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ON THE POSSIBILITY OF ABNORMAL OCCUPATION IN ^{3}HE AND ^{4}HE

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ABSTRACT

The possibility of abnormal occupation in the plane-wave Hartree-Fock ground state of helium systems is studied with reference to several semiphenomenological intermolecular potentials. Also studied is a particular type of non-plane-wave Slater determinant and found to have lower energy than the plane-wave determinant but only at very high densities.

RESUMEN

Se aborda la posibilidad de tenerse en el determinante de Slater de Hartree-Fock con ondas planas una ocupación anormal para la descripción del estado fundamental de fluidos del helio utilizando varios potenciales intermoleculares. También se considera el uso de determinantes con orbitales que no son ondas planas, sino que se localizan espacialmente, y éstos resultan tener menor energía pero sólo a densidades muy elevadas.

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I. INTRODUCTION

The possibility of taking plane-wave orbitals in a Hartree-Fock determinant to fill momentum space differently from the normal Fermi sphere arrangement has recently been investigated(1) for several two-body potentials, with the result that such an "abnormal" occupation may yield, in some circumstances, energies lower than the corresponding "normal" ones.

Some criteria have been established in Ref.1 which allow one to decide, on the basis of properties of the Fourier transform of the relevant two-body interaction, when such abnormal occupation may prevail energy-wise.

Non-plane-wave Slater determinants (or permanents) have also been studied recently(2), and found to be superior, energy-wise, to the plane-wave ones in some special fermionic and bosonic cases. These consist of spatially localized single particle orbitals constructed in such a way that the repulsive cores of the particles are avoided, thus lowering the energy expectation value of the determinant with respect to that of plane waves where the particles overlap excessively with each other.

It is clear then that, within the single-determinantal approximation, several instances have been encountered of both Fermi and Bose many-body systems for which a spatially non-homogeneous ground state leads to a tighter bound ground state than the homogeneous, plane-wave one.

The purpose of the present note is to study, in the spirit of Refs.1 and 2, ^{3}He and ^{4}He systems employing several semiphenomenological potentials in common use, with a view to establish whether: a) abnormal occupation is favored within the variational class of plane wave determinants; b) a non-plane-wave single determinantal ground state built up with Wannier-like functions(2) may be found below, energy-wise, the normal plane-wave one. Clearly this study is very preliminary to the general objective, namely, to know the best (i.e., lowest energy) single determinantal state for a given many body system, which is tantamount to having the unique Hartree-Fock state for that system.

II. FOURIER TRANSFORMS

Consider N fermions (bosons) which interact pair-wise with a central potential $v(r)$ with $r \equiv |\vec{r}_1 - \vec{r}_2|$ whose Fourier transform is

$$\tilde{v}(q) \equiv \int d^3r \;\; e^{-i\vec{q}.\vec{r}} \, v(r). \tag{1}$$

Studying the properties of this Fourier transform the following theorem can be proved(1) concerning Fermi systems: If $\tilde{v}(q)$ is monotonically decreasing, and hence non-negative since there is no abnormal plane-wave occupation. A similar theorem that applies in the Bose case reads(1): If $\tilde{v}(q) \geqslant 0$, $\forall q$ then there is no abnormal occupation.

In order to study the possibility of abnormal plane-wave occupation in He systems, one must apply these theorems on the basis of a given potential $v(r)$. Consequently, we analyze the Fourier transforms of the five different semiphenomenological He-He potentials considered in Ref.3 They are:

(i) the Frost-Musulin potential(4), MFM,

$$v(r) = -\varepsilon \,[\, 1 + c(1-r_m/r) \,]\; \exp[\; c(1-r/r_m) \;] \;\; ; \tag{2}$$

(ii) the Frost-Musulin potential of Bruch and McGee(5), FDD-1, whose short-range ($r \leqslant r_s$) part is given by expression (2) and whose long-range one is

$$v_{\ell r}(r) = -(c_6 r^{-6} + c_8 r^{-8}) \;\text{ for } r \geqslant r_s \quad ; \tag{3}$$

(iii) the Morse potential of Bruch and McGee(5), MDD-2, which has a short-range part

$$v_{sr}(r) = -\varepsilon \left\{ \; 2 \exp\,[\, c(1-r/r_m)] - \exp\,[\, 2c(1-r/r_m)] \; \right\} \text{for } r \leqslant r_s, \tag{4}$$

and a long-range part given by expression (3);

(iv) the Sposito potential(6), S, which has the same analytic form as the MDD-2;

(v) the Beck potential(7), B,

$$v(r) = A \exp(-\alpha r - \beta r^6) - B(r^2 + a^2)^{-3} \,[\, 1 + \frac{b+3a^2}{r^2+a^2} \,] \;. \tag{5}$$

The values of the different parameters are listed in Table II of Ref. 3.

Due to spherical symmetry the Fourier transform (1) reduces to

$$\tilde{v}(q) = \frac{4\pi}{q}\int_0^\infty dr\ r\ \sin qr\ v(r) \quad . \tag{6}$$

The calculation of $\tilde{v}(q)$ for the MFM potential is straightforward and one obtains a simple analytic form,

$$\tilde{v}_{MFM}(q) = \frac{4\pi\varepsilon c e^c}{q^2+c^2/r_m^2}\left[\ r_m - \frac{2(1+c)}{r_m(q^2+c^2/r_m^2)}\ \right] \quad . \tag{7}$$

In the case of the FDD-1, MDD-2 and S potentials, since we deal with different analytic expressions for $v(r)$ depending on whether r is smaller or larger than r_s, the Fourier transform is split into two terms:

$$\tilde{v}(q) \equiv \tilde{v}_{sr}(q) + \tilde{v}_{\ell r}(q) \quad , \tag{8}$$

which arise, respectively, from the short-, $v_{sr}(r)$, and long-range, $v_{\ell r}(r)$, parts of the potential. The calculation of $\tilde{v}_{sr}(q)$ causes no problem. On the other hand, care must be taken when one evaluates $\tilde{v}_{\ell r}(q)$ since the corresponding formula contains the sine integral $si(qr_s)$, which can be written as

$$si(qr_s) = -f(qr_s)\cos qr_s - g(qr_s)\ \sin qr_s \tag{9}$$

(cf. for example Ref.8). As expression (9) is multiplied by a polynomial in q for obtaining $\tilde{v}_{\ell r}(q)$, the main source of error that arises if the functions $f(qr_s)$ and $g(qr_s)$ are not carefully calculated is a divergence for large q.

Finally, for the Beck potential, B, it is necessary to integrate numerically the first term of expression (5) and for this the Gaussian quadrature was used.

The results for the Fourier transforms are shown in Fig.1 The values obtained for the MDD-2 potential agree with previous ones(9).

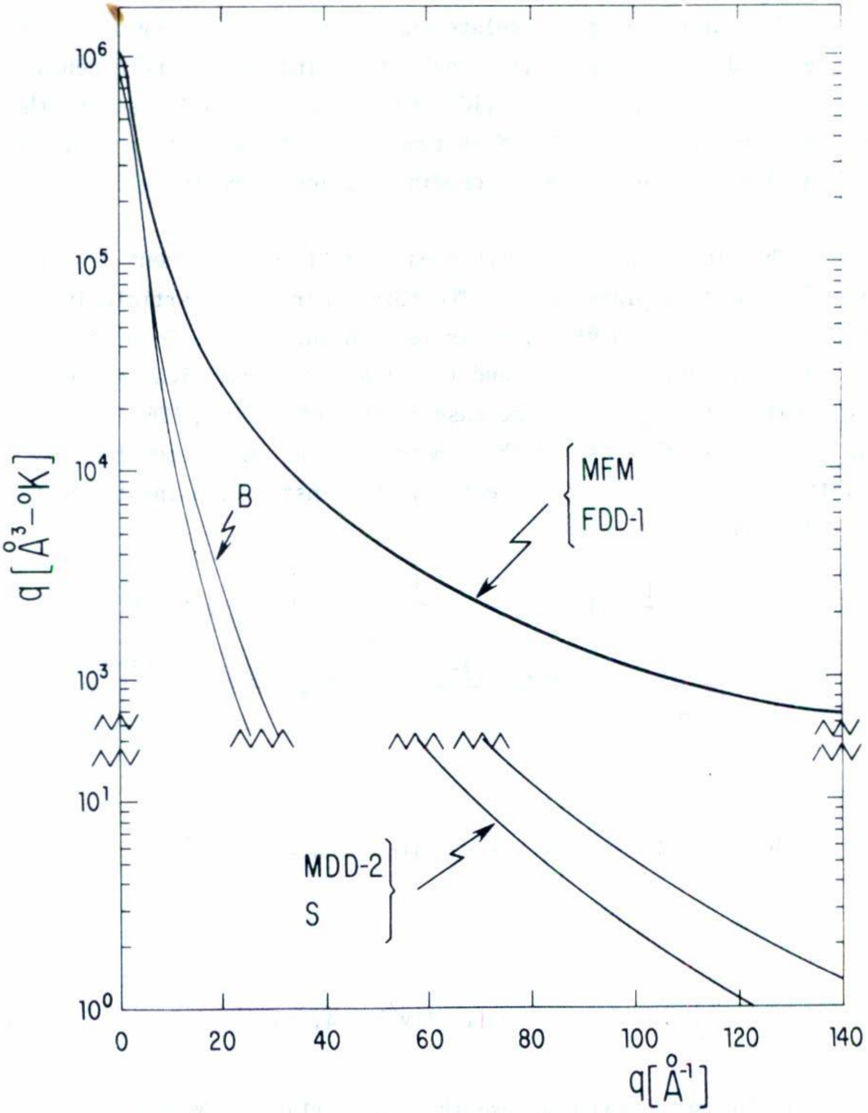

Fig. 1 Fourier transforms of various He-He potentials as a function of momentum.

III. ZERO ORDER GROUND STATE ENERGY

Our purpose is to calculate the ground state energy of ^{3}He and ^{4}He in zero order$^{(10)}$, i.e., with single-determinantal (or permanental) states, both in a "fluid" and "solid" phase. So, we shall evaluate the total energy per particle $\varepsilon \equiv E/N$ as function of the density ρ utilizing the potentials analyzed in the preceeding section. The formalism is that of Ref.2.

The fluid phase is represented by a Slater permanent or determinant of normalized plane-waves. The total energy per particle in the Bose case is $\varepsilon_{fl}(B) = \frac{1}{2}\rho\,\tilde{v}(o)$, as is well-known. In the Fermi case $\varepsilon_{fl}(F)$ can be evaluated using Eqs. (4) and (5) of Ref.2. Analytical expressions can be obtained for $\varepsilon_{fl}(F)$ in the case of the MFM, FDD-1, MDD-2 and S potentials, while in the case of the B potential one must recur to numerical calculations as in the previous section. For instance, using the MFM potential one arrives at

$$\begin{aligned}\varepsilon_{fl}(F) = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2\rho)^{2/3} + \varepsilon e^c \Bigg\{ & \frac{4\pi r_m^3\rho}{c^3}\,[c^2 - 2(1+c)] \\ & - \frac{c^3}{24\pi^3 r_m^3\rho}\left[(1+c)h\left(\frac{2r_m(3\pi^2\rho)^{1/3}}{c}\right) + \frac{c^2}{4}g\left(\frac{2r_m(3\pi^2\rho)^{1/3}}{c}\right)\right]\Bigg\} \quad , \end{aligned} \tag{10}$$

where

$$h(y) \equiv -1 + \frac{1-y^4}{1+y^2} + (1+\tfrac{3}{2}y^2)\ln(1+y^2) - y^3\tan^{-1}y \quad , \tag{11}$$

and

$$g(y) \equiv \tfrac{3}{2}y^4 - y^2 + (1+3y^2)\ln(1+y^2) - 4y^3\tan^{-1}y \quad . \tag{12}$$

In the solid phase we use the non-overlapping Wannier-like functions of Ref. 2 and obtain

$$\varepsilon_{sol} = \frac{2\pi^2\hbar^2}{m\,[\,(K/\rho)^{1/3} - a\,]^2} + \frac{1}{2}\sum_{\vec{R}} < \vec{R}\,\vec{R}'|v(r)|\,\vec{R}\,\vec{R}' > \quad , \tag{13}$$

where K is a constant which depends on the structure of the solid lattice, a is a variational parameter and $\vec{R}$ represents the lattice sites. The second term of ε_{sol} can be evaluated applying the method outlined by Bernardes$^{(11)}$, as was done in Ref. 12. As an example we give the result obtained for the simple MFM potential

$$\varepsilon_{sol} = \frac{2\pi^2\hbar^2}{m\,[\,(K/\rho)^{1/3}-a\,]^2} - \frac{\varepsilon}{2}\sum_{n=1}^{\infty} C_n[\,c(1-r_m/f_n) + F_n(\rho)\,] \cdot\exp\,[\,c(1-f_n/r_m)\,] \quad . \tag{14}$$

with

$$F_n(\rho) = 1 + \sum_{\substack{k,k'=0 \\ (k+k'\neq 0)}}^{\infty} A_k\, A_{k'} \left\{ \frac{c}{2r_m}\,[\,(K/\rho)^{1/3}-a\,] \right\}^{2(k+k')} \cdot[\,-2(k+k')(1+c)\,\frac{r_m}{c} - cr_m + (1+c)f_n\,] \quad , \tag{15}$$

where C_n is the number of n-th nearest neighbors, $f_n \equiv S_n/S_1$, whit S_n being the distance between n-th nearest neighbors, and the A_k are defined in Eq. (45) of Ref. 12. For the other potentials the expressions for ε_{sol} are more complicated. Moreover, to determine the solid phase energy per particle, ε_{sol} must be minimized with respect to the variational parameter a.

We calculate $\varepsilon_{fl}(B)$, $\varepsilon_{fl}(F)$, and ε_{sol} in the range of densities $0.01\ \text{Å}^{-3} \leqslant \rho \leqslant 1\ \text{Å}^{-3}$ utilizing the five previously mentioned potentials. Three different solid structures are taken: sc(K=1) , fcc($K=\sqrt{2}$) and bcc($K=3\sqrt{3}/4$) . The results are weakly dependent on the particular potential for both fluid and solid phases. This behavior can be easily understood in the fluid case. For bosons ε_{fl} is fixed by the value of the Fourier transform at the origin and, as can be seen in Fig. 1, $\tilde{v}(o)$ is very similar for all potentials. In the case of fermions taking into account Eqs. (4) and (5) of Ref. 2 and looking at Fig. 1, one can realize that $\varepsilon_{fl}(F)$ is mainly determined by the values of the Fourier transforms at small q, and in that region the $\tilde{v}(q)$ are still very close to one another. On the other hand, it is interesting to note that the minimum ε_{sol} is attained for $a/(K/\rho)^{1/3} \simeq 0.8$ to 0.9 independently of the potential used and the crystal structure considered.

Since the results for all the potentials are equivalent in the spirit of our search, it is enough to report those obtained with any one of them. Thus, we plot in Fig.2 the results for the B potential, because it is currently considered as one of the most popular ones.

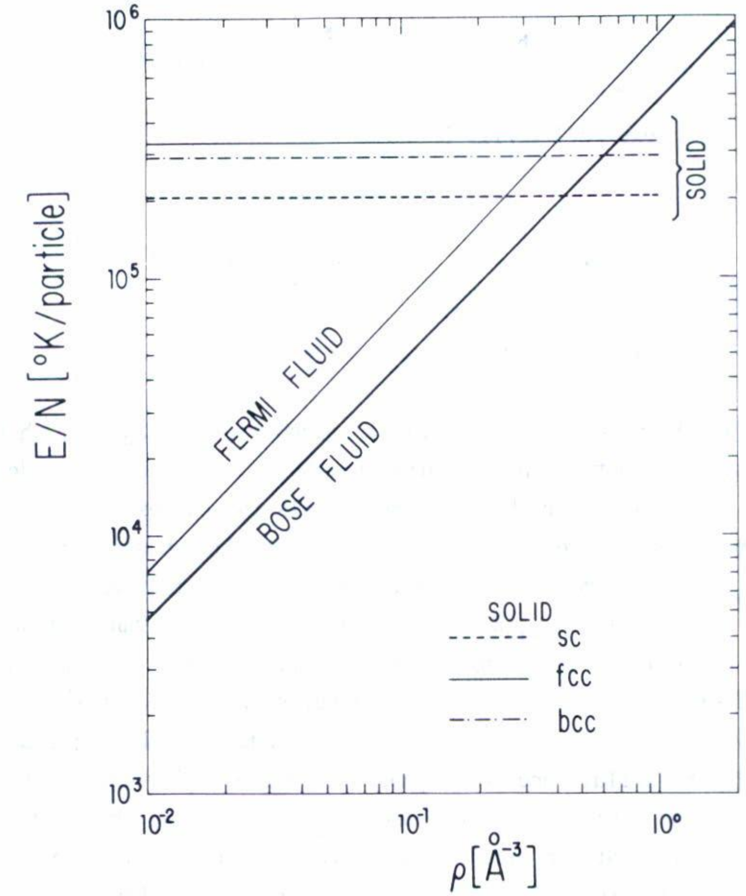

Fig.2 "Fluid" and "solid" energies per particle as a function of density calculated using the B (Beck) potential. Both Bose and Fermi fluid curves are shown.

IV. DISCUSSION AND CONCLUSIONS

The simple analytic expression obtained for the Fourier transform of the MFM potential is a monotonically decreasing function. In the case of the FDD-1, MDD-2 and S potentials, oscillating terms appear in the Fourier transforms due to the splitting of the potentials in two parts (short- and long-range). However, the oscillations are not strong enough to change the monotonic behavior, as can be seen in Fig.1.

In short, all five Fourier transforms calculated in this work are positive definite and monotonically decreasing. Consequently, no abnormal occupation is possible, either in the Fermi or in the Bose case, according to the theorems mentioned in section II.

The possibility has also been investigated of finding, in the spirit of Ref.2 a Slater determinant built up with Wannier-like single-particle wave functions which yields a lower energy than the corresponding plane-wave one.

Fig.2 shows that in the physical range of densities(10) 0.015 Å^{-3} $\leqslant \rho \leqslant 0.025$ Å^{-3} both bosonic and fermionic ε_{f1} lie below the ε_{sol} evaluated with any structure. Only at high densities $\rho \gtrsim 0.25$ Å^{-3} does one obtain lower energy per particle in the solid phase than in the fluid one, i.e., both for ^{3}He and ^{4}He a crystalline structure is preferred (in zero order) for densities beyond the physical range.

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