Alternate, well-founded way to treat center-of-mass correlations: Proposal of a local center-of-mass correlations potential

Jérémie Messud*

Université Bordeaux, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France

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The recently developed "internal" density functional theory provides an existence theorem for a local potential that contains the center-of-mass correlations effects. The knowledge of the corresponding energy functional would provide a much more effective way than projection techniques to treat these correlations. The aim of this article is to construct such a functional. We propose a well-founded method, suitable for fermions as well as for bosons, which does not require any free parameters.

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I. INTRODUCTION

One of the most obvious symmetries of isolated self-bound systems (such as atomic nuclei, helium droplets, or molecular systems where nuclei are treated explicitly) is translational invariance. Translational invariance of self-bound Hamiltonians ensures Galilean invariance of the wave function, so that the center-of-mass (c.m.) properties can be separated from the "internal" properties (which are of experimental interest). As a consequence, one laboratory coordinate is redundant for the description of the internal properties, which produces c.m. correlations.

A numerically manageable and successful way to describe self-bound systems is to use mean-field-like calculations with effective interactions. The corresponding equations are often justified starting from the Hartree-Fock (HF) framework, which sacrifices by construction "Galilean invariance for the sake of the Pauli principle," to quote Ref. [1]. As a consequence, c.m. correlations are treated incorrectly (in an equivalent manner, the redundant coordinate problem is treated incorrectly). This introduces a spurious coupling between the internal properties and the c.m. motion in an HF framework that affects the energy and other observables [2].

A way to overcome this problem in the stationary case is to perform the projected HF, where projection before variation on c.m. momentum restores translational or Galilean invariance of the wave function. Peierls and Yoccoz proposed a single-projection method to restore translational invariance [3]. Later, Peierls and Thouless proposed a double-projection method to restore the more fundamental Galilean invariance [4]. To our knowledge, all numerical calculations that treat c.m. correlations by projection before variation have been done using the Peierls and Yoccoz method [5–8], thus not restoring the full Galilean invariance. Moreover, the price is the abandonment of the independent-particle description and a large numerical cost [1,4,9,10]. Indeed, projection techniques require "an order of magnitude more computing time than the underlying mean-field-like calculations," to quote Ref. [7], which is prejudicial for the description of intermediate-sized systems. This led to the development of various approximate methods to treat c.m. correlations; see Ref. [11] for an overview. For instance, a common method is to add a $-\langle \frac{\mathbf{P}^2}{2mN} \rangle$ term in the energy functional (more details are given in Sec. II C). But the success of those methods is not systematic, and the approximations done not completely justified.

In the time-dependent case, the spurious c.m. motion problem remains [12,13], but the situation is trickier, as the projected HF method becomes unmanageable even for very small self-bound systems [12]. It thus remains an open problem to develop a rigorous and numerically inexpensive scheme to treat c.m. correlations, which would go beyond standard approximations and remain usable in the time-dependent case.

The search for such a scheme has not yet been pursued extensively, perhaps because it is sometimes thought that the c.m. correlations problem concerns only very small self-bound systems. But c.m correlations can have a non-negligible effect even for intermediate-sized systems. For instance, it has been shown that c.m. correlations are non-negligible for all nuclei heavier than ^{16}O [6,7,14]. This reinforces the necessity to develop a numerically manageable method to treat them.

A rigorous alternative and *a priori* numerically much less costly way to take these correlations into account has been revealed by the recently developed "internal" density functional theory (DFT) and Kohn-Sham (KS) scheme [15–17]. Differing from the standard DFT [18–21], it is formulated in the c.m frame of a self-bound system and proves that the c.m. correlations can be included in the energy functional and thus in a local KS potential [15–17]. In addition to the fact that it gives a much more fundamental justification than the HF framework for the use of mean-field-like calculations with effective interactions for the description of self-bound systems, it shows that there would be no need for a c.m. projection if the ultimate functional were known. The internal DFT gives an existence theorem but not a constructive method. The aim of the present article is to propose such a constructive method.

The article is organized as follows. Section II provides a brief review of the internal DFT formalism and underlines the limitations of the commonly used methods to treat c.m. correlations. Section III develops a new general form for a local c.m. correlations potential that introduces no free parameter.

*Present address: CGGVeritas, F-91341 Massy, France; jeremie.messud@cggveritas.com

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Finally, Sec. IV gives convincing numerical results on various model systems.

II. THE INTERNAL DFT AND C.M. CORRELATIONS FUNCTIONAL

A. Brief review of the internal DFT formalism

We start from a self-bound system composed of N identical particles of mass m and follow the considerations of Ref. [15]. The coordinates of the particles in any chosen inertial frame of reference (such as the laboratory) are denoted $\{\mathbf{r}_i\}$. The c.m. coordinate of the system is denoted

$$\mathbf{R} = \frac{1}{N}\sum_{j=1}^{N}\mathbf{r}_j.$$

The system is described by the following translationally invariant N-body Hamiltonian:

$$H = \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} + \sum_{\substack{i,j=1\\ i>j}}^{N} u(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i=1}^{N} v^{\text{int}}(\mathbf{r}_i - \mathbf{R}), \quad (1)$$

composed of the usual kinetic energy term, a two-body potential u which describes the particle-particle interaction (generalization of the following considerations to three-body, etc., interactions is straightforward) and an arbitrary translationally invariant potential v^{int}. The latter potential is an "internal" potential, i.e., it is defined in the c.m. frame and acts only on the internal properties. Of course, the potential is 0 in the purely isolated self-bound case. Nevertheless, its form is suitable for modeling the internal effects of fields used in experiments (polarization potentials, etc.) [16].

We introduce the Jacobi coordinates ξ_α, defined as $\xi_1 = \mathbf{r}_2 - \mathbf{r}_1$, $\xi_2 = \mathbf{r}_3 - \frac{\mathbf{r}_2+\mathbf{r}_1}{2}, \ldots, \xi_{N-1} = \frac{N}{N-1}(\mathbf{r}_N - \mathbf{R})$. This permits us to separate the Hamiltonian (1) into $H = H_{\text{CM}} + H_{\text{int}}$, where $H_{\text{CM}} = -\hbar^2/(2mN)\Delta_{\mathbf{R}}$ is a one-body Hamiltonian describing the c.m. motion and acting in the $\mathbf{R}$ space only, and H_{int} is an $(N-1)$ body-Hamiltonian describing the internal properties and acting in the $\{\xi_\alpha\}$ space only:

$$H_{\text{int}} = \sum_{\alpha=1}^{N-1}\frac{\tau_\alpha^2}{2\mu_\alpha} + U(\xi_1,\ldots,\xi_{N-1}) + V^{\text{int}}(\xi_1,\ldots,\xi_{N-1}).$$

H_{int} contains the interaction u and the potential v^{int}, because they can be rewritten as functions of the $\{\xi_\alpha\}$ only [denoted $U(\xi_1,\ldots,\xi_{N-1})$ and $V^{\text{int}}(\xi_1,\ldots,\xi_{N-1})$, respectively] and the internal kinetic energy, which is expressed in terms of the conjugate momentum τ_α of ξ_α and the reduced masses $\mu_\alpha = m\frac{\alpha}{\alpha+1}$. As $[H_{\text{CM}}, H_{\text{int}}] = 0$, the eigenstate ψ of H can be written as a product of the form

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \Gamma(\mathbf{R})\,\psi_{\text{int}}(\xi_1,\ldots,\xi_{N-1}), \quad (2)$$

where Γ and ψ_{int} are defined by the equations

$$-\frac{\hbar^2}{2M}\Delta_{\mathbf{R}}\Gamma = E_{\text{cm}}\Gamma, \quad (3)$$

$$H_{\text{int}}\psi_{\text{int}} = E_{\text{int}}\psi_{\text{int}}. \quad (4)$$

Γ is the c.m. wave function that describes the motion of the isolated system as a whole in any inertial frame of reference. Because $\Gamma(\mathbf{R})$ is the solution of the free Schrödinger equation, it should be an arbitrary stationary plane wave, i.e., infinitely spread and not normalizable. This leads to the delocalization of $\mathbf{R}$ and arbitrary c.m. energy. This does not correspond to experimental situations where the system is no longer isolated: interactions with other systems of the experimental apparatus localize the c.m. However, this is not a problem, as internal properties that are of experimental interest are fully described by ψ_{int}. Note that ψ_{int} is, by definition, always normalizable for the ground state of a self-bound system. The internal density associated with ψ_{int} is [15,22,23]

$$\begin{aligned}\rho_{\text{int}}(\mathbf{r}) &= N\left(\frac{N}{N-1}\right)^3\int d\xi_1\cdots d\xi_{N-2}\\ &\quad\times\left|\psi_{\text{int}}\left(\xi_1,\ldots,\xi_{N-2},\frac{N\mathbf{r}}{N-1}\right)\right|^2\\ &= N\int d\mathbf{r}_1\cdots d\mathbf{r}_N\;\delta(\mathbf{R})|\psi_{\text{int}}(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2\\ &\quad\times\delta(\mathbf{r}-(\mathbf{r}_i-\mathbf{R})). \end{aligned}\quad (5)$$

$\rho_{\text{int}}(\mathbf{r})$ is normalized to N and $\mathbf{r}$ is defined in the c.m. frame (see the δ relation in the previous equation).[1] Note that even if ψ_{int} can be written as a function of the $(N-1)$ Jacobi coordinates only, it can also be written as a function of the N coordinates $\mathbf{r}_i$. In this case, one of the coordinates would be redundant [24], which is expressed by the $\delta(\mathbf{R})$ in the previous equation.

The stationary internal DFT theorem demonstrated in various ways in Refs. [15,25,26] states that for a nondegenerate ground state and a given kind of particle, ψ_{int} can be expressed as a unique functional of ρ_{int}, i.e., $\psi_{\text{int}}[\rho_{\text{int}}]$. As a consquence, the ground-state internal energy of a self-bound system $E_{\text{int}} = (\psi_{\text{int}}[\rho_{\text{int}}]|H_{\text{int}}|\psi_{\text{int}}[\rho_{\text{int}}])$ can also be expressed as a unique functional of ρ_{int}.

A practical way to compute ρ_{int} is given by the internal KS scheme, developed in Ref. [15]. To set up this scheme, we assume that there exists, *in the c.m. frame*, a local single-particle potential (i.e., an N-body noninteracting system) that can reproduce the exact density ρ_{int} of the interacting system. We develop ρ_{int} on the corresponding basis $\{\varphi_{\text{int}}^i\}$ of one-body orbitals expressed in the c.m. frame:

$$\rho_{\text{int}}(\mathbf{r}) = \sum_{i=1}^{N}\left|\varphi_{\text{int}}^i(\mathbf{r})\right|^2. \quad (6)$$

We refer the reader to Ref. [17], Sec. III C, for a justification of the introduction of N orbitals in the KS scheme, even if only $(N-1)$ coordinates are sufficient to describe internal properties. We implicitly supposed that the particles are fermions, but a KS scheme to describe boson condensates can be set up in a similar manner by choosing all the φ_{int}^i to be identical.

[1] More generally, we can introduce a $\delta(\mathbf{R}-\mathbf{a})$ where $\mathbf{a}$ is an arbitrary translation vector, which would lead to perfectly equivalent results. We chose $\mathbf{a} = \mathbf{0}$ for simplicity, so that the formalism is formulated in the c.m. frame.

The KS assumption implies $\varphi^i_{\rm int}[\rho_{\rm int}]$ [21]; thus, we can rewrite $E_{\rm int}$ as [15]

$$E_{\rm int}[\rho_{\rm int}] = \sum_{i=1}^{N}\left(\varphi^i_{\rm int}\left|\frac{\mathbf{p}^2}{2m}\right|\varphi^i_{\rm int}\right) + E_{\rm HXC}[\rho_{\rm int}] + \int d\mathbf{r}\, v_{\rm int}(\mathbf{r})\rho_{\rm int}(\mathbf{r}), \tag{7}$$

where we have introduced the "interaction energy functional":[2]

$$E_{\rm HXC}[\rho_{\rm int}] = \frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\, \gamma_{\rm int}[\rho_{\rm int}](\mathbf{r},\mathbf{r}')\, u(\mathbf{r}-\mathbf{r}') + E_{\Delta\rm kin}[\rho_{\rm int}], \tag{8}$$

where

$$E_{\Delta\rm kin}[\rho_{\rm int}] = \left(\psi_{\rm int}\left|\sum_{\alpha=1}^{N-1}\frac{\tau_\alpha^2}{2\mu_\alpha}\right|\psi_{\rm int}\right) - \sum_{i=1}^{N}\left(\varphi^i_{\rm int}\left|\frac{\mathbf{p}^2}{2m}\right|\varphi^i_{\rm int}\right) \tag{9}$$

$$= \int d\mathbf{r}_1\cdots d\mathbf{r}_N\,\delta(\mathbf{R})\,\psi^*_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \times \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N) - \sum_{i=1}^{N}\left(\varphi^i_{\rm int}\left|\frac{\mathbf{p}^2}{2m}\right|\varphi^i_{\rm int}\right). \tag{10}$$

$E_{\rm HXC}$ traditionally contains the Hartree energy plus the quantum exchange-correlations energy [15]. We do not explicitly use this decomposition here because common functionals that describe self-bound systems (such as the Skyrme force in nuclear physics [2]) approximate $E_{\rm HXC}$ as a whole.

We now give particular attention to the $E_{\Delta\rm kin}$ term. We call the "interacting" kinetic energy the kinetic energy of the self-bound system, i.e., $\int d\mathbf{r}_1\cdots d\mathbf{r}_N\delta(\mathbf{R})\,\psi^*_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$, and the "noninteracting" kinetic energy the kinetic energy of the KS system, i.e., $\sum_{i=1}^{N}(\varphi^i_{\rm int}|\frac{\mathbf{p}^2}{2m}|\varphi^i_{\rm int})$. We see from Eq. (10) that $E_{\Delta\rm kin}$ is the difference between those two energies. It thus contains the exchange and "standard" correlations[3] part of the "interacting" kinetic energy term, but also its c.m. correlations part [owing to $\delta(\mathbf{R})$]. It is the only term of the functional that explicitly contains the c.m. correlations and represents the main difference from the traditional DFT.

Varying $E_{\rm int}[\rho_{\rm int}]$, Eq. (7), with respect to $\varphi^{i*}_{\rm int}$, and imposing orthonormality of the $\{\varphi^i_{\rm int}\}$ leads to "internal" KS equations

$$\left(-\frac{\hbar^2}{2m}\Delta + U_{\rm HXC}[\rho_{\rm int}] + v_{\rm int}\right)\varphi^i_{\rm int} = \epsilon_i\varphi^i_{\rm int}, \tag{11}$$

where $U_{\rm HXC}[\rho_{\rm int}](\mathbf{r}) = \delta E_{\rm HXC}[\rho_{\rm int}]/\delta\rho_{\rm int}(\mathbf{r})$ is local as expected. Equations (11) have the same form as the traditional KS equations formulated for non–translationally invariant Hamiltonians [19], but we have justified their use in the c.m. frame for self-bound systems described with translational-invariant Hamiltonians and shown that the functional form of $U_{\rm HXC}[\rho_{\rm int}]$ differs by the inclusion of c.m. correlations [15].

Moreover, we see from Eq. (10) that one has to be cautious with the meaning that is given to the noninteracting kinetic energy in mean-field-like calculations. Indeed, the noninteracting kinetic energy cannot be considered as a first-order approximation of the interacting kinetic energy in the general case. The difference is equal to $E_{\Delta\rm kin}$, which can be large when c.m. correlations effects are strong, i.e., for small and intermediate-sized self-bound systems. For large self-bound systems, $E_{\Delta\rm kin}$ decreases (in relative value) so that the noninteracting and interacting kinetic energies values approach each other.

Finally, we mention that the internal DFT formalism has been generalized to time-dependent self-bound systems in Ref. [16], for instance, for the description of the collision of two nuclei or laser irradiation, and multicomponent self-bound systems in Ref. [17] for the description of self-bound systems composed of different kinds of particles (atomic nuclei, mixtures of ^{3}He and ^{4}He droplets, and molecular systems where the nuclei are treated explicitly). The latter work permits us to recover the traditional DFT formalism when one kind of particle is much heavier than the others [17], underlining why the traditional DFT is well suited to describe electrons (only) in molecular systems but not to describe self-bound systems.

B. Proposed method to obtain a c.m. correlations functional

We split the $E_{\rm HXC}$ functional defined by Eq. (8) in a more interesting way for our purpose:

$$E_{\rm HXC}[\rho_{\rm int}] = E^{\rm stand}_{\rm HXC}[\rho_{\rm int}] + E_{\rm cm}[\rho_{\rm int}]. \tag{12}$$

$E^{\rm stand}_{\rm HXC}$ is the "standard" many-body interaction energy (we recall that "standard" means every interaction energy except that of the c.m. correlations), which is mostly described by the parametrized functionals commonly used for mean-field-like calculations of self-bound systems (see Refs. [2,9] for a description of functionals used for nuclear systems and Ref. [27] for a description of functionals used for helium droplet systems).

$E_{\rm cm}$ is the pure c.m. correlations energy, which is, by construction, mostly *not* taken into account in commonly used functionals (except through a renormalization of the mass in the noninteracting kinetic energy term), which can affect the results; see Ref. [11]. The goal of this article is to build a well-founded form for $E_{\rm cm}$ that can be used to describe all self-bound systems by simple addition to the commonly used functionals (which rigorously implies a refitting of those functionals) and is numerically manageable.

The idea is simple: we start from $E_{\rm HXC}$, Eq. (8), and neglect all the "standard" interaction terms. Then, by definition (12), we are left with $E_{\rm cm}$. This is equivalent to starting from $E_{\Delta\rm kin}$, Eq. (10), and neglecting all the exchange and standard correlations terms. We thus have to find a good approximation of $E_{\Delta\rm kin}$ to proceed. We propose to search for an approximation as a functional of the KS orbitals $\varphi^i_{\rm int}$. We adopt this approach because it provides a lot of flexibility

[2] $\gamma_{\rm int}(\mathbf{r},\mathbf{r}')$ is the local part of the two-body *internal* density matrix defined in Ref. [15], which is trivially a functional of $\rho_{\rm int}$.

[3] Henceforth, "standard" correlations mean all correlations except the c.m. correlations.

while being fully coherent with DFT (indeed, the KS orbitals are functionals of the internal density, i.e., $\varphi^i_{\rm int}[\rho_{\rm int}]$, as soon as they satisfy KS equations [21], which can be constrained explicitly by use of the optimized effective potential (OEP) method [28–30]).

C. The commonly used form for the c.m. correlations functional

We first show how the proposed method permits us to recover the commonly used $-\langle\frac{\mathbf{P}^2}{2mN}\rangle$ form for $E_{\rm cm}$ and to understand its limitations. We rewrite $E_{\Delta\rm kin}$, Eq. (9), in the following equivalent way:[4]:

$$\begin{aligned}
&E_{\Delta\rm kin}[\rho_{\rm int}]\\
&=\int d\mathbf{R}\delta(\mathbf{R})\left(\psi_{\rm int}\left|\sum_{\alpha=1}^{N-1}\frac{\tau_\alpha^2}{2\mu_\alpha}\right|\psi_{\rm int}\right)-\sum_{i=1}^{N}\left(\varphi^i_{\rm int}\left|\frac{\mathbf{p}^2}{2m}\right|\varphi^i_{\rm int}\right)\\
&=\int d\mathbf{R}d\xi_1\cdots d\xi_{N-1}\,(\sqrt{\delta(\mathbf{R})}\psi_{\rm int}(\xi_1,\ldots,\xi_{N-1}))^*\\
&\quad\times\sum_{\alpha=1}^{N-1}\frac{\tau_\alpha^2}{2\mu_\alpha}(\sqrt{\delta(\mathbf{R})}\psi_{\rm int}(\xi_1,\ldots,\xi_{N-1}))\\
&\quad-\sum_{i=1}^{N}\left(\varphi^i_{\rm int}\left|\frac{\mathbf{p}^2}{2m}\right|\varphi^i_{\rm int}\right)\\
&=\int d\mathbf{r}_1\cdots d\mathbf{r}_N\,(\sqrt{\delta(\mathbf{R})}\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N))^*\\
&\quad\times\left(\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}-\frac{\mathbf{P}^2}{2mN}\right)(\sqrt{\delta(\mathbf{R})}\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N))\\
&\quad-\sum_{i=1}^{N}\left(\varphi^i_{\rm int}\left|\frac{\mathbf{p}^2}{2m}\right|\varphi^i_{\rm int}\right).
\end{aligned}\tag{13}$$

$\sqrt{\delta(\mathbf{R})}\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is interpreted as the c.m.-frame N-body "wave function" [recall that $\psi_{\rm int}$ has the dimension of an $(N-1)$-body wave function; see Eq. (2)]. This wave function is obviously not translationally invariant [$\delta(\mathbf{R})$ fixes the c.m. in position space and amounts to moving in the c.m. frame] and antisymmetric under the exchange of two particles (as $\psi_{\rm int}$ is antisymmetric). It is non-null only for the $\{\mathbf{r}_i\}$ that satisfy $\mathbf{R}=\sum_{i=1}^N\mathbf{r}_i=0$, so that the $\{\mathbf{r}_i\}$ become the c.m.-frame coordinates.

Within the internal DFT formalism, the commonly used approximation to treat c.m. correlations can be recovered by supposing that the KS Slater determinant, denoted $\psi^{\rm aux}$, is a good first-order approximation of the c.m.-frame N-body wave function:

$$\sqrt{\delta(\mathbf{R})}\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\approx\psi^{\rm aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N),\tag{14}$$

where

$$\psi^{\rm aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\frac{1}{\sqrt{N!}}\sum_P(-1)^p\Pi_{i=1}^N\varphi^{P(i)}_{\rm int}(\mathbf{r}_i).$$

(P are the possible permutations of the coordinates and p is the number of transpositions of P.) Inserting this approximation into (13) and following the method described in Sec. II B (the standard correlations are, by construction, neglected and the exchange terms naturally cancel), we obtain

$$\begin{aligned}
E_{\Delta\rm kin}\to E_{\rm cm}[\{\varphi^k_{\rm int}\}]&=-\left(\psi^{\rm aux}\left|\frac{\mathbf{P}^2}{2mN}\right|\psi^{\rm aux}\right)\\
&=-\sum_{i=1}^{N}\left(\varphi^i_{\rm int}\left|\frac{\mathbf{p}^2}{2mN}\right|\varphi^i_{\rm int}\right)\\
&\quad-\frac{1}{2mN}\sum_{i,j=1}^{N}(\varphi^i_{\rm int}|\mathbf{p}|\varphi^i_{\rm int})(\varphi^j_{\rm int}|\mathbf{p}|\varphi^j_{\rm int}).
\end{aligned}\tag{15}$$

We recover the commonly used form for the c.m. correlations functional. Note that, in practice, the term in the last line in Eq. (15) is often neglected to reduce the numerical cost [11].

The internal DFT formalism permits us to shed new light on the validity of approximation (15). It holds if and only if approximation (14) holds at least to first order. But in general this cannot be the case because $\psi^{\rm aux}$ is far from being null when $\sum_{i=1}^N\mathbf{r}_i\neq 0$. Moreover, $\psi^{\rm aux}$ contains a c.m. vibration typical of Slater determinants [i.e., $(\psi^{\rm aux}|\mathbf{P}^n|\psi^{\rm aux})\neq 0$ for $n\geqslant 2$] [1,2], whereas $\sqrt{\delta(\mathbf{R})}\psi_{\rm int}$ does not contain such a vibration [i.e., $(\psi^{\rm int}|\mathbf{P}^n|\psi^{\rm int})=0,\forall n$]. Thus, we cannot expect to obtain a systematically satisfying improvement with this form [11].

In the next section, we propose an improved form for the c.m. correlations energy functional, where the c.m. correlations [the $\delta(\mathbf{R})$ term] appear explicitly.

III. A GENERAL NEW FORM FOR A LOCAL C.M. CORRELATIONS POTENTIAL

A. The idea and the result

We adopt a different point of view from that in Sec. II C. We start with $E_{\Delta\rm kin}[\rho_{\rm int}]$ written as in Eq. (10) [instead of Eq. (13)] and do the replacement [instead of Eq. (14)]:

$$\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\to\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\psi^{\rm aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N),\tag{16}$$

where $\Gamma^{\rm aux}(\mathbf{R})$ is any non-null one-body "wave function" that implicitly depends on the number of particles N. The reasons for its introduction are as follows.

(i) $\psi_{\rm int}$ has the dimension of an $(N-1)$–body wave function, whereas the KS Slater determinant $\psi^{\rm aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ has the dimension of an N-body wave function. Dividing $\psi^{\rm aux}$ by $\Gamma^{\rm aux}$ permits us to recover the correct dimension while preserving antisymmetry.

(ii) The KS Slater determinant $\psi^{\rm aux}$ contains a c.m. vibration, whereas $\psi_{\rm int}$ must not contain such a vibration, as mentioned in Sec. II C. This is not a problem from the KS point of view, where $\psi^{\rm aux}$ represents nothing more than an auxiliary quantity that must only reproduce the

[4]We mention that the square root of the δ function is not defined. To be perfectly rigorous, we should have introduced $\lim_{\Gamma^{\rm aux}\to\delta}\sqrt{\Gamma^{\rm aux}(\mathbf{R})}$, where $\Gamma^{\rm aux}$ is a normalized function, instead of $\sqrt{\delta(\mathbf{R})}$. We nevertheless use the latter notation to lighten the text, which does not affect the conclusions.

correct $\rho_{\rm int}$. But if we want to replace $\psi_{\rm int}$ by a form constructed from $\psi^{\rm aux}$ in Eq. (10), the c.m. vibration has to be "subtracted" from $\psi^{\rm aux}$. $\Gamma^{\rm aux}$ represents the proposed way to achieve this "subtraction."

(iii) The $\delta(\mathbf{R})$ term, and thus the c.m. correlations, will appear explicitly in the functional.

(iv) As we will see, the final result has a clear physical meaning and leads to convincing numerical results, which shows its pertinence.

In the particular harmonic oscillator case (i.e., when the interaction u is parabolic), we always can achieve the separation $\psi^{\rm aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\Gamma^{\rm aux}(\mathbf{R})\times F(\xi_1,\ldots,\xi_{N-1})$ [13]. Thus, the $\Gamma^{\rm aux}$ term introduced in Eq. (16) permits us to directly "subtract" all the c.m. vibration contained in $\psi^{\rm aux}$, and $\frac{1}{\Gamma^{\rm aux}}\psi^{\rm aux}$ leads to a good approximation of $\psi_{\rm int}$.

However, in the general case, we do not expect $\frac{1}{\Gamma^{\rm aux}}\psi^{\rm aux}$ to be, strictly speaking, a good approximation of $\psi_{\rm int}$. Indeed, $\psi_{\rm int}$ is translationally invariant, whereas $\frac{1}{\Gamma^{\rm aux}}\psi^{\rm aux}$ is not anymore. In other terms, $\psi^{\rm aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ cannot be separated into $\Gamma^{\rm aux}(\mathbf{R})\times F(\xi_1,\ldots,\xi_{N-1})$. This is not a problem because in every integral where $\psi_{\rm int}$ appears (which represent observables), a $\delta(\mathbf{R})$ term that breaks translational invariance also appears explicitly. What we expect is that the replacement, (16), i.e., the introduction of $\Gamma^{\rm aux}$, allows sufficient flexibility to lead to a satisfying result for both $E_{\rm cm}$ and $\rho_{\rm int}$. Then, even if the subtraction is not "direct" because there is no separation of the c.m. motion, it is "indirect" because it leads to the correct final result. Note that, because of the $\delta(\mathbf{R})$ that appears in all integrals that represent observables, only the values and variations of $\Gamma^{\rm aux}$ around $\mathbf{R}=\mathbf{0}$ can contribute.

We now insert approximation (16) into (10) and keep only the real part of the result [indeed, the straightforward result leads to a complex $E_{\Delta\rm kin}$ in the general case, which is fundamentally because form (16) cannot be rewritten as a function of the $\{\xi_\alpha\}$ only]. We then obtain an approximation of the exact $E_{\Delta\rm kin}$ where the "standard" correlations have been neglected by construction. As discussed in Sec. II B, it remains to neglect the exchange terms to obtain $E_{\rm cm}$. The calculation is detailed in Appendix A. The final result is

$$\begin{aligned}E_{\Delta\rm kin}\to E_{\rm cm}\big[\{\varphi^k_{\rm int}\}\big]=&-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int d\mathbf{r}\;\varphi^{i*}_{\rm int}(\mathbf{r})\Delta_{\mathbf{r}}\varphi^{i}_{\rm int}(\mathbf{r})\times\left(\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\;\big|\varphi^{l\neq i}_{\rm int}(\mathbf{r}')\big|^2\times f_{i,l\neq i}\big[\{\varphi^{k\neq i,l}_{\rm int}\}\big](\mathbf{r}+\mathbf{r}')-1\right)\\&-\frac{\hbar^2}{2mN}\;\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\times\int d\mathbf{r}\;\big|\varphi^{i}_{\rm int}(\mathbf{r})\big|^2\int d\mathbf{r}'\;\big|\varphi^{l\neq i}_{\rm int}(\mathbf{r}')\big|^2\times f_{i,l\neq i}\big[\{\varphi^{k\neq i,l}_{\rm int}\}\big](\mathbf{r}+\mathbf{r}')\\&+\text{Pure Imaginary}\big[\{\varphi^k_{\rm int}\}\big],\end{aligned}\tag{17}$$

where the functional Pure Imaginary counteracts the pure imaginary part of the second and third lines of Eq. (17) and becomes null in the real (stationary) case. We keep this functional for the general (time-dependent) case.

The "two-particle c.m. correlations functional" is defined as:

$$f_{i,l\neq i}\big[\{\varphi^{k\neq i,l}_{\rm int}\}\big](\tilde{\mathbf{r}})=N^D\int\Pi^N_{\substack{j=1\\j\neq i,l}}d\mathbf{r}_j\,\delta\left(\sum_{\substack{k=1\\k\neq i,l}}^{N}\mathbf{r}_k+\tilde{\mathbf{r}}\right)\Pi^N_{\substack{j=1\\j\neq i,l}}\big|\varphi^j_{\rm int}(\mathbf{r}_j)\big|^2,\tag{18}$$

where D is the dimension in which the calculation is done ($D=1,2,$ or 3). In the following, we note $f_{i,l\neq i}$ instead of $f_{i,l\neq i}[\{\varphi^{k\neq i,l}_{\rm int}\}]$ to lighten the notations. The meaning and properties of this functional are detailed in Sec. III B.

The potentials $U^l_{\rm cm}$ corresponding to $E_{\rm cm}$ are defined by ($l=1\cdots N$)

$$\begin{aligned}U^l_{\rm cm}(\mathbf{r})\varphi^l_{\rm int}(\mathbf{r})=\frac{\delta E_{\rm cm}\big[\{\varphi^k_{\rm int}\}\big]}{\delta\varphi^{l*}_{\rm int}(\mathbf{r})}=&-\frac{\hbar^2}{2m}\left\{\Delta_{\mathbf{r}}\varphi^l_{\rm int}(\mathbf{r})\times\left(\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\big|\varphi^{m\neq l}_{\rm int}(\mathbf{r}')\big|^2 f_{l,m\neq l}(\mathbf{r}+\mathbf{r}')-1\right)\right.\\&\left.+\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\varphi^l_{\rm int}(\mathbf{r})\sum_{\substack{i=1\\i\neq l}}^{N}\int d\mathbf{r}'\varphi^{i*}_{\rm int}(\mathbf{r}')\Delta_{\mathbf{r}'}\varphi^{i}_{\rm int}(\mathbf{r}')\times f_{i,l\neq i}(\mathbf{r}+\mathbf{r}')\right\}\\&-\frac{\hbar^2}{2mN}\;\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\times\varphi^l_{\rm int}(\mathbf{r})\int d\mathbf{r}'\big|\varphi^{m\neq l}_{\rm int}(\mathbf{r}')\big|^2\times f_{l,m\neq l}(\mathbf{r}+\mathbf{r}')\\&+\frac{\delta}{\delta\varphi^{l*}_{\rm int}(\mathbf{r})}\text{Pure Imaginary}\big[\{\varphi^k_{\rm int}\}\big],\end{aligned}\tag{19}$$

where the last line is obviously null in the real (stationary) case. Note that the potentials $U^l_{\rm cm}$ are not the same for all states. This is because $E_{\rm cm}[\{\varphi^k_{\rm int}\}]$ is orbital dependent, which requires extra measures to recover a common potential or, equivalently, to preserve orthonormalization. A way to overcome this problem and remain fully coherent with DFT

is to use the OEP method, which permits us to find the potential common to all states that reproduces most accurately the effect of the $U^l_{\rm cm}$ potentials. We refer the reader to Refs. [28–30] for the exhaustive equations. As the full OEP result is very costly numerically, it is often simplified. The Krieger-Li-Iafrate (KLI) approach is a popular one, and in a further step of simplification, the Slater approximation [31,32] is used. As our goal is to find a numerically inexpensive form for the local c.m. potential, we hereafter detail only the Slater approximation:

$$U^{\rm Slat}_{\rm cm}(\mathbf{r}) = \frac{1}{\rho_{\rm int}(\mathbf{r})}\sum_{i=l}^{N}\left|\varphi^l_{\rm int}(\mathbf{r})\right|^2 U^l_{\rm cm}(\mathbf{r}). \tag{20}$$

B. Properties of $f_{i,l\neq i}$ and numerical considerations

The definition, (18), of the two-particle c.m. correlations functional $f_{i,l\neq i}$ shows that

(i) it is real and has the dimension of a density;
(ii) it is normalized to N^D, i.e., $\int d\tilde{\mathbf{r}} f_{i,l\neq i}(\tilde{\mathbf{r}}) = N^D$;
(iii) $\lim_{\tilde{\mathbf{r}}\to\pm\infty} f_{i,l\neq i}(\tilde{\mathbf{r}}) = 0$; and
(iv) it is a "multiconvolution" of all single densities, unless these are associated with orbitals i and l.

Points (i)–(iii) permit us to make explicit the physical meaning of $\frac{1}{N^D} f_{i,l\neq i}(\mathbf{r}+\mathbf{r}')$: it is the probability that particle $l \neq i$ has position $\mathbf{r}'$, given that particle i has position $\mathbf{r}$. Indeed, because of the c.m. correlations, the positions of those particles are not independent; every single orbital $\varphi^i_{\rm int}$ is coupled to every single orbital $\varphi^{l\neq i}_{\rm int}$ through $f_{i,l\neq i}$. This coupling appears in the c.m. correlations energy, (17), and potentials, (19).

To better understand this coupling, note that $f_{i,l\neq i}$ can be rewritten as

$$\begin{aligned} f_{i,l\neq i}(\tilde{\mathbf{r}}) &= 2^D\delta(\tilde{\mathbf{r}}) \quad \text{if} \quad N=2,\\ &= 3^D\left|\varphi^{k\neq i,l}_{\rm int}(-\tilde{\mathbf{r}})\right|^2 \quad \text{if} \quad N=3,\\ &= N^D\int \Pi^N_{\substack{j=1\\ j\neq i,l,m}} d\mathbf{r}_j\, \Pi^N_{\substack{j=1\\ j\neq i,l,m}} \left|\varphi^j_{\rm int}(\mathbf{r}_j)\right|^2 \\ &\quad\times\left|\varphi^m_{\rm int}\left(-\sum_{\substack{k=1\\ k\neq i,l,m}}^{N}\mathbf{r}_k - \tilde{\mathbf{r}}\right)\right|^2 \quad \text{if} \quad N\geqslant 4,\\ &\ldots \\ &\quad \text{Constant, for very large } N \text{ (limit of a Fermi gas).} \end{aligned} \tag{21}$$

We see that, in the two-particle case, $f_{1,2}$ is proportional to the steep δ function. Thus, if particle 1 has position $\mathbf{r}$, particle 2 will have position $-\mathbf{r}$, so that the c.m. remains stuck at $\mathbf{R}=\mathbf{0}$. In the three-particle case, $f_{i,l\neq i}$ has a larger width, because the introduction of a third particle allows more freedom to the motion of the two other particles, while preserving $\mathbf{R}=\mathbf{0}$. For $N\geqslant 4$, the width of $f_{i,l\neq i}$ will increase as N grows, because of the multiconvolution form of $f_{i,l\neq i}$. Indeed, a larger number of particles allows more liberty to the motion of two of them while preserving $\mathbf{R}=\mathbf{0}$. For very large N, the system tends to a Fermi gas, so that $f_{i,l\neq i}$ tends to become constant and delocalized in the whole space, i.e., the motions of the particles tend to become independent. The c.m. correlations can then be neglected, as expected.

Practically speaking, we see that the numerical cost of the whole scheme lies in the calculation of $f_{i,l\neq i}$ for $N\geqslant 4$, i.e., the calculation of the multiconvolution of Eq. (21). At first sight, it seems to be disadvantageous for large N. But a mathematical property of the convolutions under Fourier transforms makes it manageable. In Appendix B, we recall the so-called "multiconvolution theorem." Its direct application to $f_{i,l\neq i}$ for $N\geqslant 4$ gives

$$f_{i,l\neq i}(\tilde{\mathbf{r}}) = N^D \times \mathcal{T}^{-1}\Big[\Pi^N_{\substack{k=1\\ k\neq i,l}}\mathcal{T}\big[\left|\varphi^k_{\rm int}\right|^2\big]\Big](-\tilde{\mathbf{r}}),$$

where $\mathcal{T}$ denotes the Fourier transform as defined in Appendix B, Eq. (B1). This permits us to drastically shorten the numerical calculation of $f_{i,l\neq i}$, which becomes manageable even for large systems. Indeed, once all the $\mathcal{T}[|\varphi^k_{\rm int}|^2]$ are calculated, $f_{i,l\neq i}$ is given by the inverse Fourier transform of their direct product, so that the numerical cost of $f_{i,l\neq i}$ equals the numerical cost of $(N+1)$ fast Fourier transforms when $N\geqslant 4$.

C. Properties of $\Gamma^{\rm aux}$ and numerical considerations

To completely characterize $E_{\rm cm}$, we still need to characterize the values of $|\Gamma^{\rm aux}(\mathbf{0})|^2$ and $\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}|_{\mathbf{R}=\mathbf{0}}$; see Eq. (17).

1. First step: Value of $|\Gamma^{\rm aux}(\mathbf{0})|^2$

$|\Gamma^{\rm aux}(\mathbf{0})|^2$ is imposed by the normalization condition on approximation (16) we used for $\psi_{\rm int}$:[5]

$$\begin{aligned} 1 &= (\psi_{\rm int}|\psi_{\rm int}) = \int d\mathbf{r}_1\cdots d\mathbf{r}_N\delta(\mathbf{R})|\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2\\ \Rightarrow |\Gamma^{\rm aux}(\mathbf{0})|^2 &= \int d\mathbf{r}d\mathbf{r}'\left|\varphi^i_{\rm int}(\mathbf{r})\right|^2\left|\varphi^{l\neq i}_{\rm int}(\mathbf{r}')\right|^2 f_{i,l\neq i}(\mathbf{r}+\mathbf{r}'). \end{aligned} \tag{22}$$

Numerically speaking, this condition will be satisfied self-consistently, starting from a reasonable initial value for $|\Gamma^{\rm aux}(\mathbf{0})|^2$ and rescaling it at every numerical loop so that it satisfies the last line in Eq. (22).

2. Second step: Value of $\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}|_{\mathbf{R}=\mathbf{0}}$

To characterize this value, we define a pertinent continuous set of normalized functions $\{\Gamma^{\rm aux}(\mathbf{R})\}$ that are twice derivable. We then choose, at each numerical step, the particular $\Gamma^{\rm aux}$ function of the set whose norm squared in $\mathbf{R}=\mathbf{0}$ is the one that has been obtained in the first step (the set should unambiguously define this value). Then we calculate $\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}|_{\mathbf{R}=\mathbf{0}}$ with it. This permits us to completely define the c.m. correlation energy, (17), and potential, (19), without introducing any free parameter.

[5]The last line in Eq. (22) is obtained by introducing the form, (16), for $\psi_{\rm int}$ in the first line in Eq. (22) and neglecting the exchange terms.

We mention a particular relation that should satisfy the $\Gamma^{\rm aux}$ functions chosen to constitute the set. Recall that $\Gamma^{\rm aux}$ depends implicitly on N. As demonstrated in Appendix C, $\Gamma^{\rm aux}$ should satisfy the following properties as N increases:

$$\lim_{N\to+\infty} |\Gamma^{\rm aux}(\mathbf{0})|^2 \to +\infty,$$
$$\lim_{N\to+\infty} \frac{1}{N} \times \frac{1}{\Gamma^{\rm aux*}(\mathbf{0})} \Delta_{\mathbf{R}} \frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}} \times |\Gamma^{\rm aux}(\mathbf{0})|^2 \to 0. \tag{23}$$

The remaining task is to choose a pertinent continuous set of $\{\Gamma^{\rm aux}(\mathbf{R})\}$ that satisfies those properties.

3. Practical proposition

The most simple [4] set for $\Gamma^{\rm aux}$ that meets all the previously mentioned criteria (and is exact in the case where the interaction u is parabolic) is the Gaussian set:

$$\Gamma^{\rm aux}(\mathbf{R}) = \left(\frac{K_N}{\pi}\right)^{D/4} \exp\left\{-\frac{K_N}{2}\sum_{i=1}^{D} R_i^2\right\}, \tag{24}$$

where R_i are the coordinates of $\mathbf{R}$ in D dimensions and K_N is the parameter that defines $\Gamma^{\rm aux}$ for every given N. With this form,

$$|\Gamma^{\rm aux}(\mathbf{0})|^2 = \left(\frac{K_N}{\pi}\right)^{D/2}, \tag{25}$$

$$\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})} \Delta_{\mathbf{R}} \frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}} = \pi^{D/2} \times D \times K_N^{1-D/2}. \tag{26}$$

For a given system composed of N particles, $|\Gamma^{\rm aux}(\mathbf{0})|^2$ is still obtained at each numerical loop with the first step (Sec. III C1), which defines K_N by Eq. (25) and $\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}|_{\mathbf{R}=\mathbf{0}}$ by Eq. (26).

We emphasize that the choice of a Gaussian set for $\Gamma^{\rm aux}$ absolutely does not constrain the $\varphi^i_{\rm int}$ to show a Gaussian behavior (even asymptotically). Indeed, it simply gives a method to define the value of $\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}|_{\mathbf{R}=\mathbf{0}}$ given the value of $|\Gamma^{\rm aux}(\mathbf{0})|^2$, where only the behavior of $\Gamma^{\rm aux}$ around $\mathbf{R}=\mathbf{0}$ enters into account. The numerical results presented thereafter show that the Gaussian set choice gives good results. Nevertheless, the search for other sets, i.e., with other variations around $\mathbf{R}=\mathbf{0}$, should be continued to obtain the most precise description of self-bound systems in fully realistic calculations. This investigation goes beyond the scope of this paper.

4. Initial condition

With this method, there is no need to analytically define K_N as a function of N; K_N is obtained numerically for every given N as indicated previously. It would nevertheless be interesting to obtain an approximate analytical form to start the numerical iterations with a pertinent initial condition. With that aim, we note that conditions (23), together with equalities (25) and (26), implies the following conditions on K_N:

$$\lim_{N\to+\infty} K_N^{D/2} \to +\infty, \qquad \lim_{N\to+\infty} \frac{1}{N} K_N \to 0. \tag{27}$$

A straightforward form for K_N that satisfies those two constraints is

$$K_N = A \times N^a, \quad \text{where} \quad 0 < a < 1. \tag{28}$$

In practice, $a \in [0.6; 0.9]$ should be a reasonable choice in nuclear physics.[6]

D. "By-products"

1. An explicit density functional for fermions

The functional proposed in Sec. III A is, by construction, not an explicit functional of $\rho_{\rm int}$ (but an orbital-dependent functional). It is well suited for stationary calculations but not for time-dependent ones because the Slater approximation does not permit us to preserve energy conservation, as this approximation is not perfectly variational [33]. Only the full time-dependent OEP result [34] will achieve energy conservation, but with a much higher numerical cost. It would be interesting to find an explicit functional of $\rho_{\rm int}$ that would overcome this time-dependent case problem.

In this section, we propose a further step of approximation that will allow us to obtain such a functional. We use the local density approximation (LDA) on the result of Sec. III A, which consists of assuming that the system is locally homogeneous [21,35]. Despite its simplicity, this approximation has proven to be very satisfying for the description of a wide range of systems, and not just large ones [2,21]. To make the LDA, we first make the replacement

$$\left|\varphi^i_{\rm int}(\mathbf{r})\right|^2 \to \frac{1}{N}\rho_{\rm int}(\mathbf{r}) \tag{29}$$

everywhere the single density terms $|\varphi^i_{\rm int}|^2$ appear in $E_{\rm cm}$, Eq. (17). In the obtained functional, the only remaining term that is not an explicit functional of $\rho_{\rm int}$ is $\sum_{i=1}^N \varphi^{i*}_{\rm int}(\mathbf{r})\Delta_{\mathbf{r}}\varphi^i_{\rm int}(\mathbf{r})$. As we consider a system composed of fermions, we can make the Thomas-Fermi approximation [21], i.e., the replacement

$$\sum_{i=1}^{N} \varphi^{i*}_{\rm int}(\mathbf{r})\Delta_{\mathbf{r}}\varphi^i_{\rm int}(\mathbf{r}) \to -\frac{3}{5}C\rho^{5/3}_{\rm int}(\mathbf{r}), \tag{30}$$

[6]The corresponding energy associated with $\Gamma^{\rm aux}$ is $E_{\Gamma^{\rm aux}} = -\frac{\hbar^2}{2Nm}(\Gamma^{\rm aux}|\Delta_{\mathbf{R}}|\Gamma^{\rm aux}) = \frac{\hbar^2}{2Nm}\frac{D}{4}K_N = \frac{\hbar^2}{2m}\frac{D}{4}A \times N^{a-1}$. $E_{\Gamma^{\rm aux}}$ is proportional to N^{a-1}. Even if $E_{\Gamma^{\rm aux}}$ has, strictly speaking, no physical meaning, it is reasonable to assume that its variation according to N should approximately be proportional to the variation of the energy associated with the c.m. vibration obtained in mean-field-like calculations (see Ref. [11]). For the nuclear case, the c.m. vibration energy evaluated for harmonic oscillator states is proportional to $N^{-1/3}$; this variation can be reproduced with $a = 2/3$. The c.m. correlation energy evaluated with an *a posteriori* fit with mean-field-like calculations is proportional to $N^{-0.2}$; this variation can be reproduced with $a \approx 0.8$ [11].

where $C = (\frac{3\pi^2}{\gamma})^{2/3}$ and γ is the degeneracy. We obtain as the final result the c.m. correlations energy written as an explicit functional of $\rho_{\rm int}$:

$$E_{\rm cm}^{\rm LDA}[\rho_{\rm int}] = \frac{\hbar^2}{2m}\int d\mathbf{r}\ \frac{3}{5}C\rho_{\rm int}^{5/3}(\mathbf{r})\left(\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\ \frac{1}{N}\rho_{\rm int}(\mathbf{r}')\times f_2[\rho_{\rm int}](\mathbf{r}+\mathbf{r}')-1\right)$$
$$-\frac{\hbar^2}{2mN}\,\Re e\left(\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\right)\int d\mathbf{r}\ \frac{1}{N}\rho_{\rm int}(\mathbf{r})\int d\mathbf{r}'\ \frac{1}{N}\rho_{\rm int}(\mathbf{r}')\times f_2[\rho_{\rm int}](\mathbf{r}+\mathbf{r}'), \tag{31}$$

where the "two-particle average c.m. correlations functional" is defined by

$$\begin{aligned} f_2(\tilde{\mathbf{r}}) &= 2^D\delta(\tilde{\mathbf{r}}) \quad \text{if} \quad N=2,\\ &= 3^D\frac{1}{N}\rho_{\rm int}(-\tilde{\mathbf{r}}) \quad \text{if} \quad N=3,\\ &= N^D\frac{1}{N^{N-2}}\int d\mathbf{r}_1\cdots d\mathbf{r}_{N-3}\ \rho_{\rm int}(\mathbf{r}_1)\times\cdots\times\rho_{\rm int}(\mathbf{r}_{N-3})\ \rho_{\rm int}\left(-\sum_{k=1}^{N-3}\mathbf{r}_k-\tilde{\mathbf{r}}\right) \quad \text{if} \quad N\geqslant 4,\\ &\cdots\\ &\quad \text{Constant, for very large } N \text{ (limit of a Fermi gas).} \end{aligned} \tag{32}$$

(We note f_2 instead of $f_2[\rho_{\rm int}]$ to lighten the notation.) Considerations similar to those in Sec. III B permit us to interpret $\frac{1}{N^D}f_2(\mathbf{r}+\mathbf{r}')$ as the average probability that one particle has position $\mathbf{r}'$ given that another particle has position $\mathbf{r}$.

The corresponding unique c.m. correlations potential is given by

$$\frac{\delta E_{\rm cm}^{\rm LDA}[\rho_{\rm int}]}{\delta\rho_{\rm int}(\mathbf{r})} = U_{\rm cm}^{\rm LDA}[\rho_{\rm int}](\mathbf{r}) = \frac{\hbar^2}{2m}\left\{C\rho_{\rm int}^{2/3}(\mathbf{r})\times\left(\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\frac{1}{N}\rho_{\rm int}(\mathbf{r}')f_2(\mathbf{r}+\mathbf{r}')-1\right)\right.$$
$$\left.+\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\ \frac{3}{5}C\rho_{\rm int}^{5/3}(\mathbf{r}')\times\ \frac{N-1}{N}f_2(\mathbf{r}+\mathbf{r}')\right\}$$
$$-\frac{\hbar^2}{2mN}\Re e\left(\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\right)\times\int d\mathbf{r}'\frac{1}{N}\rho_{\rm int}(\mathbf{r}')\times f_2(\mathbf{r}+\mathbf{r}'). \tag{33}$$

Still, we see that the numerical cost lies in the calculation of f_2 for $N\geqslant 4$. To reduce this cost, we use the "multiconvolution theorem" recalled in Appendix B. Its direct application to f_2 for $N\geqslant 4$ gives [using the definition Eq. (B1) for the Fourier transform $\mathcal{T}$]

$$f_2(\tilde{\mathbf{r}}) = N^D\frac{1}{N^{N-2}}\times\mathcal{T}^{-1}[(\mathcal{T}[\rho_{\rm int}])^{N-2}](-\tilde{\mathbf{r}}).$$

This permits us to speed up drastically the numerical calculation of f_2, which becomes manageable even for very large systems. Indeed, we simply calculate $\mathcal{T}[\rho_{\rm int}]$, raise it to power $(N-2)$, and calculate its inverse Fourier transform. Thus, the numerical cost of the calculation of f_2 is equal to two fast Fourier transforms for all $N\geqslant 4$.

Moreover, this scheme is perfectly variational, contrary to that in Sec. III A and, thus, is suitable for stationary calculations as well as for time-dependent ones (it will achieve energy conservation if a time-independent $v_{\rm int}$ is used).

2. *An explicit density functional for bosons*

Until now, we have only considered systems of fermions. The c.m. correlations energy functional for boson condensates is obtained by replacing $\varphi_{\rm int}^i\to\varphi_{\rm int}$, thus $\rho_{\rm int}=N|\varphi_{\rm int}|^2$, in Eq. (17). Setting $\varphi_{\rm int}=\sqrt{\rho_{\rm int}/N}$, we obtain

$$E_{\rm cm}[\rho_{\rm int}] = -\frac{\hbar^2}{2m}\int d\mathbf{r}\ \sqrt{\rho_{\rm int}(\mathbf{r})}\Delta_{\mathbf{r}}\sqrt{\rho_{\rm int}(\mathbf{r})}\times\left(\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\ \frac{1}{N}\rho_{\rm int}(\mathbf{r}')\times f_2(\mathbf{r}+\mathbf{r}')-1\right)$$
$$-\frac{\hbar^2}{2mN}\Re e\left(\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\right)\times\int d\mathbf{r}\ \frac{1}{N}\rho_{\rm int}(\mathbf{r})\int d\mathbf{r}'\ \frac{1}{N}\rho_{\rm int}(\mathbf{r}')\times f_2(\mathbf{r}+\mathbf{r}'), \tag{34}$$

where f_2 is defined as in Eq. (32) and the corresponding c.m. correlations potential is given by

$$\frac{\delta E_{\rm cm}[\rho_{\rm int}]}{\delta\rho_{\rm int}(\mathbf{r})} = U_{\rm cm}[\rho_{\rm int}](\mathbf{r}) = -\frac{\hbar^2}{2m}\left\{\frac{1}{\sqrt{\rho_{\rm int}(\mathbf{r})}}\Delta_{\mathbf{r}}\sqrt{\rho_{\rm int}(\mathbf{r})}\times\left(\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\frac{1}{N}\rho_{\rm int}(\mathbf{r}')f_2(\mathbf{r}+\mathbf{r}')-1\right)\right.$$
$$\left.+\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\int d\mathbf{r}'\ \sqrt{\rho_{\rm int}(\mathbf{r})}\Delta_{\mathbf{r}}\sqrt{\rho_{\rm int}(\mathbf{r})}\times\frac{N-1}{N}f_2(\mathbf{r}+\mathbf{r}')\right\}$$
$$-\frac{\hbar^2}{2mN}\Re e\left(\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\right)\times\int d\mathbf{r}'\frac{1}{N}\rho_{\rm int}(\mathbf{r}')\times f_2(\mathbf{r}+\mathbf{r}'). \tag{35}$$

TABLE I. Energies of the various formalisms [in units where $\hbar = m = 1$; benchmark: total energy = 0.50 and interacting kinetic energy $(\psi_{\rm int}|\frac{\tau^2}{2\mu}|\psi_{\rm int}) = 0.25$].

Formalism	Noninteracting kinetic energy	E_H	E_C	$-\langle\frac{\mathbf{P}^2}{2mN}\rangle$ or $E_{\Delta\rm kin}$ or $E_{\rm cm}$	Total energy
H only	0.353	0.353	0	0	0.71
H + standard correlations	0.5	0.25	0.25	0	1.00
H + standard correlations + standard c.m. correction	0.706	0.177	0.177	−0.353	0.71
Internal DFT with c.m. correlations functional	1.225	0.120	0.120	−0.918	0.55
Exact internal DFT	1.000	0.125	0.125	−0.750	0.50

This potential is common to all states, is an explicit functional of $\rho_{\rm int}$, and is strictly variational (so that it may be used in the time-dependent case).

IV. NUMERICAL RESULTS

We consider one-dimensional (1D) calculations which will allow us to better understand some features of the internal DFT formalism and more easily include various particle-particle interactions.

A. Model system composed of two particles with a strong interaction

1. The model and the benchmark

We consider a self-bound system composed of two different particles, to maximize the c.m. correlations effects. We suppose that the two particles have the same mass m and are coupled by a strong interaction, which models features of a proton and a neutron. The first particle has laboratory coordinates $r^{(1)}$, $p^{(1)}$, and the second particle has laboratory coordinates $r^{(2)}$, $p^{(2)}$. The reduced mass is $\mu = m/2$, and the Jacobi coordinates are $\xi = r^{(1)} - r^{(2)}$, $\tau = p^{(1)} - p^{(2)}$. We suppose that the interaction between the two particles is parabolic (harmonic oscillator) so that the laboratory Hamiltonian is $H = \sum_{i=1}^{2} \frac{p^{(i)2}}{2m} + \frac{1}{4}m\omega^2(r^{(1)} - r^{(2)})^2$, and the internal Hamiltonian is

$$H_{\rm int} = \frac{\tau^2}{2\mu} + \frac{1}{2}\mu\omega^2\xi^2. \tag{36}$$

Its ground state can be written analytically ($\psi_{\rm int}$ should not be antisymmetrized because we deal with two different particles):

$$\psi_{\rm int}(\xi) = \left(\frac{\mu\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left\{-\frac{1}{2}\frac{\mu\omega}{\hbar}\xi^2\right\}. \tag{37}$$

The corresponding energy is $E_{\rm int} = \frac{1}{2}\hbar\omega$ and the c.m.-frame one-body densities for each kind of particle are [$R = (r^{(1)} + r^{(2)})/2$; $l = 1 \cdots 2$] [17]

$$\rho_{\rm int}^{(l)}(r) = \int dr^{(1)}dr^{(2)}\delta(R)|\psi_{\rm int}(r^{(1)} - r^{(2)})|^2\delta(r - (r^{(l)} - R))$$
$$= 2|\psi_{\rm int}(2r)|^2 = \sqrt{\frac{2m\omega}{\pi\hbar}} \exp\left\{-\frac{2m\omega}{\hbar}r^2\right\}. \tag{38}$$

This is our benchmark.

It can be shown analytically using a harmonic oscillator basis that the Hartree (H) solution (there is no exchange because the two particles are different) leads to $E_{\rm int} = \frac{1}{\sqrt{2}}\hbar\omega$ and $\rho_{\rm int}^{(l)}(r) = \sqrt{\frac{m\omega}{\sqrt{2}\pi\hbar}} \exp(-\frac{m\omega}{\sqrt{2}\hbar}r^2)$. Thus the H energy is $2/\sqrt{2}$ ($\approx$1.4) times more important than that of the benchmark, and the density is 1.7 times more spread. The H solution is much more delocalized than the benchmark because the c.m. correlations are neglected.[7]

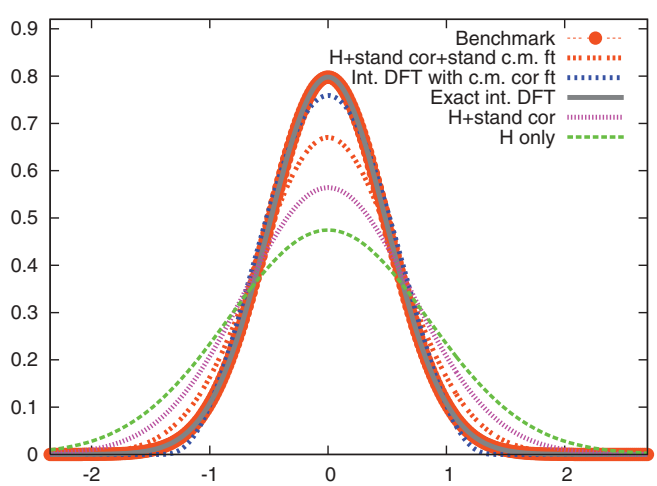

FIG. 1. (Color online) Internal densities $\rho_{\rm int}^{(l)}$ of the various formalisms. x axis: position, in units where $\hbar = m = 1$.

2. The internal DFT exact functional

Applying the multicomponent internal DFT formalism developed in Ref. [17] (whose equations have a form relatively

[7]The c.m. correlations tend to localize the densities compared to the independent particle approximation, which can be understood as follows: if c.m. correlations are taken into account, when one particle moves in a direction where the potential well is higher, the other particle will have to move in the opposite direction where the potential well is also higher. The first particle will thus feel the repulsion present in the independent particle approximation, but also the repulsion felt by the second particle through the c.m. correlations.

TABLE II. Energies of the various formalisms in the $N = 2$ case [in units where $\hbar = m = 1$; benchmark: total energy $= -0.59$ and interacting kinetic energy $(\psi_{\rm int}|\frac{\tau^2}{2\mu}|\psi_{\rm int}) = 0.12$].

Formalism	Noninteracting kinetic energy	$E_H \times (1 - \frac{1}{N})$	$-\langle \frac{\mathbf{P}^2}{2mN} \rangle$ or $E_{\rm cm}$	Total energy
H only	0.133	−0.626	0	−0.49
H + standard c.m. correction	0.260	−0.712	−0.065	−0.52
Internal DFT with c.m. correlations functional	0.535	−0.776	−0.418	−0.66

similar to that of the "one kind of particle" internal DFT equations recalled in Sec. II A), we can rewrite the internal energy ($\varphi_{\rm int}^{(1)}$ and $\varphi_{\rm int}^{(2)}$ being the KS orbitals):

$$E_{\rm int}\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right] = \sum_{l=1}^{2}\left(\varphi_{\rm int}^{(l)}\left|\frac{p^2}{2m}\right|\varphi_{\rm int}^{(l)}\right) + E_H\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right] + E_C\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right] + E_{\Delta\rm kin}\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right], \quad (39)$$

where[8]

$$E_H\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right] = \int dr dr' \rho_{\rm int}^{(1)}(r)\rho_{\rm int}^{(2)}(r')\frac{1}{4}m\omega^2(r-r')^2, \quad (40)$$

$$\begin{aligned} E_C\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right] &= \int dr\, dr' \gamma_{\rm int}^{(12)}(r,r')\frac{1}{4}m\omega^2(r-r')^2 - E_H\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right] \\ &= \int dr \frac{1}{2}\left(\rho_{\rm int}^{(1)}(r) + \rho_{\rm int}^{(2)}(r)\right)m\omega^2 r^2 - E_H\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right], \end{aligned} \quad (41)$$

$$\begin{aligned} E_{\Delta\rm kin}\left[\rho_{\rm int}^{(1)}, \rho_{\rm int}^{(2)}\right] &= \left(\psi_{\rm int}\left|\frac{\tau^2}{2\mu}\right|\psi_{\rm int}\right) - \sum_{i=1}^{2}\left(\varphi_{\rm int}^{(i)}\left|\frac{p^2}{2m}\right|\varphi_{\rm int}^{(i)}\right) \\ &= -\frac{3}{2}\hbar\omega + \frac{3}{2}\int dr\left(\rho_{\rm int}^{(1)}(r) + \rho_{\rm int}^{(2)}(r)\right)m\omega^2 r^2. \end{aligned} \quad (42)$$

E_H is the H energy, E_C is the "standard" correlations energy linked to the particle-particle interaction, and $E_{\Delta\rm kin}$ is the energy associated with the correlations contained in the interacting kinetic energy. It is the only term that contains explicitly the c.m. correlations.[9]

[8]To obtain these results, we pose $\varphi_{\rm int}^{(i)} = \sqrt{\rho_{\rm int}^{(i)}}$ and use $\gamma_{\rm int}^{(12)}(r,r') = \int dr^{(1)}dr^{(2)}\delta(R)|\psi_{\rm int}(r^{(1)}-r^{(2)})|^2 \times \delta(r-(r^{(1)}-R))\delta(r'-(r^{(2)}-R)) = \frac{1}{2}(\rho_{\rm int}^{(1)}(r) + \rho_{\rm int}^{(2)}(r))\delta(r+r')$.

[9]Note that even if, in the general case, the functional $E_C + E_{\Delta\rm kin}$ is universal [15,16], forms (41) and (42) are limited to the two-different-particle case because exchange effects are not taken into account. Thus they cannot be used to describe a system composed of an arbitrary number of particles of each kind. The universal functional, applicable to an arbitrary number of particles, is more involved but should permit us to recover (41) and (42) to the limit of a system composed by two different particles.

3. *The c.m. correlations functional*

We now approximate $E_{\Delta\rm kin}$ by the functional $E_{\rm cm}$ proposed in Sec. III, with $\Gamma^{\rm aux}(R) = (\frac{K}{\pi})^{1/4}\exp\{-\frac{K}{2}R^2\}$. We obtain

$$\begin{aligned} E_{\rm cm} &= -\frac{\hbar^2}{2m}\int dr\left[\varphi_{\rm int}^{(1)*}(r)\Delta_r\varphi_{\rm int}^{(1)}(r)\left(2\sqrt{\frac{\pi}{K}}\left|\varphi_{\rm int}^{(2)}(-r)\right|^2 - 1\right)\right. \\ &\quad \left. + \varphi_{\rm int}^{(2)*}(r)\Delta_r\varphi_{\rm int}^{(2)}(r)\left(2\sqrt{\frac{\pi}{K}}\left|\varphi_{\rm int}^{(1)}(-r)\right|^2 - 1\right)\right] \\ &\quad - \frac{\hbar^2}{2m}\sqrt{K\pi}\int dr\left|\varphi_{\rm int}^{(1)}(r)\right|^2\left|\varphi_{\rm int}^{(2)}(-r)\right|^2. \end{aligned} \quad (43)$$

The corresponding local c.m. correlations potentials are ($l = 1, 2$)

$$\begin{aligned} U_{\rm cm}^{(l)}(r)\varphi_{\rm int}^{(l)}(r) &= -\frac{\hbar^2}{2m}\left(2\sqrt{\frac{\pi}{K}}\left|\varphi_{\rm int}^{(m\neq l)}(-r)\right|^2 - 1\right)\Delta_r\varphi_{\rm int}^{(l)}(r) \\ &\quad - \frac{\hbar^2}{2m}\left(2\sqrt{\frac{\pi}{K}}\varphi_{\rm int}^{(m\neq l)*}(-r)\Delta_r\varphi_{\rm int}^{(m\neq l)}(-r)\right. \\ &\quad \left. + \sqrt{K\pi}\left|\varphi_{\rm int}^{(m\neq l)}(-r)\right|^2\right). \end{aligned} \quad (44)$$

(There is no need for the Slater approximation because we deal with one particle only of each kind.)

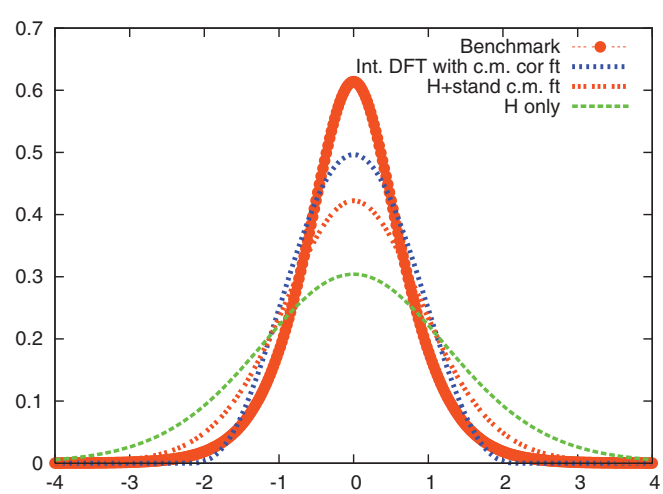

FIG. 2. (Color online) Internal density $\rho_{\rm int}/2$ of the various formalisms in the $N = 2$ case. x axis: position, in units where $\hbar = m = 1$.

TABLE III. "Internal DFT with c.m. correlations functional" energies for various N's (in units where $\hbar = m = 1$).

N	Noninteracting kinetic energy	$E_{\rm cm}$	Total energy	K	Interacting kinetic energy
2	0.535	−0.418	−0.66	1.94	0.117
3	0.463	−0.185	−1.90	1.74	0.278
4	0.702	−0.196	−3.97	2.74	0.507
5	1.014	−0.217	−6.84	4.01	0.799
6	1.390	−0.239	−10.56	4.54	1.151

Remember that, in making this approximation, we are neglecting the "standard" correlations part of $E_{\Delta\rm kin}$. In realistic 3D cases these correlations are mostly taken into account in the parametrized functionals that are commonly used. In our case, there is no simple way to include them in the rest of the functional, so it will not be possible to perfectly match the benchmark. Nevertheless, as they remain only a correction, the benchmark should be reasonably matched, at least much better than with the commonly used $-\langle\frac{\mathbf{P}^2}{2mN}\rangle$ approximation (see discussion in Sec. II C).

4. Numerical results

We use a unit system where $\hbar = m = 1$ and choose $\omega = 1$. Table I and Fig. 1 present numerical results for the following formalisms:

(i) E_H, called "H only";
(ii) $E_H + E_C$, called "H + standard correlations";
(iii) $E_H + E_C - \langle\frac{\mathbf{P}^2}{2mN}\rangle$, called "H + standard correlations + standard c.m. correction";
(iv) $E_H + E_C + E_{\rm cm}$, called "internal DFT with c.m. correlations functional" (we obtain $K \approx 3.9$ with the method described in Sec. III C);
(v) $E_H + E_C + E_{\Delta\rm kin}$, called "exact internal DFT"; and
(vi) benchmark (described in Sec. IV A1).

First, we see from Table I and Fig. 1 that the exact internal DFT perfectly reproduces the total energy and densities of the benchmark so that noninteracting v-representability [15,21] is perfectly achieved. [This is not a surprise; when one deals with only one particle of each kind, it is always possible to reach $\varphi_{\rm int}^{(l)} = \sqrt{\rho_{\rm int}^{(l)}}$.]

From Table I, we see that the noninteracting kinetic energy cannot be compared to the interacting kinetic energy. In particular, there is a factor 4 between the "exact internal DFT" noninteracting kinetic energy (=1) and the interacting kinetic energy (=0.250). Indeed, as discussed in Sec. II A, it is the "noninteracting kinetic energy + $E_{\Delta\rm kin}$" that is comparable to the interacting kinetic energy. Exact internal DFT then perfectly reaches the benchmark: $1.000 - 0.750 = 0.250$. The internal DFT with $E_{\rm cm}$ gives $1.225 - 0.928 = 0.307$, which fairly well reproduces the benchmark, considering that the "standard" correlations part of $E_{\Delta\rm kin}$ has been neglected. The result with standard c.m. correction gives $0.706 - 0.353 = 0.353$, which is worse.

From the point of view of the total energy, the "internal DFT with c.m. correlations functional" is much closer to the benchmark than the other approximate schemes. From the point of view of the densities, Fig. 1 shows that the internal DFT with c.m. correlations functional is very close to the benchmark and represents a great improvements compared to the other results. Nevertheless, we see some differences, which

TABLE IV. "H only" energies for various values of N (in units where $\hbar = m = 1$).

N	Total energy
2	−0.491
3	−1.75
4	−3.79
5	−6.66
6	−10.37

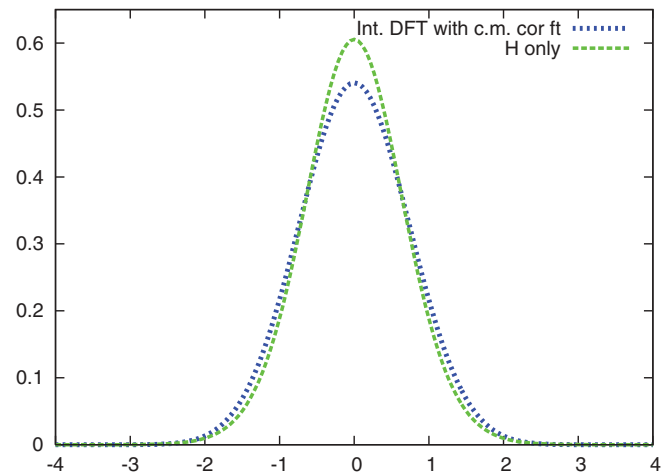

FIG. 3. (Color online) Internal density $\rho_{\rm int}/6$ of the various formalisms in the $N = 6$ case. x axis: position, in units where $\hbar = m = 1$.

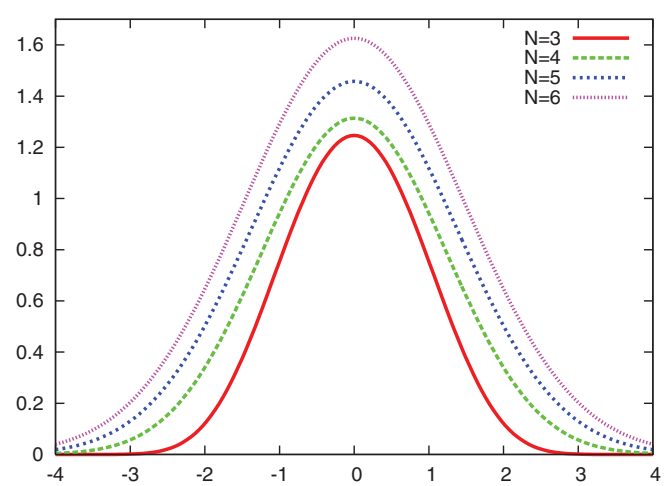

FIG. 4. (Color online) f_2 for $N = 3$ to 6. $N = 2$ is the δ function. x axis: position, in units where $\hbar = m = 1$.

are explained by the fact that the standard correlations part of $E_{\Delta\text{kin}}$ is not taken into account in our model.

B. Model system of identical bosons (smooth interaction)

We now consider a 1D system composed of N identical bosons of mass m and positions $\{r_i\}$ without spin in a condensate state and with an attractive two-body interaction of the form ($e > 0$)

$$u(r - r') = -\frac{1}{\sqrt{(r - r')^2 + e}}, \tag{45}$$

where the greater e, the smoother the potential. This allows us to model features of ^{4}He droplets.

The internal DFT energy functional is given by (φ_{int} is the one-body orbital describing the bosons and $\rho_{\text{int}} = N|\varphi_{\text{int}}|^2$)

$$E_{\text{int}}[\rho_{\text{int}}] = N\left(\varphi_{\text{int}}\left|\frac{p^2}{2m}\right|\varphi_{\text{int}}\right) + E_H[\rho_{\text{int}}] \times \left(1 - \frac{1}{N}\right) + E_C[\rho_{\text{int}}] + E_{\text{cm}}[\rho_{\text{int}}], \tag{46}$$

where $E_H[\rho_{\text{int}}] \times (1 - \frac{1}{N})$ represents the H energy, where the self-interaction has been subtracted and $E_C[\rho_{\text{int}}]$ is the standard correlations energy. We once again neglect E_C because we have no simple way to evaluate it as a functional of ρ_{int}. Note that more is neglected than in the previous model (of Sec. IV A), because E_C contains all the standard correlations, whereas in Sec. IV A we were able to keep a part of them. We thus can expect that the benchmark will be a little less matched here than in Sec. IV A; nevertheless, as E_C is small (even if not always completely negligible), the benchmark should remain reasonably matched.

The c.m. correlations energy is defined as in Sec. III D2, where Γ^{aux} is defined as in Sec. III C:

$$\begin{aligned} E_{\text{cm}}[\rho_{\text{int}}] = &-\frac{\hbar^2}{2m}\int dr\ \sqrt{\rho_{\text{int}}(r)}\Delta_{\mathbf{r}}\sqrt{\rho_{\text{int}}(r)} \\ &\times\left(\sqrt{\frac{\pi}{K(N)}}\int dr'\ \frac{1}{N}\rho_{\text{int}}(r')f_2(r + r') - 1\right) \\ &-\frac{\hbar^2}{2mN}\sqrt{\pi K(N)}\int dr\ \frac{1}{N}\rho_{\text{int}}(r) \\ &\times\int dr'\ \frac{1}{N}\rho_{\text{int}}(r')f_2(r + r'), \end{aligned} \tag{47}$$

and f_2 is defined by Eq. (32). The internal KS equation is

$$\left(-\frac{\hbar^2}{2m}\Delta + U_H[\rho_{\text{int}}] \times \left(1 - \frac{1}{N}\right) + U_{\text{cm}}[\rho_{\text{int}}]\right)\varphi_{\text{int}} = \epsilon\varphi_{\text{int}},$$

where

$$\begin{aligned} U_{\text{cm}}[\rho_{\text{int}}](r) = &-\frac{\hbar^2}{2m}\left\{\frac{1}{\sqrt{\rho_{\text{int}}(r)}}\Delta_r\sqrt{\rho_{\text{int}}(r)} \times \left(\sqrt{\frac{\pi}{K(N)}}\int dr'\frac{1}{N}\rho_{\text{int}}(r')f_2(r + r') - 1\right)\right. \\ &\left.+\sqrt{\frac{\pi}{K(N)}}\int dr'\ \sqrt{\rho_{\text{int}}(r')}\Delta_{\mathbf{r}}\sqrt{\rho_{\text{int}}(r')} \times \frac{N - 1}{N}f_2(r + r')\right\} \\ &-\frac{\hbar^2}{2mN}\sqrt{K(N)\pi}\int dr'\frac{1}{N}\rho_{\text{int}}(r') \times f_2(r + r'). \end{aligned} \tag{48}$$

For the $N = 2$ case, we can compute a benchmark. Indeed, by use of Jacobi coordinates, the internal Hamiltonian can be rewritten as $H_{\text{int}} = \frac{\tau^2}{2\mu} - \frac{1}{\sqrt{\xi^2+e}}$, where $\mu = m/2$ is the reduced mass. It is then possible to calculate numerically the exact many-body ground state ψ_{int} and the c.m.-frame one-body density $\rho_{\text{int}}(r) = 4|\psi_{\text{int}}(2r)|^2$.

The next results are given for:

(i) $E_H \times (1 - \frac{1}{N})$, called "H only."
(ii) $E_H \times (1 - \frac{1}{N}) - \langle\frac{\mathbf{P}^2}{2mN}\rangle$, called "H + standard c.m. correction."
(iii) $E_H \times (1 - \frac{1}{N}) + E_{\text{cm}}$, called "internal DFT with c.m. correlations functional."
(iv) Benchmark (for the $N = 2$ case only).

Table II and Fig. 2 report the energies and densities for the $N = 2$ case. We again see that the internal DFT noninteracting kinetic energy cannot be compared to the interacting kinetic energy. It is the internal DFT "noninteracting kinetic energy + E_{cm}" ($0.535 - 0.418 = 0.117$) that is comparable to the interacting kinetic energy (0.12). The result with standard c.m. correction gives $0.260 - 0.065 = 0.195$, which is worse. We also see that the internal DFT with c.m. correlations functional reproduces the benchmark fairly well, at least much better than the other schemes. We nevertheless see some differences, which are explained by the fact that E_C has been neglected. (See discussion at the beginning of this section.)

Table III shows that the part of the c.m. correlations energy in the total internal DFT energy decreases as N grows (63% for $N = 2$; 2% for $N = 6$). As a consequence, and even if shell effects play a role, the internal DFT noninteracting kinetic energy tends to become closer to the interacting kinetic energy as N grows (factor 4.6 for $N = 2$; factor 1.2 for $N = 6$). The "H only" and internal DFT densities become closer as N increases (see Fig. 3 for $N = 6$). Tables III and IV show that the H only total energy also becomes closer to the internal DFT total energy as N increases.

Finally, we see from Table III that K grows as N grows and from Fig. 4 that the maximum value of f_2 also grows as N grows (but the maximum value $\frac{1}{N^D} f_2$ diminishes), confirming the reasoning in Sec. III C.

V. CONCLUSION

The internal DFT provides an existence theorem for a c.m. correlations energy functional associated with a local potential. In this article, we have constructed such a functional, without involving any free parameters. The use of this functional is justified by the strong formal background, and variants suitable for fermionic as well as bosonic systems have been proposed. The resulting scheme is numerically manageable and represents a well-founded alternative to projection techniques to treat c.m. correlations. It can be added directly to actual energy functionals, although a refitting of them then would be necessary. Moreover, this scheme permits us to recover the precise value of the interacting kinetic energy and represents a manageable way to include the c.m. correlations in time-dependent calculations of self-bound systems.

We have presented convincing numerical results on 1D model systems. These results show that the developed functional represents a great improvement compared to the "standard c.m. correction" commonly used in nuclear physics (of the form $-\langle \frac{\mathbf{P}^2}{2mN} \rangle$), especially from the point of view of the energies. The next step will be to include the proposed functional in realistic 3D calculations, for instance, in mean-field-like calculations of nuclei with Skyrme interaction [2,9]. As the "standard" correlations are mostly taken into account in the commonly used functionals, the 3D results should be even more convincing than the 1D ones.

Even if the proposed Gaussian set for Γ^{aux} has been proved to give satisfying results, the search for other forms, i.e., with other variations around $\mathbf{R} = \mathbf{0}$, should continue to provide the most precise description of atomic nuclei, helium droplets, or small molecular systems where a quantum treatment of the nuclei is necessary.

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APPENDIX A: DETAILS OF THE CALCULATION THAT LEADS TO E_{cm}

We evaluate $\int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) \psi^*_{\text{int}}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \times \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} \psi_{\text{int}}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ using approximation (16) for ψ_{int} and obtain

$$
\begin{aligned}
&\int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) \frac{1}{\Gamma^{\text{aux}*}(\mathbf{R})} \psi^{\text{aux}*}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} \frac{1}{\Gamma^{\text{aux}}(\mathbf{R})} \psi^{\text{aux}}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \\
&= -\frac{\hbar^2}{2m} \frac{1}{|\Gamma^{\text{aux}}(\mathbf{0})|^2} \frac{1}{N!} \sum_{P,P'} (-1)^{p+p'} \sum_{i=1}^N \int d\mathbf{r}_i \; F_i^{P,P'}\big[\{\varphi_{\text{int}}^k\}\big](\mathbf{r}_i) \times \varphi_{\text{int}}^{P(i)*}(\mathbf{r}_i) \Delta_{\mathbf{r}_i} \varphi_{\text{int}}^{P'(i)}(\mathbf{r}_i) \\
&\quad - \frac{\hbar^2}{2m} \frac{1}{N^2} \frac{1}{\Gamma^{\text{aux}*}(\mathbf{0})} \Delta_{\mathbf{R}} \frac{1}{\Gamma^{\text{aux}}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}} \frac{1}{N!} \sum_{P,P'} (-1)^{p+p'} \sum_{i=1}^N \int d\mathbf{r}_i \; F_i^{P,P'}\big[\{\varphi_{\text{int}}^k\}\big](\mathbf{r}_i) \times \varphi_{\text{int}}^{P(i)*}(\mathbf{r}_i) \varphi_{\text{int}}^{P'(i)}(\mathbf{r}_i) \\
&= -\frac{\hbar^2}{2m} \frac{1}{|\Gamma^{\text{aux}}(\mathbf{0})|^2} \sum_{i=1}^N \bigg\{ \int d\mathbf{r} \; F_i\big[\{\varphi_{\text{int}}^{k\neq i}\}\big](\mathbf{r}) \times \varphi_{\text{int}}^{i*}(\mathbf{r}) \Delta_{\mathbf{r}} \varphi_{\text{int}}^{i}(\mathbf{r}) \\
&\quad + \frac{1}{N!} \sum_{P,P'\neq P} (-1)^{p+p'} \int d\mathbf{r} \; F_i^{P,P'\neq P}\big[\{\varphi_{\text{int}}^k\}\big](\mathbf{r}) \times \varphi_{\text{int}}^{P(i)*}(\mathbf{r}) \Delta_{\mathbf{r}} \varphi_{\text{int}}^{P'(i)}(\mathbf{r}) \bigg\} \\
&\quad - \frac{\hbar^2}{2mN} \frac{1}{\Gamma^{\text{aux}*}(\mathbf{0})} \Delta_{\mathbf{R}} \frac{1}{\Gamma^{\text{aux}}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}} \frac{1}{N} \sum_{i=1}^N \bigg\{ \int d\mathbf{r} \; F_i\big[\{\varphi_{\text{int}}^{k\neq i}\}\big](\mathbf{r}) \times \big|\varphi_{\text{int}}^{i}(\mathbf{r})\big|^2 \\
&\quad + \frac{1}{N!} \sum_{P,P'\neq P} (-1)^{p+p'} \int d\mathbf{r} F_i^{P,P'\neq P}\big[\{\varphi_{\text{int}}^k\}\big](\mathbf{r}) \times \varphi_{\text{int}}^{P(i)*}(\mathbf{r}) \varphi_{\text{int}}^{P'(i)}(\mathbf{r}) \bigg\},
\end{aligned}
\tag{A1}
$$

where we have defined ($D = 1$, 2, or 3 is the dimension in which the calculation is done)

$$
F_i^{P,P'}\big[\{\varphi_{\text{int}}^k\}\big](\mathbf{r}) - N^D \int \Pi_{\substack{j=1\\ j\neq i}}^N d\mathbf{r}_j \delta\Bigg(\sum_{\substack{k=1\\ k\neq i}}^N \mathbf{r}_k + \mathbf{r}\Bigg) \Pi_{\substack{j=1\\ j\neq i}}^N \varphi_{\text{int}}^{P(j)*}(\mathbf{r}_j) \varphi_{\text{int}}^{P'(j)}(\mathbf{r}_j),
$$

and its diagonal part,

$$F_i\big[\{\varphi_{\rm int}^{k\neq i}\}\big](\mathbf{r}) = \frac{1}{N!}\sum_P F_i^{P,P}\big[\{\varphi_{\rm int}^{k}\}\big](\mathbf{r}) = N^D \int \Pi_{\substack{j=1\\ j\neq i}}^N d\mathbf{r}_j \delta\left(\sum_{\substack{k=1\\ k\neq i}}^N \mathbf{r}_k + \mathbf{r}\right)\Pi_{\substack{j=1\\ j\neq i}}^N \left|\varphi_{\rm int}^j(\mathbf{r}_j)\right|^2. \tag{A2}$$

F_i is the probability that particle i has position $\mathbf{r}$, according to the c.m. coupling with every other particle and their probability distributions. In the following, we note F_i instead of $F_i[\{\varphi_{\rm int}^{k\neq i}\}]$ to lighten the notations.

$F_{P,P'\neq P}$ is caused solely by exchange effects. In the following, as explained in Secs. II B and III A, we neglect the pure exchange effects and thus $F_{P,P'\neq P}$. We obtain

$$\int d\mathbf{r}_1\cdots d\mathbf{r}_N \delta(\mathbf{R})\psi_{\rm int}^*(\mathbf{r}_1,\ldots,\mathbf{r}_N)\sum_{i=1}^N \frac{p_i^2}{2m}\psi_{\rm int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$$
$$\to -\frac{\hbar^2}{2m}\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}\sum_{i=1}^N\int d\mathbf{r}\ F_i(\mathbf{r})\times\varphi_{\rm int}^{i*}(\mathbf{r})\Delta_{\mathbf{r}}\varphi_{\rm int}^i(\mathbf{r}) - \frac{\hbar^2}{2mN}\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\times\frac{1}{N}\sum_{i=1}^N\int d\mathbf{r}\ F_i(\mathbf{r})\times\left|\varphi_{\rm int}^i(\mathbf{r})\right|^2.$$

We now insert this result into $E_{\Delta\rm kin}$, Eq. (10), and keep only the real part, i.e., $\Re e(E_{\Delta\rm kin})$, as justified in Sec. III A. We are left with only the c.m. correlations contribution,

$$\begin{aligned}E_{\Delta\rm kin}\to E_{\rm cm}\big[\{\varphi_{\rm int}^k\}\big] = &-\frac{\hbar^2}{2m}\sum_{i=1}^N\int d\mathbf{r}\left(\frac{1}{|\Gamma^{\rm aux}(\mathbf{0})|^2}F_i(\mathbf{r})-1\right)\times\varphi_{\rm int}^{i*}(\mathbf{r})\Delta_{\mathbf{r}}\varphi_{\rm int}^i(\mathbf{r})\\ &-\frac{\hbar^2}{2mN}\frac{1}{\Gamma^{\rm aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{\rm aux}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}}\int d\mathbf{r}\ F_i(\mathbf{r})\times\left|\varphi_{\rm int}^i(\mathbf{r})\right|^2\\ &+\text{Pure Imaginary}\big[\{\varphi_{\rm int}^k\}\big],\end{aligned} \tag{A3}$$

where Pure Imaginary$[\varphi_{\rm int}^k\}]$ is a pure imaginary functional which counteracts the imaginary part of the first two lines of (A3).

F_i is interesting in terms of the physics in energy considerations, although it is not a fundamental quantity for the potential (obtained by variation of $E_{\rm cm}$). We thus introduce a more fundamental quantity which appears in both the c.m. correlations energy and potential, namely the "two-particle c.m. correlations functional" defined in Eq. (18), which is linked to F_i by the relation

$$\forall l\neq i:\quad F_i(\mathbf{r}') = \int d\mathbf{r}\left|\varphi_{\rm int}^l(\mathbf{r})\right|^2 f_{i,l\neq i}(\mathbf{r}+\mathbf{r}'). \tag{A4}$$

When (A4) is inserted into (A3), we obtain form (17) for the c.m. correlation energy.

APPENDIX B: THE MULTICONVOLUTION THEOREM

We define the Fourier transform $\mathcal{T}$ of an integrable function $L:\Re e\to\Im m$ as

$$\forall\mathbf{r},\mathbf{s}\in\Re e:\quad \mathcal{T}[L](\mathbf{s}) = \int d\mathbf{r}\ e^{-2\pi i\mathbf{s}.\mathbf{r}}\ L(\mathbf{r}) \tag{B1}$$

and the inverse Fourier transform $\mathcal{T}^{-1}$ of a function $\tilde{L}:\Re e\to\Im m$ as

$$\forall\mathbf{r},\mathbf{s}\in\Re e:\quad \mathcal{T}^{-1}[\tilde{L}](\mathbf{r}) = \int d\mathbf{s} e^{2\pi i\mathbf{s}.\mathbf{r}}\tilde{L}(\mathbf{s}).$$

We start from $(K+1)$ integrable functions $g_i:\Re e\to\Im m$ and define the "multiconvolution":

$$C[\{g_i\}](\tilde{\mathbf{r}}) = \int d\mathbf{r}_1\cdots d\mathbf{r}_K\ g_1(\mathbf{r}_1)\times\cdots\times g_K(\mathbf{r}_K)\times g_{K+1}\left(-\sum_{i=1}^K\mathbf{r}_i-\tilde{\mathbf{r}}\right).$$

We can show easily that

$$\mathcal{T}[C](\mathbf{s}) = \Pi_{i=1}^{K+1}\mathcal{T}[g_i](-\mathbf{s}), \tag{B2}$$

which leads to

$$\begin{aligned}C[\{g_i\}](\tilde{\mathbf{r}}) &= \mathcal{T}^{-1}\big[\Pi_{i=1}^{K+1}\mathcal{T}[g_i](-\mathbf{s})\big](\tilde{\mathbf{r}})\\ &= \mathcal{T}^{-1}\big[\Pi_{i=1}^{K+1}\mathcal{T}[g_i]\big](-\tilde{\mathbf{r}}).\end{aligned}$$

This is the "convolution theorem" [36] generalized to multiconvolutions, which states that the Fourier transform of a multiconvolution is the product of the Fourier transforms of each function that enters into the multiconvolution. Note that this relationship is only valid for form (B1) of the Fourier transform. For forms normalized in other ways, a constant scaling factor will appear.

APPENDIX C: SOME PROPERTIES OF $\Gamma^{\rm aux}$ WHEN N BECOMES VERY LARGE

The limit where the c.m. correlations become negligible is obtained when N becomes very large, as mentioned in

Sec. III B. Indeed, $f_{i,l\neq i}$ then tends to become constant and delocalized in the whole space. We define

$$\lim_{N\to+\infty} f_{i,l\neq i} = \text{Constant}. \tag{C1}$$

The normalization condition, (22), thus implies, when N is very large,

$$\begin{aligned}&\lim_{N\to+\infty} |\Gamma^{\text{aux}}(\mathbf{0})|^2\\ &= \lim_{N\to+\infty} \int d\mathbf{r}\, d\mathbf{r}' \left|\varphi^i_{\text{int}}(\mathbf{r})\right|^2 \left|\varphi^{l\neq i}_{\text{int}}(\mathbf{r}')\right|^2 f_{i,l\neq i}(\mathbf{r}+\mathbf{r}')\\ &= \text{Constant}.\end{aligned} \tag{C2}$$

(Remember that Γ^{aux} is implicitly dependent of N.) When these results are inserted into E_{cm}, Eq. (17), we see that its second line becomes null and that its third line becomes proportional to $\frac{1}{N} \times \frac{1}{\Gamma^{\text{aux}*}(\mathbf{0})} \Delta_{\mathbf{R}} \frac{1}{\Gamma^{\text{aux}}(\mathbf{R})}|_{\mathbf{R}=\mathbf{0}} \times |\Gamma^{\text{aux}}(\mathbf{0})|^2$, which must tend to 0 when N becomes very large so that E_{cm} can be neglected. This implies the first relation that Γ^{aux} should satisfy:

$$\lim_{N\to+\infty} \frac{1}{N} \times \frac{1}{\Gamma^{\text{aux}*}(\mathbf{0})} \Delta_{\mathbf{R}} \frac{1}{\Gamma^{\text{aux}}(\mathbf{R})}\bigg|_{\mathbf{R}=\mathbf{0}} \times |\Gamma^{\text{aux}}(\mathbf{0})|^2 \to 0.$$

We denote $\mathcal{R}$ the region of space where the system has a nonzero density and V the corresponding volume. For very large systems, we have

$$\begin{aligned}\left|\varphi^i_{\text{int}}(\mathbf{r})\right|^2 &\approx \frac{1}{V} \quad \text{for} \quad \mathbf{r}\in\mathcal{R},\\ &\approx 0 \quad \text{for} \quad \mathbf{r}\notin\mathcal{R}.\end{aligned} \tag{C3}$$

Inserting those results in definition (21) of $f_{i,l\neq i}$ gives

$$\begin{aligned}f_{i,l\neq i}(\mathbf{r}) &\approx \frac{N^D}{V} \quad \text{for} \quad \mathbf{r}\in\mathcal{R},\\ &\approx 0 \quad \text{for} \quad \mathbf{r}\notin\mathcal{R}.\end{aligned} \tag{C4}$$

In the general case, we have $V < kN$, where k is a constant (as for saturating systems, like nuclear ones [2], where V becomes close, but still inferior, to kN). Thus,

$$\lim_{N\to+\infty} f_{i,l\neq i}(\tilde{\mathbf{r}}) = +\infty, \tag{C5}$$

whatever the dimension in which the calculation is done [but $\lim_{N\to+\infty} \frac{1}{N^D} f_{i,l\neq i}(\mathbf{r}) = \lim_{N\to+\infty} \frac{1}{V} = 0$]. As a consequence of Eqs. (C1), (C2), and (C5), we deduce a second relation that Γ^{aux} should satisfy:

$$\lim_{N\to+\infty} |\Gamma^{\text{aux}}(\mathbf{0})|^2 \to +\infty. \tag{C6}$$

[1] K. W. Schmid, Eur. Phys. J. A **12**, 29 (2001).
[2] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer-Verlag, New York, 1980).
[3] R. E. Peierls and J. Yoccoz, Proc. Phys. Soc. **70**, 381 (1957).
[4] R. E. Peierls and D. J. Thouless, Nucl. Phys. **38**, 154 (1962).
[5] S. Marcos, H. Flocard, and P. H. Heenen, Nucl. Phys. A **410**, 125 (1983).
[6] S. Marcos, H. Flocard, and P. H. Heenen, Phys. Lett. B **134**, 287 (1984).
[7] K. W. Schmid and P. G. Reinhard, Nucl. Phys. A **530**, 283 (1991).
[8] J. Dobaczewski, J. Phys. G: Nucl. Part. Phys **36**, 105105 (2009).
[9] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev. Mod. Phys. **75**, 121 (2003).
[10] R. R. Rodríguez-Guzmán and K. W. Schmid, Eur. Phys. J. A **19**, 45 (2004); **19**, 61 (2004).
[11] M. Bender, K. Rutz, P.-G. Reinhard, and J. A. Maruhn, Eur. Phys. J. A **7**, 467 (2000).
[12] A. S. Umar and V. E. Oberacker, J. Phys. G: Nucl. Part. Phys. **36**, 025101 (2009).
[13] J. M. Irvine, J. Phys. G: Nucl. Phys. **6**, L175 (1980).
[14] K. W. Schmid, Eur. Phys. J. A **12**, 29 (2001).
[15] J. Messud, M. Bender, and E. Suraud, Phys. Rev. C **80**, 054314 (2009).
[16] J. Messud, Phys. Rev. C **80**, 054614 (2009).
[17] J. Messud, Phys. Rev. A **84**, 052113 (2011).
[18] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[19] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[20] W. Kohn, Rev. Mod. Phys. **71**, 1253 (1999).
[21] R. M. Dreizler and E. K. U. Gross, *Density Functional Theory* (Springer-Verlag, Berlin, 1990).
[22] B. G. Giraud, Phys. Rev. C **77**, 014311 (2008).
[23] K. Yabana, Prog. Theor. Phys. **76**, 414 (1986).
[24] K. Dietrich, Nucl. Phys. A **606**, 63 (1996).
[25] J. Engel, Phys. Rev. C **75**, 014306 (2007).
[26] N. Barnea, Phys. Rev. C **76**, 067302 (2007).
[27] M. Barranco, R. Guardiola, S. Hernańdez, R. Mayol, J. Navarro, and M. Pi, J. Low Temp. Phys. **142**, 1 (2006).
[28] R. T. Sharp and G. K. Horton, Phys. Rev. **90**, 317 (1953).
[29] J. D. Talman and W. F. Shadwick, Phys. Rev. A **14**, 36 (1976).
[30] S. Kümmel and L. Kronik, Rev. Mod. Phys. **80**, 3 (2008).
[31] J. B. Krieger, Y. Li, and G. J. Iafrate, Phys. Rev. A **45**, 101 (1992).
[32] J. B. Krieger, Y. Li, and G. J. Iafrate, Phys. Rev. A **46**, 5453 (1992).
[33] J. Messud, P. M. Dinh, P.-G. Reinhard, and E. Suraud, Ann. Phys. (Berlin) **523**, 270 (2011).
[34] C. A. Ullrich, U. J. Gossmann, and E. K. U. Gross, Phys. Rev. Lett. **74**, 872 (1995).
[35] R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules* (Oxford University Press, New York, 1989).
[36] Y. Katznelson, *An Introduction to Harmonic Analysis* (Cambridge University Press, Cambridge, 2004).