

Density functional theory for self-bound systems

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The density functional theory is extended to account for self-bound systems. To this end the Hohenberg-Kohn theorem is formulated for the intrinsic density and a Kohn-Sham-like procedure for an N -body system is derived using the adiabatic approximation to account for the center of mass motion.

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Introduction. The formulation of a density functional theory (DFT) for self-bound systems is a question of current interest in nuclear physics [1,2]. Nuclear application of the DFT through the Skyrme model or using different density functionals is the only viable way to study heavy nuclei. The basic physical quantity in the DFT is the single particle density. This quantity, being well defined for an N -body system being localized by an external field is essentially zero for a freely moving self-bound system [1]. Therefore, when treating finite self-bound many-particle systems the DFT should be modified to account for center of mass motion. This modification can be looked for along two possible lines. One is to add an external potential, confine the system so that the DFT applies, and remove the center of mass effects at the end of the calculation [2]. The other possibility is to derive the Hohenberg-Kohn (HK) theorem [3] for the intrinsic density and construct a Kohn-Sham (KS) [4] type procedure for calculating the density and energy [1]. In this article we follow the second path. We first derive the HK theorem for the intrinsic density. This theorem, as the original HK theorem, is a specific case of a more general theorem by Valiev and Fernando who proved the existence of an energy functional for any Hermitian operator [1,5]. Here we rederive this proof using our notation for completeness and clarity. Once we have the HK theorem at our disposal, we follow the KS procedure, and construct a KS-like Schrödinger equation, which can be separated into a single particle equation using a Born-Oppenheimer type approximation for the “slow” center of mass coordinate. In this last step one is forced to introduce some approximations because the desired KS orbitals break the translation invariance.

For clarity we restrict our discussion to a particle system interacting via two-body forces which only depend on the relative distance between the particles. Furthermore, in deriving the KS-like equations we follow the Hartree rather than the Hartree-Fock scheme.

HK theorem for the intrinsic density. Consider a system of N particles moving under the influence of a two-body potential

$$U = \sum_{i \neq j}^N u(\mathbf{r}_i - \mathbf{r}_j) \quad (1)$$

and an intrinsic “one”-body potential

$$V_{\text{in}} = \sum_i^N v_{\text{in}}(\mathbf{r}_i - \mathbf{R}), \quad (2)$$

where $\mathbf{R} = \frac{1}{N} \sum_i^N \mathbf{r}_i$ is the center of mass coordinate. The Hamiltonian describing the internal motion of the system is

$$H = T_{\text{in}} + U + V_{\text{in}}, \quad (3)$$

where the intrinsic kinetic energy operator is given by

$$T_{\text{in}} = \sum_i^N \frac{\mathbf{p}_i^2}{2} - \frac{\mathbf{P}^2}{2N}. \quad (4)$$

Here $\mathbf{P} = \sum_i^N \mathbf{p}_i$ is the center of mass momentum. Following HK we assume a nondegenerate ground state Ψ . The intrinsic translational invariant density

$$n_{\text{in}}(\mathbf{r}) = \langle \Psi | \sum_i^N \delta(\mathbf{r}_i - \mathbf{R} - \mathbf{r}) | \Psi \rangle \quad (5)$$

is clearly a functional of $v_{\text{in}}(\mathbf{r})$. Following the HK method we can prove that conversely (up to a constant) $v_{\text{in}}(\mathbf{r})$ is a functional of $n_{\text{in}}(\mathbf{r})$. We start by assuming that another potential $v'_{\text{in}}(\mathbf{r})$ with a ground state Ψ' gives rise to the same intrinsic density $n_{\text{in}}(\mathbf{r})$. The two wave functions Ψ, Ψ' must be different unless $v_{\text{in}} - v'_{\text{in}} = \text{const}$, because they correspond to two different Hamiltonians H and $H' = T_{\text{in}} + U + V'_{\text{in}}$. Utilizing the variational principle one gets

$$E' = \langle \Psi' | H' | \Psi' \rangle < \langle \Psi | H' | \Psi \rangle = \langle \Psi | H + V'_{\text{in}} - V_{\text{in}} | \Psi \rangle \quad (6)$$

or

$$E' < E + \int d\mathbf{r} n_{\text{in}}(\mathbf{r})(v'_{\text{in}}(\mathbf{r}) - v_{\text{in}}(\mathbf{r})). \quad (7)$$

Interchanging primed and unprimed quantities, we get

$$E < E' + \int d\mathbf{r} n_{\text{in}}(\mathbf{r})(v_{\text{in}}(\mathbf{r}) - v'_{\text{in}}(\mathbf{r})). \quad (8)$$

Adding the last two equations we reproduce the famous inconsistency

$$E + E' < E' + E. \quad (9)$$

Thus we have shown that $v_{\text{in}}(\mathbf{r})$ is a functional of the intrinsic density $n_{\text{in}}(\mathbf{r})$. Because $v_{\text{in}}(\mathbf{r})$ fixes H , we see that the intrinsic N -body ground state is a functional of $n_{\text{in}}(\mathbf{r})$.

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Because Ψ is a functional of the intrinsic density we can define the functional

$$F[n_{\text{in}}(\mathbf{r})] = \langle \Psi | T_{\text{in}} + U | \Psi \rangle, \quad (10)$$

which is a universal functional valid for any number of particles as we can repeat the proof for any number of particles N , which by itself is a functional of $n_{\text{in}}(\mathbf{r})$. The HK variational principle for the ground state energy

$$E[n_{\text{in}}(\mathbf{r})] \equiv \int d\mathbf{r} n_{\text{in}}(\mathbf{r}) v_{\text{in}}(\mathbf{r}) + F[n_{\text{in}}(\mathbf{r})] \quad (11)$$

follows trivially from the original proof [3].

KS equations. Once it has been established that the energy of the finite self-bound many-body system is a functional of the intrinsic density the next step is to construct extended KS equations for such a system. The ground state energy of the N -body system interacting via two-body potential u can be written in the form

$$E = \frac{1}{2} \iint d\mathbf{r} d\mathbf{r}' n_{\text{in}}(\mathbf{r}) u(\mathbf{r} - \mathbf{r}') n_{\text{in}}(\mathbf{r}') + G[n_{\text{in}}(\mathbf{r})], \quad (12)$$

where G is a universal functional of the intrinsic density. Following KS we write

$$G[n_{\text{in}}(\mathbf{r})] = T_s[n_{\text{in}}] + E_{\text{xc}}[n_{\text{in}}], \quad (13)$$

where $T_s[n_{\text{in}}]$ is the intrinsic kinetic energy of a system of particles interacting with a “one”-body potential $v_{\text{in}}[n_{\text{in}}]$ and $E_{\text{xc}}[n_{\text{in}}]$ is the exchange-correlation functional. Due to the HK variational principle for the energy, Eq. (12), we obtain the equation

$$\int d\mathbf{r} \delta n_{\text{in}}(\mathbf{r}) \left[\frac{\delta T_s[n_{\text{in}}]}{\delta n_{\text{in}}(\mathbf{r})} + \varphi(\mathbf{r}) \right] = 0, \quad (14)$$

subject to the condition

$$\int d\mathbf{r} \delta n_{\text{in}}(\mathbf{r}) = 0. \quad (15)$$

Here

$$\varphi(\mathbf{r}) = \varphi_{\text{xc}}(\mathbf{r}) + \int d\mathbf{r}' u(\mathbf{r} - \mathbf{r}') n_{\text{in}}(\mathbf{r}') \quad (16)$$

and

$$\varphi_{\text{xc}}(\mathbf{r}) = \frac{\delta E_{\text{xc}}[n_{\text{in}}]}{\delta n_{\text{in}}(\mathbf{r})}. \quad (17)$$

Equations (14) and (15) are precisely the same equations one obtains starting with the Hamiltonian

$$H = \sum_i^N \frac{\mathbf{p}_i^2}{2} - \frac{\mathbf{P}^2}{2N} + \sum_i \varphi(\mathbf{r}_i - \mathbf{R}). \quad (18)$$

Unfortunately this Hamiltonian cannot be separated into single particle orbitals like the original KS Hamiltonian. However, because the center of mass coordinate is a slow coordinate we can replace all the center of mass operators by their expectation values. To do so, let us assume that φ is a smooth function that can be expanded in the following manner,

$$\varphi(\mathbf{r} - \mathbf{R}) \cong \varphi(\mathbf{r}) - R_a \partial_a \varphi(\mathbf{r}) + \frac{1}{2} R_a R_b \partial_{ab}^2 \varphi(\mathbf{r}) - \dots, \quad (19)$$

where

$$\partial_a \varphi(\mathbf{r}) = \frac{\partial \varphi(\mathbf{r})}{\partial r_a} \quad (20)$$

$$\partial_{ab}^2 \varphi(\mathbf{r}) = \frac{\partial^2 \varphi(\mathbf{r})}{\partial r_a \partial r_b},$$

and summation over the spatial directions $a, b = \{x, y, z\}$ is assumed. Replacing the center of mass terms by their expectation values and choosing a coordinate system such that $\langle \mathbf{R} \rangle = 0$, we obtain

$$H \cong \sum_i^N \frac{\mathbf{p}_i^2}{2} - \frac{\langle \mathbf{P}^2 \rangle}{2N} - N \langle R_a^2 \rangle \partial_{aa}^2 \varphi|_0 + \sum_i \left\{ \varphi(\mathbf{r}_i) + \frac{1}{2} \langle R_a R_b \rangle \partial_{ab}^2 \varphi(\mathbf{r}_i) \right\}, \quad (21)$$

retaining only the leading center of mass corrections. The $\partial_{aa}^2 \varphi|_0$ correction accounts for a linear term in $\nabla \varphi$ which upon summation over all particles is proportional to \mathbf{R} . Clearly this Hamiltonian is a sum of N single particle Hamiltonians leading to the KS type orbitals in the Hartree approximation

$$\left[-\frac{1}{2} \nabla^2 + \varphi(\mathbf{r}) + \frac{1}{2} \langle R_a R_b \rangle \partial_{ab}^2 \varphi(\mathbf{r}) \right] \psi_i = \epsilon_i \psi_i. \quad (22)$$

To be more concrete let us consider the local density approximation (LDA) in which it is assumed that $\varphi_{\text{xc}}(\mathbf{r}) = \varphi_{\text{xc}}(n_{\text{in}}(\mathbf{r}))$. In this approximation the leading correction to the single particle potential due to the center of mass is

$$\delta \varphi(\mathbf{r}) = \frac{1}{2} \langle R_a R_b \rangle \partial_{ab}^2 \varphi(\mathbf{r}), \quad (23)$$

where

$$\partial_{ab}^2 \varphi(\mathbf{r}) = \frac{d\varphi_{\text{xc}}}{dn_{\text{in}}} \partial_{ab}^2 n(\mathbf{r}) + \frac{d^2 \varphi_{\text{xc}}}{dn_{\text{in}}^2} \partial_a n(\mathbf{r}) \partial_b n(\mathbf{r}) + \int d\mathbf{r}' u(\mathbf{r} - \mathbf{r}') \partial_{ab}^2 n(\mathbf{r}'). \quad (24)$$

Here $n(\mathbf{r})$ is the laboratory one-body density given by

$$n(\mathbf{r}) = \sum_i^N |\psi_i(\mathbf{r})|^2. \quad (25)$$

Equations (16), (17), and (22)–(25) together with

$$\langle R_a R_b \rangle = \frac{\langle r_a r_b \rangle}{N} = \frac{1}{N^2} \sum_i^N \langle \psi_i | r_a r_b | \psi_i \rangle \quad (26)$$

form a closed set of equations to be solved self-consistently, just as in the case of a system bounded by an external potential.

The nature of the center of mass expansion depends on the system at hand. This point is most easily demonstrated in the Hartree picture where the expectation value of all the odd moments of R_a can be set to zero and the second even moment is given by

$$\langle R_a R_b R_c R_d \rangle = \frac{1}{N^2} (\langle r_a r_b \rangle \langle r_c r_d \rangle + \langle r_a r_c \rangle \langle r_b r_d \rangle + \langle r_a r_d \rangle \langle r_b r_c \rangle) + O\left(\frac{1}{N^3}\right). \quad (27)$$

From Eqs. (26) and (27) it is clear that the leading orders in the expansion (19) can be regarded as a Taylor series in $\langle r^2 \rangle / N$ and that in the limit $N \rightarrow \infty$ the original KS equations are recovered. For a collapsing system where the size of the system does not depend on the number of particles the expansion (19) behaves as a $1/N$ series. For noncollapsing systems, such as nuclei, the rms radius grows as $\sqrt[3]{N}$ and the expansion converges much slower as $1/\sqrt[3]{N}$, unless the r dependence of the potential scales as the rms matter radius, i.e., $\varphi \approx \varphi(r/\sqrt[3]{Na})$.

Example. As an example for our procedure consider a system of N fermions moving in a harmonic oscillator potential,

$$H = \sum_i^N \frac{\mathbf{p}_i^2}{2} + \sum_i \frac{1}{2} \omega^2 \mathbf{r}_i^2. \quad (28)$$

Using the relation

$$\sum_i^N (\mathbf{r}_i - \mathbf{R})^2 = \sum_i^N \mathbf{r}_i^2 - N \mathbf{R}^2, \quad (29)$$

we can rewrite this Hamiltonian as a sum of a center of mass term,

$$H_{\text{cm}} = \frac{\mathbf{P}^2}{2N} + \frac{1}{2} N \omega^2 \mathbf{R}^2, \quad (30)$$

and an internal Hamiltonian written in the form (18)

$$H_{\text{in}} = \sum_i^N \frac{\mathbf{p}_i^2}{2} - \frac{\mathbf{P}^2}{2N} + \frac{1}{2} \sum_i^N \omega^2 (\mathbf{r}_i - \mathbf{R})^2. \quad (31)$$

Following Eq. (21), we evaluate the center of mass corrections

$$\begin{aligned} N \langle R_a R_a \rangle \partial_{aa}^2 \varphi|_0 &= N \langle \mathbf{R}^2 \rangle \omega^2, \\ \frac{1}{2} \langle R_a R_b \rangle \partial_{ab}^2 \varphi(\mathbf{r}_i) &= \frac{1}{2} \langle \mathbf{R}^2 \rangle \omega^2, \end{aligned} \quad (32)$$

and we get the approximated internal Hamiltonian

$$H_{\text{in}} \cong \sum_i^N \frac{\mathbf{p}_i^2}{2} - \frac{\langle \mathbf{P}^2 \rangle}{2N} - \frac{1}{2} N \omega^2 \langle \mathbf{R}^2 \rangle + \sum_i \frac{1}{2} \omega^2 \mathbf{r}_i^2. \quad (33)$$

Comparing Eq. (33) with Eq. (30) it is clear that for the harmonic oscillator case the corrections to the internal Hamiltonian ensure the right cancellation of the center of mass energy.

Discussion. It is already known for some time that the HK theorem can be generalized to any Hermitian operator, including the intrinsic density. The challenge, however, is to find a useful KS-like procedure that reduces the self-bound many-body system into a set of single quasiparticle orbitals. From the onset it is clear that such orbitals break the translational symmetry, and therefore some approximations are called for. In this brief report we have demonstrated that starting with the HK theorem for the intrinsic density one can reach this goal by treating the center of mass coordinate as an adiabatic variable. This approximation recovers the KS equation in the limit $N \rightarrow \infty$ and includes center of mass recoil effects in the orbital equations and to the ground state energy. We have demonstrated that for the case of N -particles moving in a harmonic-oscillator potential this procedure yields the right center of mass correction.

We argue that the importance of the center of mass corrections might vary for different systems. Regardless whether the effect is small or large the current approach helps bridge the gap between the DFT and its application to finite self-bound systems.

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