Abnormal occupation in boson matter

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We delineate the conditions of interaction and density in extended Bose systems under which the single permanent of plane waves yielding the lowest energy expectation value deviates from the zero-momentum condensate. A potential $v(r)$ independent of relative orbital angular momentum L does not favor abnormal occupation at any density, provided its Fourier transform is non-negative. However, abnormal occupation can occur for simple reasonable choices of $v(r)$, in particular, a repulsive square barrier. Considering L-dependent interactions, truncation of the partial wave expansion of the potential will ordinarily promote abnormal occupation in some density region. Several specific examples of abnormal momentum distributions are studied, and numerical results are given for potentials relevant to alpha-particle matter and liquid ^{4}He.

[NUCLEAR STRUCTURE Infinite alpha matter, Hartree-Fock method, abnormal occupation of plane wave orbitals.]

I. INTRODUCTION

The normal starting point for the microscopic treatment of an infinitely extended quantum system consists of a "vacuum state" in which the particles fill the lowest-momentum orbitals consistent with their Bose or Fermi nature. Thereafter, correlations due to the interactions between the particles are introduced, either by perturbation theory[1] or by correlation-operator approaches (including variational[2–5] and coupled-cluster[6] methods). In the process, an interacting ground state is built containing admixtures of excited states of the noninteracting system in which the momentum distribution deviates substantially from the normal one. In the case of weakly interacting particles, the amplitudes of these admixtures will be small, and the normal "vacuum" provides an appropriate starting point. However, it is by no means clear from the outset that such is the case when the particles interact strongly, as in the following systems of great current interest: nuclear matter, neutron-star matter, finite nuclei, and the helium systems. It may well provide advantageous—either from the practical standpoint or as a reflection of some underlying physical structure—to start with a vacuum corresponding to abnormal occupation of the given single-particle states.

It is our aim in the present paper to reach, by example, a better understanding of the conditions under which an abnormal vacuum is preferred in extended systems of identical spinless bosons, interacting through short-range potentials having finite matrix elements in a plane-wave basis. Some preliminary results of this work have been reported in Ref. 7. In Sec. II we formulate the problem of the determination of the optimal permanent of plane-wave orbitals in an independent-particle description of such systems (determination of an "optimal vacuum"). Five simple forms of abnormal occupation are proposed for examination. Section III is concerned with two-body interactions

v_{ij}, which are independent of relative orbital angular momentum L. Abnormal occupation of any sort is excluded for a potential of this type if its Fourier transform is non-negative. However, abnormal occupation is shown to occur for some quite reasonable choices of v_{ij}, most notably the repulsive square barrier. In Sec. IV we consider L-dependent potentials, and note that truncation of the partial wave expansion of v_{ij} will ordinarily lead to abnormal occupation in some density regime. Numerical results are presented for certain interactions relevant to alpha-particle matter and liquid helium, based on the simple choices of abnormal momentum distribution specified in Sec. II. Section V addresses in general terms the significance—physical versus merely technical—of the theoretical phenomenon of abnormal occupation in strongly interacting quantum systems.

II. FORMULATION OF THE PROBLEM

We consider a nonrelativistic system of N identical bosons of mass m interacting pairwise via potentials v_{ij}. Thus the Hamiltonian of the system is written

$$H=t+v=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i{}^2+\sum_{i<j}^{N}v_{ij}\ , \tag{2.1}$$

where t and v are the total kinetic and potential energy operators, respectively. We seek to determine the *optimal* independent-particle wave function Φ in the subspace of symmetric functions, that is, the function $\Phi=\Phi_0$, which gives the expected energy

$$N\epsilon\equiv E\equiv\frac{\langle\Phi\,|\,H\,|\,\Phi\rangle}{\langle\Phi\,|\,\Phi\rangle}\equiv\langle H\rangle=\langle t\rangle+\langle v\rangle\ , \tag{2.2}$$

its absolute minimum value. Without loss of generality, the independent-particle wave functions over which the variation is performed may be taken as permanents of orthonormal single-particle wave functions ϕ_α,

$$\Phi=\mathrm{perm}[\phi_\alpha(\vec{r}_j)]_{n_\alpha}\ , \tag{2.3}$$

where n_α is the occupation number of orbital α. Two constraints delimit the set $\{n_\alpha\}$, namely, the n_α can assume only positive-integral (or zero) values

$$n_\alpha\equiv 0,1,2\ ,\dots,\ N\ , \tag{2.4}$$

and

$$\sum_\alpha n_\alpha=N\ . \tag{2.5}$$

The general Hartree-Bose problem so formulated may be decomposed, for conceptual purposes, into two parts: (i) the determination, for a given single-particle basis $\{\phi_\alpha\}$, of the optimal set $\{n_\alpha^0\}$ of occupation numbers and (ii) the determination of the optimal choice of single-particle basis, $\{\phi_\alpha^0\}$. We do not propose to solve the full problem here; rather, we shall examine only the first aspect of it, in nontrivial special cases of physical interest. Other facets of the general Hartree-Bose and Hartree-Fock problems are being addressed in a number of parallel investigations (see, e.g., Refs. 8–14). Here we restrict attention to the plane-wave choice of single-particle wave functions, $\phi_\alpha=\phi_{\vec{k}}=V^{-1/2}e^{i\vec{k}\cdot\vec{r}}$, these being normalized and satisfying periodic boundary conditions in a cube of volume V. At an appropriate stage in the subsequent analysis we shall pass to the thermodynamic limit, i.e., $N,V\rightarrow\infty$ with the density $\rho=N/V$ constant. It is to be noted that the chosen wave function Φ will then describe a uniform (liquid or gaseous) phase of an infinitely extended system.

The evaluation of (2.2) is now straightforward:

$$\langle t\rangle=\sum_{\vec{k}}(\hbar^2k^2/2m)n_{\vec{k}}\ , \tag{2.6}$$

while, for $N>>1$ (cf. Ref. 15),

$$\langle v\rangle=\frac{1}{2}\sum_{\vec{k}_1\vec{k}_2}(1-\tfrac{1}{2}\delta_{\vec{k}_1,\vec{k}_2})n_{\vec{k}_1}n_{\vec{k}_2}\langle\vec{k}_1\vec{k}_2\,|\,v_{12}\,|\,\vec{k}_1\vec{k}_2+\vec{k}_2\vec{k}_1\rangle\ , \tag{2.7}$$

where

$$\langle\vec{k}_1\vec{k}_2\,|\,v_{12}\,|\,\vec{k}_1'\vec{k}_2'\rangle=V^{-2}\int d^3r_1\int d^3r_2\,e^{-i\vec{k}_1\cdot\vec{r}_1}e^{-i\vec{k}_2\cdot\vec{r}_2}v_{12}e^{i\vec{k}_1'\cdot\vec{r}_1}e^{i\vec{k}_2'\cdot\vec{r}_2}\ . \tag{2.8}$$

By convention, *normal* occupation in a Hartree-Bose description of a many-boson system means that all the particles are put in the orbital with lowest single-particle energy. In our case this implies

$$n_{\vec{k}} = N\delta_{\vec{k},\vec{0}} , \tag{2.9}$$

i.e., all the bosons reside in a zero-momentum condensate. With (2.9) we have, trivially, in the case that $v_{12} = v(r_{12})$,

$$\langle t \rangle = 0, \quad \langle v \rangle = \tfrac{1}{2} N \rho \nu(0) , \tag{2.10}$$

where

$$\nu(q) \equiv \int d^3r\, e^{-i\vec{q}\cdot\vec{r}} v(r) . \tag{2.11}$$

We observe that $\nu(0)$ must be taken positive (or zero), otherwise collapse would ensue for sufficiently large ρ (which can be considered a variational parameter), even though the energy is extensive.

While the normal distribution (2.9) certainly minimizes the kinetic energy, there is no *a priori* reason why it should remain optimal when interactions are present. It is in fact the main purpose of this article to present and study a number of examples in which choices of the set $\{n_k\}$ different from (2.9)—corresponding to *abnormal* occupation— *lower* the energy per particle relative to the normal value. The following special choices of abnormal distribution will be considered. All contain a zero-momentum condensate with occupation number ξN, where $0 \le \xi \le 1$.

(i) Single wing (SW)

$$n_{\vec{k}} = N[\xi \delta_{\vec{k},\vec{0}} + (1-\xi)\delta_{\vec{k},\vec{k}_0}] , \tag{2.12}$$

(ii) Double wing (DW)

$$n_{\vec{k}} = N[\xi \delta_{\vec{k},\vec{0}} + \tfrac{1}{2}(1-\xi)\delta_{\vec{k},\vec{k}_0} + \tfrac{1}{2}(1-\xi)\delta_{\vec{k},-\vec{k}_0}] , \tag{2.13}$$

(iii) Spherical shell (SS)

$$n_{\vec{k}} = N\xi \delta_{\vec{k},\vec{0}} + \frac{2\pi^2 \rho(1-\xi)}{k_0{}^2} \frac{1}{2\sigma} [\theta(k_0+\sigma-k) - \theta(k_0-\sigma-k)], \quad k_0 > 0, \ \sigma \to 0^+ , \tag{2.14}$$

(iv) Bose sphere (BS)

$$n_{\vec{k}} = N\xi \delta_{\vec{k},\vec{0}} + \theta(k_B - k), \quad k_B > 0 , \tag{2.15}$$

(v) Gaussian (G)

$$n_{\vec{k}} = N\xi \delta_{\vec{k},\vec{0}} + \frac{8\pi^{3/2}(1-\xi)\rho}{k_0{}^3} e^{-k^2/k_0{}^2} , \quad k_0 > 0 . \tag{2.16}$$

These choices are depicted in schematic fashion in Fig. 1.

Several comments and caveats on the use of (i)–(v) are in order before we proceed. The total momentum of the many-body state associated with (i) is clearly nonzero, a defect which may be repaired by going to (ii). There remains in (ii) a preferred axis $\hat{k}_0$ (or $-\hat{k}_0$), however, for the interactions to be assumed, the energy expectation value in cases (i) and (ii) turns out to be independent of this axis. For choice (iii) the issue of a preferred orientation in momentum space is obviated.

Without closer inspection it would appear that each of (i)–(v) contains two parameters, ξ and k_0 or k_B, which may be varied independently to minimize $\langle H \rangle$. Recall, however, that all variation of $\{n_{\vec{k}}\}$ are subject to the two constraints (2.4)–(2.5) mentioned above, which become

$$n_{\vec{k}} \equiv 0,1,2 ,\ldots, N , \tag{2.17}$$

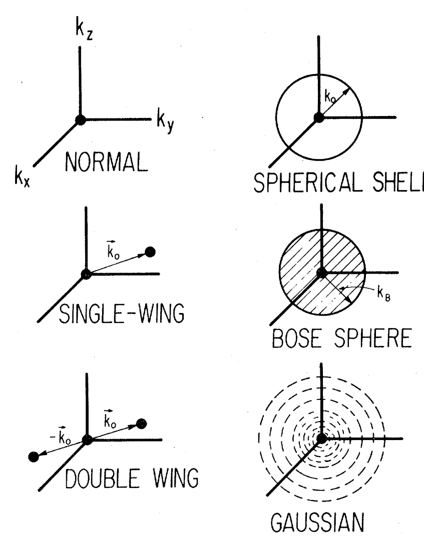

FIG. 1. Schematic representation of various abnormal occupations investigated in this paper, compared to the normal one.

$$\sum_{\vec{k}} n_{\vec{k}} = N \Longrightarrow \frac{1}{(2\pi)^3 \rho} \int d^3k \, n_{\vec{k}} = 1 \ . \tag{2.18}$$

We remark that (2.17) and (2.18) are satisfied by construction for all choices except (iv) [where (2.17) is satisfied but (2.18) must still be imposed explicitly] and (v) [where (2.18) holds but (2.17) cannot strictly be met]. The remedy is simple in the Bose sphere case: (2.18) implies k_B and ξ are related by

$$\rho = k_B{}^3/6\pi^2(1-\xi) \ , \tag{2.19}$$

so that there remains only one independent variational parameter. [If we desired a further integral parameter n could be introduced as a factor of $\theta(k_B - k)$, then $\rho = nk_B{}^3/6\pi^2(1-\xi)$. However, the optimal choice turns out to be $n=1$.] In the Gaussian case, nonintegral values of $n_{\vec{k}}$ are of course inevitable, so the use of this distribution is not rigorous. The seriousness of the violation of constraint (2.17) may, however, be alleviated by taking the amplitude $C = 8\pi^{3/2}(1-\xi)\rho/k_0{}^3$ of the Gaussian term to be large, $C >> 1$.

Use of spherical-shell distribution requires special care. The limit $\sigma \to 0^+$ leading to an infinitesimally thin shell must be taken *after* the energy (2.2) is evaluated via (2.6) and (2.7) for *finite* σ. [Taking the limit $\sigma \to 0^+$ *before* inserting $n_{\vec{k}}$ into (2.6) and (2.7) has unphysical consequences.] Of course, the true optimal $n_{\vec{k}}$ may in general be much more complicated than any of (i)–(iv).

Finally we note that a straightforward solution of the variational equations for E—obtainable by varying with respect to $n_{\vec{k}}$, Eqs. (2.6) and (2.7), subject to the conditions (2.17) and (2.18)—does not seem tractable as too many Lagrange multipliers would be involved.

III. L-INDEPENDENT POTENTIALS

In this section we derive some general and some specific conclusions with regard to the occurrence of abnormal occupation in the presence of certain simple radial potentials. If v_{12} is the same in all states of relative orbital angular momentum L, we have

$$\langle \vec{k}_1\vec{k}_2 \,|\, v_{12} \,|\, \vec{k}_1\vec{k}_2 + \vec{k}_2\vec{k}_1 \rangle = V^{-1}[\nu(0) + \nu(|\vec{k}_1 - \vec{k}_2|)] \ . \tag{3.1}$$

Accordingly, the potential energy expectation value (2.7) can be rewritten as

$$\langle v \rangle = \tfrac{1}{2} N\rho\nu(0) + \frac{1}{2V} \sum_{\vec{k}_1 \neq \vec{k}_2} n_{\vec{k}_1} n_{\vec{k}_2} \nu(|\vec{k}_1 - \vec{k}_2|) \ . \tag{3.2}$$

Suppose the Fourier transform $\nu(q)$ of the given potential is non-negative for all q (more precisely, except on a set of measure zero). It then follows that

$$\Delta\epsilon \equiv \epsilon_{\text{abnormal}} - \epsilon_{\text{normal}} > 0 \ , \tag{3.3}$$

for *any* abnormal $n_{\vec{k}}$, since the second term in (3.2) cannot become negative. One may thus conclude that for a number of familiar potentials abnormal occupation will *not* occur. These include (setting $\vec{r}_{12} = \vec{r}$)

(a) repulsive delta interaction

$$v_{12} = v_0 \delta(\vec{r}) \ , \quad (v_0 > 0) \ , \tag{3.4}$$

(b) repulsive Gaussian

$$v_{12} = v_0 e^{-\lambda^2 r^2} \ , \quad (v_0 > 0), \tag{3.5}$$

(c) Bruch-McGee interaction between ^{4}He atoms (Ref. 16)

$$\begin{aligned} v_{12} &= \epsilon_0 (B_0{}^2 e^{-2r/a_0} - 2B_0 e^{-r/a_0}), \\ &\quad r \le 3.6828 \text{ Å} \\ &= -\frac{C_6}{r^6} - \frac{C_8}{r^8} \ , \quad r > 3.6828 \text{ Å} \ , \end{aligned} \tag{3.6}$$

where $\epsilon_0 = 9.25$ K, $a_0 = 0.494\,13$ Å, $B_0 = 455.674$, $C_6 = 6842$ KÅ^6, and $C_8 = 26\,930$ KÅ.^{8} One finds $\nu(0) = 702\,285$ KÅ.^{3};

(d) Mimura-Puff fit of ^{4}He interatomic potential (Ref. 17)

$$v(r) = E_0 \left[\frac{a}{r} \right] (e^{-r/a} - \gamma e^{-\beta r/a}) \ , \tag{3.7}$$

where $E_0 = 894\,000$ K, $\gamma = 0.2560$, $a = 0.3760$ Å, and $\beta = 0.8000$. In this case $\nu(0) = 358\,312$ KÅ^3.

(e) v_0, v_1, and v_2 "homework" models of the two-nucleon interaction (Refs. 3–5, 18)

(f) Jellium interaction

$$\begin{aligned} \nu(q) &= 4\pi e^2/q^2, \quad q > 0 \ . \\ \nu(0) &= 0 \ . \end{aligned} \tag{3.8}$$

We turn now to simple L-independent noncollapsing potentials which *do* favor abnormal occupation.

(g) Repulsive square barrier

$$v_{12}=v_0\theta(a-r)\ ,\quad (v_0>0)\ . \tag{3.9}$$

The Fourier transform of this potential,

$$v(q)=4\pi v_0 a^3\frac{j_1(qa)}{qa}\ , \tag{3.10}$$

assumes negative values over finite intervals. Defining a dimensionless energy per particle $e=\epsilon(2ma^2/\hbar^2)$ and coupling strength $\Lambda=(4\pi/3)(2ma^2/\hbar^2)v_0\rho a^3$, we have, for the single-wing choice of abnormal occupation, (2.12),

$$\Delta e=(1-\xi)(k_0a)^2+3\Lambda\xi(1-\xi)j_1(k_0a)/k_0a\ .\quad \text{(SW)} \tag{3.11}$$

A numerical search would be required to determine

$$\Delta e(\bar{k}_0,\bar{\xi})\equiv\mathop{\mathrm{Min}}_{k_0,\xi}\Delta e(k_0,\xi)\ . \tag{3.12}$$

However, the essential physical effect is demonstrated if we obtain an *upper bound*

$$\Delta e(\tilde{k}_0,\tilde{\xi})\geq\Delta e(\bar{k}_0,\bar{\xi}), \tag{3.13}$$

and show that this upper bound can be made negative for large enough Λ.

(i) Choice of $\tilde{k}_0$: Take $\tilde{k}_0a=5.76\ldots$ (position of the first minimum of $j_1(x)/x$]. (ii) Determination of $\tilde{\xi}$: We note that $[\partial(\Delta e)/\partial\xi]_{\xi=\tilde{\xi}}=0$ implies $\tilde{\xi}=(-A+B)/2B$, where $A\equiv(\tilde{k}_0a)^2=33.22$ and $B\equiv3\Lambda j_1(\tilde{k}_0a)/\tilde{k}_0a=-0.086\,17\Lambda$. The restriction $\tilde{\xi}\leq1$ requires $-B\geq A$, or $\Lambda\geq390.4$. Thus

$$(\Delta e)_{\rm SW}\leq\frac{(A+B)^2}{4B}=-\frac{(33.22-0.086\,17\Lambda)^2}{0.3447\Lambda}, \tag{3.14}$$

i.e., $(\Delta e)_{\rm SW}$ is surely negative for $\Lambda>390.4$.

Similar results are obtained for the double wing and spherical-shell choices of $n_{\vec{k}}$, (2.13) and (2.14). With the former choice

$$(\Delta e)_{\rm DW}=(1-\xi)(k_0a)^2+3\Lambda[\xi(1-\xi)j_1(k_0a)/k_0a+(1-\xi)^2j_1(2k_0a)/8k_0a]. \tag{3.15}$$

Again taking $\tilde{k}_0a=5.76\ldots$ and defining $C\equiv3\Lambda j_1(2\tilde{k}_0a)/8\tilde{k}_0a=-0.003\,282\Lambda$ and A and B as before, the value of ξ minimizing Δe is $\tilde{\xi}=(-A+B-2C)/2(B-C)$. Again $\tilde{\xi}\leq1$ implies $\Lambda\geq390.4$. Then

$$(\Delta e)_{\rm DW}\leq\frac{(A+B)^2}{4(B-C)}=-\frac{(33.22-0.086\,17\Lambda)^2}{0.3316\Lambda}, \tag{3.16}$$

the upper bound again being negative for $\Lambda>390.4$.

In the spherical-shell case,

$$(\Delta e)_{\rm SS}=(1-\xi)(k_0a)^2+3\Lambda\xi(1-\xi)j_1(k_0a)/k_0a+3\Lambda(1-\xi)^2[1-j_0(2k_0a)]/4(k_0a)^2. \tag{3.17}$$

With $\tilde{k}_0a=5.76\ldots$ and $D\equiv-3\Lambda[1-j_0(2\tilde{k}_0a)]/2(\tilde{k}_0a)^2=-0.048\,53\Lambda$, the value of $\tilde{\xi}$ is $(-A+B+D)/(2B+D)$. The condition $\tilde{\xi}\leq1$ once more calls for $\Lambda\geq390.4$. Finally,

$$(\Delta e)_{\rm SS}\leq\frac{(A+B)^2}{4B+2D}=-\frac{(33.22-0.086\,17\Lambda)^2}{0.4418\Lambda}, \tag{3.18}$$

so that the double-wing choice gives the lowest upper bound of the three cases.

Is the occurrence of abnormal occupation for the repulsive square barrier (3.9) due to its *infinite sharpness*? To show that the answer is no, we consider the following example.

(h) Smoothed repulsive square barrier (Fermi or Woods-Saxon function)

$$v_{12}=v_0\left[\exp\left[\frac{r-a}{\delta}\right]+1\right]^{-1},\quad (v_0,a,\delta>0)\ . \tag{3.19}$$

The Fourier transform of this interaction is

$$v(q)=-v_0\frac{4\pi}{q}J'(q)\ , \tag{3.20}$$

where the prime denotes derivative and

$$J(q)\equiv\int_0^\infty dr\cos(qr)\left[\exp\left[\frac{r-a}{\delta}\right]+1\right]^{-1}$$
$$=\frac{\cos qa}{q}\int_{-a/\delta}^{\infty}dx\frac{\sin(qx\delta)}{(e^x+1)(e^{-x}+1)}+\frac{\sin qa}{q}\times\int_{-a/\delta}^{\infty}dx\frac{\cos(qx\delta)}{(e^x+1)(e^{-x}+1)}\ . \tag{3.21}$$

Taking $\delta/a<<1$ extends both lower limits to $-\infty$. The first integral then vanishes by symmetry, leaving $J(q)\simeq\pi\delta\sin(qa)/\sinh(\pi q\delta)$ and

$$v(q) \simeq -\frac{4\pi^2\delta}{q} v_0 \left[\frac{a\cos qa}{\sinh \pi q\delta} - \frac{\pi\delta \sin qa \cosh \pi q \delta}{(\sinh \pi q\delta)^2} \right]$$
$$\simeq 4\pi a^3 v_0 \left\{ \frac{j_1(qa)}{qa} + \left[\frac{\delta}{a}\right]^2 \frac{\pi^2}{6} \left[\cos qa + \frac{\sin qa}{qa}\right] + 0\left[\left[\frac{\delta}{a}\right]^4\right] \right\}. \tag{3.22}$$

Now, since the sum of the first two terms in this last expression is *still negative* at $qa = 5.76\ldots$ for $\delta = (0.1)a$, we see that abnormal occupation can produce an energy lowering even if the repulsive barrier is *not* perfectly sharp.

Another example of a purely radial potential for which abnormal occupation can occur is provided by the work of Biswas and Warke[19]:

(i) Repulsive Yukawa-attractive exponential interaction

$$v_{12} = \frac{ae^{-\mu r}}{r} - \frac{be^{-\lambda r}}{2\lambda} . \tag{3.23}$$

Conditions on the parameters a, μ, b, and λ for which DW occupation is energetically preferable to the undepleted zero-momentum condensate over certain density ranges, and for which the system does not obviously experience collapse, are derived in Ref. 19. In this case it is not the sharp or nearly sharp edges in the potential which induce abnormal occupation, but rather an appropriate balance of (smooth) repulsive and attractive components.

IV. L-DEPENDENT POTENTIALS

We focus now on (generally) L-dependent interactions

$$v_{12} = \sum_L v_L(r) P_L , \tag{4.1}$$

where P_L projects onto the subspace of the two-particle system corresponding to relative angular momentum L. Defining $k = (\frac{1}{2}) | \vec{k}_1 - \vec{k}_2 |$ (relative wave number) and

$$\langle \vec{k}_1 \vec{k}_2 | v_{12} | \vec{k}_1 \vec{k}_2 + \vec{k}_2 \vec{k}_1 \rangle \equiv 2V^{-1} \tilde{v}(k) , \tag{4.2}$$

an elementary calculation yields

$$\tilde{v}(k) = 4\pi \sum_{L \text{ even}} (2L+1) \int_0^\infty r^2 dr\, j_L{}^2(kr) v_L(r) . \tag{4.3}$$

Note that in the event of normal occupation we only need the potential matrix element with all k's equal to zero. Thus

$$\epsilon_{\text{normal}} = \tfrac{1}{2} \rho \tilde{v}(0) , \tag{4.4}$$

where

$$\tilde{v}(0) = 4\pi \int_0^\infty r^2 dr\, v_0(r) , \tag{4.5}$$

i.e., just the volume integral of the S-wave component of the potential. It is now a straightforward matter to derive expressions for the energy shift $\Delta\epsilon = \epsilon_{\text{abnormal}} - \epsilon_{\text{normal}}$ corresponding to the specific proposals (2.12)–(2.16) for abnormal occupation. The results are listed below:

$$(\Delta\epsilon)_{\text{SW}} = (1-\xi)(\hbar^2 k_0{}^2/2m) + \xi(1-\xi)\rho[2\tilde{v}(k_0/2) - \tilde{v}(0)] , \tag{4.6}$$

$$(\Delta\epsilon)_{\text{DW}} = (1-\xi)(\hbar^2 k_0{}^2/2m) + \xi(1-\xi)\rho[2\tilde{v}(k_0/2) - \tilde{v}(0)] + (\tfrac{1}{4})(1-\xi)^2 \rho[2\tilde{v}(k_0) - \tilde{v}(0)] , \tag{4.7}$$

$$(\Delta\epsilon)_{\text{SS}} = (1-\xi)(\hbar^2 k_0{}^2/2m) - (\tfrac{1}{2})(1-\xi^2)\rho\tilde{v}(0) + 2\xi(1-\xi)\rho\tilde{v}(k_0/2) + \tfrac{1}{2}\rho(1-\xi)^2 \int_{-1}^{1} d\mu\, \tilde{v}(k_0\sqrt{1-\mu}/\sqrt{2}) , \tag{4.8}$$

$$(\Delta\epsilon)_{\text{BS}} = (\tfrac{3}{5})(1-\xi)(\hbar^2 k_B{}^2/2m) - (\tfrac{1}{2})(1-\xi^2)\rho\tilde{v}(0) + 6\xi(1-\xi)\rho \int_0^1 dt\, t^2 \tilde{v}(k_B t/2) + 24(1-\xi)^2 \rho \int_0^1 dt\, t^2 P(t) \tilde{v}(k_B t), \tag{4.9}$$

with

$$P(t) \equiv 1 - \tfrac{3}{2}t + \tfrac{1}{2}t^3 , \tag{4.10}$$

$$(\Delta\epsilon)_G = \tfrac{3}{2}(1-\xi)(\hbar^2 k_0^2/2m) + \xi(1-\xi)\rho[\mathscr{I}(k_0/2) - \tilde{v}(0)] + \tfrac{1}{2}(1-\xi)^2\rho[\mathscr{I}(k_0/\sqrt{2}) - \tilde{v}(0)] , \tag{4.11}$$

with

$$\mathscr{I}(q) \equiv 8\pi^{-1/2} \int_0^\infty dx\, x^2 e^{-x^2} \tilde{v}(qx) . \tag{4.12}$$

In the case of the Gaussian distribution, the transformation $\vec{\kappa} = \sqrt{(1/2)}(\vec{k}_1 - \vec{k}_2)$, $\vec{K} = \sqrt{(1/2)}(\vec{k}_1 + \vec{k}_2)$ was used to arrive at the above formula involving the single integral $\mathscr{I}(q)$.

Reverting momentarily to the special case of an L-independent potential with $v_L(r) = v(r)$, all L, formulas corresponding to (4.6)–(4.11) may be easily generated directly, or may be derived from (4.6)–(4.11) by invoking the sum rule[20]

$$\sum_{L \text{ even}} (2L+1) j_L{}^2(kr) = \frac{1}{2}\left[1 + \frac{\sin 2kr}{2kr}\right] . \tag{4.13}$$

In effect, the generic quantity $2\tilde{v}(Q/2) - \tilde{v}(0)$ appearing in the above results is to be replaced by $v(Q)$.

An important feature of formulas (4.6)–(4.11) should be emphasized. If the partial-wave expansion (4.3) is truncated at some L, i.e., $v_L \equiv 0$, $L > L_{\max}$, a lowering of the energy ($\Delta\epsilon < 0$) can always be arranged, for any of the stated choices of abnormal occupation, provided (i) $\tilde{v}(k)$ falls off the k for large k (which will normally be so) and (ii) $\tilde{v}(0) > 0$ (which is required anyway to prevent collapse). One need merely take k_0 or k_B large enough so that potential terms involving k_0 or k_B can be neglected compared to the other terms, and increase ρ or $k_B{}^3$ to the point that the kinetic part of $\Delta\epsilon$ is overwhelmed by the potential contribution proportional to $-\rho\tilde{v}(0)$. (Take ξ anywhere in the range $0 < \xi < 1$.) The *total* energy per particle $(\frac{1}{2})\rho\tilde{v}(0) + \Delta\epsilon$ will remain positive. Attention is drawn to the special case that $v_L(r) = v(r)$, $L \le L_{\max}$, with $v(k) > 0$ for all k. We note that $\tilde{v}(0)$ and $v(0)$ are then identical. Letting $L_{\max} \to \infty$ in such a case, the combination $2\tilde{v}(Q/2) - \tilde{v}(0)$ sums to $v(Q)$ and any energy decreases due to the $-\rho\tilde{v}(0)$ terms in the various $\Delta\epsilon$ formulas are eradicated.

A. Ali-Bodmer (AB) interaction in alpha matter

An interesting physical example of bosons interacting via an L-dependent two-body potential is provided by the idealized alpha-particle model of nuclear matter considered in Ref. 21. (For discussion of the physical relevance of such models, see Refs. 21 and 22.) The interaction between the "elementary" alpha particles making up the system may be taken in the form (4.1) with

$$v_L(r) = \sum_{i=A,R} V_{Li} \exp(-\lambda_{Li}{}^2 r^2) , \tag{4.14}$$

as in the model of the α-α interaction devised by Ali and Bodmer[23] (AB). For $\tilde{v}(k)$ we then obtain

$$\tilde{v}(k) = \frac{\pi^2}{k} \sum_{i=A,R} \sum_{\substack{L \\ (\text{even})}} (2L+1) V_{Li} \lambda_{Li}{}^{-2} e^{-k^2/2\lambda_{Li}{}^2} I_{L+1/2}(k^2/2\lambda_{Li}{}^2) , \tag{4.15}$$

where the modified Bessel function $I_{L+1/2}$ is given by[20]

$$I_\mu(z) = \sum_{s=0}^{\infty} \frac{(z/2)^{2s+\mu}}{s!\Gamma(\mu+s+1)} \sim [\Gamma(\mu+1)]^{-1}(z/2)^\mu \quad (z \to 0) , \quad \sim e^z/\sqrt{2\pi z} \quad (z \to \infty) , \tag{4.16}$$

or

$$I_{L+1/2}(z) = \sqrt{2z/\pi}\, z^L \left[\frac{1}{z}\frac{d}{dz}\right]^L \frac{\sinh z}{z} . \tag{4.17}$$

The result (4.15) is derived from the relation

$$\int_0^\infty dr\, r^2 j_L{}^2(Qr) e^{-\lambda^2 r^2} = \frac{\pi}{4Q\lambda^2} I_{L+1/2}(Q/2\lambda^2) \exp(-Q^2/2\lambda^2) . \tag{4.18}$$

We also note that

$$\tilde{v}(0) = \pi^{3/2} \sum_{i=A,R} V_{0i} \lambda_{0i}{}^{-3} . \tag{4.19}$$

A numerical study of abnormal occupation has been carried through, based on (4.14) with the choice of parameters V_{Li}, λ_{Li} denoted by d_0', d_2, $d_4(0.7,10)$ in Ref. 23 (the standard AB potential).

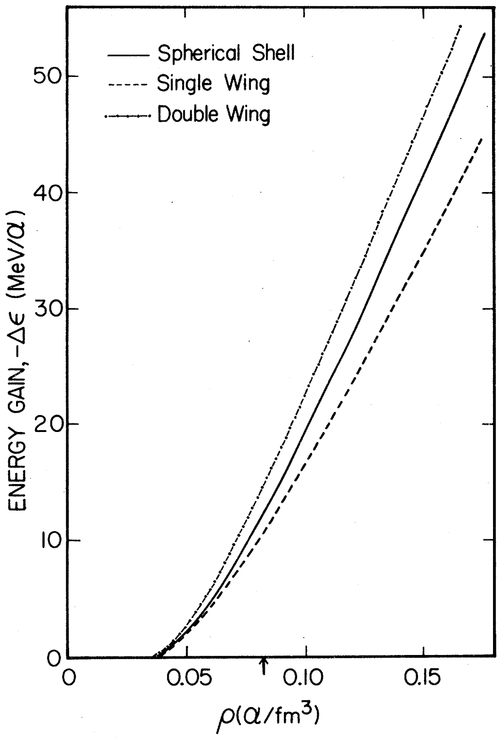

FIG. 2. Energy lowering $-\Delta\epsilon$ in Ali-Bodmer alpha matter for single-wing, double-wing, and spherical-shell abnormal occupations, relative to the energy for normal occupation. (The energy drop is maximized, at each density ρ, with respect to the free parameters in the assumed momentum distribution.) The vertical arrow marks the equilibrium density of alpha matter obtained in Ref. 21.

To be specific, we take $V_{0R}=475$ MeV, $V_{2R}=320$ MeV, and $V_{4R}=10$ MeV, together with $V_{LA}=-130$ MeV, $\lambda_{LR}=0.7\ \mathrm{fm}^{-1}$, and $\lambda_{LA}=0.475\ \mathrm{fm}^{-1}$, $L\leq 4$. It is supposed that $V_{Li}=0$, $L>4$, so

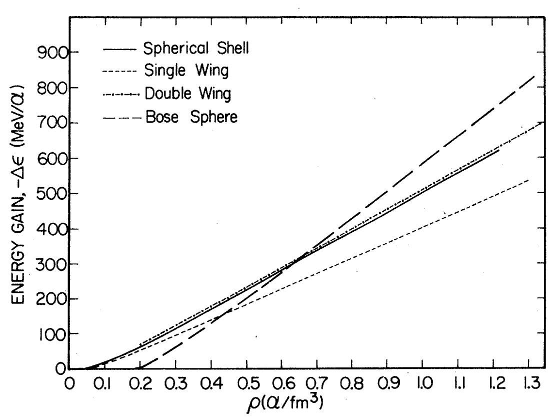

FIG. 3. Energy drop $-\Delta\epsilon$ in Ali-Bodmer alpha matter for four different abnormal occupations, extended to higher densities (see Fig. 2).

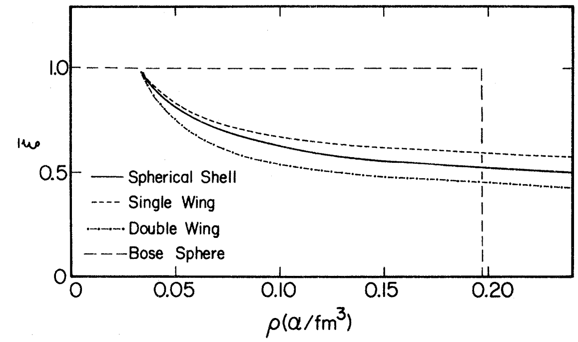

FIG. 4. Optimal zero-momentum condensate fraction $\bar{\xi}$ in Ali-Bodmer alpha matter, corresponding to minimization of the energy, at each density, with respect to the free parameters of the assumed abnormal momentum distributions.

that we are dealing with a truncated partial-wave decomposition of the two-body interaction v_{12}.

The results of minimizing $\Delta\epsilon$ with respect to the independent parameters ξ and k_0 in the SW, DW, and SS abnormal distributions and the single parameter ξ in the BS distribution are summarized in Figs. 2–5. The arrow in Fig. 2 marks the equilibrium density of ideal alpha matter as determined by Johnson and Clark via hypernetted-chain variational theory,[21] assuming an L-independent α-α interaction in which the AB S-wave component acts in *all* (even) angular momentum states. We note that the indicated density corresponds to roughly double the empirical saturation density of nuclear matter, hence much of the density range displayed in the figures lies outside the domain of applicability of the alpha-particle model.

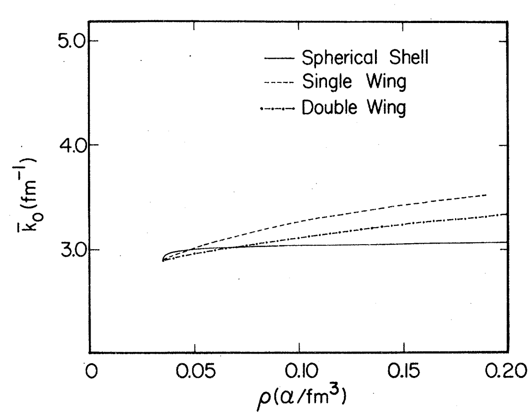

FIG. 5. Optimal value $\bar{k}_0$ of parameter k_0 (or k_B in the Bose-sphere case) in Ali-Bodmer alpha matter, corresponding to minimization of the energy, at each density, with respect to the free parameters of the assumed abnormal momentum distributions.

Even so, the single-wing, double-wing, and spherical-shell energy shifts plotted in Fig. 2 show that abnormal occupation is already favored at physically relevant densities: for the SW, DW, and SS occupation functions the critical density $\rho_{\rm crit}$, beyond which $\Delta\epsilon$ (at optimal k_0, ξ) is negative, is approximately 0.035 alphas per fm^3, which is slightly below the accepted equilibrium density of nuclear matter. Beyond this $\rho_{\rm crit}$, we find $(-\Delta\epsilon)_{\rm SW} < (-\Delta\epsilon)_{\rm SS} < (-\Delta\epsilon)_{\rm DW}$. The difference between $(-\Delta\epsilon)_{\rm DW}$ and $(-\Delta\epsilon)_{\rm SS}$ appears to approach a constant value as the density increases, the separation of the corresponding curves being hardly noticeable on the scale of Fig. 3. (We might mention that upon artificially reducing the particle mass from the alpha mass to the nucleon mass, $\rho_{\rm crit}$ in the SS case increases to about 0.14 alphas per fm^3.)

For the BS choice, $\Delta\epsilon$ remains positive until the density reaches some five times ordinary nuclear density ($\rho_{\rm crit}=0.197$ fm^{-3} in this case). On the other hand, at very high densities the BS ansatz is found to be more advantageous than even the DW or the SS distribution (see Fig. 3). This is a remarkable result, considering that the Bose sphere $n_{\vec{k}}$ has only one independent variational parameter rather than two. It may well be worthwhile to introduce an additional parameter into the BS distribution as indicated earlier.

Looking next at Fig. 4, we observe that in the SW, DW, and SS cases, $\bar{\xi}$ for $\rho > \rho_{\rm crit}$ falls off smoothly with ρ from unity at $\rho_{\rm crit}$ to a value around 0.5, flattening out for large ρ. This behavior may be understood qualitatively in terms of the origin of the energy decrease $-\Delta\epsilon$ in exchange of particles between different $\vec{k}$ states. Considering the simplest example, namely condensates at $\vec{k}=\vec{0}$ and $\vec{k}=\vec{k}_0$ (single-wing choice), we get the maximum number of exchanges with $\xi=\frac{1}{2}$, as is reflected in the factor $\xi(1-\xi)$ in the second term (potential term) of (4.6). If the first term (kinetic term) could be ignored, we would have, optimally, $\xi=\bar{\xi}=\frac{1}{2}$ at any k_0 for which $2\tilde{v}(k_0/2) - \tilde{v}(0)$ is negligible. The effect of the kinetic term is of course to push $\bar{\xi}$ toward a value somewhat greater than one half, however, with increasing density the potential term becomes dominant and this effect recedes. The behavior of $\bar{\xi}$ vs ρ in the DW and SS cases can be understood similarly.

We note that the AB potential has the property that $\tilde{v}(k)$ is *negative* over a considerable range in k. [More precisely, as k increases $\tilde{v}(k)$ rises from $\tilde{v}(0)=956.83$ MeV fm^3 to a maximum of 1636 MeV fm^3 at $k=0.49$ fm^{-1}, falls off to zero around $k=1.2-1.3$ fm^{-1}, and thereafter makes a negative swing with a minimum of some -417 MeV fm^3 at about $k=2.2$ fm^{-1}.] This property favors abnormal occupation, and has the consequence that the optimal k_0 in the SW, DW, and SS distribution is smaller than would otherwise be the case (see forthcoming examples). This optimal k_0 (denoted $\bar{k}_0$) is plotted against ρ in Fig. 5. Returning our attention to Fig. 4, we see that in the BS case there is a sudden and complete depletion of the zero-momentum condensate as ρ passes $\rho_{\rm crit}$, which contrasts with the behavior of the SW, DW, and SS examples.

Curves for the Gaussian choice of $n_{\vec{k}}$ have not been presented, since energy decreases for that distribution are of doubtful validity due to violation of the requirement (2.17) of integral occupation numbers. However, it is perhaps of interest to quote results for the critical density as a function of the amplitude parameter $C=8\pi^{3/2}(1-\xi)\rho/k_0{}^3$. We obtain $\rho_{\rm crit}=0.55$, 3.73, 37.3, and 372.7 fm^{-3} for $C=1$, 10, 100, and 1000, respectively. The infraction of constraint (2.17) is the less severe, the larger C. Clearly, the Gaussian choice is not relevant to the present problem.

In order to further illuminate the L-truncation phenomenon, we have examined the issue of abnormal occupation (specifically, in the SW case) for an α-α interaction consisting of the AB potential supplemented by a term in which the Ali-Bodmer $v_4(r)$ acts equally in *all* even partial waves $L \geq 6$. The preference for abnormal occupation displayed by the AB potential (as previously defined) is erased: $\Delta\epsilon$ remains positive for 0.01 fm^{-3} $\leq \rho \leq 300$ fm^{-3}.

B. Truncated Bruch-McGee (BM) potential in liquid ^{4}He

As a second L-dependent example derived from a physical problem, consider a system of ^{4}He atoms interacting via a potential of form (4.1) *truncated* at the $L=0$ term. For $v_0(r)$ we assume the Bruch-McGee potential (3.6) [which, in a relatistic treatment of bulk ^{4}He, would normally be taken to act equally in *all* (even) partial waves]. We remark that, in contrast to the AB interaction, $\tilde{v}(k)$ for the truncated BM potential is positive for all k.

From the previous argument it is clear that the L-dependent interaction so defined *will* promote abnormal occupation at densities ρ beyond some $\rho_{\rm crit}$. One is curious to see how this critical density compares with the experimental equilibrium density of liquid ^{4}He at zero temperature, $\rho_{\text{exp}}=0.0218$ atoms per Å^3. It is sufficient for our purposes to examine the simple case of the single-wing distribution, realizing that we will obtain only an upper bound on the true ρ_{crit}. We find in fact that even ρ_{crit} (SW) is less than 0.01 Å^{-3}, in the range $\rho=0.01-0.09$ Å^{-3} the best k_0 increases from $6-10$ Å^{-1}, while the corresponding optimal ξ declines from about 0.6 to slightly over 0.5. The SW energy reduction can be *very* substantial (e.g., some -4000 K at $\rho=0.03$ Å^{-3}, increasing with ρ), but of course the total energy never goes negative.

Needless to say, truncating its partial-wave expansion (4.1) at $L=0$ severely mutilates the Bruch-McGee potential. What happens to ρ_{crit} as we truncate at higher and higher values $L_{\max}$ of L? To look into this equation we find it computationally convenient—and certainly adequate at the qualitative level deemed appropriate—to work instead with the simpler model (3.7) of the He atom-He atom interaction used by Mimura and Puff.

C. Truncated Mimura-Puff (MP) potential in liquid ^{4}He

Again adopting the SW choice of $n_{\vec{k}}$, we have truncated the partial-wave expansion (4.1) of the L-independent MP potential successively at $L_{\max}=0,2,4,6,\ldots,18$. A coarse search at $\rho=0.01$ Å^{-3} revealed no instances of abnormal occupation surviving past $L_{\max}=0$, for which a negative $\Delta\epsilon$ was found with $k_0=6$ Å^{-1}, $\xi=0.5-0.9$. At $\rho=0.03$, 0.05, 0.07, 0.09 Å^{-3}, abnormal occupation survives (at least) to $L_{\max}=4$, 6, 8, 10, respectively. As expected, the most favorable k_0 (most favorable ξ) marches up (down) with density toward a saturation value. It may further be remarked that $\tilde{v}(k)>0$ for all k, for all truncations. The transform $\tilde{v}(k)$ becomes more repulsive as $L_{\max}$ is increased, at fixed k; it becomes less repulsive as k is increased, at given $L_{\max}$.

V. CONCLUDING REMARKS

Restricting attention to Bose trial ground-state wave functions which are permanents of plane-wave orbitals, we have used a selection of simple prescriptions for abnormal occupation ($n_{\vec{k}} \neq N\delta_{\vec{k},0}$) of these orbitals (i) to demonstrate that abnormal occupation is indeed advantageous in a variety of model many-body systems of some intrinsic physical interest and (ii) more broadly, to elucidate the circumstances under which abnormal occupation may be expected to prevail. One phenomenon uncovered by our investigations is especially worthy of note: the promotion of abnormal occupation by truncation of the partial-wave expansion of the two-body interaction. More generally, abnormal occupation seems to be favored by circumstances of interaction, density, and particle mass which tend to produce spatial order.

The momentum distribution $n_{\vec{k}}$ corresponding to an *arbitrary* permanent of plane waves can be mimicked to any desired accuracy by a finite collection of shells (of finite and/or infinitesimal thickness) and condensates $\xi_i\delta_{\vec{k},\vec{k}_i}$. One may then construct successive approximations to the truly optimal $n_{\vec{k}}$ (within the class corresponding to plane-wave permanents), either by (a) standard analytic and numerical means or (b) by a systematic computer search. The latter approach was adopted in a recent investigation[13] of the analogous Fermi problem, in which abnormal occupation consists in deviation from the filled Fermi sea. Of course, the Bose problem is rather more difficult because of the possibility of multiple occupation of single-particle states, especially as manifested in condensates at various momenta $\hbar\vec{k}$ each containing, in the thermodynamic limit, a finite fraction of the particles. At any rate, work is presently continuing along line (a), with the option of implementing approach (b).

One may entertain the viewpoint that abnormal occupation serves to simulate, within the independent-particle picture, the effects of strong correlations (e.g., strong short-range correlations) among the particles. It then becomes important to determine whether or not abnormal occupation "survives" when such dynamical correlations are explicitly incorporated into the trial wave function. That is: if an independent-particle wave function Φ_a corresponding to abnormal occupation is energetically favored over the function Φ_n corresponding to normal occupation, is the correlated state $F\Phi_a$ still preferred over an "optimally" determined $F\Phi_n$? (Here, it is supposed that F stays within some judiciously chosen class of *tractable* correlation operators, to avoid trivialities.) If the answer to this question is no, then the fundamental significance of work such as that described here is greatly diminished, its justification lying primarily in the simplicity with which it allows correlation effects to be introduced in some physical settings. If the answer is yes, then the phenomenon of abnormal occupation does indeed promise unique insights into the nature of many-body ground states.

A partial answer to the above question is being sought within the framework of Jastrow correlation operators and HNC and other integral equation method.[3–5] The first concrete evidence—obtained for a certain group of model Fermi systems resembling nuclear matter[14]—is negative. However, the broader issue of the significance and implications of the phenomenon of abnormal occupation across the diverse subfields of many-body physics remains an open and challenging one.

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