Combining phase-space and time-dependent reduced density matrix approach to describe the dynamics of interacting fermions

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The possibility to apply phase-space methods to many-body interacting systems might provide accurate descriptions of correlations with a reduced numerical cost. For instance, the so-called stochastic mean-field phase-space approach, where the complex dynamics of interacting fermions is replaced by a statistical average of mean-field like trajectories is able to grasp some correlations beyond the mean-field. We explore the possibility to use alternative equations of motion in the phase-space approach. Guided by the BBGKY hierarchy, equations of motion that already incorporate part of the correlations beyond mean-field are employed along each trajectory. The method is called Hybrid Phase-Space (HPS) because it mixes phase-space techniques and the time-dependent reduced density matrix approach. The novel approach is applied to the one-dimensional Fermi-Hubbard model. We show that the predictive power is improved compared to the original stochastic mean-field method. In particular, in the weak-coupling regime, the results of the HPS theory can hardly be distinguished from the exact solution even for long time.

I. INTRODUCTION

The accurate description of the evolution of interacting fermions is an extremely challenging problem when the number of particles increases. One of the difficulties is the number of degrees of freedom (DOFs) to be followed in time that scales exponentially with the number of particles. A natural way to reduce the complexity is to assume that some DOFs are more relevant than others and to follow in time only these DOFs. A typical illustration of this strategy is the Time-Dependent Hartree-Fock (TDHF) approach where one-body DOFs are assumed to contain the relevant information on the system evolution. This reduction of information is evident when we consider as a starting point the Bogolyubov-Born-Green-Kirkwood-Yvon (BBGY) hierarchy [1–6]. Then, the TDHF theory is recovered by assuming that two-body, three-body, ... DOFs can all be written in terms of the one-body density (see for instance [7]). The BBGY approach also provides strong guidance to go beyond the mean-field approximation by including gradually higher order effects related to two-body, three-body, ... DOFs. This has led to a variety of approaches that can be referred to as the Time-Dependent Reduced Density Matrix (TDRDM). More precisely such approach can be called TDnRDM where the n is the maximal order of the reduced density matrix that is considered in the description. Solving the TDnRDM with n > 1, even today, remains a complicated numerical task and the approximation used to truncate the BBGY hierarchy has to be analyzed with special care (see for instance the recent discussions in [8, 9] and references therein).

Phase-space approaches offer an alternative scheme allowing to describe correlations beyond mean-field. In these approaches, a complex dynamical problem is replaced by a set of simpler dynamical evolutions. Then, the complexity of the dynamics can eventually be described by a proper weighted average over the simpler evolutions [10]. An example of such approach that has been applied in bosonic interacting systems with some success is the Truncated-Wigner Approximation (TWA) [11]. Less attempts have been made to develop and apply Phase-Space approaches in Fermi systems. We mention the so-called Stochastic Mean-Field (SMF) theory that was proposed already some times ago [12] and tested also with some success [13–15] (for a review see [16]). Another approach, that turns out to be rather close to the SMF technique, is the fermion-TWA (f-TWA) of Ref. [17].

In the SMF phase-space approach proposed in Ref. [12], the initial quantum fluctuations in many-body space are mimicked by a Gaussian statistical ensemble of initial one-body densities. Then, each initial condition follows a TDHF like trajectory that plays the role of the ”simple” evolution. We already have shown in Refs. [18, 19] that the approach can benefit from relaxing the Gaussian approximation for the initial statistical ensemble. Our aim here is to explore if alternative equations of motion for individual trajectory can be proposed that would improve the predictive power of this phase-space method. To further progress, we realized that a more careful analysis of the connection between the phase-space approach proposed in Ref. [12] and the BBGY hierarchy should be made. For this reason, we start the discussion below by recalling basic aspects of this hierarchy that will be useful later. Then, we propose a novel phase-space
approach inspired from both SMF and BBGKY that we called Hybrid Phase-Space (HPS). We show that it indeed improves the description of interacting systems.

II. MANY-BODY DYNAMICS: BBGKY VERSUS PHASE-SPACE METHODS

A. BBGKY and truncation schemes

In the present article, we consider a general two-body Hamiltonian written in the second quantized form as:

$$H = \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{4} \sum_{ijkl} \tilde{v}_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l.$$  (1)

Here $\tilde{v}_{12}$ denotes the antisymmetric matrix elements. The initial condition is given in terms of the N-body density matrix $D(t_0)$ that contains the information on the initial state of a set of independent or correlated fermions. Our aim is to provide an accurate description of the system evolution for time $t > t_0$. The exact solution to this problem can be obtained by solving the Liouville-von Neumann equation given by:

$$i\hbar \dot{D}(t) = [H, D(t)],$$  (2)

where $\dot{D}(t)$ denotes the time-derivative of $D(t)$. In many realistic situations, the direct use of Eq. (2) is intractable due to the number of components of $D(t)$, that are directly connected to the number of DOFs to follow in time. A standard way to reduce the complexity is to assume that there is a hierarchy in the importance of selected degrees of freedoms compared to others. Often, the one-body DOFs are assumed to be more important than two-body DOFs and that are supposed to be more important than three-body DOFs and so on and so forth. The usual method to focus on the k-body DOFs consists in introducing the k-body reduced density matrix (kRDM), defined through:

$$\langle k' \cdots 1 | R_{1 \cdots k} | 1 \cdots k \rangle = \langle \hat{a}_{k'}^\dagger \cdots \hat{a}_1^\dagger \hat{a}_1 \cdots \hat{a}_k \rangle.$$  

In the following, we will mainly focus on the one-, two- and three-body density matrices, denoted respectively by $R_1$, $D_{12}$ and $T_{123}$. Assuming that the number of particles in the system is $N$, these densities are linked to each other through the partial trace relations:

$$(N - 1)R_1 = Tr_2 D_{12}, \quad (N - 2)D_{12} = Tr_3 T_{123}.$$  (3)

Starting from Eq. (2), one can derive the well-known BBGKY hierarchy of equations of motion (EOMs) [1–9], showing that the kRDM evolution is coupled to the (k+1)RDM. For the present discussion, we will only need the two first equations of the hierarchy that are given respectively by:

$$i\hbar \dot{R}_1 = [t_1, R_1] + \frac{1}{2} Tr_2 [\tilde{v}_{12}, D_{12}],$$  (4)

and

$$i\hbar \dot{D}_{12} = [H_{12}, D_{12}] + \frac{1}{2} Tr_3 [\tilde{v}_{13} + \tilde{v}_{23}, T_{123}],$$  (5)

with $H_{12} = t_1 + t_2 + \frac{1}{2} \tilde{v}_{12}$. The BBGKY hierarchy has been and is still a continuous source of inspiration to obtain approximate treatments of the N-body dynamical problem. The standard strategy is to truncate the hierarchy at a given order $k$ while using a prescription for the densities of orders higher than $k$ so that they can be written as a functional of lower orders reduced densities. The simplest example is the Time-Dependent Hartree-Fock (TDHF) theory that is recovered from Eq. (4) assuming that the 2RDM is given by $D_{12} = R_1 R_2 (1 - R_{12})$. The resulting equation then writes:

$$i\hbar \dot{R}_1 = [t_1, R_1] + Tr_2 [\tilde{v}_{12}, R_1 R_2]$$  (6)

$$\equiv [h_1[R], R_1],$$  (7)

where $h_1[R] = t_1 + Tr_2[\tilde{v}_{12} R_2]$ denotes the mean-field. Staying at the mean-field level is generally not sufficient to describe interacting systems and most often two-body or higher correlations between particles should be included explicitly. For instance, large efforts are devoted to obtain closed EOMs between the 1RDM and 2RDM or solely for the 2RDM matrix [20–23]. One delicate issue is the prescription used to truncate the BBGKY hierarchy that might strongly impact the quality of the results [24, 25]. Related to this issue is the possible breakdown of some important conservation laws when writing the 3RDM in terms of the 2RDM and 1RDM [6]. We note that an interesting solution to this problem was recently given with the purification technique proposed in Refs. [8, 9].

B. Phase-Space approach applied to Fermi systems

In the present work, we will call "Phase-Space" approach a technique where a complex quantum dynamical problem is replaced by an ensemble of simpler dynamical problems with a statistical ensemble of initial conditions. The statistical properties of the initial ensemble are chosen at best to reproduce the initial properties of the complex system to be simulated. As mentioned in the introduction, very few practical phase-space theories to simulate fermionic interacting systems have been proposed so far [12, 17].

Here, we will use the SMF theory that we are familiar with as a starting point. In this approach, a statistical ensemble of one-body densities is considered. Each realization of the initial statistical ensemble, denoted by
where \( R^{(n)}_\alpha \) labels the event, is then evolved assuming that the 1RDM follows a mean-field like trajectory that is independent from the other trajectories

\[
i \hbar \dot{R}^{(n)}_\alpha = \left[ H, R^{(n)}_\alpha \right]. \tag{8}
\]

There are two important ingredients in this phase-space method:

(a) the statistical properties of the initial ensemble,

(b) the choice of the equation of motion for the 1RDM.

In \cite{12 17}, Gaussian probabilities are assumed for the matrix elements of the 1RDM such that their first and second moments match the quantum mean and fluctuations of the quantum statistical average over the events, for instance the classical statistical average. An important property resulting from Eqs. (9) is that the original quantum framework is replaced by a statistical treatment. For instance, any one-body theory is assumed to be independent of the statistical average. An important aspect of the SMF theory is that the statistical properties of the initial ensemble, it was shown in Ref. \cite{12} that the initial ensemble of 1RDM should fulfill the following conditions at initial time (omitting \( t_0 \) for compactness):

\[
\begin{align*}
R^{(n)}_{\alpha \beta} & = \delta_{\alpha \beta} n_\alpha, \\
\delta R^{(n)}_{\alpha \beta} \delta R^{(n)}_{\gamma \delta} & = \frac{1}{2} \delta_{\alpha \gamma} \delta_{\beta \delta} \left[ n_\alpha (1 - n_\beta) + n_\beta (1 - n_\alpha) \right],
\end{align*}
\tag{9}
\]

where \( \delta R^{(n)}_{ij} = R^{(n)}_{ij} - \overline{R}^{(n)}_{ij} \) and where \( \overline{X}^{(n)} \) denotes here the statistical average. An important result of the SMF theory is that the original quantum framework is replaced by a statistical treatment. For instance, any one-body observable \( O \) becomes a fluctuating quantity \( O^{(n)} \) given at time \( t \) by:

\[
O^{(n)}(t) = \text{Tr}(O R^{(n)}(t)) = \sum_{ij} O_{ij} R^{(n)}_{ji}(t).
\]

The fluctuations properties are then obtained using classical statistical average over the events, for instance the mean value is given by \( O^{(n)}(t) = \text{Tr}(O R^{(n)}(t)) \) while the second central moment, denoted by \( \Sigma^2_O(t) \), is obtained through:

\[
\Sigma^2_O(t) = \frac{O^{(n)}(t) O^{(n)}(t) - O^{(n)}(t)^2}{\sum_{ij} O_{ij} O_{kl} \delta R^{(n)}_{ij}(t) \delta R^{(n)}_{kl}(t)}.
\tag{10}
\]

An important property resulting from Eqs. (9) is that the statistical average of the mean value and fluctuations matches the quantum mean and fluctuations of the quantum problem at initial time.

Applications of the SMF approach have shown several appealing features. One of the attractive aspects is that its predictive power can compete for instance with the TD2RDM approach while only requiring the propagation of the one-body density. In general, it was found that the approach is highly competitive when the interaction between particles is not too strong and, whatever the strength of the interaction, it properly describes the short time evolution as well as the average asymptotic behavior. An illustration of application is given below.

1. Illustration of application in the 1D Fermi-Hubbard model

In order to illustrate the SMF predictive power, we follow Ref. \cite{15} and apply the approach to the 1D Fermi-Hubbard model. The reason why we specifically focused on this model is because it was one of the most difficult to describe within the phase-space approach compared to other applications \cite{13 14 18} and, even in the weak-coupling, the long-time evolution was impossible to reproduce. Therefore, it is a perfect test-bench for quantifying the departure from the exact evolution and/or for testing possible improvements beyond SMF.

In this model, the Hamiltonian describes interacting fermions of spin \( \sigma \) that can move in a set of doubly-degenerated sites labelled by \( i \) and associated to creation/annihilation operators \((\hat{c}^\dagger_{i \sigma}, \hat{c}_{i \sigma})\). The Hamiltonian is given here by

\[
H = -J \sum_{i, \sigma} \left\{ \hat{c}^\dagger_{i \sigma} \hat{c}_{i+1 \sigma} (1 - \delta_{i, N_s}) + \hat{c}^\dagger_{i \sigma} \hat{c}_{i-1 \sigma} (1 - \delta_{i, N_s}) \right\} + U \sum_{i} \hat{c}^\dagger_{i \sigma} \hat{c}_{i \sigma} \hat{c}_{i \sigma} \hat{c}_{i \sigma}^\dagger,
\tag{11}
\]

where we use sharp boundary conditions. The model can be interpreted as a schematic Hamiltonian describing interacting particles on a lattice where particles can tunnel from one site to neighboring ones, the tunneling being described in an effective way by the \( J \) term. The \( U \) term acts as a local Coulomb interaction between 2 electrons that are on the same site. For more detailed interpretation of the Hubbard model, see for instance \cite{26 27}. The exact solutions, that are shown below, are obtained here by directly solving the coupled equations between the coefficients of the decomposition of the time-dependent state on a full many-body basis using the spin symmetry of the initial state (see discussion in appendix \[A\]).

Following Ref. \cite{15}, we consider the case where the number of particles \( N \) is equal to the number of sites \( N_s \) (assumed to be even in the following) and suppose that all particles are initially located on one side of the mesh. The initial state then corresponds to a Slater determinant with occupation numbers, denoted by \( n_{i \sigma} = 1 \) if \( i < N_s/2 \) and 0 otherwise. These occupation probabilities are related to the one-body density through \( n_{i \sigma} \equiv R^\sigma_{ii} \), where we used the notation \( R^\sigma_{ij} = \langle \hat{c}^\dagger_{i \sigma} \hat{c}_{j \sigma} \rangle \). The mean-field equation of the one-body density components are given in appendix B of \cite{15} as well as the statistical properties of the initial ensemble of one-body density matrices.
used when applying the SMF approach. For the sake of completeness, the SMF equation for the Fermi-Hubbard model are recalled in appendix A.

For small number of sites, the problem can be solved exactly and can be confronted to approximate treatments. We compare in Fig. 1 the exact solution obtained for 4 (resp. 8) particles on 4 (resp. 8) sites with both the mean-field and stochastic mean-field solution using the Gaussian assumption for the initial statistical ensemble and for a coupling strength $U/J = 0.1$. In the following, we will use the convention $\hbar = 1$ and time will be given in $J^{-1}$ units.

We clearly see that a significant improvement in the description of the evolution is achieved in the SMF approach compared to the TDHF case. For instance, the damping of $n_1(t)$ is remarkably well reproduced up to $t \simeq 40J^{-1}$ and deviation from the exact solution is only observed for long time evolution. In general, it is found [16] that the predictive power of SMF is rather good in the weak coupling regime and degrades when the coupling increases. In addition, while it uses only mean-field like EOMs, it is found to be able to compete with other approaches like those based on the truncation of the BBGKY hierarchy we have discussed previously. We have shown in Ref. [15] and more recently in [19], that the approach can be sometimes further improved by relaxing the Gaussian approximation on the initial fluctuations. In the specific case of the Hubbard model, we have tried to replace the initial Gaussian ensemble by a two-point distribution as proposed in [19] but the improvements were marginal. Below, we propose a novel approach that combines the SMF with the BBGKY hierarchy truncation technique.

2. $k$-body density matrix in SMF and BBGKY like hierarchy on symmetric moments

As noted in Ref. [28], an explanation of the SMF success is that this approach is equivalent to solve an untruncated infinite set of coupled equations of motion on the moments defined as:

$$M_{1\ldots k} = \frac{R_1^{(n)} \cdots R_k^{(n)}}{R_1^{(n)} \cdots R_k^{(n)}} M_{1\ldots k}^{(n)}.$$  \hspace{1cm} (12)

As explained in the appendix B these moments play a special role in the SMF approach in many respects that we recall below:

• First of all, $M_{1\ldots k}^{(n)}$ do contain the information on $k$-body correlations between observables. Indeed, let us consider a set of one-body observables $\{O^\alpha\}$ with $\alpha = 1, \ldots, k$. In the phase-space method, we have:

$$O^{1,\ldots,k} = \sum_{ij,\ldots,mm} O_{ij}^{1,\ldots,k} \sum_{mn} \frac{R_{ij}^{(n)} \cdots R_{mm}^{(n)}}{R_{ij}^{(n)} \cdots R_{mm}^{(n)}}.$$  \hspace{1cm} (13)

• Similarly to the set of density matrices defined by Eq. (3), the moments are linked with each other through a partial trace relation that holds event-by-event:

$$\text{Tr}_{k+1} M_{1\ldots k}^{(n)}(t) = N \times M_{1\ldots k}^{(n)}(t),$$  \hspace{1cm} (14)

where we used the fact that $\text{Tr} R_1^{(n)}(t) = N$ for all trajectories and at all time. Since this property holds for each event, it is also valid in average.

• The SMF phase-space approach can also be interpreted as the following mapping at initial time:

$$\langle \{\tilde{N}_{ij}\} \rangle \rightarrow R_{ij}^{(n)},$$  \hspace{1cm} (15)

$$\langle \{\tilde{N}_{ij}, \tilde{N}_{kl}\} \rangle \rightarrow R_{ij}^{(n)} R_{kl}^{(n)}.$$  \hspace{1cm} (16)
where \( \hat{N}_i \) = \( \hat{a}_i \dagger \hat{a}_i \) and where \( \{\ldots\}_+ \) denotes the quantum expectation value of the fully symmetric moments (for further details see appendix \[3\]).

In the quantum problem, these quantum symmetric moments contain the same information as the density matrices. This is illustrated for the one-, two- and three-body densities with Eqs. \([B2]-[B4]\).

For a Gaussian distribution of the initial fluctuations, the mapping is exact at initial time only for the first two moments and only approximate for higher moments. From this mapping, one can also define in a clean way the equivalent to the density matrices within the SMF framework. The expression of the event-by-event two-body and three-body density matrices are respectively given by Eq. \([B4]\) and \([B5]\). In particular, consistently with the Gaussian approximation, we again deduce that the average one- and two-body densities matches the exact quantum densities at initial time.

- Finally, starting from the TDHF equation of motion on \( R_1^{(n)} \) and using the explicit form of the mean-field Hamiltonian, it is rather simple to show \([28]\) that, event by event, the set of moments follow a set of coupled equations where at a given order \( k \), the moment \( M_1^{(n)}(t) \) is coupled to the moment \( M_{1-k+1}^{(n)}(t) \). Then, by averaging over the events, an equivalent hierarchy is obtained on the average moments. For the following discussion, we give the explicit form of the first two equations of the hierarchy. The first equation reads:

\[
\frac{i}{\hbar} \dot{R}_1^{(n)} = \left[ t_1, R_1^{(n)} \right] + \text{Tr}_2 \left[ \tilde{v}_{12}, M_{12}^{(n)} \right],
\]

while the equation on the second moment is given by:

\[
\frac{i}{\hbar} \frac{d}{dt} M_{12}^{(n)}(t) = \left[ t_1 + t_2, M_{12}^{(n)} \right] + \text{Tr}_3 \left[ \left( \tilde{v}_{13} + \tilde{v}_{23} \right), M_{123}^{(n)} \right].
\]

These equations and their average counterparts illustrate how non-trivial effects beyond the mean-field picture are incorporated within SMF. Taking the average over trajectories, we readily obtain the first two equations of the hierarchy coupling \( R_1 \) to \( M_{12} \), \( M_{12} \) to \( M_{123} \), and so on and so forth.

### III. Hybrid Phase-Space Method

The clear advantage of the SMF theory highlighted above is its predictive power despite the fact that only the mean-field machinery is involved. We indeed recurrently observed that the approach can compete with other techniques where two-body DOFs are explicitly evolved in time. The approach is however not exact and leads to deviations with the exact results, for instance for long time evolution even in the weak coupling regime (see Fig. \[1\]). Its predictive power degrades when the strength of the two-body interaction increases.

The building blocks of the approach are the two assumptions made for the items (a) and (b) discussed in section \[11\], respectively the Gaussian assumption for the initial statistical ensemble and the mean-field like dynamics of \( R_1^{(n)} \) along each path. In recent years, we have already explored the possibility to relax the Gaussian approximation for the initial probabilities in Refs. \[18]-[19].

Our conclusion is that, although a systematic way of deciding the form of the initial probabilities is still missing, non-Gaussian probabilities that are better optimized to reproduce the initial system can lead to non-negligible improvements in the description of its evolution. Unfortunately, the alternative prescription proposed in Ref. \[19\] leads to only small improvement compared to the Gaussian case for the Fermi-Hubbard model.

The original motivation of the present work was to use the BBGKY hierarchy as a guidance to propose an equation of motion for \( R^{(1)} \) that could provide an alternative to the mean-field like equation used in SMF and eventually increase the predictive power. A first hint in this direction was given in Ref. \[29]-[30] for bosonic like systems where higher order equations of the BBGKY hierarchy were used to extend the TWA approach and leads to an improved description of the evolution. It turns out that the method we propose below not only reaches the goal for item (b) but might also be useful to better describe the initial state.

#### A. Critical analysis of the standard SMF approach and its connection with the BBGKY hierarchy

The strategy we follow to change the EOMs used in SMF is to make connection between the hierarchy of equation on the moments obtained from the average SMF evolution and the BBGKY hierarchy obtained for the k-body densities in the quantum many-body problem. As we have seen in the SMF approach, the hierarchy of dynamical equations on moments is relatively simple. In parallel, in the BBGKY hierarchy, the set of equations on the densities are relatively simple too. Unfortunately, the opposite is not true. Starting from the SMF average moments, we can obtain the corresponding average density (see for instance Eqs. \([B4]-[B5]\)). The expressions and as a consequence the equation of motion for the average density are complex. On the other hand, starting from the BBGKY hierarchy, one can express the quantum symmetric moments in terms of the densities (see discussion in the appendix \[3\]), but in this case, it is the EOMs on the quantum moments that become rapidly extremely complex. This complexity has prevented us from finding a systematic constructive way to improve the EOMs to be used in the phase-space approach. Below, we propose a more pragmatic approach.
B. Hybrid Phase-Space (HPS) method guided by the BBGKY hierarchy

Besides the Gaussian assumption for the initial noise, the first evident source of errors in SMF can be seen by taking the average evolution of $R_{1}^{(n)}$. Indeed, taking the average of Eq. (18) and using the relation between the average moment $M_{123}^{(n)}$ and the average density $D_{12}^{(n)}$ obtained by averaging Eq. (B4), we immediately see that the evolution does not match the first BBGKY equation that is given by:

$$\mathcal{T}_{123}^{(n)}(t) = \mathcal{D}_{12}^{(n)}(t)R_{1}^{(n)}(t)(1 - P_{13} - P_{23}).$$

(20)

Using this expression in Eq. (18), we obtain that the equation of motion on $\mathcal{D}_{12}^{(n)}(t)$ can be recast as:

$$i\hbar \frac{\partial \mathcal{D}_{12}^{(n)}}{\partial t} = \left[ H_{12}, \mathcal{D}_{12}^{(n)} \right] + \frac{1}{2} \left( 1 - R_{1}^{(n)} - R_{2}^{(n)} \right) \bar{v}_{12} \mathcal{D}_{12}^{(n)}$$

$$- \frac{1}{2} \mathcal{D}_{12}^{(n)} \bar{v}_{12} \left( 1 - R_{1}^{(n)} - R_{2}^{(n)} \right).$$

(21)

This equation, together with Eq. (17) will be the EOMs we will use in the following and that will replace the mean-field propagation in the phase-space method.

In order to generalize the SMF approach, we still need to specify the statistical properties to be used for $R_{1}^{(n)}(t_{0})$ and $D_{12}^{(n)}(t_{0})$. One of our targeted goals is to fulfill the three requirements given by Eq. (19). In particular the matching of the initial three-body density is not possible in the original phase-space approach when the Gaussian assumption is made on the initial ensemble. A natural generalization would be to assume that

$$D_{12}^{(n)}(t) = D_{12}^{(n)}(t) + \Delta_{12}^{(n)}(t),$$

(22)

where $D_{12}^{(n)}(t)$ can be for instance given by expression (B4) while $\Delta_{12}^{(n)}(t)$ has statistical properties chosen to ensure at time $t_{0}$ that the second and third equations in (19) are respected. One actually can also try to impose simultaneously that $\text{Tr}_{2}(D_{12}^{(n)}(t)) = (N - 1)R_{1}^{(n)}(t)$. This implies automatically $\text{Tr}_{2}(\Delta_{12}^{(n)}(t)) = 0$ at all time. We explored this strategy and tried to find a convenient statistical initial ensemble for $\Delta_{12}^{(n)}(t)$ with one or several of these constraints, but did not found any simple way.

In the absence of a clear prescription, we finally simplified the problem and assumed that $R_{1}^{(n)}$ has the same initial statistical property as before given by Eqs. (9) while the quantity $\mathcal{D}_{12}^{(n)}(t)$ is not fluctuating initially with:

$$\mathcal{D}_{12}^{(n)}(t_{0}) = D_{12}(t_{0}).$$

(23)

for all events. Then each initial condition is propagated using the equations (17) and (21). It should be noted in particular that, although $\mathcal{D}_{12}^{(n)}(t)$ is not fluctuating at

$^2$ This expression holds at initial time for a statistical ensemble of independent particles at zero or finite temperature. In this case, we have:

$$T_{123} = R_{1}R_{2}R_{3}(1 - P_{12})(1 - P_{13} - P_{23}) = D_{12}R_{3}(1 - P_{13} - P_{23}).$$
initial time, it should be labelled by \( \langle n \rangle \) due to the initial fluctuations of \( R_1^{(n)} \) that is used in Eq. (21). In the absence of fluctuation on \( D_{12} \) at \( t_0 \) and with the condition (23), it is immediate to verify that the two first constraints in (19) are fulfilled while for the third one we have:

\[
T_{123}^{(n)}(t_0) = D_{12}(t_0) R_{3}^{(n)}(t_0)(1 - P_{13} - P_{23}),
\]

\[
= D_{12}(t_0) R_{3}(t_0)(1 - P_{13} - P_{23}).
\]

Therefore if \( T_{123}(t_0) = D_{12}(t_0) R_{3}(t_0)(1 - P_{13} - P_{23}) \) in the initial conditions, the third constraint in (19) is also fulfilled. This of course restrict the type of initial condition that could be considered. For instance, this will not allow to treat systems with initial residual non-zero three-body correlations. But systems that are initially described as a Slater determinant or a statistical ensemble of independent particles or eventually with only residual two-body correlations can be considered in the present approach.

An important remark is that we keep the spirit of the formalism is the average of these quantities. In particular fluc-
tuations or equivalently correlations between observables will still be performed using classical average over the sampled trajectories. Accordingly, as shown in the appendix B, one can define a fluctuating two-body or three-body density \( D_{12}^{(n)}(t) \) or \( T_{123}^{(n)}(t) \) along each path that are given by Eq. (B1) and (B2), and the only meaningful two-body density one could extract from the present formalism is the average of these quantities. In particular, \( D_{12}^{(n)}(t) \) obtained by solving the Eq. (21) or \( T_{123}^{(n)}(t) \) obtained by using Eq. (20) should not be confused in average with the two- and three-body densities obtained by the phase-space method. Note that, even if at initial time we have \( D_{12}^{(n)}(t_0) = D_{12}^{(n)}(t_0) = D_{12}(t_0) \), there is no reason that this equality is preserved for \( t > t_0 \). We prefer to interpret these quantities as intermediate objects leading to a source term in Eq. (17) that has the effect to introduce effects beyond the mean-field.

The present method, by using an initial statistical ensemble and where quantities are obtained by performing a classical statistical average clearly enters into the category of phase-space approaches. However, because we use intermediate quantities that do not fluctuate at initial time, we do not follow fully the strategy of the original SMF approach and for this reason we will hereafter be called Hybrid Phase-Space (HPS) method.

FIG. 2. Time evolution of the (a) occupation probability of the leftmost site \( b \) center of mass \( q(t) \) of the interacting particles and (c) one-body entropy \( S(t) \) for \( U/J = 0.1 \) and \( N = N_s = 4 \) assuming that all particles are located on the left of the mesh initially. In each panel, the exact solution is displayed by a black solid line, the results of the original SMF phase-space approach are shown by a blue dashed line. The results of the HPS approach are shown with red filled circles. In the SMF and HPS phase-space technique, results are obtained using 10000 trajectories.

In the present section, we apply the HPS method to the 1D Fermi-Hubbard model with different particle numbers and two-body interaction strengths. As we mentioned previously, this model is a perfect test-bench for improving the SMF phase-space method because, even in the weak-coupling limit, the SMF approach was not predictive for the long time evolution. For this model case, we give in appendix A the explicit forms of the equations of motion that are used respectively for the SMF and for the HPS approaches as well as the properties of the initial fluctuations.

We compare the exact evolution and approximate phase-space evolution in Figs. 2 and 3 obtained respectively for the case where \( N = N_s = 4 \) and \( N = N_s = 8 \) in the weak-coupling regime \( U/J = 0.1 \) and when all particles are located on one side of the mesh at initial time. Therefore, the initial condition in the mean-field consists in a Slater determinant with initial spin symmetry. In panel (a) of this figure, we display the occupation probability of the leftmost site. In the exact case, the occupation probability of the site \( i \) verifies \( n_{i}(t) = R_{ii}^{\sigma}(t) \). Due to the initial condition, it verifies \( n_{i}(t) = n_{i}(t) \), allowing us to denote it simply by \( n_{i} \). In the phase-space approach, the occupation probability has the same spin symmetry and is defined through the average over events \( n_{i}(t) = R_{ii}^{\sigma}(n)(t) \). In panel (b) of these figures,
we show a quantity \( q(t) \) that could be interpreted as the equivalent to the center of mass of the particles. This quantity is defined as:

\[
q(t) = \frac{1}{2N_s} \sum_{i, \sigma} \left( i - \frac{1}{2} \right) R^{\sigma \sigma}_{ii}(t).
\]  

(24)

The factor 2 comes from the fact that we sum over spins. Finally in panel (c), we show the one-body entropy that is computed as:

\[
S(t) = -k_B \text{Tr} \{ R_1(t) \ln R_1(t) + (1 - R_1(t)) \ln(1 - R_1(t)) \}.
\]

In practice, the entropy is computed by diagonalizing the average one-body density at time \( t \). The entropy \( S(t) \) quantifies the departure from the pure Slater determinant case for which \( S(t) = 0 \).

In Figures 2 and 3, we see that the new phase-space method proposed here is much better than the original SMF approach and not only reproduces the short time evolution but also the evolution over much longer time. In the case of weak coupling, we observe that the HPS evolution is almost on top of the exact evolution and only at very large time \( U/J > 60 \), very small deviations with the exact results are observed. In particular, the new phase-space approach does not suffer from the over-damping that is generally observed in SMF [13] and that is clearly seen in Fig. 2. By comparing the two figures, we also see that the agreement with the exact solution is improved when the number of particles increases.

The fact that the long-time evolution is also reproduced by the new phase-space approach is quite surprising. Indeed, in the HPS approach as in the original SMF, the different trajectories are independent from each other. As shown in ref. [31, 32], the long-time evolution of small systems can be treated in terms of a set of mean-field trajectories only if the quantum interferences between the trajectories are accounted for.

Such interferences are indeed present in the Fermi-Hubbard model as illustrated in Fig. 4. In this figure, we show the evolution of the local density \( n_i(t) = R^{\sigma \sigma}_{ii}(t) \) for one of the spin orientation as a function of time obtained for \( U/J = 0.1 \) and \( N = N_s = 8 \) assuming that all particles are located on one side of the mesh initially. The exact solution (a) is compared to the SMF (b) and HPS (c) phase-space methods.

In Fig. 5 and Fig. 6 for \( N = 4 \) and Fig. 7 and Fig. 8 for \( N = 8 \), we show the evolution of the leftmost site
In each case, all particles are initially located on one side of the mesh. The exact solution is displayed using a black solid line, the result of the original SMF phase-space approach is shown by a blue dashed line and the results of the HPS approach are shown with red filled circles.

A similar observation can be made for the SMF approach with a time-scale $\tau_{\text{SMF}}$ over which the approach is reproducing the exact evolution. We clearly see in these figures that whatever the coupling $U/J$ is, we have always $\tau_{\text{SMF}} < \tau_{\text{HPS}}$.

Finally, as a further illustration of the complex correlations that were missing in the SMF and that could be grasped by the HPS method, we also tried slightly different initial conditions. We assumed for $N = 8$ particles that initially half the particles (here 4) are on the left site of the lattice while the other half is located on the right side. (see Eq. (A4)). The dynamics can be seen as a minimal version for two colliding Fermi systems. We show in Fig. 9 the local density evolution for the weak coupling regime with $U/J = 0.1$. We compare in this
Our conclusion is therefore that the novel phase-space method has globally a much better predictive power than the original phase-space approach based on the mean-field propagation. In particular, it seems extremely good in the weak coupling regime even for the long time evolution. The increase of predictive power, as discussed in section [III], can directly be traced back to the better account of the initial conditions with in particular the three-body density that is properly reproduced and a partial account for the two-body correlations in the evolution of each trajectory. Note finally that we also applied the HPS to higher coupling strength ($U/J > 1$) but we observed that some trajectories are hard to converge unless very small numerical time-step are used. Therefore, in its present form, the HPS method is essentially restricted to weak- to medium-coupling regime.

V. CONCLUSION

In this work, we explored the possibility to improve the predictive power of the SMF phase-space approach by relaxing the assumption that the equation of motion in this phase-space approach identifies with TDHF. Our strategy was to use the BBGKY hierarchy as a guidance and improve the evolution along each trajectory by including at least partially effects beyond the mean-field approximation. To do so, it was rather natural to us to assume that we consider not only a one-body density with initial fluctuations but also a two-body density that can fluctuate at initial time as proposed in Eq. (22). Then, the two densities would follow a set of coupled equations that could be inspired from the TD2RDM approach. Unfortunately, the different attempt we made were unsuccessful and having both the one- and two-body densities that fluctuate lead to unstable trajectories preventing from performing the statistical average.

We then propose here an alternative method where a set of one-body densities are still considered initially but where the TDHF approximation is corrected by an additional term that approximately describe the effect of correlations that built-up in time on the one-body evolution. This method mixes concepts taken from phase-space and BBGKY techniques and is called for this reason Hybrid...
Phase-Space approach. The applications of the novel approach to the one-dimensional Fermi-Hubbard model clearly demonstrates that the predictive power is improved compared to the original SMF technique. In particular, the new method is very effective in the weak-coupling regime and can even predict the long time evolution. This long-time evolution description was not possible with the original SMF technique. Overall, we see that the predictive power is increased for all coupling strength that are considered in this work.

It should be noted that we observed in practice that the number of trajectories to be sampled in the HPS and SMF approach to obtain similar statistical errors are more or less the same. Still the numerical effort in the HPS approach is significantly increased due to the fact that the TDHF trajectory originally used in SMF is replaced by a TD2RDM like equation that is more numerically demanding. Despite the extra numerical effort, the improved results obtained here are rather encouraging and the possibility to mix fluctuating with non-fluctuating initial conditions might open new perspectives.

Appendix A: Equation of motion used for the Fermi-Hubbard Model

The EOMs in the Fermi-Hubbard model with sharp boundary conditions (see the Hamiltonian (11)) can conveniently be written in the basis set of site orbitals with spin associated with the fermionic operators ($\hat{c}_{i \sigma}^\dagger, \hat{c}_{i \sigma}$). We denote by $N = N^\uparrow + N^\downarrow$ the number of particles where $N^\uparrow$ (resp. $N^\downarrow$) is the number of particles with spin up (resp. down). For $N_s$ sites, the size of the Hilbert N-body space is given by $\binom{N_s}{N^\uparrow} \times \binom{N_s}{N^\downarrow}$. Some symmetries can eventually be used to reduce the numerical complexity of the problem:

- The number of particles $N = \sum_i (n^\uparrow_i + n^\downarrow_i)$ is conserved, i.e. $[N, H] = 0$.
- The projection on the $z$-axis of the total spin $S_z = \frac{1}{2} \sum_i (n^\uparrow_i - n^\downarrow_i)$ is conserved: $[S_z, H] = 0$.
- As a consequence of the two symmetries above, the number of $+\frac{1}{2}$ particles and $-\frac{1}{2}$ particles are both conserved.

These symmetries imply that the Hamiltonian matrix will be block diagonal where a given block corresponds to a given value of $N$ and $S_z$ projection. In particular, if the system has a given particle number and $S_z$ at initial time, its time-evolution only requires the corresponding part of the Hamiltonian in this sub-block, reducing significantly the numerical effort for the exact solution.

The symmetries of the initial state that are preserved in time automatically implies some symmetries on the matrix elements of the one-, two-, ··· density matrices. Denoting the spin up (resp. spin down) with a + (resp. −), and considering that the initial state corresponds to the $S_z = 0$ (symmetry spin up/spin down) case, we have schematically:

$$
\begin{align*}
R^{++} &= R^{--} \\
R^{+-} &= R^{-+} = 0 \\
D^{+-+-} &= D^{---} \\
D^{++++} &= D^{----} = D^{+-+} + D^{--+} \\
D^{++-} &= D^{--+}
\end{align*}
$$

where $R$ and $D$ denote respectively the one and two-body density matrices (note that here the labels associated to site number are implicit). We can see that one only needs to propagate $R^{++}$ or $R^{--}$, and a careful analysis shows that $D^{+-+-}$ is the only component of the two-body density matrix that will affect the dynamics when propagating both the one-body and two-body degrees of freedom in the BBGKY hierarchy. Note that the quantity $D^{(n)}_{12}$ introduced in this article follows the same symmetry properties as $D_{12}$.

We give below the different EOMs that are used in the present work (with the convention $\hbar = 1$):
Omitting the spin indices on $R$ for clarity since no confusion can be made, and considering that the latin subscript $i,j,\ldots$ denotes the $i^{th}, j^{th}, \ldots$, site starting from the left of the 1D lattice, one can write the EOMs for the TDHF, SMF and HPS theories:

For an initial state that corresponds to a Slater determinant, we have the initial conditions:

\begin{equation}
R_{ij}(t_0) = \begin{cases} 1 & \text{if } i = j \text{ and } i \leq N_s = N \\ 0 & \text{otherwise} \end{cases}
\end{equation}

Assuming that all particles are located on the left side of the lattice, the initial density is given by:

\begin{equation}
R_{ij}(t_0) = \begin{cases} 1 & \text{if } i = j \text{ and } i \notin [N^+/2, N_s - N^+/2] \\ 0 & \text{otherwise} \end{cases}
\end{equation}

In another test, the initial conditions were modified to simulate the collision of two groups of particles of equal sizes initially disposed on each extremities of the mesh:

\begin{equation}
R_{ij}(t_0) = \begin{cases} 1 & \text{if } i = j \text{ and } i \notin [N^+/2, N_s - N^+/2] \\ 0 & \text{otherwise} \end{cases}
\end{equation}

SMF EOM – In the original SMF phase-phase approach, the EOM remains the TDHF one except that the initial density is fluctuating at initial time. We then have:

\begin{equation}
i\dot{R}_{ij}^{(n)} = -J \left( R_{i+1,j}^{(n)}(1 - \delta_{iN_s}) + R_{i-1,j}^{(n)}(1 - \delta_{i1}) - R_{i,j+1}^{(n)}(1 - \delta_{jN_s}) - R_{i,j-1}^{(n)}(1 - \delta_{j1}) \right) + UR_{ij}^{(n)} \left( R_{ii}^{(n)} - R_{jj}^{(n)} \right),
\end{equation}

where the initial at initial time:

\begin{equation}
\begin{aligned}
\dot{R}_{ij}^{(n)}(t_0) &= R_{ij}^{(n)}(t_0) + \delta R_{ij}^{(n)}(t_0), \\
R_{ij}^{(n)}(t_0) &= R_{ij}(t_0).
\end{aligned}
\end{equation}

The properties of $\delta R_{ij}^{(n)}(t_0)$ are specified in section II B. We would like to mention that we assume in the present SMF application as well as in the HPS presented below that spin up-spin down symmetry is respected along each path. Fluctuations that break the spin symmetry at initial time are allowed by the statistical properties of the one-body density $R_{ij}^{(n)}$ within SMF. For the SMF, this was tested and discussed in Ref. [15]. The conclusion is that allowing the breaking of spin symmetry at initial time increases the numerical effort while not increasing/decreasing the predicting power. For this reason, we consider here the case where the spin symmetry is respected event-by-event.

HPS EOM – In the HPS equation of motion, only $D^{+-+-}_{ijkl}$ is coupled to $R^{(n)} = R^{++(n)} = R^{--(n)}$. For this reason, we use the compact notations $D^{(n)}_{ijkl} = D^{+-+-}_{ijkl}$. The EOMs then read

\begin{equation}
i\dot{R}_{ij}^{(n)} = -J \left( R_{i+1,j}^{(n)}(1 - \delta_{iN_s}) + R_{i-1,j}^{(n)}(1 - \delta_{i1}) - R_{i,j+1}^{(n)}(1 - \delta_{jN_s}) - R_{i,j-1}^{(n)}(1 - \delta_{j1}) \right) + UR_{ij}^{(n)} \left( R_{ii}^{(n)} - R_{jj}^{(n)} \right),
\end{equation}

\begin{equation}
i\dot{D}_{ijkl}^{(n)} = -J \left( D_{i+1,jkl}^{(n)}(1 - \delta_{iN_s}) + D_{i-1,jkl}^{(n)}(1 - \delta_{i1}) + D_{ij+1,kl}^{(n)}(1 - \delta_{jN_s}) + D_{ij-1,kl}^{(n)}(1 - \delta_{j1}) - D_{ijkl}^{(n)}(1 - \delta_{kl}) \right) + \frac{1}{U} \left( \delta_{ik} D_{jkk}^{(n)} - R_{ik} D_{jkl}^{(n)} \right) D_{ijkl}^{(n)}
\end{equation}

For an initial state that corresponds to a Slater determinant, we have the initial conditions:

\begin{equation}
\begin{aligned}
\dot{R}_{ij}^{(n)}(t_0) &= R_{ij}^{(n)}(t_0) + \delta R_{ij}^{(n)}(t_0), \\
\dot{R}_{ij}^{(n)}(t_0) &= R_{ij}(t_0), \\
\dot{D}_{ijkl}^{(n)}(t_0) &= R_{ik}(t_0)R_{jl}(t_0).
\end{aligned}
\end{equation}
Appendix B: General remark on SMF and some properties

In Ref. [28], it has been shown that the SMF approach can be linked to a hierarchy of equations of the moments of the one-body density that resembles the BBGKY hierarchy. In the present section, we precise the link between the moments and the SMF approach. In SMF, one-body observables are treated as classical fluctuating objects that are given along each trajectory by:

\[ A^{(n)}(t) = \sum_{ij} A_{ij} R_{ji}^{(n)}(t) \]  

(B1)

where \( R_{ji}^{(n)}(t) \) are the densities with initial fluctuations followed by TDHF evolution.

The SMF approach makes a mapping between quantum expectation values and classical statistical average. More precisely, let us consider a set of one-body operators, denoted by \( \hat{A}, \hat{B}, \hat{C}, \ldots \). The following mapping is made:

\[
\langle \hat{A} \rangle \quad \rightarrow \quad \langle \hat{A}^{(n)} \rangle = \sum_{ij} A_{ij} R_{ji}^{(n)},
\]

\[
\langle \{ \hat{A}, \hat{B} \} \rangle \quad \rightarrow \quad \langle \{ \hat{A}^{(n)}, \hat{B}^{(n)} \} \rangle = \sum_{ijkl} A_{ij} B_{kl} R_{ji}^{(n)} R_{ki}^{(n)},
\]

\[
\langle \{ \hat{A}, \hat{B}, \hat{C} \} \rangle \quad \rightarrow \quad \langle \{ \hat{A}^{(n)}, \hat{B}^{(n)}, \hat{C}^{(n)} \} \rangle = \sum_{ijklmn} A_{ij} B_{kl} C_{mn} R_{ji}^{(n)} R_{ki}^{(n)} R_{mj}^{(n)},
\]

\[
\vdots
\]

where we have used the notation:

\[
\langle \{ \hat{A}, \hat{B} \} \rangle = \frac{1}{2} \langle \hat{A} \hat{B} + \hat{B} \hat{A} \rangle,
\]

\[
\langle \{ \hat{A}, \hat{B}, \hat{C} \} \rangle = \frac{1}{6} \langle \hat{A} \hat{B} \hat{C} + \hat{A} \hat{C} \hat{B} + \hat{B} \hat{A} \hat{C} + \hat{B} \hat{C} \hat{A} + \hat{C} \hat{B} \hat{A} + \hat{C} \hat{A} \hat{B} \rangle
\]

\[
\vdots
\]

The above quantum average can be connected to the one-, two- and higher order many-body densities simply by setting \( \hat{A} = \hat{N}_{ij}, \hat{B} = \hat{N}_{lk}, \hat{C} = \hat{N}_{nm} \) where we have introduced the notations \( \hat{N}_{ij} = a_i^\dagger a_i \). A lengthy but straightforward calculation gives:

\[
R_{ij} = \langle \hat{N}_{ij} \rangle,
\]

\[
D_{ij,kl} = \langle \{ \hat{N}_{ij}, \hat{N}_{kl} \} \rangle - \frac{1}{2} \langle \delta_{ik} R_{kj} + \delta_{kj} R_{it} \rangle,
\]

\[
T_{ijn;ikm} = \langle \{ \hat{N}_{ij}, \hat{N}_{ik}, \hat{N}_{nm} \} \rangle - \frac{1}{2} \langle \delta_{jk} D_{ln;im} + \delta_{lm} D_{nj;ki} + \delta_{jm} D_{ni;ik} + \delta_{ij} D_{nk;im} + \delta_{ni} D_{j;mk} + \delta_{nk} D_{ij;mi} \rangle
\]

\[
- \frac{1}{6} \langle \delta_{jk} \delta_{lm} R_{ni} + \delta_{lj} \delta_{mj} R_{nk} + \delta_{lm} \delta_{ni} R_{jk} + \delta_{lk} \delta_{mj} R_{in} + \delta_{nl} \delta_{jk} R_{lm} + \delta_{jm} \delta_{nk} R_{li} \rangle,
\]

\[
\vdots
\]

Where \( R_1, D_{12} \) and \( T_{123} \) denote the one-, two-, three-body density matrix respectively. We see in particular that the information content of the symmetric moments \( \langle \hat{N}_{ij} \rangle, \langle \{ \hat{N}_{ij}, \hat{N}_{kl} \} \rangle, \langle \{ \hat{N}_{ij}, \hat{N}_{ik}, \hat{N}_{nm} \} \rangle, \ldots \) is equivalent to the information content of the one-, two-, three-body density matrix.

These relationships on the quantum densities and quantum symmetric moments and the mapping between these moments and the density \( R^{(n)} \) show that the equivalent of the two-, three- ... body density can also be constructed in the SMF theory. Based on the above relationships, we introduce the matrices \( D_{12}^{(n)}, T_{123}^{(n)} \ldots \) that are defined from the quantity \( R^{(n)} \) used in SMF using:

\[
D_{ij,kl}^{(n)} = R_{ij}^{(n)} R_{kl}^{(n)} - \frac{1}{2} \langle \delta_{ik} R_{kj}^{(n)} + \delta_{kj} R_{it}^{(n)} \rangle,
\]

(B4)

\[
T_{ijn;ikm}^{(n)} = + R_{ij}^{(n)} R_{ik}^{(n)} R_{nm}^{(n)}
\]

\[
- \frac{1}{2} \langle \delta_{jk} R_{in}^{(n)} R_{mk}^{(n)} + \delta_{lm} R_{kn}^{(n)} R_{ij}^{(n)} + \delta_{jm} R_{ni}^{(n)} R_{kl}^{(n)} + \delta_{ij} R_{kn}^{(n)} R_{mn}^{(n)} + \delta_{ni} R_{mj}^{(n)} R_{kl}^{(n)} + \delta_{nk} R_{ml}^{(n)} R_{ij}^{(n)} \rangle
\]

\[
+ \frac{1}{3} \langle \delta_{jk} \delta_{lm} R_{in}^{(n)} + \delta_{lj} \delta_{mj} R_{nk}^{(n)} + \delta_{lm} \delta_{ni} R_{jk}^{(n)} + \delta_{lk} \delta_{mj} R_{in}^{(n)} + \delta_{nl} \delta_{jk} R_{lm}^{(n)} + \delta_{jm} \delta_{nk} R_{li}^{(n)} \rangle,
\]

(B5)
Properties of the density matrices

The density matrices $D^{(n)}$ and $T^{(n)}$ defined in Eq. (B4) and (B5) do automatically fulfill some important properties. For instance, after a rather lengthy but straightforward calculation, it is possible to show that we have

$$
\text{Tr} R_1^{(n)}(t) = N,
$$

$$(N-1) \text{Tr} D_{12}^{(n)}(t) = R_2^{(n)}(t),
$$

$$(N-2) \text{Tr} T_{123}^{(n)}(t) = R_{12}^{(n)}(t),
$$

\ldots

These are important properties that holds for the exact evolution and are automatically fulfilled on an event-by-event basis and therefore also hold when averaging over events. Such requirement are known to be a critical issue when performing TD$n$RDM calculations \cite{28}. In SMF, the statistical properties of the initial conditions are constructed to insure that the first and second moments of the quantum fluctuations match the one obtained through the statistical average. This automatically implies that we have the properties:

$$
\bar{R}_1^{(n)}(t = 0) = R_1(t = 0),
$$

$$
\bar{D}_{12}^{(n)}(t = 0) = D_{12}(t = 0).
$$

(B6)

However, the three-body average density does not a priori match the quantum three-body density, especially if a Gaussian approximation is made for the initial statistical ensemble (see for instance the discussion in \cite{19}).

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3 Note that we did not check for higher-order densities but we anticipate that similar relations holds

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