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Citation: [AIP Conference Proceedings](#) **850**, 149 (2006); doi: 10.1063/1.2354646

View online: <http://dx.doi.org/10.1063/1.2354646>

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A Density Functional for Liquid ^3He Based on the Aziz Potential

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Abstract. We propose a new class of density functionals for liquid ^3He based on the Aziz helium-helium interaction screened at short distances by the microscopically calculated two-body distribution function $g(r)$. Our aim is to reduce to a minimum the unavoidable phenomenological ingredients inherent to any density functional approach. Results for the homogeneous liquid and droplets are presented and discussed.

Keywords: density functional, helium, pair correlation

PACS: 67.60.-g, 67.70.+n, 61.46.+w

The total energy of a system consisting of N identical particles that interact pairwise can be universally expressed as

$$\begin{aligned} E &= Tr_{1,\dots,N}(H\rho_N) \\ &= Tr_1(h_1\rho) + \frac{1}{2}Tr_{1,2}(V\rho_2) \end{aligned} \quad (1)$$

where Tr_i denotes tracing with respect to the quantum numbers of particle i , H is the N -body Hamiltonian with h_1 the one-body contribution and V the pair potential. Here ρ and ρ_2 are, respectively, the one- and two-particle density operators corresponding to the full density matrix ρ_N . The two-body density of particles 1 and 2 is usually expressed in terms of the pair correlation function $g(1, 2)$ as $\rho_2(1, 2) = \rho(1)\rho(2)g(1, 2)$. Since Hohenberg-Kohn's theorem[1] states that the total energy of an N -particle system is a functional of ρ –and only ρ –, one of the main problems in many-body theory is to relate the pair correlation function to the one-body density. In a microscopic approach, this can be achieved by means of hierarchically coupled equations that contain summations of diagrams.

A phenomenological approach to circumvent the ignorance of the true pair distribution as a function of the single-particle (sp) density, preserving to some extent the many-body character of the system, is provided by Density Functional (DF) theories. These are mean field descriptions of the fully correlated system, where the interaction of two and more particles are included through parametrized functions of the sp density.

Recently, a DF has been proposed[2] for inhomogeneous ^4He that incorporates the available knowledge about the pair correlation function into a representation

of the potential energy. In these works, one adopts the so-called "hybrid" DF

$$\begin{aligned} E &= \int d\mathbf{r} \tau(\mathbf{r}) + \int d\mathbf{r} \sum_{n=2}^4 \frac{c_n}{n} \rho(\mathbf{r}) [\bar{\rho}(\mathbf{r})]^n \quad (2) \\ &+ \frac{1}{2} \int \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}) g(|\mathbf{r} - \mathbf{r}'|) V_{LJ}(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}') \\ &+ \frac{1}{2} \int \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}) \mathcal{G}(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}') \end{aligned}$$

where $\tau(\mathbf{r})$ is the kinetic energy density, $\bar{\rho}(\mathbf{r})$ is a coarse-grained density obtained by averaging ρ with respect to the function $\rho_0 h(|\mathbf{r} - \mathbf{r}'|) = \rho_0 [1 - g(|\mathbf{r} - \mathbf{r}'|)]$, and the pair interaction term contains the full Lennard-Jones potential. The correlation kinetic energy is

$$\mathcal{G}(|\mathbf{r} - \mathbf{r}'|) = \frac{\hbar^2}{2m} \left[|\nabla \sqrt{g(|\mathbf{r} - \mathbf{r}'|)}|^2 + |\nabla' \sqrt{g(|\mathbf{r} - \mathbf{r}'|)}|^2 \right] \quad (3)$$

After introducing an analytical form for the pair correlation function, that reproduces experimental data at saturation density ρ_0 , we fit the coefficients c_n , $n = 2$ to 4 by using the energy per atom, density and incompressibility modulus at saturation. A good agreement is obtained for density profiles of adsorbed films, as compared with Monte Carlo calculations, as well as a good figure for the surface tension and for various wetting data.

The purpose of the present work is to apply the above philosophy to construct a hybrid DF for inhomogeneous liquid ^3He . A complete DF for this system should be able to describe both the density (spin-symmetric or S) and the spin (spin-antisymmetric or A) channels of the homogeneous liquid; given the complexities of the A -channel, we postpone this issue for a later study and

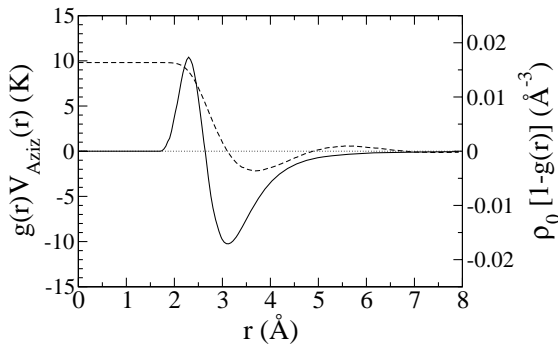


FIGURE 1. Screened Aziz potential $g(r)V_A(r)$ (full line) and direct pair correlation $h(r)$ (dashed line) as functions of radial distance between particles.

here concentrate in spin-saturated ^3He . Accordingly, we propose the following DF

$$\begin{aligned}
 E &= \int d\mathbf{r} \frac{\hbar^2}{2m} \left(1 - \frac{\tilde{\rho}(\mathbf{r})}{\rho_c}\right)^2 \sum_{i=1}^N |\nabla\phi_i(\mathbf{r})|^2 \quad (4) \\
 &+ \int d\mathbf{r} \frac{c}{2} \rho(\mathbf{r}) [\tilde{\rho}(\mathbf{r})]^{1+\gamma} \\
 &+ \frac{1}{2} \int \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}) g(|\mathbf{r}-\mathbf{r}'|) V_A(|\mathbf{r}-\mathbf{r}'|) \rho(\mathbf{r}') \\
 &+ \frac{f}{2} \int \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}) \mathcal{G}(|\mathbf{r}-\mathbf{r}'|) \rho(\mathbf{r}')
 \end{aligned}$$

Here $\phi_i(\mathbf{r})$ are sp wave functions to be determined by solving the mean field Kohn-Sham (KS) equations [3] and the sp density is $\rho(\mathbf{r}) = \sum_{i=1}^N |\phi_i(\mathbf{r})|^2$. The two-body interaction V_A is the full Aziz HFD-B(HE) potential[5]. The density-dependent factor in the kinetic energy term and the repulsive correlation energy with strength c are chosen as in the Orsay-Paris (OP) DF,[4] and $f = 0.93$ is a constant parameter selected so as to preserve the OP value of the integral of the pairwise potential energy. In this way, the predicted equation of state coincides with the OP and experimental ones.

The main difficulty here is the lack of experimental information on the pair correlation; however, the key ingredients are the equal and opposite pair correlation functions $g_{\uparrow\uparrow}(|\mathbf{r}-\mathbf{r}'|)$ and $g_{\uparrow\downarrow}(|\mathbf{r}-\mathbf{r}'|)$ that can be computed within a diffusion Monte Carlo frame[6]. With these data, we numerically construct the density-density correlation function $g(|\mathbf{r}-\mathbf{r}'|) = [g_{\uparrow\uparrow}(|\mathbf{r}-\mathbf{r}'|) + g_{\uparrow\downarrow}(|\mathbf{r}-\mathbf{r}'|)]/2$, later employed as the input for the KS equations. In Fig. 1 we show the effective potential $g(r)V_A(r)$ and the direct pair correlation $h(r) = 1 - g(r)$, in full and dashed lines, respectively.

In order to assess the reasonability of this DF, we have computed density profiles and energetics of $^3\text{He}_N$ clusters for increasing number of atoms N . A byproduct of this calculation is the predicted value of the surface

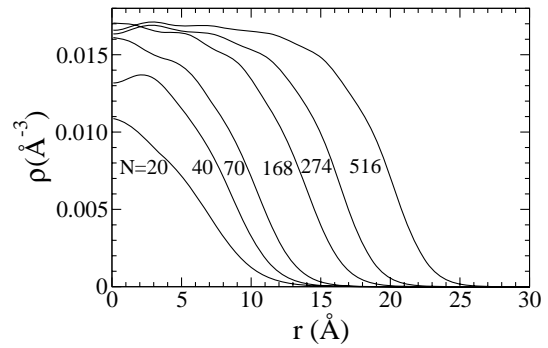


FIGURE 2. Radial density profiles of spherical $^3\text{He}_N$ clusters for various numbers of atoms N .

tension, which in this case reads $0.121 \text{ K } \text{Å}^{-2}$, to be compared with an experimental figure of $0.113 \text{ K } \text{Å}^{-2}$. Typical results are displayed in Fig. 2, where we plot density profiles for $N = 20, 40, 70, 168, 274$ and 516 .

In summary, we are proposing a new DF for the spin-symmetric channel of nonhomogeneous liquid ^3He , which incorporates some desirable features of a true many-body system, namely the two-body correlation function, here determined by a rigorous simulation. This method permits to represent the two-body interaction by a realistic pair potential, avoiding the arbitrary core suppression of earlier DF's and eliminating both the core and the coarse-graining radius as parameters. Additionally, no gradients of the sp density need to be introduced through parametric functions. We believe that the present results encourage further research, especially, examining the dynamical response of the liquid and seeking to improve the description of the spin-antisymmetric channel.

We are indebted to Jordi Boronat for kindly providing his numerical data on the pair correlation functions. This work was partially supported by grants 2001SGR00064 and FIS2004-00912, Spain, and PICT 03-08450 (AN-PCYT), Argentina.

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