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Mass formula for ^{3}He clusters

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We have obtained an analytic expression for the total energy of ^{3}He clusters composed of N atoms. It is a variational solution of an energy density functional, where the extended Thomas-Fermi method has been used for the kinetic-energy density. The energy is calculated as an expansion in decreasing powers of the cluster radius, $R \propto N^{1/3}$. Contributions of volume (R^3), surface (R^2), curvature (R), constant (R^0), ($1/R$), and ($1/R^2$) are identified in the formula. Simple analytical formulas are also derived for relevant quantities such as chemical potentials, fusion and fission potentials, surface thickness, unit radii, and relative compression. Our results are compared with other available theoretical calculations.

I. INTRODUCTION

The study of the stability and structure of rare-gas clusters has received growing attention in the past few years.[1-5] At present, although the experimental values of the binding energy,[6] density,[7] compressibility,[7] and surface tension[8] of the two heliums are known, the experimental information about helium drops is still rather poor.[3,9,10] On the theory side, previous studies[4,11-23] of ^{3}He and ^{4}He clusters have mainly dealt with the description of ground-state properties along two principal routes. First we find microscopic-type calculations such as those in Refs. 4 and 11, where a Monte Carlo method is performed using the Aziz *et al.*[24] atomic potential as input. Second, we find the density-functional method equipped with phenomenological zero-range interactions.[13,15,16,21] This second strategy is more economical and, usually, provides a clearer picture of the structure of these systems.

The aim of this work is to obtain an analytical formula for the total energy, and other physical observables, of a cluster composed of N atoms of ^{3}He, using a variational ansatz for the structure of the cluster. This work can be considered as a continuation of another dealing with ^{4}He clusters.[21] As the ^{3}He atom is a fermion, the many-body equation with which one would have, in principle, to deal with, are of the Hartree-Fock type. But this type of calculation is difficult and does not permit to obtain analytic expressions, therefore we will resort to the widely used semiclassical approximation for the kinetic-energy density and apply the extended Thomas-Fermi (ETF) method. The use of this approximation is justified because the genuine quantum-mechanical effects are not very pronounced. We will use a functional of phenomenological nature which has already been successfully used in the description of atomic nuclei.[25] With respect to the variational ansatz, we have used a function proposed by some of us in the description of the physics of metallic clusters.[26-28]

The paper is organized as follows. Section II presents the energy functional to be used in the ETF method; from this functional we will obtain the energy of the clusters as a function of two variational parameters. The other parameters of the model are fixed so as to reproduce the experimental data for ^{3}He, and take into account higher-order inhomogeneity corrections (ETF parameters). In this second section we impose the condition that the total energy of a cluster must be a minimum. This leads to mathematical conditions which fix analytically the variational parameters and the other coefficients of the mass formula. Section III presents our results and a comparison with other available theoretical calculations; in particular, the value of the coefficients in the mass formula, fission, and fusion potentials, the chemical potential, skin depth, unit radii, relative compression, and profile of densities are all discussed as a function of N. Finally, in Sec. IV we give our conclusions.

II. DENSITY FUNCTIONAL AND CALCULATION OF THE ENERGY OF THE CLUSTERS

In the present work, as in Ref. 21, we will use the following functional for the total energy of the clusters:

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$$E[n]=\int\left[\frac{\hbar^2}{2m^*}\mathcal{T}+\frac{b}{2}n^2+\frac{c}{2}n^p+d(\nabla n)^2\right]d\mathbf{r}\ ,$$

$$=E_{\text{kin}}+E_a+E_r+E_d\ , \tag{2.1}$$

where $n(\mathbf{r})$ is the particle density and m^* is the effective mass of a ^{3}He atom. Functionals of the type (2.1) have been extensively used in the description of atomic nuclei and can be derived from a phenomenological interaction of the Skyrme type.[25] The coefficients of the functional are determined by fitting an appropriate set of experimentally known quantities. For the effective mass we use

$$\frac{1}{m^*}=\frac{1}{m}\left[1-\frac{n}{n_c}\right]^2, \tag{2.2}$$

with $n_c=0.0406$ Å^{-3}, and m being the mass of the ^{3}He atom. Equation (2.2) accounts very accurately for the variation of the specific heat with pressure[29] and is necessary for a proper description of ^{3}He at $T=0$. On the contrary, the use of m^* is not necessary when dealing with ^{4}He; that is because there $m^*=m$.

The first term in Eq. (2.1), E_{kin}, represents the cluster kinetic energy and it was obtained by performing ETF calculations based on the following kinetic-energy density,[30] $\mathcal{T}(\mathbf{r})$:

$$\mathcal{T}(\mathbf{r})=\alpha n^{5/3}+\beta\frac{(\nabla n)^2}{n}+\delta\nabla^2 n\ , \tag{2.3}$$

with $\alpha=\frac{3}{5}(3\pi^2)^{2/3}$, $\beta=\frac{1}{18}$, and $\delta=\frac{1}{3}$. This functional can be obtained through a development of the cluster kinetic energy as a power series of $\hbar$, when dealing with a fermionic assembly moving in a smoothly varying local potential. In this respect we find a clear difference with respect to what we used in Ref. 21. There, the ground state of the system was formed by a Bose condensate and, hence, $\mathcal{T}(\mathbf{r})$ could be written down exactly. The coefficient $\beta=\frac{1}{18}$ accounts for high-order inhomogeneity corrections involving the high-order density dependence of the effective mass.[31] The validity of Eq. (2.3) is justified in this system because in a microscopic quantum-mechanical analysis of it, neither shell effects nor Friedel-oscillations have been observed to occur; hence, a semiclassical description is quite close to the quantum-mechanical one.[15]

The term with b represents the attractive component of the interatomic potential—at long distance—while c stands for the short-distance repulsive interaction. The value of the coefficients b, c, and p is chosen so as to fit the bulk properties of ^{3}He. The fourth term of the functional represents a repulsive effect at the surface, and d will be fixed so as to fit the experimental value of the surface tension, once the trial function for the density is given.

A. Bulk parameters

In order to fix the bulk parameters, let us consider a fermionic assembly of N particles, which form a sphere of constant density and radius R. If the energy is given by Eq. (2.1), then

$$E=\frac{3\hbar^2}{10m}\left[\frac{9\pi}{4}\right]^{2/3}\frac{N^{5/3}}{R^2}\left[1-\frac{3N}{4\pi n_c R^3}\right]^2$$

$$+\frac{3b}{8\pi}\frac{N^2}{R^3}+\frac{c}{2}\left[\frac{3}{4\pi}\right]^{p-1}\frac{N^p}{R^{3(p-1)}}\ , \tag{2.4}$$

where it is assumed that $b<0, c>0$ and $p>1$. This expression for the energy had a parallel counterpart in the bosonic case; there the expression was simpler because the kinetic-energy term was absent. For a fixed N, the condition of extremum, $dE/dR=0$, leads to

$$0=r^{3p-5}+\frac{5b}{2(12\pi^5)^{1/3}}\frac{m}{\hbar^2}r^{3p-6}-5r_c^3r^{3p-8}$$

$$+4r_c^6r^{3p-11}+\frac{5(p-1)c}{2(12\pi^5)^{1/3}}\left[\frac{3}{4\pi}\right]^{p-2}\frac{m}{\hbar^2}\ , \tag{2.5}$$

where we have adopted the convention $R=rN^{1/3}$ and $r_c=(3/4\pi n_c)^{1/3}$. The solution of Eq. (2.5) provides a value for r, r_0, which depends exclusively on the parameters of the potential; moreover, we obtain a unit radius not dependent on n, i.e., a saturating behavior.[32] To assure stability, we must analyze the second derivative $d^2E/dR^2|_{r=r_0}$, too,

$$\left.\frac{d^2E}{dR^2}\right|_{r=r_0}=\frac{9}{4\pi}\frac{N^{1/3}}{r_0^4}\left\{\frac{3}{5}(12\pi^5)^{1/3}\frac{\hbar^2}{m}\right.$$

$$\times\left[(\tfrac{5}{3}-p)-5(\tfrac{8}{3}-p)\frac{r_c^3}{r_0^3}\right.$$

$$\left.+4(\tfrac{11}{3}-p)\frac{r_c^6}{r_0^6}\right]$$

$$\left.+\frac{3b}{r_0}(1-p/2)\right\}. \tag{2.6}$$

If $b=c=0$, there are two possible solutions for Eq. (2.5), $r_0=r_c$ and $r_0=4^{1/3}r_c$. The first one corresponds to a minimum (with $E=0$) and the second one to a maximum. If $c=0$, b values increasingly negative imply a decrease of the r_0 value, corresponding to the minimum (so that $r_0<r_c$). On the other hand, if $b=0$, an increasing c implies an increasing value for r_0, corresponding to the minimum ($r_0>r_c$), but such state will have $E>0$ and will eventually decay. Thus, we can see how the two, attractive and repulsive, terms are necessary to provide a unit radius $r_0>r_c$ such that a stable equilibrium (minimum of the energy), without decay ($E<0$), can be implemented.

Our next task will be to apply these ideas to the ^{3}He case and then to determine the bulk properties of our model. Eq. (2.5) gives $r_0(n_0)$ which, inserted into Eq. (2.4) will give the binding energy per particle

$$\left.\frac{E}{N}\right|_{r=r_0}=\left.\frac{E}{N}\right|_0\ .$$

In a parallel way, we can also calculate the compressibility of the liquid ^{3}He, K_0. From its definition, we have

$$K_0^{-1}=K^{-1}\Big|_{r=r_0}=\frac{n_0 r_0^2}{9}\left[\frac{\partial^2(E/N)}{\partial r^2}\right]_{r=r_0} . \tag{2.7}$$

The last three equations will provide the basic properties of our system when saturation is reached, i.e., bulk properties ($N\rightarrow\infty$). Using[15,16] $b=-683.0$ K Å^3, $c=1.405\,057\times10^6$ K Å$^{3(p-1)}$, and $p=4.1$, we can fit the experimental values of the density (or unit radius), $n_0=1.6347\times10^{-2}$ Å^{-3} ($r_0=2.4443$ Å), binding energy $E/N|_0=-2.49$ K, and compressibility $K_0=5.056$ K^{-1} Å^3 for ^{3}He.

B. Trial function for the density: Semi-infinite medium

As a trial function to implement the variational calculation, we are going to use a function proposed by some of us, and which has been used both in Ref. 21 and in analytical calculation of metallic clusters. Its form is

$$n(\mathbf{r})=\bar{n}\begin{cases}1-R\,(1+s/R)e^{-R/s}\dfrac{\sinh(r/s)}{r}\;, & r\le R\\[2ex] R\left[\cosh(R/s)-\dfrac{\sinh(R/s)}{R/s}\right]\dfrac{e^{-r/s}}{r}\;, & r>R\;;\end{cases} \tag{2.8}$$

$\bar{n}$, R, s are the variational parameters which have to be fixed.

From now on, we will assume that any helium drop formed by N atoms has a spherical symmetry and, of course, the density function $n(\mathbf{r})$ verifies the normalization condition

$$\int n(\mathbf{r})d\mathbf{r}=N\;, \tag{2.9}$$

hence, there are two independent parameters at our disposal; suppose that they are R and s. It is easy to see that, due to (2.8) and (2.9) R can be interpreted as the equivalent sharp radius. It is useful to use the convention $R=rN^{1/3}$, r being the equivalent-sharp unitary radius, and as $\bar{n}=3/4\pi r^3$; thus, our final variational parameters are r and s.

Inserting Eq. (2.8) into (2.1) and using $\hbar^2/m=16.044$ K Å^2, we can obtain the leptodermic development of the four terms composing the cluster energy, i.e., E_{kin}, E_a, E_r, and E_d. As the expressions are rather long they are omitted (available on request).

By adding all the contributions with the same order in N, we can express the energy as

$$E(r,s,N)=N\left[\sum_{n=0}^{\infty}f_n(r,s)N^{-n/3}\right]\;, \tag{2.10}$$

where, as usual, f_0 represents the volume term, f_1 the surface term, f_2 that of curvature, etc.

The total energy must be an extremum, minimum, with respect to variations in the parameters r and s, i.e.,

$$\frac{\partial}{\partial r}E(r,s,N)=\sum_{n=0}^{\infty}(f_n)_r^{(1)}(r,s)\Big|_{r_m,s_m}N^{-n/3}=0\;, \tag{2.11a}$$

$$\frac{\partial}{\partial s}E(r,s,N)=\sum_{n=0}^{\infty}(f_n)_s^{(1)}(r,s)\Big|_{r_m,s_m}N^{-n/3}=0\;, \tag{2.11b}$$

where r_m and s_m indicate the values of r and s at the minimum. Now, after performing a Taylor expansion in Eqs. (2.11) around r_0 and s_0, of the form

$$r_m=r_0+\sum_{i=1}^{\infty}{}^{r}\Delta_i N^{-i/3}\;, \tag{2.12a}$$

$$s_m=s_0+\sum_{i=1}^{\infty}{}^{s}\Delta_i N^{-i/3}\;, \tag{2.12b}$$

then for the lowest n, by noting that f_0 does not depend on s, we will have

$$(f_0)_r^{(1)}(r=r_0)=0\;, \tag{2.13a}$$

$$(f_1)_s^{(1)}(r=r_0,s=s_0)=0\;. \tag{2.13b}$$

Equation (2.13a) expresses something already known: with the chosen values of b, c, and p, the volume energy per atom for bulk matter is an extremum in r_0 (see Sec. II A). Equation (2.13b) corresponds to the minimization of the surface tension of the semi-infinite medium and allows us to calculate $s=s_0(n_c,d,\beta,\delta)$. To fix d, we will use the experimental value of the surface tension $\sigma_0=0.113$ K Å^{-2}. We know that

$$\sigma=\lim_{N\rightarrow\infty}\frac{E(r_m,s_m,N)-Nf_0(r_0)}{4\pi r_m^2N^{2/3}}\;.$$

By looking at Eq. (2.10) and doing a Taylor expansion around r_0 and s_0, as defined, we have

$$\sigma=\frac{f_1(r_0,s_0(n_c,d,\beta,\delta))}{4\pi r_0^2}\;. \tag{2.14}$$

In this way, having Eqs. (2.13b) and (2.14) fitted to the experimental surface tension, we obtain expressions for $s_0(n_c)$ and $d(n_c,\beta,\delta)$.

Using for n_c, β, and δ, the values fixed at the beginning of this section, we obtain

$$s_0=2.4171\text{ Å}\;, \tag{2.15a}$$

$$d=1.8831\times10^3\text{ K Å}^5\;. \tag{2.15b}$$

At this point, all the parameters entering the density functional are fixed. The value of d given in (2.15b) differs only slightly from that found by Stringari and Treiner[15,16] ($d^{\text{ST}}=2.222\times10^3$ K Å^5). These authors use an identical density functional and analyze it through the Euler-Lagrange equations.

C. Condition of extremum for the energy

Now we are ready to proceed to the minimization. The idea consists of obtaining $s_m(r_m)$ as a certain $s_0(r_0)$ plus corrections; this is shown in Eqs. (2.12), in such a way that Eqs. (2.11) are fulfilled at all orders in N. The reader interested in details is referred to Ref. 21; here only the last formula is written. The energy at the minimum can be expressed, in a self-explanatory notation, as

$$E=a_v(r_0)N+a_s(r_0,s_0)N^{2/3}+a_c(r_0,s_0)N^{1/3}$$
$$+a_0(r_0,s_0)N^0+\sum_{n=-1}^{-\infty} a_n(r_0,s_0)N^{n/3}\ , \qquad (2.16)$$

where the new coefficients have been tabulated in Table I.

III. RESULTS AND DISCUSSION

In Fig. 1, we have plotted E/N as a function of N, including the contribution of the successive terms given by Eq. (2.16). To make the comprehension of the figure easier, we have plotted the results with two different scales both in abscissas (ordinary, for $N<100$, and the other logarithmic, for $N>100$) as in ordinates (both ordinary). From this figure we observe how the contribution of a_0 together with that of a_{-1}, and specially that of a_{-2}, allows the existence of bound states from a minimum N value, namely $N_m \approx 38$. A value of N lower than N_m would correspond to a metastable state which we will refer to later.

Previous calculations related to ^{3}He are the one by Pandharipande, Pieper, and Wiringa[4] and the one by Stringari and Treiner,[15] which are also written in Table I, to have a first-sight comparison. The calculation of Ref. 4 uses a Hamiltonian containing the HFDHE2 (Hartree-Fock dispersion) interatomic potential of Aziz *et al*,[24] and the results are obtained through a variational Monte Carlo (VMC) method. The values in Table I are fitted to VMC energies for the interval $20 \le N \le 240$.

Referring to a_v and a_s the different results show a remarkable concordance, specially for a_s, while there exists a marked discrepancy with respect to a_c. At this point it is worth emphasizing that while our calculation is completely analytical and that we are able to calculate as many coefficients as we wish, in Ref. 4, the values are obtained using a best fit with an accuracy of χ^2, of the order of one per degree of freedom, and coming only up to a_c. Normally, one would expect that the curvature correction to the energy of a convex surface would be positive, and indeed these authors admit the lack of physical meaning of the a_c found in the fit. They are also aware of the high influence that the degree of the assumed polynomial has on the value of a_c. In the case of having extended the calculation up to terms in N^0, the value of the obtained a_c would have been positive; this would have been confirmed if one had extended the calculations further, i.e., up to $N^{-1/3}$ or $N^{-2/3}$. It is also likely that in these cases the a_v of these authors would have got near ours. The discrepancies existing in the coefficients are, however, not very important for the cluster energy as one can observe in Fig. 2. As a general tendency in the figure, our values are higher than those of Ref. 4, for $N>50$.

TABLE I. Energy coefficients (in K) of the mass formula for ^{3}He clusters.

	Present work	Reference 4	Reference 15
a_v	−2.49	−2.09[a]	−2.49[b]
a_s	8.48	9.90[a]	8.42[b]
a_c	5.31	−9.90[a]	4.09[b]
a_0	−16.08		−19.80[c]
a_{-1}	−0.01		
a_{-2}	−31.32		

[a] Fit to VMC energies for $20 \le N \le 240$.

[b] Asymptotic properties of EL energies for bulk and semi-infinite liquid.

[c] Fit to QM energies. This is required to reproduce the energy of light magic clusters.

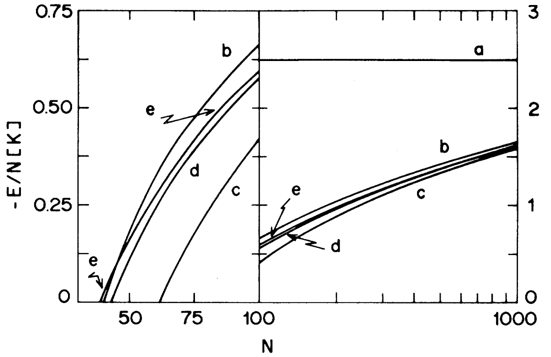

FIG. 1. Energy per atom in a ^{3}He cluster: Contribution of the different terms of the mass formula (see the text). Curve *a*: a_v; curve *b*: $a_v+a_sN^{-1/3}$, ; curve *c*: $a_v+a_sN^{-1/3}+a_cN^{-2/3}$; curve *d*: $a_v+a_sN^{-1/3}+a_cN^{-2/3}+a_0N^{-1}$; curve *e*: $a_v+a_sN^{-1/3}+a_cN^{-2/3}+a_0N^{-1}+a_{-1}N^{-4/3}+a_{-2}N^{-5/3}$.

With respect to Ref. 15, those authors are precisely the density functional given in Eq. (2.1) and their results are derived through a quantum-mechanical (QM) calculation. The values presented in Table I for a_v, a_s, and a_c are obtained by these authors from the asymptotic properties of Euler-Lagrange (EL) energies for the bulk and semi-infinite liquids, whereas a_0 is obtained by fitting QM energies so as to reproduce the energy of light magic clusters. a_v and a_s should be coincident with ours because the two calculations give the bulk properties of the system and also fit the surface tension of the semi-infinite

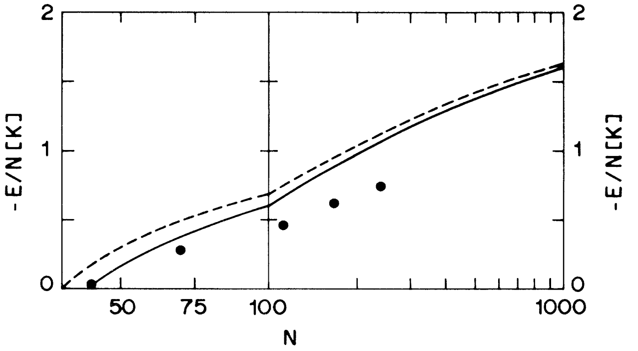

FIG. 2. Energy per atom in a ^{3}He cluster. The continuous line represents the present work. The (●) represent the VMC energies of Ref. 4. The dotted line represents the asymptotic properties of the EL and QM energies (Ref. 15).

medium. However, a small discrepancy is observed with regard to a_s, which is probably traced to a misprint or to the existence of a rounding error in any of the magnitudes involved in the computation of this coefficient. Within the general agreement, with respect to a_c and a_0 we find a greater discrepancy. Again one should remember that the a_0 of Ref. 15 was obtained through a numerical adjustment and no more coefficients were calculated. In Fig. 2 we have also drawn the E/N values from Ref. 15. There, one observes how for small N, they lie between those of Refs. 4 and 15, and for large N, our values tend to coincide with those of Ref. 15 (asymptotically the coincidence is complete). It is, likewise, interesting to find out what is the minimum value of N, N_m, necessary to have a stable ^{3}He cluster. As already mentioned, in our calculation we find $N_m \approx 38$, to be compared with $N_m = 40$ obtained in Ref. 4 and with $N_m = 30$ of Ref. 15. This greater proximity to the result of Ref. 4 is not strange because in the range of small N, E/N in the two cases is quite similar (see Fig. 2).

Now let us define the fusion potential, $\phi_{\rm FU}$, as the energy released when a cluster of N atoms captures 1 atom more; i.e., in the transit $N \rightarrow N+1$. Analogously, the fission potential $\phi_{\rm FI}$ is the energy to be added to an N, atom cluster, to strip one atom $[N \rightarrow (N-1)+1]$. Hence, $\phi_{\rm FU} = E(N) - E(N+1)$ and $\phi_{\rm FI} = E(N-1) - E(N)$, respectively. Using Eq. (2.16) and the coefficients quoted in Table I, we will have

$$\phi_{\rm FU}[K] = 2.49 - 5.66N^{-1/3} - 1.77N^{-2/3} + 0.94N^{-4/3} ,$$
$$\phi_{\rm FI}[K] = 2.49 - 5.66N^{-1/3} - 1.77N^{-2/3} - 0.95N^{-4/3} . \tag{3.1}$$

In Fig. 3 these values, together with the QM results of Ref. 15, are plotted. Unfortunately, these potentials have not been computed in Ref. 4. In Fig. 3 we observe that the agreement for $\phi_{\rm FI}$ is better than that for $\phi_{\rm FU}$. As N gets higher values, the difference between $\phi_{\rm FU}$ and $\phi_{\rm FI}$, in our analysis, comes down quickly; in Ref. 15 this occurs more slowly. When $N \rightarrow \infty$, $\phi_{\rm FU}$ and $\phi_{\rm FI}$ tend to the same asymptotic value.

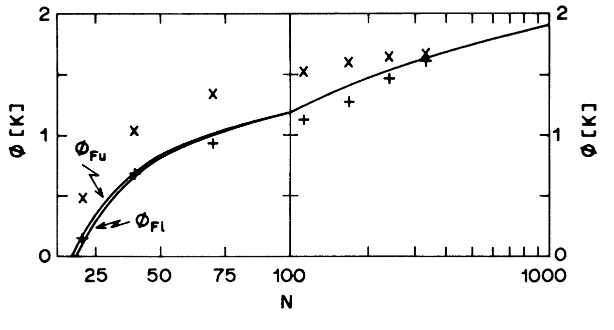

FIG. 3. Fusion and fission potentials. (×) for fusion and (+) for fission represent the QM values of Ref. 15.

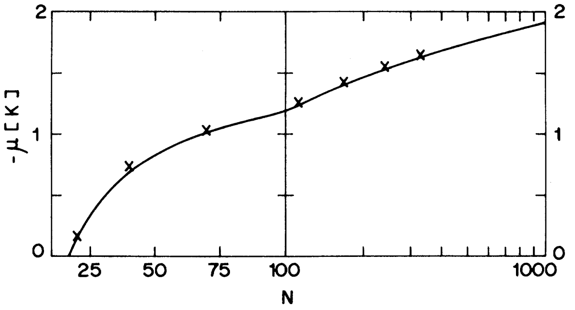

FIG. 4. Chemical potential. Crosses represent EL values of Ref. 15.

Another interesting observable is the chemical potential, which is defined at zero temperature as $dE(N)/dN$. In our analysis, we find

$$\mu[K] = -2.49 + 5.66N^{-1/3} + 1.77N^{-2/3} + 0.3\times10^{-3}N^{-4/3} , \tag{3.2}$$

and it is obvious that $\mu = (\phi_{\rm FU} + \phi_{\rm FI})/2$. Due to the smallness of the coefficient of the $N^{-4/3}$ term in Eq. (3.2), this term in the sum can be neglected.

In Fig. 4, μ is plotted vs N and compared with the results obtained in Ref. 15 by numerical integration of the EL equation (these results are denoted by crosses); the agreement is excellent. Observing Figs. 2 and 4 we note that, for small N, μ may be negative in spite of having E/N positive; this corresponds to metastable states. The minimum number of atoms to form a metastable cluster, in our analysis, is $N_m^{\rm met} \approx 17$; Strinari and Treiner predict ≈ 16, while Pandharipande, Pieper, and Wiringa, although they have not explicitly calculated it, estimate $N_m^{\rm met} \approx 20$. Thus, the agreement is notable.

Two other interesting physical magnitudes are the surface thickness, $t(N)$, and the unitary radius $\hat{r}_0(N)$. $t(N)$ is defined as the distance between the points where the density has 0.9 and 0.1 its central density,

$$t(N) = r_{10}(N) - r_{90}(N) . \tag{3.3}$$

$\hat{r}_0(N)$ is defined as

$$\hat{r}_0(N) = [\tfrac{5}{3}\langle r^2(N)\rangle]^{1/2} N^{-1/3} , \tag{3.4}$$

with $\langle r^2(N)\rangle = (1/N)\int n(r) r^2 d\mathbf{r}$ being the mean quadratic radius. Using the trial function (2.8), it is easy to prove that

$$t = 2s_m \ln(5) + O(1/R^2) , \tag{3.5}$$

and

$$t(N)[\text{Å}] = 7.78 - 3.21N^{-1/3} + O(1/R^2) . \tag{3.6}$$

In Table II, we give the values obtained by means of Eq. (3.6) and compare them with those given by the repeatedly mentioned authors. The agreement is fairly good, however the discrepancy, for small and intermediate N, with the results of Ref. 15 are more sensitive. Asymptotically, Stringari and Treiner find $t(\infty) = 8.3$ Å, and Pandharipande, Pieper, and Wiringa suggest a number close to 8 Å; our result is 7.8 Å.

Inserting Eq. (2.8) into (3.4), we obtain

TABLE II. Surface thickness (in Å), $t(N)$, for ^{3}He clusters.

N	Present work	Reference 4	Reference 15
20	6.6		8.6[b]
40	6.8		8.8[b]
70	7.0		8.8[b]
112	7.1		9.5[b]
168	7.2	~8[a]	9.6[b]
240	7.3	~8[a]	9.5[b]
330	7.3		9.4[b]
∞	7.8		8.3[b]

[a] VMC values.
[b] QM values.

$$\hat{r}_0(N)=r_m\left[1+10\frac{s_m^2}{r_m^2}N^{-2/3}\right]^{1/2}, \tag{3.7}$$

where again the values of r and s at the minimum are used.

The result given by Eq. (3.7) is exact.[33] Considering now Eqs. (2.12) we obtain

$$\hat{r}_0(N)[\text{Å}]=2.44-0.23N^{-1/3}+12.66N^{-2/3}+O(1/R^2)\ . \tag{3.8}$$

In Table III, the values coming from Eq. (3.8) are given together with the VMC values of Ref. 4 and the QM values of Ref. 15. Our results coincide pretty well with those of Ref. 4 and are slightly higher than those of Ref. 15; this discrepancy quickly disappears as N grows.

It is interesting to study the behavior of the density at the origin (center of the droplet) as N grows. The habitual strategy is by analyzing the relative compression $\delta n/n_0$, which is defined as

$$\frac{\delta n}{n_0}=\frac{n_c}{n_0}-1\ , \tag{3.9}$$

which, bearing in mind Eq. (2.8), can be expressed as

$$\frac{\delta n}{n_0}=\left[\frac{r_0}{r_m}\right]^3-1-\left[\frac{r_0}{r_m}\right]^3\left[\frac{r_m}{s_m}N^{1/3}+1\right]e^{-(r_m/s_m)N^{1/3}}\ . \tag{3.10}$$

TABLE III. Unit radii (in Å), $\hat{r}_0(N)$, for ^{3}He clusters.

N	Present work	Reference 4	Reference 15
20	4.1		4.0[b]
40	3.5	3.3[a]	3.1[b]
70	3.1	3.0[a]	2.9[b]
112	2.9	2.9[a]	2.8[b]
168	2.8	2.8[a]	2.7[b]
240	2.7	2.7[a]	2.6[b]
330	2.7		2.6[b]
∞	2.4		2.4[b]

[a] VMC values.
[b] QM values.

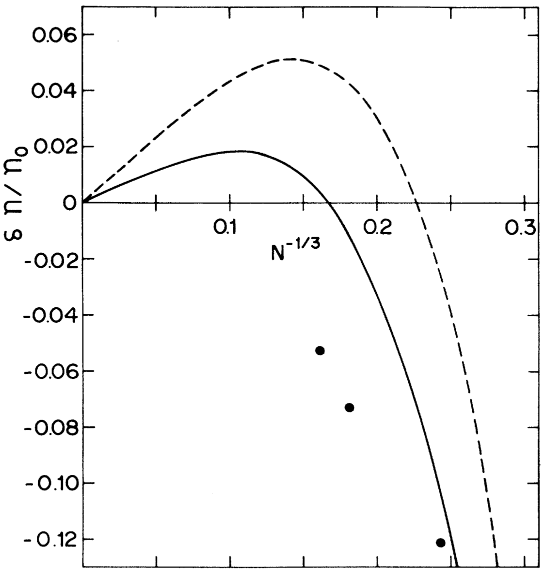

FIG. 5. Relative compression, $\delta n/n_0$, as a function of $N^{-1/3}$ for ^{3}He clusters. The dashed line corresponds to the properties of the EL equation of Ref. 15. The (●) corresponds to the VMC calculations of Ref. 4.

We have found

$$\frac{\delta n}{n_0}=0.278N^{-1/3}-0.811N^{-2/3}-0.348N^{-1}-7.85N^{-4/3}-(1.01N^{1/3}+1.60-2.60N^{-1/3})\times e^{-1.01N^{1/3}+0.323-1.87N^{-1/3}}\ . \tag{3.11}$$

In Fig. 5, Eq. (3.11) is plotted together with the result found in Ref. 15 and others which are deduced from the microscopic calculation of Ref. 4. As the reader can see, our results are intermediate between these two.

Finally, in Fig. 6 we have plotted the density profile of the cluster with $N=186$ and its comparison with the results of the other authors. It can be observed there in the zone where most of the atoms are lodged how our results are intermediate between those of these authors, while in

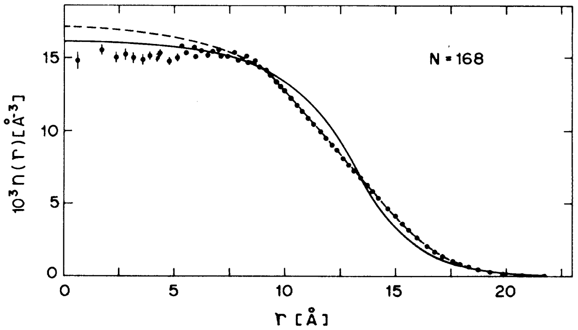

FIG. 6. Density profile of a ^{3}He cluster with $N=168$ atoms. The dashed line represents the QM calculations of Ref. 15 whereas (●) corresponds to the microscopic calculation of Ref. 4.

the periphery of the cluster our results are more acute. This last observation can be traced to the fact that we have obtained a skin depth somewhat smaller.

IV. CONCLUSION

We have obtained an analytical expression for the total energy of ^{3}He clusters, from an explicit density ansatz and a phenomenological density functional for the energy; the ETF method is used to obtain the kinetic-energy density. The trial function for the density depends on two parameters which are fixed by imposing the condition that the energy cluster must be a minimum; the other parameters of the model have been fixed by adjusting the bulk and semi-infinite media and take into account higher-order inhomogeneity corrections (Kirzhnits terms). The leptodermic development has allowed the computation of the energy as a series in decreasing powers of $R(N^{1/3})$. Specifically, the volume, surface, curvature, constant, $1/R$ and $1/R^2$ terms have been computed. We have also presented analytic expressions for the fusion and fission potentials, chemical potential, surface thickness, unitary radii and the relative compression. Our resulting mass formula is in good agreement with the prediction obtained by other not so economical theoretical methods.

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