Optimizing stochastic trajectories in exact quantum jump approaches of interacting systems

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Abstract

The quantum jump approach, where pairs of state vectors follow Stochastic Schroedinger Equation (SSE) in order to treat the exact quantum dynamics of two interacting systems, is first described. In this work the non-uniqueness of such stochastic Schroedinger equations is investigated to propose strategies to optimize the stochastic paths and reduce statistical fluctuations. In the proposed method, called the 'adaptative noise method', a specific SSE is obtained for which the noise depends explicitly on both the initial state and on the properties of the interaction Hamiltonian. It is also shown that this method can be further improved by introduction of a mean-field dynamics. The different optimization procedures are illustrated quantitatively in the case of interacting spins. A significant reduction of the statistical fluctuations is obtained. Consequently a much smaller number of trajectories is needed to accurately reproduce the exact dynamics as compared to the SSE without optimization.

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Recently the description of open quantum systems with Stochastic Schroedinger Equation (SSE) has received much attention \[1, 2, 3\]. This is due firstly to the possibility of substituting the description of a complex system based on the evolution of its density matrix by a description based on the stochastic evolution of wave-packets. Therefore these methods reduce significantly the number of degrees of freedom to be taken into account. A second reason is the increasing computational facilities that allow for massive numerical applications. The Monte-Carlo wave-function techniques are presently extensively used to treat Markovian master equations in the Lindblad form \[1, 2, 3, 6, 7, 8, 9, 10\]. In that case the system density evolution (noted $\rho_S$) is simulated using SSE on system state-vectors $\ket{\Phi}$. Then the dissipative evolution is recovered by averaging symmetric densities $\rho = \ket{\Phi} \bra{\Phi}$ over different stochastic trajectories, i.e. $\rho_S = \mathbb{P}$. Following this strategy, various quantum jump approaches based on SSE have been proposed \[1, 2, 11\].

Large theoretical efforts have been also devoted to the introduction of non-Markovian effects using quantum jumps. A possible way to treat this problem is to use stochastic equations that contain a non-local memory kernel \[12, 13, 14\]. In that case the average evolution of the density matrix is still given by averaging over symmetric densities $\rho = \ket{\Phi} \bra{\Phi}$, but state vectors evolve according to integro-differential stochastic equations. An alternative method that avoids the evaluation of non-local memory kernels is to introduce pairs of state-vectors leading to densities of the type $\rho = \ket{\Psi_1} \bra{\Psi_2}$. Then it is possible to treat non-Markovian effects approximately \[15\] using time-local SSE. More recently \[16\] SSE using pairs of state vectors have been proposed as a way to simulate the dynamics of interacting systems exactly, with the difference that $\ket{\Psi_1}$ and $\ket{\Psi_2}$ are separable states of the system and its environment. Such an exact reformulation has already been applied to different model cases \[16\] and appears as a candidate to treat the correlated dynamics of self-interacting mesoscopic systems \[17, 18\] and of systems interacting with an environment \[19\].

A common aspect to all stochastic methods used to simulate Markovian and non-Markovian dynamics is that the equation of motion of the density matrix does not define uniquely the stochastic equation of state vectors (see discussion in ref. \[11\]). A specific choice of equation is generally retained by imposing additional conditions along the stochastic path. For instance in the Markovian limit, nonlinear state-dependent stochastic equations have been obtained by invoking either normalization conditions of state-vectors, orthogonal-
jump processes \[20, 21\] or measurement arguments \[22, 23\]. In addition the introduction of mean-field dynamics \[17, 18\] significantly improves the stochastic description. Further freedom exists due to the fact that the noise itself can be multiplied by an arbitrary phase-factor without breaking the stochastic reformulation. Again, this fact has been noted in different studies on Markovian dynamics \[11\] and is sometimes used to pass from one stochastic equation to another \[2, 24\]. In the non-Markovian case it can also provide appropriate modifications of the stochastic dynamics \[25\].

Although an infinite number of stochastic formulations can generally describe the dynamics of an open system, the physical interpretation as well as the nature of the process can be completely different from one SSE to another. In addition, a series of works dedicated to Markovian dynamics with symmetric densities have pointed out that stochastic formulations are not equivalent as far as numerical implementation is concerned \[10, 18, 26\]. For instance numerical efficiency can be significantly improved by considering evolution of normalized states. The flexibility of SSE approaches has however not been explored yet when pairs of states vectors are used. It is clear that, in order to be able to apply the latter theory to a large variety of physical problems, specific accurate methods must be developed.

The main purpose of this paper is to investigate more systematically the freedom in the formulation of stochastic process using pairs of states in order to optimize the quantum jumps and reduce the number of trajectories necessary to describe the dynamics of interacting systems accurately. The paper is organised as follows: first the procedure to reinterpret the dynamics of interacting systems in terms of a Monte-Carlo evolution of pairs of wave-packets is described. The existence of an infinite number of SSE dynamics leading to a large freedom in defining stochastic trajectories is illustrated. In section II general strategies using this freedom to optimize the quantum jumps and minimize the statistical fluctuations are described. In this case we show that the optimal noise depends explicitly on the initial state and on the properties of the interaction. In section III we show that the combination of mean-field dynamics with the optimization of the noise leads to an additional reduction of the statistical fluctuations. Lastly, the method is illustrated quantitatively with a schematic model of interacting spin systems.
I. SSE FOR THE EXACT DYNAMICS OF INTERACTING SYSTEMS

Here we give a guideline for the exact reformulation of correlated dynamics in terms of diffusive wave-function processes using pairs of wave-packets. Note that a formal derivation of the equation given below can be obtained using the Hubbard-Stratonovich transformation [27, 28], see for instance ref. [19].

A. SSE with pairs of wave-packets

Following [16] we start from a general Hamiltonian describing the interaction of a system and its environment given by:

\[ H_I = \sum_\alpha A_\alpha \otimes B_\alpha \]  

Here we assume that the Hamiltonian is possibly already written in the interaction picture. \( A_\alpha \) and \( B_\alpha \) are operators acting respectively on the system and on the environment. Starting from an initial uncorrelated state:

\[ |\Psi\rangle = |\Phi\rangle \otimes |\chi\rangle, \]  

where \( |\Phi\rangle \) and \( |\chi\rangle \) are state vectors for the system and the environment respectively, the evolution of the system can be replaced by the set of stochastic Schrödinger equations:

\[
\begin{align*}
    d|\Phi\rangle &= \gamma \sum_\alpha a_\alpha(t) A_\alpha |\Phi\rangle \\
    d|\chi\rangle &= \gamma \sum_\alpha b_\alpha(t) B_\alpha |\chi\rangle
\end{align*}
\]  

where \( \gamma \) is a parameter defined formally as \( \gamma = \sqrt{\frac{e}{i\hbar}} \). Here \( a_\alpha(t) \) and \( b_\alpha(t) \) are complex stochastic Gaussian variables that follow the Ito stochastic rules [29]. Note that although we consider diffusive Gaussian processes, other stochastic methods could be used like piecewise deterministic processes (PDP’s) [16, 30]. Indeed, the results presented in this work can be adapted to PDP quantum mechanics. In the following, we note \( \overline{X} \) the average of \( X \) over the stochastic variables. Under the condition:

\[ a_\alpha(t)b_\alpha(t) = 1, \]  

the average evolution corresponds to the exact Schrödinger equation

\[ \frac{d|\Psi\rangle}{dt} = \frac{\hbar}{i} H_I |\Psi\rangle. \]
An interesting aspect of this random process is that stochastic equations \[^{3}\] preserve the separability of the total state given by eq. \[^{2}\] so that the procedure can be iterated to simulate the evolution on large time scales.

A second attractive aspect is that the stochastic formulation can be extended to provide an exact treatment of the Liouville-von Neumann equation of the density matrix. In that case, we consider

\[
D = |\Psi_1\rangle \langle \Psi_2|
\]

where $|\Psi_1\rangle$ and $|\Psi_2\rangle$ is a pair of different system+environment states both given by eq. \[^{2}\]. Both states follow independent stochastic equations given (for both) by eq. \[^{3}\]. Noting $\rho(t) = D(t)$, its evolution reads

\[
i\hbar \frac{d\rho}{dt} = [H_I, \rho]
\]

which is nothing but the exact Liouville-von Neumann equation. Again, eq. \[^{6}\] is preserved along each stochastic path. The latter reformulation of exact dynamics is not limited to initially uncorrelated states. Indeed if the initial density matrix is correlated, it can be replaced by an ensemble of couples of states. The initial density reads: $\rho(t = 0) = E(|\Psi_1\rangle \langle \Psi_2|)$ where the average here means the average over initial dyadics. Then the complete dynamics is obtained by averaging both on the initial ensemble and on the stochastic paths.

The random process presented in this section describes the exact dynamics of a system coupled to an environment. Therefore, although the SSE on wave-functions is Markovian, it contains all non-Markovian effects. It is also worth noticing that this method significantly differs from quantum jump processes used in the Markovian limit \[^{1}, 2, 4, 5, 6, 7, 8, 9, 10\] or in the non-Markovian limit with a non-local memory kernel \[^{12}, 13, 14\]. The first reason is that pairs of state vectors that evolve according to independent SSE should be considered. A second important aspect is that quantum jumps applied to Markovian dynamics require in general to follow only states of the system. Indeed the effect of the environment has already been approximated in the Lindblad equation describing the system density matrix evolution. Here wave-packets of both system and environment should be followed in time and the system evolution can be obtained using the $\rho_S = Tr_E(\rho)$ where $Tr_E(.)$ denotes the partial trace over the environment. However the necessity to follow environment degrees of freedom may lead to additional difficulties.
B. Statistical Fluctuations

The possibility to perform exact dynamics of interacting systems is of particular interest to discuss dissipative effects due to the coupling of a system with its environment. In particular it does not have the limitations of Lindblad Master equations \[10, 16\]. However large numerical efforts are needed to treat exactly a physical process due to the number of trajectories required to reduce statistical fluctuations of the observables. This is why so far it has essentially been applied to rather schematic models.

Following \[18\], a measure of the increase of statistical fluctuations is given by:

\[
\Lambda_{\text{stat}} = E \left( \frac{1}{2} \left( |D(t) - \bar{D}(t)|^2 \right) \right) = E \left( \frac{1}{2} \left( \text{Tr} (D^+ (t) D(t)) \right) \right) - \text{Tr} \left( \rho^2 (t) \right)
\]

(8)

where \( ||A||^2 = \text{Tr} (A^+ A) \) is the Hilbert-Schmidt norm. In addition, if the initial state is a pure state, \( \text{Tr} (\rho^2 (t)) = 1 \).

The growth of statistical fluctuations is of particular importance for numerical implementations since it is directly connected to the number of trajectories required to properly reproduce the evolution of a physical system using SSE. Now let us make explicit the evolution of the statistical noise associated to the SSE defined by eq. (8). We consider the contribution of a single initial couple of state vectors \( D = |\Psi_1 \rangle \langle \Psi_2 | \) and we note \( \lambda_{\text{stat}} = \overline{\text{Tr} (D^+ (t) D(t))} \) its contribution to \( \Lambda_{\text{stat}} \). It is assumed for simplicity that each wave-packet is initially normalized. Starting from \( D \), the infinitesimal increase of \( \lambda_{\text{stat}} \) is given by:

\[
d\lambda_{\text{stat}} = d \langle \Psi_1 | \Psi_1 \rangle + d \langle \Psi_2 | \Psi_2 \rangle
\]

(9)

in which each contribution reads:

\[
d \langle \Psi_i | \Psi_i \rangle = \frac{dt}{\hbar} \sum_{\alpha} \left( |a_{\alpha}(t)|^2 \langle A_{\alpha}^+ A_{\alpha} \rangle_{\Phi_i} + |b_{\alpha}(t)|^2 \langle B_{\alpha}^+ B_{\alpha} \rangle_{\chi_i} + 2 \mathbb{R} \left\{ a_{\alpha}(t) b_{\alpha}^*(t) \langle A_{\alpha} \rangle_{\Phi_i} \langle B_{\alpha}^+ \rangle_{\chi_i} \right\} \right)
\]

(10)

with \( i = 1, 2 \). Therefore statistical fluctuations depend explicitly on the properties of the random variables \( a_{\alpha} \) and \( b_{\alpha} \). In several works \[16, 17, 18\] specific choices of noise have been made. In all cases it was possible to demonstrate that the fluctuations have an upper bound that grows exponentially in time. Conjointly, the numerical implementation depends strongly on the retained SSE as well as the possible appearance of instabilities in
II. OPTIMAL QUANTUM JUMPS AND THE REDUCTION OF STATISTICAL FLUCTUATIONS

Let us now detail the properties of invariance of the SSE approaches. Starting from a general complex noise \( a_\alpha \) and \( b_\alpha \) that fulfills the necessary condition given by (11), any new couple of random variables \((a'_\alpha(t), b'_\alpha(t))\) defined by means of the transformation

\[
\begin{align*}
  a'_\alpha(t) &= c_\alpha a_\alpha(t) \\
  b'_\alpha(t) &= \frac{1}{c_\alpha} b_\alpha(t)
\end{align*}
\]  

with

\[
c_\alpha = e^{i\theta_\alpha} \sqrt{u_\alpha}
\]  

also gives the correct exact dynamics. In the following, \( u_\alpha \) and \( \theta_\alpha \) will be referred to respectively the scaling factor and the phase factor. Invariance of the stochastic reformulation with respect to application of a scaling or a phase shows that an infinite number of SSE’s exists to simulate the exact dynamics of interacting systems, as it has been shown in most of the stochastic theories in Hilbert Space \[2, 11, 25\]. Such an invariance and in particular the invariance with respect to a phase factor has already been noted in several works \[2, 25\] and has been used for different purposes.

Let us now apply a scaling and a phase factor on the statistical errors. We see that, while statistical fluctuations associated to the initial stochastic equations are given by eq. (10), the new SSE leads to different statistical fluctuations given by

\[
\begin{align*}
  \overline{d \langle \Psi | \psi \rangle} &= \frac{d\Phi}{\Phi} \sum_\alpha \left( u_\alpha |a_\alpha(t)|^2 \langle A_\alpha^+ A_\alpha \rangle_\Phi + \frac{1}{u_\alpha} |b_\alpha(t)|^2 \langle B_\alpha^+ B_\alpha \rangle_\chi \\
  &\quad + 2 \Re \left\{ e^{i2\theta_\alpha} a_\alpha(t) b_\alpha^*(t) \langle A_\alpha \rangle_\Phi \langle B_\alpha^+ \rangle_\chi \right\} \right)
\end{align*}
\]  

where the indices \( i = 1, 2 \) have been omitted for simplicity. Thus, the growth of statistical fluctuations may significantly differ depending on the noise. In this section we show that the scaling factor as well as the phase factor can be properly adjusted to obtain minimal
Statistical fluctuations thus reducing the number of stochastic trajectories in numerical implementations. It may be seen in the last equation that the parameters of the transformation act independently on the two parts of eq. (13) and as such, they can be adjusted separately. For a component $\alpha$ of the interaction Hamiltonian, the two functions $\Omega_\alpha$ and $\Gamma_\alpha$ are defined as:

$$\Omega_\alpha(u_\alpha) = u_\alpha |a_\alpha(t)|^2 \langle A_\alpha^+ A_\alpha \rangle_\phi + \frac{1}{u_\alpha} |b_\alpha(t)|^2 \langle B_\alpha^+ B_\alpha \rangle_\chi$$  \hspace{1cm} (14)

$$\Gamma_\alpha(\theta_\alpha) = 2 \Re \left\{ e^{i2\theta_\alpha} a_\alpha(t) b_\alpha^*(t) \langle A_\alpha \rangle_\phi \langle B_\alpha^+ \rangle_\chi \right\}$$  \hspace{1cm} (15)

Starting from a given statistical noise $(a_\alpha(t), b_\alpha(t))$, the strategy is to find the optimal $u_\alpha$ and $\theta_\alpha$ that minimize respectively these two functions.

### A. Optimal scaling factor

In eq. (14) both $\langle A_\alpha^+ A_\alpha \rangle_\phi$ and $\langle B_\alpha^+ B_\alpha \rangle_\chi$ are fixed parameters that depend on the initial state. For a given initial state vector, $\Omega_\alpha$ is minimal for

$$u_\alpha = \left( \frac{|b_\alpha|^2 \langle B_\alpha^+ B_\alpha \rangle_\chi}{|a_\alpha|^2 \langle A_\alpha^+ A_\alpha \rangle_\phi} \right)^{1/2}$$  \hspace{1cm} (16)

Under this specific choice the lower limit of $\Omega_\alpha$ reads:

$$\Omega_\alpha = 2 \sqrt{|a_\alpha(t)|^2 \cdot |b_\alpha(t)|^2 \langle A_\alpha^+ A_\alpha \rangle_\phi \langle B_\alpha^+ B_\alpha \rangle_\chi}$$  \hspace{1cm} (17)

This expression is valid for any $a_\alpha$ and $b_\alpha$ fulfilling the condition (4). Due to eq. (14), we also have $|a_\alpha(t)|^2 \cdot |b_\alpha(t)|^2 \geq 1$. Thus it is better to start with a noise such that $|a_\alpha(t)|^2 \cdot |b_\alpha(t)|^2 = 1$.

Coming back to the general case, it is important to note that the optimization depends on the state on which the expectation values are taken. In particular, if

$$\left( \frac{|b_\alpha|^2 \langle B_\alpha^+ B_\alpha \rangle_\chi}{|a_\alpha|^2 \langle A_\alpha^+ A_\alpha \rangle_\phi} \right) = 1,$$  \hspace{1cm} (18)

the minimal value of $\Omega_\alpha$ corresponds exactly to expression (13). In this case, no reduction of the statistical fluctuation is obtained. Such a case will be presented in a forthcoming section. Generally speaking, the more the optimal value of $u_\alpha$ differs from one, the larger the reduction of the statistical noise.
B. Optimal phase factor

Let us now turn to the second term in eq. (13). In order to minimize the statistical noise, the second term should be negative. It is always possible to fix conveniently $\theta_\alpha$ in order to have the minimum value for $\Gamma_\alpha$, i.e:

$$\Gamma_\alpha = -2 \left| \overline{a_\alpha b_\alpha^*} \right| \cdot \left| \langle A_\alpha \rangle_\Phi \langle B_\alpha^+ \rangle_\chi \right|$$

(19)

The absolute value of the expression depends explicitly on $\left| \overline{a_\alpha b_\alpha^*} \right|$. Let us now give an explicit expression for $a_\alpha$ and $b_\alpha$. We define

$$\begin{cases}
a_\alpha = x_\alpha + iy_\alpha \\
b_\alpha = x'_\alpha + iy'_\alpha
\end{cases}$$

(20)

where all components are real Gaussian stochastic variables. Using condition (11), we obtain:

$$\left| \overline{a_\alpha b_\alpha^*} \right|^2 = -1 + 2 \left( x_\alpha x'_\alpha + y_\alpha y'_\alpha + y_\alpha x'_\alpha + x_\alpha y'_\alpha \right)$$

(21)

which leads to the inequality

$$\left| \overline{a_\alpha b_\alpha^*} \right|^2 \leq -1 + 2 |a_\alpha^2| \cdot |b_\alpha^2|.$$  

(22)

In order to reduce the fluctuations, expression (21) must be maximized. The maximal value is obtained if $a_\alpha$ and $b_\alpha^*$ are fully correlated, i.e. $b_\alpha^* \propto a_\alpha$. Therefore a convenient choice for the couple $(a_\alpha, b_\alpha)$ is

$$\begin{cases}
a_\alpha = \sqrt{\delta} e^{i\varphi} x_\alpha \\
b_\alpha = \frac{1}{\sqrt{\delta}} e^{-i\varphi} x_\alpha
\end{cases}$$

(23)

where $x_\alpha^2 = 1$ and $\delta$ is a real parameter. The latter expression leads to $\left| \overline{a_\alpha b_\alpha^*} \right|^2 = -1 + 2 |a_\alpha^2| \cdot |b_\alpha^2| = 1$. Since any noise given by the expression (23) can be obtained from an initial real noise $x_\alpha$ through the transformation (11), we simply assume that $a_\alpha = b_\alpha = x_\alpha$. Then, if we define $\theta_{AB}$ as:

$$\langle A_\alpha \rangle_\Phi \langle B_\alpha^+ \rangle_\chi = e^{i\theta_{AB}} \left| \langle A_\alpha \rangle_\Phi \langle B_\alpha^+ \rangle_\chi \right|$$

(24)

the optimal phase factor given by

$$2\theta_\alpha = \pi - \theta_{AB}$$

(25)

leads to the minimum value

$$\Gamma_\alpha = -2 \left| \langle A_\alpha \rangle_\Phi \langle B_\alpha^+ \rangle_\chi \right|. $$

(26)
C. Summary

In this section starting from the diffusive equation given in section I A, we have shown that the noise can be optimized to reduce the statistical fluctuations. For any given initial state $|\Psi\rangle = |\Phi\rangle \otimes |\chi\rangle$, an optimal reduction of the statistical fluctuations corresponds to a diffusive process with a specific complex Gaussian noise given by

$$
\begin{align*}
a_\alpha(t) &= e^{i\theta_\alpha} \sqrt{u_\alpha x_\alpha} \\
b_\alpha(t) &= e^{-i\theta_\alpha} \frac{1}{\sqrt{u_\alpha}} x_\alpha
\end{align*}
$$

with $x_\alpha^2 = 1$. In these expressions both the scaling factor and the phase factor, given respectively by equations (16) and (25) depend explicitly on the initial state vector as well as on the Hamiltonian. Along the optimal path, the normalization evolution reads:

$$
d\langle \Psi|\Psi \rangle = 2\frac{dt}{\hbar} \sum_\alpha \left( \sqrt{\langle A_+^A A_\alpha \rangle_{\Phi} \langle B_+^B B_\alpha \rangle_{\chi}} - \sqrt{\langle A_+^A \rangle_{\Phi} \langle A_\alpha \rangle_{\Phi} \langle B_+^B \rangle_{\chi} \langle B_\alpha \rangle_{\chi}} \right)
$$

$$
\equiv 2\frac{dt}{\hbar} \sum_\alpha F_\alpha
$$

The procedure described here for a single initial state can be applied to the complete description of correlated systems. In this case, an ensemble of wave-packets is considered simultaneously, each state evolving according to its own stochastic equation with a noise adapted at each time-step. Since for all states the trajectories are optimally chosen, we do expect that the total statistical fluctuations obtained by averaging over the ensemble of states will also be reduced. In the following, this method will be referred to as the ’adaptative noise method’.

III. NOISE ON TOP OF MEAN-FIELD DYNAMICS

Before giving an example of application of the adaptative noise procedure, we would like to mention that the flexibility on the noise is not the only way to optimize quantum jumps. It is possible to introduce a deterministic part in addition to the stochastic contribution that partially treats the coupling of the system with the environment without breaking the separability of the state vector. One ends up with non-linear, state dependent, stochastic equations. Such non-linear equations have been obtained in the Markovian limit by assuming jumps orthogonal to the state $|20, 21, 30\rangle$ or ”optimal” measurement arguments $|22, 23\rangle$. 
In all cases we expect that the numerical accuracy will be improved. Closely related is the introduction of mean-field dynamics associated to the interacting system \[17, 18, 19\].

In this section the latter method is used. The mean-field associated to the general Hamiltonian given by (1) as well as the associated stochastic dynamics are described. As will be seen, the introduction of mean-field gives non-linear equations equivalent to other techniques. Lastly we discuss how the attractive aspects inherent to mean-field theories and to the adaptative noise can be combined to take advantage of both methods.

### A. Optimized Stochastic mean-field dynamics

Starting from the interaction Hamiltonian the associated mean-field dynamics can be obtained using the variational principle

\[
\delta \langle \Psi | i\hbar \partial_t - H_I | \Psi \rangle = 0 \tag{30}
\]

where \(|\Psi\rangle\) is a separable state given by equation (2). Using the variational principle we obtain the mean-field equation of motion for each component of the total state vector.

\[
\begin{cases}
  i\hbar \partial_t |\Phi\rangle = \sum_{\alpha} \langle B_{\alpha} \rangle_{\chi} A_{\alpha} |\Phi\rangle = h_{MF}^S |\Phi\rangle \\
  i\hbar \partial_t |\chi\rangle = \sum_{\alpha} \langle A_{\alpha} \rangle_{\Phi} B_{\alpha} |\chi\rangle = h_{MF}^E |\chi\rangle
\end{cases} \tag{31}
\]

where \(h_{MF}^S\) and \(h_{MF}^E\) denotes the mean-field Hamiltonians acting respectively on the system and the environment. The mean-field dynamics differs from the exact dynamics since part of the coupling is not accounted for. Using mean-field expressions, the complete Hamiltonian can be recast as

\[
H_I |\Psi\rangle = \left\{ h_{MF}^S \otimes 1_E + 1_S \otimes h_{MF}^E - \langle A_{\alpha} \rangle_{\Phi} \langle B_{\alpha} \rangle_{\chi} + \sum_{\alpha} (A_{\alpha} - \langle A_{\alpha} \rangle_{\Phi}) \otimes (B_{\alpha} - \langle B_{\alpha} \rangle_{\chi}) \right\} |\Psi\rangle \tag{32}
\]

In this expression \(1_S\) and \(1_E\) correspond to the unity operators acting respectively on the system and on the environment spaces. Similarly to the case presented previously, the last term in eq. (32) can be reinterpreted as an average over stochastic paths, leading to a new set of stochastic evolution:

\[
\begin{cases}
  d |\Phi\rangle = \left\{ \frac{dt}{i\hbar} \left( h_{MF}^S - \frac{1}{2} \sum_{\alpha} \langle A_{\alpha} \rangle_{\Phi} \langle B_{\alpha} \rangle_{\chi} + \gamma \sum_{\alpha} a_{\alpha} (A_{\alpha} - \langle A_{\alpha} \rangle_{\Phi}) \right) \right\} |\Phi\rangle \\
  d |\chi\rangle = \left\{ \frac{dt}{i\hbar} \left( h_{MF}^E - \frac{1}{2} \sum_{\alpha} \langle A_{\alpha} \rangle_{\Phi} \langle B_{\alpha} \rangle_{\chi} + \gamma \sum_{\alpha} b_{\alpha} (B_{\alpha} - \langle B_{\alpha} \rangle_{\chi}) \right) \right\} |\chi\rangle
\end{cases} \tag{33}
\]
Thus the introduction of the mean-field prior to a stochastic formulation induces a modification of the operator entering the stochastic contribution. In the latter case \( A_\alpha \) and \( B_\alpha \) are replaced by \( A'_\alpha = (A_\alpha - \langle A_\alpha \rangle_\Phi) \) and \( B'_\alpha = (B_\alpha - \langle B_\alpha \rangle_\chi) \). Similar equations have been obtained in ref. \[19\] using the Hubbard-Stratonovich transformation in conjunction with the Girsanov transformation. More generally when mean-field is introduced prior to stochastic formulation, stochastic terms generally found in the treatment of Markovian \[21, 22, 23, 24, 30\] as well as non-Markovian dynamics \[13, 14\] appear naturally. Such a similitude is not surprising since for instance mean-field naturally gives rise to orthogonal jumps. When mean-field is introduced, the evolution of the statistical fluctuations (noted \( \Lambda_{\text{stat}}^{\text{MF}} \)), associated to the stochastic mean-field dynamics with an initial state \( |\Psi\rangle \), differs from eq. (10) and reads:

\[
d\Lambda_{\text{stat}}^{\text{MF}} = \frac{dt}{\hbar} \sum_\alpha |a_\alpha|^2 \left( \langle A'^+_\alpha A_\alpha \rangle_\Phi - \langle A'^+_\alpha \rangle_\Phi \langle A_\alpha \rangle_\Phi \right) + |b_\alpha|^2 \left( \langle B'^+_\alpha B_\alpha \rangle_\chi - \langle B'^+_\alpha \rangle_\chi \langle B_\alpha \rangle_\chi \right). \tag{34}
\]

It is first observed that the quantum fluctuations for operators \( A_\alpha \) and \( B_\alpha \) with respect to the state vectors \( |\Phi\rangle \) and \( |\chi\rangle \) appear naturally in this expression. The main advantage of mean-field \[17, 18\] is that the latter expression is always much smaller than the first term of eq. (10) leading generally to smaller statistical fluctuations.

Let us now combine the advantage of the mean-field with the optimization proposed in this work. At variance with the general case presented previously, we have \( \langle A'_\alpha \rangle_\Phi = \langle B'_\alpha \rangle_\chi = 0 \), leading to \( \Gamma_\alpha = 0 \). As a consequence, only an optimization through the scaling factor can be performed. In the stochastic mean-field case, the optimal value is obtained simply by replacing respectively \( A_\alpha \) and \( B_\alpha \) by \( A'_\alpha \) and \( B'_\alpha \) in expression (16). This leads to a reduced statistical fluctuation given by

\[
\overline{d\langle \Psi | \Psi \rangle} = 2 \frac{dt}{\hbar} \sum_\alpha \sqrt{\langle A'^+_\alpha A_\alpha \rangle_\Phi - \langle A'^+_\alpha \rangle_\Phi \langle A_\alpha \rangle_\Phi} \left( \langle B'^+_\alpha B_\alpha \rangle_\chi - \langle B'^+_\alpha \rangle_\chi \langle B_\alpha \rangle_\chi \right) \tag{35}
\]

\[
\equiv 2 \frac{dt}{\hbar} \sum_\alpha F_{\alpha}^{\text{MF}}. \tag{36}
\]

Using now the fact that

\[
(F_\alpha^2) - (F_{\alpha}^{\text{MF}})^2 = \left( \sqrt{\langle A'^+_\alpha A_\alpha \rangle_\Phi \langle B'^+_\alpha \rangle_\chi \langle B_\alpha \rangle_\chi} - \sqrt{\langle B'^+_\alpha B_\alpha \rangle_\chi \langle A'^+_\alpha \rangle_\Phi \langle A_\alpha \rangle_\Phi} \right)^2 \geq 0, \tag{37}
\]

we see that an optimized stochastic mean-field dynamics will always further reduce statistical fluctuations.
B. Alternative optimization of the phase factor

In the stochastic mean-field dynamics presented above, there still exists a freedom on the phase factor to reduce the statistical errors. More generally although the method proposed in chapter II appears as the natural way to obtain an optimal phase factor, it can obviously not be used if $\Gamma_\alpha = 0$. In this section we propose an alternative strategy to obtain the phase factor. We assume that $\Gamma_\alpha$ cancels out. The optimized statistical fluctuations reduce to

$$d\langle \Psi | \Psi \rangle = 2\frac{dt}{\hbar} \sum_\alpha \sqrt{\langle A_\alpha^+ A_\alpha \rangle_\Phi \langle B_\alpha^+ B_\alpha \rangle_\chi}.$$  

(38)

Here, the SSE without or with mean-field are considered indifferently. In the latter case, $A_\alpha$ and $B_\alpha$ must be replaced by $A'_\alpha$ and $B'_\alpha$ in the following expressions. For a single time step a modification of the phase does not affect directly the expression (38). However the phase factor can be adjusted to act on the value of $c_2^\alpha = \langle A_\alpha^+ A_\alpha \rangle_\Phi \langle B_\alpha^+ B_\alpha \rangle_\chi$ along the trajectory. Indeed, starting from the SSE given by equation (3), we have

$$\overline{dc_2^\alpha} = -\frac{dt}{\hbar} \sum_\beta \langle A_\beta^+ A_\alpha A_\beta \rangle_\Phi \langle B_\alpha^+ B_\alpha \rangle_\chi \overline{c_2^\alpha} + \frac{dt}{\hbar} \sum_\beta \langle A_\alpha^+ A_\beta \rangle_\Phi \langle B_\beta^+ B_\alpha B_\beta \rangle_\chi$$

$$+ \frac{dt}{\hbar} \sum_\beta \overline{ab_\beta} \langle A_\beta^+ A_\alpha A_\beta \rangle_\Phi \langle B_\alpha^+ B_\alpha B_\beta \rangle_\chi - \frac{dt}{\hbar} \sum_\beta \overline{ab_\beta} \langle A_\alpha^+ A_\beta \rangle_\Phi \langle B_\alpha^+ B_\beta B_\alpha \rangle_\chi$$

$$+ 2\frac{dt}{\hbar} \sum_\beta \Re \left\{ \sum_\beta \overline{ab_\beta} \langle A_\beta^+ A_\beta \rangle_\Phi \langle B_\alpha^+ B_\alpha B_\beta \rangle_\chi \right\}$$

(39)

In this expression, only the last term is influenced by a phase-factor. The others are invariant with respect to a phase transformation. In order to reduce the statistical fluctuations, it is suitable to drive the system towards small values of $c_2^\alpha$ during the evolution. This can be achieved by means of a proper adjustment of $\theta_\alpha$. Similarly to section IIIB we define:

$$\langle A_\alpha^+ A_\alpha A_\beta \rangle_\Phi \langle B_\beta^+ B_\alpha B_\beta \rangle_\chi = e^{i\theta_{AB}} \left| \langle A_\alpha^+ A_\alpha A_\beta \rangle_\Phi \langle B_\beta^+ B_\alpha B_\beta \rangle_\chi \right|$$

(40)

and the new optimal phase factor is then given by $2\theta_\alpha = \pi - \theta'_{AB}$ leading to

$$\Re \left\{ \overline{ab_\beta} \langle A_\alpha^+ A_\alpha A_\beta \rangle_\Phi \langle B_\beta^+ B_\alpha B_\beta \rangle_\chi \right\} = - \left| \langle A_\alpha^+ A_\alpha A_\beta \rangle_\Phi \langle B_\beta^+ B_\alpha B_\beta \rangle_\chi \right|$$

(41)

As previously we assume that $|\overline{ab_\beta}| = 1$. The method presented here provides an indirect way to reduce statistical fluctuations when the second term of equation (10) is of no

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1 in the mean-field case, additional terms exist due to the deterministic part in the SSE. These terms are not reported here but will not change the conclusion.
use. This is always the case in stochastic mean-field dynamics. Therefore in the forthcoming applications of stochastic mean-field, the phase will always be deduced from the latter alternative method.

IV. ILLUSTRATION

In this chapter we apply the different optimization procedures described previously on an illustrative example consisting of a system of spins in interaction. We show in this example that the statistical fluctuations can be significantly reduced leading to more efficient stochastic calculations. A systematic study shows that the reduction of statistical fluctuations depends on the parameters of the model.

The analytical model proposed in [16] is considered. The model considers a spin described by its Pauli operator \( \sigma \) coupled with an environment of spins with spin operators \( \sigma^{(\alpha)} \) \((\alpha = 1, \cdots, N)\) where \( N \) is the number of spins. The interaction Hamiltonian is given by

\[
H = 2 \sum_{\alpha} C_{\alpha} \left( \sigma_{+} \sigma^{-}_{-}^{(\alpha)} + \sigma_{-} \sigma_{+}^{(\alpha)} \right)
\]

(42)

where \( C_{\alpha} \) is the coupling constant. This model is a simplified version of the one used for the description of a single electron spin in a quantum dot given in [31]. Its simplicity is particularly suitable for the present study, enabling us to focus mainly on statistical fluctuations. In addition it has a similar form to the one generally taken in the description of open quantum systems [10, 32]. Here, it is assumed that \( C_{\alpha} = C/N \). In this case starting from an initial density \( \rho(t = 0) = |\Psi(0)\rangle \langle \Psi(0)| \) with

\[
|\Psi(0)\rangle = |+\rangle \otimes |-, \cdots, -\rangle,
\]

(43)

the dynamical evolution is known analytically [16]. In particular the exact system density evolution obtained by performing the partial trace on the environment, i.e. \( \rho_{S}(t) = Tr_{E}(\rho(t)) \), is given by

\[
\rho_{S}(t) = \rho_{++} |+\rangle \langle +| + \rho_{--} |--\rangle \langle --|
\]

(44)

with \( \rho_{++} = 1 - \rho_{--} = \cos^{2}(2Ct) \). We consider the model as a benchmark for the different SSE considered in this work. In the present case the interaction operators discussed in the previous chapters read: \( A_{\alpha} = \sqrt{\frac{2C}{N}} \sigma_{\pm} \) and \( B_{\alpha} = \sqrt{\frac{2C}{N}} \sigma_{\pm}^{(\alpha)} \).
We now consider four different classes of simulations. In the first type of calculations mean-field is not accounted for. Two calculations will be performed without (noted SSE) and with optimization (OSSE). The SSE case can be considered as the reference case and corresponds to \( a_\alpha = b_\alpha = x_\alpha \). In the second type of calculations the mean-field is introduced and the cases without and with optimization are again considered. They will be referred to as Stochastic Mean-field (SMF), again with \( a_\alpha = b_\alpha = x_\alpha \) and Optimized Stochastic Mean-field (OSMF).

A. Statistical fluctuations

Let us first consider the case \( N = 1 \) and \( C = 0.5 \). In order to illustrate quantitatively the effect of the different optimization, we perform an ensemble of stochastic trajectories all starting from the same initial state vector \( |\Psi(0)\rangle \). The evolution in time of the average quantity \( \langle \Psi | \Psi \rangle \) is shown in figure 1. The SSE, OSSE, SMF and OSMF calculations are represented respectively by filled circles, filled triangles, open stars and open squares. In each case an ensemble of \( N_{\text{traj}} = 10^5 \) trajectories are performed. Let us first focus on the stochastic dynamics without optimization. We see that \( \langle \Psi | \Psi \rangle \) increases much faster in the standard SSE case than in Stochastic mean-field dynamics. As expected the introduction of the mean-field alone reduces statistical fluctuations. When optimization procedures are introduced, the evolution of \( \langle \Psi | \Psi \rangle \) is significantly further reduced. It is worth noticing that the OSSE gives a much lower increase than the SMF dynamics. This indicates that the effect of optimization on the standard SSE already gives a much better result than the one using stochastic mean-field without optimization. Finally Fig. 1 shows that the maximal reduction is obtained when both the mean-field and the optimization are taken into account.

We would like to mention that the present model has several specific aspects. First if the phase factor is not optimized (i.e. the phase is set to zero), no improvement is observed. Indeed if the original noise is set to \( a_\alpha = b_\alpha = x_\alpha \), then \( \langle A^+_\alpha A_\alpha \rangle_\Phi = \langle B^+_\alpha B_\alpha \rangle_\chi \) along the trajectory, leading to an optimal scaling factor constantly equal to one. Therefore the strong reduction is due to the combined action of the phase factor and the scaling factor. Note that in the present model, it is possible to show that for a given initial state \( \theta_{AB} = \theta'_{AB} \), the optimal phases are the same in the two optimized calculations.

In order to quantify the statistical fluctuation growth, each curve is fitted using the func-
FIG. 1: Evolution of $\langle \Psi | \Psi \rangle$ (in log scale) as a function of time $t$ multiplied by the coupling constant $C$ for $N = 1$ and $C = 0.5$ (in arbitrary units). The calculations correspond to SSE (filled circles), OSSE (filled triangles), SMF (open stars) and OSMF (open squares). Averages have been obtained with $10^5$ trajectories.

The evolution $\langle \Psi | \Psi \rangle \propto e^{\lambda_s t}$. A measurement of the increase is directly given by $\lambda_s$. We have obtained $\lambda_s \simeq 2.6, 1.3, 0.78$ and $0.53$ for the SSE, SMF, OSSE and OSMF cases respectively. The reduction of the statistical errors has a direct effect on the capacity of the different stochastic formulations to efficiently reproduce the exact dynamics: the slower the increase the more efficient the stochastic equation. This is illustrated in figure 2 where the evolution of the occupation probability $n_+ = \langle + | \rho_S(t) | + \rangle$ is shown as a function of time for the four calculations and compared to the exact result. In all cases the same number of trajectories $N_{\text{traj}} = 10^4$ was used. In each case the standard deviation on $n_+$ calculated with the set of trajectories is shown in the form of error bars. Large values are observed in the case of standard SSE. In addition the SSE calculation is unable to reproduce the exact dynamics over the considered time interval. The optimized calculations give a good reproduction of the exact dynamics while in the SMF a small departure from the exact solution is observed at large time. A precise comparison indicates (as expected) that the OSMF gives the best agreement. These results show again that the reduction of the statistical fluctuations improves the stochastic methods. For a given number of trajectories, the associated standard deviations are proportionally reduced. This is illustrated in figure 3 where the standard deviations of $n_+$ obtained with the four types of calculations are displayed. Standard deviations follow the same trends as the statistical fluctuations displayed in figure 1.
FIG. 2: The occupation probability $n_+$ obtained by averaging over stochastic trajectories is shown as a function of time $t$ multiplied by the coupling constant $C$ and compared to the exact dynamics (solid line) with $10^4$ trajectories. Top: Results obtained using the SSE with (open squares) and without (filled circles) optimization. Bottom, results obtained using the SMF techniques with (open squares) and without (filled circles) optimization. In each case the error bars represent the standard deviations.

that all stochastic methods lead to the exact result for an infinite number of trajectories. However in order to have the same standard deviations with the standard SSE as the one displayed in figure 2 using OSMF, several millions of trajectories are needed.

B. Variation of parameters

We now systematically study the effect of the different optimizations on the behavior of statistical fluctuations when the parameters of the model change. In a first series of calculations, the effect of the variation of the coupling constant $C$ for a fixed number of bath states ($N = 1$) is considered. In the second series of calculations the number of states was varied while $C = 0.5$. $\lambda_s$ was obtained by fitting the statistical fluctuations. We show in figure 4 and figure 5 the values of $\lambda_s$ respectively as a function of $C$ and $N$ for the SSE.
FIG. 3: Evolution of the standard deviations of $n_+$ as a function of time $t$ multiplied by the coupling constant $C$ obtained for $10^5$ trajectories using SSE (filled circles), OSSE (filled triangles), SMF (open stars) and OSMF (open squares).

and the OSMF calculations. In figure 4 for both stochastic calculations, $\lambda_s$ exhibits a linear behavior with $C$ in agreement with the expressions (10) and (36). However the statistical fluctuations increase much more rapidly with $C$ in the SSE case than in the OSMF case. Therefore it is found that the effect of the optimization increases when the coupling increases. Similarly $\lambda_s$ increases faster with the number $N$ of states in the bath in SSE compared to the optimized cases. Again the optimization is more efficient when $N$ increases.

In this section we have illustrated by a model case the optimization procedure described previously. We have shown that the combined effect of using the mean-field and the adaptive noise significantly improves the quantum jump simulations. Lastly, we have shown that the improvement depends explicitly on the coupling strength as well as on the number of states in the bath.

V. CONCLUSION

In this work the freedom in the stochastic reformulation of the exact dynamics of interacting systems using pairs of wave-packets has been used to optimize stochastic trajectories. For a given initial state an optimal complex noise that minimizes statistical fluctuations is obtained. It is shown that the properties of the stochastic variables depend on the specific
FIG. 4: Evolution of $\lambda_s$ as a function of the coupling constant $C$ obtained using SSE (filled circles) and OSMF (open squares). The result of a fit is displayed with solid (for SSE) and dashed (for OSMF) lines and corresponds respectively to $\lambda_s \propto 5.5C$ and $\lambda_s \propto 1.15C$.

FIG. 5: Evolution of $\lambda_s$ as a function of the number of states $N$ in the bath for $C = 0.5$ obtained using SSE (filled circles) and OSMF (open squares). The result of a fit is displayed with solid and dashed lines for the SSE and OSMF cases and corresponds to $\lambda_s \propto 1.8\sqrt{N}$ and $\lambda_s \propto 1.0\sqrt{N}$.

state to which it is applied as well as on the interaction properties, hence the denomination 'adaptative noise method'. We have also shown that the method can be combined with the introduction of a mean-field prior to the stochastic reformulation. The combination of the mean-field and the adaptative noise is expected to lead in general to a further reduction of
The statistical fluctuations.

The different optimization procedures have been studied with a schematic model consisting of a single spin interacting with a bath of spins. In this model the optimization of jumps significantly reduces the statistical fluctuations. Accordingly it has been shown that for a given number of trajectories, a much better reproduction of the exact dynamics is obtained compared to the standard SSE without optimization. Although promising, more complex models should be used to fully demonstrate the power of the method.

At last we would like to mention that the work described here cannot be directly applied to stochastic Many-Body theories to treat self-interacting bosonic or fermionic systems as proposed in ref. [17, 18]. In this case, the operators $A_\alpha$ and $B_\alpha$ are identical and are applied to the same state. Work is currently in progress to modify the original stochastic reformulation in order to take advantage of the optimization procedure described here.

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