Towards a nonequilibrium Green’s function description of nuclear reactions

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Abstract. Semiclassical time-dependent approaches are nowadays able to describe energetic central collisions of heavy isotopes with minimal assumptions. Simulations in the mean-field picture have provided insight on both nuclear structure and low-energy many-body reaction mechanisms. In this context, nonequilibrium Greens functions techniques have the potential to improve the description of the time evolution of nuclear systems by introducing effects beyond the mean-field. We describe a first attempt to use the Kadanoff-Baym dynamics for one-dimensional nuclear systems, with a particular emphasis on the process of correlation build-up.

1. Introduction

Nonequilibrium Green’s function (NGF) techniques [1, 2, 3, 4] represent a powerful tool to describe the evolution of correlated quantum many-body systems. The study of the Kadanoff-Baym (KB) dynamics in different quantum many-body systems is an on-going challenge for theorists. The first direct implementations of NGF in homogeneous nuclear systems saw light almost 30 years ago [2]. Posterior advances include, among others, the extension to homogeneous electronic systems [5], small atoms [6] and molecules [7], quantum dots [8] and, more recently, the study of double excitations [9, 10]. Within nuclear physics, NGF techniques have been mostly used for derivations rather than exploited directly [11, 12, 4]. With so few quantitative studies on the impact of correlations in the time evolution of nuclear systems, one might wonder whether nuclear reactions simulations based on the mean-field picture or on semiclassical approaches are valid at all. To clarify these issues, we would like to develop nuclear reaction simulations beyond the Hartree-Fock approximation. Green’s functions out of equilibrium, as described by the two-time Kadanoff-Baym approach, are an ideal tool for this purpose.

Our interest on the many-body aspects of nuclear dynamics ties well with the recent advances in nuclear structure theory. Effective field theories based on the chiral expansion together with renormalization techniques have provided access to perturbative QCD-inspired nuclear interactions [13]. As a direct consequence, first principles many-body calculations of medium-mass and heavy nuclei are becoming possible. These are based on a variety of methods, from coupled cluster [14] to equilibrium Green’s function techniques [15]. The extension of similar \textit{ab initio} methods to the realm of central nuclear collisions is an exciting prospect, as these have been mostly studied within phenomenological approaches.
On a more general scale, the advancement of dynamical quantum many-body methods is necessary for our understanding of systems that range from ultracold atoms [16] to nuclei [17] or atoms [6]. Simulations with NGF techniques can provide a systematic understanding of correlation effects via conserving approximations [18]. Moreover, different approximations may account for the effects of different types of correlations. The description, however, remains of a single-particle type and other many-body effects are averaged out. Not surprisingly, in the semiclassical limit the KB equations yield the Boltzmann equation (BE). In the few body limit, KB dynamics seem to run into some trouble, possibly associated to the small number of degrees of freedom [19].

Historically, just a handful of methods have been developed to describe central nuclear reactions. Few of these are general enough to be employed in generating practical predictions. The time-dependent Hartree-Fock (TDHF) method has been exhaustively employed in describing low-energy reactions [20]. Nowadays, TDHF simulations can be performed in full 3D and involve nuclei as heavy as uranium [21]. However, the validity of TDHF requires correlations to play a negligible role in the dynamics [12]. At low energies, one might argue that the role of correlations is minimized by antisymmetrization. Conversely, one would expect correlations to dominate at higher energies, where the Pauli principle weakens.

In the semiclassical limit, the two-time Kadanoff-Baym (KB) equations reduce to a single-time, Boltzmann equation (BE). The BE has been extensively used to analyze reactions at intermediate and high-energies [22, 23]. This approach deals with the increasing complexity of the reaction by using simplifying assumptions on an average, single-particle level. Because of their semiclassical nature, however, these descriptions have remained genuinely disconnected from the quantum methods employed for nuclear structure. More importantly, there is no systematic way of improving upon the BE-type approaches.

Correlations can lead to a fast thermalization of the occupation of single-particle states and to enhanced stopping, compared to what can be found in TDHF [24, 25, 26]. Similarly, quantum effects may dominate in high-density regions and thus affect reaction observables. Specifically aiming at increasing incident energies, it is therefore important to develop a quantal approach to central nuclear reactions that, besides the mean-field effects, can also incorporate correlations. The NGF approach that we try to develop can also remove some of the serious limitations of both TDHF and the BE. Unfortunately, even at the single-particle level, NGF techniques require handling vast amounts of information that can easily overwhelm the capabilities of computing systems, rendering this approach impractical.

Here we summarise our first attempts to implement NGF’s to idealised, one-dimensional (1D) nuclear systems. The study of 1D nuclear systems (nuclear slabs) is academic, but offers an initial benchmark for ideas involved in the time evolution. Furthermore, 1D calculations provide simple and clear visualisations. First, we describe the application of mean-field dynamics in the context of nuclear collisions. In this case, the use of Green’s functions techniques illustrates the importance of off-diagonal matrix elements in the space representation for the dynamics of central nuclear collisions. Further, we explore 1D simulations of the time evolution of correlated systems within the second order Born approximation.

2. Kadanoff-Baym equations
We describe the dynamics of correlated nuclear systems using the KB equations. Within this approach, the time evolution can incorporate different levels of correlations. For certain intrinsically-consistent many-body approximations to the self-energy, one can show that the time evolution induced by the self-consistent KB equations preserves the conservation laws obeyed by the system as a whole [18, 2]. We will use both the mean-field approximation and the second-order, direct Born approximation, which do preserve conservation laws.

The KB equations are nominally derived without any particular assumption on the physical
The expectation values, \( \langle \cdot \rangle \equiv \langle \cdot \rangle_t \), at different times. Those containing single-particle information are related to the expectation values of products of two single-particle annihilation and creation operators at different time arguments,

\[
G^<(x_1, t_1; x_2, t_2) = i \langle \hat{a}^\dagger(x_2, t_2) \hat{a}(x_1, t_1) \rangle, \quad (1)
\]

\[
G^>(x_1, t_1; x_2, t_2) = -i \langle \hat{a}(x_1, t_1) \hat{a}^\dagger(x_2, t_2) \rangle. \quad (2)
\]

The expectation values, \( \langle \cdot \rangle \equiv \Tr \{ \hat{\rho}_i \cdot \} \), are taken with respect to an initial density matrix, \( \hat{\rho}_i \), at \( t = t_0 \). We consider initial uncorrelated states, even though the theory can incorporate correlations in the initial state [2].

The KB equations for 1D systems, governing the evolution of Green’s functions in their arguments,

\[
\left\{ \frac{i\hbar}{\partial t_1} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} \right\} G^\Sigma(11') = \int dx_1 \Sigma_{HF}(11) G^\Sigma(11'),
\]

\[+ \int_{t_1}^{t_1'} \partial t_1' \Sigma^+(11) G^\Sigma(11') + \int_{t_0}^{t_1} dt \Sigma^<(11) G^-(11'), \]

\[
\left\{ -i\hbar \frac{\partial}{\partial t_1'} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1'^2} \right\} G^\Sigma(11') = \int dx_1 G^\Sigma(11) \Sigma_{HF}(11'),
\]

\[+ \int_{t_0}^{t_1'} dt \Sigma^+(11) G^\Sigma(11') + \int_{t_0}^{t_1} dt \Sigma^<(11) G^<(11'), \]

follow from considerations of the equations of motion for creation and destruction operators [1]. The simplified notation \( 1 = (x_1, t_1) \) has been introduced. The retarded (+) and advanced (-) functions are defined according to \( F^\pm(1, 2) = F^\Sigma(1, 2) \pm \Theta [\pm(t_1 - t_2)] [F^> (1, 2) - F^<(1, 2)] \), with \( F^\Sigma \) standing for a possible singular contribution at \( t_1 = t_2 \). The generalized self-energy \( \Sigma(1, 2) \) introduces interaction effects on the time evolution and also describes excitation processes within the system [1, 2].

The self-energy in the previous equations has been separated into two different components. The first one involves the Hartree-Fock (HF) contribution, \( \Sigma_{HF}(1, 2) \), which accounts for the instantaneous, one-body interaction of the considered particle with the mean-field produced by the other particles of the system. The term involving \( \Sigma^\Sigma \) describes time-dependent excitation processes, beyond the mean-field changes. Such terms account for the effect of correlations on the time evolution and need to be included for a complete description of nuclear reactions.

1D calculations are rather economical in terms of CPU and storage. Let us consider the difficulties associated to storing density matrices (or Green’s functions) in \( D \) dimensions without explicit spin or isospin degrees of freedom. A uniform mesh of size \( N_x \) in each direction will yield matrices of size \( N_x^{2D} \). Fairly sparse meshes with \( N_x \sim 10 \) are already computationally demanding at present. For 1D this is not an issue and we will present results with \( N_x \sim 100 \), that can be carried out straightforwardly. In addition to spatial variables, NGF requires a suitable infrastructure to keep track of the time degree of freedom, as memory effects come into play. From Eq. (3), one can easily see that the time derivative of the Green’s function \( G^< \) at times \( t_1 \) and \( t_1' \) depends on the Green’s functions and self-energies at all the previous times \( t \), \( t_0 < t < t_1 \) and \( t_0 < t < t_1' \), via the time integrals on the r.h.s. Consequently, to find a solution of the KB equations, one must keep track of all the previous time-steps. For a uniform mesh of \( N_t \) points in time, the \( G^\Sigma \) functions thus require handling \( N_x^{2D} \times N_t^2 \) matrices. For \( D > 1 \), this becomes a major concern in the numerical implementation of the KB equations [27].

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3. Mean-field approximation

The KB equations simplify substantially when the correlation effects, described in terms of $\Sigma^\lessgtr$, are neglected. In that case, the evolution equations for $G^<\lessgtr$ and $G^>\lessgtr$ can be decoupled. Since the single-particle observables are more straightforwardly expressed in terms of $G^<$, we concentrate on the evolution of the latter. Thanks to the instantaneous nature of $\Sigma_{HF}$, the set of equations for the time-diagonal elements of the Wightman function, $t_1 = t_{1'},$ can also be closed and there is no need to consider explicitly time off-diagonal terms. Note, in particular, that this reduces the dimensionality of the problem to $N^2_2$, as one can update $G^<$ at every time step and there is no need to keep explicit track of expectation values involving the past.

The evolution equations simplify even more when assuming a negligible range for the nucleon-nucleon interactions. In that case, the evolution equation becomes:

$$i\hbar \frac{\partial}{\partial t} G^<(x_1, x_{1'}; t) = -\frac{\hbar^2}{2m} \left\{ \frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_{1'}^2} \right\} + U(x_1, t) - U(x_{1'}, t) \right] G^<(x_1, x_{1'}; t), \quad (5)$$

This can easily be linked to TDHF by expanding the Wightman functions in terms of single-particle states [17]. For the same initial state and mean-field parametrization, both approaches yield identical dynamics. Our goal here is not so much to provide an accurate description of 1D nuclear mean-field dynamics, but rather to explore its implementation in terms of Green’s functions.

In the following, we shall assume a spin-isospin saturated system and thus suppress the (degenerate) spin and isospin indices. In the strict 1D interpretation of the 1D calculations, the density of nucleons is $n(x, t) = \nu \rho(x, x; t)$, where $\nu = 4$ represents the spin-isospin degeneracy of the system, and the nucleon number is $A = \nu N_s$. $N_s$ is the number of shells filled in the calculation. One can connect this 1D interpretation to 3D calculations by assuming that matter is uniform in the $y$ and $z$ directions. With this, the density in the 3D interpretation, becomes proportional to the 1D density, $n(x, t) = \xi n_1(x, t)$, so with $\xi = \sqrt{\frac{3}{4}} \left( \frac{\pi n_d^2}{\nu^4} \right)^{1/3}$ [17]. The advantage of developing a 3D interpretation is that it allows one to employ well-known 3D mean-field parameterizations for 1D calculations. We choose a simple nuclear mean-field parametrization for our calculations,

$$U(t) = \frac{3}{4} t_0 n(x, t) + \frac{2 + \sigma}{16} t_3 [n(x, t)]^{1+\sigma}, \quad (6)$$

with the parameters fitted to the saturation properties of nuclear matter [17]. For such a local mean-field, the time evolution of the density matrix can be implemented numerically in a rather straightforward way using the Split Operator Method (SOM) [17, 28]. This involves a continuous switching between configuration space and momentum space which is optimally accomplished using Fast Fourier Transforms (FFT) [28]. In practical terms, we use an implementation of the SOM involving a uniform mesh in the spatial dimension, with periodic boundary conditions at the edges.

3.1. Preparation of the initial state

Before discussing the dynamics at the mean-field level, we will comment on the construction of initial states. The initial state for a reaction (or any other dynamical process) should be a ground state within the same approximation scheme as used in the dynamics. This guarantees that observables for the ground state should do not change with time. One way of preparing the initial system in a consistent manner is through an imaginary-time evolution [11, 4], employing analogous approximations for the self-energy within the imaginary- and real-time domains. Naturally, it may be worthwhile to explore alternative ways of preparing the initial state. If we
restrict ourselves, for practical purposes, to dynamics in the real time, an obvious choice is that of an adiabatic switching.

At time \( t \to -\infty \), the system may be assumed to represent the ground state for a known (or solvable) external potential, \( U_0 \). Here we will limit ourselves to a 1D Harmonic Oscillator (HO), which yields a relatively good starting point for nuclear physics purposes \[29\]. Provided that the interaction is switched on slowly enough while the external HO is steadily eliminated, the system may be evolved to the interacting ground state \[30\]. In the absence of level crossings or phase transitions, the procedure should be generally valid. We show in the following examples of this at the Hartree-Fock level. Further, we will present preliminary calculations of analogous results within the two-time dynamics at the direct Born approximation.

With the adiabatic switching, the single-particle potential acquires an explicit time dependence, and we adopt

\[
U_t = F(t - \tau_0) U_0 + [1 - F(t - \tau_0)] U ,
\]

where \( U \) is our mean-field parametrization and \( U_0 = \frac{1}{2} m \Omega^2 x^2 \) is the precursor HO potential. \( \Omega \) can be chosen to minimize the evolution of geometric characteristics foes nuclear slabs \[17\]. The switching function \( F \) above is equal to 1 at some initial argument \( t_i (\leq 0) \) and to 0 at some final argument \( t_f (\geq 0) \) when the switching over is completed. This switching function is constructed in terms of a monotonically decreasing function \( f \),

\[
F(t) = \frac{f(t) - f(t_f)}{f(t_i) - f(t_f)},
\]

for the argument values \( t_i \leq t \leq t_f \). In the switching function for Eq. (7), we have most often employed

\[
f(t) = \frac{1}{1 + e^{t/\tau}}
\]

within Eq. (8). Here, \( \tau \) represents a transition time that, for the sake of adiabaticity of the切换, should be longer than any characteristic time of the system. Notably, whenever \( f(t_i) \simeq 1 \) and \( f(t_f) \simeq 0 \), such as for \( |t_i, f| \gg \tau \) in the case of (9), then the two functions \( f \) and \( F \) practically coincide,

\[
F(t) \simeq f(t).
\]

Slower adiabatic switchings should provide better approximations to the mean-field ground states. In the top panel of Fig. 1, we show the evolution of the energy per nucleon for a HO slab initiated at time \( t = -1000 \text{ fm}/c \). We concentrate on a single case, with \( N_s = 2 \) HO shells filled (i.e. \( A = 8 \) nucleons in the 1D interpretation). We consider different transition times, \( \tau \), that characterise the adiabaticity of the transition. For any of the employed transition times \( \tau \geq 5 \text{ fm}/c \), the energy evolves to a value very close to that for the static Hartree-Fock solution (see inset). Judging the quality of the adiabatic transition on the basis of the energy alone is potentially treacherous, though, as the energy is quadratic in the deviation of wave function from the ground state. In principle, final states for the adiabatic evolution might be found, with a wavefunction poorly approximating that of the mean-field ground-state, but giving an energy close to the ground-state value.

Alternatively, the total density, \( n \), is linear in the deviation of the wavefunction from the ground-state, so it may provide a better measure of the wavefunction quality. With this in mind, in the bottom panel of Fig. 1, we show the evolution of the size of the slab, defined as twice its average extent in 1D. Indeed, for \( \tau = 5 \) and \( 10 \text{ fm}/c \), slab sizes exhibit significant
Figure 1. Time evolution of the energy per particle (upper panel) and the size of the slab (lower panel) when adiabatically switching from a starting HO configuration to a final mean-field state. Different values of the transition time $\tau$ are considered. The inset in the top panel shows a magnified portion of the time evolution of the energy. For reference, mean-field results from static Hartree-Fock solutions are shown as straight solid lines.

oscillations in the final state, indicating that the ground state has not been yet satisfactorily reached. Instead, the final state in the dynamics is an excited state of the final hamiltonian and thus fluctuates over time. For $\tau \gtrsim 30 \text{ fm/c}$, the oscillations become insignificant, with the slab sizes practically coinciding with that of the static Hartree-Fock solution.

In a nuclear reaction, the construction of the initial state involves two steps. First, the ground state of the two reacting systems has to be built. Second, the two initial states have to be boosted so as to collide with each other. The boost can be accomplished through a simple multiplication by momentum phase factors [31]:

$$G^<_{1}(x_1, x_1') = e^{ipx_1/h} G^<_{0}(x_1, x_1') e^{-ipx_{1'}/h},$$  \hspace{1cm} (11)

where $G^<_{1}$ corresponds to a moving slab at momentum per nucleon $P$, while $G^<_{0}$ is that of an idle slab. As a consequence of the boost, the kinetic energy for the slab increases by the amount $\Delta K/A = P^2/2m$. The net Wightman function of the colliding system is constructed as a sum of functions for two countermoving slabs, $G^<_{1}(x_1, x_1') = G^<_{1}(x_1, x_1') + G^>_{2}(x_1, x_1')$. We will here concentrate on symmetric collisions, with the second slab being a symmetric reflection of the first. Our conclusions, however, are general and broadly valid also for asymmetric reaction.

3.2. Collisions of slabs

The relatively simple 1D model of nuclear collisions discussed here demonstrates a surprisingly rich range of phenomena [32, 33, 17]. Qualitatively different physical processes are observed within the model when changing the center-of-mass (CM) energy for the reactions. At low
collision energies \(E_{CM}/A \sim 0.1 - 0.5 \text{ MeV}\), the nuclear slabs fuse into one compound slab that remains excited for long times. For intermediate energies \(E_{CM}/A \sim 0.5 - 15 \text{ MeV}\), a fusion process is observed, followed by a break-up into a number of smaller slabs. Higher reaction energies \(E_{CM}/A > 15 \text{ MeV}\) yield a pile-up of density at the system center, followed by a violent break-up phase with the formation of a low-density neck. The process is reminiscent of multifragmentation in nuclear reactions.

We will not explore this wide phenomenology here, but rather focus on one specific case that will highlight the importance of space off-diagonal matrix elements in \(G^<\) specifically. Let us concentrate on the collision energy range immediately above fusion reactions. When the two colliding slabs fuse, the compound system is too excited in energy to remain bound and the system undergoes a fission process into three fragments. Because of the symmetry of this specific collision, the final state is formed by a central fragment and two outgoing, symmetric slabs. Figure 2 provides the snapshots for the time evolution of one such collision at \(E_{CM}/A = 4 \text{ MeV}\). Following the fusion of the original slabs at \(t \sim 50 \text{ fm/c}\), two density peaks form at the edges of the compound system and subsequently emerge from the central region to opposite sides. The central region eventually recontracts and oscillates, as it is a highly excited state of an \(A \sim 8\) system. The \(A \sim 4\) fragments remain excited too, as evidenced in the small changes with time of their central density.

3.3. Off-diagonal structure of the density matrix

At equal arguments in a specific representation, the function \(-iG^<\) of Eq. (1) yields the single-particle density in that representation. At different arguments, the off-diagonal matrix elements reflect existing correlations between magnitudes and phases of single-particle wavefunctions. As we have discussed earlier, the task of following all the elements in 3D is likely to overwhelm present computer storage capabilities. Nevertheless, the quantities of most direct physical interest, including densities, tend to be associated with either diagonal values of the functions or values close to the diagonal [1]. In the specific physical cases where the matrix elements that lie sufficiently far from the diagonal can be ignored, NGF calculations would become possible.
Figure 3. Intensity plots representing the real (upper panels) and the imaginary part (lower panels) of the scaled density matrix, $\xi \nu \rho(x, x'; t)$, for a collision at $E_{CM}/A = 4 \text{ MeV}$.

due to a drastic reduction in dimensionality. We argue that central nuclear reactions are good examples of this, as the late stages involve limited phase coherence between different elements.

To examine and quantify the importance of elements far from the diagonal in space representation, let us explore the off-diagonal structure of $-iG^<$ in the same reaction presented in Fig. 2. The upper (lower) panels of Fig. 3 show intensity plots for the imaginary (real) parts of $G^<(x, t; x', t')$ for three different times in the reaction, chosen to represent the initial, overlap and late instants. The diagonal of the upper panels, $x = x'$, coincide with the density profiles displayed in Fig. 2. To understand off-diagonal structures, it is useful to think of the expansion of the Wightman function in terms of natural orbitals,

$$-iG^<(x_1, t_1; x_{1'}, t_{1'}) = \sum_\alpha n_\alpha \phi_\alpha(x_1, t_1) \phi^*_\alpha(x_{1'}, t_{1'}). \quad (12)$$

The wavefunctions of the initial slabs are confined to within the size of the slab and, consequently, $-iG^<$ will have a limited, square support in the $(x, x')$ plane. The left panels of Fig. 3 show this confinement around the two initial slabs. Changes in sign as one moves away from the diagonal are attributable to the boost factors.

At this collision energy, once the compound slab is formed (central panel), it remains in contact for a too short time for the single-particle orbitals to spread out evenly over the size of the compound system. In consequence, the square-like support for the density matrix of the compound system is only approximate. The two outgoing fragments and the central compound system are clearly identified as blobs near the diagonal, $x = x'$. In addition, cross-correlations develop between individual fragments, as signaled by the patches of significant values of the density matrix far away from the $x = x'$ diagonal. As an example, the structures at $x \sim 0$ and $x' \sim 15 \text{ fm}$ for $t = 200 \text{ fm}/c$ in Fig. 3, both for the real and imaginary parts of the matrix, signal the overlap of single-particle states between the central and the outgoing fragments.

The discussed correlation patches may be understood in terms of the fragmentation of natural orbitals. Orbitals can have components in each fragment rather than being split among them. Consequently, if the two fragments are in positions $x_1$ and $x_2$, when taking the product in Eq. (12) one will find non-zero elements of $G^<$ around $(x_1, x_2)$. Physically, this is a reflection of
the fact that, during the breakup, the nucleons from the original orbitals have finite probabilities of ending up in different fragments. The amplitudes for those possibilities maintain a phase relationship leading to correlations in the density matrix. The entanglement of the internal wavefunctions is thus the sole reason for the persistence of the far-away off-diagonal patches in the density matrix. The real and imaginary parts for those structures are comparable in magnitude, see Fig. 3. This points to the involvement of significant relative phases, as expected from the significant difference in momentum and position. Note that these entanglement correlations persist for fragments that are 30 fm apart for the $t = 200 \text{ fm}/c$ panels of Fig. 3.

Physics beyond the mean-field dynamics (short-range correlations, particle and gamma decays, etc.) are likely to introduce additional decoherence between the separating fragments, beyond that stemming only from different mean-field orbitals. Correspondingly, higher values for the off-diagonal elements are likely to persist more in a mean-field approach than in any simulation with correlations. As a corollary, if one finds out that the far off-diagonal elements may be disregarded within the mean-field dynamics, then it should be even more possible to disregard such elements in more realistic approaches.

We have quantified the importance of off-diagonal matrix elements using two different methods. First, we have employed an ad hoc procedure based on super-operators that eliminate off-diagonal elements in the time evolution [17]. Fig. 4 sketches the spatial structure of the super-operator. White areas, beyond $|x - x'| > x_0 + d_0$, are artificially eliminated at each time step. The remaining blue (grey) areas are left unaffected. Note that the structure is chosen to preserve the periodicity in $(x, x')$ space. Fixing $d_0 = 2 \text{ fm}$, one can progressively eliminate more and more off-diagonal matrix elements by decreasing $x_0$. For the break-up reaction explored here, the results of this procedure are shown in Fig. 5. Neither the total energy nor its kinetic or potential components (upper panel) seem to be affected by these cuts. The extent of the system, presented in the bottom panel, is also unaffected, pointing towards a good average description of the density distribution in the system. Overall, the elimination procedure we have devised indicates that off-diagonal elements play a very small feedback effect on the dynamics.

The off-diagonal suppression procedure we have just presented, though, does not directly

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**Figure 4.** The elimination procedure of off-diagonal elements in terms of superoperators eliminates off-diagonal elements in the white region, $|x - x'| > x_0 + d_0$.

**Figure 5.** Time evolution of the energy per particle (upper panel) and of the system extent (lower panel) in a collision at $E_{CM}/A = 4 \text{ MeV}$ for different values of the cutoff parameter $x_0$ at fixed $d_0 = 2 \text{ fm}$. 
involves any substantial savings in terms of storage or CPU time. The most substantial savings can be achieved by using an alternative spatial discretization scheme in a rotated coordinate frame. This rotation is the computational equivalent of a switch to Wigner space. With this, one could control the sparseness and lengths of the mesh in the relative coordinate while keeping the average (physical) direction unaffected. Our preliminary calculations indicate that this implementation reproduces well the original dynamics while simultaneously reducing substantially the total numerical effort.

4. Two-time Kadanoff-Baym evolution

We turn now our attention to beyond mean-field dynamics as obtained from the Kadanoff-Baym dynamics. We use the second order approximation in the propagator expansion. The so-called direct Born self-energy in momentum space reads:

\[
\Sigma^S(p, t; p', t') = \int \frac{dp_1 dp_2}{2\pi} V(p - p_1) V(p' - p_2) G^S(p_1, t; p_2, t') \Pi^S(p - p_1; t; p' - p_2, t')
\]  \hspace{1cm} (13)

\[
\Pi^S(p, t; p', t') = \int \frac{dp_1 dp_2}{2\pi} G^S(p_1, t; p_2, t') G^S(p_2 - p', t'; p_1 - p, t)
\]  \hspace{1cm} (14)

In this exploratory study, we have not included the exchange term despite the fact that it may induce significant effects. As it is common in nuclear physics, we use two different interactions for the mean-field self-energy and the Born term. The Hartree-Fock self-energy of Eq. (6) has a zero-range as well as a density dependence that effectively accounts for three-body correlations. The attractive component of the mean-field provides stability. The Born term requires a finite range interaction and we choose the (time-independent) form:

\[
V(p) = V_0 \sqrt{\pi \eta^2} p^2 e^{-\frac{\pi^2 \eta^2}{4}}
\]  \hspace{1cm} (15)

with \( V_0 = 40 \) MeV and \( \eta = 3 \) fm. In coordinate space representation, this interaction qualitatively reproduces the characteristic short-range repulsion and long-range attraction of the nucleon-nucleon interaction. Note that the \( p^2 \) dependence at low momenta is necessary to avoid divergences in the 1D scattering cross section.

The solution of the KB equations, Eqs. (3) and (4), is a computationally demanding task in the two-time plane [27], all the more so for inhomogeneous systems [6]. We advance the solution of these following the algorithms presented in Ref. [34]. In analogy to the mean-field case, we use Fast-Fourier transforms to switch from real to momentum space thus allowing for quick phase-factor multiplications and calculation of convolution integrals. At each time step, we demand self-consistency of the density before we proceed further on in time. Results presented here correspond to a mesh of \( N_x = 40 \) points with \( N_t = 150 \) time-steps.

In analogy to the mean-field case, we want to explore the potential of adiabatic switching to build initially correlated ground states. To that end, we follow a two-step process. First, we build a mean-field ground state using the same adiabatic switching, from a HO to a mean-field ground state, described in Sec. 3.1. Further, we turn on adiabatically the Born self-energy. Because of the two-time nature of the time propagation, the adiabatic switch-on should also develop a two-time structure. The origin of this double time dependence can be found in Eq. (13), which can be formulated also for time-dependent interactions. Replacing the time independent interaction, \( V(p) \), by the adiabatically evolving one, \( \tilde{V}(p, t) = (1 - F(t)) V(p) \), the self-energy becomes directly proportional to the product \( (1 - F(t)) \times (1 - F(t')) \). The adiabatically switched-on self-energies, however, feed back to the propagator via the KB evolution and are also sensitive to associated memory effects. Consequently, the time dependence of the self-energy can be more complex than that given by the product of adiabatic factors as time proceeds.
Fig. 6 shows preliminary results for the correlated adiabatic switching on for a slab with \( N_s = 4 \), *i.e.* \( A = 16 \) in the 1D interpretation. The upper panel shows the total energy of the system. The switch-on provides an attractive contribution to the energy of the order of \( \sim 1 \text{ MeV} \). Note that, due to numerical limitations in this preliminary implementation, we have had to restrict the time evolution to relatively short timescales. As a direct consequence, the range of adiabatic switchings is also restricted. The final energy that is reached as \( \tau \) increases does change for all the values of \( \tau \) explored in the figure, which suggests that we have not yet reached adiabatically the ground state of the final system. With correlations, however, the switching needs to be slow compared to characteristic correlation times [35]. The success of the switching procedure should be judged again with the degree to which the final state is stationary.

The lower panel of Fig. 6 focuses on the time evolution of the slab’s size in the adiabatic evolution. When correlations are turned on, the slab swells in size. With the present time extent, we can only resolve an initial oscillation in slab size. A rapid damping of this oscillation is expected as \( \tau \) increases and the evolution becomes more and more adiabatic. Naively, one expects the final state obtained in these dynamical calculations to be the same as the equivalent ground state obtained in imaginary time. We plan to carry on a detailed analytical and numerical comparison in the near future.

Note that, by introducing correlations in the dynamics, the occupation probabilities of the single-particle states, \( n_\alpha \), gradually move away from a Fermi step function to a correlated shape. Net energy is gained at the cost of populating states with higher single-particle energies. The redistribution of the state populations provides damping mechanisms in nuclear reactions. Their microscopic description is one of the major goals of our long term project.

5. Conclusions
The mean-field time evolution provides a first qualitative guidance on the dynamics of nuclear slabs. In terms of numerical implementation, it has allowed us to develop an understanding of initial state dynamics through adiabatic switching. This procedure provides good results
when implemented with standard TDHF codes. At the mean-field level, the implementation of the dynamics within the NGF theory introduces a double-argument description of the system. Correlations between spatial off-diagonal elements are generated in a nuclear collision whenever single-particle orbitals can be spread across different fragments (or, in the case of multifragmentation, among the whole system).

We have also developed the tools to simulate correlated dynamics by implementing the KB equations numerically. In this first, preliminary study, we have explored the potential of these techniques to yield correlated ground states. To this aim, we have performed an adiabatic switching of the Born self-energy on top of Hartree-Fock results. These indicate that relatively large timescales are needed for the system to thermalize. Such long times are as of now inaccessible due to numerical limitations. The hope is that these limitations can be overcome in the near future by further optimization and parallelization of our numerical codes.

In spite of their considerable general potential in describing quantal time-dependent systems, NGF techniques have been, so far, underutilized in nuclear physics. Specific potential applications within nuclear physics include the description of large-amplitude collective motion and of central nuclear collisions. The techniques could yield a seamless description for nuclear structure [36]. Quite more generally, a more thorough understanding of the interplay between spatial dynamics, temporal evolution and beyond mean-field correlations in quantum many-body systems is a challenging prospect. The overall consistent picture provided by NGF’s seems to be the best candidate to address these issues rigorously.

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