ABNORMAL BOSON OCCUPATION IN ALPHA MATTER

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Received 17 October 1978

A specific example of abnormal boson occupation is given whereby a vacuum state energy lower than the normal one for the case of Ali–Bodmer alpha particle matter is found at physical densities.

The microscopic treatment of an interacting N boson system, like ^{4}He alpha matter in its ground state, has developed along two general lines: 1) perturbation theory [1] based mainly on the infinite partial summation of one class or another of diagrams and 2) variational methods [2] based originally on the use of Bijl–Dingle–Jastrow correlation functions and evolving to the latest "hypernetted chain" techniques [3]. Both lines of approach, however, have restricted themselves exclusively to the initial starting point of a "normally occupied vacuum state", i.e.. to the (fully-symmetric) permanent of plane-wave single-particle states all *in the zero momentum state.*

Although diverse theories involving *abnormal* boson occupation have appeared [4], little if any attention has been directed to the question of the optimum *unperturbed* vacuum state to be employed in a given N boson problem. The "normal" vacuum state minimizes the ground state expectation value for the *ideal* Bose system but there is no *a priori* reason why it should also do so for the fully-interacting case focused initially on an independent-particle scheme. And indeed, it would appear very strange if it did.

In this note we wish to emphasize this fact by a specific example of abnormal occupation within the context of alpha matter, a hypothetical system that has attracted continued interest [5] because of its possible relevance to alpha-clustering [6] in the nuclear surface. Our motivation lies in the usefulness of providing an (energetically) improved and more realistic starting point for the more refined subsequent correlation-energy studies of the many-boson problem via either perturbational or vibrational approaches.

The ground state of the N boson system, described by the hamiltonian

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

is given, at the independent-particle level, by the single permanent of plane waves

$$\mathrm{perm}[e^{i\mathbf{k}_i\cdot\mathbf{r}_j}]\, n_{\mathbf{k}_i}\,, \tag{2}$$

where the occupation numbers $n_{\mathbf{k}}$ may take on any of the non-negative integer values 0, 1, ..., N, and are otherwise restricted to obey the obvious condition

$$\sum_{\mathbf{k}} n_{\mathbf{k}} = N\,. \tag{3}$$

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The ground state expectation energy with (2) (which is a Hartree–Fock energy since plane-wave orbitals, under usual periodic-boundary conditions, always satisfy the Hartree–Fock equations) is,

$$E = \langle t \rangle + \langle v \rangle \,, \tag{4}$$

where

$$\langle t \rangle = \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}}^0 n_{\boldsymbol{k}} \,, \quad \epsilon_{\boldsymbol{k}}^0 \equiv \hbar^2 k^2/2m \tag{5}$$

and for $N \gg 1$,

$$\langle v \rangle = \tfrac{1}{2} \sum_{k_1 k_2} (1 - \tfrac{1}{2}\delta_{\boldsymbol{k},\boldsymbol{k}_2}) n_{\boldsymbol{k}_1} n_{\boldsymbol{k}_2} \times \langle \boldsymbol{k}_1 \boldsymbol{k}_2 | v_{12} | \boldsymbol{k}_1 \boldsymbol{k}_2 + \boldsymbol{k}_2 \boldsymbol{k}_1 \rangle \,, \tag{6a}$$

$$\langle \boldsymbol{k}_1 \boldsymbol{k}_2 | v_{12} | \boldsymbol{k}_1' \boldsymbol{k}_2' \rangle \equiv V^{-2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \times \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_1 \cdot \boldsymbol{r}_1} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_2 \cdot \boldsymbol{r}_2} v_{12} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_1' \cdot \boldsymbol{r}_1} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_2' \cdot \boldsymbol{r}_2} \,, \tag{6b}$$

with V the normalization volume. For normal occupation, $n_{\boldsymbol{k}} = N\delta_{\boldsymbol{k},0}$, one finds immediately that

$$\langle v \rangle = \tfrac{1}{2} N \rho \nu(0) \,, \tag{7a}$$

$$\rho \equiv N/V \,, \quad \nu(q) \equiv \int \mathrm{d}^3 r \, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} v(r) \,, \tag{7b}$$

so that the energy per particle for normal occupation is just

$$\epsilon_{\text{normal}} = \tfrac{1}{2} \rho \nu(0) \,. \tag{8}$$

This being a rigorous upper bound to the exact energy per particle by the Rayleigh–Ritz variational principle, allows one to conclude that (the volume integral of the interaction) $\nu(0) > 0$ is a necessary condition to avoid collapse of the N-body system to infinite binding-per-particle and density.

Consider now, merely by way of illustration, abnormal occupation given by

$$n_{\boldsymbol{k}} = N[\xi \delta_{\boldsymbol{k},0} + (1-\xi)\delta_{\boldsymbol{k},\boldsymbol{k}_0}] \,, \quad 0 \leqslant \xi \leqslant 1 \,. \tag{9}$$

Namely, one depletes the $\boldsymbol{k} = 0$ state to a fraction ξ and populates *macroscopically* with the remaining particles, the single point in $\boldsymbol{k}$-space given by the vector $\boldsymbol{k}_0$, where ξ and $\boldsymbol{k}_0$ will be variational parameters to be chosen so as to minimize the energy at a given density. (Clearly, the total momentum of the proposed state is non-zero – a defect easily remedied by also occupying at $\boldsymbol{k} = -\boldsymbol{k}_0$. But that only complicates the analysis which at any rate will lead to a variational state superior to the normal one.) Using (5) and (9) one has

$$\langle t \rangle = N(1-\xi)\epsilon_{k_0}^0 \,. \tag{10}$$

If the interaction potential v_{12} is the same in all partial waves of relative orbital angular momentum (i.e., is l-independent), then (6b) and (7b) lead to

$$\langle \boldsymbol{k}_1 \boldsymbol{k}_2 | v_{12} | \boldsymbol{k}_1 \boldsymbol{k}_2 + \boldsymbol{k}_2 \boldsymbol{k}_1 \rangle = V^{-1} [\nu(0) + \nu(|\boldsymbol{k}_1 - \boldsymbol{k}_2|)] \tag{11}$$

and subsequently, via (6a), to

$$\langle v \rangle / N = \tfrac{1}{2} \rho \nu(0) + \xi(1-\xi)\rho\nu(k_0) \,, \quad k_0 > 0 \,. \tag{12}$$

Thus, the energy difference between the abnormally- and normally-occupied states is just

$$\Delta\epsilon \equiv \epsilon - \epsilon_{\text{normal}} = (1-\xi)\epsilon_{k_0}^0 + \xi(1-\xi)\rho\nu(k_0) \,. \tag{13}$$

We first briefly examine two examples of (l-independent) two-body interactions, both of which must of course satisfy the non-collapse condition $\nu(0) > 0$ stated above. i) The purely repulsive gaussian interaction

$$v(r) = v_0 \mathrm{e}^{-\lambda^2 r^2} \,, \quad v_0 > 0 \,, \tag{14}$$

having a non-negative Fourier transform $\nu(q)$ for all q, can never make the energy difference (13) negative. However, ii) the repulsive square barrier

$$v(r) = v_0 \theta(a - r) \,, \quad v_0 > 0 \,, \tag{15}$$

for which

$$\nu(q) = 4\pi v_0 a^3 \frac{j_1(qa)}{qa} \tag{16}$$

will make (13) negative for some value of ρ and ξ if the value of k_0 is picked, say, to correspond to the first (negative) minimum of (16) and $v_0 a^3$ is sufficiently large. Therefore, we have here an explicit example of an abnormally-occupied vacuum state which is lower in energy than the normal one.

A less trivial as well as more realistic example is provided by alpha particle matter interacting via a pairwise, l-dependent Ali–Bodmer potential [1]

$$v_{12} = \sum_{l=0,2,4} v_l(r_{12}) |l\rangle\langle l| \,, \tag{17a}$$

$$v_l(r) \equiv \sum_{\iota=\mathrm{A,R}} V_{l\iota}\, \mathrm{e}^{-\lambda_{l\iota}^2 r^2}\,, \tag{17b}$$

where $|l\rangle$ is an eigenstate of relative orbital angular momentum l, the indices A and R stand for "attractive" and "repulsive" and the parameters $V_{l\iota}, \lambda_{l\iota}$ refer to the set labelled "d" in ref. [7]. To evaluate the corresponding potential energy expectation value one uses the following integral [8]

$$\int_0^\infty \mathrm{d}r r^2 j_l^2(Qr)\, \mathrm{e}^{-\lambda_l^2 r^2} = (\pi/4Q\lambda_l^2)\, \mathrm{e}^{-Q^2/2\lambda_l^2}\, I_{l+1/2}(Q/2\lambda_l^2)\,, \tag{18}$$

where $j_l(x)$ are the spherical Bessel functions and $I_\nu(z)$ the modified Bessel functions defined [8] by

$$I_\nu(z) = \sum_{s=0}^\infty \frac{(z/2)^{2s+\nu}}{s!\Gamma(\nu+s+1)} \underset{z\ll 1}{\longrightarrow} [\Gamma(\nu+1)]^{-1}(z/2)^\nu \underset{z\gg 1}{\longrightarrow} \mathrm{e}^z/\sqrt{2\pi z} \tag{19}$$

or, alternatively, by the Rayleigh formula

$$I_{l+1/2}(z) = (2z/\pi)^{1/2}\, z^l (z^{-1}\, \mathrm{d}/\mathrm{d}z)^l\, z^{-1} \sinh z\,. \tag{20}$$

Defining the relative linear momentum for two particles as $\boldsymbol{k} \equiv \frac{1}{2}(\boldsymbol{k}_1 - \boldsymbol{k}_2)$, one finally obtains from (6b) for the Ali–Bodmer potential (17) that

$$\langle \boldsymbol{k}_1\boldsymbol{k}_2 | v_{12} | \boldsymbol{k}_1\boldsymbol{k}_2 + \boldsymbol{k}_2\boldsymbol{k}_1\rangle = 2V^{-1}\tilde{v}(k)\,, \tag{21}$$

where

$$\tilde{v}(k) \equiv \frac{\pi^2}{k} \sum_{\iota=\mathrm{A,R}} \sum_{l=0,2,4} (2l+1)\, V_{l\iota}\lambda_{l\iota}^{-2} \times \mathrm{e}^{-k^2/2\lambda_{l\iota}^2}\, I_{l+1/2}(k^2/2\lambda_{l\iota}^2) \underset{k\to\infty}{\longrightarrow} \mathrm{O}(k^{-2})\,, \tag{22}$$

where the last result follows from (19). We also note by direct calculation from (22) that

$$\tilde{v}(0) = \pi^{3/2} \sum_{\iota=\mathrm{A,R}} V_{0\iota}\lambda_{0\iota}^{-3}\,, \tag{23}$$

coincides with $v(0)$, as defined in (7b), *for the s-wave alone.* The corresponding normally-occupied-state energy per particle is then just

$$\epsilon_{\mathrm{normal}} = \tfrac{1}{2}\rho\tilde{v}(0)\,, \tag{24}$$

where, as was to be expected, only the s-wave interactions enter. Furthermore, the Ali–Bodmer force is found to satisfy the non-collapse (necessary) condition $\tilde{v}(0) > 0$, as of course it should. Higher partial-waves come into play for the abnormally-occupied case (9), leading eventually to the energy difference

$$\Delta\epsilon = (1-\xi)\epsilon_{k_0}^0 + \xi(1-\xi)\rho[2\tilde{v}(k_0/2) - \tilde{v}(0)]\,, \tag{25}$$

which is our main result. Now, in view of the rapid fall-off of $\tilde{v}(k_0/2)$ for k_0 large enough, by (22), the energy difference (25) can become negative for some ρ and ξ provided only that $\tilde{v}(0)$ be sufficiently large so as to compensate for the increased kinetic energy.

The latter indeed turns out to be the case, as shown below. But first let us mention that the l-dependent repulsive gaussian interaction case – for which *no energy decrease* was found above for the abnormal relative to the normal state – is recoverable from our final result (25) if for $\tilde{v}(q)$ in (22) one considers the force parameters V_l, λ_l to be independent of l, sums over all *even* l (since odd-l states do not contribute to the matrix element in (6a)) and applied the sum rule [8]

$$(\pi/2z)^{1/2} \sum_{l\ \mathrm{even}}^\infty (2l+1)\, I_{l+1/2}(z) = \cosh z\,. \tag{26}$$

In such a case,

$$\tilde{v}(q) = \tfrac{1}{2}[v(0) + v(2q)] \tag{27}$$

and (25) reduces to (13). Clearly then, an Ali–Bodmer s-wave interaction equally in all (even) partial waves gives no lowering of the energy for the new occupation numbers (9). The situation is completely different for the "true", i.e., l-dependent, Ali–Bodmer interaction as we now proceed to report.

A direct-variation of (25) was carried out numerically with respect to the two variational parameters $0 \leqslant \xi \leqslant 1$ and $k_0 > 0$, for several alpha matter densities ρ, in order to determine

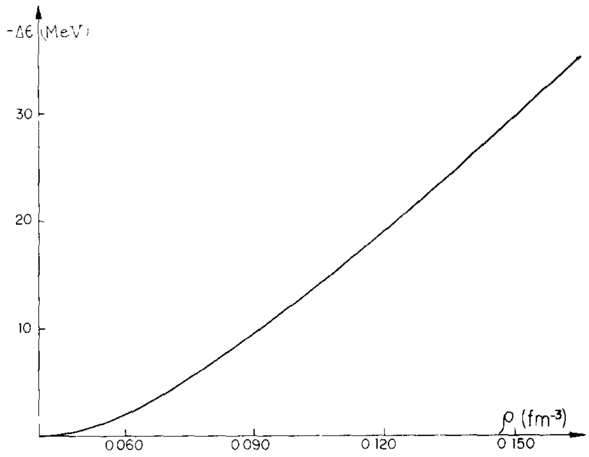

Fig. 1 Energy difference (25) between the abnormally- and normally-occupied vacuum states, minimized in variational parameters ξ and k_0, for the Ali–Bodmer l-dependent alpha–alpha interaction The energy difference is negative for all densities beyond the critical value of 0 0415 fm^{-3} (which is roughly half of equilibrium density).

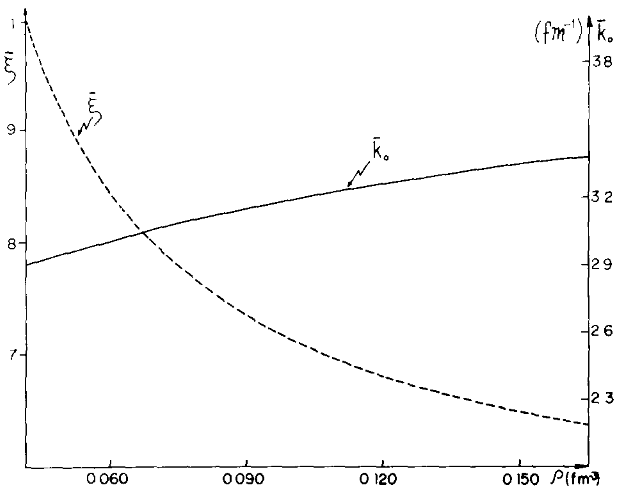

Fig 2 Values of $\bar{\xi}$ (left scale) and $\bar{k}_0$ (right scale) which minimize the energy at each density Note the relatively small variation in $\bar{k}_0$ over relevant physical densities of alpha matter.

$$\min_{0\leqslant\xi\leqslant 1, k_0>0} \epsilon(\xi, k_0; \rho) \equiv \epsilon(\bar{\xi}, \bar{k}_0, \rho) .$$

The results are shown in figs. 1 and 2. A critical density of $\rho_0 = 0.0415$ fm^{-3} (above which the abnormally occupied state is stabler, i.e., lower in energy) was found. We note that recent variational calculations [9] place the alpha matter equilibrium density at around 0.08 fm^{-3}, so that the densities for which abnormal occupation is relevant are indeed of physical interest.

The above example by no means exhausts the approach suggested here for the study of the general many-boson problem since a) an improved occupation n_k and/or b) use of non-plane-wave orbitals (giving rise to, say, spatial inhomogeneities may give an even lower vacuum state energy These possibilities are presently under study

Research supported in part by INEN, CONACYT-PNCB (México) and U.S. National Science Foundation under Grant No. DMR78-08552.

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