

Density functional theory and Kohn-Sham scheme for self-bound systemsJ er mie Messud,^{1,2} Michael Bender,^{3,4} and Eric Suraud^{1,2}¹*Universit  de Toulouse, UPS, Laboratoire de Physique Th orique (IRSAMC), F-31062 Toulouse, France*²*CNRS, LPT (IRSAMC), F-31062 Toulouse, France*³*Universit  Bordeaux, Centre d'Etudes Nucl aires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France*⁴*CNRS/IN2P3, Centre d'Etudes Nucl aires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France*

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We demonstrate how the separation of the total energy of a self-bound system into a functional of the internal one-body Fermionic density and a function of an arbitrary wave vector describing the center-of-mass kinetic energy can be used to set up an “internal” Kohn-Sham scheme.

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I. INTRODUCTION

Density functional theory (DFT) [1–3] is widely used in condensed-matter physics and quantum chemistry to calculate the properties of many-electron systems and is based on the simple local density instead of on the less tractable N -body wave function. One of the pillars of DFT is the Hohenberg-Kohn (HK) theorem [4], which in its original form, proves that for any nondegenerate system of fermions or bosons [1] put into a local external potential $v_{\text{ext}}(\mathbf{r})$, there exists a unique functional of the local one-body density $\rho(\mathbf{r})$ that gives the exact ground-state energy when $\rho(\mathbf{r})$ corresponds to the exact ground-state density. A thorough mathematical analysis of the foundations of the HK theorem was given by Lieb [5]. A crucial point is that, because the theorem is based on the Ritz variational principle, it is valid only for systems described by a normalizable wave function [6]; i.e., ones for which a bound (ground) state exists. Various extensions of the HK theorem have been proven, for example for spin-density energy functionals, for nonlocal external potentials, and for relativistic, time-dependent, or superconducting systems [3]. The Kohn-Sham (KS) [7] scheme furthermore provides a straightforward method to compute self-consistently the ground-state density in a quantum framework, defining the local single-particle potential (i.e., the noninteracting system) that reproduces the exact ground-state density through an auxiliary product state.

Self-consistent mean-field (SCMF) approaches using effective interactions are widely used to describe the low-energy structure of atomic nuclei [8] and resemble a KS scheme in many ways. Originally conceived as a Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) method based on an effective in-medium interaction, this framework has often been characterized as “nuclear DFT” [9–15]. The similarities become particularly obvious when the effective interaction is explicitly constructed as an energy functional depending on various local densities and currents [16]. There are, however, important conceptual differences that prevent the straightforward mapping of the existing nuclear SCMF schemes onto the standard KS formalism for electronic systems. For example, nuclei are self-bound, the intrinsic nuclear states obtained by SCMF methods often break several symmetries of the nuclear

Hamiltonian, and many extensions of the nuclear SCMF method aim to explicitly calculate correlation effects instead of absorbing them into the functional. The present article addresses the first of these points by aiming at a KS scheme for self-bound systems. Similar efforts leading to approximate KS schemes have been made before [17,18]. Here, we propose an alternative demonstration of the HK theorem that carefully considers the technical issues arising from the separation of the internal and center-of-mass coordinates that is required to apply it to self-bound systems and that leads to an internal KS scheme.¹

II. THE PROBLEM**A. Role of the external potential**

In electronic systems, the wave function and density are defined in the frame attached to the center-of-mass (c.m.) of the atomic nuclei. The latter also provides naturally the external potential $v_{\text{ext}}(\mathbf{r})$, whose presence is compulsory to bind electrons that repel each other. The key point of the HK theorem is that the pure electronic problem is universal, whatever the external field (provided it gives a bound state).

In self-bound systems (such as atomic nuclei or He droplets), the situation is intrinsically different because the net fermion-fermion (or boson-boson) interaction is attractive. Thus, external fields are not necessary to obtain bound states, so that we are immediately in the corresponding “pure” system, with the big difference being that such systems physically exist. The absence of an external potential, however, has as a consequence that the modeling of isolated self-bound systems is plagued by a c.m. problem. For any stationary state with arbitrary total momentum \mathbf{P} , the c.m. will be delocalized and evenly distributed over the whole space. An even more critical issue is that such laboratory wave functions are not normalizable, which prevents any attempt to formulate DFT for isolated, self-bound systems in terms of the laboratory

¹We follow here the nomenclature of [24] by referring to coordinates independent of the center-of-mass as “internal” ones, whereas we reserve the label “intrinsic” for symmetry-breaking states from which bands of rotational states and/or parity vibrations can be modeled.

density by simply taking the limit $v_{\text{ext}}(\mathbf{r}) \rightarrow 0$ in the HK theorem. Indeed, this density is an indeterminate constant [17,19], which prevents constructing from it a universal functional. It is of course the “internal density” ρ_{int} (i.e., the density relative to the system’s c.m.) that is of interest. But standard DFT concepts as formulated so far are not applicable yet in terms of a well-defined internal density.

B. The center-of-mass problem

A second key point is that in a description of an isolated, self-bound system based on a Hamiltonian and a wave function, the Hamiltonian should explicitly be invariant under translation to ensure Galilean invariance of the wave function.² Thus, the N -body wave function ψ can be separated into a wave function Γ that depends on the position $\mathbf{R} = \frac{1}{N} \sum_{j=1}^N \mathbf{r}_j$ of the c.m. only, and an “internal” wave function ψ_{int} that depends on the remaining $(N - 1)$ Jacobi coordinates ξ_α defined as $\xi_1 = \mathbf{r}_2 - \mathbf{r}_1$, $\xi_2 = \mathbf{r}_3 - \frac{\mathbf{r}_2 + \mathbf{r}_1}{2}$, \dots , $\xi_{N-1} = \frac{N}{N-1}(\mathbf{r}_N - \mathbf{R})$,

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

The function $\Gamma(\mathbf{R})$ describes the motion of the isolated system as a whole in any chosen inertial frame of reference, such as the laboratory. It is a plane wave, thus not normalizable, as we will detail thereafter. The function ψ_{int} describes the internal properties and is a function of the $(N - 1)$ Jacobi coordinates. Of course, it could also be written as a function of the N coordinates \mathbf{r}_i , but one of them would be redundant [20].

In this context, the internal density ρ_{int} associated to ψ_{int} , rather than the laboratory density ρ , becomes the natural quantity from which to construct DFT in a self-bound system. We note that for such a finite system it is impossible to construct a product state that has the required structure of ψ_{int} . In a HF framework, one directly approximates $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$ by a Slater determinant in N coordinates \mathbf{r}_i in the c.m. frame of the system. Consequently, the HF state contains (at least) one redundant coordinate, which introduces a spurious coupling between the internal properties and the c.m. motion [21]. For this reason, the HF approximation sacrifices “Galilean invariance for the sake of the Pauli principle,” to quote Ref. [22]. A rigorous remedy is to perform projected HF, where projection before variation on c.m. momentum restores Galilean invariance at the price of abandoning the independent-particle description [22,23]. This reasoning does not hold, in principle, for DFT, where the key ingredient is the density, not an explicit N -body wave function.

A demonstration of a rigorous internal HK theorem has been made recently in Refs. [17,18] in two different ways, with the aim of correctly separating the internal properties

from the c.m. motion—but neither of them led to a rigorous internal KS scheme. A source term coupled to the N -body internal density operator was introduced in Ref. [17], allowing the authors to express the exact total energy of a self-bound system as a functional of this operator. A scheme to construct a corresponding noninteracting system in a systematic manner was proposed, but its link with the KS scheme of traditional DFT remains unclear. In Ref. [18], it was shown that the internal energy of a self-bound system can be written as a functional of the internal one-body density and an approximate KS scheme was proposed that is valid only if the c.m. coordinate is treated as an adiabatic variable. A different approach to the problem is taken in Refs. [24,25], where an oscillator potential (not invariant under translation) that traps the c.m. is added to the self-bound Hamiltonian. This approach has the particular characteristic that it does not affect the internal properties of the system—the ground-state wave function is a wave packet that factorizes into the form of Eq. (1), with $\Gamma(\mathbf{R})$ now being a Gaussian and thus normalizable. The laboratory density ρ is then well defined and a KS scheme for ρ can be rigorously set up. The internal density ρ_{int} can be deduced from ρ by deconvolution. However, the resulting energy functional and KS equations are neither an internal energy functional nor internal KS equations. Thus, the question of a rigorous formulation of an internal KS scheme comparable to SCMF calculations using an effective interaction remains open. Here, we propose an approach to demonstrate the internal HK theorem that is complementary to those found in Refs. [17,18], and that has the advantage that the link to the traditional HK theorem is more clear. This directly leads to the formulation of a general internal KS scheme.

III. DFT IN INTERNAL DEGREES OF FREEDOM

A. Separation of internal and c.m. coordinates

We start from a general, translationally invariant, N -body Hamiltonian composed of the usual kinetic energy term and a two-body potential u that describes the fermion-fermion (or boson-boson) interaction:

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

For the sake of simplicity of the demonstration, we assume a momentum-independent, two-body interaction and N identical particles. The generalization to three-body interactions is straightforward, and the generalization to systems containing different types of particles will be discussed elsewhere. We rewrite the Hamiltonian using the $N - 1$ Jacobi coordinates ξ_α to decouple the internal properties from the c.m. motion. The ξ_α are to be distinguished from the N “laboratory coordinates” \mathbf{r}_i and the N “c.m. frame coordinates” $(\mathbf{r}_i - \mathbf{R})$ relative to the total c.m. \mathbf{R} . One can then separate Eq. (2) into $H = H_{\text{c.m.}} + H_{\text{int}}$, where $H_{\text{c.m.}} = -(\hbar^2/2M)\Delta_{\mathbf{R}}$ (with $M = Nm$ being the total mass) is a one-body operator acting in \mathbf{R} space only, and H_{int} is an $(N - 1)$ -body operator in ξ_α space. H_{int} contains the interaction u that can be rewritten as a

²Translational invariance, which states that the observables do not depend on the position of the c.m., is a necessary but not sufficient condition for the more fundamental Galilean invariance, which ensures that observables are the same in all inertial frames. For a relativistic description of the quantum N -body system [15], Lorentz invariance must be considered instead of Galilean invariance.

function of ξ_α , which we denote as $u(\{\xi_\alpha\})$ for simplicity, and the internal kinetic energy, which is expressed in terms of the conjugate momentum τ_α of ξ_α and the corresponding reduced mass $\mu_\alpha = m \frac{\alpha}{\alpha+1}$. Because $[H_{\text{c.m.}}, H_{\text{int}}] = 0$, the eigenstate ψ of H can be built as a product of the form of Eq. (1) with

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

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

where

$$H_{\text{int}} = \sum_{\alpha=1}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} + u(\{\xi_\alpha\}). \quad (5)$$

There is no bound state for $\Gamma(\mathbf{R})$ because the solutions are arbitrary, stationary plane waves, which leads to an arbitrary c.m. energy $E_{\text{c.m.}} = \hbar^2 \mathbf{K}^2 / (2M)$ and delocalization of \mathbf{R} . We will come back to the interpretation of $\Gamma(\mathbf{R})$ below. By definition of a self-bound system, ψ_{int} is a bound state and is therefore normalizable. The corresponding total energy $E = E_{\text{c.m.}} + E_{\text{int}}$ splits into

$$E^{(\mathbf{K})}[\psi_{\text{int}}] = \frac{\hbar^2 \mathbf{K}^2}{2M} + \frac{E_{\text{int}}[\psi_{\text{int}}]}{(\psi_{\text{int}}|\psi_{\text{int}})}, \quad (6)$$

$$E_{\text{int}}[\psi_{\text{int}}] = (\psi_{\text{int}}|H_{\text{int}}|\psi_{\text{int}}), \quad (7)$$

where the internal energy is obviously a functional of ψ_{int} , and the c.m. energy is parametrized by an arbitrary \mathbf{K} . We see that the c.m. properties (given by \mathbf{K}) and the internal properties (given by ψ_{int}) are fully decoupled. The ground state ψ_{int} of H_{int} is obtained by minimization of the total energy $E^{(\mathbf{K})}[\psi_{\text{int}}]$ for a given \mathbf{K} , or equivalently of $E_{\text{int}}[\psi_{\text{int}}]$, under the normalization constraint.

The previous steps allow us to uniquely identify and separate the c.m. motion. In traditional electronic DFT the problem does not show up as the electronic properties are defined in the frame attached to the c.m. of the nuclei, where the nuclear background is accounted for by introducing an external, local, one-body potential $v_{\text{ext}}(\mathbf{r})$ that provides the key ingredient of the HK theorem. For a self-bound system, v_{ext} is not compulsory. To facilitate the proof of the HK theorem, however, we introduce an arbitrary potential v_{aux} , which serves as a mathematical auxiliary and can be safely dropped at the end to recover an isolated self-bound system.

B. An auxiliary translational invariant potential

To conserve the separation of the c.m. and the internal properties, we cannot simply use a one-body potential of the form $v_{\text{aux}}(\mathbf{r})$. The potential v_{aux} should necessarily verify two conditions: (1) translational invariance and (2) because we are interested in the internal properties, the redundant c.m. coordinate should be removed (as discussed previously). These two conditions impose the form $\sum_{i=1}^N v_{\text{aux}}(\mathbf{r}_i - \mathbf{R})$ as already used in Refs. [17,18], which corresponds to an arbitrary potential seen in the c.m. frame. It can be expressed as a function of only the Jacobi coordinates, $\sum_{i=1}^N v_{\text{aux}}(\mathbf{r}_i - \mathbf{R}) = v_{\text{aux}}(\{\xi_\alpha\})$, so it does not couple to the c.m. properties, and

the decomposition of Eq. (1) for ψ still holds with $H_{\text{int}} \rightarrow H_{\text{int}} + v_{\text{aux}}(\{\xi_\alpha\})$ in Eq. (4). Of course, the associated internal wave function is modified accordingly and consequently all internal observables are also modified, but for the sake of simplicity we keep the same notations ($\psi_{\text{int}}, E_{\text{int}}, H_{\text{int}}$).

For the next step, we evaluate the contribution of the auxiliary potential term ($\psi_{\text{int}}|v_{\text{aux}}(\{\xi_\alpha\})|\psi_{\text{int}}$) to the internal energy. First, we note that for any operator \hat{f} that can be expressed through Jacobi coordinates in position representation [we write $\hat{f}(\{\xi_\alpha\})$ when expressed through Jacobi coordinates and $\hat{f}(\{\mathbf{r}_i\})$ when expressed through the laboratory coordinates], we have the relation

$$\begin{aligned} & (\psi_{\text{int}}|\hat{f}(\{\xi_\alpha\})|\psi_{\text{int}}) \\ &= \int d\xi_1 \cdots d\xi_{N-1} \psi_{\text{int}}^*(\{\xi_\alpha\}) \hat{f}(\{\xi_\alpha\}) \psi_{\text{int}}(\{\xi_\alpha\}) \\ &= \int d\mathbf{R} d\xi_1 \cdots d\xi_{N-1} \delta(\mathbf{R}) \psi_{\text{int}}^*(\{\xi_\alpha\}) \hat{f}(\{\xi_\alpha\}) \psi_{\text{int}}(\{\xi_\alpha\}) \\ &= \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) \psi_{\text{int}}^*(\{\mathbf{r}_i\}) \hat{f}(\{\mathbf{r}_i\}) \psi_{\text{int}}(\{\mathbf{r}_i\}). \end{aligned} \quad (8)$$

We see that the ‘‘internal mean values’’ calculated with ψ_{int} expressed as a function of the $(N-1)$ $\{\xi_\alpha\}$ can also be calculated with ψ_{int} expressed as a function of the N coordinates $\{\mathbf{r}_i\}$. The transformation from the $\{\xi_\alpha\}$ to the $\{\mathbf{r}_i\}$ introduces a $\delta(\mathbf{R})$ that represents the dependence of the redundant coordinate on the others.³

For the mean value of the auxiliary potential, Eq. (8) leads to

$$\begin{aligned} & (\psi_{\text{int}}|v_{\text{aux}}(\{\xi_\alpha\})|\psi_{\text{int}}) \\ &= \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2 \sum_{i=1}^N v_{\text{aux}}(\mathbf{r}_i - \mathbf{R}) \\ &= \sum_{i=1}^N \int d\eta v_{\text{aux}}(\eta) \int d\mathbf{r}_1 \cdots d\mathbf{r}_N |\psi(\mathbf{r}_1, \dots, \mathbf{r}_N)|^2 \\ & \quad \times \delta[\eta - (\mathbf{r}_i - \mathbf{R})] \\ &= \sum_{i=1}^N \int d\mathbf{r} v_{\text{aux}}(\mathbf{r}) \frac{\rho_{\text{int}}(\mathbf{r})}{N} \\ &= \int d\mathbf{r} v_{\text{aux}}(\mathbf{r}) \rho_{\text{int}}(\mathbf{r}), \end{aligned} \quad (9)$$

where we have introduced the *internal* density

$$\begin{aligned} & \rho_{\text{int}}(\mathbf{r})/N \\ &= \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2 \delta[\mathbf{r} - (\mathbf{r}_i - \mathbf{R})] \\ &= \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2 \delta[\mathbf{r} - (\mathbf{r}_N - \mathbf{R})] \\ &= \left(\frac{N}{N-1} \right)^3 \int d\mathbf{R} d\xi_1 \cdots d\xi_{N-1} \delta(\mathbf{R}) \end{aligned}$$

³More generally, we can introduce a $\delta(\mathbf{R} - \mathbf{a})$ where \mathbf{a} is an arbitrary translation vector that represents the position of the system’s c.m. in the laboratory coordinates $\{\mathbf{r}_i\}$. For sake of simplicity of notation, we choose $\mathbf{a} = \mathbf{0}$ without loss of generality.

$$\begin{aligned}
& \times |\psi_{\text{int}}(\{\xi_\alpha\})|^2 \delta\left(\xi_{N-1} - \frac{N\mathbf{r}}{N-1}\right) \\
& = \left(\frac{N}{N-1}\right)^3 \int d\xi_1 \cdots d\xi_{N-2} \\
& \times \left| \psi_{\text{int}}\left(\xi_1, \dots, \xi_{N-2}, \frac{N\mathbf{r}}{N-1}\right) \right|^2. \quad (10)
\end{aligned}$$

The density $\rho_{\text{int}}(\mathbf{r})$ is normalized to N and a function of the c.m. frame coordinates. The laboratory density is obtained by convolution with the c.m. wave function as in Refs. [24,26]. The potential v_{aux} that is N -body with respect to the laboratory coordinates [and $(N-1)$ -body when expressed with Jacobi coordinates] becomes one-body (and local) when expressed with the c.m.-frame coordinates. The energy $E_{\text{int}}[\psi_{\text{int}}]$ [7] and thus the total energy $E^{(\text{K})}[\psi_{\text{int}}]$ given by Eq. (6) are then to be complemented by

$$E_{\text{int}} \rightarrow E_{\text{int}} + \int d\mathbf{r} v_{\text{aux}}(\mathbf{r})\rho_{\text{int}}(\mathbf{r}). \quad (11)$$

C. The Hohenberg-Kohn theorem

The internal energy E_{int} remains obviously a functional of ψ_{int} . Because an arbitrary one-body potential in the c.m. frame of the form $\int d\mathbf{r} v_{\text{aux}}(\mathbf{r})\rho_{\text{int}}(\mathbf{r})$ enters in its definition, and because the ground state of H_{int} is obtained by minimization of E_{int} , we can directly apply the usual proof of the HK theorem [4] and claim that for a nondegenerate ground state ψ_{int} and for a given fermion or boson type (i.e., a given interaction u), ψ_{int} and thus the internal energy E_{int} of a self-bound system [Eq. (11)] can be expressed as unique functionals of ρ_{int} . As already emphasized, the HK theorem is valid only for arbitrary “external” potentials that lead to *bound* ground states [5]. As a direct consequence, the internal DFT scheme is valid only for potentials v_{aux} that lead to *bound* internal ground states ψ_{int} . For self-bound systems, described by our formalism in the limit $v_{\text{aux}} \rightarrow 0$, ψ_{int} should by definition be a bound ground state, so that the previous conclusions still hold without breaking the consistency of the scheme.

D. The internal Kohn-Sham scheme

To recover the “internal” KS scheme, we assume, as in the traditional KS scheme, that there exists *in the c.m. frame* a local single-particle potential (i.e., a N -body noninteracting system) that reproduces the density ρ_{int} of the interacting system. We develop ρ_{int} in the corresponding basis φ_{int}^i of one-body orbitals expressed in c.m. frame coordinates \mathbf{r}^4 :

$$\rho_{\text{int}}(\mathbf{r}) = \sum_{i=1}^N |\varphi_{\text{int}}^i(\mathbf{r})|^2. \quad (12)$$

⁴Even if only $(N-1)$ coordinates are sufficient to describe the internal properties, we still deal with a system of N particles. Thus, we have to introduce N orbitals in the KS scheme if we want them to be interpreted (to first order) as single-particle orbitals and obtain a scheme comparable to SCMF calculations using effective interactions.

The KS assumption implies $\varphi_{\text{int}}^i[\rho_{\text{int}}]$ [1], so we can rewrite E_{int} as⁵

$$\begin{aligned}
E_{\text{int}}[\rho_{\text{int}}] & = \sum_{i=1}^N \left(\varphi_{\text{int}}^i \left| \frac{\mathbf{p}^2}{2m} \right| \varphi_{\text{int}}^i \right) + E_H[\rho_{\text{int}}] \\
& \quad + E_{\text{XC}}[\rho_{\text{int}}] + \int d\mathbf{r} v_{\text{aux}}(\mathbf{r})\rho_{\text{int}}(\mathbf{r}), \\
E_{\text{XC}}[\rho_{\text{int}}] & = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \gamma_{\text{int}}(\mathbf{r}, \mathbf{r}') u(\mathbf{r} - \mathbf{r}') - E_H[\rho_{\text{int}}] \\
& \quad + \left(\varphi_{\text{int}} \left| \sum_{\alpha=1}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} \right| \varphi_{\text{int}} \right) - \sum_{i=1}^N \left(\varphi_{\text{int}}^i \left| \frac{\mathbf{p}^2}{2m} \right| \varphi_{\text{int}}^i \right), \quad (13)
\end{aligned}$$

where we added and subtracted the internal Hartree energy $E_H[\rho_{\text{int}}] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho_{\text{int}}(\mathbf{r})\rho_{\text{int}}(\mathbf{r}')u(\mathbf{r} - \mathbf{r}')$ for the direct part and the noninteracting kinetic energy $\sum_{i=1}^N (\varphi_{\text{int}}^i | \frac{\mathbf{p}^2}{2m} | \varphi_{\text{int}}^i)$. For convenience, we introduced the local part of the two-body internal density matrix,

$$\begin{aligned}
\gamma_{\text{int}}(\mathbf{r}, \mathbf{r}') & = \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2 \\
& \quad \times \delta[\mathbf{r} - (\mathbf{r}_i - \mathbf{R})] \delta[\mathbf{r}' - (\mathbf{r}_{j \neq i} - \mathbf{R})] \\
& = \frac{N(N-1)}{2} \left(\frac{N-1}{N-2}\right)^3 \left(\frac{N}{N-1}\right)^3 \int d\xi_1 \cdots d\xi_{N-3} \\
& \quad \times \left| \psi_{\text{int}}\left(\xi_1, \dots, \xi_{N-3}, \frac{\mathbf{r}' + (N-1)\mathbf{r}}{N-2}, \frac{N\mathbf{r}'}{N-1}\right) \right|^2, \quad (14)
\end{aligned}$$

using steps similar to those used in Eq. (10) and using $\mathbf{r}_N - \mathbf{R} = \frac{N-1}{N}\xi_{N-1}$ and $\mathbf{r}_{N-1} - \mathbf{R} = \frac{N-2}{N-1}\xi_{N-2} - \frac{\xi_{N-1}}{N}$. The quantity γ_{int} , which normalizes as required to $N(N-1)/2$, is a function of the c.m.-frame coordinates and gives the two-body density matrix $\gamma(\mathbf{r}, \mathbf{r}')$ in the laboratory by convolution with the c.m. wave function $\Gamma(\mathbf{R})$. Applying Eq. (8) to the $u(\{\xi_\alpha\})$ part of H_{int} and inserting Eq. (14) gives directly

$$(\psi_{\text{int}} | u(\{\xi_\alpha\}) | \psi_{\text{int}}) = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \gamma_{\text{int}}(\mathbf{r}, \mathbf{r}') u(\mathbf{r} - \mathbf{r}'). \quad (15)$$

Following steps similar to those used in Eq. (8), one can show that the interacting kinetic energy can be rewritten as

$$\begin{aligned}
& \left(\psi_{\text{int}} \left| \sum_{\alpha=1}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} \right| \psi_{\text{int}} \right) \\
& = \left(\psi_{\text{int}} \left| -\frac{\hbar^2 \Delta_{\mathbf{R}}}{2M} + \sum_{\alpha=1}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} \right| \psi_{\text{int}} \right) \\
& = \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) \psi_{\text{int}}^*(\{\mathbf{r}_i\}) \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} \psi_{\text{int}}(\{\mathbf{r}_i\}). \quad (16)
\end{aligned}$$

⁵To keep close contact with standard DFT, we make here the usual separation of the energy into direct (Hartree) and exchange-correlation parts. Owing to the complexity of the nucleon-nucleon interaction in the vacuum, strong correlations in the nuclear medium, and the appearance of three-body forces, it is common practice in nuclear applications to construct approximate expressions for the entire functional. This, however, does not affect the conclusions of the present article.

Equation (16) makes it clear that the difference with the non-interacting kinetic energy $\sum_{i=1}^N \int d\mathbf{r} \varphi_{\text{int}}^{i*}(\mathbf{r}) \frac{p^2}{2m} \varphi_{\text{int}}^i(\mathbf{r})$ comes not only from the correlations neglected in the traditional independent-particle framework, but also from the c.m. correlations [the $\delta(\mathbf{R})$ term in the previous expression]. The inclusion of the c.m. correlations in the functional is the main difference with the traditional KS scheme. Still, the key point is that the internal, pure exchange-correlation energy $E_{\text{XC}}[\rho_{\text{int}}]$ can be expressed as a functional of ρ_{int} . Varying $E_{\text{K}}[\rho_{\text{int}}]$ in Eq. (6) or, equivalently, $E_{\text{int}}[\rho_{\text{int}}]$ in Eq. (13) with respect to $\varphi_{\text{int}}^{i*}$ and imposing normality of the $\{\varphi_{\text{int}}^i\}$,

$$\frac{\delta}{\delta \varphi_{\text{int}}^{i*}(\mathbf{r})} \left[E_{\text{int}}[\rho_{\text{int}}] - \sum_{i=1}^N \epsilon_i (\varphi_{\text{int}}^i | \varphi_{\text{int}}^i) \right] = 0, \quad (17)$$

leads to the “internal” Kohn-Sham equations for the $\{\varphi_{\text{int}}^i\}$

$$\left(-\frac{\hbar^2}{2m} \Delta + U_H[\rho_{\text{int}}] + U_{\text{XC}}[\rho_{\text{int}}] + v_{\text{aux}} \right) \varphi_{\text{int}}^i = \epsilon_i \varphi_{\text{int}}^i, \quad (18)$$

with $U_H[\rho_{\text{int}}](\mathbf{r}) = \delta E_H[\rho_{\text{int}}]/\delta \rho_{\text{int}}(\mathbf{r})$ and $U_{\text{XC}}[\rho_{\text{int}}](\mathbf{r}) = \delta E_{\text{XC}}[\rho_{\text{int}}]/\delta \rho_{\text{int}}(\mathbf{r})$, which is local as expected. Equation (18) has the same form as the traditional KS equations formulated for nontranslationally invariant Hamiltonians [7]. Here, however, we have justified its use in the c.m. frame for self-bound systems described with translationally-invariant Hamiltonians and have shown that the functional form of $U_{\text{XC}}[\rho_{\text{int}}]$ differs because of the inclusion of the c.m. correlations. Together with Eqs. (6) and (13), Eq. (18) completely defines the total energy $E_{\text{K}}[\rho_{\text{int}}]$ as the sum of the c.m. kinetic energy and the internal energy.

E. The laboratory density

It is instructive to calculate the laboratory density ρ . Following Ref. [24], one obtains

$$\rho(\mathbf{r}) = \int d\mathbf{R} |\Gamma(\mathbf{R})|^2 \rho_{\text{int}}(\mathbf{r} - \mathbf{R}). \quad (19)$$

As $\Gamma(\mathbf{R})$ is a plane wave, $\rho(\mathbf{r})$ is constant. This confirms that the usual definition of the “laboratory density” lacks a meaningful interpretation for isolated, self-bound systems. Of course, this

full delocalization does not occur in an experiment because observed self-bound systems are not *isolated* anymore. The observables related to $\Gamma(\mathbf{R})$ (i.e., position, momentum, or kinetic energy) are used to transform all observables into the c.m. frame, thereby explicitly using the Galilean invariance. The key point is that the decoupling of the c.m. motion allows one to deduce the internal properties that preserve Galilean invariance, whereas $\Gamma(\mathbf{R})$ is left to the choice of experimental conditions.

IV. SUMMARY AND CONCLUSIONS

In summary, we have shown in a way complementary to those proposed in Refs. [17,18] that the many-body internal wavefunction ψ_{int} and thus the internal energy of a self-bound system can be expressed as unique functionals of the total one-body internal density ρ_{int} . Next, we have shown rigorously that the internal properties of the system are described by an internal KS scheme. The key difference with the traditional HK/KS functional is the inclusion of the c.m. correlations. However, the question about the validity of the Kohn-Sham hypothesis, known as the “noninteracting v -representability” problem [1], remains to be answered, as in traditional DFT. The internal DFT scheme proposed here provides a justification for the application of DFT to isolated ^3He and ^4He droplets [27]. The present article establishes also the first step toward a Kohn-Sham scheme applicable to nuclear-structure physics. Further necessary developments are the generalization to two (or more) species of interacting particles, and the treatment of broken rotational and space-inversion symmetry that requires the formulation of the theory in terms of the so-called “intrinsic” one-body density, as defined in Ref. [28].

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