

# Stochastic Schroedinger equation from optimal observable evolution

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In this article, we consider a set of trial wave-functions denoted by  $|Q\rangle$  and an associated set of operators  $A_\alpha$  which generate transformations connecting those trial states. Using variational principles, we show that we can always obtain a quantum Monte-Carlo method where the quantum evolution of a system is replaced by jumps between density matrices of the form  $D = |Q_a\rangle\langle Q_b|$ , and where the average evolutions of the moments of  $A_\alpha$  up to a given order  $k$ , i.e.  $\langle A_{\alpha_1} \rangle, \langle A_{\alpha_1} A_{\alpha_2} \rangle, \dots, \langle A_{\alpha_1} \dots A_{\alpha_k} \rangle$ , are constrained to follow the exact Ehrenfest evolution at each time step along each stochastic trajectory. Then, a set of more and more elaborated stochastic approximations of a quantum problem is obtained which approach the exact solution when more and more constraints are imposed, i.e. when  $k$  increases. The Monte-Carlo process might even become exact if the Hamiltonian  $H$  applied on the trial state can be written as a polynomial of  $A_\alpha$ . The formalism makes a natural connection between quantum jumps in Hilbert space and phase-space dynamics. We show that the derivation of stochastic Schroedinger equations can be greatly simplified by taking advantage of the existence of this hierarchy of approximations and its connection to the Ehrenfest theorem. Several examples are illustrated: the free wave-packet expansion, the Kerr oscillator, a generalized version of the Kerr oscillator, as well as interacting bosons or fermions.

## I. INTRODUCTION

Starting from the pioneering works of Feynman on path integrals [1], large efforts have been devoted to the possibility to replace a quantum problem by a stochastic process [2–7]. One of the greatest interest of stochastic formulations can be summarized as follow: let us consider a quantum system where the number of degrees of freedom to follow is too high to authorize an exact treatment. In some cases, it is possible to recover the exact solution by averaging over an ensemble of trajectories where the number of degrees of freedom to consider along each path is significantly reduced. Then the exact problem can be recast into a set of problems that can be carried out. Such a stochastic formulation is for instance at the heart of quantum Monte-Carlo techniques in particular when considering interacting systems [2–4].

Essentially two strategies exist to introduce stochastic formulations. The first technique consists of selecting a limited number of degrees of freedom associated to specific observable, which contains already a large amount of information on the system. Then, the system evolution is recovered by averaging over stochastic evolution of these observable. This technique will be called here as 'Phase-Space technique' [8]. New developments along this line have been proposed to treat interacting fermionic systems [9].

Alternatively, several works have shown that one can take advantage of the Stochastic Schroedinger Equation (SSE) approach [5–8, 10–21] to simulate exactly quantum systems [22–26]. In that case, a specific class of trial wave-functions is selected and the exact Schroedinger equation is mapped into a stochastic process between trial states. Again, trial wave-functions are chosen to be much simpler than the exact wave-function, although

complex enough to incorporate already some important features of the problem. SSE have generally an equivalent stochastic evolution in phase-space: for instance, the stochastic process proposed in ref. [23] can be equivalently replaced by a stochastic process for the one-body density evolution [27] associated with N-body densities  $D = |\Phi_1\rangle\langle\Phi_2|$  where both states corresponds to trial wave-functions, i.e. Hartree-Fock states.

In this work, we would like to address more systematically the possibility to obtain SSE for a given quantum problem using the phase-space evolution. Following ref. [29], we consider trial state vectors denoted by  $|Q\rangle$ , where  $Q = \{q_\alpha\}_{\alpha=1,N}$  (with  $N$  eventually infinite) correspond to a set of variables which completely determines the state. The ensemble of states obtained by taking all possible values of  $Q$  is denoted by  $\mathcal{S}_Q$ . The second important hypothesis is that we assume the existence of an ensemble of operators  $\{A_\alpha\}_{\alpha=1,N}$ , that generate local transformations between the state of  $\mathcal{S}_Q$ , i.e. one state  $|Q\rangle$  transforms into another state  $|Q + \delta Q\rangle$  of  $\mathcal{S}_Q$  through the transformation

$$|Q + \delta Q\rangle = e^{\sum_\alpha \delta q_\alpha A_\alpha} |Q\rangle. \quad (1)$$

At the deterministic level, variational principles [29, 30] provide a systematic way to replace the exact problem by an approximate dynamics in restricted space  $\mathcal{S}_Q$ . A first example of extension of variational methods to obtain stochastic Schroedinger equation has been given in ref. [28].

In this article we propose an alternative procedure to obtain SSE from variational principles. Some aspects related to standard variational methods are first recalled. Schroedinger equations obtained in this way are intimately connected to the phase-space evolution and can be regarded as the best projected approximation for the

dynamics within the subspace of observable  $\langle A_\alpha \rangle$ . We show that variational techniques can be helpful to obtain stochastic formulations of a given problem which has a natural interpretation in terms of observable evolution. Starting from variational methods, we prove the existence of a hierarchy of approximations of a quantum problem using SSE methods where the expectation values of the moments of the  $A_\alpha$  up to a given order  $k$ , i.e.  $\langle A_{\alpha_1} \rangle, \langle A_{\alpha_1} A_{\alpha_2} \rangle, \dots, \langle A_{\alpha_1} \dots A_{\alpha_k} \rangle$ , follow in average the exact Ehrenfest evolution at each time step along each stochastic trajectory. Therefore, this generalization of the deterministic case can be regarded as the best approximation of the dynamics on an enlarged subspace of observable.

In the second part of this article, the existence of such a hierarchy and its connection to the Ehrenfest evolution are used to deduce SSE in several illustrative examples.

## II. GENERAL REMARKS ON VARIATIONAL PRINCIPLES

Variational principles are powerful tools to provide approximate solutions for the static or dynamical properties of a system when few degrees of freedom are supposed to dominate[29–34]. The selection of few relevant degrees of freedoms generally strongly reduces the complexity of the considered problem. Before introducing stochastic mechanics, we consider standard variational principles and recall specific aspects which will be helpful in the following discussion. We assume that the system is given at time  $t_0$  by  $|\Psi(t_0)\rangle = |Q\rangle$  where  $|Q\rangle$  belongs to  $\mathcal{S}_Q$ . The wave-function, denoted by  $|\Psi(t)\rangle$ , which evolves according to a given Hamiltonian  $H$  has a priori no reason to remain in the subspace  $\mathcal{S}_Q$ . However, a good approximation of the dynamics restricted to wave-functions of  $\mathcal{S}_Q$  is obtained by minimizing the action[29, 30]

$$S = \int_{t_0}^{t_1} ds \langle Q | i\hbar \partial_t - H | Q \rangle, \quad (2)$$

with respect to the variation of  $Q$  and with the additional boundary condition  $|\delta\Phi(t_0)\rangle = 0$  and  $\langle\delta\Phi(t_1)| = 0$ . The variation with respect to  $\langle\delta Q|$  leads then to the equation

$$\langle\delta Q| i\hbar \partial_t^\leftarrow - H | Q \rangle = 0, \quad (3)$$

while the variation with respect to  $|\delta Q\rangle$  gives the hermitian conjugate equation

$$\langle Q | i\hbar \partial_t^\rightarrow + H | \delta Q \rangle = 0. \quad (4)$$

Here  $\partial_t^\leftarrow$  and  $\partial_t^\rightarrow$  means that the derivative is acting respectively to the left and right hand side.

### A. observable evolution

Due to relation (1), the above Schroedinger equation corresponds to specific evolutions of the expectation values  $\langle A_\alpha \rangle$  of the operators  $A_\alpha$ . Using  $|\delta Q\rangle =$

$\sum_\alpha \delta q_\alpha A_\alpha |Q\rangle$ , variations with respect to  $|\delta Q\rangle$  are replaced by a set of independent variations  $\{\delta q_\alpha\}_{\alpha=1,N}$ , leading to:

$$i\hbar \langle dQ | A_\alpha | Q \rangle = -dt \langle Q | H A_\alpha | Q \rangle, \quad (5)$$

while variation with respect to  $\delta q_\alpha^*$  gives

$$i\hbar \langle Q | A_\alpha | dQ \rangle = dt \langle Q | A_\alpha H | Q \rangle. \quad (6)$$

Combining the two equations gives

$$i\hbar \frac{d\langle A_\alpha \rangle}{dt} = \langle [A_\alpha, H] \rangle, \quad (7)$$

which is nothing but the exact Ehrenfest equation of motion for the set of operators  $A_\alpha$ . Therefore, starting from a density  $D(t_0) = |Q\rangle \langle Q|$ , for one time step the evolution of  $\langle A_\alpha \rangle$  corresponds to the exact evolution although the state is constrained to remain in the  $\mathcal{S}_Q$  space. This property is however a priori only true for observable which are linear combination of  $A_\alpha$ .

### B. Links with effective Hamiltonian and projected dynamics

The evolution deduced from the variational method can equivalently be interpreted as an effective Hamiltonian dynamics. Indeed, we have

$$|dQ\rangle = \sum_\alpha dq_\alpha A_\alpha |Q\rangle \equiv \frac{dt}{i\hbar} H_1 |Q\rangle, \quad (8)$$

where we have introduced the effective Hamiltonian  $H_1$ . This Hamiltonian differs from  $H$  unless  $H$  applied on the trial wave-function is itself a linear combination of  $A_\alpha$ . The expression of  $H_1$  can be obtained using the evolution of  $dq_\alpha$ . From eq. (6) we obtain

$$i\hbar \sum_\alpha dq_\alpha \langle A_\beta A_\alpha \rangle = dt \langle A_\beta H \rangle. \quad (9)$$

Writing  $\langle Q | A_\beta A_\alpha | Q \rangle = M_{\beta\alpha}$ ,  $dq_\alpha$  can formally be obtained by inverting the last expression into

$$dq_\alpha = \frac{dt}{i\hbar} \sum_\beta M_{\alpha\beta}^{-1} \langle Q | A_\beta H | Q \rangle. \quad (10)$$

Plugging last equation into (8) leads to  $H_1 = \mathcal{P}_1 H$ , where  $\mathcal{P}_1$  is defined as

$$\mathcal{P}_1 = \sum_{\alpha\beta} A_\alpha |Q\rangle M_{\alpha\beta}^{-1} \langle Q | A_\beta, \quad (11)$$

and plays the role of a "projector" onto the subspace of operators  $A_\alpha$ . In particular, for any observable  $B$ , the operator  $B' = (1 - \mathcal{P}_1)B$  fulfills  $\langle A_\alpha B' \rangle = 0$ . Similarly, if we denote by  $B'' = B(1 - \mathcal{P}_1)$ , we have  $\langle B'' A_\alpha \rangle = 0$ . Writing the full Hamiltonian as

$$H = \mathcal{P}_1 H + (1 - \mathcal{P}_1) H,$$

we see that the effective evolution of  $|dQ\rangle$  given by eq. (8) where  $H_1$  is obtained from the minimization of the action can be interpreted as the approximate evolution when the part of the Hamiltonian that do not contribute to the  $\langle A_\alpha \rangle$  is neglected. As a matter of fact, the second part is responsible from the deviation of the projected dynamics from the exact one. In summary, we have recalled here that the variational dynamics can be regarded as a projected dynamics into the subspace of relevant observable [39, 40]. In the following, we show that aspects of variational principles presented here can be adapted to obtain Monte-Carlo methods.

### III. STOCHASTIC QUANTUM MECHANICS FROM VARIATIONAL PRINCIPLES

Several recent studies have shown that the exact evolution of complex quantum systems can be replaced by a set of stochastic evolutions of simpler trial wave-functions. In this context, at a given intermediate time, the exact density is replaced by the average over "densities" of the form [22–26]

$$D(t) = |Q_a\rangle \langle Q_b|, \quad (12)$$

where both states belongs to  $\mathcal{S}_Q$ . In all cases, the main advantage of these reformulations was to prove that the stochastic methods can be performed imposing that both states remain in  $\mathcal{S}_Q$ . As in previous section, this condition implies that we restrict variations of each state to

$$|Q_a + \delta Q_a\rangle = e^{\sum_\alpha \delta q_\alpha^{[a]} A_\alpha} |Q_a\rangle, \quad (13)$$

$$|Q_b + \delta Q_b\rangle = e^{\sum_\alpha \delta q_\alpha^{[b]} A_\alpha} |Q_b\rangle, \quad (14)$$

where now  $\delta q_\alpha^{[a]}$  and  $\delta q_\alpha^{[b]}$  may also contain a stochastic part.

The aim of the present section is to show that, given a class of trial states, a hierarchy of Monte-Carlo formulations of a quantum problem can be systematically obtained using variational methods. The description of the system can be gradually improved by introducing a set of noises, written as

$$\begin{cases} \delta q_\alpha^{[a]} = \delta q_\alpha^a + \delta \xi_\alpha^{[2]} + \delta \xi_\alpha^{[3]} + \dots \\ \delta q_\alpha^{[b]*} = \delta q_\alpha^{b*} + \delta \eta_\alpha^{[2]} + \delta \eta_\alpha^{[3]} + \dots \end{cases} \quad (15)$$

where the second, third... terms represent stochastic variables added on top of the deterministic contribution. Those are optimized to not only insure that the average evolution of  $\langle A_\alpha \rangle$  matches the exact evolution at each time step but also that the average evolutions of higher moments  $\langle A_\alpha A_\beta \rangle$ ,  $\langle A_\alpha A_\beta A_\gamma \rangle$ ,... follow the exact Ehrenfest dynamics.

#### A. Step 1: deterministic evolution

Assuming first that stochastic contributions  $\xi_\alpha^{[i]}$  and  $\eta_\alpha^{[i]}$  are neglected in eq. (15), we show how variational

principles described previously can be used for mixed densities given by eq. (12). It is worth noticing that variational principle have also been proposed to estimate transition amplitudes [30] (see also discussion in [41]). In that case, different states are used in the left and right hand side of the action. This situation is similar to the case we are considering. We are interested here in the short time evolution of the system, therefore we disregard the time integral in equation (2) and consider directly the action

$$S = Tr(\{i\hbar \partial_t^\dagger - i\hbar \partial_t^\dagger - H\} D), \quad (16)$$

where  $Tr(\cdot)$  stands for the usual trace. Starting from the above action, one can generalize the different aspects discussed in section II to the case of densities formed with couples of trial states. For instance, the minimization with respect to the variations  $\langle \delta Q_b |$  and  $|\delta Q_a\rangle$  leads to the two conditions

$$\begin{cases} i\hbar \langle Q_b | A_\alpha | dQ_a \rangle = \langle Q_b | A_\alpha H | Q_a \rangle, \\ i\hbar \langle dQ_b | A_\alpha | Q_a \rangle = \langle Q_b | H A_\alpha | Q_a \rangle, \end{cases} \quad (17)$$

from which we deduce that

$$i\hbar \frac{d}{dt} \langle A_\alpha \rangle = \langle [A_\alpha, H] \rangle, \quad (18)$$

where  $\langle A_\alpha \rangle = \langle Q_b | A_\alpha | Q_a \rangle$ . Therefore, the minimization of the action again insures that the exact Ehrenfest evolution is followed by the  $A_\alpha$  observable over one time step. Similarly, the evolution of both  $|Q_a\rangle$  and  $|Q_b\rangle$  are given by

$$\begin{cases} |dQ_a\rangle = \sum_\alpha dq_\alpha^a A_\alpha |Q_a\rangle = \frac{dt}{i\hbar} \mathcal{P}_1 H |Q_a\rangle \\ \langle dQ_b| = \langle Q_b | \sum_\alpha dq_\alpha^{b*} A_\alpha = -\frac{dt}{i\hbar} \langle Q_b | H \mathcal{P}_1 \end{cases}$$

where  $\mathcal{P}_1$  now reads

$$\mathcal{P}_1 = \sum_{\alpha\beta} A_\alpha |Q_a\rangle M_{\alpha\beta}^{-1} \langle Q_b | A_\beta. \quad (19)$$

In opposite to previous section,  $\mathcal{P}_1$  cannot be interpreted as a projector onto the space of observable due to the fact that  $M_{\alpha\beta} = \langle Q_b | A_\alpha A_\beta | Q_a \rangle$  is not anymore a metric for that space. However, we still have the property that the total Hamiltonian can be split into two parts, one which corresponds to the effective dynamic solution of the minimization, and one which is neglected, which identifies the irrelevant part for the  $\langle A_\alpha \rangle$  evolutions. It is worth noticing that the variational approximation presented here for mixed densities has been already used without justification in ref. [26] to optimize stochastic trajectories.

#### B. Step 2 : Introduction of gaussian stochastic processes

In this section, we show that the description of the dynamics can be further improved by introducing diffusion

in the Hilbert space  $\mathcal{S}_Q$ . We consider that the evolutions of  $q_\alpha^{[a]}$  and  $q_\alpha^{[b]}$  now read

$$\begin{aligned} dq_\alpha^{[a]} &= dq_\alpha^a + d\xi_\alpha^{[2]}, \\ dq_\alpha^{[b]*} &= dq_\alpha^{b*} + d\eta_\alpha^{[2]}, \end{aligned}$$

where  $d\xi_\alpha^{[2]}$  and  $d\eta_\alpha^{[2]}$  correspond to two sets of stochastic gaussian variables (following Ito rules of stochastic calculus [42]) with mean values equal to zero and variances verifying

$$d\xi_\alpha^{[2]} d\xi_\beta^{[2]} = d\omega_{\alpha\beta}, \quad (20)$$

$$d\eta_\alpha^{[2]} d\eta_\beta^{[2]} = d\sigma_{\alpha\beta}, \quad (21)$$

$$d\xi_\alpha^{[2]} d\eta_\beta^{[2]} = 0 \quad (22)$$

We assume that  $d\omega_{\alpha\beta}$  and  $d\sigma_{\alpha\beta}$  are proportional to  $dt$ . Note that equation (22) reflects that the stochastic contributions to the evolutions of  $|Q_a\rangle$  and  $\langle Q_b|$  are independent. The advantage of introducing the Monte-Carlo method can be seen in the average evolutions of the states. Keeping only linear terms in  $dt$  in eq. (14) gives for instance

$$\overline{|dQ_a\rangle} = \left\{ \sum_\alpha dq_\alpha^a A_\alpha + \sum_{\alpha < \beta} d\omega_{\alpha\beta} (A_\alpha A_\beta + A_\beta A_\alpha) \right\} |Q_a\rangle \quad (23)$$

In the previous section, we have recalled that using trial state leads to an approximate treatment of the dynamics associated to effective Hamiltonian which can only be written as a linear superposition of the  $A_\alpha$ . Last expression emphasizes that, while the states remain in the  $\mathcal{S}_Q$  space during the stochastic process, the average evolution can now simulate the evolution with an effective Hamiltonian containing not only linear but also quadratic in  $A_\alpha$ .

The goal is now to take advantage of this generalization and reduce further the distance between the average evolution and the exact one. The most natural generalization of the last section is to minimize the average action

$$S = \overline{Tr(\{i\hbar\partial_t^\dagger - i\hbar\partial_t - H\} D)}, \quad (24)$$

with respect to the variations of different parameters, i.e.  $\delta q_\alpha^a$ ,  $\delta q_\alpha^{b*}$ ,  $\delta\omega_{\alpha\beta}$  and  $\delta\sigma_{\alpha\beta}$ . In the following, a formal solution of the minimization procedure is obtained. We show that variational principles applied to stochastic process generalize the deterministic case by imposing that not only that expectation values  $\langle A_\alpha \rangle$  but also the second moments  $\langle A_\alpha A_\beta \rangle$ , follow the exact Ehrenfest evolution.

### 1. Effective Hamiltonian dynamics deduced from the minimization

The variations with respect to  $\delta q_\alpha^{b*}$  and  $\delta\sigma_{\alpha\beta}$  give two sets of coupled equations between  $dq_\alpha^a$  and  $d\omega_{\alpha\beta}$ . The

formal solution of the minimization can however be obtained by making an appropriate change on the variational parameters prior to the minimization. In the following, we introduce the notation  $B_\nu = A_\alpha A_\beta + A_\beta A_\alpha$  where  $\nu$  denotes  $(\alpha, \beta)$  with  $\alpha < \beta$ . Starting from the general form of the effective evolution (23), we dissociate the part which contributes to the evolution of the  $\langle A_\alpha \rangle$  from the rest. This could be done by introducing the projection operator  $\mathcal{P}_1$ . Equation (23) then reads

$$\overline{|dQ_a\rangle} = \left\{ \sum_\alpha dz_\alpha^a A_\alpha + \sum_\nu d\omega_\nu (1 - \mathcal{P}_1) B_\nu \right\} |Q_a\rangle \quad (25)$$

where the new set of parameters  $dz_\alpha^a$  is given by

$$dz_\alpha^a = dq_\alpha^a + \sum_{\beta\nu} d\omega_\nu M_{\alpha\beta}^{-1} \langle Q_b | A_\beta B_\nu | Q_a \rangle. \quad (26)$$

Similarly, the average evolution  $\langle dQ_b|$  transforms into

$$\overline{\langle dQ_b|} = \langle Q_b| \left\{ \sum_\alpha dz_\alpha^{b*} A_\alpha + \sum_\nu d\sigma_\nu B_\nu (1 - \mathcal{P}_1) \right\} \quad (27)$$

where  $dz_\alpha^{b*}$  is given by

$$dz_\alpha^{b*} = dq_\alpha^{b*} + \sum_{\beta\nu} d\sigma_\nu \langle Q_b | B_\nu A_\beta | Q_a \rangle M_{\beta\alpha}^{-1}. \quad (28)$$

In the following, we write  $B'_\nu = (1 - \mathcal{P}_1) B_\nu$  and  $B''_\nu = B_\nu (1 - \mathcal{P}_1)$ . The great interest of this transformation is to have  $\langle A_\alpha B'_\nu \rangle = 0$  and  $\langle B''_\nu A_\alpha \rangle = 0$  for all  $\alpha$  and  $\nu$ . Accordingly, the variations with respect to  $\delta z_\alpha^{b*}$  and  $\delta z_\alpha^a$  lead to

$$\begin{cases} i\hbar \overline{\langle Q_b | A_\alpha | dQ_a \rangle} = \langle Q_b | A_\alpha H | Q_a \rangle \\ i\hbar \overline{\langle dQ_b | A_\alpha | Q_a \rangle} = \langle Q_b | H A_\alpha | Q_a \rangle, \end{cases} \quad (29)$$

which gives closed equations for the variations  $dz_\alpha^a$  and  $dz_\alpha^{b*}$  which are decoupled from the evolution of  $d\omega_\nu$  and  $d\sigma_\nu$ . These equations are identical to the ones derived in step 1 and can be again inverted as

$$\sum_\alpha dz_\alpha^a A_\alpha |Q_a\rangle = \frac{dt}{i\hbar} \mathcal{P}_1 H |Q_a\rangle, \quad (30)$$

$$\langle Q_b| \sum_\alpha dz_\alpha^{b*} A_\alpha = -\frac{dt}{i\hbar} \langle Q_b| H \mathcal{P}_1. \quad (31)$$

On the other hand, the variations with respect to  $\delta\sigma_\nu$  and  $\delta\omega_\nu$  lead to

$$\begin{cases} i\hbar \overline{\langle Q_b | B''_\nu | dQ_a \rangle} = \langle Q_b | B''_\nu H | Q_a \rangle, \\ i\hbar \overline{\langle dQ_b | B'_\nu | Q_a \rangle} = \langle Q_b | H B'_\nu | Q_a \rangle, \end{cases} \quad (32)$$

which again gives closed equations for  $d\omega_\nu$  and  $d\sigma_\nu$ . These equations can be formally solved by introducing the two projectors  $\mathcal{P}_2$  and  $\mathcal{P}'_2$  associated respectively to

the subspaces of operators  $B_\nu(1-\mathcal{P}_1)$  and  $(1-\mathcal{P}_1)B_\nu$ .  $\mathcal{P}_2$  differs from  $\mathcal{P}'_2$  due to the fact that  $B_\nu$  operators and  $A_\alpha$  operators do not a priori commute. Then, the effective evolution given by eq. (23) becomes

$$\begin{aligned}\overline{|dQ_a\rangle} &= \frac{dt}{i\hbar} \left( \sum_\alpha dz_\alpha^a A_\alpha + (1-\mathcal{P}_1) \sum_\nu d\omega_\nu B_\nu \right) |Q_a\rangle \\ &= \frac{dt}{i\hbar} (\mathcal{P}_1 + \mathcal{P}_2) H |Q_a\rangle,\end{aligned}\quad (33)$$

while

$$\overline{\langle dQ_b|} = -\frac{dt}{i\hbar} \langle Q_b| H (\mathcal{P}_1 + \mathcal{P}'_2). \quad (34)$$

In both cases, the first part corresponds to the projection of the exact dynamics on the space of observable  $\langle A_\alpha \rangle$ . The second term corresponds to the projection on the subspace of the observable  $\langle A_\alpha A_\beta \rangle$  "orthogonal" to the space of the  $\langle A_\alpha \rangle$ .

## 2. Interpretation in terms of observable evolution

The variation with respect to an enlarged set of parameters does a priori completely determine the deterministic and stochastic evolution of the two trial state vectors. The associated average Schrodinger evolution corresponds to a projected dynamics. The interpretation of the solution obtained by variational principle is rather clear in terms of observable evolution. Indeed, from the two variational conditions, we can easily deduce that

$$\begin{aligned}\overline{d\langle A_\alpha \rangle} &= \langle [A_\alpha, H] \rangle, \\ \overline{d\langle B_\nu \rangle} &= \frac{dt}{i\hbar} \langle [B_\nu, H] \rangle.\end{aligned}$$

In summary, using the additional parameters associated with the stochastic contribution as variational parameters for the average action given by eq. (24), one can

further reduce the distance between the simulated evolution and the exact solution. When gaussian noises are used, this is equivalent to impose that the evolution of the correlations between operators  $A_\alpha$  obtained by averaging over different stochastic trajectories also matches the exact evolution.

## C. Step 3: Generalization

If the Hamiltonian  $H$  applied to the trial state can be written as a quadratic Hamiltonian in terms of  $A_\alpha$  and if the trial states form an overcomplete basis of the total Hilbert space, then the above procedure can provide with an exact stochastic reformulation of the problem. If it is not the case, the above methods can be generalized by introducing higher order stochastic variables. Considering now the more general form

$$\begin{cases} \delta q_\alpha^{[a]} = \delta q_\alpha^a + \delta \xi_\alpha^{[2]} + \delta \xi_\alpha^{[3]} + \dots \\ \delta q_\alpha^{[b]*} = \delta q_\alpha^{b*} + \delta \eta_\alpha^{[2]} + \delta \eta_\alpha^{[3]} + \dots \end{cases}$$

we suppose now that the only non vanishing moments for  $d\xi_\alpha^{[k]}$  and  $d\eta_\alpha^{[k]}$  are the moments of order  $k$  (which are then assumed to be proportional to  $dt$ ). For instance, we assume that  $d\xi_\alpha^{[3]}$  verifies

$$\overline{d\xi_\alpha^{[3]}} = \overline{d\xi_\alpha^{[3]} d\xi_\beta^{[3]}} = 0, \quad (35)$$

$$\overline{d\xi_\alpha^{[3]} d\xi_\beta^{[3]} d\xi_\gamma^{[3]}} \neq 0. \quad (36)$$

Then without going into details, we can easily generalize the method presented in step 2 and deduce that the average evolutions of the trial states will be given by

$$\begin{aligned}\overline{|dQ_a\rangle} &= \frac{dt}{i\hbar} \{\mathcal{P}_1 + \mathcal{P}_2 + \mathcal{P}_3 + \dots\} H |Q_a\rangle \\ \overline{\langle dQ_b|} &= -\frac{dt}{i\hbar} \langle Q_b| H \{\mathcal{P}_1 + \mathcal{P}'_2 + \mathcal{P}'_3 + \dots\}\end{aligned}$$

where the first terms contain all the information on the evolution of the  $\langle A_\alpha \rangle$ , the second terms contain all the information on the evolution of the  $\langle A_\alpha A_\beta \rangle$  which is not accounted for by the first term, the third terms contain all the information on the evolution of the  $\langle A_\alpha A_\beta A_\gamma \rangle$  which is not contained in the first two terms, ... The procedure described here gives an exact Monte-Carlo formulation of a given problem if the Hamiltonian  $H$  applied on  $|Q_a\rangle$  or  $\langle Q_b|$  can be written as a polynomial of  $A_\alpha$ . If the polynomial is of order  $k$ , then the sum stops at  $\mathcal{P}_k$ .

## D. Summary and discussion on practical applications

In this section, we propose a systematic method to replace a general quantum problem by stochastic processes

within a restricted class of trial state vectors associated to a set of observable  $A_\alpha$ . Using variational techniques, we show that a hierarchy of stochastic approximations

can be obtained. This method insures that at the level  $k$  of the hierarchy, all moments of order  $k$  or below of the observable  $A_\alpha$  evolve according to the exact Ehrenfest equation over a single time step. The Monte-Carlo formulation might become exact if the Hamiltonian applied to the trial state writes as a polynomial of the  $A_\alpha$  operators.

Aside of the use of variational techniques, we end up with the following important conclusion: *Given an initial density  $D = |Q_a\rangle\langle Q_b|$  where both states belongs to a given class of trial states associated to a set of operators  $A_\alpha$ , we can always find a Monte-Carlo process which preserves the specific form of  $D$  and insures that expectations values of all moments of the  $A_\alpha$  up to a certain order  $k$  evolve in average according to the Ehrenfest theorem associated to the exact Hamiltonian at each time step and along each trajectory.*

This statement will be referred to as the "existence theorem" in the following. Such a general statement is very useful in practice to obtain stochastic processes. Indeed, the use of variational techniques might become rather complicated due to the large number of degrees of freedom involved. An alternative method is to take advantage of the natural link made between the average effective evolution deduced from the stochastic evolution and the phase-space dynamics. Indeed, according to the existence theorem, we know that at a given level  $k$  of approximation, the dynamics of each trial state can be simulated by an average effective Hamiltonian insuring that all moments of order  $k$  or below matches the exact evolution. In general, it is easier to express the exact evolution of the moments and then 'guess' the associated SSE.

The second important remark is that the above method can also be used to provide a SSE which maintains  $Tr(D) = 1$  along each path. In that case, the action (24) can still be used but the density  $D$  should be replaced by

$$D = \frac{|Q_a\rangle\langle Q_b|}{\langle Q_b | Q_a \rangle}. \quad (37)$$

All the equations given above can then be equivalently derived. The main difference being that  $A_\alpha$  is now replaced by  $(A_\alpha - \langle A_\alpha \rangle)$  in the variations of the states (equation (14)). As we will see, the possibility to use constant trace formulation usually simplifies the use of the Ehrenfest theorem to guess the involved stochastic equations.

#### IV. APPLICATIONS

In the following, we give few examples which have been studied recently in the context of Monte-Carlo techniques to illustrate how formal results obtained in previous section can be applied. In each case, the link between the phase-space evolution and the associated SSE is pointed out.

##### A. The free wave-packet expansion

We first consider a system initially in the ground state of a harmonic oscillator described by the Hamiltonian  $H_0 = \hbar\omega (a^+a + \frac{1}{2})$  where  $a$  and  $a^+$  are the usual creation/annihilation operators with  $[a, a^+] = 1$ . Denoting by  $\eta = m\omega/\hbar$ , the initial wave-packet corresponds to a gaussian wave-function of width  $\langle x^2 \rangle = \frac{1}{2\eta}$ . At time  $t = 0$ , the harmonic constraint is released. During the free expansion, the wave-packet remains gaussian and verifies [43]

$$\langle x^2 \rangle = \frac{1}{2\eta} + \frac{\hbar^2\eta}{2m^2}t^2, \quad (38)$$

where  $m$  is the mass of the system.

##### 1. Stochastic formulation

We show that this free expansion can be simulated by quantum diffusion between gaussian wave-functions of fixed widths. Let us assume that, at a given intermediate time step of the stochastic process, the density is given by averaging over densities of the form (which includes the initial condition)

$$D = \frac{|\alpha\rangle\langle\beta|}{\langle\beta|\alpha\rangle}, \quad (39)$$

where  $|\alpha\rangle$  and  $\langle\beta|$  are Bargmann states of the initial oscillator defined as  $|\alpha\rangle = e^{\alpha a^+}|0\rangle$  [8]. These states verify  $a|\alpha\rangle = \alpha|\alpha\rangle$  and  $\langle\beta|a^+ = \langle\beta|\beta^*$ . We use Bargmann states instead of coherent states to simplify the discussion. In particular, we have the transformation properties

$$|\alpha + d\alpha\rangle = e^{d\alpha a^+}|\alpha\rangle, \quad \langle\beta + d\beta| = \langle\beta|e^{d\beta^* a}, \quad (40)$$

which illustrates that the generator of transformations between Bargmann states are the  $a$  and  $a^+$  operators.

Once the harmonic constraint is released the Hamiltonian becomes the free Hamiltonian

$$H = \frac{p^2}{2m} = -\frac{\hbar\omega}{4}(a^+ - a)^2. \quad (41)$$

The action of  $H$  on  $|\alpha\rangle$  and  $\langle\beta|$  can be written respectively as

$$\begin{aligned} H|\alpha\rangle &= -\frac{\hbar\omega}{4}(a^{+2} - 2\alpha a^+ + \alpha^2)|\alpha\rangle, \\ \langle\beta|H &= -\frac{\hbar\omega}{4}\langle\beta|(a^2 - 2\beta^*a + \beta^{*2}), \end{aligned}$$

which corresponds to polynomial of order 2 in  $a^+$  and  $a$  respectively. Therefore, we expect that the exact dynamics can be simulated with gaussian stochastic process

between densities given by eq. (39). The associated stochastic evolution of  $\alpha$  and  $\beta^*$  are written as

$$\begin{cases} d\alpha = \overline{d\alpha} + d\xi^{[2]}, \\ d\beta^* = \overline{d\beta^*} + d\eta^{[2]}, \end{cases}$$

where  $\overline{d\alpha}$  and  $\overline{d\beta^*}$  correspond to the deterministic part of the evolution, while  $d\xi^{[2]}$  and  $d\eta^{[2]}$  are two independent gaussian stochastic variables with zero mean and following Ito rules [42]. In order to precise the nature of the stochastic evolution, one can use the fact that the first and second moments of the  $a$  and  $a^+$  operators follow in average the exact evolution over one time step. Noting that, for  $D$  given by eq. (39), we have  $\langle a^+ \rangle = \text{Tr}(a^+ D) = \beta^*$  and  $\langle a \rangle = \text{Tr}(a D) = \alpha$ , the Ehrenfest theorem applied to  $\langle a^+ \rangle$  and  $\langle a \rangle$  gives the two equations

$$\overline{d\alpha} = \overline{d\beta^*} = i \frac{\hbar\eta}{2m} (\beta^* - \alpha). \quad (42)$$

The application of the Ehrenfest theorem respectively to  $\langle a^2 \rangle$ ,  $\langle a^{+2} \rangle$  and  $\langle a^+ a \rangle$  gives

$$\begin{aligned} \overline{d(\alpha^2)} &= \frac{i\hbar\eta}{m} dt \left\{ (\beta^* - \alpha)\alpha + \frac{1}{2} \right\}, \\ \overline{d(\beta^{*2})} &= \frac{i\hbar\eta}{m} dt \left\{ (\beta^* - \alpha)\beta^* - \frac{1}{2} \right\}, \\ \overline{d(\alpha\beta^*)} &= \frac{i\hbar\eta}{m} dt \{ (\beta^* - \alpha)(\alpha + \beta^*) \}. \end{aligned}$$

Last condition is automatically fulfilled if we assume that  $d\xi^{[2]}$  and  $d\eta^{[2]}$  are independent stochastic variables. According to Ito rules, we also have

$$\begin{aligned} \overline{d(\alpha^2)} &= 2\alpha\overline{d\alpha} + d\xi^{[2]}d\xi^{[2]}, \\ \overline{d(\beta^{*2})} &= 2\beta^*\overline{d\beta^*} + d\eta^{[2]}d\eta^{[2]}, \end{aligned}$$

from which we deduce

$$d\xi^{[2]}d\xi^{[2]} = -d\eta^{[2]}d\eta^{[2]} = \frac{i\hbar\eta}{2m} dt. \quad (43)$$

A stochastic evolution of  $\alpha$  and  $\beta^*$  compatible with the above conditions is then

$$d\alpha = i\hbar \left\{ \frac{\eta}{2m} (\beta^* - \alpha) + \sqrt{\frac{\eta}{2m}} dW_1 \right\}, \quad (44)$$

$$d\beta^* = i\hbar \left\{ \frac{\eta}{2m} (\beta^* - \alpha) + \sqrt{\frac{\eta}{2m}} dW_2 \right\}, \quad (45)$$

where  $dW_1$  and  $dW_2$  are independent stochastic variables with zero mean and  $dW_1 dW_1 = -dW_2 dW_2 = \frac{dt}{i\hbar}$ . The above  $c$ -number dynamic defines a stochastic evolution of the trial states through the relation (40) or equivalently can be interpreted as a diffusion process in the space of densities given by expression (39).

## 2. Recovering the exact dynamics from the average evolution

Let us now check that the stochastic dynamics properly describes the exact evolution. For this, it is convenient to consider the stochastic complex variables defined as  $X = \text{Tr}(Dx)$  and  $P = \text{Tr}(Dp)$ . For densities given by eq. (39),  $X$  and  $P$  are related to  $\alpha$  and  $\beta^*$  through the relations

$$\begin{cases} X = \frac{1}{\sqrt{2\eta}}(\alpha + \beta^*), \\ P = i\hbar\sqrt{\frac{\eta}{2}}(\beta^* - \alpha). \end{cases}$$

Accordingly,  $X$  and  $P$  are stochastic complex variables. Starting from eq. (45), we obtain

$$\begin{cases} dX = \frac{P}{m} dt + d\chi_1, \\ dP = d\chi_2, \end{cases} \quad (46)$$

where the new stochastic variables  $d\chi_1$  and  $d\chi_2$  verify

$$\begin{aligned} \overline{d\chi_1} &= \overline{d\chi_2} = 0, \\ \overline{d\chi_1 d\chi_1} &= \overline{d\chi_2 d\chi_2} = 0, \\ \overline{d\chi_1 d\chi_2} &= \frac{\hbar^2\eta}{2m} dt. \end{aligned}$$

The Langevin equations (46) identifies with the classical equation of motion of the free particle with extra complex gaussian noises. Assuming that initially  $X(0) = P(0) = 0$ , and using Ito rules of stochastic calculus, we deduce that

$$\overline{X^2(t)} = \frac{\hbar^2\eta}{2m^2} t^2.$$

Since along each stochastic path  $\text{Tr}(Dx^2) = \frac{1}{2\eta} + X^2$ , we finally end up with

$$\overline{\text{Tr}(Dx^2)} = \frac{1}{2\eta} + \frac{\hbar^2\eta}{2m^2} t^2,$$

which is nothing but the exact result given by eq. (38).

With this simple example, we have illustrated how a quantum problem can be transformed into a Monte-Carlo process between densities formed of two Bargmann states. A remarkable aspect of the method used here is that at no time it is needed to minimize directly the action. We only took advantage of both the existence theorem and Ehrenfest evolution to obtain the Stochastic Schroedinger evolution of trial states. It should however be kept in mind that the above stochastic process is intimately connected to the projection technique described in previous section.

## B. The Kerr oscillator

As a second example, we consider the model Hamiltonian known as the Kerr oscillator

$$H = \hbar\omega a^+ a + \frac{1}{2}\hbar K (a^+)^2 a^2. \quad (47)$$

Using either the positive-P representation [8] or more recent works based on quantum-field theoretical techniques [44], it can be shown that the quantum problem of a system evolving with  $H$  can be replaced by an ensemble of stochastic c-number evolutions. Let us follow the same strategy as in previous example, and assume that at a given time step the density can be recovered by averaging over densities given by eq. (39). Using similar arguments as before, we know that the exact Hamiltonian dynamics can be simulated by a gaussian diffusion process on  $\alpha$  and  $\beta^*$ , which have the general form given by eq. (42). The Ehrenfest theorem applied on  $\langle a \rangle$  and  $\langle a^+ \rangle$  gives directly

$$\begin{aligned}\overline{d\alpha} &= -idt \{ \omega + K [\beta^* \alpha] \} \alpha, \\ \overline{d\beta^*} &= idt \{ \omega + K [\beta^* \alpha] \} \beta^*,\end{aligned}$$

while the evolutions of  $\langle a^2 \rangle$ ,  $\langle a^{+2} \rangle$  and  $\langle a^+ a \rangle$  lead respectively to

$$\begin{aligned}\overline{d\alpha^2} &= -2idt \{ \omega + K [\beta^* \alpha] \} \alpha^2 - iK dt \alpha^2, \\ \overline{d\beta^{*2}} &= 2idt \{ \omega + K [\beta^* \alpha] \} \beta^{*2} + iK dt \beta^2, \\ \overline{d(\alpha\beta^*)} &= 0.\end{aligned}$$

From the two sets of equations, we deduce

$$\begin{aligned}d\xi^{[2]} d\xi^{[2]} &= -iK dt \alpha^2, \\ d\eta^{[2]} d\eta^{[2]} &= iK dt \beta^{*2}.\end{aligned}$$

Therefore, a stochastic Monte-Carlo process compatible with the above condition is given by

$$\begin{aligned}d\alpha &= -idt \{ \omega + \alpha K [\beta^* \alpha] \} + \sqrt{K\hbar} \alpha dW_1 \\ d\beta^* &= idt \{ \omega + K [\beta^* \alpha] \} \beta^* + \beta^* \sqrt{K\hbar} dW_2\end{aligned}$$

where again  $dW_1$  and  $dW_2$  are independent stochastic variables with zero mean and  $dW_1 dW_1 = -dW_2 dW_2 = \frac{dt}{i\hbar}$ . The above stochastic process is exactly the same as the one derived in ref. [44] using a completely different technique. Indeed, although the presented framework uses phase-space arguments, it has a strong connection with the Hamiltonian dynamics. A great advantage here is that the guess of the Monte-Carlo process is rather

straightforward compared to ref. [44]. Note that above stochastic equations are non-linear stochastic differential equation which might be numerically difficult to handle [45].

### C. The generalized Kerr Hamiltonian

Up to now, we have presented examples where the exact Hamiltonian can be recovered using gaussian noises. To illustrate further the simplicity of the method, we consider the following Hamiltonian

$$H = \hbar\omega a^+ a + \frac{1}{2}\hbar K_1 (a^+)^2 a^2 + \frac{1}{6}\hbar K_2 (a^+)^3 a^3, \quad (48)$$

which will be referred hereafter as the generalized Kerr Hamiltonian. According to the existence theorem, in order to simulate exactly the Hamiltonian, it is necessary to include an extra contribution to the c-number evolution

$$\begin{aligned}d\alpha &= \overline{d\alpha} + d\xi^{[2]} + d\xi^{[3]}, \\ d\beta^* &= \overline{d\beta^*} + d\eta^{[2]} + d\eta^{[3]},\end{aligned}$$

where first and second moments of  $d\xi^{[3]}$  and  $d\eta^{[3]}$  cancel out while third moments are proportional to  $dt$ . As in previous section, the use of the Ehrenfest theorem for the first and second moments leads respectively to

$$\begin{aligned}\overline{d\alpha} &= -idt \left\{ \omega + K_1 [\beta^* \alpha] + \frac{1}{2} K_2 [\beta^* \alpha]^2 \right\} \alpha, \\ \overline{d\beta^*} &= idt \left\{ \omega + K_1 [\beta^* \alpha] + \frac{1}{2} K_2 [\beta^* \alpha]^2 \right\} \beta^*,\end{aligned}$$

and

$$\begin{aligned}d\alpha^{[2]} d\alpha^{[2]} &= -idt \alpha^2 (K_1 + K_2 [\beta^* \alpha]), \\ d\beta^{*[2]} d\beta^{*[2]} &= idt \beta^{*2} (K_1 + K_2 [\beta^* \alpha]).\end{aligned}$$

In order to determine the extra contribution, one should use the third moments. The evolution of  $\langle a^{+3} \rangle$  gives for instance

$$\overline{d(\beta^*)^3} = i\beta^{*3} \left\{ 3 \left[ \omega + K_1 [\beta^* \alpha] + \frac{1}{2} K_2 [\beta^* \alpha]^2 \right] + 3 (K_1 + K_2 [\beta^* \alpha]) + K_2 \right\}.$$

Using the identity

$$\overline{d(\beta^*)^3} = 3\beta^{*2} \overline{d\beta^*} + 3\beta^* d\beta^{*[2]} d\beta^{*[2]} + d\beta^{*[3]} d\beta^{*[3]} d\beta^{*[3]},$$

gives

$$d\beta^{*[3]} d\beta^{*[3]} d\beta^{*[3]} = idt \hbar K_2 \beta^{*3}.$$

Similarly, the evolution of  $\langle a^3 \rangle$  gives

$$d\alpha^{[3]} d\alpha^{[3]} d\alpha^{[3]} = -idt \hbar K_2 \alpha^3.$$



Therefore, the exact evolution of the generalized Kerr oscillator can be simulated with coherent states using

the stochastic process on the c-numbers

$$\begin{aligned} d\alpha &= -idt \left\{ \omega + K_1 [\beta^* \alpha] + \frac{1}{2} K_2 [\beta^* \alpha]^2 \right\} \alpha + (d\xi_2 + d\xi_3) \alpha, \\ d\beta^* &= idt \left\{ \omega + K_1 [\beta^* \alpha] + \frac{1}{2} K_2 [\beta^* \alpha]^2 \right\} \beta^* + (d\eta_2 + d\eta_3) \beta^*, \end{aligned}$$

where the  $d\xi_i$  and  $d\eta_i$  are independent stochastic variables verifying

$$\begin{aligned} \overline{d\xi_i} &= \overline{d\eta_i} = 0, \\ \overline{d\xi_3 d\xi_3} &= \overline{d\eta_3 d\eta_3} = 0, \\ \overline{d\xi_2 d\xi_2} &= \overline{d\eta_2 d\eta_2} = -idt(K_1 + K_2 [\beta^* \alpha]), \\ \overline{d\xi_3 d\xi_3 d\xi_3} &= \overline{d\eta_3 d\eta_3 d\eta_3} = -idt K_2. \end{aligned}$$

The exactness of the above stochastic process can be checked using the fact that for any density given by equation (39) and the stochastic evolution of  $\alpha$  and  $\beta^*$  given above, we have the average relation

$$\overline{e^{d\alpha(a^+ - \langle a^+ \rangle)} D + D e^{d\beta^*(a - \langle a \rangle)}} = D + \frac{dt}{i\hbar} [H, D], \quad (49)$$

where  $H$  is the total Hamiltonian given by eq. (48). This relation shows that the average evolution identifies with the exact evolution for a given  $D$  and a single time step. Note that here the use of  $(a^+ - \langle a^+ \rangle)$  and  $(a - \langle a \rangle)$  is related to the constant trace,  $Tr(D) = 1$ , imposed along each paths.

#### D. Interacting Boson systems

In recent years, several works have demonstrated that bosons [22] or fermions [23] interacting through a two-body potential can be simulated exactly by a Monte-Carlo method using simple trial state vector. Let us first consider the general case of  $N$  interacting bosons described by the general two-body Hamiltonian

$$H = \sum_{ij} \langle i | T | j \rangle a_i^+ a_j + \frac{1}{2} \sum_{ijkl} \langle ij | v_{12} | lk \rangle a_i^+ a_j^+ a_l a_k, \quad (50)$$

where the  $a_i$  and  $a_i^+$  correspond to a complete set of creation/annihilation operators which obey bosons commutation rules. It has been shown in ref. [22], that Bose-Einstein condensates wave-functions can be used as trial wave-functions. In that case, the generator of the transformations between two non-orthogonal wave-function are the single-particle operators  $a_i^+ a_j$ . Since  $H$  can be written as a quadratic polynomial in terms of these operators, we can have guessed the existence of

such a stochastic reformulation. We show here that the proposed method also leads to an exact reformulation of the exact problem in terms of jumps between densities

$$D = |N : \phi_a\rangle \langle N : \phi_b|, \quad (51)$$

where both  $|N : \phi_a\rangle$  and  $|N : \phi_b\rangle$  stand for two Bose-Einstein condensates wave-function and where  $Tr(D) = 1$  along each path.

##### 1. Phase-space stochastic dynamics

Let us assume that the system is at initial time  $t_0$  in a specific Bose condensate wave-function  $|N : \phi\rangle$ , where  $|\phi\rangle$  is the associated single-particle state. Due to the nature of the initial state, all the information is contained in the one-body degrees of freedom. It is then convenient to define the one-body density matrix  $\langle j | \rho_1 | i \rangle = \langle a_i^+ a_j \rangle$ , whose matrix elements can be written as

$$\rho_1 = N |\phi\rangle \langle \phi| = N P_\phi, \quad (52)$$

$P_\phi$  being the projector on the single particle state  $|\phi\rangle$ . According to the existence theorem, we know that an exact Monte-Carlo reformulation can be obtained using the first and second moments of a complete set of one-body operators. This is equivalent to express the evolution of the one and two-body densities over one time step. Indeed, the two-body density denoted by  $\rho_{12}$  is defined as usual as  $\langle ij | \rho_{12} | kl \rangle = \langle a_k^+ a_l^+ a_j a_i \rangle$ . For a pure Bose-Einstein condensate,  $\rho_{12}$  reads

$$\rho_{12} = N(N-1) P_\phi(1) P_\phi(2), \quad (53)$$

where  $P_\phi(i)$  means that the projection is made on the  $i^{th}$  particle. The evolution of  $\rho_1$  and  $\rho_{12}$  over one time step are given by the first two equations of the Bogolyubov-Born-Green-Kirwood-Yvon (BBGKY) hierarchy [46–48], which reduces in the present case to the two equations of motion

$$i\hbar \frac{d}{dt} \rho_1 = [h_{MF}(1), \rho_1], \quad (54)$$

$$i\hbar \frac{d}{dt} \rho_{12} = [h_{MF}(1) + h_{MF}(2), \rho_{12}] + B_{12}. \quad (55)$$

$h_{MF}$  denotes the mean-field Hamiltonian given by

$$h_{MF} = T + (N - 1)Tr_2(v_{12}P_\phi(2)), \quad (56)$$

where  $Tr_2$  corresponds to the partial trace on the second particle.  $B_{12}$  is the extra contribution which treats correlations beyond mean-field and reads

$$B_{12} = (1 - P_\phi(1))(1 - P_\phi(2))v_{12}\rho_{12} - \rho_{12}v_{12}(1 - P_\phi(1))(1 - P_\phi(2)). \quad (57)$$

Due to this extra contribution, the exact many-body density differs from a pure Bose-Einstein wave-function after one time step evolution.

Starting from the initial densities given by eq. (52) and (53), it is possible to guess a phase-space stochastic

dynamics that simulates exactly the evolution of  $\rho_1$  and  $\rho_{12}$ . This is indeed the case if we assume that  $P_\phi$  evolves according to a stochastic equation that verifies

$$\begin{aligned} \overline{dP_\phi} &= \frac{dt}{i\hbar} [h_{MF}, P_\phi], \\ \overline{dP_\phi(1)dP_\phi(2)} &= \frac{dt}{i\hbar} (1 - P_\phi(1))(1 - P_\phi(2))v_{12}P_\phi(1)P_\phi(2) \\ &\quad - P_\phi(1)P_\phi(2)v_{12}(1 - P_\phi(1))(1 - P_\phi(2)). \end{aligned}$$

Following ref. [22, 23] we can write  $v_{12}$  as a sum of squares of hermitian one-body operators:  $v_{12} = \sum_k O_\lambda(1)O_\lambda(2)$ . We see that a proper choice for the stochastic evolution of  $P_\phi$  is

$$dP_\Phi = \frac{dt}{i\hbar} [h_{MF}, P_\phi] + \sum_\lambda d\xi_\lambda^{[2]}(1 - P_\phi)O_\lambda P_\phi + \sum_\lambda d\eta_\lambda^{[2]}P_\phi O_\lambda(1 - P_\phi), \quad (58)$$

where  $d\xi_\lambda^{[2]}$  and  $d\eta_\lambda^{[2]}$  are two sets of independent stochastic variables with mean zero and verifying  $d\xi_\lambda^{[2]}d\xi_{\lambda'}^{[2]} = \delta_{\lambda\lambda'}\frac{dt}{i\hbar}$  and  $d\eta_\lambda^{[2]}d\eta_{\lambda'}^{[2]} = -\delta_{\lambda\lambda'}\frac{dt}{i\hbar}$

## 2. Equivalent stochastic process in Hilbert space

The above phase-space stochastic dynamics can be simulated through a stochastic Schroedinger equation on single-particle wave-functions. Then,  $P_\phi(t) = |\phi\rangle\langle\phi|$  transforms into a set of couples of wave-packets  $P_\phi(t + dt) = |\phi + d\phi_a\rangle\langle\phi + d\phi_b| = |\phi_a\rangle\langle\phi_b|$ , where states evolves over one time step according to

$$\begin{cases} d|\phi_a\rangle = \left(\frac{dt}{i\hbar}h_{MF} + \sum_\lambda d\xi_\lambda^{[2]}(1 - P_\phi)O_\lambda\right)|\phi_a\rangle \\ d\langle\phi_b| = \langle\phi_b|\left(-\frac{dt}{i\hbar}h_{MF} + \sum_\lambda d\eta_\lambda^{[2]}O_\lambda(1 - P_\phi)\right). \end{cases}$$

where  $|\phi_a(t_0)\rangle = |\phi_b(t_0)\rangle = |\phi\rangle$ . It turns out that the above stochastic process preserves  $P_\phi^2 = P_\phi$  for each trajectory, i.e.  $\langle\phi_a|\phi_b\rangle = 1$ .

This stochastic evolution corresponds to quantum jumps in many-body space which transform the initial pure Bose-Einstein condensate into an ensemble of densities given by

$$D = |N : \phi_a\rangle\langle N : \phi_b|, \quad (59)$$

with  $\langle\phi_a|\phi_b\rangle = 1$  (which implies  $Tr(D) = 1$ ) and is a priori valid only for the first time step. Let us now assume that we start from one of this many-body densities. It could be shown without difficulty that all the above equation remains valid except that now  $P_\phi = |\phi_a\rangle\langle\phi_b|$ . Therefore, the single-particle SSE given above can be used to

describe the long time evolution of the system. Note finally that the Monte-Carlo equations presented here differs from the "constant trace" scheme described in ref. [22] in particular due to the use of a common mean-field Hamiltonian in the evolution of  $|\phi_a\rangle$  and  $\langle\phi_b|$ .

## E. Interacting Fermions systems

We consider now a system of fermions interacting through a two-body Hamiltonian

$$H = \sum_{ij} T_{ij}a_i^+a_j + \frac{1}{4} \sum_{ijkl} \langle ij|v_{12}|kl\rangle a_i^+a_j^+a_la_k, \quad (60)$$

where the creation/annihilation operators now obey fermionic commutation rules and where  $v_{12}$  is antisymmetric. Since the derivation of a Monte-Carlo theory is very similar to the boson case, we only give here the important steps.

Let us assume that at a given time step, the exact density can be recovered by averaging over an ensemble of densities

$$D = |\Phi_a\rangle\langle\Phi_b|, \quad (61)$$

where both states correspond to Hartree-Fock states. If we denote by  $\{|\beta_i\rangle\}_{i=1,N}$  and  $\{|\alpha_i\rangle\}_{i=1,N}$  the set of  $N$  single-particle states, we assume in addition that for each couples of Hartree-Fock states, associated singles-particle wave-functions verify  $\langle\beta_j|\alpha_i\rangle = \delta_{ij}$ . Accordingly, the one-body density matrix associated to a given  $D$  reads [27, 49, 50]

$$\rho_1 = \sum_i |\alpha_i\rangle\langle\beta_i|. \quad (62)$$

We can easily verify that  $\rho_1^2 = \rho_1$  and  $Tr(D) = 1$ . For each  $D$  given by eq. (61), the two-body density is given by  $\rho_{12} = (1 - P_{12})\rho_1\rho_2$  where  $P_{12}$  corresponds to the

permutation operator. The evolution of  $\rho_1$  and  $\rho_{12}$  over one time step are given by the two first equations of the BBGKY hierarchy which reads in that case

$$i\hbar \frac{d}{dt} \rho_1 = [h_{MF}, \rho_1], \quad (63)$$

$$i\hbar \frac{d}{dt} \rho_{12} = [h_{MF}(1) + h_{MF}(2), \rho_{12}] + (1 - \rho_1)(1 - \rho_2)v_{12}\rho_1\rho_2 - \rho_1\rho_2v_{12}(1 - \rho_1)(1 - \rho_2), \quad (64)$$

where the mean-field Hamiltonian now reads  $h_{MF} = T + Tr_2(v_{12}\rho_2)$ . This expression identifies with the one obtained for bosons except that  $P_\phi$  is now replaced by the one-body density. Again, introducing a complete set of hermitian operators  $O_\lambda$ , the previous expression can be simulated by a stochastic dynamics in phase-space given by eq. (58) (where again  $P_\phi$  is replaced by  $\rho_1$ ) equivalent to a stochastic process for single-particle wave-functions given by

$$d|\alpha_i\rangle = \left( \frac{dt}{i\hbar} h_{MF} + \sum_\lambda d\xi_\lambda^{[2]} (1 - \rho_1) O_\lambda \right) |\alpha_i\rangle, \\ d\langle\beta_i| = \langle\beta_i| \left( -\frac{dt}{i\hbar} h_{MF} + \sum_\lambda d\eta_\lambda^{[2]} O_\lambda (1 - \rho_1) \right).$$

This stochastic equation on single-particle wave-functions, which has been found using a different technique in ref. [51], preserves the property  $\langle\beta_j|\alpha_i\rangle = \delta_{ij}$ . Therefore, it corresponds in many-body space to a Monte-Carlo procedure which transforms the initial set of densities into another set of densities with identical properties.

### 1. Possible Extensions for Many-Body systems

In the context of many-body systems, the above derivations are restricted to particles interacting through two-body interactions. The method presented here can also be used to provide Monte-Carlo formulations when particles interact through three-body or more interactions. Then higher order noises are necessary and evolution of the three-body or more density matrices should be estimated along stochastic paths.

Another possible application of the method is to include pairing correlation in the trial states. In that case, the relevant degrees of freedom along the path are not only the one-body density  $\rho_{ij} = Tr(a_i^\dagger a_j D)$  but also the abnormal density defined as  $\kappa_{ij} = Tr(a_j a_i D)$  (see for instance [30, 52]). Although we do not develop here explicitly the formalism, it would be interesting to make the connection between the technique described above

and the recent related works which use either directly a stochastic simulation in phase-space [9] or stochastic Schroedinger equations [53, 54].

We guess that the result is the one obtained recently in ref. [54]. In that case, it has been shown that the exact two-body problem can be mapped into a quantum Monte-Carlo process between densities  $D = |\Phi_a\rangle\langle\Phi_b|$  written as a product of two Hartree-Fock Bogolyubov states with  $\langle\Phi_b|\Phi_a\rangle = 1$  along the path.

## V. DISCUSSION

Different examples given above illustrate how one can take advantage of both phase-space evolution and Monte-Carlo process in Hilbert space. Most often, the exact problem is replaced by a set of coupled non-linear stochastic equations. Therefore, we would like to mention that we can end with same difficulties encountered sometimes in that case [8] with the appearance of unstable trajectories. This is the case for instance with the stochastic nonlinear equations derived in section (IV B), which are numerically difficult to integrate [45].

Another example is given by the two-mode Hamiltonian of ref. [55] given by

$$H = \frac{\hbar\Omega}{2} (c_1^\dagger c_2 + c_2^\dagger c_1) + \hbar K [(c_1^\dagger)^2 c_1^2 + (c_2^\dagger)^2 c_2^2],$$

where  $(c_1^\dagger, c_1)$  and  $(c_2^\dagger, c_2)$  correspond respectively to the creation/annihilation operators of two orthogonal single particles states denoted by  $|u_1\rangle$  and  $|u_2\rangle$ , and obey boson commutation rules. This Hamiltonian has been used to mimic the dynamics of two coupled condensates. The exact static and dynamical solutions associated to this Hamiltonian can be obtained exactly and it has been retained as a test case in ref. [22] for Monte-Carlo methods. The framework presented here leads to an alternative stochastic processes between densities  $D = |N : \phi_a\rangle\langle N : \phi_b|$ , where single-particle states  $|\phi_a\rangle$  and  $|\phi_b\rangle$  can be decomposed as

$$|\phi_a\rangle = \alpha_a(t)|u_1\rangle + \beta_a(t)|u_2\rangle, \\ |\phi_b\rangle = \alpha_b(t)|u_1\rangle + \beta_b(t)|u_2\rangle.$$

A direct application of the formalism developed for bosons in section IV D with  $O_1 = \sqrt{\hbar K} c_1^\dagger c_1$  and  $O_2 =$

$\sqrt{\hbar K} c_2^\dagger c_2$  leads to stochastic equations for  $\alpha_a$  and  $\beta_a$

$$\begin{aligned} d\alpha_a &= -\frac{idt\Omega}{2}\beta_a - 2idtK(N-1)[\alpha_b^*\alpha_a]\alpha_a + \sqrt{2K\hbar}\left[d\xi_1^{[2]} - dW\right]\alpha_a, \\ d\beta_a &= -\frac{idt\Omega}{2}\alpha_a - 2idtK(N-1)[\beta_b^*\beta_a]\beta_a + \sqrt{2K\hbar}\left[d\xi_2^{[2]} - dW\right]\beta_a. \end{aligned}$$

where  $dW = d\xi_1^{[2]}\alpha_b^*\alpha_a + d\xi_2^{[2]}\beta_b^*\beta_a$ . These equations have to be completed with similar equations for  $\alpha_b^*$  and  $\beta_b^*$ . It could in particular be checked that  $Tr(P_\phi) = \alpha_b^*\alpha_a + \beta_b^*\beta_a$  is constant along each path.

An illustration of the result obtain by a direct numerical integration of these equation is shown in figure 1 for the special case where all bosons are initially in the same state  $|u_2\rangle$  and for the same parameters values taken as in ref. [22], i.e.  $N = 17$ ,  $K = 0.1\Omega$  and  $\Omega dt = 10^3$ . Figure 1 presents the evolution of  $p_1 = \langle c_1^\dagger c_1 \rangle$  as a function of time. The stochastic calculation does perfectly

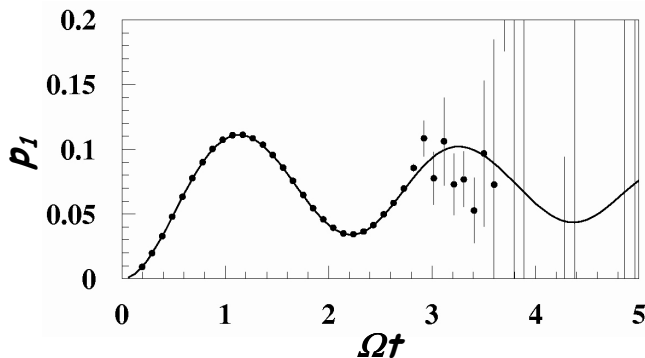


FIG. 1: Evolution of  $p_1 = \langle c_1^\dagger c_1 \rangle$  as a function of time (circles) obtained by averaging over  $10^4$  stochastic trajectories. The result is compared to the exact evolution (solid lines). Error bars represent standard deviation.

reproduce the exact results up to  $\Omega t \simeq 2.8$  with a rather small number of trajectories. After this time, large deviations with respect to the exact evolution occur, and could not be reduced by increasing the number of trajectories. A careful analysis show that some trajectories becomes hard to integrate numerically. Indeed, for some trajectories while  $Tr(P_\phi) = 1$ ,  $||\alpha_b^*\alpha_a||$  and  $||\beta_b^*\beta_a||$  may become very large. Accordingly, the implementation of the above stochastic equations requires the time step to be very small or, alternatively to develop specific numerical techniques.

This last example illustrates that the stochastic equations might be difficult to integrate numerically due to their non-linearity. This is a problem which seems to be recurrent in the context of quantum stochastic me-

chanics both with Stochastic Schroedinger Equation [22] or stochastic evolution in phase-space [8]. Therefore, to take fully advantage of these techniques one should develop specific numerical methods. This has been done for instance in refs. [22, 45, 56] using the fact that stochastic equations are generally not unique. Such a non-uniqueness also exists in the formalism described here.

## VI. CONCLUSION

The main goal of this paper is to show that one can take advantage of the phase-space evolution to construct Monte-Carlo processes in Hilbert space of a restricted class of trial wave-functions. In the first part of this work, we show that given a class of trial wave-functions  $|Q_a\rangle$  associated to a set of specific operators  $A_\alpha$ , it is always possible to obtain a hierarchy of stochastic approximations of a quantum problem in terms of quantum jumps between densities formed of couples of trial states  $D = |Q_a\rangle\langle Q_b|$ . At the level  $k$  of the hierarchy, the existence of such a stochastic process is proved using variational techniques. The quantum diffusion obtained in such a way has a clear interpretation in phase-space evolution. Indeed, at a given level  $k$  we show that moments of  $A_\alpha$  calculated by averaging expectation values  $\langle A_{\alpha_1} \rangle, \langle A_{\alpha_1} A_{\alpha_2} \rangle, \dots, \langle A_{\alpha_1} \dots A_{\alpha_k} \rangle$  over different trajectories match the exact evolution. The stochastic formulation can eventually be exact if the Hamiltonian applied to the trial state can be recast as a polynomial of  $A_\alpha$ .

The proof of the existence of such a hierarchy of stochastic formulation is very helpful to bridge stochastic mechanics in Hilbert space and phase-space evolution. In the second part of this article, several examples illustrates how the Ehrenfest theorem can directly be used to guess stochastic Schroedinger equations. Finally, a critical discussion on numerical aspects is given.

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