Density functional theory with spatial-symmetry breaking and configuration mixing

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This article generalizes the notion of the local density of a many-body system to introduce collective coordinates as explicit degrees of freedom. It is shown that the energy of the system can be expressed as a functional of this object. The latter can in turn be factorized as the product of the square modulus of a collective wave function and a normalized collective-coordinate-dependent density. Energy minimization translates into a set of coupled equations, i.e., a local Schrödinger equation for the collective wave function and a set of Kohn-Sham equations for optimizing the normalized density at each point in the collective space. These equations reformulate the many-body problem exactly provided one is able to determine density- and collective-wave-function-dependent terms of the collective mass and potential which play a similar role to the exchange-correlation term in electronic Kohn-Sham density functional theory.

I. INTRODUCTION

Density-functional-based models, being the only microscopic, fully quantum-mechanical tool currently available to provide insight on the structure of nuclei up to the heaviest ones, are the focus of intense investigation to improve their accuracy and precision. For example, recent developments in effective field theory methods and the theoretical foundations of nuclear density functional theory (DFT) have triggered attempts to bridge *ab initio* many-body methods, based on chiral effective field theory and high-precision two- and three-nucleon interactions, and DFT, using the former to build parts of the latter [1–8]. Another current line of work consists in enriching the form of empirical energy functionals in a systematic way [9–11].

One puzzling fact about nuclear DFT is that it owes much of its power to the use of symmetry-breaking density configurations. The method thus deviates from the symmetry-conserving Hohenberg-Kohn (HK) [12] and Kohn-Sham (KS) [13] framework. The most basic example of a broken symmetry is the translational invariance of the Hamiltonian, which is troublesome for self-bound finite systems best described by a localized density. KS frameworks have recently been built for a trapped system [14] and for a functional of the internal density, i.e., expressed in the reference frame of the nuclear center of mass [15,16]. A density-functional framework allowing to break arbitrary symmetries was put forward in Ref. [17], relying however on an unspecified restriction of the variational space for a trial wave function. Another example of a broken symmetry is the nonconservation of particle number in the BCS treatment of pairing. As an alternative, exact solutions of the pairing Hamiltonian and symmetry-restored Hartree-Fock-Bogolyubov equations have been formulated as a functional (function, in fact) of occupation numbers in a given single-particle basis [18–20], and functions of occupation numbers have been studied as an alternate route to building mass tables [21]. These works keep the HK/KS formalism unchanged except for a variation in its basic degree of freedom: the system's single-particle density.

However, formally integrating into DFT the breaking of rotational invariance, as well as the violation of particle-number conservation, remains to be done. Although effort is currently being put into building functionals of the scalar, symmetry-conserving density [22], it is likely that breaking these symmetries is essential to describe what is understood as nuclear deformation, and treat pairing in finite systems, while keeping computational complexity to a minimum.

The cost-efficiency of KS-like schemes comes from the idea of using a Slater determinant to reproduce the local density ρ of a given correlated wave function, thereby capturing essential quantum effects, and encode the missing correlations into a functional $E_{\mathrm{xc}}[\rho]$ [23,24]. Thus, no explicit mention is made of a many-body wave function. Nonetheless, current expectations about nuclear DFT were mostly raised by the success encountered during its first life as mean-field theory performed with effective density-dependent interactions, together with beyond-mean-field extensions such as the generator coordinate method (GCM) performed on top of symmetry-restored mean-field states [25–28]. This was commonly understood as an approximate wave function method, which requires the restoration of broken symmetries for consistency with the underlying Hamiltonian, and allows multiple symmetry-restored configurations to be mixed to describe zero-point collective motion, or shape coexistence, and make extensive spectroscopic predictions in nuclei where these degrees of freedom are important. The somewhat *ad hoc* extension from a Hamiltonian picture to a density-functional-based one leads to pathologies in the theory [29], which can be formally addressed [30,31] at the expense of additional complexity and constraints on the form of the functional, such as forbidding terms other than polynomials of the density [32–34]. This is referred to as the multireference energy density functional (MR-EDF) model.

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An alternate formalism uses a collective "Bohr" Hamiltonian [35–42], initially developed as a model for a quantum vibrating liquid droplet, as an alternative or approximation to the Hill-Wheeler equations of the GCM. The mean-field energy landscape in the space of deformation parameters is then used as a potential (with or without zero-point energy corrections) and mass parameters determined from the Slater determinants enter a corresponding kinetic operator.

MR-EDF and collective Hamiltonians are powerful tools, well adapted to the idiosyncrasies of the nuclear many-body problem, yet they do not have a clear connection to the first-principles formulation thereof, which may limit their future development. Here, I attempt to improve on this situation.

The present article aims to formulate a density functional theory allowing to break spatial symmetries (e.g., translation, rotation) and treat collective motion in a spirit similar to the GCM, MR-EDF, or collective Hamiltonian-based methods, while keeping the theory exact in the DFT sense, i.e., provided we can determine the exact functional. First, the relevant mathematical objects are defined, then the existence of a functional is summarily proven in Sec. II. A useful form of the latter is given in Sec. III. The example of translational motion is used as an illustration in Sec. IV. Finally, a minimal Kohn-Sham-like scheme for introducing auxiliary Slater determinants is presented in Sec. V. Results are discussed throughout and summarized in Sec. VI.

II. DEFINITIONS AND EXISTENCE OF A FUNCTIONAL

Consider a system of N fermions with Hamiltonian $\hat{H} = \hat{T} + \hat{U} + \hat{V}$, where $\hat{T}$, $\hat{U}$, and $\hat{V}$ are respectively kinetic, interaction, and external potential terms. Trial N-body anti-symmetric wave functions Ψ depend on N coordinate three-vectors $\vec{r}_i$, $i = 1 \ldots N$ (omitting, in this first presentation, internal degrees of freedom of the particles for the sake of clarity). Let us write

$$\mathbf{R} \equiv (\vec{r}_1, \ldots, \vec{r}_N), \tag{1}$$

$$d^{3N}\mathbf{R} \equiv d^3\vec{r}_1 \cdots d^3\vec{r}_N. \tag{2}$$

The kinetic and external-potential terms of $\hat{H}$ can be written as (in units where $\hbar = m = 1$)

$$\hat{T} = -\frac{1}{2}\hat{\Delta} = -\frac{1}{2}\sum_i \Delta_i, \tag{3}$$

$$\hat{V}(\mathbf{R}) = \sum_i v_{\text{ext}}(\vec{r}_i), \tag{4}$$

while, for now, we shall keep $\hat{U}$ as an arbitrary interaction term. It is assumed that $\hat{H}$ has a nondegenerate ground state.

Now consider a set of differentiable real functions $Q_\mu(\vec{r})$ indexed by $\mu = 1 \ldots n$. We will use these to define local operators,

$$\hat{Q}_\mu(\mathbf{R}) \equiv \sum_i Q_\mu(\vec{r}_i), \tag{5}$$

their expectation values q_μ in a many-body wave function defining a set of collective coordinates. Now, for any given set of values $\underline{q} = (q_1, \ldots, q_n)$, each q_μ being taken in the interval

of possible values of $Q_\mu(\mathbf{R})$, we can define the operator

$$\hat{P}(\underline{q}, \mathbf{R}) \equiv \prod_\mu \delta(\hat{Q}_\mu(\mathbf{R}) - q_\mu). \tag{6}$$

This operator selects configurations of the N particles for which the collective coordinates defined by the functions $\hat{Q}_\mu$ correspond exactly to the given values ($\underline{q}$). It effectively projects Ψ onto an eigenspace of the $\hat{Q}_\mu$. Using the definition above, it is trivial to prove the projectorlike property

$$\hat{P}(\underline{q}, \mathbf{R})\, \hat{P}(\underline{q}', \mathbf{R}) = \delta^{(n)}(\underline{q} - \underline{q}')\, \hat{P}(\underline{q}, \mathbf{R}) \tag{7}$$

as well as the closure relation

$$\int d^n\underline{q}\; \hat{P}(\underline{q}, \mathbf{R}) = 1, \tag{8}$$

where the q_μ integral runs over the interval of possible values of $\hat{Q}_\mu(\mathbf{R})$. Note that, due to possible algebraic inequalities between the values of these functions, we may have $\hat{P}(\underline{q}, \mathbf{R}) = 0$ in some domain of $\underline{q}$ space. Such a domain is understood to be excluded in the following. We can now use $\hat{P}$ to define the *generalized density*,

$$D(\underline{q}, \vec{r}) \equiv N \int d^{3N}\mathbf{R}\; \delta^{(3)}(\vec{r} - \vec{r}_1)\; \hat{P}(\underline{q}, \mathbf{R})\Psi^*(\mathbf{R})\, \Psi(\mathbf{R}). \tag{9}$$

Comparing with the usual density,

$$\rho(\vec{r}) = N \int d^{3N}\mathbf{R}\; \delta^{(3)}(\vec{r} - \vec{r}_1)\; \Psi^*(\mathbf{R})\, \Psi(\mathbf{R}), \tag{10}$$

we see that $D(\underline{q}, \vec{r})$ is, up to a factor N, the probability density of finding one particle at $\vec{r}$ and the collective configuration of the N particles at $\underline{q}$. As $\hat{P}$ is an N-body operator, D contains information from up to N-body components of the density matrix associated with Ψ.

It is possible to split this information by defining, first, a collective wave function (cwf)

$$f(\underline{q}) \equiv e^{i\theta(\underline{q})} \left[\frac{1}{N} \int d^3\vec{r}\; D(\underline{q}, \vec{r}) \right]^{1/2}, \tag{11}$$

$$= e^{i\theta(\underline{q})} \left[\int d^{3N}\mathbf{R}\, \Psi^*(\mathbf{R})\hat{P}(\underline{q}, \mathbf{R})\Psi(\mathbf{R}) \right]^{1/2}, \tag{12}$$

where $\theta(\underline{q})$ is a chosen phase depending on the problem at hand. We shall assume there exists a natural and unambiguous choice. For ground states, $\theta(\underline{q}) = 0$ seems appropriate; otherwise, an irreducible representation of a symmetry group of $\hat{H}$ in $\underline{q}$ space may provide the dependence of $\theta(\underline{q})$ on some or all coordinates (this will be further discussed Secs. III and IV).

Second, we can define the $\underline{q}$-dependent density (defined first almost everywhere, then elsewhere by continuity)

$$d(\underline{q}, \vec{r}) \equiv |f(\underline{q})|^{-2} D(\underline{q}, \vec{r}), \tag{13}$$

which captures the conditional probability density of finding a particle at $\vec{r}$ if the collective configuration is $\underline{q}$. The meaning of $d(\underline{q}, \vec{r})$ can be made more explicit by introducing the "slice" wave function

$$\Psi(\underline{q}, \mathbf{R}) \equiv f^{-1}(\underline{q})\, \hat{P}(\underline{q}, \mathbf{R})\, \Psi(\mathbf{R}), \tag{14}$$

which satisfies, using Eqs. (7) and (12)

$$\int d^{3N}\mathbf{R}\,\Psi^*(\underline{q},\mathbf{R})\,\Psi(\underline{q}',\mathbf{R}) = \delta^{(n)}(\underline{q}-\underline{q}'), \qquad (15)$$

$$\int d^n\underline{q}\,f(\underline{q})\,\Psi(\underline{q},\mathbf{R}) = \Psi(\mathbf{R}). \qquad (16)$$

This wave function is nonzero on a manifold of dimension $3N - n$ determined by the values of the collective coordinates. Then, $d(\underline{q},\vec{r})$ is the density of this state [using Eq. (7) again],

$$\delta^{(n)}(\underline{q}-\underline{q}')\,d(\underline{q},\vec{r})$$
$$= N \int d^{3N}\mathbf{R}\,\delta^{(3)}(\vec{r}-\vec{r}_1)\Psi^*(\underline{q},\mathbf{R})\,\Psi(\underline{q}',\mathbf{R}). \quad (17)$$

Moreover, the quantities defined above satisfy the normalization relations, obtained from their respective definitions and the closure relation, Eq. (8),

$$\int d^n\underline{q}\int d^3\vec{r}\,D(\underline{q},\vec{r}) = N, \qquad (18)$$

$$\int d^n\underline{q}\,f^*(\underline{q})\,f(\underline{q}) = 1, \qquad (19)$$

$$\forall\underline{q}, \quad \int d^3\vec{r}\,d(\underline{q},\vec{r}) = N, \qquad (20)$$

and the following relations:

$$\int d^n\underline{q}\,D(\underline{q},\vec{r}) = \rho(\vec{r}), \qquad (21)$$

$$\int d^3\vec{r}\,D(\underline{q},\vec{r}) = N\,|f(\underline{q})|^2, \qquad (22)$$

which exhibit the role of D as a joint probability distribution and those of ρ and $|f|^2$ as the corresponding marginal distributions. Finally, we can see that the value of $\underline{q}$ is encoded in $d(\underline{q},\vec{r})$ through

$$\int d^3\vec{r}\,Q_\mu(\vec{r})\,d(\underline{q},\vec{r}) \qquad (23)$$

$$= |f(\underline{q})|^{-2}\int d^{3N}\mathbf{R}\,\hat{Q}_\mu(\mathbf{R})\,\hat{P}(\underline{q},\mathbf{R})\Psi^*(\mathbf{R})\,\Psi(\mathbf{R}) = q_\mu, \qquad (24)$$

thus reducing the variational domain for d. We could have used a two-body or higher operator for $\hat{Q}$, but this would prevent us from obtaining a simple expression like Eq. (24) for this purpose.

Now, let us see how the energy of the system can be expressed as a functional of D. Let $w(\underline{q},\vec{r})$ be a real function uniformly bounded from below and

$$\hat{w}(\underline{q},\mathbf{R}) = \sum_i w(\underline{q},\vec{r}_i), \qquad (25)$$

$$\hat{W}(\mathbf{R}) = \int d^n\underline{q}\,\hat{w}(\underline{q},\mathbf{R})\,\hat{P}(\underline{q},\mathbf{R}). \qquad (26)$$

This N-body operator applies on each slice of a wave function a different, $\underline{q}$-dependent, local, single-particle potential $w(\underline{q},\vec{r})$:

$$\hat{W}(\mathbf{R})\,\Psi(\mathbf{R}) = \int d^n\underline{q}\,f(\underline{q})\,\hat{w}(\underline{q},\mathbf{R})\,\Psi(\underline{q},\mathbf{R}). \qquad (27)$$

Its expectation value is, using Eqs. (13), (17), and (27),

$$\langle\Psi|\hat{W}|\Psi\rangle = \int d^n\underline{q}\,d^n\underline{q}'\,f^*(\underline{q})\,f(\underline{q}')$$
$$\times\int d^{3N}\mathbf{R}\,\Psi^*(\underline{q},\mathbf{R}')\,\hat{w}(\underline{q}',\mathbf{R})\,\Psi(\underline{q}',\mathbf{R}), \quad (28)$$

$$= \int d^n\underline{q}\int d^3\vec{r}\,w(\underline{q},\vec{r})\,D(\underline{q},\vec{r}), \qquad (29)$$

i.e., this potential is purely multiplicative with respect to the generalized density D, just as a local one-body potential $v(\vec{r})$ is with respect to $\rho(\vec{r})$. In fact, such a one-body potential is a special case of $\hat{W}$ with no dependence on $\underline{q}$ [$w(\underline{q},\vec{r}) = v(\vec{r})$ in Eq. (25)].

Let us add such a potential to the Hamiltonian and define the following functional, which implies solving for the ground state of $\hat{H} + \hat{W}$:

$$F[w] = \min_\Psi\langle\Psi|\hat{H} + \hat{W}|\Psi\rangle. \qquad (30)$$

To obtain a physically useful theory, we first need to ensure that w and Ψ, hence all physical observables, are functionals of D. The proof is identical to the usual case [12,43,44] and shall not be repeated here.

Using the Hellmann-Feynman theorem and Eq. (29), we have

$$\frac{\delta F[w]}{\delta w(\underline{q},\vec{r})} = D(\underline{q},\vec{r}). \qquad (31)$$

We can thus use a Legendre transform to write a functional of D,

$$E[D] = \min_w\left[F[w] - \int d^n\underline{q}\int d^3\vec{r}\,w(\underline{q},\vec{r})D(\underline{q},\vec{r})\right] \quad (32)$$

$$= \min_{\Psi\to D}\langle\Psi|\hat{H}|\Psi\rangle, \qquad (33)$$

where $\Psi \to D$ means that the variational domain for Ψ is restricted to wave functions having the generalized density D. It thus appears that the energy of the system can be written as a functional of D, in a similar fashion to the HK result. The ground-state energy of the system can then be found by minimizing the functional $E[D]$.

Since D depends on more variables than just the coordinates of one particle, it introduces additional degrees of freedom compared to standard DFT. Moreover, as seen in Sec. II, given a phase choice, D can be unambiguously decomposed into a cwf f and a $\underline{q}$-dependent normalized density d. We can thus also write

$$E[D] = E[f,d]. \qquad (34)$$

This alternate formulation will become useful when deriving the formal basis for a practical many-body method in the next few sections. For now, let me give a few examples of collective coordinates that can be usefully incorporated.

For instance, assuming a vanishing external potential ($\hat{V} = 0$), using x/N, y/N and z/N for $Q_\mu(\vec{r})$ (x,y,z being the Cartesian components of $\vec{r}$), the collective coordinates q_μ are the components of the center-of-mass (CoM) coordinate vector $\vec{R}$. The generalized density is then $D(\vec{R},\vec{r}) = |f(\vec{R})|^2\,d(\vec{R},\vec{r})$,

where, provided $\hat{U}$ is translation invariant, $f = \Omega^{-1/2}$ with Ω a normalization volume, $d(\vec{R}, \vec{r}) = \rho_{\text{int}}(\vec{r} - \vec{R})$, and ρ_{int} is the internal density of the system, nonvanishing if the system is self-bound. In this case, ρ_{int} is the only physically relevant degree of freedom present in D; the energy is a functional of the internal density, which is the result of Ref. [16] that we recover here as a limit case.

More generally, when the cwf $f(q)$ is known from symmetry arguments and the coordinate-dependent density for one value of the coordinates, $d(\underline{q}, \vec{r})$, can be deduced from its value at some natural reference point $d(\underline{0}, \vec{r})$ by a symmetry transformation, the latter is obviously a sufficient degree of freedom.

Suppose we now add the functions $(y^2 + z^2, x^2 + z^2, x^2 + y^2, -xy, -yz, -zx)$ to the set of $Q_\mu(\vec{r})$. We can now use as coordinates the components of the inertia tensor of the nucleus in the laboratory frame,

$$\mathbb{J} \equiv \int d^3\vec{r} \begin{pmatrix} y^2 + z^2 & -xy & -xz \\ -yx & x^2 + z^2 & -yz \\ -zx & -zy & x^2 + y^2 \end{pmatrix} d(\vec{R}, \mathbb{J}, \vec{r}). \tag{35}$$

From this and the CoM position, using the Huygens-Steiner theorem from solid mechanics, we can recover the inertia tensor in the CoM frame $\mathbb{J}_0$,

$$\mathbb{J}_0 \equiv \mathbb{J} - N(R^2 \mathbb{I} - \vec{R} \otimes \vec{R}), \tag{36}$$

where $\mathbb{I}$ is the identity matrix and $\otimes$ is the tensor (outer) product of vectors. In turn, $\mathbb{J}_0$ can be translated into a root-mean-square matter radius ($r_{\text{rms}} \equiv [\text{Tr}(\mathbb{J}_0)/2N]^{1/2}$) and a quintuplet of quadrupole deformation parameters and Euler angles $(\beta, \gamma, \varphi, \vartheta, \psi)$ [36,41]. We can thus treat deformation and rotation degrees of freedom dynamically.

At this point we might find that the number of collective coordinates in our theory, i.e., eight independent components of $(\vec{R}, \mathbb{J}_0)$ is actually too large for practical applications. For example, fluctuations of the radius are not usually considered an essential dynamical degree of freedom. We can define a functional with coordinates removed as follows. Consider a reduced set $\underline{\check{q}}$ of $\check{n} < n$ coordinates, and the generalized density $\check{D}(\underline{\check{q}}, \vec{r})$ depending on this reduced set. The energy can be written as

$$E[\check{D}] = \min_{D \to \check{D}} E[D], \tag{37}$$

where $D \to \check{D}$ means that for all $\vec{r}$,

$$\int dq_{\check{n}+1} \cdots dq_n \, D(\underline{q}, \vec{r}) = \check{D}(\underline{\check{q}}, \vec{r}). \tag{38}$$

This operation can be performed after a nonlinear transformation among the coordinates $\underline{q}$, such as the one mentioned above to obtain the canonical Bohr coordinates from the inertia tensor. Using this, we can remove in succession r_{rms}, then, if desired, γ and ψ (to obtain a functional describing only axially symmetric deformation). Alternatively, we may remove β and γ and keep only Euler angles as coordinates. In this case, again, the cwf as well as the transformations of the density

$d(\vec{R}, \varphi, \vartheta, \psi; \vec{r})$ are known analytically, and we can express the energy as a function of a single, deformed intrinsic density.

Note that Eq. (38) has a similar form to Eq. (21). We could, in principle, use this procedure starting with the full N-body local density $\Psi^*(\mathbf{R})\Psi(\mathbf{R})$ and, integrating out collective coordinates, yield a succession of generalized-density functionals, all the way down to the Hohenberg-Kohn functional of $\rho(\vec{r})$ if we remove all of them. This formalism thus appears very general and flexible. In particular, it gives us a choice between a "single-reference" description of many-body systems in terms of a single density (if symmetries define the dependence on $\underline{q}$ of the relevant quantities), of a "multireference" description explicitly coupling single-particle and collective motion.

Another important point to stress is that this theory is symmetry conserving. Let $\vec{S}(\vec{r})$ be an orthogonal transformation of the coordinates. Then, define

$$\mathcal{S}(\mathbf{R}) = (\vec{S}(\vec{r}_1), \vec{S}(\vec{r}_2), \ldots, \vec{S}(\vec{r}_N)), \tag{39}$$

and suppose the set of collective coordinates is chosen so that we can define

$$\underline{\mathcal{S}}(\underline{Q}(\mathbf{R})) \equiv \underline{Q}(\mathcal{S}(\mathbf{R})). \tag{40}$$

Then, the projector $\hat{P}(\underline{q}, \mathbf{R})$ is invariant under the simultaneous transformation of single-particle and collective coordinates,

$$\hat{P}(\underline{\mathcal{S}}(\underline{q}), \mathcal{S}(\mathbf{R})) = \delta^{(n)}(\underline{\hat{Q}}(\mathcal{S}(\mathbf{R})) - \underline{\mathcal{S}}(\underline{q})), \tag{41}$$

$$= \delta^{(n)}(\underline{\hat{Q}}(\mathbf{R}) - \underline{q}). \tag{42}$$

If, furthermore, the transformation leaves the many-body wave function invariant up to a phase η,

$$\Psi(\mathcal{S}(\mathbf{R})) = \eta \Psi(\mathbf{R}), \tag{43}$$

we have, from the definition of D,

$$D(\underline{\mathcal{S}}(\underline{q}), \vec{S}(\vec{r})) = D(\underline{q}, \vec{r}). \tag{44}$$

This simultaneous transformation thus leaves D invariant as well, the same property being obtained for d if f is invariant under $\underline{\mathcal{S}}$. Of course, for a given, fixed value of $\underline{q}$, $D(\underline{q}, \vec{r})$ and $d(\underline{q}, \vec{r})$, understood as functions of $\vec{r}$ alone, do not have to be symmetry invariant. This brings a solution to the usual conundrum around using the symmetry-conserving HK framework to justify nuclear DFT.

For completeness, the case of a wave function transforming as a nontrivial representation of a symmetry group should be mentioned. In general, D is not invariant in this case. Ideally, the collective coordinates should be chosen so as to replicate the group structure in the transformations of f and d. This deserves a more detailed discussion, which involves the phase choice entering the definition of f and needs to be done on a case-by-case basis.

One remaining hurdle is pairing: treating superfluid systems by breaking the conservation of particle number to yield a nonzero pair density would require an operator $\hat{P}(\underline{q})$ projecting on the associated U(1) gauge angle [yielding a particle-number breaking slice $|\Psi(\underline{q})\rangle$]. This, in turn, requires the definition of a gauge-angle operator; technicalities of such phase operators have been worked out in the field of quantum optics [45] starting from a particle-number representation. In our case,

this would entail a switch to a Fock-space representation, which is envisionable yet cumbersome (the present derivation is pervaded with N-body operators), and, moreover, the definition of a particle-number basis corresponding to each point (or state) in the N-body Hilbert space, i.e., choosing one definite particle-addition operator. Such a procedure relies on an arbitrary choice (what is the $N + 2$-body component of the N-particle system's correlated wave function?) that has to be studied in detail, and is beyond the scope of the present work, the remainder of which shall be concerned with normal systems. Let me simply suggest that pairing should probably be treated with a different, simpler scheme, which shall be described in a future paper.

III. COLLECTIVE SCHRÖDINGER EQUATION

The rest of this article shall be devoted to deriving the formal basis for a practical many-body method based on the result from the previous section. Here I focus on the dependence of the energy on the cwf f and derive a form of the functional that allows us to optimize the latter. Let us define a trial wave function

$$\Psi' = \int d^n\underline{q}\; g(\underline{q}) |\Psi(\underline{q})\rangle, \tag{45}$$

where g is a trial cwf, whereas in the following f, d, and $\Psi(\underline{q},\mathbf{R})$ are defined through Eqs. (12)–(14) from a starting wave function $\Psi(\mathbf{R})$. This will allow us to examine the dependence of the energy on the cwf and put $E[g,d]$ in a convenient form, then set $g = f$ at the end. The trial energy is

$$E = \langle\Psi'|\hat{T} + \hat{U} + \hat{V}|\Psi'\rangle, \tag{46}$$

$$= \int d^n\underline{q}\, d^n\underline{q}'\; g^*(\underline{q})\, g(\underline{q}')\langle\Psi(\underline{q})|\hat{T} + \hat{U} + \hat{V}|\Psi(\underline{q}')\rangle, \tag{47}$$

Let us first give the interaction matrix element. Here we assume a local interaction (which can nevertheless contain three-body or higher operators),

$$\langle\Psi(\underline{q})|\hat{U}|\Psi(\underline{q}')\rangle = \frac{\delta(\underline{q} - \underline{q}')}{\langle\hat{P}(\underline{q})\rangle} \int d^{3N}\mathbf{R}$$
$$\times \hat{P}(\underline{q},\mathbf{R})\, \hat{U}(\mathbf{R})\, \Psi^*(\mathbf{R})\, \Psi(\mathbf{R}), \tag{48}$$

with a similar expression for $\hat{V}$, where we define

$$\langle\hat{P}(\underline{q})\rangle = \int d^{3N}\mathbf{R}\; \hat{P}(\underline{q},\mathbf{R})\, \Psi^*(\mathbf{R})\Psi(\mathbf{R}) \tag{49}$$

$$= |f(\underline{q})|^2. \tag{50}$$

The kinetic matrix element, in turn, is (after integrating by parts; here and below we assume Dirichlet boundary conditions or an infinite integration domain, allowing us to drop boundary terms)

$$\langle\Psi(\underline{q})|\hat{T}|\Psi(\underline{q}')\rangle$$
$$= \frac{1}{2}\int d^{3N}\mathbf{R}\hat{\mathbf{\nabla}}\Psi^*(\underline{q},\mathbf{R}) \cdot \hat{\mathbf{\nabla}}\Psi(\underline{q}',\mathbf{R}). \tag{51}$$

$$= \frac{1}{2\,f^*(\underline{q})\,f(\underline{q}')}\int d^{3N}\mathbf{R}\{\hat{\mathbf{\nabla}}\hat{P}(\underline{q},\mathbf{R}) \cdot \hat{\mathbf{\nabla}}\hat{P}(\underline{q}',\mathbf{R})$$
$$\times \Psi^*(\mathbf{R})\, \Psi(\mathbf{R}) + \hat{P}(\underline{q},\mathbf{R})\, \hat{\mathbf{\nabla}}\hat{P}(\underline{q}',\mathbf{R}) \cdot [\hat{\mathbf{\nabla}}\Psi^*(\mathbf{R})\, \Psi(\mathbf{R})$$
$$- \Psi^*(\mathbf{R})\, \hat{\mathbf{\nabla}}\Psi(\mathbf{R})] - \delta^{(n)}(\underline{q} - \underline{q}')\, \hat{P}(\underline{q},\mathbf{R})\, \Psi^*(\mathbf{R})\, \hat{\Delta}\,\Psi(\mathbf{R})\}. \tag{52}$$

The gradient of $\hat{P}$ can be derived using Eq. (6) and the chain rule,

$$\hat{\mathbf{\nabla}}\hat{P}(\underline{q},\mathbf{R}) = -\sum_\mu \hat{\mathbf{\nabla}}Q_\mu(\mathbf{R})\, \partial_\mu \hat{P}(\underline{q},\mathbf{R}), \tag{53}$$

where ∂_μ indicates differentiation with respect to q_μ. Applying the result of Eq. (52) in Eq. (47), using integration by parts to transfer ∂_μ on the cwf, and reducing the double integral with Eq. (7), we can write the kinetic energy as

$\langle\Psi'|\hat{T}|\Psi'\rangle$

$$= \frac{1}{2}\int d^n\underline{q}\left\{\sum_{\mu\nu}F_{\mu\nu}\,\partial_\mu(f^{*-1}(\underline{q})\,g^*(\underline{q}))\partial_\nu(f^{-1}(\underline{q})\,g(\underline{q}))\right.$$
$$- i\sum_\mu J_\mu f^{*-1}(\underline{q})\,g^*(\underline{q})\partial_\mu(f^{-1}(\underline{q})\,g(\underline{q}))$$
$$- \int d^{3N}\mathbf{R}\;\hat{P}(\underline{q},\mathbf{R})\,\Psi^*(\mathbf{R})\,\hat{\Delta}\,\Psi(\mathbf{R})$$
$$\left.\times f^{*-1}(\underline{q})\,g^*(\underline{q})\,f^{-1}(\underline{q})\,g(\underline{q})\right\}, \tag{54}$$

where we introduce

$$F_{\mu\nu}(\underline{q}) \equiv \int d^{3N}\mathbf{R}\;\hat{P}(\underline{q},\mathbf{R})$$
$$\times \hat{\mathbf{\nabla}}\hat{Q}_\mu(\mathbf{R}) \cdot \hat{\mathbf{\nabla}}\hat{Q}_\nu(\mathbf{R})\,\Psi^*(\mathbf{R})\,\Psi(\mathbf{R}), \tag{55}$$

$$J_\mu(\underline{q}) \equiv \frac{i}{2}\int d^{3N}\mathbf{R}\;\hat{P}(\underline{q},\mathbf{R})\,\hat{\mathbf{\nabla}}\hat{Q}_\mu(\mathbf{R})$$
$$\cdot [\hat{\mathbf{\nabla}}\Psi^*(\mathbf{R})\,\Psi(\mathbf{R}) - \Psi^*(\mathbf{R})\,\hat{\mathbf{\nabla}}\Psi(\mathbf{R})]. \tag{56}$$

It is straightforward to check that $F_{\mu\nu}$ is positive semidefinite by contracting it with an arbitrary vector and using its definition, which yields the result as the integral of a positive semidefinite function. Using Eq. (53) and the steady-state continuity equation for the probability current of $\Psi(\mathbf{R})$, we can easily check that J_μ itself satisfies

$$\sum_\mu \partial_\mu J_\mu(\underline{q}) = 0. \tag{57}$$

Its definition and this property suggests its role as a collective current.

Finally, replacing f everywhere by its expression involving $\theta(\underline{q})$ and $\langle P(\underline{q})\rangle$, using integration by parts again, *then* setting $g = f$, we have

$$E[f,d] = \int d^n\underline{q}\; f^*(\underline{q})\left[-\frac{1}{2}\sum_{\mu\nu}\partial_\mu\,\mathcal{A}_{\mu\nu}(\underline{q})\,\partial_\nu + \mathcal{U}(\underline{q})\right.$$
$$\left.- \frac{i}{2}\sum_\mu(\partial_\mu\mathcal{V}_\mu(\underline{q}) + \mathcal{V}_\mu(\underline{q})\,\partial_\mu)\right]f(\underline{q}), \tag{58}$$

where we made ∂_μ act on all factors to its right. The potentials entering Eq. (58) are defined as follows. First, the collective mass term is

$$\mathcal{A}_{\mu\nu}(\underline{q}) \equiv \frac{F_{\mu\nu}(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle}. \tag{59}$$

This collective-mass term does not explicitly involve the interaction; it consists of a part of the kinetic energy. This is expected since a local potential does not couple slices with different $\underline{q}$, the latter being nonzero on different, nonoverlapping manifolds in the many-body coordinate space: a local operator only contributes to the local collective potential. The dependence of $\mathcal{A}_{\mu\nu}$ on the interaction is thus implicit, due to dependence on the wave function itself in $\langle \hat{P}(\underline{q}) \rangle$ and $F_{\mu\nu}(\underline{q})$.

To the contrary, the GCM and its collective-Hamiltonian based approximations typically use, as building blocks, Slater determinants which are not localized in collective coordinate space (hence their nonorthogonality and, in the GCM, the need to remove zero-norm states when solving the Hill-Wheeler equations). Our collective mass and the one found in collective-Hamiltonian models may thus have slightly different meanings.

Second, the collective potential is

$$\mathcal{U}(\underline{q})$$

$$\equiv \sum_{\mu\nu} F_{\mu\nu}(\underline{q}) \left[\frac{1}{2} \frac{\partial_\mu \theta(\underline{q}) \, \partial_\nu \theta(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle} + \frac{1}{8} \frac{\partial_\mu \langle \hat{P}(\underline{q}) \rangle \, \partial_\nu \langle \hat{P}(\underline{q}) \rangle}{\langle \hat{P}(\underline{q}) \rangle^3} \right]$$

$$+ \frac{1}{4} \sum_{\mu\nu} \partial_\mu \left[\frac{F_{\mu\nu}(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle^2} \partial_\nu \langle \hat{P}(\underline{q}) \rangle \right] - \frac{1}{2} \sum_\mu \frac{J_\mu(\underline{q}) \, \partial_\mu \theta(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle}$$

$$+ \frac{1}{\langle \hat{P}(\underline{q}) \rangle} \int d^{3N} \mathbf{R} \; \hat{P}(\underline{q}, \mathbf{R}) \Psi^*(\mathbf{R}) \left[-\frac{1}{2} \hat{\Delta} + \hat{U}(\mathbf{R}) \right] \Psi(\mathbf{R})$$

$$+ \int d^3 \vec{r} \; v_{\text{ext}}(\vec{r}) \, d(\underline{q}, \vec{r}). \tag{60}$$

If Ψ is an eigenstate of $\hat{H}$, the last two terms of Eq. (60) boil down to the energy E. In fact, all terms proportional to $F_{\mu\nu}$ and J_μ entering Eq. (58) cancel each other, as is made obvious by setting $f = g$ prematurely in Eq. (54), and these expressions could be simplified to a trivial form. However this particular separation of the energy is useful in isolating the dynamics of the system with respect to the chosen coordinates, while integrating out uninteresting ones. We shall see below, with an example, that it yields a meaningful physical value for the collective mass and potential.

This potential contains a piece of the kinetic energy, as well as all interaction and external-potential terms of the Hamiltonian (the latter being contained in the last line). Here, we assumed a local interaction term. A nonlocal one would simply make the potential itself nonlocal in the collective space, i.e., $\mathcal{U}(\underline{q}, \underline{q}')$. Such a nonlocal interaction is commonly found as the result of a renormalization-group (RG) evolution [46–48] of a starting, local model of the nucleon-nucleon interaction. This suggests that our collective Hamiltonian is not renormalization-scale invariant. Since $D(\underline{q}, \vec{r})$ involves components of many-body density matrices of the system,

it is sensitive to details of the wave function and should not be considered an observable in the RG sense, or at best a scheme-dependent one [49], and the same has to be deduced for quantities entering Eq. (58). However, the main purpose of the present formalism is the description of low-energy collective states and observables which should not be sensitive to such details. The generalized density, as the cwf, should thus be largely scale-invariant *in practice*, for appropriate choices of the collective coordinates. We are thus presented with a scale-dependent collective Hamiltonian with largely scale-independent solutions, indicating that scale dependence mainly occurs through reshuffling of contributions to the energy between nonlocality in $\mathcal{U}$ and the collective mass term. In practice, it should be safe to limit ourselves to parametrizations of a local collective potential.

Finally, the potential multiplying the current operator is

$$\mathcal{V}_\mu(\underline{q}) \equiv \sum_\nu F_{\mu\nu}(\underline{q}) \frac{\partial_\nu \theta(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle} + \frac{J_\mu(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle}. \tag{61}$$

Here, the first term in the definition of $\mathcal{V}$ as well as the term involving J_μ in Eq. (60) are proportional to the derivative of the phase introduced in Eq. (11) and ensure invariance of the energy with respect to gauge transformations of f. The notion that the energy (especially the kinetic energy) should not depend on the complex phase of the wave function may be counterintuitive. It is worth reminding here that we are dealing with a functional of a generalized *density*, and that the cwf f, if useful for formulating a theory of collective motion, has been introduced somewhat artificially. Thinking in terms of the correlated many-body wave function of the system, the functional $E[D] = E[f,d]$ yields the lowest energy of all states having D as their generalized density; the state which minimizes this energy is unique and we can access no other. For example, in the case of translational motion examined above, plane waves with nonzero momentum are excluded from the theory, as they have the same density, in terms of the CoM coordinate vector, as the zero-momentum state.

The second term in Eq. (61) involves the current $J_\mu(\underline{q})$. We can use the freedom of choosing the phase $\theta(\underline{q})$ mentioned above to cancel it with the first term if we can make the phase satisfy

$$\sum_\nu F_{\mu\nu}(\underline{q}) \partial_\nu \theta(\underline{q}) = -J_\mu(\underline{q}), \tag{62}$$

which amounts to introducing in the cwf the current which is present in the underlying many-body wave function. Cancelling this term is useful to simplify the functional into a form that is more convenient to later derive a Schrödinger equation for f,

$$E[f,d] = \int d^n \underline{q} \; f^*(\underline{q}) \left[-\frac{1}{2} \sum_{\mu\nu} \partial_\mu \mathcal{A}_{\mu\nu}(\underline{q}) \partial_\nu + \mathcal{U}(\underline{q}) \right] f(\underline{q}). \tag{63}$$

The phase will then simply come out from the solution to that equation.

The collective inverse mass $\mathcal{A}_{\mu\nu}(\underline{q})$ and the collective potential $\mathcal{U}(\underline{q})$ depend on the wave function Ψ: they are,

for each $\underline{q}$, functionals of f and d. A collective Schrödinger equation can be obtained by minimizing E with respect to f, with a constraint on the norm, Eq. (19), viz.

$$\frac{\delta(E[f,d] - E'||f||^2)}{\delta f^*}$$

$$= 0 = \left[-\frac{1}{2} \sum_{\mu\nu} \partial_\mu \mathcal{A}_{\mu\nu}(\underline{q}) \partial_\nu + \mathcal{U}(\underline{q}) + \mathcal{U}_{\rm ra}(\underline{q}) - E' \right] f(\underline{q}),$$

(64)

where ∂_μ acts on all factors to its right, with a rearrangement potential that appears because of the functional derivation of $\mathcal{A}$ and $\mathcal{U}$,

$$\mathcal{U}_{\rm ra}(\underline{q}) \equiv \int d^n \underline{q}' \, f^*(\underline{q}')$$

$$\times \left[-\frac{1}{2} \sum_{\mu\nu} \partial'_\mu \frac{\delta \mathcal{A}_{\mu\nu}(\underline{q}')}{\delta |f|^2(\underline{q})} \partial'_\nu + \frac{\delta \mathcal{U}(\underline{q}')}{\delta |f|^2(\underline{q})} \right] f(\underline{q}'),$$

(65)

where ∂'_μ differentiates with respect to q'_μ. Note that in general, a distinction has to be made between E (energy) and E' (eigenvalue of the collective Hamiltonian) due to the rearrangement energy.

The remaining issue is then to optimize the $\underline{q}$-dependent density $d(\underline{q},\vec{r})$. This will be dealt with in Sec. V.

IV. EXAMPLE: TRANSLATIONAL MOTION

An illustrative example is useful at this point. Consider the case, already mentioned above, of a translationally invariant Hamiltonian, where we use the components of the CoM coordinate vector $\vec{R}$ as collective coordinates: $Q_1(\vec{r}) = x/N$, $Q_2(\vec{r}) = y/N$, $Q_3(\vec{r}) = z/N$. As mentioned above, translational symmetry allows us to write the energy as a functional of the internal density without further consideration for collective motion. However, applying the formalism of the previous section to this case is useful, since all quantities entering the collective Hamiltonian can be derived analytically.

Using these definitions,

$$\hat{\nabla} \hat{Q}_\mu(\mathbf{R}) \cdot \hat{\nabla} \hat{Q}_\nu(\mathbf{R}) = \frac{\delta_{\mu\nu}}{N},$$

(66)

$$F_{\mu\nu}(\underline{q}) = \frac{\delta_{\mu\nu}}{N} \langle P(\underline{q}) \rangle,$$

(67)

$$\mathcal{A}_{\mu\nu}(\underline{q}) = \frac{\delta_{\mu\nu}}{N}.$$

(68)

The mass of the system entering the kinetic term is thus N times the mass of the constituent particle itself, as expected.

Assuming $v_{\rm ext}(\vec{r}) = 0$ and $\hat{U}$ invariant under translations and Galilei transformations, we can write the Hamiltonian as

$$\hat{H} = \hat{T}_{\rm cm} + \hat{T}_{\rm int} + \hat{U},$$

(69)

$$\hat{T}_{\rm cm} = -\frac{1}{2N} \left(\sum_i \hat{\nabla}_i \right)^2,$$

(70)

and any eigenstate wave function of the system as

$$\Psi(\mathbf{R}) = \Psi_{\rm cm}(\vec{R}) \, \Psi_{\rm int}(\boldsymbol{\Xi}),$$

(71)

where $\boldsymbol{\Xi}$ is a vector of Jacobi coordinates allowing us to describe internal motion of the particles.

For $D(\vec{R},\vec{r})$ independent of $\vec{R}$, the value of $\Psi_{\rm cm}(\vec{R})$ that minimizes the c.m. kinetic energy is $\Psi_{\rm cm}(\vec{R}) = \Omega^{-1/2}$. To access a state with non-vanishing c.m. kinetic energy, we need to choose a trial $f(\vec{R})$ such that the c.m.-coordinate density $|f|^2(\vec{R})$ is inhomogeneous. One such choice is

$$f(\vec{R}) = \sqrt{\frac{2}{\Omega}} \, \sin(\vec{K} \cdot \vec{R}).$$

(72)

For d, let us set $d(\vec{R},\vec{r}) = \rho_{\rm int}(\vec{r})$, where $\rho_{\rm int}$ is the internal density of an eigenstate of the internal Hamiltonian $\hat{T}_{\rm int} + \hat{U}$ with eigenvalue $E_{\rm int}$. We have

$$|f(\vec{R})|^2 = \langle P(\vec{R}) \rangle = \frac{2}{\Omega} \, \sin^2(\vec{K} \cdot \vec{R}),$$

(73)

with the phase

$$\theta(\vec{R}) = \begin{cases} 0 & \text{for } 0 \leqslant \vec{K} \cdot \vec{R} - 2m\pi < \pi \\ \pi & \text{for } \pi \leqslant \vec{K} \cdot \vec{R} - 2m\pi < 2\pi \end{cases}$$

(74)

for integer m. The wave function minimizing the energy for this choice of f has $\Psi_{\rm cm}(\vec{R}) = f(\vec{R})$. Note that J_μ, Eq. (57), is, in this case, the average momentum of the system. This quantity is zero for this state, thus

$$J_\mu(\vec{R}) = 0.$$

(75)

We can derive the collective potential by using the above and Eqs. (73) and (74) in Eq. (60); after some trigonometry and much cancellation,

$$\mathcal{U}(\underline{q}) = +\frac{\pi^2 K^2}{2N} \sum_m \delta^2(\vec{K} \cdot \vec{R} - m\pi) - \frac{K^2}{2N} + E.$$

(76)

Here, $\delta^2(x)$ refers to the pseudodistribution which yields zero for functions having a node at $x = 0$, and infinity otherwise [which is the result obtained by making $\theta(\vec{R})$ vary smoothly from 0 to π on an interval whose width is then taken to zero]. The expectation value of $\mathcal{U}$ is thus

$$\int d^n \underline{q} \, f^*(\underline{q}) \mathcal{U}(\underline{q}) f(\underline{q}) = E - \frac{K^2}{2N} = E_{\rm int}.$$

(77)

In the Schrödinger equation, this term will constrain the cwf to have nodes at $\vec{K} \cdot \vec{R} = m\pi$, i.e., the same as our original choice for f. Since the phase $\theta(\vec{R})$ which introduces this term is indissociable from the choice of f (the only reasonable phase choices are ones that make f continuous), the expectation value of this operator, in fact, vanishes for any trial cwf. It can thus be dropped from the collective Schrödinger equation. Similarly, $\mathcal{V}_\mu$ vanishes except for a similar singularity at the nodes of the wave function, and the same observation applies.

Finally, $\mathcal{U}_{\rm ra}$ is in this case proportional to $1/\Omega$ and thus negligible. The collective Schrödinger equation we obtain thus involves a kinetic term with the mass of the nucleus and a constant potential equal to the internal energy. The cwf

f chosen initially is a trivial solution with eigenvalue and expectation value equal to the total energy of the system.

V. INTRODUCING ORBITALS: KOHN-SHAM SCHEME

In this section I attempt to introduce single-particle orbitals in the formulation of the previous sections. This introduction is intended to be "minimal," i.e., as simple as possible—other formulations could be envisioned.

Let us start by writing the collective potential of Eq. (63) as

$$\mathcal{U}[f,d](\underline{q}) = T_s[\rho_{\underline{q}}] + \mathcal{U}^{\text{ext}}[\rho_{\underline{q}}] + \mathcal{U}^{\text{ic}}[f,d](\underline{q}), \quad (78)$$

where, for convenience, we define $\rho_{\underline{q}}(\vec{r}) \equiv d(\underline{q},\vec{r})$ and T_s is the usual Kohn-Sham kinetic energy functional

$$T_s[\rho_{\underline{q}}] = \min_{\{\phi_i(\underline{q})\} \to \rho_{\underline{q}}} \left[-\frac{1}{2} \int d^3\vec{r} \sum_{i=1}^{N} \phi_i^*(\underline{q};\vec{r}) \, \Delta \, \phi_i(\underline{q};\vec{r}) \right], \quad (79)$$

the $\phi_i(\underline{q},\vec{r})$ being a set of orthogonal single-particle orbitals. The notation $\{\phi_i(\underline{q})\} \to \rho_{\underline{q}}$ restricts the variational domain to sets of orbitals satisfying

$$\rho_{\underline{q}}(\vec{r}) = d(\underline{q},\vec{r}) = \sum_{i=1}^{N} \phi_i^*(\underline{q},\vec{r}) \, \phi_i(\underline{q},\vec{r}). \quad (80)$$

Note that we use the unmodified mass of the particle in the kinetic operator. It is common, in nuclear functionals, to include a CoM motion correction, either by simply multiplying the particle mass by $(1 - 1/N)$ or also including, in addition, the two-body part of the internal kinetic-energy operator in the energy. Bear in mind that the decomposition (78) and (79) is merely a choice, which should be judged on its practical merits. From first-principle arguments, the use of such a CoM correction in a functional of the internal density is not required [16,50]. Note that we built our formalism starting from a many-body ground-state wave function with a vanishing CoM kinetic energy, and do not need to remove the latter. The Slater determinant formed by the KS orbitals has a nonvanishing CoM energy, but it is only a theoretical auxiliary. Moreover, since its explicit particle-number dependence breaks size consistency, such a correction is undesirable in applications to reactions [51] or fission [52,53], hence its omission here.

The term $\mathcal{U}^{\text{ext}}$ captures the contribution from the external potential,

$$\mathcal{U}^{\text{ext}}[\rho_{\underline{q}}] = \int d^3\vec{r} \, v_{\text{ext}}(\vec{r}) \, \rho_{\underline{q}}(\vec{r}), \quad (81)$$

while $\mathcal{U}^{\text{ic}}$ is the interaction and correlation contribution not accounted for by the previous terms. In canonical electronic DFT, interaction and correlation terms in the functional are further split into Hartree and exchange-correlation terms. We shall keep the formalism more compact and general with respect to the form of the interaction by omitting this step.

The density $d(\underline{q},\vec{r})$ can be optimized by minimizing the energy with respect to the orbitals with a normalization constraint, as well as a constraint on the average value of the collective coordinates to satisfy Eq. (24),

$$\frac{\delta\left[E - e_k(\underline{q})(\underline{q}k|\underline{q}k) - \sum_\mu l_\mu(Q_\mu|\rho_{\underline{q}})\right]}{\delta\phi_k^*(\underline{q};\vec{r})} = 0, \quad (82)$$

$$l_\mu \equiv \frac{\partial E}{\partial(Q_\mu|\rho_{\underline{q}})}, \quad (83)$$

which, per Eqs. (63), (78), and (79), yields

$$\left[-\tfrac{1}{2}\Delta + v_{\text{ext}}(\vec{r}) + v_s(\underline{q};\vec{r}) - \lambda_\mu Q_\mu(\vec{r}) - \varepsilon_i(\underline{q})\right]\phi_i(\underline{q};\vec{r}) = 0, \quad (84)$$

where we have redefined the single-particle energy as $\varepsilon_k(\underline{q}) \equiv |f(\underline{q})|^{-2} e_k(\underline{q})$ and the Legendre multiplier as $\lambda_\mu \equiv |f(\underline{q})|^{-2} l_\mu$.

The auxiliary potential $v_s(\underline{q},\vec{r})$ is

$$v_s(\underline{q};\vec{r}) \equiv |f(\underline{q})|^{-2} \frac{\delta E[f,d]}{\delta d(\underline{q},\vec{r})} \quad (85)$$

$$= |f(\underline{q})|^{-2} \int d^n\underline{q}' \, f^*(\underline{q}')$$

$$\times \left[-\frac{1}{2}\partial_\mu' \frac{\delta \mathcal{A}_{\mu\nu}(\underline{q}')}{\delta d(\underline{q},\vec{r})} \partial_\nu' + \frac{\delta \mathcal{U}^{\text{ic}}(\underline{q}')}{\delta d(\underline{q},\vec{r})} \right] f(\underline{q}'). \quad (86)$$

This formulation raises the usual problem of noninteracting v representability [44], i.e., of the existence of a map between $v(\underline{q},\vec{r})$ and $d(\underline{q},\vec{r})$ subject to Eq. (84) at each $\underline{q}$, which presents itself in the same way in the present formalism as we use the KS kinetic-energy functional T_s.

Per the Hohenberg-Kohn theorem applied to the noninteracting system, Eqs. (79) and (84) unambiguously define a unique potential $v_s(\underline{q},\vec{r})$ and a unique set of orbitals and associated energies which, for each value of $\underline{q}$, are functionals of $\rho_{\underline{q}}(\vec{r})$. These orbitals are labeled by an index k which can be smaller or greater than N. In the following we use i as an index on the first N (occupied) orbitals, a as an index on unoccupied (or virtual) orbitals, while k indexes the whole basis. This in turn allows us to introduce orbital-dependent terms in the functional. Let us use this possibility by expressing the collective mass as

$$\mathcal{A}_{\mu\nu}[f,d](\underline{q}) = \mathcal{A}_{\mu\nu}^{\text{In}}[d](\underline{q}) + \mathcal{A}_{\mu\nu}^{\text{ic}}[f,d](\underline{q}). \quad (87)$$

In the last expression, $\mathcal{A}_{\mu\nu}^{\text{In}}$ is the Inglis cranking-formula collective mass [27,54], while $\mathcal{A}_{\mu\nu}^{\text{ic}}$ is the remaining interaction-correlation component,

$$\mathcal{A}^{\text{In}}(\underline{q}) \equiv [B^{\text{in}}(\underline{q})]^{-1}, \quad (88)$$

$$B_{\mu\nu}^{\text{In}}[f,d](\underline{q}) = 2 \sum_{ai} \frac{(\underline{q}i|v_{\underline{q}}^{(\mu)}|\underline{q}a)(\underline{q}a|v_{\underline{q}}^{(\nu)}|\underline{q}i)}{[\varepsilon_a(\underline{q}) - \varepsilon_i(\underline{q})]^3}, \quad (89)$$

where

$$v_{\underline{q}}^{(\mu)}(\vec{r}) \equiv \frac{\partial v(\underline{q},\vec{r})}{\partial q_\mu}, \quad (90)$$

$$(\underline{q}k|v_{\underline{q}}^{(\mu)}|\underline{q}l) = \int d^3\vec{r} \, \phi_k^*(\underline{q},\vec{r}) \, v_{\underline{q}}^{(\mu)}(\vec{r}) \, \phi_l(\underline{q},\vec{r}). \quad (91)$$

Orbital-dependent terms have been extensively used in quantum-chemistry applications of DFT, first as a way of replacing nonlocal exchange terms [55,56], see also [57], then as a tool for introducing explicit correlations in the functional through perturbation theory [58,59]. Let me refer to the reviews in Refs. [8,60,61] and simply use a straightforward generalization of their main result [make all quantities depend on $\underline{q}$ and add a factor $|f(\underline{q})|^{-2}$ to the definition of v_s] to derive the contribution $v_{In}(\underline{q},\vec{r})$ of $\mathcal{A}_{\mu\nu}^{In}$ to the auxiliary potential. This can be obtained by inverting the optimized effective potential (OEP) equation,

$$|f(\underline{q})|^2 \int d\vec{r}' \; \chi_s(\underline{q};\vec{r},\vec{r}') \, v_{In}(\underline{q};\vec{r}') = \Lambda_{In}(\underline{q};\vec{r}), \quad (92)$$

where

$$\Lambda_{In}(\underline{q};\vec{r}) = \sum_k \left\{ -\int d\vec{r}' \left[\phi_k^*(\underline{q};\vec{r}) \, G_k(\underline{q};\vec{r},\vec{r}') \, \frac{\delta E_{In}}{\delta \phi_k^*(\underline{q};\vec{r}')} \right. \right.$$
$$\left. \left. + \text{c.c.} \right] + |\phi_k(\underline{q};\vec{r})|^2 \, \frac{\delta E_{In}}{\delta \varepsilon_k(\underline{q})} \right\}, \quad (93)$$

and E_{In} is the cranking contribution to the energy,

$$E_{In}[f,d] = -\frac{1}{2} \int d^n\underline{q} \; f^*(\underline{q}) \sum_{\mu\nu} \partial_\mu \big(\mathcal{A}_{\mu\nu}^{In}[d](\underline{q}) \partial_\nu f(\underline{q}) \big), \quad (94)$$

χ_s being the static KS response function and G_k the KS Green's function,

$$\chi_s(\underline{q};\vec{r},\vec{r}') = -\sum_k \phi_k^*(\underline{q};\vec{r}) \, G_k(\underline{q};\vec{r},\vec{r}') \, \phi_k(\underline{q};\vec{r}') + \text{c.c.}, \quad (95)$$

$$G_k(\underline{q};\vec{r},\vec{r}') = \sum_{l \neq k} \frac{\phi_l(\underline{q};\vec{r}) \, \phi_l^*(\underline{q};\vec{r}')}{\varepsilon_l(\underline{q}) - \varepsilon_k(\underline{q})}. \quad (96)$$

The functional derivatives of the orbital-dependent energy with respect to ϕ_k^* and ε_k, using t as a shorthand for either, are

$$\frac{\delta E_{In}}{\delta t} = \frac{1}{2} \int d^n\underline{q} \; f^*(\underline{q})$$
$$\times \underline{\partial} \left[(B^{In})^{-1}(\underline{q}) \frac{\delta B^{In}(\underline{q})}{\delta t} (B^{In})^{-1}(\underline{q}) \, \underline{\partial} f(\underline{q}) \right], \quad (97)$$

where the derivatives of B^{In} are given by

$$\frac{\delta B_{\mu\nu}^{In}}{\delta \phi_k^*(\underline{q};\vec{r})}$$
$$= 2 \begin{cases} \sum_a v_{\underline{q}}^{(\mu)}(\vec{r}) \, \phi_a(\underline{q};\vec{r}) \frac{(\underline{q}a|v_{\underline{q}}^{(\nu)}|\underline{q}k)}{[\varepsilon_a(\underline{q})-\varepsilon_k(\underline{q})]^3} & (k \leqslant N), \\ \sum_i \frac{(\underline{q}k|v_{\underline{q}}^{(\mu)}|\underline{q}i)}{[\varepsilon_k(\underline{q})-\varepsilon_i(\underline{q})]^3} v_{\underline{q}}^{(\nu)}(\vec{r}) \, \phi_i(\underline{q};\vec{r}) & (k > N), \end{cases} \quad (98)$$

and

$$\frac{\delta B_{\mu\nu}^{In}}{\delta \varepsilon_k(\underline{q})} = 6 \begin{cases} \sum_a \frac{(\underline{q}k|Q_\mu|\underline{q}a)(\underline{q}a|Q_\nu|\underline{q}k)}{[\varepsilon_a(\underline{q})-\varepsilon_k(\underline{q})]^4} & (k \leqslant N), \\ -\sum_i \frac{(\underline{q}i|Q_\mu|\underline{q}k)(\underline{q}k|Q_\nu|\underline{q}i)}{[\varepsilon_k(\underline{q})-\varepsilon_i(\underline{q})]^4} & (k > N), \end{cases} \quad (99)$$

This completes the sets of equations needed to solve for energy-minimizing $f(\underline{q})$ and $d(\underline{q},\vec{r})$. The solution should proceed by alternating between Eq. (84) at a set of points in $\underline{q}$ space and (65), starting from an initial guess and iterating to convergence, using standard tools for the self-consistent solution of Kohn-Sham equations. This is obviously more involved than standard DFT, owing to the multiplication of the computational load by the number of $\underline{q}$ mesh points, but this problem appears relatively easy to treat with parallel processing, as only the cwf and fields have to be communicated between neighboring points, as well as densities, unless one assumes a lack of dependence of $\mathcal{U}(\underline{q})$ on densities at $\underline{q}' \neq \underline{q}$. The largest data sets, i.e., orbitals, stay local.

In the treatment of Hill-Wheeler or collective Hamiltonian equations, feedback from collective motion to the single-particle "mean field" is usually ignored [28]. Above, we have a recipe for going beyond that approximation, which would be of interest for the description of rotational bands in collective nuclei [62,63], as well as the dynamics of fission processes [64].

If we nevertheless neglect the feedback from collective motion, the formalism can be put into a more conventional form. Assuming the $\mathcal{A}$ term from the equation for $v_s(\underline{q},\vec{r})$, Eq. (87), to be negligible, the latter then only contains a functional derivative of $\mathcal{U}$. The collective potential $\mathcal{U}(\underline{q})$ generally depends on $d(\underline{q}',\vec{r})$ and $f(\underline{q}')$ for all $\underline{q}'$, due to the coupling between different slices $\Psi(\underline{q})$ in the many-body Schrödinger equation. If we further assume that this coupling is weak, we can reduce the dependence of $\mathcal{U}$ on the density at $\underline{q}$, i.e.,

$$\mathcal{U}(\underline{q})[f,d] = \mathcal{U}(\underline{q})[\rho_{\underline{q}}] = \mathcal{U}[\rho_{\underline{q}}] \quad (100)$$
$$= T_s[\rho_{\underline{q}}] + \mathcal{U}_{ext}[\rho_{\underline{q}}] + \mathcal{U}_{ic}[\rho_{\underline{q}}], \quad (101)$$

where the second equality in Eq. (100) is justified by the fact that the value of $\underline{q}$ is encoded in $\rho_{\underline{q}}(\vec{r}) = d(\underline{q},\vec{r})$, Eq. (24). We then obtain

$$v_s(\underline{q},\vec{r}) = \frac{\delta \mathcal{U}_{ic}}{\delta \rho_{\underline{q}}}. \quad (102)$$

Then, $\mathcal{U}_{ic}[\rho_{\underline{q}}]$ plays the role of the usual Skyrme, Gogny, or relativistic functional, which can be used in the standard way, with an independent, *a posteriori* solution of the collective Schrödinger equation. This form, however, relies on the assumptions above.

More generally, a practical application of the present theory requires a parametrization of $\mathcal{U}_{ic}$ and $\mathcal{A}_{\mu\nu}^{ic}$. Let me stress the latter: the cranking formula used above is by no means assumed correct by itself. It could be replaced by a term derived using adiabatic time-dependent Hartree-Fock (ATDHF) [37,41,65,66] or the Gaussian overlap approximation to the GCM (GCM-GOA) [26,38–40]. Even then, such terms rely entirely on the single-particle orbitals at each position in the collective space and cannot be expected to correctly reproduce the physics of the underlying correlated many-body state. The collective mass $\mathcal{A}_{\mu\nu}$ is an integral part of the functional, and, in the absence of a rigorous *ab initio* derivation, it is perfectly reasonable to parametrize it and adjust the parameters to experimental data.

VI. SUMMARY AND OUTLOOK

The energy of a many-body system is expressible as a functional of a *generalized density*, which extends the concept of the local particle density to include a dependence on coordinates describing collective motion of the particles. The generalized density can be decomposed as the product of the square of a cwf and a density parametrized by the collective coordinates, which is allowed to break spatial symmetries of the Hamiltonian. By decomposing the kinetic contribution to the energy, the functional can be written into a form that allows us to write a Schrödinger equation for the cwf. When the collective coordinates are chosen to be the components of the inertia tensor of the system, the collective Hamiltonian takes the form of a generalized Bohr Hamiltonian. Single-particle quantum effects can be reintroduced with single-particle orbitals determined from a single-particle potential deduced from the parametrizations of the collective mass and potential. With the assumption of weak coupling between single-particle degrees of freedom at different points in the collective space, the functional can be reduced to a form similar to current nuclear energy density functionals augmented by a collective Hamiltonian; equations have been derived for going beyond this scheme and optimizing single-particle and collective degrees of freedom simultaneously.

Extending the formalism to superfluid systems presents a significant challenge, and it is likely that a simpler scheme

can be found for this particular case. Derivations have been carried out ignoring spin and isospin degrees of freedom; reintroducing these [50], as well as introducing spin and kinetic densities [67,68], seems to pose no major obstacle. Developing a time-dependent version of the theory presented here in the vein of Refs. [69,70] could prove useful for the treatment of excitations of deformed and highly collective nuclei, as well as nuclear reactions [71]. Finally, it would be interesting to derive from first principles, for a few nuclei, the collective Hamiltonian proposed here. This is made difficult by the N-body operators involved, but probably feasible using a many-body method that uses the $3N$-dimensional coordinate representation natively, such as variational or Green's function Monte Carlo [72,73].

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