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Dynamical models for fragment formation

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Abstract. The various dynamical models for fragment formation in nuclear collisions are discussed in order to bring out their relative advantages and shortcomings. After discussing the general requirements for dynamical models that aim to describe fragment formation, we consider the various mean-field models that incorporate fluctuations and then turn to models based on molecular dynamics.

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1 Introduction

Nuclear collisions in the medium-energy regime (from several tens to several hundreds MeV/nucleon) typically yield several intermediate-mass fragments (IMFs) (see Tamain [1]). Thus, at relatively low energies dissipative binary reactions may create IMFs at midrapidity, while higher-energy central collisions create expanding systems that produce clusters copiously; and peripheral collisions produce excited projectile-like fragments that multifragment. The IMFs typically carry a major part ($\sim 50\%$) of the nucleons involved.

Since the fragments are formed in dynamical reactions where equilibrium is not guaranteed *a priori*, there is a need for developing microscopic dynamical descriptions for fragment formation. This poses a significant theoretical challenge because of the basic quantal nature of the many-body nuclear system. Although it is possible to derive such models by truncating a hierarchy of quantum many-body equations, it is difficult to ensure that the error would remain small throughout the rather long duration of fragmentation reactions. Therefore, most of the currently employed models have been developed by performing certain drastic simplifications while seeking to retain a quantitatively useful description for those aspects that are deemed to be of most interest. Consequently, models with different characteristics have been developed and applied to fragmentation reactions with reasonable successes in specific cases.

The purpose of this paper is to summarize the main requirements for models that aim to describe fragment formation and to elucidate their relative merits and shortcomings. First, sect. 2 discusses those model features that are of largest importance. Then, within that framework, we discuss in sect. 3 models that have been developed on the basis of mean-field theory, while sect. 4 covers those that involve molecular dynamics.

Since this paper focuses on fragment formation, we do not intend to evaluate the overall utility of individual models. Indeed, treatments that do not seek to describe fragment formation, such as the nuclear Boltzmann equation (see Fuchs and Wolter [2]) are not addressed here, even if they may have proven to be very important generally for the study of heavy-ion reactions. (An early guide to microscopic models for intermediate-energy nuclear collisions was given in ref. [3].) Neither does this paper cover the statistical models for fragment formation (see Botvina and Mishustin [4]) which provide us with a powerful tool for understanding fragmentation.

2 General requirements

We discuss here the general features that are required by any dynamical model aiming to describe nuclear fragmentation.

2.1 General framework for the time evolution

Ideally, any such model should be derivable from the underlying quantum many-body description by means of well-defined approximations. Most of the models for nuclear dynamics are based on the mean-field picture, exemplified by the time-dependent Hartree-Fock (TDHF)

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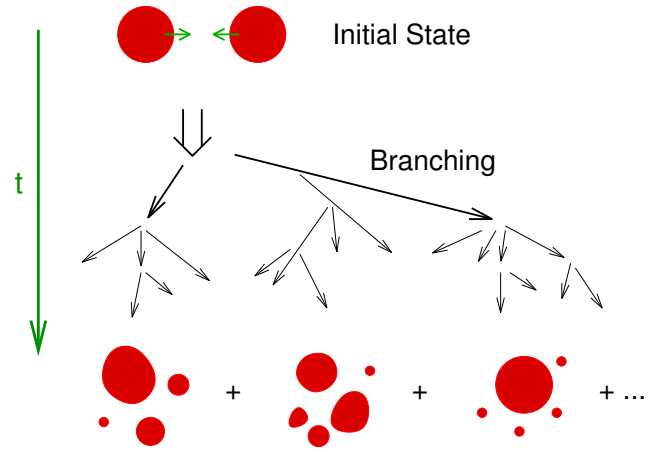

Fig. 1. A schematic picture of a fragmentation reaction in which a given initial channel may develop into many different fragmentation channels during the dynamical evolution.

treatment or its semiclassical analogue, the Vlasov equation. However, the direct two-nucleon collisions grow increasingly important when the collision energy reaches and surpasses the Fermi energy, as the Pauli exclusion principle becomes ever less effective in blocking the two-nucleon collisions. Therefore, the models should incorporate both single-particle motion in a mean field and Pauli-suppressed two-nucleon collisions. This is indeed the case for most of the models discussed here.

2.2 Dynamical bifurcations

The most important special challenge associated with fragmentation is the occurrence of dynamical bifurcations, the feature that a given initial configuration may lead to many different fragmentations, as illustrated in fig. 1. Since the number of final channels is huge, even if only the most important fragmentations are considered, a standard coupled-channel treatment would be practically impossible. On the other hand, this very feature makes it natural to employ concepts and methods from transport theory. Consequently, most models involve some stochastic agent as a simple way to produce spontaneous fluctuations and the associated trajectory branchings.

2.3 Basic quantum statistics

Any quantitatively useful model of nuclear systems must take account of the basic quantum-statistical feature that causes Pauli blocking and endows the nucleons with Fermi motion. Therefore, the initial nucleon momenta are usually sampled from a Fermi distribution, even if the specific model does not inherently contain such a feature. This ensures that the one-body phase-space density is reasonably consistent with the corresponding single-nucleon wave functions. Furthermore, the final states of the direct two-body collisions are usually suppressed by suitable Pauli-blocking factors, thus helping to prevent the nucleons to revert to the Maxwell-Boltzmann form characteristic of classical systems. Even though the various models tend to include these basic features, the specific manner in which this is actually done varies greatly from one model to another.

2.4 Macroscopic nuclear properties

The dynamical models should have stationary solutions that reproduce the most important macroscopic nuclear properties, such as density distributions and binding energies, whereas shell and pairing effects are not very important because the produced fragments are usually excited by several MeV/nucleon. This requirement can be met if the model yields proper values of the nuclear saturation density and the associated binding energy (including its isospin dependence), together with especially the nuclear surface tension. It is thus important that these key quantities be known for the various models.

2.5 Thermal nuclear properties

Because of the complexity of the fragmentation process, statistical features play a large role in determining the relative fragment yields. It is therefore quantitatively important that the nuclear level densities, as reflected in the specific heat, have realistic magnitudes. In particular, in a quantum system the excitation energy grows quadratically with temperature, $E^* = aT^2$, while the relation tends to be linear in a classical system. The desirability of this characteristic property poses a significant problem for the dynamical models and, as we shall discuss, most models are inadequate in this particular regard.

2.6 Interactions

It is preferable that the models contain only a minimal number of parameters. In fact, the mean-field Hamiltonian should in principle be known from static nuclear properties and thus not be subject to adjustment. It is in the context of fragment production especially important that the employed interaction yields a liquid-gas phase transition in uniform matter.

With regard to the residual two-body interaction, it is most often represented by means of differential scattering cross-section which may, in principle, be modified by the local density and temperature. Although such medium modifications might be calculable, they may also be taken as somewhat adjustable.

In any case, both the long-range interaction responsible for the mean field and the residual interaction causing the collisions should already have been fixed from applications that do not involve fragmentation. So, consequently, there should ideally be no new parameters associated with the treatment of fragmentation processes.

2.7 Particle emission from hot nuclei

The fragments produced after the violent stage of the reactions are still excited by typically several MeV/nucleon. Such fragments de-excite by light-particle emission over a time scale that is very long in comparison with that of the collision. Although it would be impractical to propagate the dynamical models for such long times, it would still be desirable that the models in principle describe the de-excitation processes. However, this is generally not the case, in large part because of the rather rough character of the dynamical models relative to the more refined treatments required for such emission processes. Indeed, the proper description of particle emission from hot nuclei usually requires a quantum-mechanical treatment. Therefore, when particle-stable fragments are needed, it is necessary to apply suitable de-excitation treatments to each of the (pre)fragments formed in the course of the collision.

2.8 Correlations and fragmentation mechanisms

It is desirable that the models can describe many-body correlations beyond those of the mean-field description. This is particularly important for a proper description of light fragments, such as alpha particles. One of the most important advantages of treatments based on molecular dynamics is that such correlations are included automatically (though not necessarily correctly, of course). It is important to recognize that one-body models also contain non-trivial correlation features when augmented by a stochastic agency that produces an entire ensemble of one-body systems from a single initial configuration. Thus, while the mean-field models may not be suitable for the description of very light fragments, they may be quite reasonable for fragments that lend themselves to a mean-field description, such as typical IMFs.

3 Mean-field models with fluctuations

Significant advances in our understanding of nuclear dynamics have been achieved within the mean-field framework. Just as the Hartree-Fock treatment provides a useful starting point for the discussion of static nuclear properties, its time-dependent version, TDHF, presents a good conceptual starting point for the treatment of nuclear dynamics. An early study of multifragmentation within the TDHF framework was made by Knoll and Strack [5], who considered the evolution of individual Slater determinants that had been sampled from a statistical ensemble representing a hot source.

The main shortcoming of pure mean-field treatments is the omission of the short-range residual interaction. An attempt to include this important physical ingredient is presented by the stochastic TDHF model [6] in which the many-body system continually jumps from one Slater determinant to another. Though conceptually appealing, this approach has not yet been developed into a practical tool (but it provides a basis for deriving the Boltzmann-Langevin treatment discussed below).

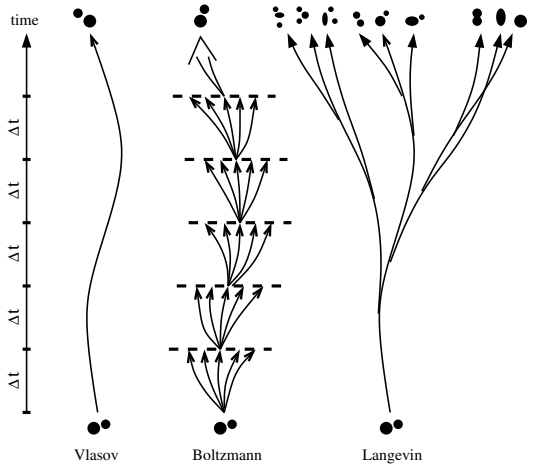

Fig. 2. Characterization of dynamical models. The various semiclassical treatments of microscopic nuclear dynamics can be characterized by the manner in which the single-particle phase-space density is being propagated from one time step to the next. In the Vlasov treatment, the particles experience only the self-consistent effective field, leading to a single dynamical history $f(\boldsymbol{r}, \boldsymbol{p}, t)$. At the Boltzmann level, the various possible outcomes of the residual collisions are being averaged at each step, leading then to a different but still single dynamical trajectory. Finally, the Boltzmann-Langevin model allows the various stochastic collision outcomes to develop independently, thus leading to a continual trajectory branching and a corresponding ensemble of histories.

Indeed, the residual interaction is more readily included within the framework of semi-classical descriptions of the Nordheim type [7], often referred to as Boltzmann-Übling-Uhlenbeck (BUU) or Vlasov-Übling-Uhlenbeck models, in which the collisionless mean-field evolution is augmented by a Pauli-blocked Boltzmann collision term. There are various techniques for solving the nuclear Boltzmann equation. One common approach introduces a (usually large) number of pseudo-particles for each nucleon present, $\mathcal{N}$, with correspondingly reduced interacting cross-sections. This method makes it possible to achieve an arbitrarily fine coverage of phase space and, in principle, the resulting solution approaches the exact solution as $\mathcal{N}$ is increased. However, it requires a fairly cumbersome programming to prevent the computational task from increasing quadratically with $\mathcal{N}$. Therefore, it is often preferable to use the parallel-ensemble method, in which $\mathcal{N}$ individual A-body systems are treated in parallel in a common mean field that is obtained by averaging, at each time, over the $\mathcal{N}$ systems (see fig. 2). This treatment retains some correlation, so although it does not converge to the Boltzmann solution it may well present a more useful model.

In the standard Boltzmann treatment, only the average effect of the collisions between the particles is included, thus yielding a deterministic evolution of the one-

particle phase-space density $f(\boldsymbol{r},\boldsymbol{p})$ (see fig. 2). While this simplification may be suitable in many physical scenarios in which the macroscopic dynamics is stable (such as the early stages of a nuclear collision when the system is hot and compressed), it is inadequate for processes involving instabilities, bifurcations, or chaos. In particular, if the combined expansion and cooling brings the system into the spinodal zone of the phase diagram, it is essential to admit the occurrence of fluctuations and allow their subsequent self-consistent development.

Various attempts to overcome this problem have been made. On the more formal side, transport theory was invoked to treat the effect of many-body correlations as a stochastic process and thus derive a transport equation for the one-particle phase-space density $f(\boldsymbol{r},\boldsymbol{p})$ [8–10]. In particular, in ref. [10] the general transport equation was reduced to coupled equations for the mean evolution of $f(\boldsymbol{r},\boldsymbol{p})$ and its fluctuations around this average trajectory. The evolution is then determined by the transport coefficients, namely the *drift* coefficients $V[f](\boldsymbol{r},\boldsymbol{p})$ that govern the average change of $f(\boldsymbol{r},\boldsymbol{p})$ (and is given by the usual Boltzmann equation) and the *diffusion* coefficients $D[f](\boldsymbol{r},\boldsymbol{p};\boldsymbol{r}',\boldsymbol{p}')$ governing the correlation between changes at two different phase-space locations. These coefficients are given in terms of the differential cross-section and this fundamental relationship ensures that they satisfy the fluctuation-dissipation theorem. While this approach yields a more exhaustive description, it is applicable only when the dynamics is macroscopically stable so all dynamical histories remain fairly similar.

However, in many situations of actual interest in heavy-ion physics, such as multifragmentation processes, the dynamical trajectories branch into configurations that are qualitatively different, as illustrated in fig. 2. It is therefore necessary to devise methods that can admit and propagate arbitrary fluctuations. This need has led to the development of the nuclear Boltzmann-Langevin (BL) model which is briefly described below.

3.1 Boltzmann-Langevin model

The Boltzmann-Langevin equation of motion for $f(\boldsymbol{r},\boldsymbol{p})$ can be written on a condensed form as [11,12]

$$\dot{f} \equiv \frac{\partial f}{\partial t} - \{h[f], f\} = C[f] \equiv \bar{C}[f] + \delta C[f]\,. \qquad (1)$$

Here the mean-field evolution of $f(\boldsymbol{r},\boldsymbol{p})$ on the left is governed by the effective one-body Hamiltonian $h[f](\boldsymbol{r},\boldsymbol{p})$, which depends self-consistently on $f(\boldsymbol{r},\boldsymbol{p})$. The collision term $C[f]$ on the right represents the effect of the two-body collisions and is therefore stochastic in nature. As such, it can be separated into its average, $\bar{C}[f]$, which is the term retained in the standard Boltzmann equation, and its fluctuating part, $\delta C[f]$. The two parts can be expressed in terms of the elementary collision process $\boldsymbol{p}_1\boldsymbol{p}_2 \rightarrow \boldsymbol{p}_1'\boldsymbol{p}_2'$, for which the expected number of occurrences within a small time interval, $\bar{\nu}$, is equal to the associated variance σ_ν^2, as in a standard random walk. This fundamental relationship leads to the fluctuation-dissipation theorem.

After it had been demonstrated [11] that the fluctuating collision term $C[f]$ produces the correct quantum-statistical equilibrium fluctuations and correlations in a uniform gas, the transport theory was turned into a practical tool by the development of a numerical method for the direct simulation of the stochastic part $\delta C[f]$ [12]. With this model, the dynamical clusterization in the presence of instabilities was then addressed [13] and explicit numerical studies were made for two-dimensional matter in the phase-space region of spinodal instability. The fluctuating part of the collision term acts as a source of irregularities in the density which may then be amplified by the self-consistent mean field. The corresponding dispersion relation (the growth rate $\gamma_k = 1/t_k$ as a function of the wave number of the distortion) was extracted from the numerical simulations and shown to exhibit a maximum which identifies the characteristic length scale for the clusterization, as reflected in the Fourier transform of the spatial density. A more detailed treatment of the linear response in stochastic mean-field theories and the onset of instabilities was subsequently made [14].

It thus appears that the Boltzmann-Langevin model offers a suitable one-body framework for the study of unstable nuclear dynamics, such as fragmentation processes. Nevertheless, it appears that an accurate description of the agitation of unstable modes in nuclear matter generally requires the inclusion of memory time effects resulting from the basic quantal nature of the system [15].

Furthermore, the numerical treatment of the fluctuating collision term presents a formidable challenge and is not yet feasible in three dimensions. Therefore a number of approximate treatments have been developed. However, typically, these approaches introduce the fluctuations by fiat in a manner that is inconsistent with the general relaxation properties of the one-body density, as expressed through the fluctuation-dissipation theorem. We discuss those various approaches in the following.

3.2 Brownian one-body dynamics

A powerful approximate treatment of the BL model was obtained by approximating the effect of the fluctuating part of the collision term, δC, by that of a suitable stochastic one-body potential, $\delta U(\boldsymbol{r},t)$,

$$\delta C[f] \rightarrow -\delta\boldsymbol{F}[f]\cdot\frac{\partial f}{\partial \boldsymbol{p}}\,, \qquad (2)$$

with the Brownian force $\delta\boldsymbol{F} \equiv \partial\delta U/\partial\boldsymbol{r}$ being tuned at each point in time and space to ensure that the dynamics of important collective modes emulates the results of the complete Boltzmann-Langevin model [16].

In the resulting Brownian one-body (BOB) model for nuclear dynamics, the stochastic force is adjusted to ensure the correct growth of the fastest-growing unstable spinodal mode, as obtained by making a local-density approximation. Since the local adjustment of the Brownian

force can be made on the basis of simple analytical approximations [17,18], the BOB scheme can be implemented by making a relatively straightforward modification of a standard BUU code [16], thus providing a powerful tool for studies of fragment formation.

The BOB model was subsequently applied to dynamical scenarios where spinodal fragmentation occurs. One study considered the multifragmentation of an initially compressed gold nucleus [19] and found, in accordance with an earlier BUU-based study [20], that the system quickly expands into a hollow and unstable configuration, where the irregularities resulting from the stochastic force are then amplified by the self-consistent mean field, resulting in several intermediate-mass fragments, together with a large number of unbound nucleons.

It thus appears that the stochastic mean-field model framework is suitable for the treatment of nuclear fragmentation dynamics, provided that the self-consistent propagation of fluctuations has been suitably incorporated.

3.3 Other approximate Boltzmann-Langevin methods

An attempt to introduce spontaneous fluctuations in a practically realizable manner was made by Bauer *et al.* [21]. Their method can be implemented relatively easily into standard BUU codes that use the pseudo-particle method of solution and it consists essentially in forcing similar two-body collisions to occur for neighboring pseudo-particles so that effectively two entire nucleons are involved in each particular collision event. Employing an idealized two-dimensional nucleon gas as a test case, Chapelle *et al.* [22] examined this intuitively appealing method. They found that it is able to produce fluctuations of the correct general magnitude, provided that a suitable coarse graining of the phase space is performed, and that these display some of the correlation features expected from the basic characteristics of the two-body collision process. These features can be improved by suitable tuning of the phase-space metric (the concept of a distance in phase space is required for the selection of the "neighboring" pseudo-particles). However, for any tuning, the detailed momentum dependence of the variance in phase-space occupancy deviates significantly from what is dictated by quantum statistics. Therefore this simple prescription may be unsuitable for problems in which these properties are important.

On a more formal basis, Ayik and Gregoire [9] proposed an approximate method for numerical implementation of the Boltzmann-Langevin theory. The method reduces the Boltzmann-Langevin equation for the microscopic one-body phase-space density $f(\boldsymbol{r},\boldsymbol{p})$ to stochastic equations for a set of macroscopic variables, namely the local or global quadrupole moment of the momentum distribution. A random change of the quadrupole moment is then made at each time step and a suitable stretching of $f(\boldsymbol{r},\boldsymbol{p})$ is performed subsequently in order to reconstruct the entire phase-space density. This method was also examined by in ref. [22] and, although several variations of the proposed scheme were examined, it was generally found that the results were far from satisfactory, since the resulting correlations associated with the fluctuating one-body density will tend to reflect the symmetries and other characteristics of the employed reconstruction procedure rather than those of the underlying physical fluctuations. Therefore this method appears unsuitable for calculating quantities that depend sensitively on the details of the momentum distribution.

For the purpose of addressing catastrophic phenomena in nuclear dynamics, such as multifragmentation, Colonna *et al.* [23] explored the possibility of simulating the stochastic part of the collision integral in the Boltzmann-Langevin model by the numerical noise $\sigma_k(0)$ associated with the finite number of pseudo-particles $\mathcal{N}$ employed in the ordinary BUU treatment. This idea is based on the observation that for large times, $t \gg t_k$, the fluctuation of density undulations of a given wave number k is given by $\sigma_k^2(t) = D_k t_k \mathrm{e}^{2t/t_\nu}$ in the Boltzmann-Langevin treatment, whereas it is $\sigma_k^2(t) = (D_k t_k/\mathcal{N} + \sigma_k(0))\mathrm{e}^{2t/t_\nu}$ in the BUU pseudo-particle treatment. Since $\sigma_k(0)$ also scales as $1/\mathcal{N}$, the matching of those two asymptotic fluctuations yields a relation determining the value of $\mathcal{N}$. For idealized two-dimensional matter, which presents a suitable test case, as it is here practical to simulate the Boltzmann-Langevin equation directly, they demonstrated that $\mathcal{N}$ can be adjusted so that the corresponding BUU calculation yields a good reproduction of the spontaneous clusterization occurring inside the spinodal region. This approximate method may therefore provide a relatively easy way to introduce meaningful fluctuations in simulations of unstable nuclear dynamics. This method was subsequently extended to 3D nuclear matter, allowing the direct extraction of the growth times t_k of the unstable modes and the associated diffusion coefficients D_k [24].

Guarnera *et al.* [25] studied the spinodal fragmentation of a hot and dilute nucleus by first expanding the system into a spinodally unstable configuration and then adding a stochastic density fluctuation that is carefully tuned to reflect the degree of fluctuation in the most unstable mode, as determined by the corresponding linear-response analysis of the unstable sphere. They found that the early clusterization appears to be dominated by unstable modes whose spatial structure is similar to the fastest growing spinodal modes in infinite matter at similar density and temperature. They followed the development of the instabilities until multifragmentation had occurred and then made an analysis of the resulting fragment size distribution. As expected from the fact that only a few modes dominate, the clusterization pattern has a large degree of regularity which in turn favors breakup into fragments of nearly equal size, with a corresponding paucity of small clusters.

Subsequently, Colonna *et al.* [26] introduced a method that roughly approximates the Boltzmann-Langevin model by adding a suitable noise to the collision term in the usual BUU treatment. The noise employed corresponds to the thermal fluctuation in the local phase-space occupancy, $\sigma_f^2(\boldsymbol{r},\boldsymbol{p}) = f(1-f)$, where $f(\boldsymbol{r},\boldsymbol{p})$ is the local

Fermi-Dirac equilibrium distribution. By performing such a local momentum redistribution at suitable intervals in the course of the evolution, the inherently stochastic nature of the two-body collision processes is mimicked. The method has the advantage that it is readily tractable and it applies equally well to both stable and unstable parts of the phase diagram. The method has been applied to multifragmentation in central collisions in the Fermi energy domain [27], showing spinodal decomposition in expanding systems.

A different approach was taken by Matera and Dellafiore [28] who applied white noise to a Vlasov system. The noise term was determined self-consistently by invoking the fluctuation-dissipation theorem and, within the linear approximation, the time evolution of the density fluctuations was found to be given by the same closed form as was found in ref. [14]. The authors showed that while a white-noise form of the stochastic field is in general *not* consistent with the fluctuation-dissipation theorem, it may provide a good approximation when the free response function is sufficiently peaked.

It is important to note that all of the methods described above employ an *ad hoc* procedure to generate fluctuations. Therefore the microscopic structure in phase space of the produced correlations is typically very different from the prediction of the Boltzmann-Langevin model. However, as stressed first in ref. [23], in situations where the dynamics is dominated by only a few modes (such as the fastest growing spinodal modes) it may suffice to require equivalence with the exact Boltzmann-Langevin approach for only those few degrees of freedom. As a consequence, some of the approaches [23–25] have carefully designed the fluctuation source so as to mimic the effects of the stochastic Boltzmann-Langevin term on the dynamics of the most unstable modes and the main dynamics of the spinodal decomposition can then be simulated.

Several studies aimed directly at cases of experimental interest [25,29,30] have found that central collisions of Xe and Sn should lead to spinodal fragmentation and display corresponding correlations in the resulting IMF sizes (see Borderie and Désesequelles [31]). This system has been investigated experimentally at INDRA [32] and a signal in quantitatively good agreement with the transport calculations was indeed observed. A comprehensive review of nuclear spinodal fragmentation was given in ref. [33].

3.4 Drawbacks of mean-field dynamics

The mean-field models treat the reduced single-particle phase-space density $f(\boldsymbol{r},\boldsymbol{p})$ and they are therefore most suitable for the calculation of quantities that can be expressed as expectation values of one-body observables. But the extraction of more complicated observables (such as two-body correlations) is problematic. This inherent problem is particularly evident when fragmentation processes are considered. For example, any emerging "fragments" need not have integer particle numbers. Fortunately, this principal problem is usually unimportant in actual applications, especially when the observables of interest can be expressed in terms of moments of the mass distribution (such as the mean IMF charge).

In this connection, it is important to recognize that although mean-field models treat only the one-body phase-space density, the stochastic versions generate entire ensembles of one-body densities. Therefore, insofar as the different fragmentations may each be satisfactorily described within the one-body framework, stochastic one-body models may in fact be well suited for multifragmentation processes.

Although quantum statistics is taken into account by the inclusion of the appropriate Fermi blocking or Bose enhancement factors in the collision term, the numerical treatments are generally classical in nature and, consequently, the occupation coefficients will eventually revert to their classical (Maxwell-Boltzmann) form. (This feature was discussed in refs. [34,35] for Vlasov dynamics.) Fortunately, because the associated time scale is usually fairly long, this principal problem is of little practical import for applications to nuclear collisions. But it does make it somewhat tricky to use the models to study equilibration phenomena.

A common problem with existing semi-classical one-body microscopic models of nuclear dynamics is their failure to provide an accurate description of the thermal properties of ordinary nuclei at only moderate excitation. As a consequence of this and the basically classical nature of the equations of motion, the de-excitation of produced prefragments is not well described and to make contact with experiment it is necessary to switch from the dynamical model to an "afterburner" that treats the de-excitation of each individual prefragment. This problem is also commonly encountered with molecular dynamics.

4 Molecular dynamics

A more direct connection to the observable physical states is provided by the molecular-dynamics many-body models. These models have been developed to ever higher levels of refinement and we can here give only a rough overview with some illustrative examples.

4.1 Classical molecular dynamics

Generally, classical molecular dynamics (CMD) solves the classical equation of motion for the positions and momenta of A particles,

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r}_i = \{\boldsymbol{r}_i, \mathcal{H}\}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{p}_i = \{\boldsymbol{p}_i, \mathcal{H}\}\,, \tag{3}$$

where the many-body Hamiltonian is of the form

$$\mathcal{H}\{\boldsymbol{r}_n, \boldsymbol{p}_n\} = \sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m_i} + \sum_{i<j} V(|\boldsymbol{r}_i - \boldsymbol{r}_j|)\,. \tag{4}$$

The nucleon-nucleon potential $V(r)$ (which may depend on the particle species) generally consists of a short-range

repulsive part and a long-range attractive part, so that the resulting matter equation of state (EOS) is of the Van der Waals type. The work by Lenk and Pandharipande [36, 37] provides a good illustration of this type of model.

The CMD equation of motion is entirely deterministic. Nevertheless, the collision dynamics has a chaotic character so that small differences in the initial states may lead to quite different final states. This feature automatically gives access to many fragmentation channels. Furthermore, while it is hard to justify CMD as a good approximation for the dynamics of the nuclear many-body quantum system, CMD does have the virtue of retaining all the orders of many-body correlations at the classical level.

Indeed, CMD simulations have provided useful insight into the general features of fragmenting finite systems, such as critical phenomena [38], phase evolution [39], the caloric curve [40] and isoscaling [41]. The character of the fragment emission has also been elucidated [42]. A particularly intriguing result was obtained by Dorso *et al.* [43] who employed a criterion that considers the binding of each particle in its host cluster and found that the fragment size distribution may be extracted rather early, already when the system is still quite dense.

4.2 Quasi-classical molecular dynamics

One of the problems with classical molecular dynamics for nuclear systems is that the fermion nature of the nucleons cannot readily be incorporated. Indeed, in the ground state of the classical Hamiltonian $\mathcal{H}$ all particles have vanishing velocities. This basic feature makes it hard to emulate the most basic features of nuclear systems.

One partial remedy for this problem is the introduction of a so-called Pauli potential, a momentum-dependent repulsion that serves to emulate the exclusion principle, as first proposed by Wilets *et al.* [44,45].

This approach was pursued in more detail by Dorso *et al.* [46] with a Gaussian repulsion depending on the phase-space separation s_{ij}, with $s_{ij}^2 = r_{ij}^2/q_0^2 + p_{ij}^2/p_0^2$. They first demonstrated that such a repulsion leads to a reasonable emulation of the Fermi-Dirac momentum distribution in thermal equilibrium, over a broad energy range of interest [46]. Furthermore, when augmented by a Lennard-Jones potential, the model yields a reasonable reproduction of the nuclear equation of state and hence appears to be suitable for instructive simulations of nuclear collisions [47]. Indeed, a first application to an initially compressed and heated nucleus allowed the extraction of its thermodynamic phase evolution, showing that the spinodal region was entered, and the resulting fragmentation exhibited characteristic signs of filamentation [39].

4.3 Quantum molecular dynamics

It is possible to go beyond deterministic molecular dynamics by introducing a Pauli-blocked collision term in a manner similar to what is done in the nuclear Boltzmann

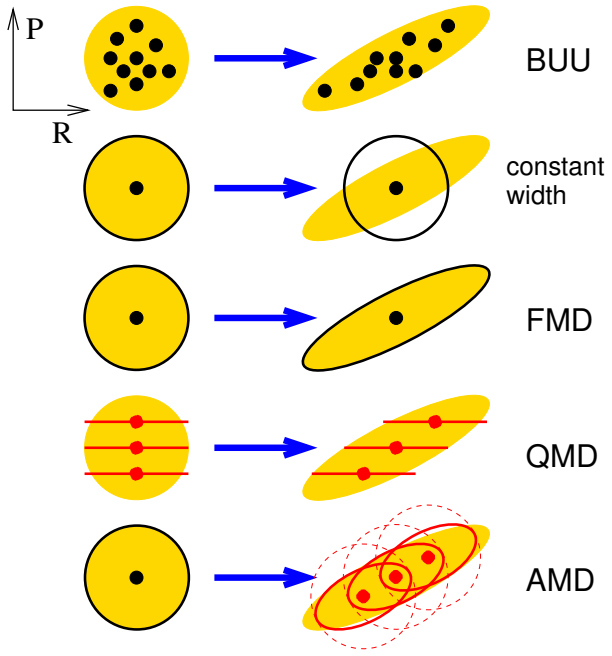

Fig. 3. Schematic depiction of the free time evolution of the phase-space distribution of a single nucleon as described by various models when the initial state is represented by a wave packet having both spatial and momentum widths. The exact evolution is indicated by the gray (yellow on-line) area.

(BUU-type) treatments. The resulting model is then technically identical to the parallel-ensemble treatment of the nuclear Boltzmann equation with $\mathcal{N} = 1$. But an important difference from the usual BUU treatment is that the fluctuations produced by the stochasticity automatically develop self-consistently for each individual collision event and thus allow the emergence of different fragmentation channels.

In addition, a Gaussian smearing is performed to obtain the spatial density of the nucleons at any point in time, which is intended to emulate the effect of individual wave packets. The resulting class of models is usually referred to as quantum molecular dynamics (QMD) [48–52]. The spatial smearing causes the force acting on each nucleon to be much smoother than the bare nucleon-nucleon force used in CMD. Furthermore, since the interaction used does not have a repulsive core the resulting force becomes rather similar to that of the mean-field description.

Even though the spatial smearing was introduced to emulate the effect of individual wave packets, the corresponding effect on the momentum distribution is ignored. Indeed, the momenta are treated as in CMD, with the kinetic energy of a nucleon taken as $\boldsymbol{p}_i^2/2m$ without any zero-point energy, while the momentum distribution is treated by a random sampling of $\boldsymbol{p}_i$. This treatment can be regarded as a practical method for including the effect of the momentum distribution on the time evolution: The nucleons will have different velocities in different events so they will be found at different positions in the final states.

In the simple example of free motion of a single nucleon, as illustrated in fig. 3, the average over the event ensemble will yield the correct free-time evolution.

A drawback of this treatment is that the initial nuclei, which are obtained by sampling the nucleon momenta $\boldsymbol{p}_i$ from a Fermi sphere, are not in their true ground states in which all nucleons would have vanishing velocities. While this undesirable feature is of little import during the violent part of the collision, it does play a significant role for the production of fragments, since their yield is largely governed by the statistical weights of the dynamical model.

QMD has been applied mainly to collisions at relatively high energy. In low-energy processes with long time scales it is difficult to keep the phase-space occupation below unity merely by means of the Pauli suppression in the two-body collisions since these become increasingly rare. In an attempt to remedy this problem, some approaches have employed a Pauli potential [53,54], but there is no quantum-mechanical foundation for such a force in the equation of motion. Furthermore, statistical particle emission from excited fragments cannot be reliably described by QMD. Therefore the dynamical QMD calculation has to be stopped at a certain time and the decay of the fragments should be calculated by a statistical decay code. The long-time simulation for equilibrated systems is beyond the limit of applicability of QMD and the result of such a simulation would not be consistent with quantum statistics.

QMD simulations of energetic nuclear collisions typically lead to copious production of fragments whose multiplicities are often comparable with the experimental data [55–59]. However, these fragments are extracted at the end of the violent stage of the collision and are generally excited by several MeV/nucleon. Therefore, the subsequent decay processes tend to significantly reduce the IMF yield [60], thus leaving a persistent discrepancy between the QMD results and the data.

Furthermore, multifragmentation of projectile-like fragments in peripheral collisions is underestimated more seriously in some QMD calculations [55,60]. However, using an algorithm based on the early cluster recognition method that invokes the single-particle binding energies in the candidate preclusters and is applicable even at high densities [43], Gossiaux *et al.* [61] were able to reproduce the observed multiplicity. This issue may be related to the fact that the effective interaction range is quite large in QMD because of the spatial smearing [61,62].

4.4 Constrained molecular dynamics

The Pauli principle requires that the phase-space density should not exceed one nucleon per phase-space volume $(2\pi\hbar)^3$ for each spin-isospin state in semiclassical descriptions. The exact treatment of the Pauli principle (see sects. 4.5 and 4.6) requires significant computational power for large systems. In order to overcome the computational difficulty, an approximate implementation of the Pauli principle has been proposed as constrained molecular dynamics (CoMD) [63,64]. In this approach, a stochastic process is added to the usual QMD in order to prevent the violation of the Pauli principle. The process is invoked when the phase-space density f_i around a nucleon i becomes greater than 1. The momenta of the nucleon i and other nucleon(s) are changed as in the two-nucleon scattering so that the Pauli principle $f_i \leq 1$ is finally satisfied after several trials. This is one of the ways to satisfy the Pauli principle, though it is not derived from first principles.

Due to the stochastic process for the Pauli principle, the condition $f_i \leq 1$ remains satisfied when a ground-state nucleus is propagated for a long time. The properties of hot nuclei may be better described by CoMD than QMD.

CoMD can reproduce the multifragmentation data at the incident energy of 35 MeV/nucleon [63,64]. The effect of the stochastic process for the Pauli principle is to reduce the Pauli-blocking factor for the two-nucleon collisions when the two nuclei overlap, which results in stronger stopping and expansion towards instability of multifragmentation. The charge distribution of intermediate-mass fragments are reasonably reproduced, except for the problems in the light-particle multiplicities.

4.5 Fermionic molecular dynamics

Fermionic molecular dynamics (FMD) [65–69] is a true quantum treatment that represents the many-body state as an antisymmetrized Slater determinant of wave packets having a Gaussian form,

$$\varphi_i(\boldsymbol{r}) \sim \exp\left[-\nu_i(\boldsymbol{r} - \boldsymbol{Z}_i)^2\right]. \tag{5}$$

The wave packet centroids $\{\boldsymbol{Z}_i\}$ and widths $\{\nu_i\}$ are complex dynamical variables whose equations of motion can be derived from the time-dependent variational principle. The nucleons are assumed to move in a mean field and their spin and isospin degrees of freedom may be included. Thus FMD is a constrained form of TDHF with nonorthogonal single-particle states for which the overlap matrix $\langle\varphi_i|\varphi_j\rangle$ should be properly considered. The derived equation of motion shows that $\{\boldsymbol{Z}_i\}$ and $\{\nu_i\}$ are not canonical variables.

Since the FMD wave function is a Slater determinant, the effective interactions developed for mean-field calculations are basically applicable to FMD. It is also possible to employ realistic nuclear forces by means of unitary correlation operators [70,71]. Furthermore, the FMD wave function provides a reasonable approximate description of ground-state nuclei [67], obtained by minimizing the energy of the constrained wave function. Properties such as binding energies and radii can be reproduced well with a reasonable effective interaction. Contrary to the molecular-dynamics models discussed above, the energy minimization yields a unique FMD ground state which is invariant under the FMD time evolution.

Even though FMD utilizes a quantum wave function, the dynamics is fully deterministic and the system remains

a single Slater determinant at all times. This is inadequate for fragmentation processes, where many different configurations are reachable. This problem could be remedied by the introduction of direct two-body collisions, which would bring the description close to Stochastic TDHF (sect. 3). While this has not yet been done in the full FMD model, it has been successfully carried out in AMD (sect. 4.6) where the width parameters $\{\nu_i\}$ are kept fixed.

Since the many-body state is described by a Slater determinant, FMD incorporates the Pauli principle perfectly, of course. Furthermore, the dynamical growth of the imaginary part of the width parameter ν_i produces a correlation between positions and momenta in the course of time, thereby ensuring that the single-particle motion is described correctly for both free motion (see fig. 3) and for nucleons in a harmonic-oscillator potential.

The deterministic character of FMD has the drawback that it does not offer a natural description of dynamical bifurcations. An important example is nucleon emission which occurs with some probability, while the nucleon remains in the source with the complementary probability. A reasonable description would yield an increasing width of the emitted part of the wave packet, while the residual packet should remain rather compact, something that is clearly beyond the reach of a single Gaussian wave packet. Clearly, such branchings could be described by the introduction of suitable stochasticity in the dynamics (see sects. 4.6 and 4.7).

By enclosing the system in a large harmonic-oscillator potential well and coupling the system weakly to a virtual thermometer while examining its long-time behavior, it has been possible to study the thermodynamic properties of FMD [72]. The model was shown to exhibit a liquid-gas phase transition and the associated caloric curves were extracted. They are similar to those obtained experimentally, with a low-temperature liquid-like region, an intermediate plateau associated with the coexistence region, and a high-temperature gas-like region. However, the contact with experiment could be firmed up by deriving the temperature from observed quantities such as isotope ratios and kinetic energies of gaseous nucleons.

There have been several other works based on molecular dynamics with dynamical wave packet widths. It was found that the inclusion of a dynamical width improves the agreement with data in some cases, such as fusion cross-section above the Coulomb barrier [73]. Kiderlen *et al.* [74] studied the fragmentation of excited systems. In response to the initial pressure, the excited system begins to expand but clusters were *not* produced even though Gaussian wave packets with many-body correlations were employed. When the excited system expands, the widths of wave packets grow and then, in turn, the interaction between the packets weakens. The mean field for such a configuration is very shallow and smooth and there is then little chance for clusters to appear. This feature conflicts with the general expectation that clusters should appear in such situations. Similarly, studies of spinodal instability [75] showed that the zero sound is significantly affected when the width grows large and this spreading of the nucleon wave packet then inhibits cluster formation.

4.6 Antisymmetrized molecular dynamics

Antisymmetrized molecular dynamics (AMD) [76–78] is similar to FMD in that the system is represented by a Slater determinant and that a part of the equation of motion is derived from the time-dependent variational principle. An important difference from FMD is that stochastic terms have been added to the equation of motion so that many configurations can appear through the reaction dynamics.

On the other hand, AMD usually treats the width parameters $\{\nu_i\}$ of the single-particle wave packets as a constant parameter common to all the nucleons. This simplification reduces the computational burden but limits the flexibility of the description, compared to the FMD description, as long as the stochastic extension terms are ignored. Nevertheless, the constant width parameter guarantees that there is no spurious coupling of the internal motion and the center-of-mass motion of a cluster or a nucleus. Furthermore, the presence of trajectory branching due to the stochasticity avoids the creation of spurious correlations in the wave function. For example, for the nucleon emission process, channels with and without nucleon emission will not mix in a single AMD wave function.

It is a very attractive feature of AMD that it provides, with a conventional effective interaction and a reasonable value of the width parameter, a quite good description of not only the basic properties of ground-state nuclei but also many detailed structure features, such as the excitation level spectra of light nuclei [79], with some extensions such as the parity and angular-momentum projections.

Recent versions of AMD [80–82] seek to take account of the dynamics of the wave packet width and shape by splitting the wave packet into components by means of a stochastic term that is calculated based on the single-particle motion in the mean field (see fig. 3). It assumes that the coherence of the single-particle wave function is lost and it branches into incoherent Gaussian wave packets at a certain time due to many-body effects. This quantum branching process makes possible the coexistence of the single-particle dynamics in the mean field and the fragment formation, which requires spatial localization and the emergence of many configurations. The resulting extended AMD may be regarded as a specific case of the stochastic mean-field equation (sect. 3) with the correlations of the fluctuation $\delta C[f]$ designed in such a way that a Gaussian wave packet appears.

The introduction of two-nucleon collisions is similar to QMD (sect. 4.3), with some differences described below. The antisymmetrization implies that the wave packet centroids $\{\boldsymbol{Z}_i\}$ cannot be interpreted as the positions and momenta of nucleons. Rather, the physical coordinates are introduced as nonlinear functions of the centroids [77] and the two-nucleon collisions are performed by using these physical coordinates. There then appear Pauli-forbidden phase-space regions into which the physical coordinates

will never enter, for any values of the centroid variables $\{\boldsymbol{Z}_i\}$. These regions are regarded as Pauli-blocked and not allowed as final state of a collision. Another difference from QMD is the fact that the physical momentum in AMD is the momentum centroid of a Gaussian phase-space distribution, while the momentum variable in QMD usually represents the definite momentum of a nucleon.

The equilibrium properties of AMD have been studied by solving the time evolution of a many-nucleon system in a container for a long time to obtain a microcanonical ensemble. When the liquid phase, in the form of a nucleus, is embedded in a nucleon gas of temperature T, the characteristic quantum relation $E^*_{\rm liq} \sim T^2$ was obtained [83] and the resulting caloric curves show that AMD is consistent with the liquid-gas phase transition [84–86].

The wave packet branching plays an essential role for obtaining such physically reasonable equilibrium properties in AMD. The importance of a stochastic term has also been demonstrated within the Quantal Langevin model discussed below (sect. 4.7). On the other hand, as mentioned above (sect. 4.5), in FMD the nucleon emission from a nucleus in the liquid-gas phase coexistence region is described by a deterministic motion of the nucleon wave packet with a variable width. The differences between these approaches have not yet been fully explored.

Although it has not been studied very carefully, the approximate reproduction of the quantum relation $E^*_{\rm liq} \sim T^2$ suggests that statistical nucleon emission from an excited fragment may be qualitatively well described in AMD, while a quantitative description would require that the model gives the correct value for the nuclear level density parameter a. If this were indeed the case, then AMD should be able to describe the statistical decay of fragments produced in collisions if the time evolution could be calculated for a sufficiently long time. Fortunately, the final results do not depend very much on the time at which the dynamical calculation is connected to the statistical decay calculation.

When the wave packet branching is included by means of a stochastic term, the resulting state must be adjusted to ensure energy conservation. This is achieved by means of a dissipative term in the equation of motion. Although this dissipative term has been constructed carefully in order to obtain a reasonable time evolution, its form has not been derived from a basic principle.

AMD has been successfully applied to fragmentation reactions, such as central collisions in the energy region of several tens of MeV/nucleon for light and heavy systems [80,87]. The fragment isospin composition obtained in dynamical collisions is consistent with statistical predictions, such as the isoscaling relation and the dependence on the symmetry energy term of the effective force [88,89]. These results are consistent with the idea that the fragment isospin composition is determined when the density is low ($\rho \approx \frac{1}{2}\rho_0$), and reflects the symmetry energy of dilute nuclear matter.

The description of few-body correlations in AMD is probably rather crude in some situations. In particular, when the incident energy is high ($\gtrsim 50\,\mathrm{MeV/nucleon}$), the nucleon multiplicity is strongly overestimated, which is probably because of the too small probability of forming light clusters from highly excited matter. The correlation needed to form light clusters should probably be treated more quantum mechanically than the accidental merging of randomly distributed wave packets.

4.7 Quantal Langevin dynamics

A more formal development of trajectory branching in wave packet dynamics has led to the Quantal Langevin (QL) model [90,91]. The motivation for this work lies in the fact that the nuclear liquid-gas phase transition differs significantly from the usual liquid-gas phase transition in macroscopic matter primarily in the role played by quantum statistics. For usual macroscopic matter, the total energies are to a good approximation linear functions of the temperature in both the liquid and gas phases. Thus the effective number of degrees of freedom is essentially constant in each phase. In contrast to this familiar situation, the liquid phase of a nucleus exhibits an increase in the number of activated degrees of freedom as the temperature is raised. In particular, the excitation energy of a nucleus at low temperature increases like $E^* = aT^2$ (where the level density parameter is $a \approx A/(8\,\mathrm{MeV})$), which is a typical quantal behavior, while the gas phase is characterized by the usual classical relation $E^*/A = \frac{3}{2}T$. The two curves intersect at $T \approx 12\,\mathrm{MeV}$, which is much higher than the transition temperature suggested by experimental data. This indicates that the quantal statistical nature of the nuclear system plays an important role for the phase transition and, presumably, for the associated nuclear multifragmentation processes.

Part of the reason for the persistent shortcoming of wave packet dynamics for the description of multifragmentation (see sect. 4.3) may be found in the fact that the equation of motion for the wave packet centroids is not consistent with the quantal statistical nature, because quantum fluctuations inherent in the wave packets are neglected. The presence of quantum fluctuations is signaled by the fact that a given wave packet is a superposition of many energy eigenstates. Therefore the fluctuations should be taken into account in such a way that the different components are properly explored in the course of time.

This fundamental problem can be clearly brought out by making a cumulant expansion of the canonical weight of a given wave packet, at the temperature $T = 1/\beta$ [92],

$$\ln \mathcal{W}_\beta = \ln\langle \exp(-\beta \hat{H})\rangle = \beta\mathcal{H} + \frac{1}{2}\beta^2\sigma_H^2 + \mathcal{O}(\beta^3)\,. \quad (6)$$

Here $\mathcal{H} \equiv \langle \hat{H}\rangle$ is the usual expectation value of the energy in the given wave packet and it is evident that the weight $\mathcal{W}_\beta$ is affected by its energy spread σ_H. Truncation of the cumulant expansion at second order, corresponding to a Poisson energy distribution in each packet (as a Gaussian would have) leads to a much improved global description of the quantum-statistical properties of the many-body system.

This approach was extended to dynamical scenarios by the introduction of a Langevin force emulating the transitions between the wave packets [90,91]. The corresponding transport process in wave packet space can be described as a Langevin process and the general form of the associated transport coefficients was derived. The ensuing diffusive wave packet evolution exhibits appealing physical properties, including relaxation towards the appropriate microcanonical quantum-statistical equilibrium distribution in the course of the time evolution. Specific expressions for the transport coefficients were subsequently derived on the basis of Fermi's golden rule and it was verified that they satisfy the associated fluctuation-dissipation theorem.

This approach is not specific to nuclear dynamics but has general applicability. For example, it was used to study the effect of quantum fluctuations on the critical properties of noble gases [93]. In nuclear physics it has been applied to hyperfragment formation from Ξ^- absorption on ^{12}C where it was found that quantum fluctuations affect the outcome qualitatively [94,95] and to multifragmentation [96] which is of particular interest here and will be briefly summarized below.

The Langevin force enables the wave packet system to explore its entire energy spectral distribution, rather than being restricted to its average value. This leads to a much improved description of the quantum-statistical features. In particular, the resulting specific heat now exhibits the characteristic evolution from a quantum fluid towards a classical gas as a function of temperature [92], in contrast to the behavior emerging with the usual treatment. Since a change of a fragment's specific heat is associated with a change in its statistical weight, the effect is clearly relevant for the fragment production problem.

The key new features of the results obtained with the quantal Langevin model are the occurrence of larger fluctuations and an enhancement of stable configurations, such as bound fragments, as a result of the need to take account of the spectral distortion of the wave packets. The former feature arises from the fact that the wave packet parameter of each nucleon is populated according to the strength of the eigen components for the given energy expectation value, and therefore the wave packet parameter can have larger fluctuations than when the energy is fixed to the expectation value. On the other hand, in order to project out the appropriate energy component from the wave packet, it is necessary to take account of its internal distortion. The combination of these two basic features then enhances the average IMF multiplicity at the final stage, especially in central collisions, as was demonstrated for Au+Au at 100–400 MeV/nucleon [96]. While the larger fluctuations allow the system to explore more configurations and thus enhances the yield of primary fragments, the latter stabilizes the fragments, since the compensation for the quantum distortion effectively acts as a cooling mechanism.

These studies suggest that the underlying quantal nature of the nuclear many-body system may indeed play a significant role in fragmentation reactions.

5 Concluding remarks

The development of a suitable dynamical description of fragment formation in nuclear collisions is a daunting task that poses many interesting challenges and makes contact with other areas of modern many-body and mesoscopic physics. We have here given a brief overview of the most commonly employed models and sought to bring out their relative merits and shortcomings. Although much progress has been made over the past couple of decades, we are still far from having models that are formally well founded, practically applicable, and sufficiently realistic to be quantitatively useful. As our discussion has brought out, the description of nuclear fragmentation dynamics requires that proper account be taken of the basic quantal nature of the system. This requirement renders purely classical equations of motion inadequate and calls for the development of quantal transport theory. Further advances along this line are likely to be of broad physical interest.

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