The emergence of collective behaviors as well as the existence of large amplitude motions are both central features in the fields of nuclear structure and reactions. From a theoretical point of view, describing such phenomena requires increasing the complexity of the many-body wavefunction of the system, to account for long-range correlations. One of the challenge when going in this direction is to keep the approach tractable within our current computational resources while gaining the maximum of predictive power for the phenomenon under study. In the Generator Coordinate Method (GCM), the many-body wave function is a linear superposition of (generally non-orthogonal) many-body states (the generator states) labeled by a few collective coordinates. Such a method has been widely used in structure studies to restore the symmetries broken by single-reference approaches. In the domain of reactions, its time-dependent version (TDGCM) has been developed and applied to predict the dynamics of heavy-ion collisions or fission where the collective fluctuations play an essential role. In this review, we present the recent developments and applications of the TDGCM in the context of nuclear reactions. We recall the formal derivations of the TDGCM and its most common approximate treatment, the Gaussian Overlap Approximation. We also emphasize the Schrödinger Collective-Intrinsic Model (SCIM) variant focused on the inclusion of quasiparticle excitations into the description. Finally, we highlight several exploratory studies related to a TDGCM built on time dependent generator states.

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I. INTRODUCTION

Since the early days of nuclear physics, the variety of shapes that atomic nuclei can take is a core notion of our interpretation of nuclear processes. The fission reaction provides a typical example as it was quickly interpreted as the elongation of a charged liquid drop of nuclear matter, leading to a scission point [1]. Descriptions in terms of vibrations and rotations of the nuclear shape also lead to quantitative reproductions of the low energy spectra [2] of atomic nuclei. These successes of the theory suggest that the shape of the nuclear density is somehow a relevant degree of freedom (DoF) to describe several phenomena. In addition to the classical picture of the time evolution of a well defined nuclear shape, taking into account its associated quantum fluctuation is of particular importance. For instance, these fluctuations directly drive the width of the probability distribution of particles transferred during low energy heavy-ion collisions, as well as the modal characteristics of the fragment distribution produced by fission. The incorporation of these fluctuations into a quantum description leads to a many-body wave function describing the system that is a mixture of states with different shapes. With this intuition, one may attempt a direct description of nuclei in terms of shape DoFs. However, transforming the $3A$ positions and $A$ spins of the nucleons into a new system of coordinates involving a set of deformations parameters is both cumbersome and problem-dependent [3, 4]. Another possibility consists in keeping the nucleons coordinates and build an ad-hoc quantum mixture of many-body states with different relevant shapes. This is precisely the starting point of the Generator Coordinate Method (GCM).

The GCM method was first developed in the seminal papers of Hill and Wheeler in the context of nuclear fission in 1953 [5], and later on generalized in Ref. [6]. The global philosophy is (i) to generate a set of many-body states parameterized by a set of shape variables (the generator states), (ii) to derive an equation of motion for the many-body wave function of the system in the restricted Hilbert space spanned by the generator states. At first, this method used to introduce shape degrees of freedom, such as the multipole moments of the one-body density. It turns out to be very versatile and has been applied since with different families of generator states. The static GCM has demonstrated over the years its ability to describe the low excitation spectrum of nuclei [7, 8]. For this kind of application, the generator states are, in general, parameterized by some gauge variables associated with the breaking and restoration of symmetry groups (Euler angles for rotational symmetry, gauge angle for the particle-number symmetry). Similar approaches based on generator states labeled by a few multipole moments of the one-body density also provided predictions of the giant monopole, dipole, and quadrupole resonances [9–14].

Studies based on the time-dependent flavor of the GCM are less abundant in the literature. The goal of this review is, therefore, to recall the formal developments related to the Time-Dependent Generator Coordinate Method (TDGCM) and highlight their current applications in the field of nuclear physics. In Sec. II, we present some general aspects of the time-dependent generator coordinate method in its standard and full-fledged implementation. In Sec. III, we focus on the Gaussian overlap approximation framework that is commonly used in most of the state of the art applications of the TDGCM. In particular, we discuss the fact that such an approach has difficulties accounting for the diabatic aspects of nuclear collective motions. We then devote the two last sections to two possible extensions of the TDGCM aiming at overcoming this issue. The Sec. IV highlights the Schrödinger Collective Intrinsic Model (SCIM),
a framework based on the symmetric moment approximation of the TDGCM. Finally, Sec. V A reports alternative methods involving a TDGCM-like ansatz built on time-dependent generator states.

II. GENERAL FORMALISM OF THE TDGCM

A. Generator states

Predicting the structure and dynamics of medium to heavy nuclei starting from the nucleons degrees of freedom is a challenging task. The difficulty arises from a large number of correlations present in the many-body wave function of nuclear systems. A feature that helps us tackle this problem, is the existence of two nearly separable time scales in nuclear processes. On one hand, we have the typical time for the motion of individual nucleons inside the nucleus which is roughly $10^{-22}$s. On the other hand, the time scales associated with collective deformations of the system are roughly 10 times bigger than the former ($1 \text{zs} = 10^{-21}$s). Such separation in time scale motivated attempts to describe the dynamics in terms of shape coordinates only. As mentioned in the introduction, one possibility is to transform the $3A$ positions of the nucleons into a set of collective coordinates plus some residual intrinsic DoFs. Such an approach could then be combined with an adiabatic approximation similar to the Born-Oppenheimer approximation in electronic systems to reduce the dynamics to the collective DoFs only. The GCM proceeds with an alternative approach that introduces collective deformations DoFs without relying on a transformation of the set nucleons DoFs.

The first step of the method consists in building a family of many-body states $\{|\phi(q)\rangle\}$ parametrized by a vector of labels $q = q_0 \cdots q_{p-1}$. We can summarize the essence of such a construction in the following few points:

- The labels $q_i$ are referred to as the generator coordinates or collective coordinates. They are continuous real numbers that can for instance characterize the shape of the nuclear density. The vector $q$ takes arbitrary values in a $P$-dimensional subspace $E \subset \mathbb{R}^P$.
- The states $\{|\phi(q)\rangle\}$ are the generator states. They are many-body states associated with the system of $A$ nucleons under study. In the standard TDGCM framework, these states are time-independent.
- The function $q \rightarrow |\phi(q)\rangle$ should be continuous. In other words, for any sequence of collective coordinates $\{q_k\}$ that converges to $q$, the corresponding sequence $|\phi(q_k)\rangle$ must converge to $|\phi(q)\rangle$. This property is required for a sound mathematical construction of the GCM framework as detailed in Ref. [15].

The choice of a family of generator states fulfilling these properties is then arbitrary which gives great versatility to the GCM method $^1$. To describe at best a physical process, the exact dynamics should as much as possible take place in the sub-Hilbert space spanned by the generator states. Therefore, building a pertinent family of generator states requires a good $a$ priori knowledge of the dynamics of the system.

To handle nuclear deformations, a standard procedure consists in defining the generator states as the solutions of a constrained Hartree-Fock-Bogoliubov equation. In this approach, each collective coordinate is typically associated to a multipole moment observable (i.e. the quadrupole moment of the one-body density). The generator state $|\phi(q)\rangle$ is then obtained by minimizing the Routhian

$$R[\phi(q)] = E_{\text{HFB}}[\phi(q)] - \sum_i \lambda_i \left( \langle \phi(q)|\hat{Q}_i|\phi(q)\rangle - q_i \right)^2,$$

where the $\hat{Q}_i$ refer to the chosen multipole operators and $\lambda_i$ are their associated Lagrange multipliers. This method presents the benefit of controlling the principal components of the shape of the states through a small set of DoFs while other DoFs are determined automatically from the HFB variational principle. It is often qualified as an adiabatic method because the generator states will minimize their HFB energy under a small number of constrained. One drawback of this method is that it does not ensure by constructing the continuity of the function $q \rightarrow |\phi(q)\rangle$. This could severely affect some applications as mentioned in Sec. II F and III C.

In the context of nuclear structure, the now-standard strategy of symmetry breaking and restoration provides a different yet natural way of building generator states. In this context, we typically define the generator states as the

$^1$ For some applications, it may be convenient to add one or several discrete generator coordinates. We will then note the generator states as $|\phi_k(q)\rangle$ where $k$ is a vector of discrete labels. A typical example of a discrete label could be the $K$ quantum number associated with the projection of the total spin onto a symmetry axis of the nucleus. Another example is provided in Sec. IV.
result of applying a parametrized group of symmetry operators on a reference (and symmetry breaking) HFB state $|\phi\rangle$. Typically, for the particle-number symmetry, the relevant collective coordinate is the gauge angle $\theta$ \cite{16} and the generator states $|\phi(\theta)\rangle$ read

$$|\phi(\theta)\rangle = \exp\left(i\theta(\hat{A} - A)\right) |\phi\rangle .$$

(2)

Note that the two aforementioned strategies to create the generator states are often mixed when dealing with several collective coordinates \cite{8}.

\section{Griffin-Hill-Wheeler ansatz}

Once the family of generator states is chosen, the Griffin-Hill-Wheeler (GHW) ansatz assumes that the many-body state of the system reads at any time

$$|\Psi(t)\rangle = \int_{q \in E} d\mathbf{q} |\phi(\mathbf{q})\rangle f(\mathbf{q}, t).$$

(3)

The function $f(\mathbf{q}, t)$ gives the complex valued weights of this quantum mixture of states. It should belong to the space of square-integrable functions that we note here $L^2(E)$. The expectation value of any observable $\hat{O}$ for a GHW state has the compact form

$$\langle \hat{O}(t) \rangle = \int \int d\mathbf{q} d\mathbf{q}' f^*(\mathbf{q}, t) \mathcal{O}(\mathbf{q}, \mathbf{q}') f(\mathbf{q}', t).$$

(4)

We used here the notation $\mathcal{O}(\mathbf{q}, \mathbf{q}')$ for the kernel of the observable defined by

$$\mathcal{O}(\mathbf{q}, \mathbf{q}') = \langle \phi(\mathbf{q}') | \hat{O} | \phi(\mathbf{q}) \rangle .$$

(5)

Important kernels that we will discussed through this review are the norm kernels and the energy (or Hamiltonian) kernels. They are defined as

$$\mathcal{H}(\mathbf{q}, \mathbf{q}') = \langle \phi(\mathbf{q}') | \hat{H} | \phi(\mathbf{q}) \rangle \quad \text{(Hamiltonian)},$$

(6)

$$\mathcal{N}(\mathbf{q}, \mathbf{q}') = \langle \phi(\mathbf{q}') | \hat{H} | \phi(\mathbf{q}) \rangle \quad \text{(norm)}.$$ 

(7)

We emphasize that the choice of collective coordinates $\mathbf{q}$ is somehow arbitrary. From one choice of collective coordinate, we may switch to a different one while keeping invariant the space of GHW states. We can show this by defining a change of variable $\varphi$

$$a = \varphi(\mathbf{q}).$$

(8)

Then we may consider the GHW ansatz built on the transformed generator states $|\tilde{\phi}(a)\rangle = |\phi(\varphi^{-1}(a))\rangle$

$$|\tilde{\psi}(t)\rangle = \int_{a \in \varphi(E)} da |\tilde{\phi}(a)\rangle \tilde{f}(a, t).$$

(9)

Any GHW state defined by Eq. (3) can be cast into a Eq. (9) with the weight function

$$\tilde{f}(a, t) = f(\varphi^{-1}(a), t) |\det(J_{\varphi}(a))|^{-1}. \quad \text{(10)}$$

Here $J_{\varphi}$ is the Jacobian matrix of the coordinate transformation. Also, the formula for the expectation value observables are invariant by this change of coordinate. Typically we have in the $a$ representation

$$\langle \tilde{O}(t) \rangle = \int \int da da' \tilde{f}^*(a, t) \mathcal{O}(a, a') \tilde{f}(a', t),$$

(11)

with

$$\mathcal{O}(a, a') = \langle \tilde{\phi}(a) | \hat{O} | \tilde{\phi}(a') \rangle .$$

(12)

Although applying such change of variable does not change the physics of the ansatz, it does change the intermediate objects of the GCM framework. In some cases, it may be essential to change the variables so to obtain good mathematical properties of the kernel operators [15, 16].

As a final remark, we would like to highlight that the integral Eq. (3) may not be well defined for some weight functions and family of generator states. The Ref. [15] gives a mathematically rigorous presentation of the GCM framework. We retain from this work that a sufficient condition for the GHW ansatz to be valid is that norm kernel defines a bounded linear operator on $L^2(E)$. 
C. Griffin-Hill-Wheeler equation

The time-dependent Schrödinger equation in the entire many-body Hilbert space,

$$\left(\hat{H} - i\hbar \frac{d}{dt}\right) |\Psi(t)\rangle = 0,$$

(13)
drives the exact time evolution of a many-body system $|\Psi(t)\rangle$. We assume here that all the interactions between the nucleons are encoded into the Hamiltonian $\hat{H}$ acting on the full many-body space. From this starting point, the TDGCM equation of motion can be obtained by assuming:

1. That the wave function of the system keeps the form of Eq. (3) at any time.

2. That at any time we have

$$\langle \Phi | \left(\hat{H} - i\hbar \frac{d}{dt}\right) |\Psi(t)\rangle = 0$$

(14)

for every GHW state $|\Phi\rangle$.

In other words, we impose that the residual $(\hat{H} - i\hbar \frac{d}{dt}) |\Psi(t)\rangle$ is orthogonal to the space of GHW states. This last assumption is equivalent to a Frenkel’s variational principle whose link to other time-dependent variational principles is discussed in Ref. [17]. By injecting the GHW ansatz (3) into (14), we obtain

$$\int \int dq dq' f_\Phi^*(q') \left(\hat{H}(q', q) - i\hbar N(q', q) \frac{d}{dt}\right) f(q, t) = 0.$$  

(15)

Here $f_\Phi$ is the mixing function defining the GHW state $|\Phi\rangle$. Solving Eq. (15) for any state $|\Phi\rangle$ is equivalent to looking for a function $f$ verifying the so-called Griffin-Hill-Wheeler equation in its time-dependent form

$$\forall q' : \int dq \left(\hat{H}(q', q) - i\hbar N(q', q) \frac{d}{dt}\right) f(q, t) = 0.$$  

(16)

When the many-body Hamiltonian is Hermitian, this equation of motion preserves the norm of the wave function as well as the total energy of the system. Otherwise, their evolution reads

$$\frac{d}{dt} \langle \Psi(t)|\Psi(t)\rangle = i\hbar \langle \Psi(t)|[\hat{H}^\dagger - \hat{H}]|\Psi(t)\rangle,$$

(17)

$$\frac{d}{dt} E(t) = i\hbar \langle \Psi(t)|[\hat{H}^\dagger - \hat{H}]\hat{H}|\Psi(t)\rangle.$$  

(18)

Such a situation typically appears when an imaginary absorption term is added to the Hamiltonian to simulate an open system in a finite simulation box. Finally, note that the time-dependent GHW equation is a continuous system of integrodifferential equations. Its non-local nature in the $q$ representation brings a serious hurdle to its numerical solving.

D. Mapping to the collective wave functions

The equation of motion Eq. (15) and an initial condition for the system is sufficient to determine the dynamics in the TDGCM framework. It is possible to numerically integrate in time this equation with an implicit scheme such as Crank-Nicolson [18]. However, the TDGCM framework offers another natural approach that turns out to be both enlightening from the mathematical perspective and more stable from a numerical point of view. This method resorts on a mapping between the GHW states and some functions of the collective coordinate $q$. The rigorous mathematical construction of this mapping in a general case is detailed in Ref. [15]. Here we will only build this mapping in the case where the norm kernel $N$ is of Hilbert-Schmidt type [19]. It is the case as long as the domain $E$ of the collective coordinates is bounded and is therefore applicable in most of the practical applications.

To start with, we recall that any kernel $O(q, q')$ also defines a linear operator acting on the space of functions $L^2(E)$ as

$$(O f)(q) = \int_{q' \in E} dq' O(q, q') f(q').$$  

(19)
as long as this integral is mathematically defined. The Hilbert-Schmidt property of the norm operator implies the existence of a complete, discrete and orthonormal family of functions \( \{ u_i(q) \} \) of \( L^2(E) \) that diagonalize the linear operator associated with the norm kernel.

\[
\forall i > 0: \quad \mathcal{N} u_i = \lambda_i u_i
\]

Due to the fact that \( \mathcal{N} \) is a Hermitian positive semidefinite operator, its eigenvalues are real and positives. We adopt here the convention where they are sorted by decreasing order and assume that only the first \( r \) eigenvalues are not zero. From this diagonalization, we can split the space of functions \( f \) into two orthogonal subspaces: the one associated with the vanishing eigenvalues and the one associated with the strictly positive eigenvalues. Formally we write down the two projectors

\[
Q(q, q') = \sum_{i \leq r} u_i(q) u_i^*(q') \quad (21)
\]
\[
\mathcal{P}(q, q') = \sum_{i > r} u_i(q) u_i^*(q') \quad (22)
\]

with

\[
Q + \mathcal{P} = \mathbb{1}_{L^2(E)}. \quad (23)
\]

The set \( \mathcal{P}L^2(E) \) is the space associated to the null eigenvalues of the norm operator \( \mathcal{N} \). Any GHW state built from a weight function belonging to this space gives the null many-body state. Its orthogonal complement is the subspace \( Q(E) = QL^2(E) \). We call collective wave functions, the functions living in this subspace.

We can define uniquely the positive hermitian square-root of \( \mathcal{N} \) (which is also Hermitian) with

\[
\mathcal{N}(q, q') = \int_{a \in E} \mathcal{N}^{1/2}(q, a) \mathcal{N}^{1/2}(a, q') \, da. \quad (24)
\]

For any GHW states, we can therefore associate its collective wave function \( g(q) \in Q(E) \) by the equation

\[
g = \mathcal{N}^{1/2} f. \quad (25)
\]

Conversely, the operator \( \mathcal{N}^{1/2} \) is invertible in \( Q(E) \). Therefore for any collective wave function \( g \in Q(E) \), one can build its corresponding GHW state with the weight function

\[
f = \mathcal{N}^{-1/2} g. \quad (26)
\]

Finally, this mapping between \( Q(E) \) and the GHW states is isometric as we may show that for any pair of GHW states \( \Psi \) and \( \Phi \) we have the property

\[
\langle \Psi | \Phi \rangle = \langle g_\Psi | g_\Phi \rangle = \int_{q \in E} g_\Psi(q) g_\Phi(q) \, dq. \quad (27)
\]

Going further, any many-body observable \( \hat{O} \) can be mapped into a collective operator \( \tilde{O} \) acting on the space \( Q(E) \). This operator is defined by \(^2\)

\[
\tilde{O} = \mathcal{N}^{-1/2} \hat{O} \mathcal{N}^{-1/2}. \quad (28)
\]

The isometry of the mapping gives a simple mean to compute matrix elements of observables.

\[
\langle \Phi | \tilde{O} | \Psi \rangle = \langle g_\Phi | \tilde{O} | g_\Psi \rangle \quad (29)
\]

\(^2\) Note that such a definition is possible for any observable \( \hat{O} \) due to the property \( Q\mathcal{O} = \mathcal{O} \).
Finally, we can reduce the TDGCM equation of motion (Eq. (16)) in this language. It becomes a time-dependent Schrödinger equation for the collective wave function.

\[ i\hbar \dot{g} = \tilde{H}g. \]  

This equation of motion presents several practical advantages compared to Eq. (16). The collective Hamiltonian \( \tilde{H} \) is in general still non-local, but the time derivative of \( g \) has now an explicit expression. This makes it possible to use faster time integration schemes at the cost of computing first the collective Hamiltonian through Eq. (28). Also, the collective wave function is expected to have a smoother behavior compared to the weight function \( f \). This comes directly from Eq. (26) where we see that eigenvalues of the norm kernel approaching zero add diverging components to \( f \). The equation (30) may be directly solved by discretizing the collective wave function \( g(q) \). In many cases, it is appropriate to solve it directly in the representation given by the basis \( \{ u_i(q) \}_{i \leq r} \). The collective Hamiltonian \( \tilde{H} \) as well as other collective observables are indeed easier to compute using this particular basis.

### E. Difficulties related to the energy kernel

Up to now, we discussed general features of the TDGCM approach valid for any family of generator states. In nuclear physics, most applications of the GCM rely on families of Bogoliubov vacua. A crux of the GCM approach is then the determination of the norm and Hamiltonian kernels between such many-body states. The Ref. [20] provides a general and now-standard approach to completely determine the norm kernel between Bogoliubov vacua based on the calculation of a matrix Pfaffian. On the other hand, the evaluation of the energy kernel in nuclear physics applications suffers from several major difficulties that we are now going to highlight. The origin of these flaws stems from the fact that our practical applications do not rely on a linear many-body Hamiltonian but instead on some effective Hamiltonians or energy density functionals. This topic was extensively discussed in the context of static GCM for nuclear structure [21–24]. We briefly list here the pitfalls raised by the determinations of the energy kernel in realistic nuclear applications.

#### 1. Neglecting some exchange terms

To avoid unbearable numerical costs, a common practice consists in neglecting or approximating parts of the many-body Hamiltonian. It is, for instance, widespread to use the Slater approximation of the Coulomb exchange term or to neglect the exchange part of the pairing force between nucleons [25]. Although convenient from a numerical point of view, it was shown in Ref. [26] that such approximations may introduce poles in the expression of the energy kernel. These poles lead to divergence in this quantity when calculated between some Bogoliubov vacua. The Refs. [27, 28] illustrate this behavior in a case of particle number symmetry restoration.

#### 2. Violation of symmetries by energy density functionals

In many of our realistic applications, the nucleon-nucleon interaction is encoded in the form of an energy density functional (EDF). Using such a formalism in combination with a GCM mixture of states requires a sound definition of a multireference energy density functional [21]. Such definition is often provided and implemented in the form of the reduced energy kernel \( h(q, q') = \mathcal{H}(q, q')/\mathcal{N}(q, q') \) between two non-orthogonal Bogoliubov vacua. For a two-body Hamiltonian case, the reduced energy kernels may be expressed from the generalized Wick theorem

\[ h(q, q') = \sum_{ijkl} t_{ij} \rho_{ji}^{qq'} + \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl} \rho_{kli}^{qq'} + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \kappa_{ij}^{qq'} \kappa_{kl}^{qq'}. \]  

It involves the matrix elements of the one- and two-body parts of the interaction \( t \) and \( \bar{v} \) as well as transition densities such as

\[ \rho_{ij}^{qq'} = \frac{\langle \phi(q') | \hat{a}_i^\dagger \hat{a}_j | \phi(q) \rangle}{\langle \phi(q) | \phi(q') \rangle}. \]  

In the practical implementations of the multireference EDF approach, such a kernel is defined, by analogy, as the same bilinear form whose coefficients now come from a fit procedure. The major differences compared to the EDF case are:
1. the coefficients defining the EDF may depend on some densities of the system,
2. the coefficients in the particle-particle channels may differ from the ones in the particle-hole channels,
3. the matrix $\bar{v}$ may not be antisymmetric.

As detailed in Refs. [21, 29], the violation of these Hamiltonian properties lead in some cases to a divergence of the reduced energy kernel that biases or prevent practical applications.

3. Density dependent terms of energy density functionals

In an EDF framework, the coefficients of Eq. (31) depends on the density of the system. For the non-diagonal part of the kernel, this requires defining a prescription on the densities to be used for this dependency. Several prescriptions have been developed and tested during the last two decades [30, 31]. A prescription that fulfills many important conditions expected from a Hamiltonian is the transition density defined by Eq. (32) (see Ref. [32]). On the other hand, this prescription yields densities with complex values. It is then incompatible with most of the EDFs developed at the mean-field level that contains terms with a non-integer power of the density. Finding a satisfying pair of density prescription and EDF valid for GCM calculations is still an open problem.

As a conclusion, the current usage of the GCM formalism with effective Hamiltonian or energy density functionals suffers from several formal and practical flows when it comes to determining the energy kernel. This situation has been a major hurdle to the development of GCM applications in nuclear physics in the last years. Several ongoing efforts attempt to overcome this difficulty by building new energy functionals valid for multireference calculations [33] or going toward ab initio treatments [34].

F. Fission dynamics with the exact TDGCM

The exact resolution of the time-dependent GHW equation in a realistic case has rarely been carried out. To our knowledge, the only published work tackling this task is presented in [35, 36] in the context of fission. It shows the challenges raised by an exact TDGCM calculation especially when dealing with large collective coordinate domains.

In Ref. [35], the authors used the TDGCM to describe the reaction $^{239}$Pu(n,f). This study relies on two common collective coordinates for fission, namely $q_{20}$ and $q_{30}$, that are associated with the expectation value of the quadrupole and the octupole moments of the one-body density. The set of constrained HFB solutions (a total of 20212) obtained for a wide range of these collective coordinates forms the family of generator states. Each generator state is practically obtained with a finite-range Gogny interaction in its D1S parameterization. A two-center axial harmonic oscillator basis with 12 shells has been used, where the parameters defining the basis have been optimized for each value of the collective coordinates.

The norm kernel has been calculated for each couple of generator states. The top panel of Fig. 1 presents its values between the mean-field ground-state and the surrounding points whereas the bottom panel of the figure shows its values obtained close to a more elongated configuration. We see that the overlaps are above $\epsilon_{\text{thresh}} = 1.0 \times 10^{-4}$ only in a neighborhood of $q_{20}$ in both cases. Also, the bottom panel highlight a discontinuous behavior with a norm kernel below $\epsilon_{\text{thresh}}$ around $q_{20} \approx 130 b$. This typically illustrates the fact that the function $q \rightarrow |\phi(q)|$ is not continuous in this area.

The reduced Hamiltonian $h(q_0, q)$, defined as the ratio between the collective Hamiltonian and the norm kernel

$$h(q_0, q) = \frac{\langle \phi(q) | \hat{H} | \phi(q_0) \rangle}{\langle \phi(q_0) | \phi(q) \rangle}$$

(33)

has also been calculated for all overlaps greater than $\epsilon_{\text{thresh}}$. The Fig. 1 presents the slices of the reduced Hamiltonian for the same cases as Fig. 1. The relative variation of the reduced Hamiltonian (where the norm kernel above the threshold) is extremely small, being only 2% around the ground state and 1% close to the discontinuity. This justifies the standard approximations of this quantity by a second-degree polynomial.

Finally, its is possible to determine the time evolution of the weight function $f(q, t)$ of the GHW ansatz (3). In cases where the size of the discretized space of the collective coordinate is still tractable, this task has been achieved through a direct diagonalization of the collective Hamiltonian [36]. For this two-dimensional application, the straightforward diagonalization involves a prohibitive numerical cost. It is still possible to use a Crank-Nicolson method to integrate in time the GHW equation (16). We plot in Fig. 2 a snapshot at time $t = 0.55$ zs (1zs = $10^{-21}$s) of the quantity $P(q, t)$ defined as

$$P(q, t) \equiv \langle \Psi(t) | (|\phi(q)\rangle \langle \phi(q) |) |\Psi(t)\rangle.$$

(34)
Figure 1: Left hand side: Overlaps $N(q_0, q)$ as a function of $q$ and where $q_0 = (30,3)$ in barn units corresponds to the ground state (upper panel) or $q_0 = (127,1)$ in barn units which corresponds to a point at higher elongation (lower panel). This was obtained for a $^{240}$Pu nucleus. The white parts correspond to values below a threshold of $1.0 \times 10^{-4}$. The yellow crosses correspond to $q_0$. Right hand side: same as the left hand side for the reduced energy kernel $h(q_0, q)$.

This correspond to the probability to measure the system in the state $|\phi(q)\rangle^3$. The most time-consuming part was the calculation of the norm and Hamiltonian kernels that required the use of 512 cpus for two weeks ($\sim 170,000$ cpu.h). The calculation of the time-evolution of the weight function $f(q,t)$ for times up to $0.55zs$ was done using 64 cpus.

Figure 2: The gray surface represents the HFB energy of the generator states as a function of $q_{20}$ and $q_{30}$. On top of this, the color map gives the quantity $P(q,t = 0.550 \, zs)$, for the same cases as in Fig. 1.

\[ t = 5.50 \times 10^{-22}s \]

\(^3\) Note that due to the non-orthogonality of the generator states its sum over all the points $q$ is not equal to 1.
cpus during one week (\( \sim 10,000 \) cpu.h). The short length of time for which the weight function was determined is not enough for the calculation of mass and charge probability distributions. A more realistic calculation would require at least 200,000 cpu.h, for the determination of the weight function up to 10zs only.

The major difficulty of such an application stems from the big size of the discretized space of the collective coordinates (substantially bigger for example than in the case of the static GCM calculations for nuclear structure). This makes the computation of the norm and Hamiltonian kernel intensive but still embarrassingly parallel. In addition, in the case of fission, techniques to determine the post-scission observables of the fragments still need to be developed for the exact TDGCM. For instance, some simplifying hypotheses on the way to treat open domains of collective coordinates have been used under the Gaussian Overlap Approximation \[37\] that are no longer valid in the exact TDGCM framework.

### III. GAUSSIAN OVERLAP APPROXIMATION (GOA)

In its straightforward application, the TDGCM leads to a non-local equation of motion that must be solved in most realistic calculations in a high-dimensional space. As mentioned in Sec. II, solving this equation involves a significant numerical cost that strongly hinders its applications in nuclear physics. Several approximated treatment of the TDGCM have been developed with the aim to build a local equation of motion for the collective wave function \( g(q,t) \) (cf. Eq. (30)). The Gaussian overlap approximation (GOA) is one of these approximations which leverages the fact that the overlap and Hamiltonian kernels can in some cases be parametrized in terms of Gaussians of the variable \( q \). In its static form, the GOA has been largely used and applied for nuclear structure. Especially, it provides a nice bridge between the Bohr Hamiltonian equation that was first formulated in \[38\] and a quantum treatment based on the \( 3A + A \) nucleons degrees of freedom \[39–43\]. Extensive reviews of the static version of the GOA can be found in Refs. \[16, 44\]. We focus here on its time-dependent flavor.

#### A. TDGCM+GOA with time even generator states

1. **Main assumptions**

In its most standard form, the GOA framework assumes the following situation:

1. We consider a family of normed generator states \( \{ |\phi(q)\rangle \} \) parametrized by a vector of real coordinates \( q \in \mathbb{R}^P \).
2. All the states of the set are time even, i.e. they are their own symmetric by the time-reversal operation.
3. The function \( q \to |\phi(q)\rangle \) is continuous and twice derivable.
4. The overlap between two arbitrary generator states can be approximated by the Gaussian shape

   \[
   N(q,q') \simeq \exp\left[-\frac{1}{2}(q - q')^t G(\bar{q})(q - q')\right],
   \tag{35}
   \]

   with \( \bar{q} = (q + q')/2 \) and \( G(\bar{q}) \) a real positive definite matrix.
5. The Hamiltonian kernel can be approximated by

   \[
   \mathcal{H}(q,q') \simeq N(q,q')h(q,q'),
   \tag{36}
   \]

   where \( h(q,q') \) is a polynomial of degree two in the collective variables \( q \) and \( q' \). This polynomial is referred to as the reduced Hamiltonian.

In most applications of the TDGCM+GOA, the generator states are built as constrained Hartree-Fock-Bogoliubov states of even-even nuclei which ensures the time even property. The question is then which are the situations where Gaussian shape is verified within a small error. Already from the time-reversal symmetry, we can infer that the overlaps are real and symmetric in \( (q - q') \). Therefore, the following relation is satisfied in the vicinity of \( q \)

\[
\langle \phi(q + \frac{s}{2}) |\phi(q - \frac{s}{2}) \rangle = \exp\left[\ln\left(\langle q + \frac{s}{2} |q - \frac{s}{2}\rangle\right)\right].
\tag{37}
\]
A Taylor development of this expression up to order two in $s$ already yields locally a Gaussian shape without any additional assumption.

$$\left\langle \phi(q + \frac{s}{2}) | \phi(q - \frac{s}{2}) \right\rangle = \exp \left[ -\frac{1}{2} s^t G(q) s + o(s^2) \right]$$  \hspace{1cm} (38)$$

with

$$G_{ij}(q) = \langle \partial_i \phi(q) | \partial_j \phi(q) \rangle,$$  \hspace{1cm} (39)$$

$$|\partial_i \phi(q)| = \frac{\partial |\phi(a)|}{\partial a_i} \bigg|_{q}.$$  \hspace{1cm} (40)$$

We used here some identities coming from the fact that generator states are normed. In situations where the coordinates corresponds to some collective deformations of the nucleus, it turns out that the Gaussian shape holds for larger values of $s$. This is justified from the central limit theorem in Ref. [44] for Slater determinants or in Ref. [16] for Bogoliubov vacua. It especially holds for heavy nuclei.

Finally, note that although we limit here our description to the case of time even generator states, it is possible to build a GOA framework without assuming this symmetry. Such generalization can be found for instance in Ref. [44].

2. Equation of motion

Starting from the hypothesis of the GOA, one can reduce the equation of motion Eq. (30) to a local one involving first and second order derivatives of the collective wave function. In this section we give only the main ideas to derive this local equation. For more exhaustive demonstrations, we refer the reader to Refs. [16, 44, 45].

In its historical version, the GOA framework assumes that the width of the Gaussian shape is a constant. However, in most practical cases this assumption is too restrictive. To overcome this issue, a series of papers published in the 70-80’s generalized the GOA framework to account for a varying Gaussian width [45–47]. The idea is to perform a change of collective variables to recover the constant width case. The mapping between the new collective coordinates $\alpha$ and the original ones $q$ reads

$$\alpha(q) = \int_{a \in C^q_0} G^{\frac{1}{2}}(a) \, da.$$  \hspace{1cm} (41)$$

where $C^q_0$ is the segment linking the origin to $q$. With this new labeling of the generator states, we get

$$\langle \phi(\alpha) | \phi(\alpha') \rangle \simeq \exp \left[ -\frac{1}{2} (\alpha - \alpha')^2 \right].$$  \hspace{1cm} (42)$$

We can therefore perform all the derivations with the $\alpha$ coordinates and make the inverse transformation on the final expressions only.

Starting with this simple form of the overlap, we seek an equation of motion involving a local collective Hamiltonian in the collective coordinate representation. Building this equation heavily relies on various properties of the Gaussian shape. A first important property is the fact that we can express analytically its positive Hermitian square root by

$$\sqrt{\mathcal{N}}^{1/2}(\alpha, \alpha') = C \cdot \exp \left[ -(\alpha - \alpha')^2 \right],$$  \hspace{1cm} (43)$$

where the constant $C$ only depends on the dimension of the coordinate $\alpha$. In addition, there is a simple link between the successive derivatives of a Gaussian shape and its multiplication by polynomials. For instance, we have for the two first derivatives in $\alpha$

$$\frac{\partial \sqrt{\mathcal{N}}^{1/2}}{\partial \alpha_k} = -2(\alpha_k - \alpha_k') \sqrt{\mathcal{N}}^{1/2},$$  \hspace{1cm} (44)$$

$$\frac{\partial^2 \sqrt{\mathcal{N}}^{1/2}}{\partial \alpha_k \partial \alpha_l} = [-2 \delta_{kl} + 4(\alpha_k - \alpha_k')(\alpha_l - \alpha_l')] \sqrt{\mathcal{N}}^{1/2}.$$  \hspace{1cm} (45)$$

Note that this assumes (i) that the integrals of $G^{1/2}(a)$ are independent of the integration path (ii) that the average of $G^{1/2}$ on the path is well approximated by its evaluation at the central point of the path (cf. Ref. [47]).
We now build a local collective Hamiltonian. After the change of variable Eq. (41), the Hamiltonian kernel between two arbitrary GHW states reads

\[ \langle \Phi | \hat{H} | \Psi \rangle = \int _{\alpha\alpha'} f_\Phi (\alpha) N^{1/2} (\alpha, \xi) h (\alpha, \alpha') N^{1/2} (\xi, \alpha') f_\Phi (\alpha') \, d\alpha \, d\alpha' \, d\xi \tag{46} \]

We assume then that the reduced Hamiltonian is a degree two polynomial to write down for any point \( \xi \)

\[ h (\alpha, \alpha') = h (\xi, \xi) + h _\alpha (\alpha - \xi) + h _{\alpha\prime} (\alpha' - \xi) \]

\[ + \frac{1}{2} [ h _{\alpha\alpha} (\alpha - \xi)^2 + 2 h _{\alpha\alpha'} (\alpha - \xi) (\alpha' - \xi) + h _{\alpha' \alpha'} (\alpha' - \xi)^2 ] , \tag{47} \]

where \( h _\alpha \) is a shorthand notation for the vector of the first derivatives of the reduced Hamiltonian estimated at \( \xi \)

\[ h _\alpha \equiv \left( \frac{\partial h (\alpha, \alpha')}{\partial \alpha_1} \bigg|_{\alpha=\alpha'=\xi}, \ldots, \frac{\partial h (\alpha, \alpha')}{\partial \alpha_p} \bigg|_{\alpha=\alpha'=\xi} \right) . \tag{48} \]

Similarly \( h _{\alpha\alpha}, h _{\alpha\alpha'}, h _{\alpha' \alpha'} \) are the tensors of second derivatives with respect to the collective coordinates and evaluated at point \( \xi \). The idea is then to inject this local development into Eq. (46). Using the property Eq. (44), we express the reduced kernel as a local operator containing derivatives acting on the right hand side \( N^{1/2} \). Finally, after rearranging all the terms and performing some integration by parts, we obtain the expected result.

\[ \langle \Phi | \hat{H} | \Psi \rangle = \int _{\alpha\alpha'} g _\Phi (\alpha) \hat{\mathcal{H}} (\alpha) \delta (\alpha - \alpha') g _\Phi (\alpha') \, d\alpha \, d\alpha' . \tag{49} \]

Identifying this expression with Eq. (29) tells us that the collective Hamiltonian is local. It reduces to a standard kinetic plus potential Hamiltonian acting on the collective wave function

\[ \hat{\mathcal{H}} (\alpha) = - \frac{\hbar^2}{2} \nabla _\alpha B (\alpha) \nabla _\alpha + V (\alpha) . \tag{50} \]

The potential and inertia matrix in this coordinate representation are

\[ V (\alpha) = h (\alpha, \alpha) - \frac{1}{2} \text{Tr} (h _{\alpha\alpha'}) \]

\[ B (\alpha) = \frac{1}{2\hbar^2} (h _{\alpha\alpha'} - h _{\alpha\alpha}) . \tag{51} \]

Injecting this expression of the collective Hamiltonian into Eq. (30) gives us the time evolution of the unknown function \( g (\alpha) \). The ultimate step is to transform back this equation of motion to another one acting on the original set of coordinates \( q \). Doing so we get the same equation with a transformed local collective Hamiltonian

\[ \tilde{\mathcal{H}} (q) = - \frac{\hbar^2}{2 \sqrt{\gamma (q)}} \nabla _q \left[ \sqrt{\gamma (q)} B (q) \right] \nabla _q + V (q) \tag{52} \]

The new collective Hamiltonian involves a metric \( \gamma (q) \) defined by

\[ \gamma (q) = \text{det} (G (q)) . \tag{53} \]

The inertia tensor takes the more involved form

\[ B (q) = \frac{1}{2\hbar^2} G^{-1} (q) \left[ h _{qq'} - h _{qq} + \sum _n \Gamma^n (q) h _{qn} \right] G^{-1} (q) . \tag{54} \]

The notation \( \Gamma^n (q) \) stands for the Christoffel symbol. It is a matrix related to \( G (q) \) through the relation

\[ \Gamma _{ki} (q) = \frac{1}{2} \sum _i G^{-1} _{ni} \left( \frac{\partial G _{ki}}{\partial q_l} + \frac{\partial G _{il}}{\partial q_k} - \frac{\partial G _{ik}}{\partial q_l} \right) . \tag{55} \]

\[ ^{5} \text{Note that some higher order correction terms in the potential are neglected here (see Ref. [44] for more details).} \]
Finally, the potential becomes in this set of coordinate

\[ V(q) = h(q, q) - \frac{1}{2} \text{Tr} \left( G^{-1}(q) h_{qq} \right). \]

The first term is nothing but the energy of the generator state \(|\phi(q)\rangle\). The second term is a zero point correction that contains second derivatives of the reduced Hamiltonian. With some additional work, it is possible to express this zero point correction \(\epsilon_{ZPE}\) in a slightly more practical form that involves the inertia tensor and second derivatives of the energy \(h(q, q)\) only.

\[ \epsilon_{ZPE}(q) = -\frac{\hbar^2}{2} \text{Tr} (BG) - \frac{1}{8} \text{Tr} \left( G^{-1} \frac{\partial^2 h(q, q)}{\partial q^2} \right) + \frac{1}{8} \text{Tr} \left( G^{-1} \sum_n \Gamma_n \frac{\partial h(q, q)}{\partial a_n} \right). \]

The equation of evolution (30) along with the expression of the collective Hamiltonian Eq. (52) and its components Eqs. (53), (56) and (54) define the dynamics of the system in the TDGCM+GOA framework.

3. Inertia and metric

Both the inertia tensor and the metric are quantities that depend on the derivatives of the generator states and/or of the reduced Hamiltonian. One possibility could be to determine these derivatives numerically for instance with a finite difference method. In the standard situation where the generator states are constrained HFB solutions, one can find an analytical expression of the inertia and the metric. We recall here this result at any point \(q\)

\[ G = \frac{1}{2} [M^{(1)}]^{-1} M^{(2)} [M^{(1)}]^{-1}. \]
\[ B = M^{(1)} [M^{(2)}]^{-1} M^{(1)} [M^{(2)}]^{-1} M^{(1)}. \]

The moments \(M^{(K)}\) and \(\tilde{M}^{(K)}\) involve the QRPA matrix \(M\) of the state \(|\phi(q)\rangle\) and are defined in App. A. For the complete derivation of these results we refer the reader to [48] and references therein. Note that this result neglects the term involving the Christofel symbol in the inertia. The argument for this approximation relies on the fact that the metric varies slowly with the collective coordinates. We are not aware of a systematic verification of this fact in applications.

In all TDGCM+GOA practical applications, the so called perturbative cranking approximation is used to avoid a costly inversion of the QRPA matrix required to compute the metric and inertia. It consists in approximating the QRPA matrix by a diagonal part only, in the quasiparticle basis that diagonalizes the generalized density matrix of \(|\phi(q)\rangle\). This gives a simple and well known form for the moments \(M^{(K)}\)

\[ M^{(K)}_{ij} = \tilde{M}^{(K)}_{ij} = \mathcal{Re} \sum_{\mu\nu} \frac{\langle \phi(q)|\hat{Q}_i|\mu\nu\rangle \langle \mu\nu|\hat{Q}_j|\phi(q)\rangle}{(E_\mu + E_\nu)^K},\]

where \(|\mu\nu\rangle\) is a two quasiparticles excitation built on top of the generator state and \(E_\mu\) and \(E_\nu\) are the corresponding quasiparticle energies.

The GCM+GOA framework unambiguously defines the metric and inertia as functions of the successive derivatives of the generator states and reduced Hamiltonian. However, it is known that this inertia and its approximate perturbative cranking estimation is too low to correctly describe several situations. One example is the case of a translation motion [44]. Several studies compare the GOA inertia with inertia provided by other theories yielding an equivalent collective equation of motion such as ATDHF [49, 50]. In Ref. [51], the authors extend the TDGCM+GOA framework by introducing conjugate coordinates that bring time odd components into the generator states. In particular, they show that the resulting collective Hamiltonian takes the same form as Eq. (52) but where the GOA inertia is replaced by the ATDHF inertia. This somehow justifies the common practice of using the ATDHF inertia when solving the collective equation of motion.

B. Applications in nuclear reactions

1. Low energy ion collisions

The force of TDGCM+GOA is its versatility in terms of the choice of collective coordinates and its ability to treat in the same framework the nucleons DoFs as well as more collective DoFs. As such, it seems an appropriate way to
tackle the dynamics of low energy ion collisions where the principal degree of freedom is the relative distance between the two reaction partners but also where the collision also affects the internal organization of the nucleons. Along this line, it is possible to build a family of generator states describing the two reaction partners and parameterized by their relative distance. Several papers followed this idea during the 1980’s. In particular, J.-F. Berger and D. Gogny [52] treated the frontal collision of $^{12}$Ca+$^{12}$Ca within a GCM+GOA approach. The focus in this kind of study is the determination of the cross-sections resonances for some specific output channels of the reaction. Other similar studies have been performed on the base of the GCM (without the GOA) and making the link with the resonating group method. D. Baye and Y. Salmon looked at the $^{16}$O+$^{40}$Ca back angles scattering [53] along with the work of Friedrich et al. [54]. Also Goeke et al. studied the $^{16}$O+$^{16}$O collision in the framework of the quantized adiabatic time-dependent Hartree-Fock approach which yields a collective equation of motion identical to the one of TDGCM+GOA [55].

After these first applications, treating collisions with the TDGCM+GOA framework was progressively abandoned to the profit of other methods such as the time-dependent Hartree-Fock plus pairing [56]. One difficulty that could explain this transition is the numerical cost required to build the generator states at the self-consistent mean-field level (note that this cost is nowadays completely acceptable). Beyond this, deeper problems raised for instance by the conservation of the total angular momentum of the collision or the generation of a continuous manifold of generator states appear with this method. Finally, the position of resonances as well as the absolute value of cross-sections are both observables that are very challenging to predict due to their extreme sensitivity to the kinematics of the reaction as well as the internal structure of the nuclei.

2. Fission dynamics

The prediction of the fission fragments characteristics from a dynamical description is a domain where the TDGCM+GOA performs successfully. Fission involves heavy nuclei and begins with large collective motions that are mostly adiabatic. This two factors make the TDGCM+GOA framework built on constrained HFB solutions a good candidate. In addition, the important width of the measured fission yields is the fingerprint of large quantum fluctuations of the one-body density of the compound system. Handling these fluctuations is exactly the purpose of the GCM.

The quest to predict fission yields from a dynamical TDGCM+GOA calculation began in the 1980’s with work of J.-F. Berger et al. exploring the rupture of the neck between prefragments in terms of different collective coordinates [57, 58]. The first calculation of the mass distribution of fission fragments was later on performed in the same group for $^{238}$U [37]. The dynamics of the fissioning system has been described in terms of the two collective coordinates $q_{20}$ and $q_{30}$ associated to the quadrupole and octupole moments of the compound nucleus. The Ref.[59] reports the same technique applied to a few other actinides with a qualitative reproduction of the experimental values. W. Younes and D. Gogny further proposed an alternative set of collective variables in Ref. [60]. Still, one hurdle to this approach was its numerical cost both concerning the determination of the generator states ($\approx 40000$ states in a 2-dimensional description) and the time integration of the collective Schrödinger equation. The development of new tools based on state of the art numerical methods enables today’s continuation of this work. For instance, the code FELIX [61, 62] solves efficiently the collective GOA dynamics based on a spectral element method. On the other hand, using Bayesian processes to determine the best suited parameters of a harmonic oscillator basis enabled significant speed up of some Hartree-Fock-Bogoliubov solvers.

In the last couple of years, we have seen a fast increase of the number of fission studies relying on this technique. A study on $^{240}$Pu benchmarked the new numerical methods [63], the impact of the choice of the initial state of the dynamics on the fission observables is discussed in details in Ref. [64] and the TDGCM+GOA successfully reproduced the fission yields transition in the Fermium isotopic chain [65] as shown in Fig. 3. On top of these papers based on the Skyrme and Gogny energy density functionals, Tao et al. produced similar results from generator states determined with a relativistic mean-field approach [66] and studied in details the sensitivity of the results to the pairing strength. Finally, the same team explored the inclusion of temperature into the generator states as a way to better take into account the diabatic aspects of the dynamics [67, 68] (cf. Fig. 3).

C. Main limitations

Despite its success in determining the fission fragment distribution, the TDGCM+GOA framework suffers from several shortcomings.

First, on the same ground as the exact TDGCM, its derivation relies on the knowledge of a many-body Hamiltonian whereas in all realistic applications it is used with an energy density functional (cf. Sec. II E). It is true that the GOA method does not require an explicit calculation of the off-diagonal elements of the energy kernel that are responsible
for divergent behavior in GCM. However, the formal construction of the GOA still depends on the existence and sound mathematical definition of these matrix elements to be a valid framework. In that sense, the GOA suffers from the same flaws than the exact TDGCM concerning the use of energy density functionals.

A second issue, also common with the exact TDGCM, comes from the requirement that the function $q \rightarrow |\phi(q)\rangle$ is continuous and twice differentiable. This is a necessary condition to develop the formalism and in particular to compute the GOA metric and inertia. However, the standard construction of the family of generator states from constrained HFB solutions does not guaranty this property [69]. In the treatment of fission, different studies highlight discontinuities of this function similar to the one visible in Fig. 1. In the common ($q_{20}, q_{30}$) space of collective coordinates, a line of discontinuity is present in the vicinity of scission configurations. This feature limits the domain of validity of the collective dynamics and ultimately prevents the determination of the fission fragments characteristics after their complete separation.

Finally, we have seen that most of the current applications of TDGCM+GOA rely on constrained HFB solutions for the generator states. Certain diabatic aspects of the nuclear dynamics are then difficult to grasp with the corresponding GHW many-body wave function. This is the case of the dissipation as well as the viscosity of the shape dynamics predicted with Langevin methods [70, 71] or time dependent Hartree-Fock-Bogoliubov calculations. Past and on going studies to improve the description of these effects include efforts to quantize the Langevin equation [72, 73], to couple the Langevin dynamics with the GCM [74] or to couple TDHFB trajectories with TDGCM [75]. Other techniques such as the SCIM and TDGCM based on time-dependent generator states are also promising avenues that we discuss in this review.

Figure 3: Left hand side: Primary fragment mass yields of Fermium isotopes obtained with the Gogny D1S effective interaction and compared with various experimental data sets after neutron evaporation. The open symbols stand for experimental data associated to spontaneous fission whereas full symbols are related to thermal neutron-induced fission. Reprinted figure with permission from Ref. [65]. Copyright 2019 by the American Physical Society. Right hand side: Effect of temperature on the free energy surface of $^{228}$Th in the plane of deformation ($\beta_{20}, \beta_{30}$). Reprinted figure with permission from Ref. [68]. Copyright 2019 by the American Physical Society.
Intrinsic degrees of freedom are often neglected in the microscopic modeling of the dynamics of reactions. However, the relevance of intrinsic degrees of freedom for the description of $6^+$ states, for example, in isotopes of Ti, Cr, and Fr, has been observed and discussed in [76]. On another topic, the TDHFB/SLDA methods [77, 78] and semi-classical approaches to the description of fission [79, 80] clue that dissipation and, therefore, intrinsic degrees of freedom are necessary to describe the fission fragments properties correctly. Therefore, a few collective degrees of freedom are not enough to adequately model such a reaction. Several paths can be taken to overcome this limitation without resorting to the full resolution of the GHW equation (16). A strategy in development consists in using the TDGCM+GOA with finite-temperature inertia tensors and collective potential. However, the inclusion of statistical mechanics on top of the TDGCM framework still lacks a solid formalization. The idea of the Schrödinger Collective-Intrinsic Model (SCIM) [81–83] is to derive a local Schrodinger-like equation from a generalization of the GHW ansatz (3) that contains individual quasiparticle degrees of freedom. The full SCIM formalism can be found in [81–83] in the stationary case. However, we would like to present here a derivation of the time-dependent SCIM equations consistent with the ones given for the TDGCM and the TDGCM+GOA equations.

A. Main assumptions

The SCIM involves four main assumptions. The first one is the expression of the state $|\Psi(t)\rangle$ that describes the evolution of the many-body wavefunction associated with the reaction. This expression is assumed to be a generalization of the GHW ansatz

$$|\Psi(t)\rangle = \sum_k \int dq |\phi_k(q)\rangle f_k(q,t).$$

(61)

In [82], the authors consider a family of generator states associated with one collective coordinate $q$ defined as the quadrupole moment of the system. The index $k$ iterates over the labels of the sheets of collective space that correspond in this case to two quasiparticle excitations. Fig. 4 shows the evolution of the excitation energies of the non-adiabatic points of the PES of $^{236}$U. Note that the scope of expression (61) is broader. It is used, for example, for $K$-mixing

\[\text{Figure 4: (Color online) Excitation energies as a function of the quadrupole moment constraint } q \text{ and associated with } 2\text{-qp excitations of HFB states. The system under study is } ^{236}\text{U around } \langle\hat{Q}_{20}\rangle = 70 \text{ b (figure a) and } \langle\hat{Q}_{20}\rangle = 325 \text{ b (figure b). The figures are taken from Ref. [81].}\]

in the context of stationary angular-momentum-projected GCM on a triaxial configuration basis. In this case, the index $k$ iterates over the values of $K$. The second assumption is the analyticity of the weight function $f$ of the GCM ansatz (61) that allows the symmetrization of the GHW equations. The third assumption is the vanishing of the weight function and its derivatives at the boundaries of the integration domain. An implicit corollary of this property is the continuity of the functions $q \rightarrow |\phi_k(q)\rangle$. It turns out that this assumption is in practice not verified for a broad
range of applications, for example, in the actinide region, as emphasized in Sec. III C. These three assumptions lead to the symmetrized GHW equation

\[
\sum_k \int ds \, e^{is\mathcal{P}/2} \left[ \mathcal{H}[s]_{lk}(q) - i\mathcal{N}[s]_{lk}(q) \frac{d}{dt} \right] e^{is\mathcal{P}/2} f_k(q, t) = 0, \tag{62}
\]

where the following notations are introduced

\[
\mathcal{H}[s]_{lk}(q) = \mathcal{H}_{lk}(q + s/2, q - s/2)
\]

and where the Hermitian operator

\[
\mathcal{P} = i \frac{\partial}{\partial q} \tag{65}
\]

corresponds to the conjugate moment associated with the collective variables. The symmetrized GHW equation can be written in a more compact operator format as

\[
\int ds \, e^{is\mathcal{P}/2} \left[ \mathcal{H}[s] - i\mathcal{N}[s] \frac{d}{dt} \right] e^{is\mathcal{P}/2} f(t) = 0, \tag{66}
\]

where \(f(t)\) denotes the function \(q \mapsto f_k(q, t)\). The fourth and last assumption of the SCIM is the validity of the truncation of the symmetric moment expansion (SME) of the norm and Hamiltonian kernels of (66) up to order two. It was, for instance, verified numerically in the context of the study [82]. The SME of \(\mathcal{K} = \mathcal{N}, \mathcal{H}\), in the case of one collective variable,

\[
\mathcal{K} = \sum_n \frac{1}{n!} \left\{ \mathcal{K}^{(n)}, \mathcal{P} \right\}^{(n)}, \tag{67}
\]

is obtained through the properties of the so-called Symmetric Ordered Product of Operators (SOPO) \(\{\mathcal{K}^{(n)}, \mathcal{P}\}^{(n)}\) presented in App. B where \(\mathcal{K}^{(n)}\) is the moment of order \(n\) of \(\mathcal{K}[s]\) in the variable \(s\)

\[
\mathcal{K}^{(n)} \equiv i^n \int ds^n \mathcal{K}[s]. \tag{68}
\]

The properties of the SOPO used to obtain these expressions are listed in App. B.

The expression (67) can be generalized to the case of \(P\) collective variables,

\[
\mathcal{K} = \sum_n \frac{1}{n!} \left\{ \mathcal{K}^{(n)}, \mathcal{P} \right\}^{(n)}, \tag{69}
\]

where the index \(n\) iterates over all the \(P\)-tuples of positive integers and where we have introduced the following notations

\[
n! \equiv n_0! n_1! \cdots n_{P-1}! \tag{70}
\]

\[
\{\mathcal{K}, \mathcal{P}\}^{(n)} \equiv \left\{ \cdots \left\{ \{\mathcal{K}, \mathcal{P}_0\}^{(n_0)}, \mathcal{P}_1 \right\}^{(n_1)} \cdots, \mathcal{P}_{P-1} \right\}^{(n_{P-1})} \tag{71}
\]

\[
\mathcal{K}^{(n)} \equiv \int ds \left[ \prod_k (isk)^{n_k} \right] \mathcal{K}[s]. \tag{72}
\]

Their second-order approximation in their SME development is then given by:

\[
\mathcal{N} \approx \sum_{n \leq 2} \frac{1}{n!} \left\{ \mathcal{N}^{(n)}, \mathcal{P} \right\}^{(n)}, \tag{73}
\]

\[
\mathcal{H} \approx \sum_{n \leq 2} \frac{1}{n!} \left\{ \mathcal{H}^{(n)}, \mathcal{P} \right\}^{(n)}, \tag{74}
\]
where \( \mathbf{n} \) is the sum of the elements of \( \mathbf{n} \). In the one-dimensional, the expressions reduce to

\[
N \approx \sum_{n=0}^{2} \frac{N^{(n)}}{n!} \{N^{(n)}, P\}^{(n)}
\]

(75)

\[
\mathcal{H} \approx \sum_{n=0}^{2} \frac{1}{n!} \{\mathcal{H}^{(n)}, P\}^{(n)}.
\]

(76)

**B. Schrödinger Collective-Intrinsic Equation**

The Schrödinger-like expression of the SCIM equations is given by

\[
\left[ \mathcal{H}_{\text{CI}} - i \frac{d}{dt} \right] g(t) = 0,
\]

(77)

where \( g(t) \) is defined according to

\[
g(t) = N^{1/2} f(t)
\]

(78)

and normalized as

\[
g^\dagger(t) g(t) = \int dq q^\ast(q, t) g(q, t) = 1.
\]

(79)

The operator \( N^{1/2} \) is the only positive-definite hermitian square-root of \( N^{1/2} \) and \( N^{-1/2} \) is the inverse of the latter. Finally, using the hermicity of \( N^{-1/2} \), the collective-intrinsic Hamiltonian \( \mathcal{H}_{\text{CI}} \) has the expression

\[
\mathcal{H}_{\text{CI}} = N^{-1/2} \mathcal{H} N^{-1/2},
\]

(80)

An explicit form for \( \mathcal{H}_{\text{CI}}(q) \) is given by

\[
\mathcal{H}_{\text{CI}} = \frac{1}{2} \{\mathcal{U}, \mathcal{P}\}^{(2)} + \{\mathcal{T}, \mathcal{P}\}^{(1)} + \mathcal{V}.
\]

(81)

where the expressions of \( \mathcal{U} = B/2, \mathcal{T} \) and \( \mathcal{V} \) are given in \([81–83]\). By analogy with the TDGCM+GOA collective Hamiltonian (52), the first term of (81) can be interpreted as a kinetic term and \( B \) as the inertia, related to the mass \( \mathcal{M} \) through the relation

\[
B = \mathcal{M}^{-1}.
\]

(82)

Similarly, the third term of (81) is comparable to the potential term of the TDGCM+GOA. However, the last term

\[
\{\mathcal{T}, \mathcal{P}\}^{(1)} = \frac{1}{2} \left[ \mathcal{T} \frac{\partial}{\partial q} + \frac{\partial}{\partial q} \mathcal{T} \right],
\]

(83)

contains first-order derivatives according to the collective variable, at the opposite of the TDGCM+GOA. In the Langevin equations, such a term corresponds to viscosity and arises in the SCIM from the coupling between intrinsic and collective degrees of freedom.

**C. Choice of quasiparticle excitations**

In \([81–83]\), the generator states consist in

- constrained HFB states \( |\phi_{k=0}(q = \langle \hat{Q}_{20} \rangle)\rangle \) describing the compound system at different elongations,
- intrinsic excitations of these HFB states

\[
|\phi_{k>0}(q)\rangle = \hat{X}(q) |\phi_0(q)\rangle.
\]

(84)
Note that the specific expression of $\hat{X}(q)_k$ is never used in the derivations of the Schrödinger-like equation, and it is just assumed that all the states in the collective space are time-reversal to avoid complex-valued overlaps. In practice, the intrinsic excitations taken into account in the existing developments of SCIM are considering 2-qp excitations. The included HFB states are breaking the rotational and particle number symmetries. To avoid restoring these symmetries, the quasiparticle excitations are chosen according to the following rules:

1. the operators $\hat{X}_k$ are two quasiparticles operators,
2. all the states in the collective space have to be time-reversal invariant,
3. the chosen excitations have to preserve “as much as possible” the number of particles and $K$, the projection of the total angular moment on the symmetry axis,
4. and they must be associated with an excitation energy below 10 MeV.

The time-reversal condition limits the possible excitation operators to be

$$\hat{X}(q)_k = \alpha_k \hat{\eta}^{(q)\dagger}_{k_1} \hat{\eta}^{(q)\dagger}_{k_2} - \delta_{k_1, k_2} \hat{\eta}^{(q)\dagger}_{k_1} \hat{\eta}^{(q)\dagger}_{k_2}$$

(85)

$$\alpha_k = \frac{1}{\sqrt{2}} \left( 1 + \delta_{k_1, k_2} \left( 1 - \frac{1}{\sqrt{2}} \right) \right),$$

(86)

where $\hat{\eta}^{(q)\dagger}_{k_1}$ is the creation operator of the quasiparticle $k_1$ associated with the HFB state

$$|\phi_0(q)\rangle = \prod_l \hat{\eta}^{(q)}_l |0\rangle.$$

(87)

The selected quasiparticles in $\hat{X}(q)_k$ are additionally assumed to have the same projection on the total angular moment on the symmetry axis $K_{k_1} = K_{k_2}$ so that the $K$ of the total system is unchanged. In case the HFB states are obtained with preserved parity, the same condition on $\pi$ is added.

The SCIM is a different way to get a local dynamical equation. The resulting Schrödinger-like equation and the corresponding collective-intrinsic Hamiltonian includes a viscosity term known to be relevant for the description of nuclear reaction from Langevin calculations. However, this method did not lead to any application beyond the works presented in [81–83].

V. QUANTUM MIXTURE OF TIME-DEPENDENT STATES

In its standard form, the TDGCM relies on the ansatz Eq. (3) that expands the many-body wave function on a family of time-independent generator states. The dynamics of the system is, therefore, entirely carried out by the time evolution of the collective wave function $g(q)$ driven by Eq. 30. Although successful in describing some nuclear phenomena like collective vibrations, such an expansion suffers from two significant drawbacks.

The first one resides in the large dimension of the ensemble of generator states required to describe processes like nuclear reactions correctly. Despite the efforts reported in Sec. III and IV to reduce the collective Hamiltonian to a local approximation, this high dimension quickly becomes a hurdle to the numerical applications of TDGCM. Part of this difficulty originates from the fact all the many-body configurations populated at all the times of the reaction must be represented in the set of generator states. In many situations, this expansion is not optimal in the sense that most of the associated weights are close to zero at a given time. To give an example, we may consider the translation motion of a localized particle. While the translated states at any positions are to be incorporated in a TDGCM description of its motion, the collective wave function at a given time only has a small spatial expansion. A natural idea is then to express the wave function as a linear superposition of a few time-dependent states that follow the expected translation motion of the particle. It may even happen that one well-chosen time-dependent basis state is enough to describe the dynamics of the system very accurately. The time-dependent energy density functional treatment of the giant resonances in nuclear physics provides such an example [84, 85].

The second drawback of the TDGCM is the construction of a family of generator states before the determination of the system evolution. Only the probability of the system to populate parts of this predefined space is provided by the equation of motion. For this approach to work, the physicist must, therefore, rely on an a priori knowledge of the typical states that are important for the dynamics. For nuclear reactions, it typically means that one should correctly guess what will be the output channels of the reaction and include an ensemble of states representative of these channels in the working space. Beyond the difficulty to generate states representative of the systems far from the initial state, the typical risks of this method are
• to miss important channels/states in the construction of the set of generator states,
• to include states that will not be populated at all but will still increase the numerical cost.

To overcome these difficulties, one solution consists in expanding the ansatz Eq. (3) on a set of time-dependent states as shown schematically in Fig. 5. The many-body wave function of the system now reads

$$\Psi(t) = \int_{q \in E} f(q, t) \phi(q, t).$$  \hspace{1cm} (88)

This very general ansatz brings more flexibility as the configuration basis can now vary in time. However, this flexibility comes with additional complexity in the equation of motion for the collective wave function \(g(q, t)\) and the generator states \(\phi(q, t)\). Studies in both chemistry and nuclear physics are exploring different strategies in the choice of generator states and the determination of the equation of motion of the system. We review these recent efforts in this Section.

A. The multiconfiguration time-dependent Hartree-Fock approach

In 1990, Meyer et al. introduced the multiconfiguration time dependent Hartree (MCTDH) approach to tackle the dynamics of molecules [86]. Contrary to the fermionic many-body problem, the degrees of freedom of the system are distinct from each other and correspond typically to distances between some atoms of a molecule. Their associated wave function is assumed to be at any time a mixture of product states

$$\Psi(x_1, \ldots, x_n, t) = \sum_{i_1=0}^{m_1-1} \cdots \sum_{i_n=0}^{m_n-1} c_{i_1 \cdots i_n} \times \left| \psi_{i_1}(t) \right\rangle \cdots \left| \psi_{i_n}(t) \right\rangle,$$  \hspace{1cm} (89)

where the \(\{ |\psi_{i_k}(t)\rangle \}\) form at any time a basis of the space associated to the \(kth\) degree of freedom and the \(c_{i_1 \cdots i_n}\) are the mixing coefficients between all the product states. The equation of motion of both the individual states and the mixing coefficients can then be obtained from the application of the Dirac-Frenkel variational principle. This method was since applied to different dynamical processes in chemistry [87–89] and up to five degrees of freedom in the treatment of the inelastic cross section of \(\text{H}_2\text{O} + \text{H}_2\) [90]. Note that in 2003, Wang et al. proposed an extension of this method referred to as multilayers MCTDHF to tackle more degrees of freedom (up to a few thousand) [91].
A natural extension of this work to the fermionic many-body problem consists in replacing the product states by Slater determinants in the trial wavefunction. This extension was introduced in Ref. [92] and the new ansatz reads

$$|\Psi(r_1, \cdots, r_n, t)\rangle = \sum_{i_1=0}^{m_1-1} \cdots \sum_{i_n=0}^{m_n-1} c_{i_1 \cdots i_n} |\phi_{i_1 \cdots i_n}(t)\rangle,$$  \hspace{1cm} (90)

with the time-dependent Slater determinants

$$|\phi_{i_1 \cdots i_n}(t)\rangle = \hat{a}_i^\dagger(t) \cdots \hat{a}_n^\dagger(t) |0\rangle.$$  \hspace{1cm} (91)

In this expression, $\hat{a}_i^\dagger(t)$ stands for the fermionic creation operator of a particle in a single-particle state $|\varphi_{ik}(r, t)\rangle$. This many-body wave function can then be injected into a time-dependent variational principle whose parameters are both the mixing coefficients $c_{i_1 \cdots i_n}$ and the single-particle wave functions $|\varphi_{ik}\rangle$. Note that there is no one to one mapping between the many-body state $|\psi(t)\rangle$ and the parameters of the right hand side. In practical applications, the set of single-particle wave function is assumed to be orthonormal at any time.

$$\langle \varphi_i(t) | \varphi_j(t) \rangle = \delta_{ij}$$  \hspace{1cm} (92)

This criteria still let some freedom in the choice of the $c_{ik}$ and $|\varphi_{ik}\rangle$ for a given many-body wave function, and therefore a degree of freedom in their associated equation of motion. A usual convention to fix this freedom consists in imposing the additional constraint

$$\langle \varphi_j(t) | \frac{\partial}{\partial t} | \varphi_i(t) \rangle = 0.$$  \hspace{1cm} (93)

This choice stabilizes the single-particle states against rotations among the occupied states. If such a rotation has to be described, only the mixing coefficients will be affected while the single-particle states will stay constant. This convention yields equation of motions that are often more suited for the numerical time integration.

With this criteria, the Dirac-Frenkel variational principle applied to two-body Hamiltonian system leads to the equation of motion for both the coefficients and the single-particle states

$$i\hbar \hat{\epsilon}_{i_1 \cdots i_n}(t) = \sum_{i_1=0}^{m_1-1} \cdots \sum_{i_n=0}^{m_n-1} \langle \phi_{i_1 \cdots i_n}(t) | \hat{H} | \phi_{i_1 \cdots i_n}(t) \rangle c_{i_1 \cdots i_n}(t)$$  \hspace{1cm} (94)

$$i\hbar |\varphi_n(t)\rangle = \hat{P} \left\{ \hat{\ell} |\varphi_n(t)\rangle + \sum_{pqr}s (\rho^{-1})_{np} \rho^{(2)}_{pqr} \hat{h}_{rs} |\varphi_q(t)\rangle \right\}$$  \hspace{1cm} (95)

where $\hat{\ell}$ is the one-body part of the Hamiltonian, $\hat{h}$ is the mean field potential that implicitly depends on the one-body density, $\rho$ and $\rho^{(2)}$ are the one- and two-body density matrices and $\hat{P}$ is a projection operator on the orthogonal complement of the occupied single-particle states. Such equation of motions have then been numerically solved for chemical systems with six valence electrons [92], to study the two photons ionization of helium [93] or the dynamics of di-molecular molecules [94, 95]. In nuclear physics, the multiconfiguration Hartree-Fock approach has been applied in its static version to determine the structure of light nuclei mostly in the s-d shell [96, 97]. Although it would present an interest to study photoabsorption phenomena in light nuclei or diffusion between light nuclei, this method has not yet been applied in its dynamics version for nuclear physics. Note also that a generalisation of the ansatz (90) to a superposition of Bogoliubov vacua and its corresponding equation of motion is yet to be formalized and tested.

B. Multiconfiguration with time-dependent non orthogonal states

The trial state Eq. (90) at the core of the MCTDHF method expands the wave function on a set of orthonormal Slater determinants. The orthonormality between such generator states simplifies the equation of motion as typically the norm kernel defined in Eq. (6) is the identity at any time. On the other hand, in the same manner as with an expansion on time independent states, it may be more efficient in some situations to expand the many-body wave function on a set of non orthogonal generator states (i.e. time-dependent Bogoliubov vacua with time-dependent deformations). Such a strategy was explored for instance in chemistry by mixing TDDFT trajectories with a shift in time to include memory effect [98] into the dynamics. This approach was proven to correctly include the description of dissipation in the two electrons dynamics of a Hooke’s atom.
On the side of nuclear physics, the idea of mixing time-dependent TDHF trajectories was already proposed in 1983 in the pioneering work of Reinhard et. al. [99] to treat nuclear collisions. Starting back from the ansatz Eq. (90), the authors proposed to take as the time-dependent generator states a set of TDHF trajectories starting from different initial conditions. A time-dependent variational principle is then applied to obtain the equation of motion only for the mixing function \( f(q,t) \) (or the collective wave function \( g(q,t) \)). Such principle is schematically pictured in Fig. 6. The idea behind this scheme is that the TDHF trajectories will carry most of the one-body dynamics of the system whereas the weight function will encompass part of the two-body collisional dynamics, so important to account for additional dissipation and fluctuation. In this paper, a GOA approximation was performed to determine the evolution of the collective wave function on in a one dimensional model of nuclear collision. The results showed in particular that the width of the internal excitation energy of the collision partners after collision were increased by a factor 7 compared to a TDHF trajectory alone.

Although promising, applications of this method to realistic systems were hurdled by the numerical cost associated with TDHF trajectories. But the advances both in numerical methods and the development of supercomputers lately induced a surge of interest for such methods. In particular, the inclusion of superfluidity in our time-dependent mean-field codes [77, 100] opened the possibility to predict collisions between open shell nuclei. Along this line, Scamps et. al. attempted to predict the transfer of pairs of fermions in the contact between two superfluids based on statistical mixing of TDHFB trajectories [101–103]. These semiclassical approaches manage to recover some crucial fluctuation related to the relative gauge angle between the reaction partners. On the other hand, they miss the quantum interference between the TDHFB trajectories. Depending on the details of the methods this may either lead to underestimating fluctuations of one-body observables or in the worse case predicting unphysical behavior such as particle transfer after the re-separation of the two reaction partners.

Coming back to a full quantum treatment of the problem, Regnier et. al. attempted recently the full fledged mixing of TDHFB trajectories in Ref. [104]. In this context, the time dependent variational principle on the ansatz Eq. 90 leads to the equation of motion of the collective wave function \( g(q,t) \)

\[
\frac{i\hbar}{\epsilon} \frac{\partial}{\partial t} g = \left( \hat{H} - \hat{D} + i\hbar \frac{\partial N^1/2 N^{-1/2}}{\partial t} \right) g. \tag{96}
\]

This equation involves the collective operators \( \hat{H} \) and \( \hat{D} \) defined by applying Eq. 28 to the kernels:

\[
\hat{H}(q,q') = \langle \phi(q,t) | \hat{H} | \phi(q',t) \rangle, \tag{97}
\]

\[
\hat{D}(q,q') = \langle \phi(q,t) | i\hbar \frac{\partial}{\partial t} | \phi(q',t) \rangle. \tag{98}
\]

Note that all the kernels and collective operators involved now depend on time. Compared to the TDGCM on static generator states (Eq. (30)), this equation contains two additional terms. The first one contains the time derivative of the generator states whereas the second one is linked to the time derivative of the norm kernel. These equations were numerically solved in a simple case modeling a contact between two superfluid systems. This study showed that such a method correctly recovers the quantum fluctuations missed in the statistical approaches.
At a time where performing series of independent time-dependent mean-field calculations in nuclear physics becomes possible, such a method could be a good candidate to tackle nuclear reactions with a complex interplay between one-body and many-body degrees of freedom. The caveat to its direct application on a realistic nuclear collision would still be the difficulty that current implementations of the nuclear mean-field dynamics formalisms rely on energy density functionals and not a Hamiltonian (cf. Sec. II E).

VI. CONCLUSION

This review presents four variants of the Time-Dependent Generator Coordinates Method that is rooted in a configuration-mixing principle. This class of methods is of particular interest to microscopically describe heavy-fermions systems. It allows the physicist to focus the description on the correlations of interest through the choice of the collective coordinates. Most of the time, the collective coordinates are related to some of the first multipole moments of the intrinsic one-body density or some groups of symmetry operators. Such freedom makes the TDGCM extremely versatile. On the other hand, its practical applications in nuclear physics are plagued by the usage of effective Hamiltonians or energy density functionals that lead to misbehaviors of the energy kernel, an essential ingredient shared by all the TDGCM approaches.

The Time-Dependent Generator Coordinate Method is the most direct implementation of the configuration-mixing principle. In this case, the only approximations are the expression of the nuclear Hamiltonian, and the restriction of the total Fock space to the one spanned by the configuration basis. The Griffin-Hill-Wheeler (GHW) equation (3) is the corresponding equation of motion. The main limitation of this method arises from the non-locality of the GHW equation in the collective coordinates representation, leading to intensive parallel computation. By resorting to some approximations, it is possible to rewrite the GHW equations into local equations, reducing hereafter substantially the calculation needs. The Gaussian Overlap Approximation (GOA) transforms the GHW equations to a local Schrodinger-like equation essentially under the condition that the norm kernel is of Gaussian character. The TDGCM+GOA is the most widely used implementation of the TDGCM for the description of nuclear reactions and especially for fission. The Schrodinger Collective-Intrinsic Method is based on the truncation of the GHW equation at the second order to obtain a local Schrodinger-like equation. In its current form, it still requires to calculate the full norm and Hamiltonian kernels. Finally, it is possible to generalize the standard TDGCM approach by expanding the many-body wave function on a set of time-dependent generator states. The recent progress of TDHFB solvers opens new possibilities for practical applications along this line.

Overall, most of these methods were first developed in the 1980’s, at a time when they were quickly facing untractable numerical costs. The computational power at our disposal nowadays is an incentive to revisit the TDGCM approaches and look for new opportunities in its description of nuclear reactions. One of the major challenge in this path is the determination of energy density functionals or effective Hamiltonians both compatible with the GCM formalism and yielding quantitative predictions of nuclear observables.

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Appendix A: Expression of the GOA moments

The expression Eq. (58) involves some moments $M^{(K)}$ and $\tilde{M}^{(K)}$ that we define here. We recall that we consider generator states that are Bogoliubov vacua. Any generator state is then fully characterized by its generalized density matrix $\mathcal{R}(q)$.

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$$  \(\text{(A1)}\)
In addition, each collective coordinate $q_i$ is associated to a one-body observable $\hat{Q}_i$ that is used as a constraint. In the basis of quasiparticles that diagonalizes $\mathcal{R}(q)$, this operator takes the matrix form

$$Q_i = \begin{bmatrix} Q_{i1}^{11} & Q_{i2}^{12} \\ Q_{i1}^{21} & Q_{i2}^{22} \end{bmatrix}$$

(A2)

In the same basis one can define the standard QRPA matrix $\mathcal{M}$ as detailed in Ref. [16]. With these notations, the moments $M^{(K)}$ involved in the determination of the GOA inertia and metrics are

$$M_{ij}^{(K)} = \frac{1}{2}(Q_i^{12*}, Q_i^{12})\mathcal{M}^{-K} \begin{pmatrix} Q_j^{12} \\ Q_j^{12*} \end{pmatrix},$$

(A3)

We also define here the modified moments $\tilde{M}^{(K)}$ by

$$\tilde{M}^{(K)} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} M^{(K)} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

(A4)

**Appendix B: Bestiary of SOPO properties**

The Symmetric Ordered Product of Operators (SOPO) are defined, for any two operators $A$ and $B$, as

$$\{A, B\}^{(n)} = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} B^k A B^{n-k}.$$  

(B1)

They can be equivalently defined recursively through their relation with the anti-commutator

$$\{A, B\}^{(1)} = \frac{1}{2} \{A, B\}$$

(B2)

$$\{A, B\}^{(n+1)} = \frac{1}{2} \{\{A, B\}^{(n)}, B\}.$$  

(B3)

The SOPO are used to obtain the Symmetric Moment Expansion (SME) of the symmetrized GHW equation (66), based on

$$e^{\alpha B/2} A e^{\alpha B/2} = \sum_{p=0}^{\infty} \frac{\alpha^p}{p!} \{A, B\}^{(p)},$$

(B4)

For any operators $A$, $B$ and $C$, the following relation is satisfied

$$A \{B, C\}^{(n)} = \sum_{k=0}^{n} \binom{n}{k} B^{A,C} \{B, C\}^{(k)},$$

(B5)

where the operators $B^{A,C}_{(n,k)}$ are given by

$$B^{A,C}_{(n,k)} = \frac{i^{n-k}}{2^{n-k}} \sum_{r=0}^{n-k} \left\{ (-1)^r \binom{n}{k+r} \binom{k+r}{r} A^{[r]} \ B \ C^{[n-k-r]} \right\},$$

(B6)

and where $A^{[r]}$ the short-hand notation for the local operator associated with the kernel

$$A^{[r]}(q) = \frac{\partial^r A}{\partial q^r}(q).$$

(B7)

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