Optimal plane-wave Hartree-Fock states for many-fermion systems

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The possibility of taking plane-wave orbitals of a Hartree-Fock determinant to fill k space differently from the "normal" Fermi sphere is investigated for several two-body potentials including the "homework" v_0, v_1, and v_2—taken from the Reid nucleon-nucleon force—as well as a sum-of-Gaussians potential chosen to fit the deuteron binding and size. A random-search and random-walk numerical algorithm shows that, provided the potential strengths are made large enough, a *single-shell* "abnormal" occupation is always found to be lower in energy than the normal one if sufficient attraction is present in the two-body interaction. No abnormal occupation is possible for, among other pair interactions, the electron or charged-boson fluid, the repulsive square barrier, and a common form of the He-He interaction.

[NUCLEAR STRUCTURE plane-wave Hartree-Fock; nuclear matter.]

I. INTRODUCTION

Recent microscropic treatments of ground state energies of many-body systems have been based on either (a) diagrammatic perturbation theory,[1] (b) variational schemes,[2] and (c) the "coupled-cluster" or exp$S$ method.[3] All begin from an "unperturbed vacuum state" consisting of plane-wave single-particle orbitals, satisfying periodic boundary conditions, but *normally occupied* in the determinant (fermions) or permanent (bosons), i.e., all $k=0$ states occupied by the N particles for the boson case or all k states filling the Fermi sphere for the fermion problem.

Such "normal" occupation, however, has strictly speaking been used only out of convenience since it clearly minimizes the energy for the *noninteracting* problem but not necessarily for the fully interacting, physical case. The question naturally arises of the possibility of "abnormally occupied" plane-wave determinants or permanents, and of their usefulness in correlation energy calculations using either of the three methods mentioned above.

The question has been investigated[4] before for fermions but only for one-dimensional spinless ones interacting with very schematic two-body potentials. Also, the boson case has been considered[5] in three dimensions with realistic (alpha-alpha) interactions. In both instances, however, a trial-and-error approach was employed in the choice of the occupation numbers.

Our purpose here will be to find the best possible occupation for several many-fermion systems interacting via simple though somewhat realistic potentials, all within the context of a plane-wave Hartree-Fock state, as a first step in the eventual simultaneous treatment of correlations *with* abnormal occupation by, e.g., Bijl-Dingle-Jastrow trial wave functions dealt with via a hypernetted-chain scheme[2]

II. FORMALISM OF PLANE-WAVE HARTREE-FOCK THEORY

Consider N fermions each with ν internal degrees of freedom in a box of volume V to which one applies periodic boundary conditions. They interact pairwise with a central potential $v(r)$, with $r\equiv|\vec{r}_1-\vec{r}_2|$, whose Fourier transform is

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

and presumed finite. The lowest kinetic energy expectation value between determinants of plane waves occupying the lowest allowable k states is then

$$\langle t\rangle=\frac{\hbar^2}{2m}\sum_{\vec{k}}k^2n_{\vec{k}}$$
$$=N\frac{3}{10}\frac{\hbar^2}{m}\left(\frac{6\pi^2}{\nu}\right)^{2/3}\rho^{2/3},\quad t\equiv-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 \tag{2}$$

where *normal occupation* and particle density are defined by

$$n_{\vec{k}}=\theta(k_F-k)\,, \tag{3a}$$

$$\rho=\frac{N}{V}=\frac{1}{V}\sum_{\vec{k}}n_{\vec{k}}=\frac{\nu k_F^{\,3}}{6\pi^2}\,. \tag{3b}$$

More general occupation $n_{\vec{k}}$ is given by

$$n_{\vec{k}}=0\text{ or }1,\quad\sum_{\vec{k}}n_{\vec{k}}=N\,, \tag{4}$$

and yields a total energy expectation value

$$E\equiv\langle t\rangle+N(V_D+V_E)$$
$$=\frac{\hbar^2}{2m}\sum_{\vec{k}}k^2n_{\vec{k}}+\tfrac{1}{2}N\rho\tilde{v}(0)-\sum_{\vec{k}_1,\vec{k}_2}n_{\vec{k}_1}n_{\vec{k}_2}\tilde{v}(|\vec{k}_1-\vec{k}_2|)\,. \tag{5}$$

For any $n_{\vec{k}}$ subject to (4) but different from (3a), i.e., *abnormal occupation*, the kinetic energy in (5) will of course be larger than (2), the direct energy V_D will not change, but the exchange energy V_E may conceivably be sufficiently lower than the normal V_E so as to render

$$E_{\text{ab}} < E_{\text{nor}} \tag{6}$$

for some density range.

In the Appendix it is made plausible that any abnormal occupation $n_{\vec{k}}$ should be spherically symmetric, i.e.,

$$n_{\vec{k}} = n(k). \tag{7}$$

Otherwise, it would be extremely awkward to perform a more refined calculation than the present one, *including correlations*, along any of the lines mentioned above.[1-3]

Then Eqs. (4) and (5) become, for sufficiently large box volume V,

$$C\int dk\, k^2 n(k) = \rho\,, \tag{8}$$

$$E/N = C_t \int dk\, k^4 n(k) + \tfrac{1}{2}\rho\tilde{v}(0) + C_V \int_0^\infty dr\, r^2 v(r)\left[\int dk\, k^2 j_0(kr) n(k)\right]^2, \tag{9}$$

$$C \equiv \nu/2\pi^2; \quad C_t \equiv \frac{\nu}{2\pi^2}\frac{\hbar^2}{2m\rho},$$

$$C_V \equiv -\nu/2\pi^3\rho, \quad j_0(x) \equiv \frac{\sin x}{x}. \tag{10}$$

The last term in (9) is just V_E and can alternatively be written

$$V_E = C_V \int dk \int dq\, n(k)\mathfrak{M}_{kq} n(q) \equiv C_V \langle n|\mathfrak{M}|n\rangle\,, \tag{11}$$

$$\mathfrak{M}_{kq} \equiv k^2 q^2 \int_0^\infty dr\, r^2 v(r) j_0(kr) j_0(qr)\,.$$

Since V_E^{nor}, i.e., with $n_{\vec{k}}$ given by (3a), is generally negative, a necessary condition for (6) to occur is that

$$V_E^{\text{ab}} \text{ be sufficiently negative.} \tag{12}$$

III. GENERAL RESULTS

A. Functional minimization

Consider the possibility of using a function $0 \leq d(k) \leq 1$ defined as the *density* of 1's in $n(k)$ between k and $k+dk$ such that, for any smooth function $\phi(k)$,

$$\int dk\, d(k)\phi(k) = \int dk\, n(k)\phi(k)\,. \tag{13}$$

We then attempt a functional minimization of $E[d] - \lambda\rho[d]$, where λ is a Lagrange multiplier. Letting

$$d(k) \equiv \pi^{-1}\tan^{-1}u(k) + \tfrac{1}{2} \tag{14}$$

ensures that $0 \leq d(k) \leq 1$ and transforms the problem to

$$\frac{\delta}{\delta u}\hat{E}[u] \equiv \frac{\delta}{\delta u}(E[u] - \lambda\rho[u]) = \left(C_t k^4 - \lambda C k^2 + 2C_V \int dq\, \mathfrak{M}_{kq} d(q)\right) \times \frac{d\,d(k)}{d\,u(k)} = 0\,, \tag{15}$$

where from (14) the last factor gives

$$\frac{d\,d(k)}{d\,u(k)} = \frac{1}{\pi(1+u^2)} \equiv d'(k) \geq 0\,. \tag{16}$$

To achieve a true minimum one must require

$$\frac{\delta^2\hat{E}[u]}{\delta u^2} = \frac{\delta^2\hat{E}}{\delta d(k)\delta d(q)} d'(k)d'(q) + \frac{\delta\hat{E}}{\delta d(k)}\frac{\delta d'(k)}{\delta u(q)} > 0\,. \tag{17}$$

Since the last term vanishes at the minimum, (17) will be satisfied, in view of (16), if and only if

$$\frac{\delta^2\hat{E}}{\delta d(k)\delta d(q)} = 2C_V\mathfrak{M}_{kq} > 0\,, \tag{18}$$

which in turn implies from (11) that $V_E^{\text{ab}} > 0$, thus violating (12). Since from (11), (13), and (17)

$$V_E^{\text{ab}} = \frac{1}{2}\left\langle \frac{d}{d'}\middle|\frac{\delta^2\hat{E}[u]}{\delta u^2}\middle|\frac{d}{d'}\right\rangle, \tag{19}$$

the contradiction is avoided if

$$d'(k) = 0 \Rightarrow d(k) = 0 \text{ or } 1\,, \tag{20}$$

namely, *representation of $n(k)$ by a continuous function is impossible.* Since such a representation should work if $n(k)$ were not a "reasonable" function, we are led to believe that the optimal $n(k)$ is piecewise differentiable, i.e., equal to zero or one throughout finite-sized intervals. Therefore, other techniques will be required. We first make some general statements.

B. Some *a priori* results

(a) Since the plane-wave (PW) Hartree-Fock (HF) energy is a rigorous upper bound to the exact (Schrödinger) ground state energy we have the following:

Lemma. To avoid collapse, $\tilde{v}(0) > 0$.

Theorem. If $\tilde{v}(q)$ is montonically decreasing [and hence non-negative since $\tilde{v}(\infty) = 0$] there is *no* abnor-

mal occupation.

Proof. A necessary condition for Eq. (6) to be satisfied is

$$V_E^{\text{abn}} - V_E^{\text{nor}} = -\frac{\nu}{2\rho(2\pi)^6}\int d^3k_1 \int d^3k_2 \tilde{v}(|\vec{k}_1 - \vec{k}_2|)[n_{\vec{k}_1} n_{\vec{k}_2} - \theta(k_F - k_1)\theta(k_F - k_2)] < 0\,, \tag{21}$$

or the term in $n_{\vec{k}_1} n_{\vec{k}_2}$ is more positive than that in $\theta(k_F - k_1)\theta(k_F - k_2)$. This will *not* occur since abnormal occupation populates higher $\vec{k}_1$, $\vec{k}_2$ at the expense of depopulating lower $\vec{k}_1$, $\vec{k}_2$. The average argument of $\tilde{v}(|\vec{k}_1 - \vec{k}_2|)$ will therefore be larger and the average value of $\tilde{v}$ smaller for abnormal than for normal occupation. Q.E.D.

Corollary.

(i) There is *no abnormal occupation for the electron gas problem* where $\tilde{v}(q) = 4\pi e^2/q^2$ for $q > 0$ and $\tilde{v}(0) \equiv 0$.

(ii) There is no *abnormal occupation for a single repulsive Yukawa potential* [such as the Bethe homework potential v_0 (Ref. 6)] since $\tilde{v}(q) = |\text{const}|/(\mu^2 + q^2)$.

(iii) *There is no abnormal occupation for liquid* ^3He interacting via a Bruch-McGee molecular interaction since its Fourier transform $\tilde{v}(q) > 0, \forall q$, and decreases monotonically.[8]

Remark. The theorem applies to a general $n_{\vec{k}}$, not just $n(k)$.

(b) A digression on *bosons* allows us to assert for the PW-HF permanental state expectation value ($N \gg 1$)

$$E = \frac{\hbar^2}{2m}\sum_{\vec{k}} k^2 n_{\vec{k}} + \tfrac{1}{2}N\rho\tilde{v}(0) + \frac{1}{2V}\sum_{\vec{k}_1 \neq \vec{k}_2} n_{\vec{k}_1} n_{\vec{k}_2} \tilde{v}(|\vec{k}_1 - \vec{k}_2|)\,, \quad n_{\vec{k}} = 0, 1, 2, \ldots, N\,, \tag{22}$$

$$E_{\text{nor}} = \tfrac{1}{2}N\rho\tilde{v}(0)\,, \qquad n_{\vec{k}} = N\delta_{\vec{k}}, 0\,, \tag{23}$$

the following:

Theorem. If $\tilde{v}(q) \geq 0$, $\forall q$, then there is no abnormal occupation.

Proof. See Eqs. (22) and (23).

Corollary. There is no abnormal occupation for

(i) liquid ^{4}He with a Bruch-McGee potential,[7,8]

(ii) the charged boson gas,[9]

(iii) bosons interacting via the homework potentials v_0, v_1, and v_2.[6]

IV. MODEL POTENTIALS

Since (1) is assumed finite we must exclude all hard-cored potentials from PW-HF theory though, of course, *other*[10] HF orbitals will accommodate such potentials. We shall employ the Reid so-called v_0, v_1, and v_2 homework potentials given by (in MeV, r in fm)

$$v_0(r) = 9263.14\frac{e^{-4.9r}}{r}\,, \tag{24a}$$

$$v_1(r) = 9263.14\frac{e^{-4.9r}}{r} - 2358\frac{e^{-2.8r}}{r} - 14.95\frac{e^{-0.7r}}{r}\,, \tag{24b}$$

$$v_2(r) = 14\,177.6\frac{e^{-4.2r}}{r} - 4554\frac{e^{-2.8r}}{r} + 150.67\frac{e^{-1.4r}}{r} - 14.95\frac{e^{-0.7r}}{r}\,. \tag{24c}$$

In addition, we have constructed a semirealistic potential which is a sum of two Gaussians with parameters such as to (1) reproduce the deuteron

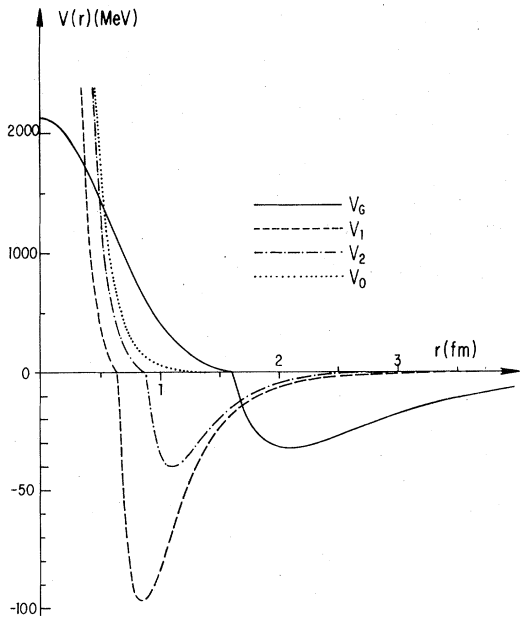

FIG. 1. The homework potentials v_0, v_1, v_2 and the sum-of-Gaussians potential v_G as given by Eq. (24). Note that the top and bottom vertical scales are different.

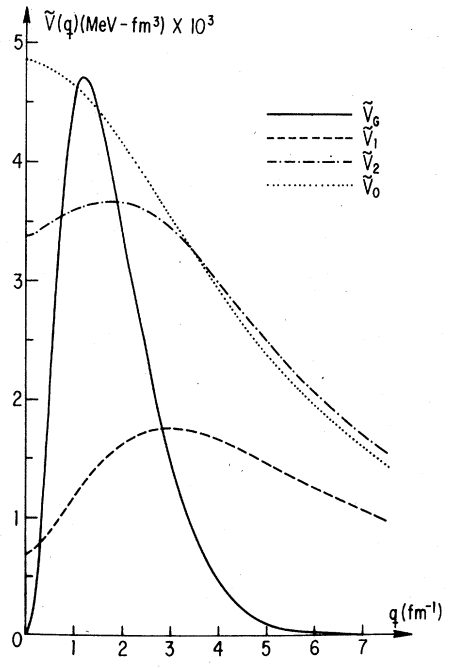

FIG. 2. Fourier transforms, Eq. (1), for the potentials of Fig. 1.

binding energy at −2.286 MeV, (2) not have any bound states with $l \geq 1$, (3) give the not unreasonably large deuteron radius of 5.119 fm, (4) make $v_c(0)$ as small as possible, and (5) make $\tilde{v}(q) > 0, \forall q$.

These last two properties enable us to employ the *rigorous lower bound*[11] on the exact (Schrödinger) ground state energy per particle given by

$$E_0^{\text{exact}}/N \geq \frac{3}{10}\frac{\hbar^2}{m}\left(\frac{6\pi^2}{\nu}\right)^{2/3}\rho^{2/3} + \tfrac{1}{2}\rho\tilde{v}(0) - \tfrac{1}{2}v(0). \qquad (25)$$

The potential, called v_G, is (in MeV, r in fm)

$$v_G(r) = 2200e^{-1.5r^2} - 66e^{-0.1449r^2} \qquad (24d)$$

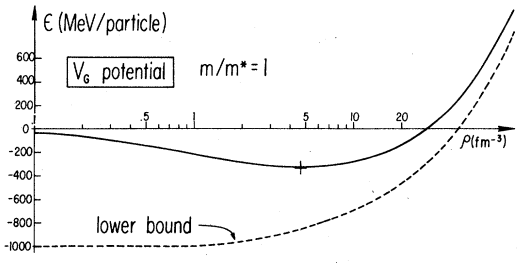

FIG. 3. Energy per particle as given by PW-HF theory with *normal* occupation (full curve) for the potential v_G of Eq. (24d) and the rigorous lower bound (dashed curve) of Eq. (25) to the exact (Schrödinger) ground state result.

and is one of the very few nucleon-nucleon potentials with the desirable feature of simultaneously *binding both the deuteron and nuclear matter* in PW-HF theory, which is *not* accomplished by any of the Reid homework potentials v_0, v_1, and v_2. The potentials (24) and (25) as well as their Fourier transforms are shown in Figs. 1 and 2. The normal PW-HF energy per particle as well as the lower bound (25) are shown for the v_G potential in Fig. 3.

V. NUMERICAL TECHNIQUES

A. Random search

In seeking the optimal $n(k)$ we must avoid being trapped in a *local* minimum of the PW-HF energy (9) and should attempt finding the *global* minimum.

Since we know that $n(k)$ will be constant throughout finite intervals (cf. Sec. III A), it is reasonable to divide k space into n shells each containing equal numbers of particles and select at random m shells out of the n shells such that the total number of particles in the m shells is always equal to N for any possible selection. Of course, the individual shells should be reasonably small so as to generate reliable distributions. Sampling a huge number of $n(k)$ configurations, although time consuming, provides a reasonable first approximation for the lowest energy configuration, subject to a more refined search as described below. In all cases *only a single minimum energy $n(k)$ configuration* was found.

B. Random walk

Having obtained, as described above, a first approximation to the $n(k)$ distribution giving the global PW-HF energy minimum, we proceed to improve upon it by recourse to a "random-walk" algorithm as follows. A specific shell out of the m occupied ones is emptied and one of the remaining n-m shells is populated. Should the resulting HF energy be lowered the new configuration is kept, otherwise it is discarded. The process is continued until no further lowering of the energy is possible. After performing the steps described in the last two subsections, one can be reasonably sure to have found the global minimum.

C. Single-shell minimization

After proceeding according to Secs. V A and V B for the model potentials described in Sec. IV, it was found that if any abnormal occupation resulted it was always of a single-shell structure, namely, one in which only those k states pertaining to a given interval (k_0, k_1) with $k_0 \geq 0$ were occupied, as found previously also in Ref. 4.

It then becomes possible to devise the following

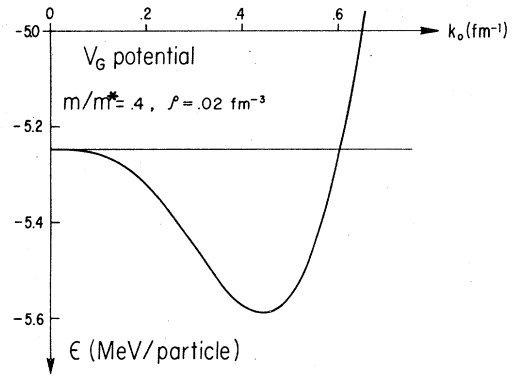

FIG. 4. Variation with binding energy per particle of the inner shell radius k_0 of the abnormal occupation given by the single-shell configuration of Eq. (26), for a given potential (the v_G), value of m/m^*, and particle density ρ.

simpler minimization procedure. For the single-shell configuration

$$n(k) = \theta(k - k_0)\theta(k_1 - k) \tag{26}$$

the PW-HF energy (9) becomes

$$\epsilon(k_0) \equiv E/N = \tfrac{1}{5}C_t(k_1^5 - k_0^5) + \tfrac{1}{2}\rho\tilde{v}(0) + C_V\int_{k_0}^{k_1} dk \int_{k_0}^{k_1} dq\, \mathfrak{M}_{kq} \tag{27}$$

where, by Eq. (8),

$$k_1 = \left(\frac{3P}{C} + k_0^3\right)^{1/3}. \tag{28}$$

It is then easy to solve

$$\frac{\partial \epsilon(k_0)}{\partial k_0} \equiv \epsilon'(k_0) = 0 \tag{29}$$

and verify if

$$\epsilon''(k_0) \geq 0. \tag{30}$$

As a by-product of this procedure one can prove the following: The normal distribution constitutes either a minimum or a saddle point of the energy as function of k_0, since here Eq. (29) gives

$$C_t k_0^2(k_1^2 - k_0^2) + 2C_V\left[\left(\frac{k_0}{k_1}\right)^2 \int_{k_0}^{k_1} dq\, \mathfrak{M}_{k_1 q} - \int_{k_0}^{k_1} dq\, \mathfrak{M}_{k_0 q}\right] = 0, \tag{31}$$

which is satisfied for $k_0 = 0$ since $\mathfrak{M}_{0q} = 0$. Q.E.D. Figure 4 shows $\epsilon(k_0)$ vs k_0 for the v_G potential and illustrates this fact.

VI. NUMERICAL RESULTS

Since the main objective of the present work is to emphasize the peculiarities and characteristic features of abnormal fermion occupation, we have used throughout effective masses m^* given in terms of the nucleon mass m. This, of course, is equivalent to fixing the mass and increasing the coupling strength of the potential. In this way we try to ascertain in which region, if any, of the ρ vs m/m^* plane there exists abnormal occupation. As mentioned in Sec. V, any abnormal occupation found to be energetically favorable was in the form of a single-shell $n(k) = \theta(k - k_0)\theta(k_1 - k)$. Figures 5–7 show below the dashed lines the zones of abnormal occupation for the interactions v_G, v_1, and v_2 respectively, in the ρ vs m/m^* plane.

On the other hand, there is no abnormal occupation for a repulsive square barrier *of arbitrary height*. This result is mentioned since *it* is *not* covered by any of the general assertions of Sec. III, since, for $v_0 > 0$,

$$v(r) = v_0\theta(c - r) \Rightarrow \tilde{v}(q) = 4\pi v_0 c^3 \frac{j_1(qc)}{qc}, \qquad j_1(x) \equiv x^{-2}\sin x - x^{-1}\cos x, \tag{32}$$

and clearly the Fourier transform oscillates. Furthermore, for the *boson* case the repulsive square barrier *does* originate abnormal occupation provided v_0 is sufficiently large.[5]

The results shown in Figs. 5–7 motivate the following.

Conjecture. Assume spherical symmetry, i.e., $n_{\vec{k}} = n(k)$. In the spirit of making general assertions,

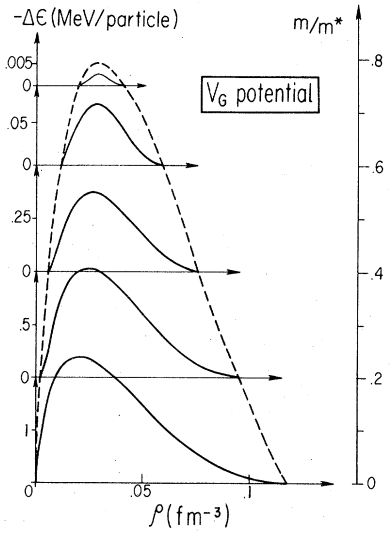

FIG. 5. Locus of points (dashed curve) in the m/m^*–ρ plane, along which the abnormally and normally occupied PW HF are equal for the v_G potential. Also shown (full curves), related to left vertical scale, is the energy gain of the abnormal to the normal case.

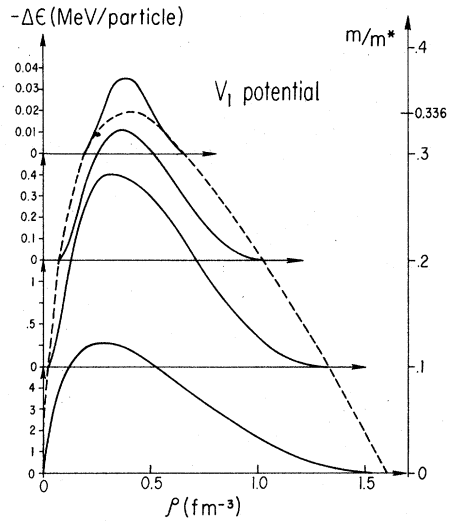

FIG. 6. Same as Fig. 5 but for the v_1 potential.

the next simple thing to consider after monotonic decreasing $\tilde{v}(q)$ is a $\tilde{v}(q)$ having a *single* maximum excluding the origin, and then there *may* be abnormal occupation. If so, we conjecture, it will be a single-shell one.

Reason. Such a $\tilde{v}(q)$ will, by Eqs. (11) as well as (1), produce an $\mathfrak{M}_{kq}$ with a single "ridge" perpendicular to the main diagonal in the kq plane. Hence $\langle n|\mathfrak{M}|n\rangle$ will be larger, i.e., V_E smaller since $C_V<0$, for n located at the ridge.

Also shown in Figs. 5–7 are the energy gains $\Delta\epsilon<0$ over the normal occupation for different values of m/m^* as function of the density ρ. For a given potential and effective mass (or interaction strength) there is a finite range of densities for which such energy gains are found. This range strongly depends on the potential involved and *shrinks to zero* as m/m^* grows beyond a certain critical value different for each potential. Along

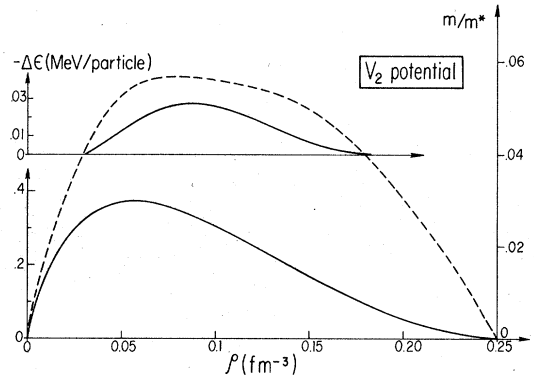

FIG. 7. Same as Fig. 5 but for the v_2 potential.

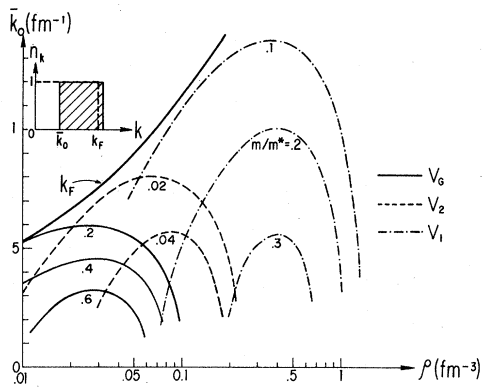

FIG. 8. Variation with particle density ρ of the inner shell radius $\bar{k}_0$ of the abnormal single-shell occupation Eq. (26) which minimizes the PW-HF energy Eq. (27) for the v_G, v_1, and v_2 pair potentials for different values of the particle mass m^* measured in units of the nucleon mass m. For reference the Fermi sphere radius $k_F = (3\pi^2\rho/2)^{1/3}$ is also graphed. Inset shows the single-shell abnormal occupation (shaded) relative to the normal one (dashed).

the dashed line $\Delta\epsilon$ is zero and decreases with m^*/m. At finite m^*/m the density region for abnormal occupation does not extend to zero density since at zero density there is only kinetic energy.

The position of the (abnormal occupation) Fermi single shell is illustrated in Fig. 8 where the inner shell-radius $\bar{k}_0$ minimizes $\epsilon(k_0)$ Eq. (27) for a given density, effective mass, and interaction. For comparison, the Fermi momentum $k_F = (3\pi^2\rho/$

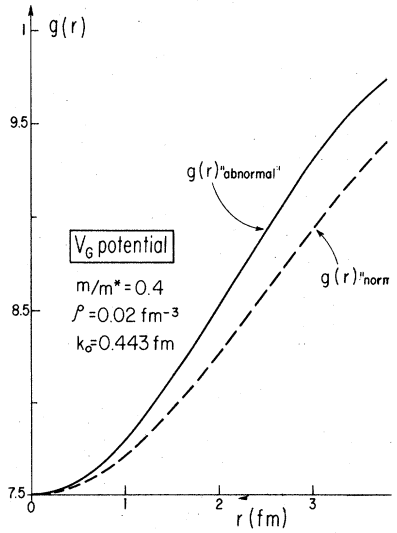

FIG. 9. The radial distribution function as defined in Eqs. (33) for normal and abnormal occupation with the v_G potential, for fixed values of m/m^*, ρ, and k_0.

$2)^{1/3}$ is also plotted. We also mention that for sufficiently large m^*/m one finds instances where $\bar{k}_0 > k_F$. Moreover, $\bar{k} \to 0$ at the boundary of the energy-gain zones of Figs. 5–7. One might ask by what physical mechanism abnormal occupation affects the energy gain. To clarify this we compare in Fig. 9 the radial distribution function $g(r)$, defined through

$$\langle v \rangle / N = \tfrac{1}{2}\rho \int d^3r\, g(r) v(r),$$
$$g(r) = 1 - \frac{1}{\nu} l^2(r), \tag{33}$$
$$l(r) \equiv \frac{\nu}{(2\pi)^3 \rho} \int d^3k\, n_{\vec{k}} e^{i\vec{k}\cdot\vec{r}},$$

for both abnormal and normal occupations. It is not possible to change the value of $g(0) = 1 - 1/\nu$ by any choice of occupation. Moreover, for small but finite interparticle distances r abnormal occupation will always *increase* the value of $g(r)$ and thus *suppress short-range correlations*. In spite of the increased $g(r)$ at very short distances, the *attractive* part of the potential (at larger values of r) is weighted by a substantially increased $g(r)$ resulting in a net energy lowering. Clearly, for this mechanism to work the potential must have long-ranged attraction. In order to avoid (N-particle) collapse there must then be a short-range repulsion. This combination will lead to a Fourier transform $\tilde{v}(q)$ behaving exactly like the one used in the above conjecture, i.e., having a single maximum at finite q.

VII. CONCLUSIONS

The conditions under which abnormal occupation exists for many-fermion systems have been given for the first time in three dimensions. For the model many-nucleon systems considered (with *any* number of species $\nu = 1, 2, 4, \ldots$), abnormal occupation was found to be energetically lower provided the mass of the particles is increased, i.e., if the interaction strength is made sufficiently large. In all cases examined the global minimum, within the space of PW determinants, corresponded to a single-shell occupation of states in k space. This was made plausible for any potential consisting of a short-ranged repulsion and a sufficiently strong long-ranged attraction.

It was shown that *no* abnormal occupation is possible at all for the electron fluid, the charged-boson fluid, a repulsive square barrier of any height and diameter, and for a purely repulsive Gaussian or Yukawa potential of any height and width. [Presumably, this argument applies also for any reasonably shaped purely repulsive potential, just on the basis of the $g(r)$ discussion of Sec. VI]. Also, there is no abnormal occupation for either ^{3}He or ^{4}He liquids, if the particles interact via a Morse interaction as modified by Bruch and McGee.

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APPENDIX: NONSPHERICAL DISTRIBUTIONS

We consider here the possibility of *nonspherical* $n_{\vec{k}} \neq n(k)$ giving lower energies than the spherical one assumed in this paper, Eq. (7). By itself this is neither reasonable as it would imply a preferred direction in the fluid, nor desirable since calculations would be appreciably complicated particularly if one wants to include correlations.

Consider the general distribution

$$n_k = \sqrt{4\pi} \sum_{lm} n_{lm}(k) Y_{lm}(\Omega) = 1 \text{ or } 0. \tag{A1}$$

After some straightforward algebra, Eqs. (11) become

$$V_E = -\frac{\nu}{2\pi^3\rho} \times \sum_{\lambda\mu} (-)^\mu \int dk_1 \int dk_2 n_{\lambda\mu}(k_1) n_{\lambda-\mu}(k_2) \mathfrak{M}^\lambda_{k_1 k_2}, \tag{A2}$$

$$\mathfrak{M}^\lambda_{k_1 k_2} \equiv \frac{k_1^2 k_2^2}{4\pi} \int_{-1}^{1} dz\, P_\lambda(z)\, \tilde{v}\left((k_1^2 + k_2^2 - 2k_1 k_2 z)^{1/2}\right). \tag{A3}$$

Now since

$$n_{lm}(k) = \frac{1}{\sqrt{4\pi}} \int d\Omega\, n_{\vec{k}} Y^*_{lm}(\Omega), \tag{A4}$$

we have either

$$n_{\vec{k}} = n(k, \Omega) = 1 \text{ or } 0 \text{ for all } \Omega, \text{ given } k, \tag{A5}$$
$$\Rightarrow n_{00}(k) = 1 \text{ or } 0, \text{ all other } n_{lm}(k) = 0$$

or

$$n_{\vec{k}} \neq \text{const, given } k \Rightarrow n_{00}(k) < 1, \text{ all other } n_{lm}(k) \neq 0. \tag{A6}$$

For $\lambda \neq 0$, the $P_\lambda(z)$ will change sign making the $\mathfrak{M}^\lambda$ *smaller* in magnitude with increasing λ. For the (smooth) potentials considered here, $\mathfrak{M}^\lambda$ gets smaller with λ very rapidly, as can easily be verified. Hence, it is most favorable to have $n_{00}(k)$ as large as possible in order in minimize (A2), which results in a spherical distribution.

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