



Many-body energy density functional

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The Hohenberg-Kohn theorem and the Kohn-Sham equations, which are at the basis of the density-functional theory, are reformulated in terms of a particular many-body density, which is translational and Galilean invariant and therefore is relevant for self-bound systems. In a similar way that there is a unique relation between the one-body density and the external potential that gives rise to it, we demonstrate that there is a unique relation between that particular many-body density and a definite many-body potential. The energy is then a functional of this density, and its minimization leads to the ground-state energy of the system. As a proof of principle, the analogous of the Kohn-Sham equation is solved in the specific case of ^4He atomic clusters, to put in evidence the advantages of this formulation in terms of physical insights.

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I. INTRODUCTION

The essential idea behind the density-functional theory (DFT) is to reduce the complexity of the solution of the many-body Schrödinger equation to a much tractable problem given in terms of the one-body density, avoiding in this way the explicit reference to the many-body wave function. In fact, Hohenberg and Kohn (HK) demonstrated that the ground-state energy of a quantum system is a functional of the one-body density $n(\vec{r})$ and could, in principle, be obtained from a minimization procedure [1]. Moreover, Kohn and Sham (KS) demonstrated that the one-body density can be represented by a noninteracting system placed inside a particular external field [2].

The success of DFT for various many-body systems, for instance, atoms, molecules, and the condensed phases, has been enormous, and its formulation and details are currently part of books in which many of the recent applications are discussed (see, for example, the books by Giuliani and Vignale [3], by Lipparini [4], and by Parr and Yang [5], and references therein). After its original formulation, many aspects were addressed along the years to put it in more solid mathematical grounds [6–8]. In the last 15 years also nuclear physicists have devoted attention to it and carried out a considerable activity, starting from the seminal works of Refs. [9,10]. Since nuclei are self-bound systems, the original formulation of the HK theorem, which starts from a Hamiltonian containing a single-particle external field, cannot be applied in a straightforward way. Such an external field, in fact, breaks the translation invariance required by a self-bound system. To this problem a series of works have been devoted proposing different solutions [11–19].

The aim of the present work is to suggest a formulation of the DFT that replaces the one-body density with a particular

many-body density and that, at the same time, fulfills the mentioned invariance. More explicitly: the traditional energy functional $E[n(\vec{r})]$ is replaced by $E[v(\rho)]$, where v is a different density, expressed in terms of the so-called hyper-radius ρ , a collective variable depending on all interparticle distances,

$$\rho^2 = \frac{2}{N} \sum_{i<j} (\vec{r}_i - \vec{r}_j)^2, \quad (1)$$

with N the number of particles (of equal masses). In a similar way that there is a unique relation between the one-body ground-state density and the external potential, we demonstrate that there is a unique relation between $v(\rho)$ and a definite many-body potential $W(\rho)$. The minimization of $E[v(\rho)]$ with respect to $v(\rho)$ leads to an equation whose solution allows to know the ground-state energy of the system, if the correct information is included in $W(\rho)$. The search for the correct KS energy functional $E[n]$ is replaced by the search for the correct $E[v]$. This approach lets us envisage the possibility that, in practical applications, the new functional $E[v(\rho)]$ might better take into account the complex many-body dynamics of a strongly interacting self-bound system.

In Sec. II we introduce the new variable ρ within the general so-called hyperspherical harmonics (HH) formalism. In Sec. III we define the associated density $v(\rho)$, the energy functional $E[v(\rho)]$, and the analogous of the KS approach, demonstrating a one-to-one relation between $v(\rho)$ and a many-body potential $W(\rho)$. As a practical application, in Sec. IV a particular energy functional is suggested for the much studied bosonic self-bound systems, namely, ^4He clusters. Surprisingly, satisfactory results are obtained. Further considerations and outlooks are found in Sec. V.

II. FORMALISM

A convenient set of translation-invariant coordinates useful to describe an interacting N -body system are the $N - 1$ Jacobi vectors $\vec{\xi}_i$, $i = 1, \dots, N - 1$ defined (for equal masses m) as

$$\vec{\xi}_{N-j} = \sqrt{\frac{2j}{j+1}} (\vec{r}_{j+1} - \vec{R}_j), \quad j = 1, \dots, N - 1, \quad (2)$$

with $\vec{R}_j = (1/j) \sum_{i=1}^j \vec{r}_i$. The $(3N - 3)$ independent Jacobi coordinates can then be transformed into a set of as many independent *hyperspherical coordinates* (HC) [20] consisting in the *hyper-radius* ρ

$$\rho = \sqrt{\sum_{i=1}^{N-1} \xi_i^2}, \quad (3)$$

and $(3N - 4)$ angles $\Omega = (\hat{\xi}_1, \dots, \hat{\xi}_{N-1}, \phi_2, \dots, \phi_{N-1})$, with the *hyperangles* ϕ_i defined by

$$\cos \phi_i = \frac{|\vec{\xi}_i|}{\sqrt{\xi_1^2 + \dots + \xi_i^2}}, \quad i = 2, \dots, N - 1. \quad (4)$$

Notice that the hyper-radius ρ is a (translation-invariant) many-body variable, involving all particle distances. In fact, it can be shown that

$$\rho^2 = \frac{2}{N} \sum_{i < j}^N (\vec{r}_i - \vec{r}_j)^2 = 2 \sum_i^N (\vec{r}_i - \vec{R}_N)^2, \quad (5)$$

with \vec{R}_N the center-of-mass position. In terms of the hyperspherical coordinates the volume element $dV^{3N-3} = d\vec{\xi}_1 \dots d\vec{\xi}_{N-1}$ becomes

$$dV^{3N-3} = \rho^{3N-4} d\rho d\Omega \quad (6)$$

(for notation and further details see, e.g., Refs. [21–23]).

Let us consider the typical translation and Galilean invariant Hamiltonian of a system characterized by mutual interactions,

$$H = T + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + \dots \equiv T + V(\rho, \Omega), \quad (7)$$

where in the kinetic term the center of mass has been subtracted,

$$T = \sum_{i=1}^N \frac{p_i^2}{2m} - \frac{P_{CM}^2}{2M_{CM}}. \quad (8)$$

Expressed in terms of the HC, ρ , and Ω , T assumes a rather familiar form:

$$T = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial \rho^2} + \frac{3N-4}{\rho} \frac{\partial}{\partial \rho} + \frac{\hat{K}^2(\Omega)}{\rho^2} \right). \quad (9)$$

The operator \hat{K} , called the hyperangular momentum, has a complete set of orthonormal eigenfunctions $\mathcal{Y}_{[K]}(\Omega)$ called hyperspherical harmonics that satisfy the following eigenvalue equation:

$$\hat{K}^2 \mathcal{Y}_{[K]}(\Omega) = K(K + 3N - 5) \mathcal{Y}_{[K]}(\Omega), \quad (10)$$

where K is called the grand angular quantum number and $[K]$ indicate all the other relative $3N - 4$ good quantum numbers.

The N -body wave function, $\Psi(\rho, \Omega)$, can in principle be expanded in terms of the HH functions up to some $[K_M]$ (in principle infinite) as

$$\Psi(\rho, \Omega) = \rho^{-(3N-4)/2} \sum_{[K]=[K_m]}^{[K_M]} u_{[K]}(\rho) \mathcal{Y}_{[K]}(\Omega_N), \quad (11)$$

where $[K_m]$ is the set of quantum numbers consistent with the minimal value of the grand angular quantum number K_m , compatible with the permutational symmetry requirements. In the case of spin-0 bosons $K_m = 0$ (and so are all other good quantum number in $[0]$); for higher values of the spin or for fermions K_m could be different from zero [24].

For normalizable wave functions one can then define the density

$$v(\rho) \equiv \int d\Omega |\Psi(\rho, \Omega)|^2 = \rho^{-(3N-4)} \sum_{[K]=[K_m]}^{[K_M]} u_{[K]}^2(\rho), \quad (12)$$

normalized as

$$\int_0^\infty d\rho \rho^{3N-4} v(\rho) = \int_0^\infty d\rho \left[\sum_{[K]=[K_m]}^{[K_M]} u_{[K]}^2(\rho) \right] = 1. \quad (13)$$

It is in terms of this density that, in the next section, the HK theorem will be reformulated.

III. THE ENERGY FUNCTIONAL

Following Levy's proof of the HK theorem [25], based on a constrained search, we start from the Hamiltonian in Eq. (7) and define the functional $E[v]$ as the minimum of the energies obtained with all wave functions Ψ that have the same $v(\rho)$:

$$E[v] = \min_{\Psi \rightarrow v} \langle \Psi | T + V | \Psi \rangle. \quad (14)$$

Since $v(\rho)$ is an integral property of $|\Psi\rangle$, there will be in principle an infinite number of normalizable functions having the same v . The functional $E[v]$ is then defined as the minimum produced by all such functions.

Calling E_0 the ground-state energy of H , and $|\Psi_0\rangle$ the corresponding wave function, the Rayleigh-Ritz variational principle establishes that

$$E[v] \geq E_0, \quad (15)$$

and

$$E[v_0] = \min_{\Psi \rightarrow v_0} \langle \Psi | T + V | \Psi \rangle = E_0, \quad (16)$$

where we have denoted by v_0 the density corresponding to the ground-state wave function $|\Psi_0\rangle$. This last statement follows from the fact that when the set of functions is selected among those having the density v_0 , the true wave function $|\Psi_0\rangle$ is included in that set and the global minimum E_0 is reached. The above statements imply that

$$\left. \frac{\delta E[v]}{\delta v} \right|_{v=v_0} = 0. \quad (17)$$

The properties of such a functional, when depending on the one-body density $n(\vec{r})$, are extensively discussed in the literature (see, for example, Refs. [3,6–8] and references therein).

Let us consider now the particular case of a system interacting through a hypercentral potential $W(\rho)$:

$$H_W = T + W(\rho). \quad (18)$$

Analogously to the central potential case for two particles, the ground-state wave function is simply

$$\Phi_0(\rho, \Omega) = \rho^{-(3N-4)/2} w_{[K_m]}(\rho) \mathcal{Y}_{[K_m]}(\Omega), \quad (19)$$

namely, it includes only the lowest term of the expansion given in Eq. (11). The hyper-radial function $w_{[K_m]}$ and the ground-state energy \mathcal{E}_0 can be obtained by solving a one-dimensional differential equation (hyper-radial equation):

$$\left[-\frac{\hbar^2}{m} \left(\frac{\partial^2}{\partial \rho^2} - \frac{(3N-4)(3N-6)}{4\rho^2} + \frac{K_m(K_m+3N-5)}{\rho^2} \right) + W(\rho) - \mathcal{E}_0 \right] w_{[K_m]}(\rho) = 0, \quad (20)$$

and the ground-state density defined in Eq. (12) is

$$v_0^W(\rho) = \rho^{-(3N-4)} w_{[K_m]}^2(\rho) \quad (21)$$

normalized as

$$\int_0^\infty d\rho \rho^{3N-4} v_0^W(\rho) = \int_0^\infty d\rho w_{[K_m]}^2(\rho) = 1. \quad (22)$$

On the other hand, after having defined $T_{\min}[v] \equiv \min_{\Psi \rightarrow v} \langle \Psi | T | \Psi \rangle$ and the density functional

$$\begin{aligned} E_W[v] &\equiv \min_{\Psi \rightarrow v} \langle \Psi | T + W | \Psi \rangle \\ &= T_{\min}[v] + \int d\rho \rho^{3N-4} v(\rho) W(\rho), \end{aligned} \quad (23)$$

\mathcal{E}_0 could as well be found by a minimization procedure, in fact,

$$\begin{aligned} \frac{\delta E_W[v]}{\delta v} &= \frac{\delta T_{\min}[v]}{\delta v} + \rho^{3N-4} W(\rho) = 0 \iff v = v_0^W \quad \text{and} \\ \mathcal{E}_0 &= E_W(v_0^W). \end{aligned} \quad (24)$$

Turning back to the energy functional of Eq. (14) we impose the following requirement:

$$E[v] = E_W[v], \quad (25)$$

assuming the W representability of the functional.¹ Namely,

$$\begin{aligned} \min_{\Psi \rightarrow v} \langle \Psi | T + V | \Psi \rangle &= \min_{\Psi \rightarrow v} \langle \Psi | T + W | \Psi \rangle \\ &= T_{\min}[v] + \int d\rho \rho^{3N-4} v(\rho) W(\rho). \end{aligned} \quad (26)$$

The energy functional $E[v]$ is now represented by a system of particles interacting through this particular potential $W(\rho)$.

Since for the ground state of $H = T + V$ one has $\frac{dE[v]}{dv} = 0$, Eq. (26) formally defines the hypercentral potential $W(\rho)$ as

$$W(\rho) = -\frac{1}{\rho^{3N-4}} \frac{\delta T_{\min}[v]}{\delta v}. \quad (27)$$

The core of requirement (26) is that $W(\rho)$ gives the same density $v(\rho)$ as $V(\rho, \Omega)$. One can show that such a $W(\rho)$ is unique.² The proof goes via a *reductio ad absurdum* procedure. One assumes that two hypercentral potentials, $W_1(\rho)$ and $W_2(\rho)$, differing by more than a constant, exist in such a way that the two Hamiltonians $H_1^W = T + W_1(\rho)$ and $H_2^W = T + W_2(\rho)$ have the same $v(\rho)$. Let us call $|\Phi_1\rangle$ and $|\Phi_2\rangle$ the respective wave functions and \mathcal{E}_1 and \mathcal{E}_2 the corresponding energies. From the Rayleigh-Ritz variational principle the following condition holds:

$$\mathcal{E}_1 < \langle \Phi_2 | H_1^W | \Phi_2 \rangle = \langle \Phi_2 | H_2^W | \Phi_2 \rangle + \langle \Phi_2 | H_1^W - H_2^W | \Phi_2 \rangle, \quad (28)$$

$$\mathcal{E}_1 < \mathcal{E}_2 + \int d\rho \rho^{3(N-4)} [W_1(\rho) - W_2(\rho)] v(\rho). \quad (29)$$

The same can be repeated starting from \mathcal{E}_2 arriving at

$$\mathcal{E}_2 < \mathcal{E}_1 + \int d\rho \rho^{3(N-4)} [W_2(\rho) - W_1(\rho)] v(\rho). \quad (30)$$

Summing both inequalities we arrive at the following contradiction, $\mathcal{E}_1 + \mathcal{E}_2 < \mathcal{E}_1 + \mathcal{E}_2$, proving that the first assumption was wrong. Accordingly, it is proven that the density $v(\rho)$ uniquely determines the hyper-radial potential $W(\rho)$ that generates it. Notice, by the way, that the same conclusion holds if a further generic $\mathcal{W}(\rho, \Omega)$ interaction is included in H_1 and H_2 .

The important conclusion is then that E_0 could be found either by $\frac{\delta E_W[v]}{\delta v} = 0$ or simply by solving Eq. (20). In the traditional KS case the problem is to guess the correct functional; here it is to guess the correct $W(\rho)$.

Equation (20) is the basic equation of the translational-invariant density-functional theory discussed here. This equation has been obtained previously in the literature (see, for example, Refs. [26–28]); however, in a different context, namely, as the result of the lowest order HH expansion of the ground-state wave function. In our case, in view of the unique relation between $W(\rho)$ and the density $v(\rho)$, this equation provides the way to obtain the right energy functional, and therefore the right ground-state energy, for any number of particles.

As a first application, in the next section the functional $E[v]$ is constructed in the case of atomic clusters of bosonic helium. The case of fermions is postponed to a forthcoming work.

IV. APPLICATION TO ATOMIC CLUSTERS

We consider clusters of atomic ^4He , largely discussed in the literature. Helium drops and the homogeneous system

¹The representability of the functional $E[n(\vec{r})]$ in terms of the external potential has been discussed many times in the literature [3,7,8].

²Here the argument is similar to that of Kohn-Sham one-body potential, namely, once the existence of W is assumed, one can show its uniqueness.

have been extensively studied using realistic He-He potentials. A rather successful one is the Aziz HFD-HE2 He-He potential [29], which we will take as reference potential and, for the purpose here, its results are considered equivalent to experimental data.

Another interesting approach to helium clusters starts from the observation that the dimer of ^4He has a binding energy of about 1 mK, three orders of magnitude less than the typical energy scale of $\hbar^2/mr_{vdW}^2 = 1.677\text{ K}$, with $\hbar^2/m = 43.281\,307\text{ K } a_0^2$ and $r_{vdW} = 5.08\, a_0$ the corresponding van der Waals length (a_0 is the Bohr radius). Moreover, the two-body scattering length has been estimated to be $a \approx 190\, a_0$, 20 times larger than r_{vdW} . In the limiting case, $a \rightarrow \infty$, the system is located at the unitary limit, well suited for an effective expansion of the interaction. In the spirit of an effective field theory devoted to describe systems with large values of the two-body scattering length [30–32], the first term of this expansion is a contact interaction between the two helium atoms. However, as it is well known, the three-body system (as well as larger systems) collapses, even if the contact interaction is set to produce an infinitesimal binding energy. This phenomenon is known as the Thomas collapse [33] and it is remedied by the introduction of a (contact) three-body force set to correctly describe the trimer energy ϵ_3 . Accordingly, the leading order (LO) of this effective theory has two terms, a two-body term and a three-body term, associated with two constants, named low-energy constants (LECs), needed to determine their strengths, usually fixed by ϵ_2 and ϵ_3 .

For the only purpose of determining $W(\rho)$, and inspired by the effective theory just described above, we introduce the following two- and three-body potentials:

$$V_{LO}^{[2]} = \sum_{i<j} A e^{-r_{ij}^2/\alpha^2}, \quad V_{LO}^{[3]} = \sum_{i<j<k} B e^{-r_{ijk}^2/\beta^2}, \quad (31)$$

where $r_{ij}^2 \equiv (\vec{r}_i - \vec{r}_j)^2$ and $r_{ijk}^2 \equiv (\vec{r}_i - \vec{r}_j)^2 + (\vec{r}_i - \vec{r}_k)^2 + (\vec{r}_j - \vec{r}_k)^2$. The natural choice is to consider $W(\rho)$ as a sort of mean hypercentral field, and we obtain it by averaging on the hyperangular part of the ground-state wave function:

$$W_A(\rho) = A \frac{N(N-1)}{2} \int d\Omega e^{-r_{12}^2/\alpha^2} |\mathcal{Y}_{[0]}(\Omega)|^2, \quad (32)$$

$$W_B(\rho) = B \frac{N(N-1)(N-2)}{6} \int d\Omega e^{-r_{123}^2/\beta^2} |\mathcal{Y}_{[0]}(\Omega)|^2 \quad (33)$$

(for spin 0 systems the minimal value of $[K_m] = 0$). From the definition of $\mathcal{Y}_{[0]}(\Omega)$ and writing the distances r_{12} and r_{123} in terms of the hyperspherical coordinates [23], the above integrals can be reduced to one-dimensional integrals that can be computed with sufficient accuracy using standard quadratures. In the particular case of the Gaussian interaction one has

$$W(\rho) = A \frac{N(N-1)}{2} \mathcal{M}\left(\frac{3}{2}, \frac{3N-3}{2}, -\frac{\rho^2}{\alpha^2}\right) + B \frac{N(N-1)(N-2)}{6} \mathcal{M}\left(3, \frac{3N-3}{2}, -\frac{3\rho^2}{\beta^2}\right), \quad (34)$$

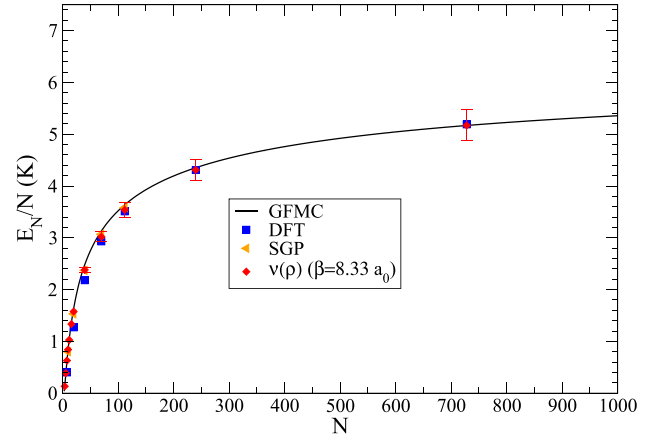


FIG. 1. Binding energy per particle obtained solving Eq. (35) with $7.5\, a_0 < \beta < 9.0\, a_0$, the (red) diamonds highlight the best case $(B, \beta) = (7.211\text{ K}, 8.33\, a_0)$, with the spread denoted by the error bars visible for $N \geq 40$. The GFMC results for the HFD-HE2 potential (black solid line), the DFT results of Ref. [37] (blue squares), and the results of the soft Gaussian potential (SGP) of Refs. [38,39] (orange triangles) are shown too.

where the function $\mathcal{M}(a, b, c)$ is a confluent hypergeometric function [34,35].

Having found an expression for $W(\rho)$ one can now give a prediction for the ground-state energy of clusters of any number N of bosons by solving the following simple equation:

$$\left[-\frac{\hbar^2}{m} \left(\frac{\partial^2}{\partial \rho^2} - \frac{(3N-4)(3N-6)}{4\rho^2} \right) + W(\rho) - \mathcal{E}_0 \right] w_0(\rho) = 0. \quad (35)$$

The four parameters in $W(\rho)$ give us the opportunity to relate the two functionals, $E_W[\nu]$ and $E[\nu]$, as follows. The helium dimer represented by the Aziz potential has a single bound state with energy $\epsilon_2 = 0.830\,12\text{ mK}$, a scattering length $a = 235.547\, a_0$, and an effective range $r_e = 13.978\, a_0$. Fitting α and A to the corresponding HFD-HE2 values, the Gaussian parameters result: $\alpha = 10.0485\, a_0$ and $A = -1.208\,018\text{ K}$.

Several choices are possible to determine the other two parameters (B, β) . One could choose, e.g., to fit the trimer and tetramer binding energies [38,39]. In view of the fact that $W(\rho)$ has to account for energies at any N , we think it more expedient to obtain couples (B, β) values, all fitting the tetramer binding energy. So we solve Eq. (35) for the four-body system and require $\mathcal{E}_0 = 0.5332\text{ K}$, the HFD-HE2 value [36]. We observe substantial independence from the three-body range β for the lowest N values with the overall best description inside the interval $7.5\, a_0 < \beta < 9.0\, a_0$, where the central value is $\beta = 8.33\, a_0$ and $B = 7.211\text{ K}$ the corresponding strength.

Having determined the parametrization of $W(\rho)$, we proceed to solve Eq. (35) for increasing values of N to determine the binding energy per atom E_N/N as a function of the number of atoms N . The results are shown in Fig. 1. The red diamonds are the results obtained with $(B, \beta) = (7.211\text{ K}, 8.33\, a_0)$, where the error bars show results with β varying inside the interval $7.5\, a_0 < \beta < 9.0\, a_0$. For the sake of comparison we show the Green function Monte Carlo (GFMC) results of

Ref. [36] (black solid line), the DFT results of Ref. [37] (blue diamond), and the results of the soft Gaussian potential (SGP) of Refs. [38,39] (orange triangles). Unexpectedly, the four-parameter hyper-radial potential $W(\rho)$ has sufficient information to reproduce the E_N/N behavior. As it is evident in Fig. 1, the results of Eq. (35) are of similar quality as those using more sophisticated potentials and methods, giving support to the formalism presented.

As we will see below, for large values of N the solutions of Eq. (35) are very much localized; the kinetic energy gets a small fraction of the total energy which tends to equal the minimum of $W(\rho)$. Using the asymptotic form of the confluent hypergeometric functions such a minimum results:

$$W_m = -\frac{3^4 A^2}{8 B} \left(\frac{\alpha}{\beta}\right)^6 N. \quad (36)$$

The potential parameters selected to reproduce the binding energy per particle for low N values predict $E_N/N \rightarrow |W_m|/N = 6.4 \pm 0.7$ K, compared to the experimental value of 7.1 K of the homogeneous system. Though this is a remarkable result considering the minimal information used to determine $W(\rho)$, the above relation gives a further condition that might be used in determining the potential parameters.

To conclude the analysis of the results, in Fig. 2 (upper panel) we show the (reduced) many-body density for selected number of particles. As can be seen from the figure, the density is extremely localized around a particular value of ρ , which increases almost linearly with N . The behavior of $v(\rho)$ indicates a very compact object, not compressible; in fact, lower values of ρ allowing the particles to be closer are discouraged as well as larger values, which would indicate possible clusterizations.

The many-body density $v(\rho)$ can be used to calculate the mean-square radius. Defining \vec{r} the position of a generic particle with respect to the center of mass, using Eq. (5) results in $\langle r^2 \rangle = \frac{1}{2N} \langle \rho^2 \rangle$, with

$$\langle \rho^2 \rangle = \int \rho^2 v(\rho) \rho^{3N-4} d\rho. \quad (37)$$

In Fig. 2 (lower panel) the unit radius, $r_0(N) = \sqrt{5/3} \langle r^2 \rangle^{1/2} / N^{1/3}$, is shown (black solid points) as a function of N with error bars corresponding to variations of β in the interval indicated above and it is compared to the GFMC results of Ref. [36] (red solid points). The agreement is evident; the r_0 values obtained from the best parametrizations of $W(\rho)$ reproduce the GFMC results better than 5%. Moreover, in the large- N limit, W_m is located at

$$\rho_m = \left(\frac{2\mathcal{B}}{|\mathcal{A}|}\right)^{1/3} N^{5/6}, \quad (38)$$

with $\mathcal{A} = \frac{A}{2} \left(\frac{3}{2}\right)^{3/2} \alpha^3$ and $\mathcal{B} = \frac{B}{6} \left(\frac{1}{2}\right)^3 \beta^6$. The unit radius tends to $r_0 \rightarrow \sqrt{5/6} \left(\frac{2\mathcal{B}}{|\mathcal{A}|}\right)^{1/3} = 4.1 \pm 0.2 a_0$, extremely close to the GFMC results at $N \rightarrow \infty$.

V. CONCLUSIONS AND OUTLOOK

In this work we formulate a density-functional approach in terms of the density $v(\rho)$. Such a density depends on the

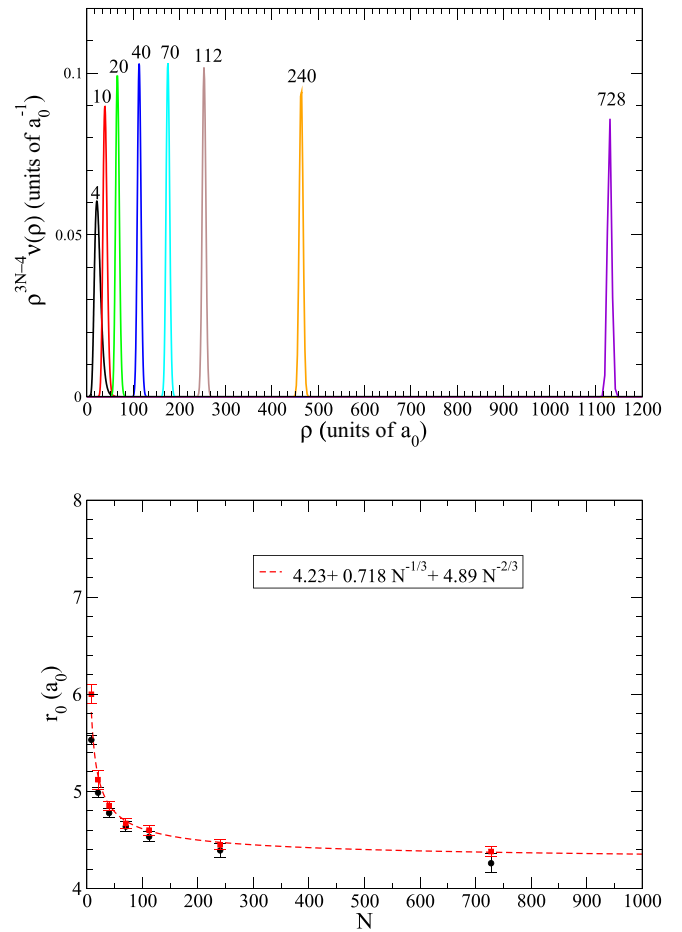


FIG. 2. The (reduced) many-body density $v(\rho)$ for selected number of particles (upper panel). The unit radius r_0 (black solid points) (lower panel) with error bars corresponding to variations of β in the interval $7.5 a_0 < \beta < 9.0 a_0$. For the sake of comparison, the GFMC results [36] are shown too (red solid points), together with a fit to these values represented by the (red) dashed line in units of a_0 .

hyper-radius ρ , a translation-invariant variable of a collective nature, because it is connected to the sum of the distances between the particles. It is shown that the functional $E[v]$ is governed by a unique (unknown) hyper-radial potential $W(\rho)$. The solution of a single hyper-radial equation with such a hyper-radial potential allows one to determine the binding energy for any number of particles in a straightforward way.

We have applied this framework to the bosonic case, focusing on ${}^4\text{He}$ clusters. The guess for $W(\rho)$ has been inspired by the effective theory approach together with a generalization of the mean-field concept. Extremely satisfying results have been found. The key point has been to use the range of the three-body interaction, β , to fine tune the hyper-radial potential $W(\rho)$. The extension to treat trapped systems is underway. Since the formalism presented here is valid for bosons as well as for fermions, an application to nuclear systems might be promising, provided that a good guess for $W(\rho)$ is found. The effective theory point of view might again be of help, as envisaged by results obtained recently in Ref. [40]. Work in that direction is in progress.

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