

Unitary evolution with fluctuations and dissipation

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We outline an extension of the classical Langevin equation to a quantum formulation of the treatment of dissipation and fluctuations of all collective degrees of freedom with unitary evolution of a many-fermion system within an extension of the time-dependent density functional theory. We illustrate the method by computing the distribution of fission fragment yields for ²⁵⁸Fm in a quantum hydrodynamic approach and a typical trajectory with full unrestricted density functional theory augmented with dissipation and fluctuations.

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I. INTRODUCTION

The description of the dynamics of a small system in interaction with a very large reservoir is one of the oldest problems in many-body physics, starting perhaps with the 1828 work of Brown on Brownian motion, followed by the illustrious theoretical studies of Einstein, Smoluchowski, Langevin, Fokker, Planck, Kramers, and a great number of many others [1]. If there are no memory effects, for a Brownian particle in the Markov approximation one can use the stochastic Langevin equation, which in one dimension reads:

$$m\ddot{x}(t) = F(x(t)) - \gamma m\dot{x}(t) + m\xi(t). \quad (1)$$

Here $\xi(t)$ is a zero mean (real) Gaussian white noise with variance $\langle\langle \xi(t)\xi(t') \rangle\rangle = \Gamma\delta(t-t')$ and angle brackets stand for statistical averaging. The strength of the damping and of stochastic forces are related by the Einstein dissipation fluctuation theorem, $m\Gamma = 2\gamma T$, where T is the temperature. (The Boltzmann constant is chosen $k_B = 1$.) Appropriate implementations of the Langevin equation or the equivalent Fokker-Planck equation have been used in nuclear physics for decades, see Refs. [2–8] and earlier references therein, in order to describe the dissipative character of the heavy-ion collisions at intermediate energies, the fission fragments yields, etc. Recently the Smoluchowski equation has been suggested as a simpler alternative to the Langevin approach by Randrup *et al.* [9–13], which assumes that the collective dynamics is overdamped, in complete agreement with our recent findings in a fully microscopic treatment of the fission dynamics at the mean-field level [14].

In the case of a quantum mechanical system one aims to replace the Schrödinger equation with a master equation [15]

$$i\hbar\dot{\rho} = [H, \rho] + \mathcal{L}(\rho), \quad (2)$$

where $\rho = \text{Tr}_{\text{res}} \rho_{\text{tot}}$ is the density matrix of the subsystem after taking the trace over the reservoir/intrinsic coordinates of the full ρ_{tot} , H is the Hamiltonian of the collective/isolated system, and $\mathcal{L}(\rho)$ is a linear superoperator acting on ρ . Such an equation for the one-body density matrix can be formally derived from a BGK hierarchy [16]. The form of the

superoperator is difficult to use in practice, it is generally nonlocal in time, and the emerging master equation is very difficult to solve. The dynamics of the system is entangled with the dynamics of the reservoir. However, in a Markov approximation one can derive a generalization of the von Neumann [17] and Landau equation [18]. The most general form of the master equation in a Hilbert space of dimension N is much simpler than Eq. (2) and of the form [19,20], and it is routinely referred to as the Lindblad equation,

$$i\hbar\dot{\rho} = [H, \rho] - i[W\rho + \rho W] + i \sum_{k,l=1}^{N^2-1} h_{kl} A_k \rho A_l^\dagger, \quad (3)$$

$$W = W^\dagger = \frac{1}{2} \sum_{k,l=1}^{N^2-1} h_{kl} A_l^\dagger A_k, \quad (4)$$

where h_{kl} and W are Hermitian positively defined matrix and operator, respectively, and A_k form a full set of linearly independent operators, apart from the unit operator. This equation was derived by requiring the preservation of the total probability ($\text{Tr}\dot{\rho} \equiv 0$) and of the positivity of ρ during the time evolution. Simpler and/or equivalent master equations have been derived over the years in quantum optics in perturbation theory [21–29]. If one were to drop the last term in Eq. (3) the probability would not be conserved, as $\hbar \text{Tr}\dot{\rho} = -2\text{Tr}(W\rho) \leq 0$. W plays the role of an optical potential, thus being responsible for simulating dissipation, which has been used in either one-channel or coupled channels situations. The loss of probability is only marginally alleviated in coupled-channel treatments (where optical potentials are also present), when the probability from the incoming channel is only partially recovered in the other channels.

The direct numerical solution of the Lindblad equation (3) or of its Monte Carlo wave function formulation [23–33] can turn into a formidable problem in cases of interest in nuclear physics, where the number of degrees of freedom (DoF) in Langevin studies is between 2 to at most 5 [4–9], which would correspond in the case of a quantum treatment to wave functions of 2–5 variables and density matrices depending on

4–10 spatial variables alone, plus time, which easily becomes prohibitive numerically. We should mention here that over the years many extensions of the time-dependent mean-field approaches have been suggested in nuclear physics, in order to incorporate fluctuations in a quantum treatment [34–41].

In this work, instead of limiting the number of collective DoF to a small number of chosen characteristics or moments of the number density $n(\mathbf{r}, t)$, we will consider the entire number density as our chosen set of collective DoF and treat them in a quantum formalism at a finite temperature, which is controlled by the intrinsic DoF. We argue that one can add carefully chosen additional terms to the usual TDDFT equations to simulate both dissipation and fluctuations of the nuclear collective motion and maintain at the same time the unitary character of the evolution, a distinctive characteristic of TDDFT. Since fluctuations are random, observables will have to be evaluated as ensemble averages over these realizations. However, in the case of steady-state situations one can also consider time-averaged observables, which should lead to the same final results.

II. DIFFICULTIES WITH INTRODUCING DISSIPATION AND FLUCTUATIONS IN MEAN-FIELD DYNAMICS

Numerically, the Lindblad equation is usually solved by means of a Monte Carlo wave function, obtained with a Hamiltonian $H - iW$ augmented with a stochastic term, which simulates the role of the last term $\sum_{k,l=1}^{N^2-1} h_{kl} A_k \rho A_l^\dagger$ in Eq. (3) [23–28,30–33]. The corresponding augmented stochastic Schrödinger equation for the single quasiparticle wave functions in a time-dependent density functional theory (TDDFT) would acquire then the form

$$i\hbar\dot{\psi}_k = [H - iW]\psi_k + S\psi_k + \sum_l \lambda_{kl}\psi_l, \quad (5)$$

where S is in general a non-Hermitian complex stochastic field, appropriately defined and λ_{kl} are Lagrange multipliers enforcing at all times the orthogonality conditions $\langle \psi_k | \psi_l \rangle = \delta_{kl}$. Unfortunately this approach cannot be used in simulating fermion systems, where one needs to evolve in time a large number of single quasiparticle wave functions ψ_k . If these orthogonality conditions are satisfied only after ensemble averaging instead one would introduce large unphysical particle number fluctuations [14], apart from expected collective energy fluctuations. With particle number fluctuations present one would have a difficult task in quantifying their role in the definition of the width of the energy fluctuations.

Upon considering dissipation and fluctuations one expects fluctuations of the collective energy, but the total particle number should be exactly conserved. The presence of the optical potential $-iW$ (and of a non-Hermitian stochastic field S) leads to a nonunitary evolution, which could in principle be restored only by introducing a large number of time-dependent Lagrange multipliers λ_{kl} , rendering this system of such coupled equation basically impossible to handle numerically.

The unravelling of the Lindblad equation (3) to a stochastic or Monte Carlo form is not a unique procedure and one may introduce various other forms for the optical potential $-iW$,

in which case W does not have to be Hermitian for example. One can also try to work with nonorthonormal quasiparticle wave functions, at the expense of making the evaluation of observables much more challenging numerically in the case of fermionic systems. Allowing for total particle fluctuations can lead to spurious mass and charge distributions in fission dynamics for example.

Our goal here is to construct a quantum approach equivalent to the classical Langevin approach. In nuclear applications of the Langevin approach practitioners typically select a few characteristics of the number density $n(\mathbf{r}, t)$ (e.g., in the case of fission: elongation of the nucleus, mass asymmetry, neck size, and two quadrupole deformations of the fragments [5]). For these collective variables one constructs a potential energy surface by minimizing the total energy with suitable constraints, an inertia and a dissipation tensor and assume the existence of coupled Langevin equations for these collective variables. The potential energy and the inertia tensor are constructed strictly speaking at zero temperature and the evolution of the intrinsic DoF is assumed to be adiabatic, thus with no intrinsic excitations, at local zero temperature when the collective variables are kept fixed.

The adiabaticity assumption in large amplitude collective motion in nuclear physics, typically conflated with the slowness of the collective motion, translates into no entropy production for the intrinsic variables, $\dot{S}_{\text{int}}(t) \equiv 0$. Since dissipation is included only in the collective motion DoF their entropy naturally increases in a Langevin approach, $\dot{S}_{\text{coll}}(t) > 0$. At the same time, the total entropy of the nuclear system, which is isolated, should in principle exactly vanish at all times, $\dot{S}_{\text{tot}}(t) \equiv 0$. This apparent contradiction finds its resolution, not in a Langevin approach to collective motion, but in an approach which allows continuous energy exchange from the collective to the intrinsic DoF, which on relatively long time scales of interest in nuclear dynamics appears irreversible. In that case one can establish that the entanglement entropy of the intrinsic DoF, $S_{\text{int}}(t) = -\text{Tr}_{\text{coll}}[\rho(t) \ln \rho(t)]$, actually increases $\dot{S}_{\text{int}}(t) > 0$. In a TDDFT approach to nuclear fission, even in the absence of explicit dissipation in the collective DoF the relation $\dot{S}_{\text{int}}(t) > 0$ is automatically fulfilled, as energy is practically irreversibly transferred from collective to intrinsic DoF [14]. Entropy is strictly speaking a quantity that is obtained only after the system explored the relevant part of the phase-space and the time average became equal to the corresponding phase-space average [42]. During the descent from saddle-to-fission a nucleus might not necessarily have enough time to relax and the intrinsic entropy might have not reached its equilibrium value at each fixed values of the collective coordinates.

The number and character of the collective variables are chosen according to various authors preferences or arguments, which are not uniformly endorsed. There exist rather compelling theoretical arguments that the actual number of relevant DoF is (much) greater than considered so far. In fission for example, on the top of the barrier the intrinsic excitation energy is rather small and the number of possible excited DoF is also small, but that is not true anymore by the time the nucleus reaches the scission configuration [14]. This aspect, however, has not been satisfactorily settled in literature.

The classical Langevin and quantum Lindblad equations both assume the Markov approximation, but at the same time they differ in one critical aspect. In the Langevin equation there are two parameters: one, γ , which controls the strength of the dissipative force, and a second one, Γ , which controls the strengths of the fluctuations. While their ratio is controlled by the temperature T , the absolute value of each of these parameters control the rate of energy exchange. In Lindblad equation (3) however the ration of the strengths of the dissipation $W = \frac{1}{2} \sum_{k,l=1}^{N^2-1} h_{kl} A_l^\dagger A_k$ and of the fluctuations $\sum_{k,l=1}^{N^2-1} h_{kl} A_k \rho A_l^\dagger$ is fixed and independent of the temperature. Diósi [43] and Akamatsu [44,45], Kajimoto *et al.* [46], Akamatsu *et al.* [47] have demonstrated, however, how in the high temperature limit one can introduce independently dissipation and fluctuations in the Lindblad equation. Efforts are under way to generalize this type of approach to finite temperatures [48–54], following the Feynman-Vernon [55] and Caldeira-Leggett [56] formalisms.

While the Lindblad equation appears as the most natural extension of a classical Markovian evolution to a quantum one, one aspect has not been resolved in the literature as far as we know. When coupling a classical system to a reservoir one expects that after a certain relaxation time the system arrives at an equilibrium. In the case of a quantum system one would expect the time averaged density matrix to reach asymptotically the limit $\rho \propto \exp(-\frac{H}{T})$. In the case of the Lindblad equation (3) that would be equivalent to the condition that

$$\sum_{k,l=1}^{N^2-1} h_{kl} [A_l^\dagger A_k H + H A_l^\dagger A_k] \equiv 2 \sum_{k,l=1}^{N^2-1} h_{kl} A_k H A_l^\dagger, \quad (6)$$

which would impose rather serious constrains on the set of operators A_k . It is not clear under what conditions a steady-state solution $\rho \propto \exp(-\frac{H}{T})$ can be achieved, unlike in the case of Fokker-Planck, Langevin or Boltzmann equations. It is not obvious what would be in general the steady-state solution of the Lindblad equation. Unlike in the case of the Langevin equation (1) there is no general prescription on how one might control the equilibrium temperature of the quantum system.

While the Lindblad approach has many appealing mathematical features, attempting to use it for describing a nuclear system appears to lead in the best case scenario to a very cumbersome formalism. We propose to go in a different direction: (i) to remove the somewhat artificial limitation of phenomenological models to a small and somewhat arbitrary number of collective variables; (ii) to develop a formalism in which the introduction of dissipation leads to a unitary evolution of the single-particle DoF and time evolution of the single-particle density satisfies the continuity equation; (iii) the energy increase due to random fluctuations is properly balanced by the dissipation; (iv) a formalism in which one can control separately the rate of fluctuations and dissipation as well as the temperature of the stationary state (as in the case of the classical Einstein fluctuation-dissipation theorem). This particular aspect is relevant in nonequilibrium processes, when the equilibration time can be longer than the time at which the system changes its macroscopic properties.

While the use of Gaussian white noise with either the Itô or Stratonovich calculus is mathematically extremely seductive [1,57], and has been advocated over the years in order to devise various generalizations of the mean-field dynamics, fluctuations in space and time corresponding to arbitrarily large fluctuations in momenta and energy are physically unjustified. Fluctuations in nuclear collective motion on a spatial scale much smaller than the average interparticle distance, which is of the order of 2 fm for nuclei, or on a temporal scale shorter than a few 10^3 s fm/c (comparable to the time it takes the fastest nucleon to traverse a big nucleus) are unwarranted. The numerical implementation of stochastic differential equations has subtleties and is more difficult to carry out than in case of differential equations. At the same time, in actual numerical implementations the high frequencies (inherent for white noise) are eliminated by using finite integration time-steps, which is equivalent to performing a short time coarse graining of the true numerical solution. Instead of introducing coarse graining in either time or space dictated by the numerical implementation we will set physics inspired limits on the character of fluctuations. Dissipation in collective motion in low-energy nuclear dynamics is mostly one-body in character [58] and very strong at the same time. These aspects were firmly confirmed recently in an unrestricted implementation of TDDFT quantum microscopic framework [14], without resorting to introducing the hard to define both the number and the character of the collective DoF, collective inertia, potential energy surface, or friction mechanisms. This is a mechanism similar to Fermi's model for high-energy cosmic rays [59]. In low-energy induced nuclear fission the two-body dissipation mechanism is inhibited due to the relatively small phase space available, corresponding to excitation energies less than about 20 MeV, and the corresponding long nucleon mean-free path [60].

The time-dependent mean-field equations can be formally obtained within a path integral approach of the propagator, as described by Negele and Orland [61], using the stationary phase approximation of a path integral representation of the many-body propagator $\int \mathcal{D}\sigma \exp(iS[\sigma]/\hbar)$, where $S[\sigma]$ is the action. There is a consensus that the TDDFT description provides a description of the average or more likely of the most probable dynamics, thus the same kind of trajectory obtained in the stationary phase approximation of the path integral [62]. What is missing in TDDFT is the contribution from fluctuations, which formally would appear as an additional contribution g_2 to the equation for the one-body density matrix ρ_1 :

$$i\hbar\dot{\rho}_1 - [h_1(\rho_1), \rho_1] = g_2. \quad (7)$$

In the mean-field approximation this type of equation can be obtained from the BGK hierarchy [16]. In the limit when g_2 vanishes this reduces to the time-dependent mean-field approximation for the one-body density matrix ρ_1 . The semiclassical limit of Eq. (7) reduces to the Boltzmann equation, if g_2 is approximated with the collision integral. Upon taking a short time average the term g_2 vanishes. It would appear natural to generalize Eq. (7) to some kind of stochastic form, to incorporate to the role of the neglected, and relatively rapid fluctuations of g_2 .

The TDDFT equations for the single-particle wave functions are obtained using a nuclear energy density functional (NEDF). The NEDF should satisfy the local Galilean covariance, which implies that the total energy of the system can be represented as a sum [63–65]

$$E_{\text{tot}}(t) = E_{\text{coll}}(t) + E_{\text{int}}(t) \equiv \int d^3\mathbf{r} \frac{mn(\mathbf{r}, t)\mathbf{v}^2(\mathbf{r}, t)}{2} + \int d^3\mathbf{r} \mathcal{E}(\tau(\mathbf{r}, t) - n(\mathbf{r}, t)m^2\mathbf{v}^2(\mathbf{r}, t), n(\mathbf{r}, t), \dots), \quad (8)$$

where $n(\mathbf{r}, t)$ is the number, $\tau(\mathbf{r}, t)$ is the kinetic, and $\mathbf{p}(\mathbf{r}, t) = mn(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t)$ are linear momentum and local collective/hydrodynamic velocity densities, and ellipses stand for various other densities. The first term in Eq. (8) is the collective/hydrodynamic energy flow E_{coll} and the second term is the intrinsic energy E_{int} in the local rest frame. For the sake of simplicity we have suppressed the spin and isospin DoF, even though they are included in the numerical examples discussed below.

III. AUGMENTED NUCLEAR TDDFT EQUATIONS INCLUDING DISSIPATION AND FLUCTUATIONS

The TDDFT evolution equations augmented to incorporate dissipation and fluctuations we introduce have the form

$$i\hbar\dot{\psi}_k(\mathbf{r}, t) = h[n]\psi_k(\mathbf{r}, t) + \gamma[n]\dot{n}(\mathbf{r}, t)\psi_k(\mathbf{r}, t) - \frac{1}{2}[\mathbf{u}(\mathbf{r}, t) \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot \mathbf{u}(\mathbf{r}, t)]\psi_k(\mathbf{r}, t) + u_0(\mathbf{r}, t)\psi_k(\mathbf{r}, t), \quad (9)$$

where $\hat{\mathbf{p}} = -i\hbar\nabla$ [not to be confused with the linear momentum density $\mathbf{p}(\mathbf{r}, t)$], the index k runs over the neutron and proton quasiparticle states and where $\psi_k(\mathbf{r}, t)$ are four-component quasiparticle wave functions and $h[n]$ is a 4×4 partial differential operator [14,66]. The fields $\mathbf{u}(\mathbf{r}, t)$ and $u_0(\mathbf{r}, t)$ generate both rotational and irrotational dynamics. One can also introduce a carefully chosen fluctuating inertia tensor $\mathbf{p} \cdot \vec{\mathbb{T}}(\mathbf{r}, t) \cdot \mathbf{p}$, a fluctuating spin-orbit interaction, a fluctuating pairing field $\delta(\mathbf{r}, t)$, and a time-symmetry-breaking stochastic field $\boldsymbol{\sigma} \cdot \mathbf{C}(\mathbf{r}, t)$. Basically, every term of the quasiparticle Hamiltonian can be rendered stochastic.

The term $\gamma[n]\dot{n} \propto -\nabla \cdot \mathbf{p}(\mathbf{r}, t)$, per continuity equation [67], plays the role of quantum friction, in which the friction coefficient $\gamma[n]$ can depend on the number density and/or its gradient, etc., and thus it can simulate volume and/or surface friction. In the presence of this quantum friction term alone $\dot{E}_{\text{tot}}(t) \leq 0$ and $\lim_{t \rightarrow \infty} \mathbf{v}(\mathbf{r}, t) = 0$ [67], similarly to the classical Langevin equation. We should add that over the years many authors have discussed various other forms of quantum friction extensions of the Schrödinger equation [68–74], some of which have similarities with our suggested form for the friction potential. However, these earlier suggestions introduce typically averages of either momenta or coordinates over the entire system, thus introducing unphysical nonlocalities into the theory. It makes no sense to have the magnitude of the dissipation in one part of the system depend on the properties of another part of the system, which can be spatially separated by a large distance.

The field $u_0(\mathbf{r}, t)$ and each of the Cartesian components of the three-dimensional (3D) velocity field $\mathbf{u}(\mathbf{r}, t)$ are uncorrelated stochastic fields of the type to be described below, see Eq. (10). By construction Eqs. (9) lead to a unitary evolution with dissipation built in (unlike the case of an optical potential). The quantum friction term and the stochastic fields do not affect the relative momenta of any pair of nucleons, and therefore they do not contribute to the thermalization of the intrinsic motion. The average value of the total local/collective momentum $\mathbf{p}(\mathbf{r}, t)$ is modified by the quantum friction and these additional stochastic fields, and thus only the collective DoF (moments of the density) are affected, as in case of the Langevin approach [4–9]. There is a one-to-one correspondence between the neutron and proton number densities $n_q(\mathbf{r}, t)$ with $q = n, p$ and all their possible moments and we call them the collective DoF. They define the shape of the nucleus, in full analogy with the generator coordinate method [75,76] or the extended generator coordinate method [77].

The TDDFT dynamics automatically incorporates the one-body dissipation mechanism [58]. The additional quantum friction term is needed to counteract the heating due to the stochastic fields $u_0(\mathbf{r}, t)$ and $m\mathbf{u}(\mathbf{r}, t)$. The strength of the quantum friction should be chosen in analogy to the Einstein fluctuation-dissipation theorem. In the case of a Brownian particle, one follows the dynamics of the Brownian particle alone, but not the effects on the dynamics of the fluid and the total energy of the fluid and Brownian particle are not conserved. In a TDDFT augmented with dissipation and fluctuations one follows the coupled dynamics of both collective and intrinsic DoF within a stochastic framework.

The generic time-dependent 3D field structure of both the scalar $u_0(\mathbf{r}, t)$ and of each Cartesian component of the vector stochastic fields $\mathbf{u}(\mathbf{r}, t)$ is of the form for $\nu = 0, x, y, z$:

$$u_\nu(\mathbf{r}, t) = \sqrt{\Gamma} \sum_{k=1}^{N_k} F(t - t_k, \tau_k) \eta_k(\mathbf{r}), \quad (10)$$

$$\eta_k(\mathbf{r}) = \sqrt{\frac{1}{N_{kb}}} \sum_{l=1}^{N_{kb}} \alpha_{kl} G(\mathbf{r} - \mathbf{r}_{kl}, a_{kl}), \quad (11)$$

where $F^2(t, \tau)$ and $G^2(\mathbf{r}, a)$ are 1D and 3D smoothed normalized δ functions of width τ and a , respectively. The finite widths τ and a impart these stochastic fields a finite memory time and a finite correlation length respectively. Here $\langle t_k - t_{k-1} \rangle \propto \langle \tau_k \rangle = O(\frac{m r_0 A^{1/3}}{\hbar k_F})$, $\langle N_{kb} \rangle = O(A)$, $\langle \alpha_{kl} \rangle = 0$, $\langle \alpha_{kl} \alpha_{mn} \rangle = \delta_{km} \delta_{ln}$, $\langle a_{kl} \rangle = O(\frac{\tau}{k_F})$, $\langle |\mathbf{r}_{kl}| \rangle = O(r_0 A^{1/3})$, $r_0 \approx 1.2$ fm, A is the mass number, k_F is the Fermi momentum, and Γ is a parameter controlling the variance of the $u_\nu(\mathbf{r}, t)$, see Eq. (13). $t_k, \tau_k, N_{kb}, a_{kl}$, and \mathbf{r}_{kl} are uncorrelated uniform random numbers in properly chosen intervals. Then

$$\int d^3\mathbf{r} \langle \eta_k(\mathbf{r}) \rangle = 0, \quad \int d^3\mathbf{r} \langle \eta_k(\mathbf{r}) \eta_l(\mathbf{r}) \rangle = \delta_{kl}, \quad (12)$$

$$\int_0^t dt' \int d^3\mathbf{r} \langle u_\nu(\mathbf{r}, t') \rangle = 0, \quad \int_0^t dt' \int d^3\mathbf{r} \langle u_\nu^2(\mathbf{r}, t') \rangle \approx \Gamma \langle N_k \rangle, \quad (13)$$

$$\int_0^t dt' \int d^3\mathbf{r} \langle u_\nu(\mathbf{r}, t') u_\nu(\mathbf{r}, t' + \Delta t) \rangle \approx 0, \quad \Delta t \gg \langle \tau_k \rangle, \quad (14)$$

where $t \approx \langle N_k \rangle \langle \tau_k \rangle$. In the limits $\lim_{\tau \rightarrow 0} F^2(t, \tau) = \delta(t)$, $\lim_{a \rightarrow 0} G^2(\mathbf{r}, a) = \delta(\mathbf{r})$, $\tau_k \rightarrow 0$, and $N_{kb} = 1$ one recovers the Gaussian white noise used in typical treatment of stochastic equations [1,57]. $u_\nu(\mathbf{r}, t)$ simulates random N_k collective jolts, administered to the system at random times t_k and of random duration τ_k . Each jolt consists of random N_{kb} bumps/sumps, randomly distributed throughout the nucleus, each with a height/depth of zero mean and unit variance and of a random diameter a_{kl} . The ratio $\Gamma/\gamma \propto T$ controls the temperature of the intrinsic system, similarly to Einstein fluctuation-dissipation theorem. There are at least two independent coupling strengths Γ (of appropriate dimension), one for $\mathbf{u}(\mathbf{r}, t)$ and the other for $u_0(\mathbf{r}, t)$.

We illustrate this approach with the case of a nucleon in a 1D harmonic oscillator $V(x) = \frac{m\omega^2 x^2}{2}$ with $\hbar\omega = 6$ MeV, a quantum friction potential as described above and a stochastic field $u_0(x, t)$ only. It is not always obvious that the time average and the phase-space average, or in other words, ergodicity is satisfied in simulations, particularly in the case of integrable systems [47,78,79]. Starting with a somewhat arbitrary initial state, after some time the harmonic oscillator reaches a steady-state solution at a temperature $T = 1/\beta$ determined from the condition

$$\begin{aligned} \frac{1}{\tau} \int_0^\tau dt E(t) &= \frac{1}{Z(\beta)} \sum_{n=0}^{\infty} e^{-\beta \varepsilon_n} \varepsilon_n, \\ Z(\beta) &= \sum_{n=0}^{\infty} e^{-\beta \varepsilon_n}, \quad \varepsilon = \hbar\omega \left(n + \frac{1}{2} \right), \\ \rho(x) &= \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau dt |\psi(x, t)|^2 \\ &\approx \frac{1}{Z(\beta)} \sum_{n=0}^{\infty} e^{-\beta \varepsilon_n} |\phi_n(x)|^2, \end{aligned} \quad (15)$$

where $\phi_n(x)$ are the 1D harmonic oscillator eigenfunctions.

In Fig. 1 we display the expectation value of the energy of the 1D oscillator as a function of the simulation time, illustrating that the system attained a steady-state regime. In Fig. 2 we show the initial, expected, and computed equilibrium density distributions. We put a minimal effort into the fine tuning of the parameters of the quantum friction potential, the stochastic field, and of the length of the simulation time.

IV. FISSION OF ^{258}Fm AND ^{240}Pu

We illustrate this approach by solving the nuclear quantum hydrodynamic equations for ^{258}Fm fission. At zero temperature within Landau's two-fluid hydrodynamics only the superfluid components survive and the dynamics reduces to that of a neutron and a proton interacting miscible classical perfect/ideal fluids [80,81] for canonically conjugate fields $n_q(\mathbf{r}, t)$ and $\phi_q(\mathbf{r}, t)$, where $\nabla \phi_q(\mathbf{r}, t) = m\mathbf{v}_q(\mathbf{r}, t)$. In a quantum hydrodynamic approach we use the semiclassical form of

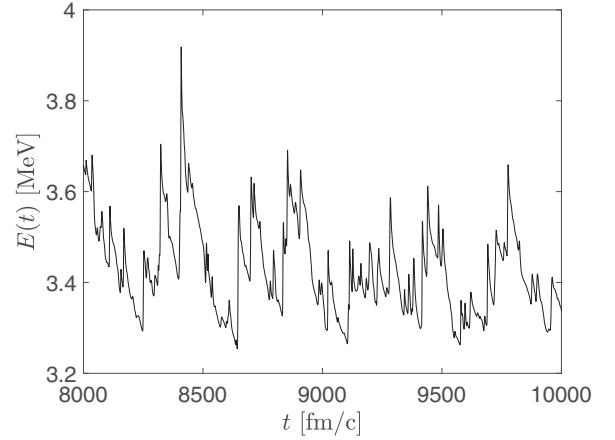


FIG. 1. The expectation value of the energy of the 1D harmonic oscillator as a function of time.

the SeaLL1 NEDF [82,83] for homogeneous nuclear matter, augmented with a Coulomb energy and gradient terms,

$$\begin{aligned} \mathcal{E}_{\text{int}} &= \mathcal{E}_{\text{kin}}(\tau_n, \tau_p) + \mathcal{E}_{\text{hom}}(n_n, n_p) + \mathcal{E}_{\text{Coul}} \\ &+ \frac{\hbar^2}{2m} (C + Dn)(\nabla n)^2, \end{aligned}$$

which reproduces the symmetric nuclear matter energy, the saturation density, the symmetry energy, and the Coulomb energy. $C = -2.8622 \text{ fm}^3$ and $D = 9 \text{ fm}^6$ are chosen to accurately reproduce the nuclear surface tension $\sigma = \int dz [\mathcal{E}_{\text{int}}(\tau(z), n(z), \dots) - \mu n(z)] \approx 1 \text{ MeV/fm}^2$, where $\mu = -15.6 \text{ MeV}$ [83] is the chemical potential for infinite symmetric nuclear matter and $n = n_n + n_p$, $n_{n,p}(z)$, and $\tau_{n,p}(z)$ are the number and kinetic energy density distribution for semi-infinite symmetric nuclear matter. Using Madelung representation [84] of the neutron and proton wave functions $\Psi_q(\mathbf{r}, t) = \sqrt{n_q(\mathbf{r}, t)} \exp[i\phi_q(\mathbf{r}, t)/\hbar]$, where $\mathbf{p}_q(\mathbf{r}, t) = n_q(\mathbf{r}, t) \nabla \phi_q(\mathbf{r}, t) = m n_q(\mathbf{r}, t) \mathbf{v}_q(\mathbf{r}, t)$, one can

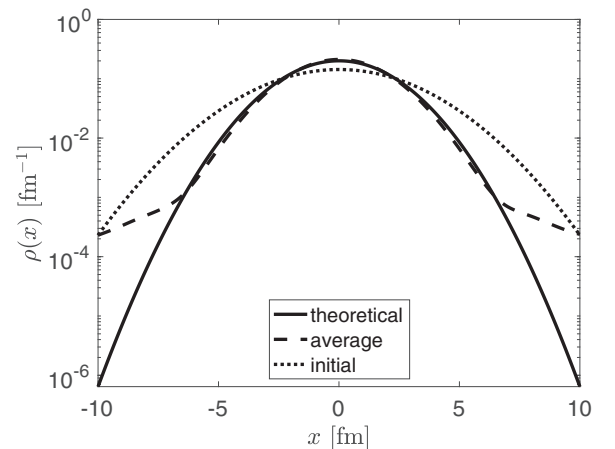


FIG. 2. The initial, final $\rho(x) = \frac{1}{\tau} \int_0^\tau dt |\psi(x, t)|^2$, and expected theoretical density distribution, using the temperature estimated from Eq. (15). By increasing the simulation time one can improve on the tails of the calculated density distribution.

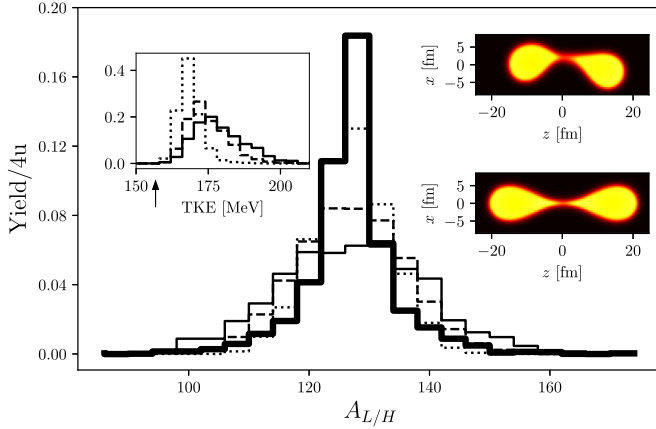


FIG. 3. The mass yields obtained solving the quantum hydrodynamics equations [82] including dissipation and fluctuations as in Eq. (16) at an excitation energy $E^* \approx 14$ MeV, obtained using different strengths $\Gamma = 0.1$ (solid), 0.05 (dash), and 0.02 (dots) MeV of the fluctuating field $u_0(\mathbf{r}, t)$ (keeping Γ/γ fixed), compared to experimental data (thick solid) [85] for spontaneous fission of ^{258}Fm . The variance of the mass (24.9, 18.4, and 12.9 amu vs experiment 15.2 amu) and of the TKE (18.3, 14.9, and 8.5 MeV vs experiment 19.3 MeV) distributions are approximately proportional to $\sqrt{\Gamma}$. In the insets we show the TKE (left inset) distributions and typical nuclear shapes at scission (right inset) with and without fluctuations and dissipation. The arrow points to the TKE for symmetric splitting in the absence of dissipation and fluctuations.

recast the quantum hydrodynamic equations into two coupled effective Schrödinger equations (here with $\mathbf{u}(\mathbf{r}, t) \equiv 0$ for simplicity) with isoscalar dissipation and fluctuations,

$$i\hbar\dot{\Psi}_q(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\Psi_q(\mathbf{r}, t) + \frac{\delta\mathcal{E}_{\text{int}}}{\delta n_q(\mathbf{r}, t)}\Psi_q(\mathbf{r}, t) + \gamma[n]\dot{n}(\mathbf{r}, t)\Psi_q(\mathbf{r}, t) + u_0(\mathbf{r}, t)\Psi_q(\mathbf{r}, t). \quad (16)$$

The hydrodynamic equations do not include pairing and shell effects and the ground states for typical nuclei have spherical symmetry. Even though we illustrate here a unitary quantum evolution with dissipation and fluctuations for two components only, the scale of this simulation is already significantly larger than any other similar simulation reported in literature so far.

The inclusion of dissipation and fluctuations easily leads to mass distributions which are close to the observed ones for spontaneous fission of ^{258}Fm , see Fig. 3, even though the goal of this first calculation is only to illustrate the method. Even though our calculations are for fission from an excited state and the purpose of this figure is to illustrate qualitative aspects of our approach. The strength of the dissipation and fluctuations terms have been adjusted to correspond to a temperature of ≈ 0.75 MeV, or an excitation energy of about 14 MeV. We have started our simulations with ^{258}Fm in its ground state. In the absence of dissipation and fluctuations only symmetric fission will be obtained with a rather narrow total kinetic energy (TKE) distribution, weakly dependent on initial conditions. The mean of the TKE distribution in a hydrodynamic approach is significantly smaller than the

observed one, as the fissioning nucleus develops unexpectedly long thin necks, reminiscent of the nuclear shapes obtained in the liquid drop model with a large viscosity [86]. Similar longer necks develop if one were to increase significantly the magnitude of the pairing strength, when the dynamics of becomes very similar to the dynamics of perfect fluids [14]. At the same time the width of the TKE distribution (≈ 20 MeV) is comparable to the observed one and to the numbers reported in Ref. [41]. Within that the nuclear shape develops a longer neck as the viscosity increases in the numerical implementation of the hydrodynamical approach of Ref. [86], a result at odds with our findings. Davies *et al.* [86] restricted the nuclear shape to a parametrization using 5 DoF only, while in the present work we have included all shape DoF. These authors also expressed some doubts concerning the accuracy of the calculated inertia and viscosity tensors at large deformations. Shell effects and pairing correlations can be accounted for by a variation of the macroscopic-microscopic formalism [5,87]. From the known neutron and proton number densities one can construct the single-particle nucleon Hamiltonian, including spin-orbit and pairing interactions, and subsequently determine the corresponding energy density, which can then be used for the next time step in Eqs. (16). The full TDDFT description is likely a more efficient solution, however.

For realistic calculations one has to resort to the full TDDFT description [14,66], using the evolution equations (9), with quasiparticle wave functions with spin and isospin DoF, and pairing correlations accounted for. Such calculations require the use of leadership computing facilities at a scale above that recently reported [14]. If one were to resort to a simpler approach, in which pairing correlations are described only at the BCS level, the calculational complexity is comparable to the a few hundred time-dependent Hartree-Fock trajectories needed to perform ensemble averages, and such simulations are quite feasible [41]. In Fig. 4 we show a

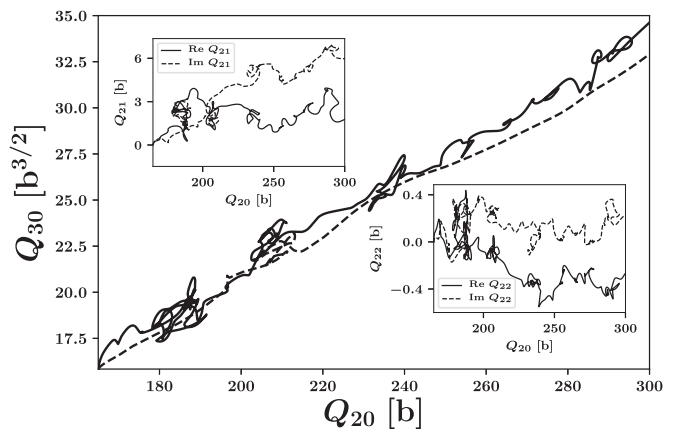


FIG. 4. In the main panel we show two typical full TDDFT trajectories for ^{240}Pu projected into the $Q_{20} = \langle 2z^2 - x^2 - y^2 \rangle$ and $Q_{30} = \langle (5z^2 - 3r^2)z \rangle$ plane obtained by evolving in time the TDDFT equations [14,66] without (dashed line) and with (full line) dissipation and fluctuations included, using the NEDF SeaLL1 [14,83]. In the insets we show the fluctuations of the moments $Q_{2m} = \langle z^{2-m}(x + iy)^m \rangle$, for $m = 1, 2$, which vanish in the absence of fluctuations and otherwise break axial symmetry.

projection onto the planes (Q_{20}, Q_{30}) and (Q_{20}, Q_{2m}) with $m = 1, 2$ of a typical full TDDFT trajectory obtained without dissipation and fluctuations and including dissipation and fluctuations using Eqs. (9), in the case of induced fission of ^{240}Pu . Fluctuations breaking axial symmetry have never been considered in Langevin-type of simulations and no information was ever presented on their magnitude and importance. To this end we integrate in time 442368 complex coupled nonlinear stochastic partial differential equations on a $3\text{D } 24^2 \times 48$ spatial lattice with a lattice constant 1.25 fm, a time step 0.03 fm/c for 130255 time steps. Only six DoF are illustrated in this figure, even though all collective DoF were allowed to fluctuate. This simulation of a unitary quantum evolution including dissipation and fluctuations is exceeding by $\approx O(10^6)$ orders of magnitude any other simulation ever reported in literature in any physics field.

V. CONCLUSIONS

The main features of the present extension of the TDDFT formalism are: (i) the present formalism is quantum; (ii) it includes all collective DoF; (iii) evolution is unitary in spite of including explicitly dissipation; (iv) all mean-field symmetries are broken during the evolution, as expected for example in a full path-integral description of the dynamics of an interacting many-fermion system [61,62], while in Langevin description for example, axial symmetry was never broken; (v) upon the inclusion of fluctuations in TDDFT, the fission dynamics remains overdamped as established in Ref. [14], collective kinetic energy (not shown) remains as small as in their absence, and trajectories become more convoluted and longer in length and time and more random in the collective space; (vi) the mean-field adjusts naturally to the changes in the nuclear shape; (vii) without fluctuations one obtains only a lower limit of fission times [14,66]. The formalism

described here is applicable to many other situations: dissipative heavy-ion collisions, nonequilibrium phenomena in cold-atom physics; dynamics of vortices in neutron star crust, quantum turbulence [88].

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