Density functional theory and Kohn-Sham scheme for self-bound systems

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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) is a widely-used framework in condensed-matter physics and quantum chemistry to calculate properties of many-electron systems, based on the simple local density instead of the less tractable Hamiltonian. One of the pillars of DFT is the Hohenberg-Kohn (HK) theorem, which in its original form proves that for any non-degenerate system of Fermions or Bosons put into a local external potential , there exists a unique functional of the local one-body density that gives the exact ground-state energy when corresponds to the exact ground-state density. A thorough mathematical analysis of the foundations of the HK theorem was given by Lieb. A crucial point is that the theorem is based on the Ritz variational principle, it is valid only for systems described by a normalisable wave function, i.e. for which a bound (ground) state exists. Various extensions of the HK theorem have been proven, for example to spin-density energy functionals, for non-local external potentials, for relativistic, for time-dependent, or for superconducting systems. The Kohn-Sham (KS) 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 non-interacting system) which reproduces the exact ground-state density through an auxiliary product state.

The self-consistent mean-field (SCMF) approaches using effective interaction that are widely used to describe the low-energy structure of atomic nuclei, resemble a KS scheme in many ways. Originally conceived as Hartree-Fock (HF) of Hartree-Fock-Bogoliubov (HFB) method based on an effective in-medium interaction, this framework has often been characterized as "nuclear DFT". The similarities become particularly obvious when the effective interaction is explicitly constructed as an energy functional depending on various local densities and currents. 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 at the explicit calculation of correlation effects instead of absorbing them into the functional. The present article addresses the first of these points, aiming at a KS scheme for self-bound systems. Similar efforts leading to approximate KS schemes have been made before. Here, we propose an alternative demonstration of the HK theorem that carefully considers the technical issues arising from the separation of internal and center-of-mass coordinates required for its application to self-bound systems, and that leads to an internal KS scheme.

II. THE PROBLEM

A. The 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 provide the external potential , 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 (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, such that we are immediately in the corresponding "pure" system, with the big difference that such systems physically exist. The absence of an external potential, however, has as a consequence that the

1 We follow here the nomenclature of to refer to coordinates independent of the center-of-mass as "internal" ones, whereas we reserve "intrinsic" for symmetry-breaking states out of which bands of rotational states and/or parity vibrations can be modeled.
modeling of isolated self-bound systems is plagued by a center-of-mass (c.m.) problem. For any stationary state with arbitrary total momentum $P$, the c.m. will be delocalized and evenly distributed in the whole space. Even more critical is that such laboratory wave function is not normalizable. This prevents any attempt to formulate DFT for isolated self-bound systems in terms of the laboratory density by simply taking the limit $v_{\text{ext}}(r) \to 0$ in the HK theorem. Indeed, this density is an indeterminate constant $\rho_{\text{int}}$, which fords to construct a universal functional from it. It is of course the “internal density” $\rho_{\text{int}}$, i.e. the density relative to the system’s c.m., which 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 Hamiltonian and wavefunction based description of an isolated self-bound system, the Hamiltonian should be explicitly translationally invariant to ensure Galilean invariance of the wave function. Hence, the $N$-body wave function $\psi$ can be separated into a wave function $\Gamma$ that depends on the position $R=\frac{1}{N}\sum_{j=1}^{N}r_j$ of the c.m. only, and an “internal” wave function $\psi_{\text{int}}$ that depends on the remaining $(N-1)$ Jacobi coordinates $\xi$ defined as $\xi_1=r_2-r_1$, $\xi_2=r_3-\frac{r_1+r_2}{2}$, \ldots, $\xi_{N-1}=-\frac{1}{N}(r_N-R)$

$$\psi(r_1,\ldots,r_N) = \Gamma(R) \psi_{\text{int}}(\xi_1,\ldots,\xi_{N-1}).$$

The $\Gamma(R)$ describes the motion of the isolated system as a whole in any chosen inertial frame of reference (as the laboratory). The $\psi_{\text{int}}$ describes the internal properties and is function of the $(N-1)$ Jacobi coordinates. Of course it could also be written as a function of the $N$ coordinates $r_i$, but one of them would be redundant.

In this context $\rho_{\text{int}}$, rather than the laboratory density $\rho$, thus becomes the natural quantity on which to construct DFT in a self-bound system. It is to be noted that for such a finite system it is impossible to construct a product state that has the required structure of $\psi_{\text{int}}$. In a HF framework, one approximates instead directly $\psi(r_1,\ldots,r_N)$ by a Slater determinant in $N$ coordinates $r_i$ in the c.m. frame of the system. Consequently, the HF state contains (at least) one redundant coordinate, that introduces a spurious coupling between the internal properties and the c.m. motion. For this reason, the HF approximation sacrifices “Galilean invariance for the sake of the Pauli principle”, to quote [21]. 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 [21, 22]. 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 [19, 25] (by two different ways), aiming at the correct separation of the internal properties from the c.m. motion, but none of them led to a rigorous internal KS scheme. A source term coupled to the $N$-body internal density operator was introduced in [19], allowing to express the exact total energy of a self-bound system as a functional of this operator. A scheme to construct a corresponding non-interacting system in a systematic manner was proposed, but its link with the KS scheme of traditional DFT remains unclear. In [25], 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, valid only if the c.m. coordinate is treated as an adiabatic variable. A different approach to the problem is taken in Refs. [23, 24], where a (non-translationally invariant) oscillator potential that traps the center-of-mass 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), $\Gamma(R)$ now being a Gaussian and with that normalizable. The laboratory density $\rho$ is then well defined and a KS scheme for $\rho$ can be rigorously set up. The internal density $\rho_{\text{int}}$ can be deduced from $\rho$ by deconvolution. However, the thus obtained 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 a complementary way than those found in [13, 23] to demonstrate the internal HK theorem, whose link with 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 $u$ which describes the

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2 Translational 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. In case of a relativistic description of the quantum $N$-body system [14], Lorentz invariance has to be considered instead of Galilean invariance.
Fermion-Fermion (or Boson-Boson) interaction
\[ H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i>j} u(r_i - r_j). \] (2)

For the sake of simplicity of the demonstration we assume a momentum-independent 2-body interaction and \( N \) identical particles. The generalization to 3-body interactions is straightforward, the generalization to systems containing different types of particles will be discussed elsewhere. We rewrite the Hamiltonian using the \( N - 1 \) Jacobi coordinates \( \xi_\alpha \), to decouple the internal properties from the c.m. motion. The \( \xi_\alpha \) are to be distinguished from the \( N \) "laboratory coordinates" \( r_i \), and the \( N \) "c.m. frame coordinates" \( (r_i - \mathbf{R}) \) relative to the total c.m. \( \mathbf{R} \). One can then separate (2) into \( H = H_{CM} + H_{int} \), where \( H_{CM} = -\frac{\hbar^2}{2M} \Delta_{\mathbf{R}} \) (with \( M = Nm \) being the total mass) is a one-body operator acting in \( \mathbf{R} \) space only, and \( H_{int} \) is a \((N - 1)\) body operator in the \( \xi_\alpha \) space. \( H_{int} \) contains the interaction \( u \) which can be rewritten as a function of the \( \xi_\alpha \) [which we denote \( u(\{\xi_\alpha\}) \) for simplicity], and the internal kinetic energy, which is expressed in terms of the conjugate momentum \( \tau_\alpha \) of \( \xi_\alpha \) and the corresponding reduced mass \( \mu_\alpha = m_\alpha / M \). As \( [H_{CM}, H_{int}] = 0 \), the eigenstate \( \psi \) of \( H \) can be built as a product of the form (1) with
\[ -\frac{\hbar^2}{2M} \Delta_{\mathbf{R}} \Gamma = E_{CM} \Gamma, \] (3)
\[ H_{int} \psi_{int} = E_{int} \psi_{int}, \] (4)

where
\[ H_{int} = \sum_{\alpha=2}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} + u(\{\xi_\alpha\}). \] (5)

There is no bound state for \( \Gamma(\mathbf{R}) \) as the solutions are arbitrary stationary plane waves, leading to arbitrary c.m. energy \( E_{CM} = \frac{\hbar^2 \mathbf{K}^2}{2M} \) and delocalization of \( \mathbf{R} \). We will come back to the interpretation of \( \Gamma(\mathbf{R}) \) below. By definition of a self-bound system, \( \psi_{int} \) is a bound, thus normalizable, state. The corresponding total energy \( E = E_{CM} + E_{int} \) splits into
\[ E^{(K)}[\psi_{int}] = \frac{\hbar^2 \mathbf{K}^2}{2M} + \frac{E_{int}[\psi_{int}]}{\psi_{int}[\psi_{int}]} \] (6)
\[ E_{int}[\psi_{int}] = (\psi_{int}[H_{int}][\psi_{int}]), \] (7)

where the internal energy is obviously a functional of \( \psi_{int} \), 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 \( \psi_{int} \)) are fully decoupled. The ground state \( \psi_{int} \) of \( H_{int} \) is obtained by minimization of the total energy \( E^{(K)}[\psi_{int}] \) for a given \( \mathbf{K} \), or equivalently of \( E_{int}[\psi_{int}] \) imposing normalization.

The previous steps have allowed 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 \( v_{ext}(\mathbf{r}) \) that provides the key ingredient of the HK theorem. In the case of 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. A translational invariant auxiliary potential

To conserve the separation of c.m. and internal properties, we cannot simply use a one-body potential of the form \( v_{aux}(\mathbf{r}) \). The potential \( v_{aux} \) should necessarily verify two conditions: (1) translational invariance and (2) as we are interested in the internal properties, the redundant c.m. coordinate should be removed (as discussed previously). These two conditions impose the form \( \sum_{\alpha=1}^{N} v_{aux}(r_{\alpha} - \mathbf{R}) \) as already used in [19, 25], which corresponds to an arbitrary potential seen in the c.m. frame. It can be expressed as a function of the Jacobi coordinates only, \( \sum_{\alpha=1}^{N} v_{aux}(r_{\alpha} - \mathbf{R}) = v_{aux}(\{\xi_\alpha\}) \), hence, it does not couple to c.m. properties, the decomposition (1) for \( \psi \) still holds with \( H_{int} \to H_{int} + v_{aux}(\{\xi_\alpha\}) \) in (4). Of course, the associated internal wave function is modified accordingly, and consequently all internal observables, but for the sake of simplicity we keep the same notations \( (\psi_{int}, E_{int}, H_{int}) \).

As the next step, we evaluate the contribution of the auxiliary potential term \( (\psi_{int}[v_{aux}(\{\xi_\alpha\})]\psi_{int}) \) to the internal energy. First, we note that for any operator \( \hat{f} \) that can be expressed through the Jacobi coordinates \( \{\xi_\alpha\} \) when expressed through the laboratory coordinates \( \{\mathbf{r}_{i}\} \) when expressed through the laboratory coordinates), we have the relation
\[ (\psi_{int}[\hat{f}(\{\xi_\alpha\})]\psi_{int}) = \int d\xi_1 \cdots d\xi_{N-1} \psi_{int}(\{\xi_\alpha\}) \hat{f}(\{\xi_\alpha\}) \psi_{int}(\{\xi_\alpha\}) \] (8)

We see that the "internal mean values" calculated with \( \psi_{int} \) expressed as a function of the \( (N - 1) \) \( \{\xi_\alpha\} \) can also be calculated with \( \psi_{int} \) 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. For the mean value of the auxiliary potential, relation leads to

\[
\langle \psi_{\text{int}} | v_{\text{aux}}(\{\xi_\alpha\}) | \psi_{\text{int}} \rangle = \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2 \sum_{i=1}^N v_{\text{aux}}(\mathbf{r}_i - \mathbf{R}) \]

\[
= \sum_{i=1}^N \int d\eta v_{\text{aux}}(\eta) \int d\mathbf{r}_1 \cdots d\mathbf{r}_N |\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 \times \delta(\eta - (\mathbf{r}_i - \mathbf{R}))
\]

\[
= \sum_{i=1}^N \int d\mathbf{r} v_{\text{aux}}(\mathbf{r}) \frac{\rho_{\text{int}}(\mathbf{r})}{N}
\]

\[
= \int d\mathbf{r} v_{\text{aux}}(\mathbf{r}) \rho_{\text{int}}(\mathbf{r})
\]

where we have introduced the internal density \(\rho_{\text{int}}(\mathbf{r})/N\)

\[
\rho_{\text{int}}(\mathbf{r}) = \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2 \delta(\mathbf{r} - (\mathbf{r}_i - \mathbf{R}))
\]

\[
= \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2 \delta(\mathbf{r} - (\mathbf{r}_N - \mathbf{R}))
\]

\[
= \left( \frac{N}{N-1} \right)^3 \int d\mathbf{R} d\xi_1 \cdots d\xi_{N-1} \delta(\mathbf{R}) \times |\psi_{\text{int}}(\{\xi_{\alpha}\})|^2 \delta(\xi_{N-1} - \frac{\mathbf{r}_N - \mathbf{R}}{N-1})
\]

\[
= \left( \frac{N}{N-1} \right)^3 \int d\xi_1 \cdots d\xi_{N-2} \left| \psi_{\text{int}}(\xi_1, \ldots, \xi_{N-2}, \frac{\mathbf{r}_N - \mathbf{R}}{N-1}) \right|^2.
\]

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 \[23\] \[27\]. The potential \(v_{\text{aux}}\) 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 \(E[\mathbf{K}][\psi_{\text{int}}]\) \[8\], are then to be complemented by

\[
E_{\text{int}} \rightarrow E_{\text{int}} + \int d\mathbf{r} v_{\text{aux}}(\mathbf{r}) \rho_{\text{int}}(\mathbf{r}).
\]

C. The Hohenberg-Kohn theorem

The internal energy \(E_{\text{int}}\) remains obviously a functional of \(\psi_{\text{int}}\). As in its definition enters an arbitrary one-body potential in the c.m. frame of the form \(\int d\mathbf{r} v_{\text{aux}}(\mathbf{r}) \rho_{\text{int}}(\mathbf{r})\), and as the ground state of \(H_{\text{int}}\) is obtained by minimization of \(E_{\text{int}}\), we can directly apply the usual proof of the HK theorem \[4\] and claim that for a non-degenerate ground state \(\psi_{\text{int}}\), and for a given Fermion or Boson type (i.e. a given interaction \(u\)), the internal energy \(E_{\text{int}}\) of a self-bound system, Eq. \[11\], can be expressed as a unique functional of \(\rho_{\text{int}}\). As already emphasized, the HK theorem is valid only for arbitrary “external” potentials that lead to bound ground states \[2\]. As a direct consequence, the internal DFT scheme is valid only for potentials \(v_{\text{aux}}\) that lead to bound internal ground states \(\psi_{\text{int}}\). As for self-bound systems, described by our formalism at the limit \(v_{\text{aux}} \rightarrow 0\), \(\psi_{\text{int}}\) should by definition be a bound ground state, 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 non-interacting system) which reproduces the density \(\rho_{\text{int}}\) of the interacting system. We develop \(\rho_{\text{int}}\) in the corresponding basis \(\varphi_{\text{int}}^i\) of one-body orbitals expressed in c.m. frame coordinates \(\mathbf{r}\)

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

The KS assumption implies \(\varphi_{\text{int}}^i[\rho_{\text{int}}]\) \[1\]; hence, we can rewrite \(E_{\text{int}}\) as \[5\]

\[
E_{\text{int}}[\rho_{\text{int}}] = \sum_{i=1}^N (\varphi_{\text{int}}^i | \mathbf{P}^2/2m | \varphi_{\text{int}}^i) + E_H[\rho_{\text{int}}]
\]

\[
+ E_{\text{XC}}[\rho_{\text{int}}] + \int d\mathbf{r} v_{\text{aux}}(\mathbf{r}) \rho_{\text{int}}(\mathbf{r})
\]

\[
E_{\text{XC}}[\rho_{\text{int}}] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \gamma_{\text{int}}(\mathbf{r}, \mathbf{r}') u(\mathbf{r} - \mathbf{r}') - E_H[\rho_{\text{int}}]
\]

\[
+ (\psi_{\text{int}} | \sum_{a=1}^{N-1} \frac{Z_a^2}{2\mu_a} | \psi_{\text{int}}) - \sum_{i=1}^N (\varphi_{\text{int}}^i | \mathbf{P}^2/2m | \varphi_{\text{int}}^i).
\]

4 Even 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.

5 To 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 common practice in nuclear applications to construct approximate expressions for the entire functional. This, however, does not affect the conclusions of the present paper.
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 non-interacting kinetic energy

$$\sum_{i=1}^{N} \left( \varphi_{\text{int}}^{i} \right)^{2} \rho_{\text{int}}^{2} \left( \frac{p_{\text{int}}^{2}}{2m} \right)$$

For convenience, we introduced the local part of the two-body internal density matrix

$$\gamma_{\text{int}}(\mathbf{r}, \mathbf{r'}) = \int d\mathbf{r}_N \cdots d\mathbf{r}_N \delta(\mathbf{R}) |\psi_{\text{int}}(\{\mathbf{r}_i\})|^2$$

(14)

$$\times \delta(\mathbf{r} - (\mathbf{r}_i - \mathbf{R})) \delta(\mathbf{r'} - (\mathbf{r}_j - \mathbf{R}))$$

$$= \frac{N(N-1)}{2} \left( \sum \frac{N}{N-1} \right) \int d\xi_1 \cdots d\xi_{N-3}$$

$$\times \left| \psi_{\text{int}}(\xi_1, \ldots, \xi_{N-3}, \mathbf{r}, \mathbf{r'}) \right|^2$$

(16)

(using similar steps as in 10 and $\mathbf{r}_N - \mathbf{R} = \frac{N-1}{N} \xi_{N-1}$ and $\mathbf{r}_N - \mathbf{R} = \frac{N-2}{N} \xi_{N-2} - \frac{\xi_{N-1}}{N}$). $\gamma_{\text{int}}$ has the required normalisation 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. (9) to the $u(\{\xi_\alpha\})$ part of $H_{\text{int}}$ and inserting Eq. (14) gives directly

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

(15)

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

$$\langle \psi_{\text{int}} | \sum_{\alpha=1}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} | \psi_{\text{int}} \rangle$$

(16)

$$= \langle \psi_{\text{int}} | - \frac{\hbar^2}{2M} \Delta + \sum_{\alpha=1}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} | \psi_{\text{int}} \rangle$$

$$= \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R}) \psi_{\text{int}}(\{\mathbf{r}_i\}) \sum_{i=1}^{N} \frac{p_{\text{int}}^2}{2m} \psi_{\text{int}}(\{\mathbf{r}_i\})$$

Equation (16) makes it clear that the difference to the non-interacting kinetic energy $\sum_{i=1}^{N} \int d\varphi_{\text{int}}^{i} \frac{p_{\text{int}}^2}{2m} \varphi_{\text{int}}^{i}(\mathbf{r})$ comes, on the one hand, 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 to the traditional KS scheme. Still, the key point is that the internal pure exchange-correlation energy $E_{XC}[\rho_{\text{int}}]$ can be expressed as a functional of $\rho_{\text{int}}$. Varying $E_{K}[\rho_{\text{int}}]$, Eq. (9), or equivalently $E_{\text{int}}[\rho_{\text{int}}]$, Eq. (13), with respect to $\varphi_{\text{int}}^{i}$, and imposing normality of the $\{\varphi_{\text{int}}^{i}\}$,

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

(17)

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

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

(18)

with $U_{H}[\rho_{\text{int}}](\mathbf{r}) = \delta E_{H}[\rho_{\text{int}}]/\delta \rho_{\text{int}}(\mathbf{r})$ and $U_{XC}[\rho_{\text{int}}](\mathbf{r}) = \delta E_{XC}[\rho_{\text{int}}]/\delta \rho_{\text{int}}(\mathbf{r})$, which is local as expected. Equation (18) has the same form as the traditional KS equations formulated for non-translationally invariant Hamiltonians [16]. Here, however, we have justified its use in the c.m. frame for self-bound systems described with translational-invariant Hamiltonians, and shown that the functional form of $U_{XC}[\rho_{\text{int}}]$ differs by the inclusion of c.m. correlations. Together with Eqs. (6) and (13), Eq. (18) defines completely the total energy $E_{K}[\rho_{\text{int}}]$ as the sum of the c.m. kinetic energy and of the internal energy.

**E. The laboratory density**

It is instructive to calculate the laboratory density $\rho$. Following Ref. [23], one obtains

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

(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 delocalisation 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 to deduce internal properties preserving Galilei 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. [19, 23] that the total energy of a self-bound system can be expressed as a functional of the total one-body internal density $\rho_{\text{int}}$. The energy in the laboratory frame contains the c.m. wave vector $\mathbf{K}$ as a parameter that can be freely chosen according to experimental conditions. Then, we have shown rigorously that the internal properties of the system are described by an internal KS scheme. The key difference to the traditional HK/KS functional is the inclusion of c.m. correlations. The question about the universal validity of the Kohn-Sham hypothesis, known as the "non-interacting v-representability" problem [1], however, remains to be answered, as in traditional DFT. The internal DFT scheme proposed here provides a justification for the application of DFT to isolated $^3$He and $^4$He droplets [28].
The present paper establishes also the first step towards 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 broken rotational and space-inversion symmetry that requires to formulate the theory in term of the so-called "intrinsic" one-body density as defined in Ref. [29].

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