and left eigenfunctions of the non-Hermitian operator Γ are given by

$$|B_n\rangle=e^{-y^2/2}|h_n\rangle , \tag{3.33a}$$

$$\langle\bar{B}_n|=\langle h_n|e^{y^2/2} . \tag{3.33b}$$

They form a biorthogonal set. Since $\langle y|h_n\rangle\sim e^{-y^2/2}$, we have, in particular,

$$\langle y|B_0\rangle\sim e^{-y^2} , \tag{3.34a}$$

$$\langle\bar{B}_0|y\rangle=1 . \tag{3.34b}$$

Also, from Eqs. (3.32), we have

$$\Gamma|B_0\rangle=\langle\bar{B}_0|\Gamma=0 . \tag{3.35}$$

We have from Eqs. (3.27) and (3.34) the relation

$$\begin{aligned}\langle\langle f(t_1)f(t_2)\rangle\rangle&=\sigma^2\lambda\langle h_0|ye^{\bar{\Gamma}|t_1-t_2|}y|h_0\rangle\\&=\sigma^2\lambda\langle h_0|y|h_1\rangle\langle h_1|y|h_0\rangle e^{-\lambda|t_1-t_2|}\\&=\frac{\sigma^2\lambda}{2}e^{-\lambda|t_1-t_2|} .\end{aligned} \tag{3.36}$$

Thus, we can recover our choice for f by requiring $\sigma=1$. Moreover, using Eq. (3.35), we may write

$$\begin{aligned}\langle\langle f(t_1)f(t_2)\rangle\rangle=\sigma^2\lambda\langle\bar{B}_0|e^{-\Gamma t_>}ye^{\Gamma t_>}\\\times e^{-\Gamma t_<}ye^{\Gamma t_<}|B_0\rangle ,\end{aligned} \tag{3.37}$$

where $t_>$ and $t_<$ are the greater and lesser of t_1 and t_2, respectively. Introducing the time-ordering operator T, we have

$$\begin{aligned}\langle\langle f(t_1)f(t_2)\rangle\rangle=\sigma^2\lambda\langle\bar{B}_0|T(e^{-\Gamma t_1}ye^{\Gamma t_1}\\\times e^{-\Gamma t_2}ye^{\Gamma t_2})|B_0\rangle .\end{aligned} \tag{3.38}$$

Equation (3.38) is now *in clear correspondence with the boson mapping*, Eq. (2.5), introduced by us. It also implies that $f(t)$ is essentially given by

$$f(t)=e^{-\Gamma t}ye^{\Gamma t} . \tag{3.39}$$

Let us now consider the dynamical equation involving the stochastic Hamiltonian, Eq. (2.3):

$$i\frac{\partial U}{\partial t}=[H_0+gf(t)(V+V^\dagger)]U . \tag{3.40}$$

Using Eq. (3.39), we have

$$\begin{aligned}i\frac{\partial U}{\partial t}\rightarrow i\frac{\partial U(y,t)}{\partial t}\\=[H_0+g\lambda^{1/2}e^{-\Gamma t}ye^{\Gamma t}(V+V^\dagger)]U(y,t) ,\end{aligned} \tag{3.41}$$

and R is then given by

$$R(t)=\int U(y,t)P(y)dy=\langle\bar{B}_0|U(y,t)|B_0\rangle , \tag{3.42}$$

with $P(y)=\sigma\lambda^{1/2}P(Z,0)$. Introducing the modified operator $\bar{U}_B$, given by

$$\bar{U}_B=e^{\Gamma t}U , \tag{3.43}$$

we have

$$i\frac{\partial\bar{U}_B(y,t)}{\partial t}=[H_0+g\lambda^{1/2}y(V+V^\dagger)+i\Gamma]\bar{U}_B(y,t) , \tag{3.44}$$

which is the celebrated Kubo-Schrödinger equation [4,7], involving the Fokker-Planck operator Γ.

Let us take a close look at the essential change in going over from Eq. (3.40) to Eq. (3.44). The stochastic evolution in $f(t)$ in Eq. (3.39) is mapped onto an evolution governed by the Fokker-Planck operator Γ in Eq. (3.44). The time dependence of $\bar{U}_B(t,0)$ is thus separated into evolution of y via Γ and the true dynamical evolution via the time dependence of $V(t)$. Finally, via Eq. (3.42), the stochastic average over f for R is mapped to integration of y over the measure $P(y)$. $U(y,t)$ is called the *marginal average* [3–7] of U.

The relation of Eq. (3.44) with our deterministic Eq. (2.10) is now clearly discernible. Introducing the Hermitian operator $\bar{\Gamma}$ from Eq. (3.31), by defining

$$U_B=e^{y^2/2}\bar{U}_B , \tag{3.45}$$

we have

$$i\frac{\partial U_B(y,t)}{\partial t}=[H_0+g\lambda^{1/2}y(V+V^\dagger)+i\bar{\Gamma}]U_B(y,t) . \tag{3.46}$$

In occupation-number representation, y may be written as

$$y=\frac{1}{\sqrt{2}}(b+b^\dagger) , \tag{3.47}$$

and $\bar{\Gamma}$ has the following expression via Eq. (3.39):

$$\bar{\Gamma}=-\lambda b^\dagger b . \tag{3.48}$$

Thus we have

$$i\frac{\partial U_B(y,t)}{\partial t}=[H_0+g(\lambda/2)^{1/2}(b+b^\dagger)(V+V^\dagger) -i\lambda b^\dagger b]U_B(y,t)\ , \tag{3.49}$$

which is nothing but Eq. (2.10), with h_B given by $-i\lambda b^\dagger b$ [i.e., Eq. (2.9a)]. Thus our deterministic equation is a *special representation* of the Fokker-Planck Eq. (3.44), where Γ is transformed to a Hermitian operator $\overline{\Gamma}$, leading to Eq. (3.49). Also, $|h_0\rangle$ is nothing but the boson vacuum $|0_B\rangle$. We reiterate here that the time ordering appearing in Eq. (3.38) appears naturally in Eq. (2.5).

In an exactly analogous manner, the complex Gaussian process may be generated by writing $f(t)$ as a sum of two independent real Gaussian variables:

$$f(t)=\frac{1}{\sqrt{2}}[f_1(t)+if_2(t)]\ , \tag{3.50}$$

with

$$\langle\langle f_i(t_1)f_j(t_2)\rangle\rangle=\delta_{ij}\frac{\lambda}{2}e^{-\lambda|t_1-t_2|}\ . \tag{3.51}$$

It then follows by reasonings similar to those for the real Gaussian processes, that the Fokker-Planck equation for the complex Gaussian process is exactly equivalent to Eq. (2.10), with

$$h_B=-\lambda(b^\dagger b+c^\dagger c)\ ,$$

with $(b,b^\dagger)$ and $(c,c^\dagger)$ bosons emerging from f_1 and f_2, respectively.

In the traditional solution of the Kubo-Schrödinger equation, Eq. (3.44), $\overline{U}_B|B_0\rangle$ is expanded in terms of the eigenfunctions of the Fokker-Planck operator $\overline{\Gamma}$ [4,7]. As an example, for the real noise we have

$$\overline{U}_B|B_0\rangle=e^{-y^2/2}\sum_n C_n|h_n\rangle\ , \tag{3.52}$$

where C_n's contain the operators of the *physical* Bose-Fermi variables. In the operator language, the transformed U_B, from Eq. (3.45), can be written as

$$U_B=\sum_n\frac{C_n}{\sqrt{n!}}b^{\dagger n}\ , \tag{3.53}$$

and C_n's are solved either by a continued-fraction expansion using a partitioning technique [7] or by a direct solution of the coupled equations for C_n [7]. In either case, R is given by C_0. This mode of *linear* expansion of U_B should be contrasted with the *exponential* representation of U_B, as appears in $\{\exp(S_B)\}\{\exp(X_B)\}$ in our cluster-cumulant theory. The cluster-cumulant theory invokes a coupled-cluster (CC) expansion, while the Fokker-Planck dynamics involves a *configuration-interaction* (CI) type of expansion. The cluster-cumulant approach is thus expected to bring in the advantages of a compact and rapidly convergent description of a CC formalism in the treatment of stochastic dynamics.

When the Lie algebra of H_B is complete, the possible cluster-cumulant operators are *finite in number,* and hence an exact solution of the cluster-cumulant equations is possible. The additional advantage is the *finiteness* of the powers of the cluster operator in the equation due to normal ordering imposed on the operators $U_{\rm ex}$ and U_M. In contrast, the corresponding CI-like expansion in Eq. (3.52) may still be infinite. This is quite similar to what happens in the CI-like expansion of a nonstochastic time-dependent problem vis-à-vis an exponential-like representation in TDCC [14]. We shall come back again to these two different modes of representation of U_B by taking up a concrete example in Sec. IV.

IV. ILLUSTRATIVE APPLICATIONS

In this section, we shall illustrate our formalism by applying it to two simple yet nontrivial problems, viz., a harmonic oscillator, which is linearly perturbed by a term involving a multiplicative real or complex OU colored noise:

$$H=\omega_0 a^\dagger a+g[f(t)a^\dagger e^{-i\omega t}+\text{H.c.}]\ . \tag{4.1}$$

We shall discuss in detail below how the closed and external operators are chosen, depending on the model space, and how a diagrammatic approach helps us to set up the cluster-cumulant equations systematically in a convenient manner. We shall also illustrate how the equations automatically factorize into various valence sectors. Since our cluster-cumulant method furnishes exact results for these problems, we shall study them for a wide range of parameters and assess the validity of the corresponding perturbative cumulant results.

A. Real noise

We consider the case of the real noise first. The Hamiltonian H_B, according to Eqs. (2.9a), (2.10), and (2.11a), is given by

$$H_B=\omega_0 a^\dagger a+g(\lambda/2)^{1/2}(b+b^\dagger) \times(a^\dagger e^{-i\omega t}+ae^{i\omega t})-i\lambda b^\dagger b\ . \tag{4.2}$$

For this problem, it is convenient to go over to the interaction representation for the unperturbed operator for the oscillator, viz., $\omega_0 a^\dagger a$.

The ground-state case. If we want to compute R governing the evolution of the unperturbed system ground state $|0_S\rangle$, then the space P is one-dimensional, spanned by the vacuum $|0_S\rangle\otimes|0_B\rangle$. Since there are no excitations in $|0_S\rangle$, this is a *zero-valence* problem. The possible external and closed operators can be discerned by collecting all the distinct operators from H_B, $\{\overline{H_B\,H_B}\}$,. . . etc. into the respective categories, depending on their actions on the state $|0_S\rangle\otimes|0_B\rangle$. Since the Lie algebra for this Hamiltonian is closed, there are a finite number of distinct operators. The only possible external operators (entering S_B) are $a^{\dagger 2}$, $a^\dagger b^\dagger$, and $b^{\dagger 2}$, viz., the ones that can excite from the model space, and the only possible closed operator (entering X_B) is unity, I. We thus write the *exact* $U_{\rm ex}$ and U_M for *UP* for this zero-valence model space as

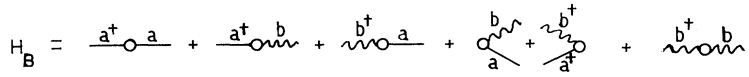


FIG. 1. Vertices for the operators of H_B for the real noise. The straight and wiggly lines denote, respectively, the system and the stochastic boson operators.

$$U_{\rm ex} \equiv \{\exp(s_0^2 a^{\dagger 2}/2 + s_2^0 b^{\dagger 2}/2 + s_1^1 a^\dagger b^\dagger)\} , \tag{4.3}$$

$$U_M \equiv \{\exp(x_0)\} . \tag{4.4}$$

We shall derive the cluster-cumulant equations for S_B and X_B by resorting to the diagrammatics. The vertices and the operators of H_B can be diagrammatically depicted as in Fig. 1, where we distinguish the system $(a^\dagger, a)$ and the stochastic $(b^\dagger, b)$ boson variables by straight and wiggly lines, respectively. The S_B and X_B vertices are likewise displayed in Fig. 2. For this zero-valence problem, all the closed operators are numbers; hence the closed operator X_B shown in Fig. 2 has no external lines to it. Similarly, the closed operator $H_{\rm eff}^B$, too, is a number and hence cannot appear in the contracted terms like $\exp(S) H_{\rm eff}$ or $H_{\rm eff} \exp(X)$ in Eqs. (2.19) and (2.20). This leads to considerable simplification of the associated cluster-cumulant equations, similar to the reduction of TDMRCC equations to the single reference case [17]. The equations for s_0^2, s_2^0, and s_1^1 can be set up by connecting an H_B vertex with one or more S_B vertices sitting on its right in all possible ways and collecting all the topologically inequivalent composites into blocks having shapes of s_0^2, s_2^0, and s_1^1. Since we are working in the interaction representation for the unperturbed oscillator, the term $\omega_0 a^\dagger a$ (the first diagram for H_B in Fig. 1) does not appear while constructing the diagrams. The full set of diagrams entering the equations for S_B is displayed in Fig. 3(a). When there are equivalent lines in a diagram, we attach a topological weight of $1/n!$ for n equivalent lines. Thus the second and third equations shown in Fig. 3(a) should have a factor $\frac{1}{2}$ on the left side. The equation for X_B should contain only completely contracted terms obtained from an H_B vertex and any number of S_B vertices. This is illustrated in Fig. 3(b).

We display below, for the sake of completeness, the cluster-cumulant equations generated from the diagrams of Fig. 3:

$$i\dot{s}_1^1 = g(\lambda/2)^{1/2}(e^{-i\delta t} + e^{i\delta t} s_1^1 s_1^1 + e^{i\delta t} s_2^0 s_0^2 + e^{i\delta t} s_0^2 + e^{-i\delta t} s_2^0) - i\lambda s_1^1 , \tag{4.5a}$$

$$i\dot{s}_2^0 = 2g(\lambda/2)^{1/2}(e^{i\delta t} s_2^0 s_1^1 + e^{i\delta t} s_1^1) - 2i\lambda s_2^0 , \tag{4.5b}$$

$$i\dot{s}_0^2 = 2g(\lambda/2)^{1/2}(e^{i\delta t} s_0^2 s_1^1 + e^{-i\delta t} s_1^1) , \tag{4.5c}$$

$$i\dot{x}_0 = g(\lambda/2)^{1/2} e^{i\delta t} s_1^1 , \tag{4.6}$$

where the detuning parameter δ is defined as $\delta = (\omega - \omega_0)$. The action of the operator R for the evolution from $|0_S\rangle$ is given by

$$R \equiv (\langle 0_B | U_B | 0_B \rangle \otimes |0_S\rangle) = \left\{ \exp(s_0^2) \frac{a^{\dagger 2}}{2} \right\} |0_S\rangle \exp(x_0) . \tag{4.7}$$

The survivality of $|0_S\rangle$ is given by

$$P_{00} = \exp(2\,{\rm Re} x_0) . \tag{4.8}$$

We have solved Eqs. (4.5) and (4.6) using a Runge-Kutta initiation followed by Adams-Moulton's predictor-corrector method [19]. No stiffness of the equations was encountered in this case for a wide range of coupling constant g and the decay time λ.

As discussed in Sec. III, we have found that iteration of our equations, written in the interaction representation for both V and the stochastic boson operators, in powers of V, yields the Fox-Kubo cumulant results. We quote the second-order expression for X_B as an illustration. The second-order cumulant expression of x_0 is given by

$$x_0 = \frac{g^2 \lambda t}{2(i\delta - \lambda)} + \frac{g^2 \lambda}{2(i\delta - \lambda)^2} (1 - e^{(i\delta - \lambda)t}) . \tag{4.9}$$

The fourth-order expressions have also been computed. They are lengthy and are not reproduced here.

Figure 4 shows the plot of the survivality of the state $|0_S\rangle$ versus time at the resonance, $\delta = 0$, for a range of values of λ and g. There are no quantum oscillations at the resonance. As expected, larger values of λ and g induce sharper decays. Figure 5 displays some typical graphs for survivality for an off-resonance case, with $\delta = 2.0$. Though the survivality eventually decays with time, the decay is preceded by oscillations during the initial time ranges. The oscillations are particularly evident for larger g's and smaller λ's.

To check the limit of validity of the Fox-Kubo perturbative cumulant theory, we now compare our exact values with the second- and fourth-order cumulant results. Figures 6(i) and 6(ii) display some second-order cumulant results vis-à-vis the exact results for various values of g and λ. Figures 6(iii) and 6(iv) show the corresponding fourth-order results. The second-order cumulant results show pronounced spurious oscillations and behave in a qualitatively different manner as compared to the exact results for large values of g ($g = 4$, in this case). The fourth-order cumulant results are much better, being substantially closer to the exact ones, though deviations are still appreciable for larger values of g. The second-order results generally show slower decay rates, while the fourth-order results overestimate the decay. The cumulant results are, generally speaking, not quite valid either for longer times or for larger couplings.

FIG. 2. S_B and X_B operators for the zero-valence problem for real noise.

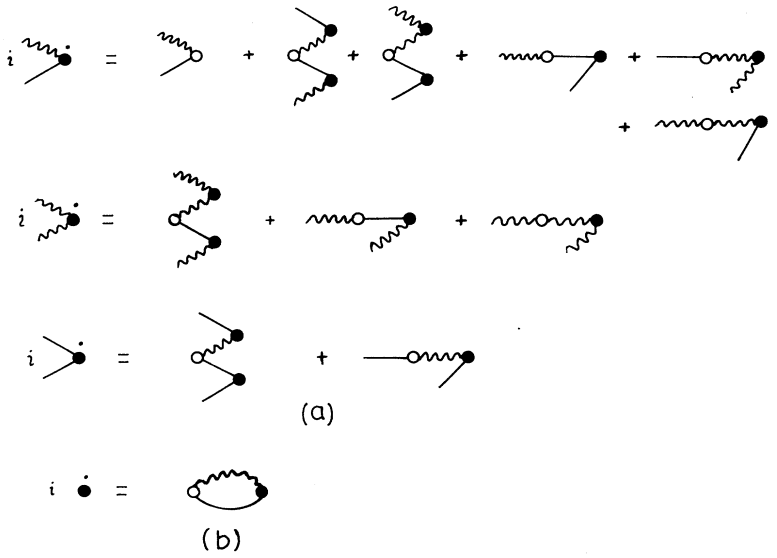


FIG. 3. Cluster-cumulant equations for the zero-valence problem for the real noise. (a) and (b) depict the equations for S_B and X_B, respectively.

The first-excited-state case. For computing the survivality of the first excited state $|1_S\rangle$, we choose the model space P to be $|1_S\rangle\otimes|0_B\rangle$. Since $|1_S\rangle$ is singly excited with respect to the system boson variable, it is a *one-valence problem.* The external operators in this case can thus contain up to one destruction operator of the system boson variables. The closed operators also can have up to one system boson destruction operator. In the category of external operators, we now have the same zero-valence operators as in the ground-state problem, viz., $a^{\dagger 2}$, $b^{\dagger 2}$, and $a^{\dagger}b^{\dagger}$, but in addition, we also have a one-valence operator $b^{\dagger}a$, with one destruction operator a. In X_B, similarly, we have the old zero-valence operator X_0 and also a new one-valence operator $a^{\dagger}a$. The

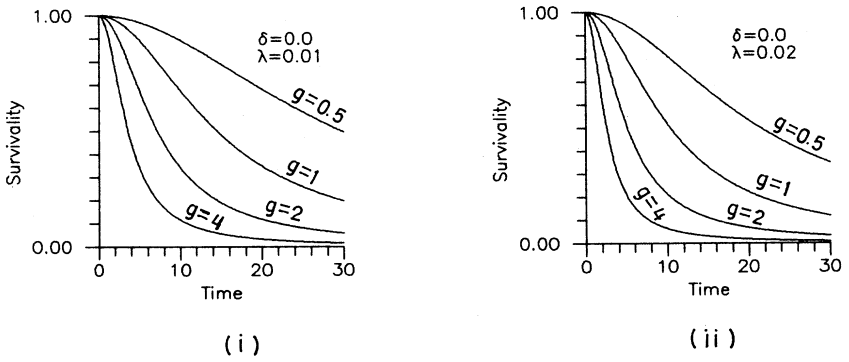
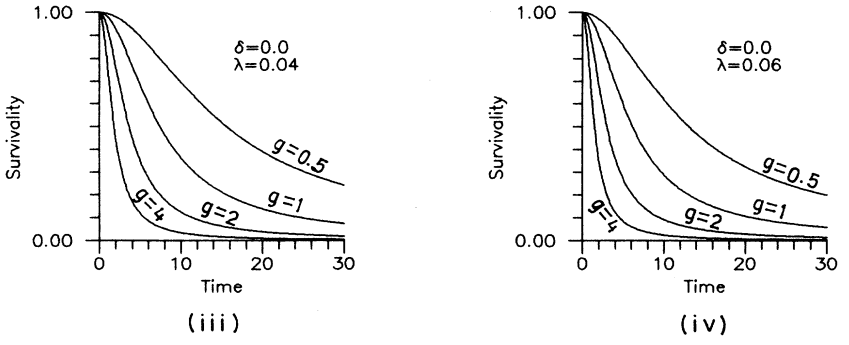


FIG. 4. Plots of the survivality of the state $|0_S\rangle$ for various values of λ and g for the real noise. $\delta=0.0$.



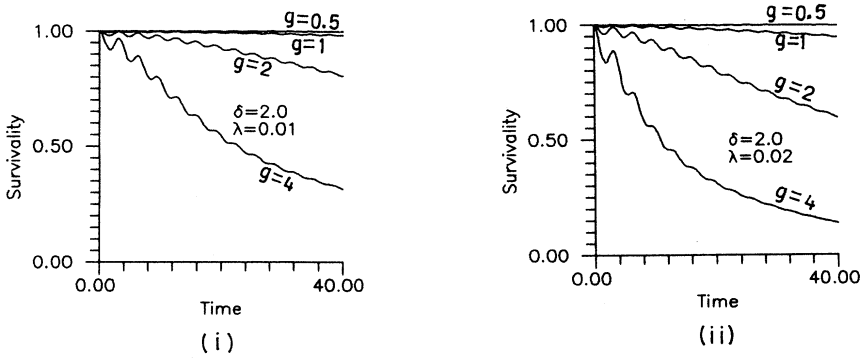
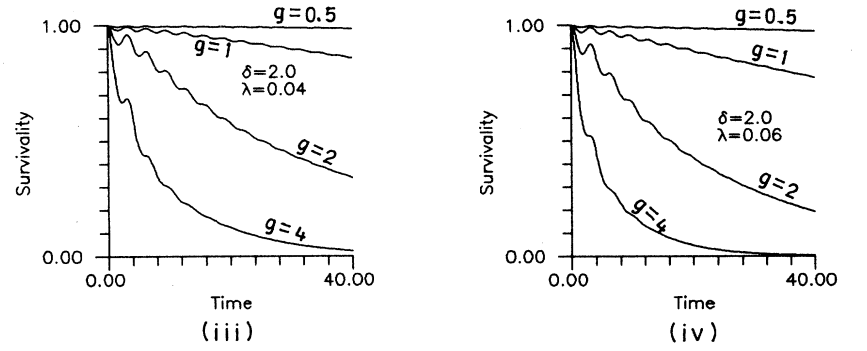


FIG. 5. Plots of the survivality of the state $|0_S\rangle$ for various values of λ and g for the real noise. $\delta=2.0$.



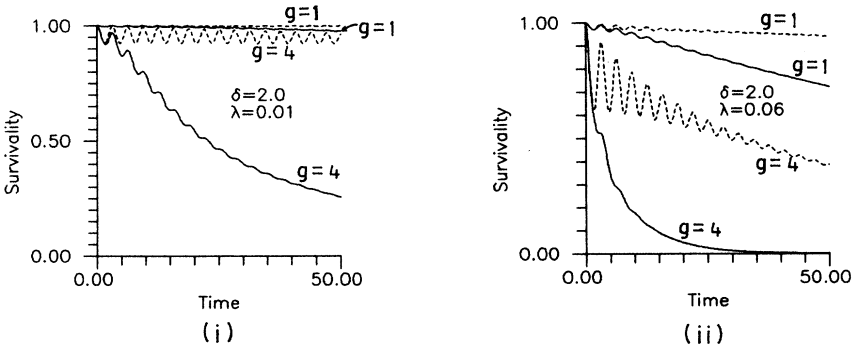
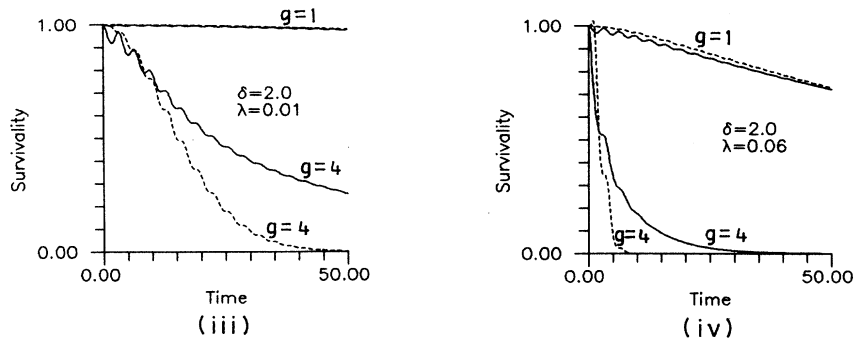


FIG. 6. Comparative graphs showing performance of the perturbative cumulant vis-à-vis exact (cluster-cumulant) results. (i) and (ii) show the second-order and (iii) and (iv) show the fourth-order cumulant results. The dotted lines represent the perturbative results.



operators U_{ex} and U_M for the one-valence problem are then of the forms

$$U_{ex}=\{\exp(s_0^2 a^{\dagger 2}/2+s_2^0 b^{\dagger 2}/2+s_1^1 a^\dagger b^\dagger+s_1^{-1} b^\dagger a)\}\ , \tag{4.10}$$

$$U_m=\{\exp(x_0+x_1 a^\dagger a)\}\ . \tag{4.11}$$

We should note here that, since the stochastic boson vacuum $|0_B\rangle$ always appears in the model spaces, we can never have the closed operator $b^\dagger b$ in U_M, viz., our model spaces are all zero valence with respect to the stochastic boson.

Owing to the normal ordering, the equations for the zero-valence cluster amplitudes are completely decoupled from those of the one-valence ones. This hierarchical decoupling, called the subsystem embedding condition (SEC) by us [13,15], is quite general and is typical of the cluster-cumulant methodology. The zero-valence sector of the problem provides us with the same values for s_0^2, s_2^0, and s_1^1 as in the ground-state case. The one-valence equations for s_1^{-1} and x_1 are the only ones we have to solve. These can again be generated conveniently by using diagrams, as illustrated in Fig. 7. Figure 7(a) displays the vertices of the new one-valence S_B and X_B operators. Since $H_{\rm eff}^B$ for the one-valence case has a one-valence operator part, the associated diagrams are displayed in Fig. 7(b). Figures 7(c) and 7(d) show, respectively, the equations for s_1^{-1} and x_1.

Again for completeness, we write below the algebraic equations for s_1^{-1} and x_1:

$$i\dot{s}_1^{-1}=g(\lambda/2)^{1/2}(e^{i\delta t}+e^{i\delta t}s_2^0-e^{-i\delta t}s_1^{-1}s_1^{-1} -e^{i\delta t}s_1^{-1}s_0^2 s_1^{-1})-i\lambda s_1^{-1}\ , \tag{4.12a}$$

$$i\dot{x}_1=g(\lambda/2)^{1/2}(e^{i\delta t}s_1^1+e^{-i\delta t}s_1^{-1}+e^{i\delta t}s_1^{-1}s_0^2 +e^{i\delta t}s_1^1 x_1+e^{-i\delta t}s_1^{-1}x_1 +e^{i\delta t}s_1^{-1}s_0^2 x_1)\ . \tag{4.12b}$$

The instructive point here is to note that, in these equations, the zero-valence cluster amplitudes s_0^2, s_2^0, s_1^1, and x_0 appear as *known time-dependent quantities.*

The survivality of the state $|1_S\rangle$ is given by

$$P_{11}=\exp(2\,\mathrm{Re}x_0)|(1+x_1)|^2\ . \tag{4.13}$$

Figure 8 displays the plot of P_{11} versus time for a range of values of g and λ for the resonance situation, $\delta=0$. Again there are no oscillations, but the decay is faster for the excited state than for the ground state for the same values of the parameters. Figure 9 shows similar plots for a typical off-resonance case, with $\delta=2.0$. The general nature of the decay is now oscillatory, with a tendency for faster decay for both larger g and λ, as expected.

To check the performance of the perturbative cumulant theory, we show in Figs. 10(i) and 10(ii) the second-order results, and in Figs. 10(iii) and 10(iv) the fourth-order results. The oscillations are stronger for the second-order results than for the fourth-order, and all of them are substantially deviant from the exact results for larger times. The deviation increases with increase in g. As λ increases, the deviation decreases for the same value

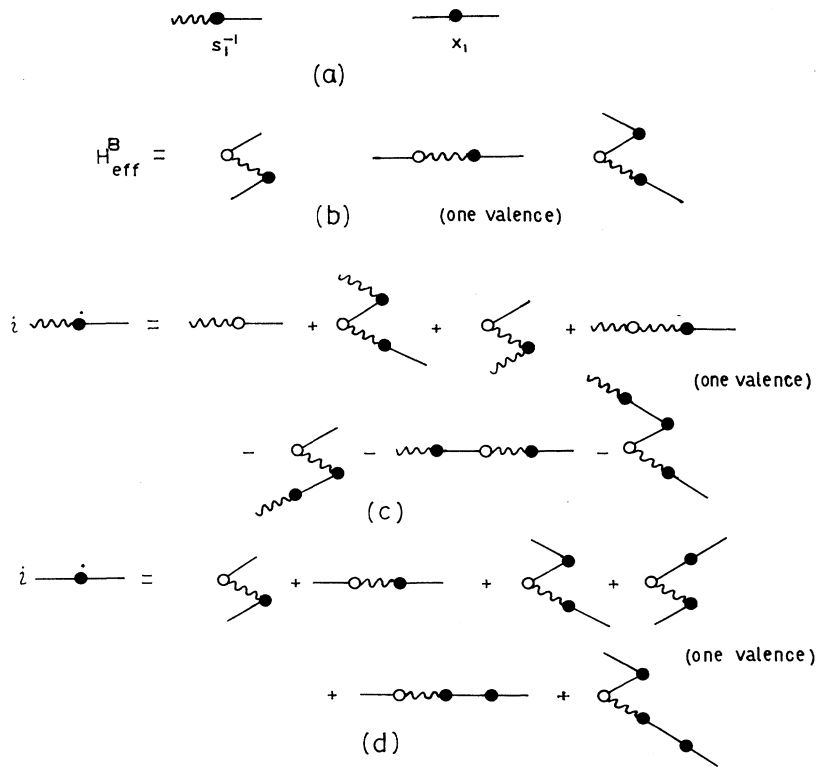


FIG. 7. (a) One-valence S_B and X_B operators for the excited state $|1_S\rangle$ for real noise. (b) The diagrams entering the one-valence part of $H_{\rm eff}^B$. (c) The diagrammatic equation for the one-valence S_B, s_1^{-1}. (d) The diagrammatic equation for the one-valence X_B, x_1.

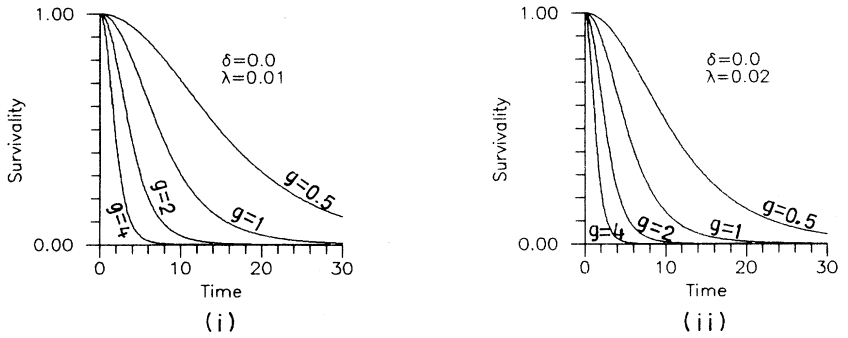
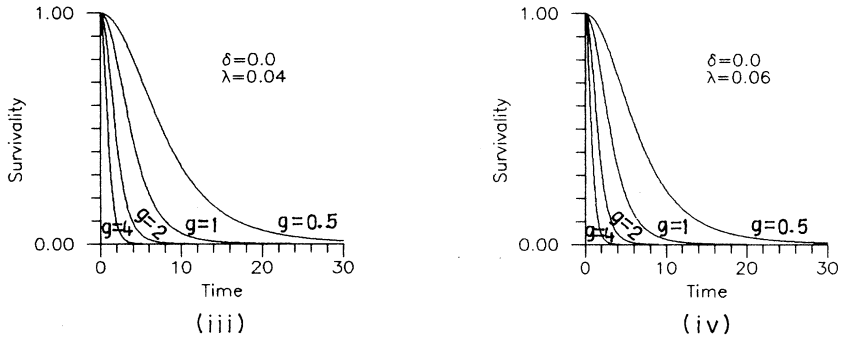


FIG. 8. Plots of the survivality of the state $|1_S\rangle$ for various values of λ and g for the real noise. $\delta=0.0$.



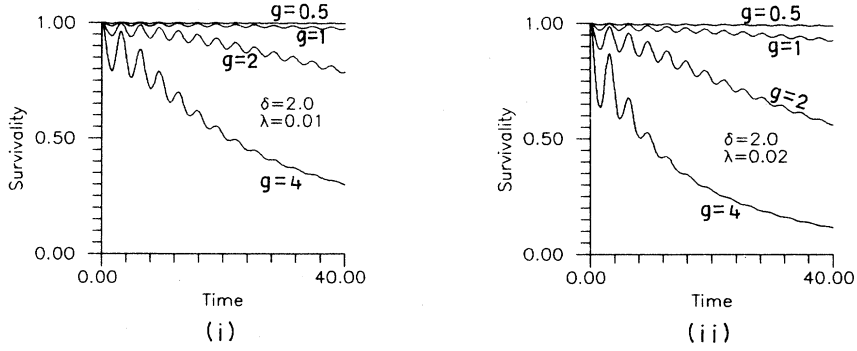
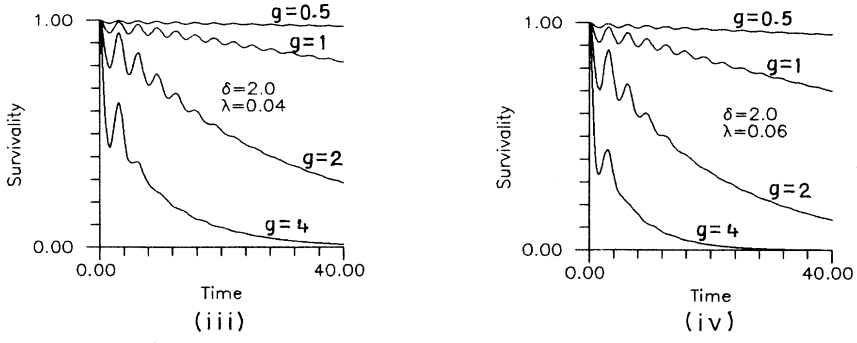


FIG. 9. Plots of the survivality of the state $|1_S\rangle$ for various values of λ and g for the real noise. $\delta=2.0$.



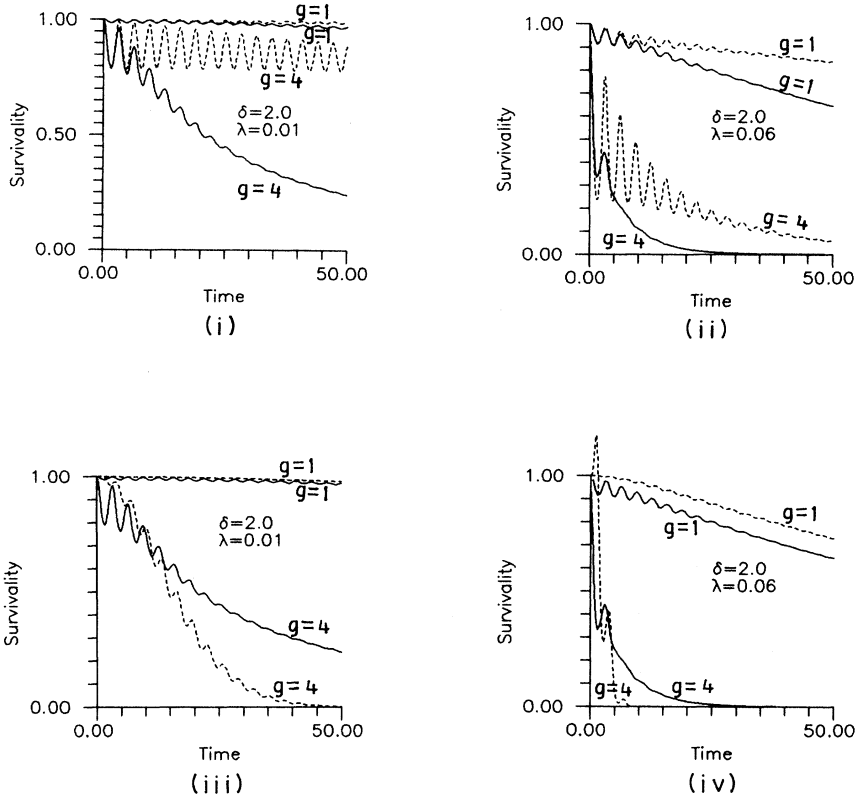


FIG. 10. Comparative graphs showing the performance of the perturbative cumulant vis-à-vis the exact (cluster-cumulant) results. (i) and (ii) show second-order and (iii) and (iv) show fourth-order results. The dotted lines represent the perturbative results.

of g, since, for larger λ, we pass the characteristic noise correlation time $\tau_c \sim 1/\lambda$ relatively more quickly, and thus multiple perturbative interactions become relatively less important. The fourth-order cumulant plot for $g=4$ and $\lambda=0.06$ shows even some spurious oscillations at very short time intervals. The multiple interactions within the interval are obviously quite important. In any case, for large coupling, $g \sim 4$, we are quite clearly beyond the validity of the perturbative regime.

For the real noise, we never encountered stiffness of the cluster-cumulant equations and thus we never needed to go over to the equivalent equations generated by the Riccati transformation, described in the Appendix.

We should note in passing that, for real noise, the choice of the doubly excited state $|2_S\rangle$ in the model space, viz., $P \equiv |2_S\rangle \otimes |0_B\rangle$, *exhausts the Lie algebra and the globally exact* U_B, and $R(t)$ for arbitrary initial functions can be generated. We do not undertake this exercise here, since this is not very illuminating. For the case of complex noise, even $|1_S\rangle$ exhausts the Lie algebra, which we describe now.

B. Complex noise

The problem for the complex noise has been treated recently using the path-integral formalism [18]. This solution involves quite complicated mathematical manipulations. In our formalism, we simply induce the corresponding boson mapping:

$$i\frac{\partial U_B}{\partial t} = \{\omega_0 a^\dagger a + g[(b+c^\dagger)a^\dagger e^{-i\omega t} + \text{H.c.}] - i\lambda(b^\dagger b + c^\dagger c)\} U_B \ . \tag{4.14}$$

The quantity inside the braces $\{\ \}$ is the mapped Hamiltonian H_B. The Lie algebra of H_B in Eq. (4.14) is closed, and hence again an *exact global solution* can be found by suitably choosing a model space.

For the ground-state problem, we again take the P space as $|0_S\rangle \otimes |0_B\rangle$. The external operators are $a^\dagger c^\dagger$ and $b^\dagger c^\dagger$, and the closed operator is x_0. For the first excited state, the P space as $|1_S\rangle \otimes |0_B\rangle$, additional external $(b^\dagger a)$ and closed $(a^\dagger a)$ operators enter. Again, in the latter case, only the additional cluster-cumulant amplitudes need to be computed. In the case of complex noise, the choice $|1_S\rangle \otimes |0_B\rangle$ happens to exhaust all the operators that can give nonvanishing effects on $|0_B\rangle$ and, as a result, we can obtain the $U_B(t)$ and the *global* $R(t)$ as

$$U_B(t) = \{\exp(s_1 a^\dagger c^\dagger + s_2 b^\dagger c^\dagger + s_3 b^\dagger a)\} \times \{\exp(x_0 + x_1 a^\dagger a)\} \ , \tag{4.15}$$

$$R(t) = \langle 0_B | U_B | 0_B \rangle = \langle 0_B | U_M | 0_B \rangle = \{\exp(x_0 + x_1 a^\dagger a)\} \ . \tag{4.16}$$

We should note that, unlike in the real-noise case [Eq. (4.7)], U_{ex} in Eq. (4.15) can never contribute to $R(t)$ in Eq. (4.16), since all its terms involve stochastic creation

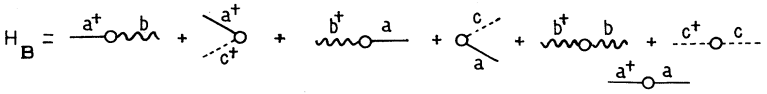


FIG. 11. Vertices for the operators of H_B for complex noise. The straight, wiggly, and dotted lines indicate the system $(a^\dagger, a)$ and the two types of stochastic boson operators $(b^\dagger, b$ and $c^\dagger, c)$.

operators $b^\dagger$ and $c^\dagger$. Equations can again be generated diagrammatically.

Figure 11 shows all the vertices of the Hamiltonian H_B. Since we have three types of bosons for the complex noise, we distinguish them as follows: straight solid lines for the system boson $(a^\dagger, a)$, and wiggly and dotted lines for the stochastic bosons $(b^\dagger, b$ and $c^\dagger, c)$, respectively. Figure 12 shows the various S_B and X_B operators for this problem. S_3 and X_1 are the one-valence operators, and the rest are all zero-valence. The zero- and one-valence components of H^B_{eff} are displayed in Figs. 13.

We derive the cluster-cumulant equations again in the interaction representation for the system boson variables. The last diagram of Fig. 11 would not thus contribute. Figure 14(a) displays the equations for S_B and X_B. Of these, Eqs. 14(a)(i), (ii), and (iv) are for the zero-valence problem and are decoupled from the rest, which are the one-valence one. In the latter, the zero-valence amplitudes appear as known time-dependent entities. We show below the algebraic expressions for the corresponding cluster-cumulant equations:

$$i\dot{s}_1 = g(\lambda/2)^{1/2}[e^{-i\delta t} + e^{i\delta t}(s_1)^2 + e^{-i\delta t}s_2] - i\lambda s_1 , \tag{4.17a}$$

$$i\dot{s}_2 = g(\lambda/2)^{1/2}(e^{i\delta t}s_1 + e^{i\delta t}s_2 s_1) - 2i\lambda s_2 , \tag{4.17b}$$

$$i\dot{s}_3 = g(\lambda/2)^{1/2}[e^{i\delta t} + e^{i\delta t}s_2 - e^{i\delta t}s_1 s_3 - e^{-i\delta t}(s_3)^2] - i\lambda s_3 , \tag{4.17c}$$

$$i\dot{x}_0 = g(\lambda/2)^{1/2}e^{i\delta t}s_1 , \tag{4.17d}$$

$$i\dot{x}_1 = g(\lambda/2)^{1/2}(e^{-i\delta t}s_3 + e^{i\delta t}s_1)(1+x_1) . \tag{4.17e}$$

For the case of complex noise, we have found [21] that a straightforward solution of the cluster-cumulant equations tends to become ill conditioned. This is due to their potential "stiffness" [19], as discussed in Sec. II C. We have bypassed this problem successfully by resorting to the inverse Riccati transformation, using the eigenvalue-independent partitioning described in the Appendix.

To do this, it is more convenient to go over to the original Schrödinger representation. The new variables are denoted by overbars on them. The cluster-cumulant equations are

$$i\dot{\bar{s}}_1 = g(\lambda/2)^{1/2}[1 + (\bar{s}_1)^2 + s_2] - (i\lambda + \delta)\bar{s}_1 , \tag{4.18a}$$

$$i\dot{s}_2 = g(\lambda/2)^{1/2}(\bar{s}_1 + s_2\bar{s}_1) - 2i\lambda s_2 , \tag{4.18b}$$

$$i\dot{\bar{s}}_3 = g(\lambda/2)^{1/2}[1 + s_2 - \bar{s}_1\bar{s}_3 - (\bar{s}_3)^2] - (i\lambda - \delta)\bar{s}_3 , \tag{4.18c}$$

$$i\dot{x}_0 = g(\lambda/2)^{1/2}\bar{s}_1 , \tag{4.18d}$$

$$i\dot{x}_1 = g(\lambda/2)^{1/2}(\bar{s}_3 + \bar{s}_1)(1+x_1) . \tag{4.18e}$$

By the "eigenvalue-independent partitioning technique" (EIP) [21], we get a set of matrix equations. From Eqs. (4.18a), (4.18b), and (4.18d) [see, e.g., Eq. (A10) of the Appendix], we have

$$i\begin{bmatrix}\dot{c}_1\\ \dot{c}_2\\ \dot{c}_3\end{bmatrix} = \begin{bmatrix}0 & -g_1 & 0\\ g_1 & -i\lambda-\delta & g_1\\ 0 & g_1 & -2i\lambda\end{bmatrix}\begin{bmatrix}c_1\\ c_2\\ c_3\end{bmatrix} , \tag{4.19}$$

where $g_1 = g(\lambda/2)^{1/2}$; with the initial conditions $c_1 = 1$, $c_2 = c_3 = 0$ at $t = 0$. $\bar{s}_1$ and s_2 are obtained from $\bar{s}_1 = c_1/c_2$ and $s_2 = c_3/c_1$ [e.g., Eq. (A7)]. From Eq. (4.18c), we have another matrix equation, with the initial condition $c_4 = 1$, $c_5 = 0$ at $t = 0$:

$$i\begin{bmatrix}\dot{c}_4\\ \dot{c}_5\end{bmatrix} = \begin{bmatrix}0 & g_1\\ g_1(1+s_2) & -(g_1\bar{s}_1 + i\lambda - \delta)\end{bmatrix}\begin{bmatrix}c_4\\ c_5\end{bmatrix} . \tag{4.20}$$

Substituting the values of $\bar{s}_1$ and s_2 from Eq. (4.19) to Eq. (4.20) and solving Eq. (4.20), the value of $\bar{s}_3$ is determined from the relation $\bar{s}_3 = c_5/c_4$. The results are presented for x_0 and x_1, after reverting to the interaction representation. We note that $x_0 = \bar{x}_0$, being a number. We should mention here that a special case of this technique has been described in a recent work by Joder [20].

For the complex noise, the amplitudes for the closed operators X_0 and X_1 show very interesting variations with time. They are also generally complex. Since their moduli appear in the expression for survivalities, we lose the information regarding the individual behavior of their real and imaginary parts in the expression for the sur-

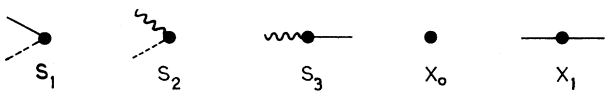


FIG. 12. Zero- and the one-valence S_B and X_B operators for the complex noise.

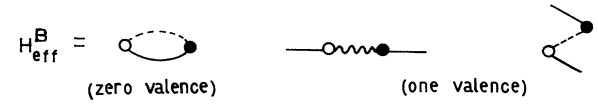


FIG. 13. Zero- and one-valence H^B_{eff} diagrams for the complex noise.

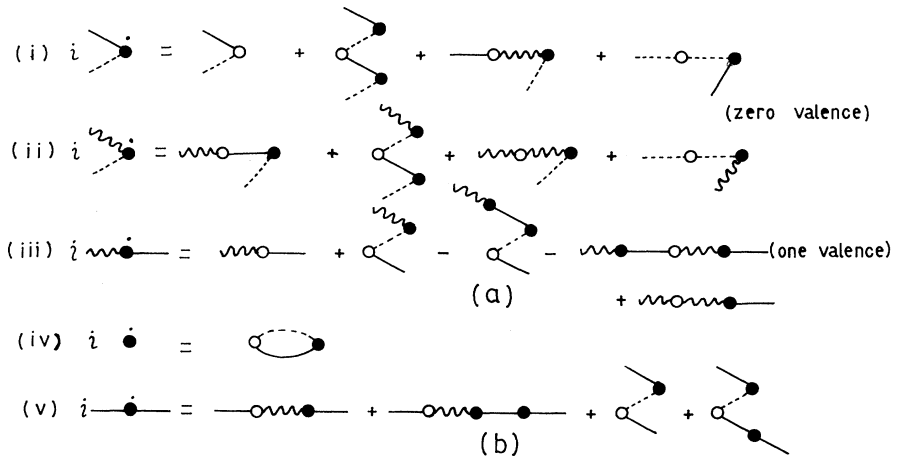


FIG. 14. Diagrams for the zero- and the one-valence cluster-cumulant equations for the complex noise. (a) shows the equations for S_B. (b) Shows the equations for X_B.

vivalities. For the complex noise, we would thus display the real and imaginary parts of x_0 and x_1 themselves.

For the resonance case, $\delta=0$, x_0 and x_1 are both real. Figure 15 shows the plots of x_0 and x_1 for various values of λ and g. The ground-state component of X_B, x_0, shows smooth decay with time, the rate being faster for larger g and λ. The analogous survivality would also thus show a smooth nonoscillatory exponential decay. The behavior for the X_B amplitude for the one-valence situation is more interesting. This clearly shows oscillatory behavior, being more pronounced for larger g and λ. x_1 reaches a value of -1.0 for longer times. Since the survivality for the excited state is of the form $\exp(2\,\mathrm{Re}x_0)(1+x_1)^2$, this reaches zero. The ground-state survivality has just the value $\exp(2\,\mathrm{Re}x_0)$, so the excited state decays much faster than the ground state.

Figure 16 displays the comparison of the second-order cumulant values with the exact results. The plots for x_0 reveal that the second-order results are quite poor when g is large. More striking is the behavior of x_1. The second-order cumulant results do not show the oscillatory behavior predicted by the exact results. For $\lambda=0.05$,

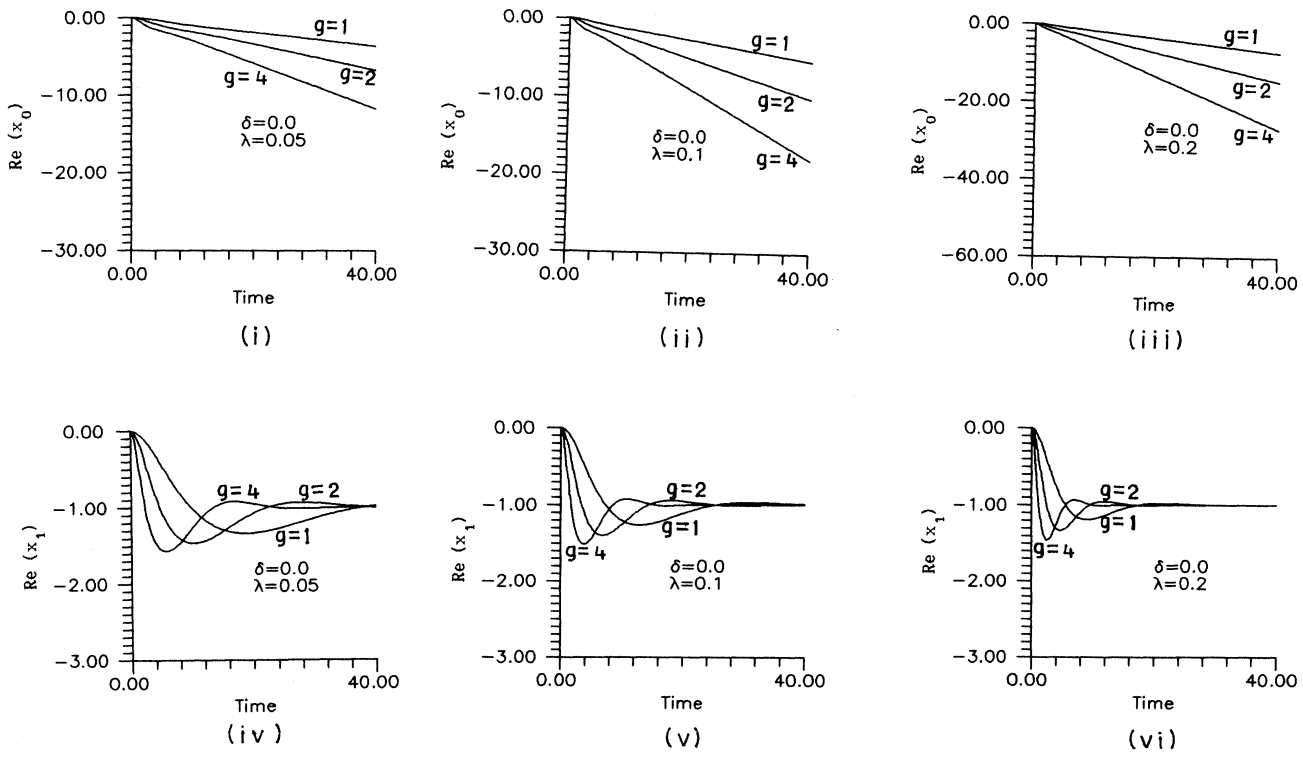


FIG. 15. Plots of x_0 and x_1 for various values of λ and g for the complex noise. $\delta=0.0$.

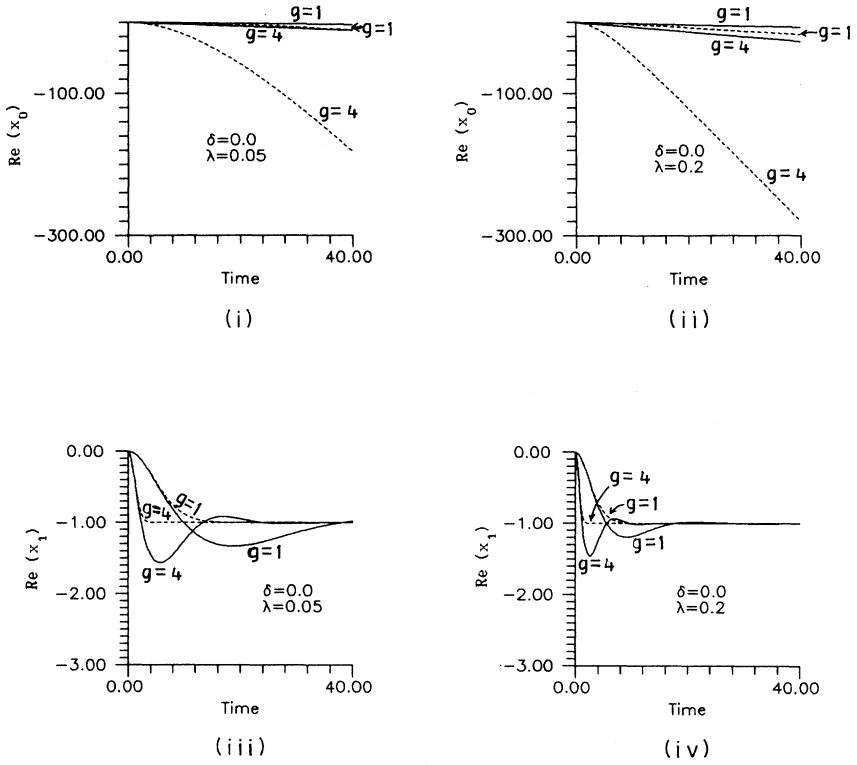


FIG. 16. Comparative graphs showing performance of the perturbative second-order cumulant vis-à-vis the exact (cluster-cumulant) results. $\delta=0.0$. The dotted lines represent the perturbative results.

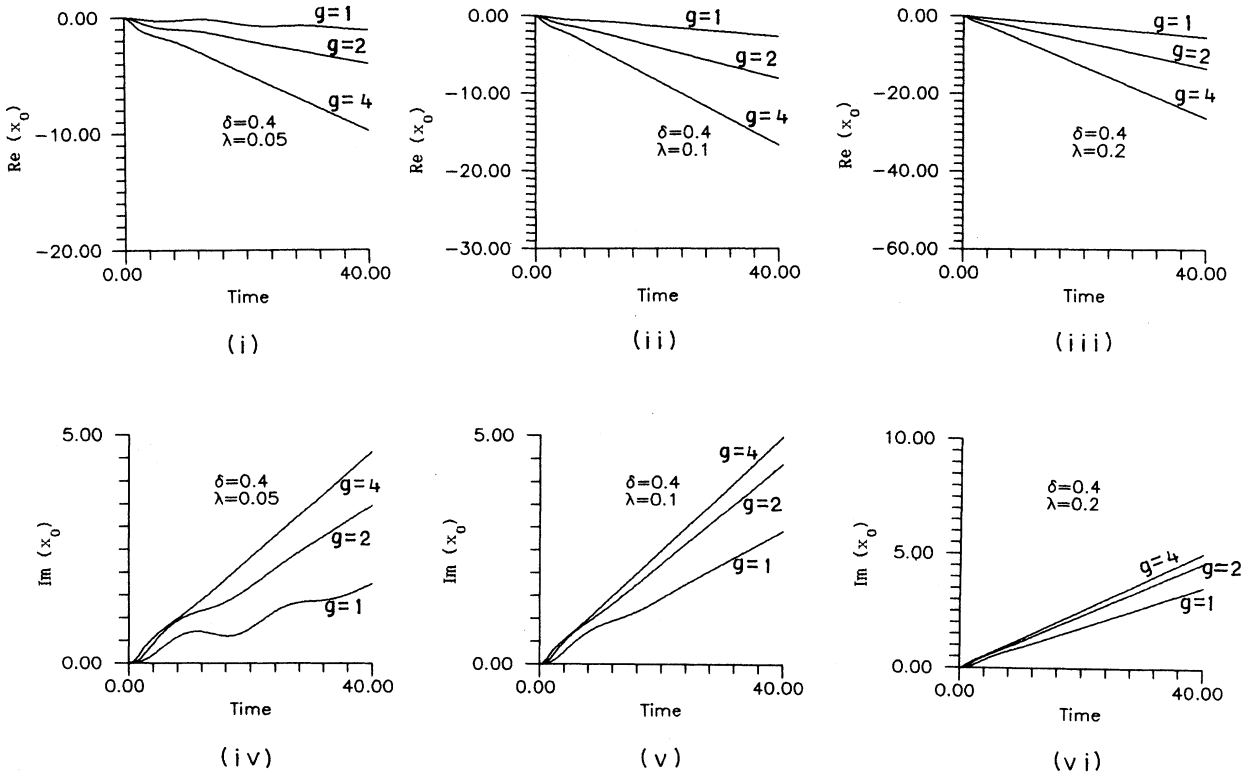


FIG. 17. Plots of the real and imaginary parts of x_0 with time for the complex noise. $\delta=0.4$.

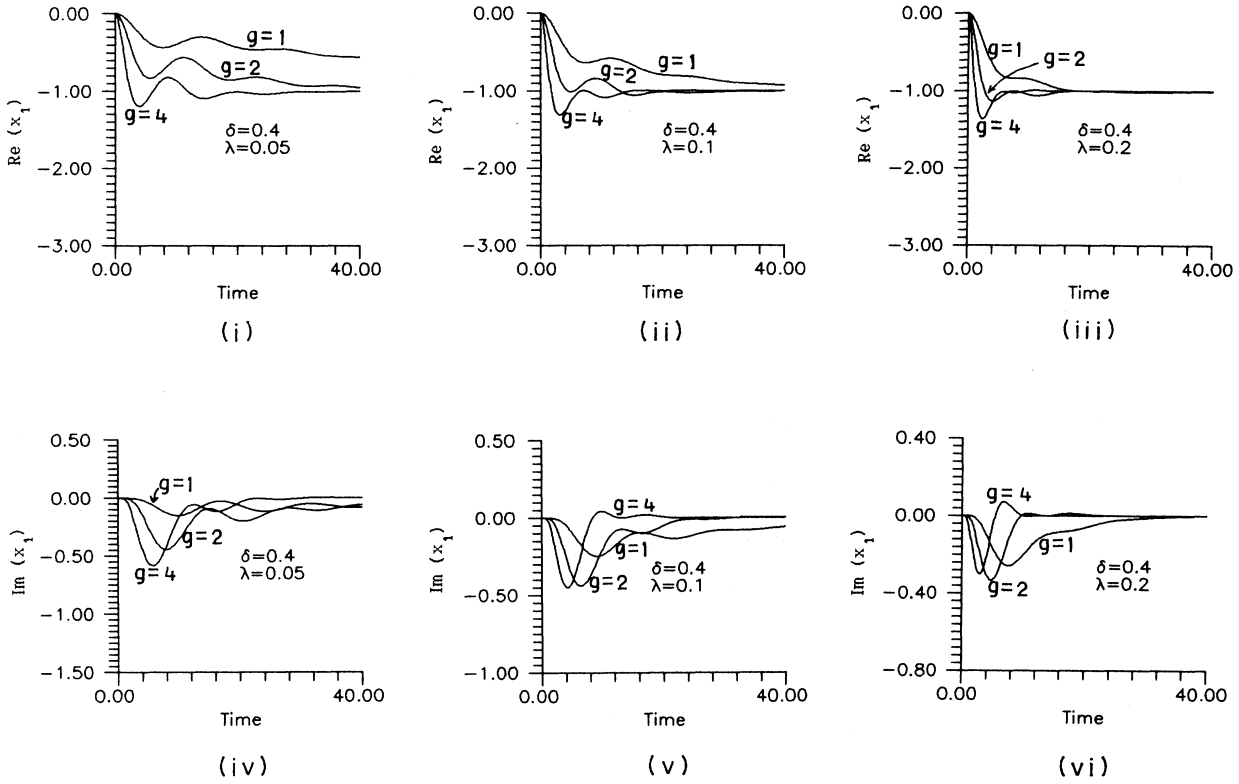


FIG. 18. Plots for the real and imaginary parts of x_1 with time for the complex noise. $\delta=0.4$.

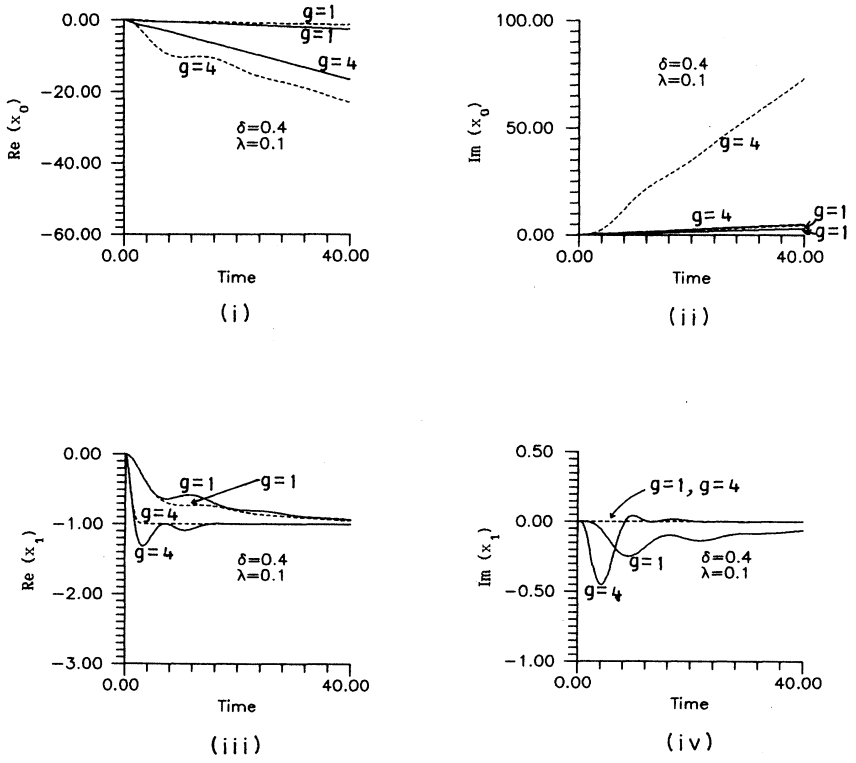


FIG. 19. Comparative graphs showing performance of the perturbative second-order cumulant results vis-à-vis the exact (cluster-cumulant) results. $\delta=0.4$. The dotted lines represent the perturbative results.

the noise correlation time τ_c is very large, ~ 2.0, and the oscillations occur within that time range as a result of the multiple interactions induced by the perturbation within that time range. The second-order cumulant results are obviously insufficient to take care of the oscillations as a result of the multiple quantum interference. The situation presumably remains the same for even higher-order perturbative cumulant results. The case of large g and small λ is again obviously way beyond the perturbative regime.

For the off-resonance case, x_0 and x_1 are complex, and we show the behavior of their real and imaginary components individually. Figures 17 and 18 display the plots for x_0 and x_1 for various values of g and λ for $\delta=0.4$. In Figs. 17, the imaginary part of x_0 induces a phase variation, which reaches a linear growth rate for larger values of g. The behavior of the real part of x_0 is quite similar to that for resonance. Figure 18 reveals that both the real and the imaginary components of x_1 show oscillatory behavior. While $\mathrm{Re}(x_1)$ reaches the value -1.0, $\mathrm{Im}(x_1)$ vanishes for larger times. This oscillation again is a nonperturbative effect, which is not captured by the second-order cumulant results, as illustrated in Fig. 19 for $\lambda=0.1$.

It is instructive to note here again the difference in structure of the operator R as obtained by us here for the colored noise, with that obtained by expansion in terms of eigenfunctions of Γ [6]. The latter, in terms of our variables, would involve an expansion of $U_B|0_B\rangle$ as

$$U_B|0_B\rangle=\sum_{m,n} U_B^{m,n}\frac{b^{\dagger m}c^{\dagger n}}{(m!n!)^{1/2}}|0_B\rangle\ , \tag{4.21}$$

which leads to an *infinite* system of coupled differential equations involving $U_B^{m,n}$. In contrast, $U_B|0_B\rangle$ in the cluster-cumulant treatment has a very compact structure, Eq. (4.15), which can be generated by solving a *finite* system of equations for S_B and X_B involving only five variables. Clearly, the ansatz, Eq. (4.21) is a *configuration-interaction* representation of U_B for colored noise, as opposed to an *exponential-like cluster expansion* in the cluster-cumulant approach, as mentioned at the end of Sec. III.

V. CONCLUDING REMARKS

We have described in this paper a nonperturbative cluster-cumulant approach for treating a stochastically averaged time-evolution operator in systems driven by colored noise. Both real and complex Ornstein-Uhlenbeck noise have been studied. The method maps the stochastic variable to a boson space, and stochastic averaging is replaced by the expectation value with respect to the boson vacuum. The mapped Hamiltonian, defined in an expanded Fock space, is deterministic and is conveniently treated by the time-dependent multireference coupled-cluster formalism developed by us recently [13,14,21].

We have found that our cluster-cumulant equations, written in the simultaneous *interaction representation* for the interaction V and the stochastic variables, generate the same perturbative cumulant results as obtained by a modified formulation, the Fox-Kubo method [4,5], suggested by us. In the algebraic structure, our approach is, however, closer to the method of Fokker-Planck dynamics involving marginal averages [4,6,7]. In fact, we have shown that our mapped Hamiltonian H_B is related to the Kubo-Schrödinger Hamiltonian [4,6,7] by a simple similarity transformation, which converts our h_B to the Fokker-Planck Hamiltonian for the OU noise. Our cluster-cumulant implementation, however, is quite different from either the Fox-Kubo cumulant expansion [4,5] and its resummed versions [9], which are perturbative, or the nonperturbative expansion methods [6,7] involving the eigenfunctions of the Fokker-Planck operator.

The path-integral approach [10,11] cannot directly be compared with ours, except in the sense of interpreting our cluster-cumulant equations in terms of expectation values with respect to the coherent state of the boson vacuum [22]. Our method offers a simple and systematic truncation scheme for nonquadratic system Hamiltonians, while the corresponding treatment in the path-integral formalism has yet to be systematized and is rather difficult to implement.

ACKNOWLEDGMENTS

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APPENDIX: AVOIDING STIFFNESS OF THE CLUSTER-CUMULANT EQUATIONS VIA THE INVERSE RICCATI TRANSFORMATION

We shall discuss here the inverse Riccati transformation method [20,21] for solving the cluster-cumulant equations, when they become stiff. By this transformation, we convert the nonlinear cluster-cumulant equations into first-order differential equations for some auxiliary variables which are linear.

We first recall that the cluster-cumulant equations are solved hierarchically starting at the zero-valence level and going upwards. Since at the zero-valence level, $\{\phi_i\}$ is just the unperturbed ground state for H_0, S_B's have only creation operators and stiffness is not encountered at this stage. Calling the associated zero-valence operator of S_B as $S_B^{(0)}$ (not to be confused with s_B^0, the operators with no stochastic boson variables), we have, from Eq. (2.22),

$$i\frac{\partial S_B^{(0)}}{\partial t}=\{\overline{H_B\exp(S_B^{(0)})}\}_{\mathrm{ex}}\ . \tag{A1}$$

The second term in Eq. (2.22) cannot contribute to the zero-valence problem, since $H_{\mathrm{eff}}^{(0)}$ in that case is a *number* (zero-body operator) and hence cannot contract with $\{\exp(S)\}$ from its left. Calling the associated zero-valence X_B as $X_B^{(0)}$, which is also a number, we have

$$i\frac{\partial X_B^{(0)}}{\partial t}=\{H_{\text{eff}}^{(0)}\}=\{\overline{H_B\exp(S_B^{(0)})}\}_{\text{cl}}^{(0)} . \tag{A2}$$

At the one-valence level, the $S_B^{(0)}$ amplitudes are *rigorously frozen* at their zero-valence values. The only new cluster-cumulant operators are of valence rank one—$S_B^{(1)}$—and appear in at most quadratic power. We encounter decaying amplitudes for the first time at the one-valence level, and it is at this stage that we invoke the *inverse Riccati transformation.* Calling the composite $\{H_B\exp(S_B^{(0)})\}$ as Z, we can write the cluster-cumulant equations for $S_B^{(1)}$ as

$$i\frac{\partial S_B^{(1)}}{\partial t}=\{Z\}_{\text{ex}}^{(1)}+\{\overline{Z\,S_B^{(1)}}\}_{\text{ex}}^{(1)}-\{\overline{S_B^{(1)}(H_{\text{eff}}^{(1)})}\} , \tag{A3}$$

$$\{H_{\text{eff}}^{(1)}\}=\{Z\}_{\text{cl}}^{(1)}+\{\overline{Z\,S_B^{(1)}}\}_{\text{cl}}^{(1)} . \tag{A4}$$

In Eq. (A3), only the linear power of $S_B^{(1)}$ can appear in the second term, since the higher powers are of valence ranks two and upwards, and hence cannot contribute. Equation (A4) indicates that $S_B^{(1)}(H_{\text{eff}})^{(1)}$ can also be only up to quadratic power of $S_B^{(1)}$. Collecting the $S_B^{(1)}$ amplitudes in a column $\sigma^{(1)}$, and calling the external and closed components of an operator symbolically as QP and PP blocks, respectively, Eq. (A3) may be written in matrix notation as

$$i\frac{\partial\sigma^{(1)}}{\partial t}=Z_{\text{QP}}+Z_{\text{QQ}}\sigma^{(1)}-\sigma^{(1)}(H_{\text{eff}})_{\text{PP}} , \tag{A5}$$

where

$$(H_{\text{eff}})_{\text{PP}}=Z_{\text{PP}}+Z_{\text{PQ}}\sigma^{(1)} , \tag{A6}$$

from Eq. (A4).

Let us now introduce block matrices C_{QP} and C_{PP} as

$$C_{\text{QP}}=\sigma^{(1)}C_{\text{PP}} . \tag{A7}$$

Our intention is to define C_{PP} in such a way that the quadratic term in $\sigma^{(1)}$ in Eq. (A5) disappears. Substituting Eq. (A6) in Eq. (A5), we find

$$i\frac{\partial C_{\text{QP}}}{\partial t}=Z_{\text{QP}}C_{\text{PP}}+Z_{\text{QQ}}C_{\text{QP}}-\sigma^{(1)}(H_{\text{eff}})_{\text{PP}}C_{\text{PP}}+i\sigma^{(1)}\frac{\partial C_{\text{PP}}}{\partial t} . \tag{A8}$$

To get rid of the quadratic term (the third one on the right side of Eq. A8), we define

$$i\frac{\partial C_{\text{PP}}}{\partial t}=(H_{\text{eff}})_{\text{PP}}C_{\text{PP}}=Z_{\text{PP}}C_{\text{PP}}+Z_{\text{PQ}}C_{\text{QP}} . \tag{A9}$$

Equations (A8) and (A9) can be compactly written as

$$i\frac{\partial}{\partial t}\begin{bmatrix}C_{\text{PP}}\\C_{\text{QP}}\end{bmatrix}=\begin{bmatrix}Z_{\text{PP}} & Z_{\text{PQ}}\\Z_{\text{QP}} & Z_{\text{QQ}}\end{bmatrix}\begin{bmatrix}C_{\text{PP}}\\C_{\text{QP}}\end{bmatrix} . \tag{A10}$$

This equation is linear in the unknowns C_{PP} and C_{QP}, and is thus much better conditioned numerically as compared to the potentially stiff Eq. (A3).

Since $S_B^{(1)}$ at $t=0$ is zero, we start from $C_{\text{QP}}=0$ and $C_{\text{PP}}=1_{\text{PP}}$, to get $C_{\text{QP}}(t)$ and $C_{\text{PP}}(t)$ at a later time t. $\sigma^{(1)}$ is then obtainable from Eq. (A7). $X_B^{(1)}$ is solved next from

$$i\frac{\partial X_B^{(1)}}{\partial t}=\{H_{\text{eff}}\}^{(1)}+\{\overline{(H_{\text{eff}}^{(1)})\,X_B^{(1)}}\}^{(1)} . \tag{A11}$$

An exactly analogous analysis may be undertaken for the higher-valence cases. For valence rank n, $S^{(n)}$ are the only unknown amplitudes, which can be grouped as a matrix $\sigma^{(n)}$. The lower-valence amplitudes $S^{(m)}$, $m<n$, are known time-dependent quantities. Again, the cluster-cumulant equations are at most quadratic in $\sigma^{(n)}$ $\sigma^{(n)}$ can be defined in terms of C_{QP} and C_{PP} exactly as in Eq. (A7). The matrix of Z involves various powers of $S_B^{(m)}$, with $m<n$, as known quantities.

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