Stochastic TDHF and the Boltzman-Langevin Equation

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Abstract

Outgoing from a time-dependent theory of correlations, we present a stochastic differential equation for the propagation of ensembles of Slater determinants, called Stochastic Time-Dependent Hartree-Fock (Stochastic TDHF). These ensembles are allowed to develop large fluctuations in the Hartree-Fock mean fields. An alternative stochastic differential equation, the Boltzmann-Langevin equation, can be derived from Stochastic TDHF by averaging over subensembles with small fluctuations.
1 Introduction

Time-Dependent Hartree-Fock (TDHF) has been the standard starting point for microscopic descriptions of collective motion with large amplitudes in nuclear dynamics and heavy-ion scattering. However, a pure TDHF description fails to reproduce the large spreading width of observables and the large fluctuations in the more energetic cases. Therefore, various versions of extended TDHF have been proposed and discussed since long, for a review see e.g. [1]. Most of these extensions try to account for an internal heating and for statistical fluctuations by adding some sort of Boltzmann collision term. But none of these approaches really succeeded because the time-evolution of the whole system remains still bound to the time-evolution of only one mean-field.

It is obvious that large spreading widths and large fluctuations can only be described if one allows fluctuations in the mean-field thus propagating a bunch of different mean-field trajectories. Such an approach was investigated in the Time-Dependent Generator-Coordinate-Method (TDGCM) where correlated states are propagated as coherent superpositions of bunches of Slater determinants [2, 3]. A formally quite similar approach was developed from a variational principle applied to the time-dependent mean-field and a time-dependent observable simultaneously [4, 5]. Both approaches give encouraging results in that one indeed can produce a significant enhancement of the spreading widths of the selected correlation channels. But they both are also very limited in that one can take into account only a few collective correlation channels in a coherent manner.

A true dynamical heavy-ion reaction will excite many degrees-of-freedom thus requiring a large manifold of different TDHF trajectories for a nearly appropriate description. It is, of course, hopeless to treat such a manifold in a completely coherent manner as in e.g. in TDGCM. On the other hand, the large number of channels suggests that phase relations between all these channels average out due to random phases. This leads to a direct statistical approach where the system is described by an ensemble of TDHF trajectories in which the members of the ensemble communicate to each other only incoherently by mutual transition rates. The simplest approach of that type was investigated in ref. [6]
where an initial hot compound system was represented by an ensemble of Slater states and this ensemble was evolved in time by propagating each state independently along its own TDHF trajectory. The results have shown that such an approach is indeed able to describe properly a wide distribution of final fragments. It is yet missing a description for the time-evolution into the compound state, i.e. for building up large internal excitations.

In this paper, we want to present and derive Stochastic TDHF which is a theory for producing and propagating an ensemble of TDHF trajectories. It was suggested years ago by Ron Cusson [7] in order to overcome the insufficiencies of TDGCM and to take up the successful ensemble approach of ref. [6]. The ensemble of Stochastic TDHF is generated from a coherent propagation of correlations in second order perturbation theory over a time interval which allows fully developed transitions from one trajectory to a neighbouring trajectory. After that time, phase information is discarded which distributes back the correlated states into a new ensemble of Slater states. One member of this ensemble is chosen stochastically according to its probability weight in the instantaneous ensemble and the same procedure is continued with this member. This propagation is traced over many time intervals producing one particular path of Stochastic TDHF. The whole procedure is repeated many times thus producing an ensemble of such trajectories which constitute the final ensemble of Stochastic TDHF.

Just recently has been proposed, in the semiclassical context, a stochastic approach to heavy-ion dynamics with large fluctuations, the Boltzmann-Langevin equation [8]. A formally similar transport equation was also studied in situations not too far from equilibrium [9]. First practical calculations of such stochastic equations are already available and they give very promising results [10, 11]. The Boltzmann-Langevin approach starts from an extended TDHF with Boltzmann collision term. This alone would produce only one single trajectory about one mean-field. An ensemble of fluctuating mean-fields is produced by a fluctuating stochastic force of the Langevin type. Such fluctuating forces are the inevitable corrolaries of dissipative terms. Based on this reasoning, a Boltzmann-Langevin equation has been postulated times ago in ref. [12]. A clear-cut derivation using the density-matrix formalism was given in ref. [8].
The two approaches, stochastic TDHF and the Boltzmann-Langevin equation, are closely related to each other. We will show in this paper that the Boltzmann-Langevin equation can be derived from stochastic TDHF by employing an appropriate averaging over "subensembles". This alternative derivation complements our understanding of the Boltzmann-Langevin equation. In particular, it provides a very transparent formulation of the conditions under which the approach can be validated.

The paper is outlined as follows. In section 2, we quickly review the TDGCM and variational approaches to correlations on top of TDHF. In section 3, we derive Stochastic TDHF and discuss conditions of validity of the approach. In section 4, we derive the Boltzmann-Langevin equation from Stochastic TDHF.

2 Short review of the Time-Dependent Generator-Coordinate-Method

We give here a short summary of the Time-Dependent Generator-Coordinate-Method (TDGCM) as outlined in ref. [3]. One considers a time-dependent correlated state as a superposition

\[ |\Psi(t)\rangle = \int d^F q \, |\Phi_q(t)\rangle \, f(q; t) \]  

where \( F \) is the number of degrees-of-freedom \( q \) for correlations. The \( \{ |\Phi_q(t)\rangle \} \) is a basis of Slater states where each state is a solution of the TDHF equation

\[ i\partial_t |\Phi_q\rangle = h_q |\Phi_q\rangle \]  

with the mean-field Hamiltonian \( h_q \) corresponding to the state \( |\Phi_q\rangle \). The time evolution of the superposition function \( f(q; t) \) is determined by time-dependent variation,

\[ \partial_t \langle f | d\Psi < H - i\partial_t |\Psi\rangle = 0. \]

One finds

\[ i\partial_t f = \hat{I}^{-1} \hat{H}_{GCM} f \]  

where \( \hat{I} \) is an integral operator corresponding to the norm overlap

\[ \hat{I} = \int d^F q' < \Phi_q |\Phi_{q'}\rangle \]

\[ \hat{I}^{-1} \hat{H}_{GCM} f \]
and \( \hat{H}_{GCM} \) is an analogous integral operator employing the reduced Hamiltonian overlap

\[
H_{GCM}(q, q') = \langle \Phi_q | H - i \partial_t | \Phi_{q'} \rangle
\]

This equation resembles a Schrödinger equation for \( f \) but it is somewhat complicated by the non-unit norm-operator \( \hat{I} \). It is important to note that in the TDGCM each basis state \( |\Phi_q\rangle \) propagates in its own mean-field \( h_q \). This allows to account for fluctuating mean-fields which is an essential effect in nuclear collective dynamics at large amplitudes. This ansatz allows much larger fluctuations in observables than a mere TDHF propagating only one mean-field [2, 3]. These fluctuations are driven by two effects: first, a possible spreading of the mean-field trajectories \( |\Phi_q\rangle \) due to nonlinear amplification of deviations by the various mean-fields (which is a particularly large effect near bifurcation points of the TDHF dynamics), and second a changing width of the collective wavefunction, or of the superposition function \( f \) respectively.

It is obvious that one cannot handle basis spaces with too large numbers of degrees-of-freedom \( F \). Thus the key question in TDGCM is an appropriate choice of the set of basis states \( \{ |\Phi_q(0)\rangle \} \). The first choice is, of course, those collective deformations which are known to develop into large amplitude collective motion, like, for example, asymmetry- or neck-degrees-of-freedom in fusion and fission. However, the optimal choice also sensitively depends on the final observable. Think of the example in which one wants to determine the final spread \( \langle \Psi(t_f) | \Delta^2 A | \Psi(t_f) \rangle \) of a one-body observable \( A \). In that case, the TDGCM wave function \( |\Psi\rangle \) exhausts the possible width optimally if the collective path \( \{ |\Phi_q(0)\rangle \} \) is chosen such that the observable \( A \) becomes the generator of the path at final time \( t_f \), i.e. \( |\Phi_q(t_f)\rangle = e^{iA_q} |\Phi_0(t_f)\rangle \). This means

\[
|\Phi_q(0)\rangle = U_{MF}(0,t_f)e^{iA_q}U_{MF}(t_f,0)|\Phi_0(t_f)\rangle
\]

where \( U_{MF} \) is the mean-field time-evolution operator. This is plausible from a practical point of view, and moreover, it can be proven by a variational approach in which the mean-field states and the time-dependent one-body operator for the observable are varied [4, 5]. In fact, this variational approach is formally equivalent to TDGCM in the Time
Dependent Random Phase Approximation (TDRPA) limit (small amplitudes) with the additional feature that it delivers automatically an optimal deformation path. The variational principle [4] was also tentatively applied to the dissipative situations occurring in heavy-ion collisions [13]. This however raises some conceptual difficulties: i) the spreading of TDHF trajectories is evaluated only through RPA modes; ii) dissipation is governed by one parameter $\tau$, characteristic of the Iterative Time Smoothing method (ITS); iii) in the case of collisional problems the momentum conservation law (associated to the isoscalar $l=1$ RPA mode) might be violated. The ITS method presumably deserves some more studies.

However, both the variational approach and TDGCM are too limited in that they can handle in practice only one or a few collective correlation channels. It is rather unlikely that internal excitations are restricted to a few degrees-of-freedom in a violent heavy-ion collision. One needs to account for a large number of degrees-of-freedom. Some savings in other features are hence required to make such a scheme tractable. On the other hand, this large number suggests that phase relations between all these degrees-of-freedom occur at random and thus can be neglected. This suggests a stochastic approach in which only probabilities are propagated rather than the much more complex probability amplitudes. The coherent propagation within TDGCM is still used, but only for a short perturbative step as an ingredient to derive the rules for the time-evolution of the probabilities. This leads eventually to the Stochastic TDHF as outlined in the next section.

The TDGCM was formulated above in terms of continuous deformation labels $q_i$. This is advantageous in the case of few collective correlation channels with large amplitudes. One can represent alternatively the correlated state $|\Psi>$ as a superposition over a discrete set of basis states $|\Phi_N>$,

$$|\Psi(t)> = \sum_N |\Phi_N(t)> f_N(t)$$

(7)

where each $|\Phi_N>$ follows again a TDHF path in its own mean-field $h_N$. The label $N$ may account, e.g., for the $1ph$, $2ph$, ... excitations about $|\Phi_0>$. Time dependent variation
with respect to $f_N$ then yields

$$i\partial_t f_M = (I^{-1})_{MM'} H_{M'N} f_N$$

(8)

where $H_{M'N}$ is the reduced Hamiltonian overlap matrix

$$H_{M'N} = <\Phi_{M'}|H - i\partial_t|\Phi_N>$$

(9)

and $I^{-1}$ is the inverse of the norm-matrix

$$I_{MM'} = <\Phi_M|\Phi_{M'}>$$

(10)

This discrete form of TDGCM is the more adapted starting point for the case of many degrees-of-freedom as will be seen in the next section.

### 3 Stochastic TDHF

#### 3.1 Correlations in perturbation theory

##### 3.1.1 Evolution of wavefunctions

We first investigate the building-up of correlations from an initial Slater state. We consider the length $t$ of this first time interval $[0,t]$ and the strength of the residual interaction just such that a perturbative treatment is still possible. The necessary conditions for the perturbative approach will be discussed at the end of this subsection.

Let us assume that we start at time $t = 0$ from a pure Slater state $|\Phi_N(0)>$. It is propagated as a Slater state according to TDHF, during the time interval $[0,t]$

$$|\Phi_N(0)> \xrightarrow{TDHF} |\Phi_N(t)> = U_N(t,0)|\Phi_N(0)>$$

(11)

where $U_N$ describes the time-evolution

$$U_N(t,t') = \mathcal{T}\{\exp(-i\int_{t'}^t dt h_N(t))\} \ , \ U_N(t,t) = \hat{1}$$

(12)
under the influence of the mean-field $h_N(\hat{t}) \equiv h(\Phi_N(\hat{t}))$. In eq. (12) $T$ denotes the time ordering operator. The mean-field $h_N$ is only part of the full Hamiltonian $H$. We have to complement it by the residual interaction $V_N$ such that

$$H = h_N + V_N$$

We assume that TDHF dominates the time-evolution for a certain period of time. Then the residual interaction $V_N$ can be considered as being small and we treat it in time-dependent perturbation theory. The full time-evolution of the initial state $|\Phi_N(0)\rangle$ can then be approximately described as

$$|\Phi_N(0)\rangle \approx \Phi_N(t) \approx -i\int V_N |\Phi_N(t)\rangle$$

where $|\Phi_N(t)\rangle$ is given in eq. (11) and $\int V_N$ is an abbreviation for the integral over the residual interaction in the interaction representation with respect to $h_N$,

$$\int V_N = \int_0^t dt' V_N(t')$$

We now expand the slightly correlated state (14) into a discrete set of Slater states $|\Phi_M(t)\rangle$

$$|\Psi_N(t)\rangle \approx |\Phi_N(t)\rangle \approx -i|\Phi_M(t)\rangle < M|\int V_N N >$$

where we have adopted the Einstein's summation convention and where we have abbreviated $< M|\int V_N N > = |\Phi_M(t)\rangle < \int V_N |\Phi_N(t)\rangle$. Furthermore, we have exploited the freedom to choose the set $\{|\Phi_M(t)\rangle\}$ to be orthonormal just at time $t$. This reduces the norm-operator as $\hat{I} \rightarrow \hat{1}$ which simplifies the treatment greatly. Thus we have obtained this way a perturbative solution of discrete TDGCM corresponding to $f_M(t) \approx \delta_{NM} - i < M|\int V_N N >$. It is to be noted that the dominating states in the expansion (17) will be the $2ph$-excitations with respect to $|\Phi_N(t)\rangle$. This freedom in choosing $|\Phi_M(t)\rangle$ is an important feature to keep in mind for future applications. Indeed it offers the possibility to concentrate the effect of the residual interaction on a small set of relevant states, thus reducing the numerical work, while exhibiting the dominant dynamical features.
3.1.2 Evolution of densities

The correlated wavefunction (17) is a coherent superposition. It is a hopeless undertaking to propagate all these correlations coherently over large time intervals which go beyond a perturbative access. We aim at an approximate treatment which neglects information on relative phases and propagates the states incoherently. In order to allow separation of coherent and incoherent parts of a state, we switch to a description in terms of density matrices. The density matrix of the correlated state $|\Psi_N(t)\rangle$ becomes up to second order in the residual interaction

$$D(t) = |\Phi_N\rangle\langle\Phi_N| - i \sum_M |\Phi_M\rangle\langle M|\hat{V}_N|N\rangle\langle N|\langle N|\hat{V}_N|M\rangle\langle M|\Phi_M\rangle + \text{h.c.}$$

$$+ \frac{1}{2} \sum_{MM'} \{ |\Phi_M\rangle\langle M|\hat{V}_N|N\rangle\langle N|\hat{V}_N|M'\rangle\langle M'|\Phi_{M'}\rangle - |\Phi_M\rangle\langle M|\hat{V}_N|M'\rangle\langle M'|\hat{V}_N|N\rangle\langle N|\Phi_N\} + \text{h.c.}$$

where "h.c." means the hermitian conjugate of the previous term. We now assume that we have a very large number of states which are coupled by $\hat{V}_N$ and that the relative phases of these states in $D$ are randomly distributed. Thus the terms in $D$ which are diagonal in the $|\Phi_M\rangle$ dominate the nondiagonal terms by far and we can approximate $D$ by its diagonal terms only

$$D(t) \approx |\Phi_N\rangle\langle\Phi_N|(1 - \sum_{M \neq N} |\langle M|\hat{V}_N|N\rangle|^2) + \sum_{M \neq N} |\Phi_M\rangle\langle M|\hat{V}_N|N\rangle|^2 < \Phi_M|$$

The transition matrix element $|\langle M|\hat{V}_N|N\rangle|^2$ therein can be evaluated easily if the mean-field does not vary much over the time interval $[0,t]$ and if the diagonal element $E_N = \langle N|\hat{h}_N|N\rangle$ is large as compared to the fluctuations $\sqrt{\langle N|\Delta^2\hat{h}_N|N\rangle}$. We assume furthermore that the time interval $[0,t]$ is also long enough to allow a fully developed transition from $|\Phi_M\rangle$ to $|\Phi_N\rangle$. With the standard steps which are already used to derive Fermi's golden rule [14] we can then derive

$$|\langle M|\hat{V}_N|N\rangle|^2 = \frac{\hbar}{\pi} |\Phi_M(0)|V_N(0)|\Phi_N(0)|^2 \delta(E_M - E_N)t = P_{NM}t$$


which defines a transition rate $P_{NM}$. After all, we end up with the density matrix

$$D(t) \approx D_N(t) + \sum_{M \neq N} [D_M(t) - D_N(t)]P_{MN}t$$

where $|\Phi_N \rangle < \Phi_N| = D_N$ has been used to compactify the notation. This means that the initial state $|\Phi_N(0) \rangle$ develops into an ensemble of Slater states

$$|\Phi_N(0) \rangle \rightarrow \mathcal{E}(t) \equiv \{|\Phi_M(t) \rangle, W_M\} , \quad W_M = \left\{ \begin{array}{ll} 1 - (\sum_{M'} P_{M'M})t & \text{for } M = N \\ P_{MN}t & \text{for } M \neq N \end{array} \right. \quad (22)$$

### 3.1.3 Conditions for the validity of the incoherent approach

In retrospective view, we can now discuss the conditions for the validity of the incoherent time-stepping developed above.

1. We have to require that the residual interaction is small enough to allow a perturbative treatment. This means $(\sum_{M \neq N} P_{MN})t \ll 1$ which, in fact, is a condition on the allowed length $t$ of the time interval $[0, t]$ for perturbative propagation

$$t \ll \frac{1}{\sum_{M \neq N} P_{MN}} \quad (23)$$

2. We have assumed that the mean-field is almost constant over the considered time interval, $h_N(t') \approx h(0)$, which means

$$t \ll t_{MF} \quad \text{where} \quad t_{MF} \quad \text{is such that} \quad h(t_{MF}) \approx h(0) \quad (24)$$

This reduces the mean-field time-evolution operator $U_N(t, t')$ to an exponential in time. This condition is related to the other assumption which we have made, namely that the diagonal part of the mean-field dominates

$$h_N |N \rangle \approx E_N |N \rangle \quad (25)$$

This reduces the mean-field propagators in the matrix element $<M|f\hat{V}_N|N>$ to a mere phase factor $\exp(-i(E_N - E_M)(t - t'))$, and allows finally to derive Fermi's golden rule in eq. (20).
3. In order to derive the $\delta(E_M - E_N) t$ from the phase factor, one has to require that the matrix element $|<M|V_N|N>|^2$ does not vary much over the relevant energy range $1/t$. This means

$$t < 1/\delta E_{\text{var}}$$

where $\delta E_{\text{var}}$ is the typical energy range over which $|<M|V_N|N>|^2$ varies.

4. Finally, it is obvious that the $\delta(E_M - E_N)$ in eq. (20) is only an approximate $\delta$-function with finite width $1/t$. This is a welcome feature in view of the fact that the spectrum $\{E_M\}$ could be also only a discrete spectrum. The notion of a $\delta$-function makes sense as long as

$$1/t \ll \Delta E$$

where $\Delta E$ is the mean energy-separation of the states $|\Phi_M>$. Altogether, the conditions (23-27) are to be fulfilled to justify the purely incoherent propagation (22). The question whether the random phase assumption is justified or not has not been tackled explicitly. It is implicitly answered in the spectral conditions which require a very large number of states. We have already mentioned that the condition (25) of a dominant diagonal mean-field is strongly related to the condition (24) of a slowly varying mean-field. This can be seen by looking at the time-variation of the mean-field Hamiltonian $h_N = h(D_N)$. The time-dependence of $h_N$ enters via the density $D_N$. Thus $\partial_t h_N = \partial_D h \partial_t D_N$, and we remind that $\partial_t D_N = -i[h_N, D_N]$. But the diagonal part $\propto E_N$ cancels in the commutator $[h_N, D_N]$. Thus $\partial_t D_N$ is driven only by the nondiagonal parts of the mean-field and correspondingly $\partial_t h$ is also directly related to the nondiagonal part of $h$. This shows the intimate connection between the two conditions (24) and (25). A detailed analysis of the various conditions for the case of a universal and time-independent basis for the whole many-body system has been given times ago in the pioneering paper of van Hove [15].

The problem with the above conditions is that they are very demanding, and they are most probably hardly fulfilled in a nuclear system or heavy-ion dynamics. In particular the conditions (24) and (25) on the mean-field are questionable because we aim at describing
violent collisions far from equilibrium. The interference of a changing mean-field during the collision process gives rise to memory effects in the collision term. Such memory effects are found to be important even at the rather modest energies of the nuclear giant resonance [16]. It is certainly an important task for future development to include such memory effects in stochastic TDHF and the Boltzmann-Langevin equation. Notwithstanding this probably necessary extension, we can only argue that the above conditions are perhaps too rigid and that the approach may hold beyond these limits. It is, of course, an important task to try to figure out less severe limits. A guideline for this task may be the observation that one computes energetic heavy-ion processes - with some success - usually in one of the various test-particle methods [22] and the collision term is evaluated there in a local-collision approximation, see e.g. [10]. This reminds the expansion about local-equilibrium as it was used extensively in ref. [18]. It may be possible to derive a more forgiving set of conditions from this local approach.

3.2 Evolution of an ensemble of Slater states

We have seen in the previous section that an ensemble of Slater states is generated within one time-step [0, t] if one neglects the phase relations between the various basis Slater states in a correlated state. We are now going to extend the single step derived above to a stochastic process describing the evolution of an ensemble of Slater states over long times. To that end, we have to introduce a more flexible notation which is adapted to trace back the path of a stochastic process. The Slater states at time t after the first time step, $|\Phi_M(t)\rangle$, are in fact the states descendant from the initial state $|\Phi_N(0)\rangle$. We indicate this by denoting the states now with a double index $|\Phi_M(t)\rangle \rightarrow |\Phi_{M_1;N_0}\rangle$ where the time can now be omitted because the highest index $M_1$ implies that this is a state after one time-step. The occupation weight of the state is generalized in a similar manner to $W_M \rightarrow W_{M_1;N_0}$. Altogether, the first time step produces the ensemble

$$\mathcal{E}(t) \equiv \{|\Phi_{M_1;N_0}\rangle ; W_{M_1;N_0} \} \quad (28)$$
We now select a state $|\Phi_{M_1;N_0} \rangle$ with probability $W_{M_1;N_0}$ as initial state for one further time step in the interval $[t, 2t]$. This is done for each member of the ensemble (28) and all steps together lead to a new ensemble

$$\mathcal{E}(2t) \equiv \{ |\Phi_{M_2;M_1,N_0} \rangle; W_{M_2;M_1,N_0} \}$$

$W_{M_2;M_1,N_0} / W_{M_1;N_0} = \begin{cases} 1 - (\sum_{M_1} P_{M_2,M_1}) t & \text{for } M_2 = M_1 \\ P_{M_2,M_1} t & \text{for } M_2 \neq M_1 \end{cases}$

where the notation of emerging states $|\Phi_{M_2;M_1,N_0} \rangle$ at time $2t$ and corresponding occupation weights $W_{M_2;M_1,N_0}$ is obvious. The process is repeated in time intervals $[(n - 1)t, nt]$. At time $nt$ we obtain the ensemble

$$\mathcal{E}(nt) \equiv \{ |\Phi_{M_n;M_{(n-1)}...M_1,N_0} \rangle; W_{M_n;M_{(n-1)}...M_1,N_0} \}$$

$$W_{M_n;M_{(n-1)}...M_1,N_0} / W_{M_{(n-1)};M_{(n-2)}...M_1,N_0} = \begin{cases} 1 - (\sum_{M_1} P_{M_n,M_{(n-1)}}) t & \text{for } M_n = M_{(n-1)} \\ P_{M_n,M_{(n-1)}} t & \text{for } M_n \neq M_{(n-1)} \end{cases}$$

Thus the density matrix of the total system becomes

$$\mathcal{D}(nt) = \sum_{M_n...M_1} |\Phi_{M_n;M_{(n-1)}...M_1,N_0} \rangle W_{M_n;M_{(n-1)}...M_1,N_0} \langle \Phi_{M_n;M_{(n-1)}...M_1,N_0}|$$

and all desired expectation values can be computed accordingly. These equations (31-33) comprise the compact formal description of stochastic TDHF.

### 3.3 Comments on practical aspects

The practical evaluation of stochastic TDHF proceeds in a Monte-Carlo fashion. At time $t$, one picks one of the $|\Phi_M(t) \rangle$ where the random choice is governed by the probability $P_{M;N}$. This $|\Phi_M(t) \rangle$ is propagated perturbatively to $|\Phi_M(2t) \rangle$ and there one picks again one particular Slater state according to the actual probability weights at $2t$. Such a stochastic path is traced until time $nt$. The procedure is repeated many times starting over and over again at $|\Phi_N(0) \rangle$. We obtain finally an ensemble $\mathcal{E}(nt) \equiv \{ |\Phi_{\text{path}}(nt) \rangle; 1/\sum_{\text{path}} \}$ in which all members have the same occupation weight. The probabilities
\[ W_{M_1 M_2 ... M_t N_0} \] are build into the states \[ |\Phi_{\text{path}}(n)\rangle \] by the rules of the selection of a stochastic path.

This short outline gives only a superficial view of the practical procedure. There are many technical problems hidden in details. For example, the set of states \[ |\Phi_M(t)\rangle \] to choose from is very large and it would be a waste of time to compute all transition rates before selecting one specific member. A sensible restriction is to assume that the residual interaction creates only \( 2p\ell\)-states and thus that the \( |\Phi_M\rangle \) are from the \( 2p\ell\)-states with respect to \( |\Phi_N\rangle \). This space is still very large. One may use the freedom of unitary transformations within the particle states and separately within the hole states in order to concentrate the transition strength into a few dominant states \( |\Phi_M\rangle \). But these more practical considerations are beyond the scope of this paper.

4 Relations to the Boltzmann-Langevin approach

4.1 Short review of the Boltzmann-Langevin approach

An alternative stochastic approach to large amplitude collective motion is provided by the Boltzmann-Langevin equation [8, 10]

\[
i \partial_t \rho_{\text{path}} = [h(\rho_{\text{path}}), \rho_{\text{path}}] + \dot{K} + \delta \dot{K}
\]

where \( h(\rho_{\text{path}}) \) is the mean-field generated from the one-body density \( \rho_{\text{path}} \), \( \dot{K} \) is a Boltzmann-like collision integral, and \( \delta \dot{K} \) is a stochastic force. The Boltzmann-Langevin equations is a stochastic differential equation producing an ensemble of one-body trajectories \( \{\rho_{\text{path}}(t)\} \) which allows large fluctuations of the mean-fields within the ensemble. This is called the global ensemble in ref. [8]. Each actual one body density \( \rho_{\text{path}} \) out of the global ensemble is the result of a mean-field propagation with collision term and occasional kicks by the stochastic force. Thus \( \rho_{\text{path}} \) represents an impure, or heated, state with non-vanishing fluctuations of the mean-field. During any time of order \( t \) (section 3.1.3) a path \( \rho_{\text{path}} \) is embedded in a so called local ensemble [8]. This ensemble

\[
\{\rho_{\text{path}} : (\rho_{\text{path}} - \rho) \text{ small}\}
\]
represents the neighbourhood of small fluctuations about a locally-averaged density $\rho$, which follows the Boltzmann equation during $t$. On this time/ensemble scale fluctuations hence average to zero and remain small. These small fluctuations in the local ensemble (35) give rise to the (small) stochastic force which then generates in the course of a (diverging) time-evolution finally the global ensemble. This distinction will become important in the latter discussion of the relations between stochastic TDHF and the Boltzmann-Langevin equations.

The collision term in eq. (34) reads in Markovian approximation

$$\dot{K}_{\nu\mu} = \pi tr_{12}\{[a_{\mu}^+ a_{\nu}, v]\delta (\mathcal{L}_0)\overline{\rho p} v \overline{\rho p} - [a_{\mu}^+ a_{\nu}, v]\delta (\mathcal{L}_0)\overline{\rho p} v \overline{\rho p}\} \quad (36)$$

where $\overline{\rho p}$ is the antisymmetrized product of one-body density matrixes $\rho$ and $\bar{\rho} = 1 - \rho$. The operator $\mathcal{L}_0$ is the mean-field Liouvillian which serves as a shorthand notation for $\mathcal{L}_0 A_{12} = [h_1 + h_2, A_{12}]$ if it acts on a two-body operator $A_{12}$. This means in detail

$$(\mathcal{L}_0 A)_{\alpha\beta\gamma\delta} = (\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_\gamma - \varepsilon_\delta) A_{\alpha\beta\gamma\delta} \quad (37)$$

where the matrix elements with respect to the instantaneous eigenbasis of the actual mean-field,

$$h(\rho) \varphi_\alpha = \varepsilon_\alpha \varphi_\alpha \quad (38)$$

have been taken. The collision term (36) has been derived e.g. in a time-dependent projector approach [17]. It is very compact and therefore most adapted to the formal considerations of this paper. A more detailed expression is given in appendix A. There, it is also shown that only the diagonal part of $\dot{K}_{\nu\mu}$ plays a role if the condition (25) is invoked. And it is this diagonal form which is also given in detail in connection with the Boltzmann-Langevin equation in ref. [8].

The stochastic force $\delta \dot{K}$ vanishes in an average, performed on a local scale in the abstract space of single-particle densities trajectories [8]. The stochastic force has the time correlation

$$< \delta \dot{K}_{\mu\nu}(t) \delta \dot{K}_{\nu'\mu'}(t') > = \dot{C}_{\mu\nu,\mu'\nu'} \delta(t - t') \quad (39)$$

$$\dot{C}_{\mu\nu,\mu'\nu'} = \pi tr_{12}\{[a_{\mu}^+ a_{\nu}, v]\delta (\mathcal{L}_0)\overline{\rho p} [v, a_{\mu}^+ a_{\nu}]\overline{\rho p}\} \quad (40)$$

15
A detailed expression for the correlation operator $\hat{C}_{\mu\nu,\mu'\nu'}$ can again be given in the instantaneous eigenbasis (38). We will skip these details here and refer to [8].

The equation (34) without the stochastic force $\delta \hat{K}$ is a standard in what one calls "extended TDHF", see e.g. ref. [1]. There are many variants related to different approximations in the handling of the mean-field as well as the collision term. Correspondingly a large amount of numerical work has been devoted to simulate such equations in the realistic (and complicated) case of heavy-ion reactions. The semiclassical approximations of these extended mean-field theories were particularly studied because of their "relative" simplicity. The various numerical versions of these calculations gave birth to a rich variety of fancy acronyms like BUU, VUU, etc. These simulations are all based on test-particle methods, which actually give reasonable approximate solutions to the Boltzmann equation [22]. The Boltzmann collision term $\hat{K}$ therein describes the approach to equilibrium in the course of the time evolution, dissipating energy from the mean-field motion into internal degrees-of-freedom. The final outcome of such an extended TDHF is a heated one-body density matrix $\rho$ which corresponds to an ensemble of Slater states. However, this approach has the severe limitation that the ensemble propagates all states in the same mean field $h(\rho)$. Accordingly, this form of extended TDHF is insufficient to describe phenomena with large fluctuations developing in the course of time. This requires to allow fluctuating mean-fields, and these are generated by the stochastic force $\delta \hat{K}$. The stochastic force $\delta \hat{K}$ is related to the collision integral through the fluctuation-dissipation theorem leading to the form (40) which obviously is very similar to eq. (36). The situation is somewhat similar to the standard example of the Langevin equation for Brownian motion [19]: the friction force dissipates energy from the particle to the heat-bath; it is to be complemented by a stochastic Langevin force which describes the reverse effect, namely the random pushing of the particle by the heat-bath. Likewise, the Boltzmann collision term acts as a dissipating force (although it preserves energy, contrarily to the friction term of the Brownian motion) and the stochastic force $\delta \hat{K}$ serves as the complementing Langevin force. The Boltzmann-Langevin equation is thus a stochastic equation which is to be solved by Monte-Carlo techniques in a way similar to Stochastic TDHF.
But this time, an ensemble \( \{ \rho_{\text{path}}; 1/\sum_{\text{path}} \} \) of one-body density matrices is generated. Nonetheless, one expects close interrelations between the Boltzmann-Langevin approach and Stochastic TDHF. In fact, the Boltzmann-Langevin equation (34) can be derived from Stochastic TDHF. This will be done in the next subsection.

### 4.2 Subensembles and mesoscopic sampling

The comparison of stochastic TDHF and the Boltzmann-Langevin equation starts from the observation that the full ensemble \( \mathcal{E} \) of Stochastic TDHF can be clustered into subensembles \( \mathcal{S}_\rho \), such that, first \( \mathcal{E} \) can be sampled from the \( \mathcal{S}_\rho \) (i.e. \( \mathcal{E} = \mathcal{S}_\rho \)), and second each \( \mathcal{S}_\rho \) is characterized by nearly the same mean-field \( h(\rho) \) and accordingly by the same density \( \rho \):

\[
\rho \leftrightarrow \mathcal{S}_\rho \equiv \{ |\Phi_M> : h_M \approx h_\rho; W_M \}
\]  

(41)

This subensemble \( \mathcal{S}_\rho \) is identified with the local ensemble (35) of the Boltzmann-Langevin approach. The Boltzmann-Langevin equation, in turn produces an ensemble of one-body density matrices

\[
\mathcal{B} \equiv \{ \rho_{\text{path}}; 1/ \sum_{\text{path}} \}
\]

where \( 1/\sum_{\text{path}} \) is the (equal) probability for each member. This global ensemble of the Boltzmann-Langevin equations is to be compared to the full ensemble (31) of stochastic TDHF.

As a note aside the local ensemble (41) is sampled from pure states only whereas the local ensemble (35) does not carry this restriction. But this is a minor difference because the sampling of ensembles is not unique anyway and because it suffices for our purposes that the average \( \rho \) and \( \Delta \rho \) are equivalent.

We want to derive the Boltzmann-Langevin equation (34, 36, 40) from stochastic TDHF. The first step is to identify a local ensemble in the Boltzmann-Langevin equation with a subensemble \( \mathcal{S}_\rho \) of Slater states according to eq. (41). The important feature of such a subensemble is that it embraces only small fluctuations of the mean-field such that we
can separate

\[ h_M = \bar{h} + \delta h_M \]  

(42)

where \( \bar{h} = h_p \) stands for the average mean-field Hamiltonian in the subensemble. We omit the index \( p \) in the following to keep notations simple. Averaging such a subensemble can be called a mesoscopic average as compared to a microscopic case in which one would consider each Slater state and to a macroscopic one in which one would average over the global ensemble. The residual interaction is split analogously to (42)

\[ V_M = \bar{V} + \delta V_M \]  

(43)

In every case, mean-field plus residual interaction constitute the full Hamiltonian. Thus we have the identities

\[ h_M + V_M = \bar{h} + \bar{V} \quad \rightarrow \quad \delta h_M = -\delta V_M \]  

(44)

The subensemble (41) corresponds to a total density operator

\[ D = \sum_M D_M W_M \quad , \quad D_M = |\Phi_M > < \Phi_M | \]  

(45)

The Boltzmann-Langevin equation is formulated in terms of reduced densities, in particular the one-body densities \( \rho \). These are obtained by tracing over the unwanted degrees-of-freedom. In order to obtain a most versatile formulation, we introduce the operators

\[ \hat{\rho} : \quad (\hat{\rho})_{\alpha \alpha'} = a_{\alpha}^{+} a_{\alpha} \]  

(46)

which projects the one-body part out of a many-body operator. In particular it projects the one-body density matrix as

\[ \rho = \text{Tr}\{\hat{\rho} D\} \quad , \quad \text{Tr} \equiv \text{tr}_{1..A} \]  

(47)

This form makes the one-body reduction easier to handle because one can exploit the freedom of cyclic permutations in the full trace \( \text{Tr} \) but not in a reduction using partial traces as \( \text{tr}_{2...A} \).
The Boltzmann equation relies on a many-body hierarchy in which one-body densities are the leading order, two-body effects the next correction, and higher order correlations are neglected. Therefore some more information on the residual interaction is needed than in stochastic TDHF, namely the assumption that \( V_M \) is a two-body force making only \( 2\text{ph} \) excitations out of \(|\Phi_M>\), i.e.

\[
V_M|\Phi_M> = \sum_{nmij} V_{nmij} a_n^+ a_i a_j a_i^+ a_j |\Phi_M>
\]

where \( n,m \) are particle states and \( i,j \) hole states with respect to \(|\Phi_M>\). We express this feature in terms of density matrices as

\[
V_M D_M = \sum_{M' \in 2\text{ph} - M} D_{M'} V_M D_M
\]

which means that the completeness relation \( \sum_{M'} D_{M'} = 1 \) can be reduced to the two \( 2\text{ph} \) space with respect to \( D_M \). Equation (48) expresses \( 2\text{ph} \) transitions from \( M \) to \( M' \). As a consequence, the one-body reduction of the transition vanishes, i.e.

\[
\text{Tr}\{\rho D_{M'} A D_M\} = 0 \quad \text{if} \quad M' \in 2\text{ph}_M
\]

where \( A \) can be any operator.

### 4.3 Derivation of the Boltzmann-Langevin equation

We start from a given subensemble (41), i.e. \( D(0) = \sum_M W_M D_M \), and propagate it one step according to Stochastic TDHF, see eq. (22). This yields eq. (21) and related equations. We repeat it in short

\[
D(t) = \sum_M W_M D_M(t) + \sum_{M'M} W_M P_{M'M} (D_{M'}(t) - D_M(t))
\]

\[
D_M(t) = U_M D_M(0) U_M^+ + i \frac{1}{\hbar} \int \langle M|V|M'\rangle \delta (E_M - E_{M'})
\]

where \( U_M = U_M(t,0) \) is the mean-field propagator (11) and the abbreviation \(|M> = |\Phi_M>\) has been used. The time-argument is irrelevant in \(|M'> or <M| because the
transition probability (20) was evaluated within the Markovian approximation, i.e. we have assumed negligible evolution of mean-field properties during the transition and we have extracted a simple phase factor \( \exp(-i(E_{M'} - E_M)(t-t')) \). We have to keep this in mind when evaluating the stochastic force in later steps.

**4.3.1 Coarse time derivatives**

Equation (21) describes one complete small time step from \( D(0) \) to \( D(t) \). However, the Boltzmann-Langevin equation is a differential equation in time. One is tempted to produce this form by taking the time-derivative. But this is not allowed in a strict mathematical sense because the final time \( t \) of the step is bound by several requirements as discussed in section 3.1. We can maintain the notion of a differential equation only if we interpret time derivatives in a coarse sense

\[
\partial_t f \approx \frac{f(t) - f(0)}{t}
\]

where \( t \) is the typical length of the time-interval \([0,t]\), according to the conditions of section 3.1. The following further steps towards a stochastic differential equation are to be understood in this sense.

**4.3.2 Preliminary form of the Boltzmann-Langevin equation**

Taking the (coarse) time derivative of eq. (21) yields

\[
i\partial_t D(t) = \sum_M W_M [h_M, D_M] + \sum_{MM'} W_{MM'} P_{MM'} (D_{M'} - D_M)
\]

In this equation, each member \( D_M \) propagates still in its own mean-field \( h_M \). We separate the leading term, propagation with the subensemble averaged mean-field Hamiltonian \( \bar{h} \), from the small fluctuation \( \delta h_M \) as introduced in eq. (42). This yields

\[
[h_M, D_M] = [\bar{h}, D_M] + [\delta h_M, D_M]
\]

We employ furthermore the eq. (44) to rewrite

\[
\]
where the first term on the right-hand-side is going to vanish if we reduce the expressions to one-body densities, see eqs. (48) and (49). We now reduce eq. (51) to the one-body level using the projection operator (46). This yields

\[ i\partial_t \rho(t) = [\hat{h}(t), \rho(t)] + \delta\dot{K} + \dot{K} \]  

(52)

\[ \delta\dot{K} = \sum_M W_M \text{Tr}\{[\hat{\rho}, \hat{V}]D_M\} \]  

(53)

\[ \dot{K} = \sum_{MM'} W_M P_{MM'}(\rho_{MM'} - \rho_M) \]  

(54)

The notation suggests already the interpretation: \([\hat{h}, \rho]\) is the leading mean-field term, \(\delta\dot{K}\) is the stochastic force, and \(\dot{K}\) is the collision term. The interpretation of the mean-field term is obvious. The assignment of the two other terms needs yet to be proven.

4.3.3 Evaluation of the collision integral

There are two strategies to derive the collision term \(\dot{K}\): first, one starts from the expression (54) and reformulates the transition rate in terms of traces of the full densities \(D_M\) and the residual interaction \(V\), and second, one goes back to the second order expression for \(D_N\) and evaluates it again in the presence of the one-body reduction using exactly the same approximations and steps as in the derivation of stochastic TDHF. We present here the derivation along the second strategy. The alternative derivation according to the first strategy is given in appendix B for completeness.

We go back to eq. (18) for the full density at time \(t\) in second order perturbation theory. The collision term stems from the second order term therein. We take the time derivative \(\partial_t\) similar as in the way to eq. (51). This withdraws one integral and removes the factor \(\frac{1}{2}\). We perform the one-body reduction as trace over the full expression together with \(\hat{\rho}\). Thus we obtain

\[ \dot{K} = \sum_M W_M \text{Tr}\{\hat{\rho}[V(t), [\hat{V}, D_M(t)]]\} \]  

(55)

where we implicitly use \(V = V_M\) as an abbreviation. We extend the time integration in
\[ \int_0^t dt' UVU^+, D_M] = \int_0^t dt' U[V, D_M]U^+ = \int_0^t dt' e^{-ih_M(t-t')}[V, D_M]e^{ih_M(t-t')} \]

where we have employed for the last step the fact that \( h_M \) is nearly constant, see condition (24). The exponentials with \( h_M \) from right and left can be summarized as an exponential with the mean-field Liouvillian \( L_0 \) as defined in eq. (37), yielding \( e^{-itL_0(t-t')}[V, D_M] \) for the integrand. We now perform the time integral and pick the \( \delta \)-function part of it which corresponds to omitting phase information as it was done in the step to Fermi's golden rule (20). This yields a \( \frac{\pi}{\hbar} \delta(L_0) \) and we obtain for the collision term in one-body reduction

\[ \hat{K} = \frac{\pi}{\hbar} \sum_M W_M \text{Tr}\{[\hat{\rho}, V]\delta(L_0)[V, D_M]\} \quad (56) \]

where \( L_0 \) is acting on everything to the right. We finally ought to implement explicitly the information that the residual interaction \( V \) makes only 2ph-transitions from the state \( D_M \). This is necessary for the further reduction of the collision integral in terms of one-body and two-body densities. We introduce the complete set \( \{\Phi_{M'}>, M' \in 2ph - M\} \) of 2ph-excitations about \( \Phi_M > \) and the corresponding full densities \( D_{M'} \). This yields the collision term in the form

\[ \hat{K} = \sum_M W_M \sum_{M' \in 2ph - M} \frac{\pi}{\hbar} \text{Tr}\{[\hat{\rho}, V]\delta(L_0)(D_MV^,D_M' - D_{M'}V^,D_M)\} \quad (57) \]

which is appropriate for the further reduction.

The transitions in the above equation are at most 2ph-transitions. Thus at most two particles are involved with the operators \( V \) and \( \hat{\rho} \) in the trace and the rest of the particles can easily be traced out. We use

\[ \sum_{M' \in 2ph - M} \text{tr}_{3...A}\{D_MVD_{M'}\} = \rho_{1,M}\rho_{2,M}V\rho_{1,M}\rho_{2,M} \quad (58) \]

where \( \rho = 1 - \hat{\rho} \) and \( \rho_{i,M} = \text{Tr}\{\hat{\rho}_iD_M\} \) is the one-body density matrix of particle \( i \) in state \( M \). The projection of the 2ph-part of \( V \) which was performed in the sequence \( D_MVD_{M'} \) is now taken over by the construction \( \rho V \rho \). A similar relation holds under inclusion of
the $\delta(\mathcal{L}_0)$. As a last step, we perform the summation over the subensemble. This yields approximately

$$\sum_M W_M \delta(\mathcal{L}_0) \rho_{1,M} \rho_{2,M} V_M \rho_{1,M} \rho_{2,M} = \delta(\mathcal{L}_0) \rho \hat{V} \rho$$

where we have neglected fluctuation terms as e.g. $\delta V_M$. We argue that the collision term is already small of second order in $V$ and combination with further small fluctuation terms is negligible. Taking all pieces together yields finally

$$\hat{K} = \frac{\pi}{\hbar} \text{tr}_2 \{[\hat{\rho}, \hat{V}] \delta(\mathcal{L}_0)(\hat{\rho} \hat{\rho} \hat{V} \hat{\rho} - \hat{\rho} \hat{V} \rho \rho)\}$$

which is the desired collision term in the form (36) of the Boltzmann-Langevin equation.

### 4.3.4 Evaluation of the stochastic force

The second term in eq. (52) describes the fluctuating force $\delta \hat{K}$ as given in eq. (53). It vanishes in the immediate average over the subensemble, i.e.

$$<\delta \hat{K}> = \sum_M W_M \text{Tr}\{[\hat{\rho}, \hat{V}, D_M]\} = \text{tr}_2 \{[\hat{V}, \sum_M W_M \rho_{12,M}]\} = \text{tr}_2 \{[\hat{V}, \rho_{1} \rho_{2}]\} = 0$$

because the residual interaction $\hat{V}$ is constructed such that it does not contribute to the mean-field $\hat{h}$, and the trace over $\rho_{1} \rho_{2}$ aims just to extract a mean-field part. This feature proves the first property of the stochastic force

$$<\delta \hat{K}> = 0$$

It remains to derive the fluctuation

$$<\delta \hat{K}(t) \delta \hat{K}(t')> = \sum_M W_M \text{Tr}\{[\hat{\rho}_{1(t)}, \hat{V}(t)] D_M(t) D_M(t') [\hat{V}(t'), \hat{\rho}_{2}]\}$$

where the one-body projectors $\hat{\rho}$ have to be distinguished by a label 1 or 2 because the fluctuation is altogether a two-body object. This is an expression of second order in $V$ similar to the collision term and similar to the transition probabilities $P_{NMt}$ in section 3.1. Thus the typical spectral properties are similar as discussed there and, in particular, we can take over the discussion of time scales. This allows the assumption that the fluctuations (61) remain within the short interval $[0, t]$ of one time step. Thus
the fluctuations are practically a \( \delta \)-function in time, see eq. (39), at the coarse time scale similar to eq. (50) for the derivatives. In other words the coarse time \( t \) which embraces the maximum size of memory effects is small compared to mean-field times \( t_{MF} \), see eq. (24).

It remains to evaluate the correlation function \( \hat{C} \). Integrating eq. (39) over time, we can write

\[
\hat{C} = \int_0^t dt' <\delta \hat{K}(t) \delta \hat{K}(t')>
\]

\[
= \int_0^t dt' \sum_M W_M \text{Tr} \{[\hat{\rho}_1, \hat{V}(t)] D_M(t) D_M(t') \{\hat{V}(t'), \hat{\rho}_2\} \}
\]

(62)

We use the time-evolution operator (11) and abbreviate it as

\[
U = U_M(t, t')
\]

to express the second part in the trace at time \( t \)

\[
\hat{C} = \int_0^t dt' \sum_M W_M \text{Tr} \{[\hat{\rho}_1, \hat{V}(t)] D_M(t) U D_M(t) [\hat{V}(t), \hat{\rho}_2] U^+ \}
\]

We now make the same assumptions as in the derivation of the transition probability, see section 3.1. The change in the mean-field is small over memory times, i.e. over the coarse time scale, and the diagonal part of the mean-field dominates, see eq. (25). Thus \( D_M \) and \( U_M \) commute and we can replace

\[
D_M U D_M = U D_M
\]

Furthermore, the time interval \([0, t]\) is long enough to develop the energy-matching delta function, i.e.

\[
\int_0^t dt' U_{...} U^{+} = \frac{\pi}{\hbar} \delta(L_0)...
\]

This yields

\[
\hat{C} = \sum_M W_M \text{Tr} \{[\hat{\rho}_1, \hat{V}(t)] \delta(L_0) D_M(t) [\hat{V}(t), \hat{\rho}_2] \}
\]

Now we have yet to implement some explicit knowledge of the fact that the residual interaction makes only 2ph-transitions. To this end, we complement the trace by the 2ph-space with respect to \( M \)

\[
\hat{C} = \sum_M W_M \sum_{M' \in 2ph-M} \text{Tr} \{[\hat{\rho}_1, \hat{V}] \delta(L_0) D_M[\hat{V}, \hat{\rho}_2] D_{M'} \}
\]

24
The further reduction proceeds similarly to the collision term: there are only two particles dynamically involved in the above trace. The remaining particles are traced out using a variant of eq. (58). This yields

$$\hat{C} = \sum_M W_M \text{tr}_{12}\{[\hat{p}_1, \hat{V}]\delta(\mathcal{L}_0)\hat{p}_1 M \hat{\rho}_{2,M} \{\hat{V}, \hat{p}_2\} \hat{p}_1 M \hat{\rho}_{2,M}\}$$

We finally perform the (sub-)ensemble average and obtain

$$\hat{C} = \text{tr}_{12}\{[\hat{p}_1, \hat{V}]\delta(\mathcal{L}_0)\hat{\rho} \{\hat{V}, \hat{p}_2\} \hat{\rho}\}$$

This is just the correlation as given in eq. (40). Thus we have shown that the $\delta \hat{K}$ of eq. (53) from stochastic TDHF yields the fluctuating force of the Boltzmann-Langevin equation.

### 4.4 On the interpretation of the stochastic force

The fluctuating force $\delta \hat{K}$ in the Boltzmann-Langevin equation comes a bit surprising for somebody who has become accustomed to the Boltzmann collision term as an appropriate extension of TDHF. Langevin forces are much better known from the typical example of Brownian motion where the observed stochastic jumps of the Brownian particle are explained by random forces from the heatbath [19]. The concept can easily be carried over to a quantal treatment of one relevant system in a heatbath of unobserved degrees-of-freedom; a typical application of this concept is the theory of the Laser [20]. It is shown in these considerations that the Langevin force always appears as the necessary complement of a damping force, and both emerge theoretically from a formal elimination of the degrees-of-freedom of the heatbath. The close relation between damping and Langevin force is expressed in the well known fluctuation-dissipation theorem [19] which provides a quantitative relation between the strength of the dissipation and the width of the fluctuations of the stochastic force.

A Boltzmann-Langevin approach, however for small fluctuations only, has been proposed times ago by Bixon and Zwanzig [12]. They start from the observation that the Boltzmann collision term acts in the same manner as a dissipating force (however, on
a huge number of relevant degrees-of-freedom and without absorbing energy), and they add the complementing Langevin force which now, of course, is a very complex matrix of forces. The Boltzmann-Langevin equation can be derived systematically in the various theoretical frameworks for nonequilibrium many-body theory, see e.g. the derivations using the density-matrix technique in ref. [8], or using the nonequilibrium Green's function techniques in ref. [21], or the derivation from stochastic TDHF given here.

The inconvenience with the Boltzmann-Langevin equation is that we do not see the origin of the random force as neatly as in the example of the Brownian particle. The reason is that we do not separate systems in relevant subsystem and heatbath. But we cut degrees-of-freedom in a many-body hierarchy. Considering one-body motion as the relevant degree-of-freedom whereas two-body and higher correlations are eliminated. That point-of-view seems to be clear from the derivations using hierarchies of density-matrices or Green's functions. This can also be understood in terms of the hierarchy of time scales we have discussed in section (3.1), namely the possibility of propagating the system over a time scale small as compared to the typical mean-field evolution but large as compared to the effects of residual interaction, which allows a statistical treatment. Note anyway that one could establish a more formal connection between these time scales and the numbers of degrees of freedom involved in the various scales of motion.

Stochastic TDHF adds some new and enlightening aspects to the Boltzmann-Langevin approach. It deals with ensembles of Slater states each one propagating in its own mean-field. This allows large fluctuations which are inevitably also large fluctuations of the mean field. The local ensemble in the Boltzmann-Langevin approach is identified with a subensemble of Slater states characterized by only small fluctuations about the given one-body density and corresponding mean field. There is now the possibility of a random choice of a particular member of the subensemble. This gives rise to a random force which is due to the small deviation of the mean-field of the chosen state from the average mean field. And this is just the Langevin force which is now nicely understood from the viewpoint of by stochastic TDHF.
5 Conclusion and outlook

We have presented stochastic TDHF as a theory for large amplitude collective motion which allows to account for large fluctuations of the mean-field. It builds up and propagates an ensemble of Slater states each one moving in its own mean-field. The unfolding of the ensemble in the course of time is achieved by the residual two-body interaction which generates transitions from one trajectory to another. The actual propagation of the ensemble is performed as a stochastic process where a certain path is chosen in each run by deciding in a Monte-Carlo fashion whether a transition is to take place or the old trajectory is to be continued. The full ensemble is built up by many repeated runs of the stochastic process.

We have derived the rules for the time-evolution of stochastic TDHF from TDHF plus correlations where the correlations are treated in second order perturbation theory. The evolution of the correlations is followed over a sufficiently large time interval. We take advantage of the fact that every many-body state, however correlated, can be represented as a coherent superposition of Slater states. It is assumed that the correlations spread over a very large number of degrees-of-freedom (i.e. neighbouring Slater states) such that phase relations between the many correlation channels occur at random and can be neglected. Thus after the end of the time interval, only the diagonal elements of the full density in a representation in terms of many Slater states are maintained; this corresponds to an incoherent summation over the various Slater states and the occupation weight of each state is determined by Fermis' golden rule for transitions caused by a weak residual interaction. Repeated application of this elementary step composes finally the ensemble of stochastic TDHF.

An alternative stochastic equation-of-motion for dissipative large amplitude collective motion is provided by the Boltzmann-Langevin equation. We have shown that one can derive the Boltzmann-Langevin approach from stochastic TDHF by subdividing the full ensemble into subensembles with only small fluctuations of the mean-field. These subensembles are the Stochastic TDHF analogon of the local ensembles of density ma-
trixes of the Boltzmann-Langevin approach. They are to represent a single member of the Boltzmann-Langevin ensemble of (heated) one-body densities. This derivation from stochastic TDHF gives some insight on the origin of the stochastic Langevin force: it can be understood as coming from the small deviation of the subensemble's mean-field from the mean-field for one particular (and randomly chosen) Slater state of the subensemble.

It is one of the advantages of stochastic TDHF that it provides a clear insight into the necessary conditions which ought to be fulfilled to validate the incoherent propagation. But this has also clarified that these conditions are probably hardly fulfilled in application to nuclear dynamics of heavy-ion reactions. In particular, the Markovian approximation is to be questioned which neglects all memory effects, i.e. the coupling of collective motion to the collision process.

The paper as it stands leaves many questions open for future investigations. The problem with the strong memory effects in nuclear physics might be solved by a combination of the coherent propagation of a few collective correlation channels according to TDGCM with the incoherent treatment of many and noncollective degrees-of-freedom according to stochastic TDHF. This is certainly manageable from a formal point-of-view. It remains to be seen whether one can work it down to a practicable approach.

It may be interesting to rederive stochastic TDHF and the Boltzmann-Langevin equation from even another formulation of many-body dynamics, from the path integral approach. This may give the opportunity to view the time-evolution globally and to all orders of the residual interaction. And it may thus provide new aspects for the coarse graining in time which is still inevitable in the present derivation.

Last but not least, it would be interesting to see how Stochastic TDHF performs compared to the Boltzmann-Langevin approach in a practical application. This will be a competition between larger ensembles with smaller members (only fully occupied states are required) in stochastic TDHF versus probably smaller ensembles with more involved members (heated one-body states) in the Boltzmann-Langevin approach.
A The detailed collision term

The compact form of the collision term in eq. (36) can be evaluated in detail using the instantaneous eigenbasis of $h$ as given in eq. (38). For then the $\delta(L_0)$ operator becomes a simple $\delta$-function of differences of the single-particle energies labelling the two-body operator on the right from $\delta(L_0)$, similar to eq. (37). Expressing all constituents of eq. (36) by matrix elements with respect to the basis (38), we obtain finally

$$\tilde{K}_{\nu\nu'} = \sum_{\alpha,\beta} \pi \delta (\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_\alpha' - \varepsilon_\beta')$$

$$\left\{ v_{\nu'\alpha'\beta'} \rho_{\alpha\gamma} \rho_{\beta\gamma} v_{\nu\alpha'\beta'} \delta_{\nu'\alpha'} - v_{\nu'\alpha'\beta'} \rho_{\alpha\gamma} \rho_{\beta\gamma} v_{\nu\alpha'\beta'} \delta_{\nu'\alpha'} - v_{\nu'\alpha'\beta'} \rho_{\alpha\gamma} \rho_{\beta\gamma} v_{\nu\alpha'\beta'} \delta_{\nu'\alpha'} + v_{\nu'\alpha'\beta'} \rho_{\alpha\gamma} \rho_{\beta\gamma} v_{\nu\alpha'\beta'} \delta_{\nu'\alpha'} \right\}$$

(64)

where $\rho_{\alpha\gamma} = \rho_{\alpha\beta} \rho_{\gamma\delta} - \rho_{\alpha\delta} \rho_{\gamma\beta}$ is the antisymmetrized product of the one-body densities.

This form of the collision integral has been derived from the time-dependent projector formalism [17]. It is a bit too general in the connection with the Markovian approximation. The assumption of slowly varying mean-field (24) is equivalent to the assumption of small nondiagonal components in the mean-field (25). We thus can assume that the mean-field Hamiltonian $h$ and the one-body density $\rho$ are simultaneously diagonal. The Hamiltonian has already been used in its diagonal representation. The density becomes

$$\rho_{\alpha\beta} = \delta_{\alpha\beta} n_\alpha , \quad \rho_{\alpha\beta} = \delta_{\alpha\beta} \bar{n}_\alpha$$

(65)

where $\bar{n}_\alpha = 1 - n_\alpha$. This allows to simplify the collision term to

$$\tilde{K}_{\nu\nu'} = \delta_{\nu\nu'} \sum_{\alpha,\delta} \pi \delta (\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_\alpha - \varepsilon_\beta) (\delta_{\nu\alpha} - \delta_{\nu\beta})$$

$$|v_{\alpha\beta\gamma\delta}|^2 (\bar{n}_\alpha \bar{n}_\beta n_\gamma n_\delta - n_\alpha n_\beta \bar{n}_\gamma \bar{n}_\delta)$$

(66)

It is this diagonal form of the collision term which has been employed in the Boltzmann-Langevin approach of refs. [8, 10]. And it has even been reduced in the local-collision approach where the single particle states are identified by their momentum and the single-particle energies $\varepsilon_\alpha$ are replaced by the local kinetic energies.
B Collision integral directly from transition rate

We start from the collision integral in the form (54). We insert the explicit definition of \( \rho_M \) in eq. (47) and write out the transition rate according to eq. (20). This yields

\[
\hat{K} = \sum_M W_M \sum_{M' \in 2ph-M} \frac{2\pi}{\hbar} \delta(E_M - E_{M'}) \langle M'|V_M|M \rangle \langle M|V_M|M' \rangle
\]

\[
\langle M'|\hat{\rho}|M' \rangle - \langle M|\hat{\rho}|M \rangle
\]

\[
= \sum_M W_M \sum_{M' \in 2ph-M} \frac{2\pi}{\hbar} \delta(E_M - E_{M'}) \text{Tr}\{VD_MVD_{M'}\hat{\rho}D_{M'} - VD_M\hat{\rho}D_MVD_M\}
\]

\[
= \sum_M W_M \sum_{M' \in 2ph-M} \frac{2\pi}{\hbar} \delta(E_M - E_{M'}) \text{Tr}\{\hat{\rho}D_MVD_{M'}VD_{M'} - \hat{\rho}D_{M'}VD_{M'}VD_M\}
\]

\[
= \sum_M W_M \sum_{M' \in 2ph-M} \frac{2\pi}{\hbar} \delta(E_M - E_{M'}) \text{Tr}\{D_{M'}\hat{\rho}D_{M'}VD_MVD_{M'} - D_{M}\hat{\rho}D_MVD_{M'}VD_{M'}\}
\]

where we have used \( |M \rangle \langle M'| = D_M \) as well as \( |M \rangle \langle M'| = D_{M'} \), the freedom of cyclic permutations in the trace Tr and the projector property of the density matrices \( D_M^2 = D_M \). The index \( M \) on \( V \) has been omitted to simplify notations.

The \( \hat{\rho} \) is a one-body operator and \( V \) is supposed to produce only 2ph-transitions from \( D_M \). Thus we can conclude to the following identities

\[
\sum \text{Tr}\{D_{M'}\hat{\rho}D_{M'}VD_MVD_{M'}\} = \sum \text{Tr}\{D_{M'}\hat{\rho}VD_{M'}VD_M\}
\]

\[
\sum \text{Tr}\{D_{M'}\hat{\rho}D_{M'}VD_MVD_{M'}\} = \sum \text{Tr}\{\hat{\rho}D_{M'}VD_MVD_{M'}\} = \sum \text{Tr}\{\hat{\rho}D_{M'}VD_{M'}VD_M\}
\]

\[
\sum \text{Tr}\{D_{M}\hat{\rho}D_{M}VD_{M'}VD_{M'}\} = \sum \text{Tr}\{D_{M}\hat{\rho}VD_{M}VD_{M'}\}
\]

\[
\sum \text{Tr}\{D_{M}\hat{\rho}D_{M}VD_{M'}VD_{M'}\} = \sum \text{Tr}\{\hat{\rho}D_{M}VD_{M}VD_{M'}\} = \sum \text{Tr}\{\hat{\rho}D_{M}VD_{M}\}
\]

where \( \sum = \sum_{M' \in 2ph-M} \). We see that the traces can be simplified in two equivalent ways. This is due to the diagonal approximation (25) for the mean-field. Both ways would lead to the same (diagonal) collision term, see eq. (66). We obtain the most symmetric expression if we resolve the trace in a symmetric manner, half the one simplification and half the other. This yields

\[
\hat{K} = \sum_M W_M \sum_{M' \in 2ph-M} \frac{\pi}{\hbar} \delta(E_M - E_{M'})
\]
\[ \text{Tr}\{\hat{\rho}_{D_{M'}}V_{D_{M}}V + D_{M'}\hat{\rho}_{V}D_{M}V - \hat{\rho}_{D_{M}}V_{D_{M'}}V - D_{M}\hat{\rho}_{V}D_{M'}V\} \]

\[ = \sum_{M} W_{M} \sum_{M' \in 2ph - M} \frac{\pi}{\hbar} \delta(E_{M} - E_{M'}) \text{Tr}\{[\hat{\rho}, V](D_{M}V_{D_{M'}} - D_{M'}V_{D_{M}})\} \]

We now want to evaluate the energy matching \(\delta(E_{M} - E_{M'})\). We aim at a final expression in the compact form of eq. (36). Therefore we implement the energies using the mean-field Liouvillian \(L_{0}\) as defined in eq. (37). We exploit the feature

\[ L_{0}D_{M}V_{D_{M'}} = (E_{M} - E_{M'})D_{M}V_{D_{M'}} \]

which is justified if we neglect the difference between \(h_{M}\) and \(h_{M'}\). This finally yields the eq. (57),

\[ \dot{K} = \sum_{M} W_{M} \sum_{M' \in 2ph - M} \frac{\pi}{\hbar} \text{Tr}\{[\hat{\rho}, V]\delta(L_{0})(D_{M}V_{D_{M'}} - D_{M'}V_{D_{M}})\} \]
References


