Theory of Solid He³. I. Comparative Study of Liquid and Solid He³†

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The ground state of solid He³ is investigated using a new method. The procedure begins with a Gaussian-Jastrow trial wave function, and calculates the energy expectation value using a cluster development that takes into account the short-range two-particle correlations between *all* particles in *each* order of the expansion. This enables a wide range of correlation functions to be used and also permits a simultaneous treatment of the liquid and the solid phases. Numerical results are presented to illustrate this method and to demonstrate the above assertions. More precise numerical calculations, which will attest to the rapid convergence of the expansion and shed light on the phase transition, and the application of this method to the study of the lattice dynamics of correlated crystals will be given in later papers.

I. INTRODUCTION

ON account of the large zero-point motion, the strong short-range repulsion and the very weak van der Waals attraction, solid He³ forms a quantum crystal and cannot be treated by the standard theories of lattice dynamics. Recent work[1–4] on the calculation of the ground-state energy of solid He³ has all been variational, employing a correlated trial wave function of the type[5]

$$\psi(1,2,\cdots,N)=\prod_i \phi_i(\mathbf{r}_i)\sum_{j<k} f_{jk}(r_{jk}),\tag{1}$$

where $\phi_i(\mathbf{r}_i)$ is generally taken (except in Ref. 4) to be a simple Gaussian centered about lattice site $\mathbf{R}_i$

$$\phi_i(\mathbf{r}_i)=\phi(|\mathbf{r}_i-\mathbf{R}_i|)=\frac{\alpha^{3/2}}{\pi^{3/4}}e^{-(\frac{1}{2})\alpha^2|\mathbf{r}_i-\mathbf{R}_i|^2}\tag{2}$$

and $f_{jk}(r_{jk})$ is generally taken (except in Ref. 2) to be of the form $f(r_{jk})$, independent of the lattice sites $\mathbf{R}_j$ and $\mathbf{R}_k$. The two-particle function $f(r)$ takes into account the short-range correlations, and the single-

particle function ϕ allows for the localization of the atoms ($\alpha>0$). Note that ψ is not antisymmetrized and ϕ is spherically symmetric. Support for these approximations as well as the Gaussian form of ϕ can be found in Refs. 1 and 6.

We wish to report here a new method of calculation which offers the following improvements: (1) it widens the range of $f(r)$'s usable in a cluster expansion of the energy, and (2) it permits a simultaneous treatment of the liquid and the solid phases. Some numerical results are given to demonstrate these improvements.

II. METHOD OF CALCULATION

The Hamiltonian of a system of N He³ atoms in volume Ω is taken to be

$$H=\frac{-\hbar^2}{2m}\sum_i \nabla_i^2+\sum_{j<k} v(r_{jk}),\tag{3}$$

where $v(r)$ is a Lennard-Jones 6-12 potential with parameters determined by deBoer and Michels. The expectation value of, H with respect to ψ, Eqs. (1) and (2), is then

$$E=E_T+E_V,$$

$$E_T=N\frac{3\alpha^2\hbar^2}{4m},$$

$$E_V=\sum_{i<j}\left[(\psi,V(r_{ij})\psi)/(\psi,\psi)\right]$$

$$=\sum_{i<j}\frac{\int\phi^2(|\mathbf{r}_1-\mathbf{R}_1|)\phi^2(|\mathbf{r}_2-\mathbf{R}_2|)\cdots\phi^2(|\mathbf{r}_N-\mathbf{R}_N|)f^2(r_{12})f^2(r_{13})\cdots f^2(r_{N-1,N})V(r_{ij})d\mathbf{r}_{12\ldots N}}{\int\phi^2(|\mathbf{r}_1-\mathbf{R}_1|)\phi^2(|\mathbf{r}_2-\mathbf{R}_2|)\cdots\phi^2(|\mathbf{r}_N-\mathbf{R}_N|)f^2(r_{12})f^2(r_{13})\cdots f^2(r_{N-1,N})d\mathbf{r}_{12\ldots N}},$$

[1] L. H. Nosanow, Phys. Rev. **146**, 120 (1966); J. H. Hetherington, W. J. Mullin, and L. H. Nosanow, *ibid.* **154**, 175 (1967).
[2] K. A. Brueckner and J. Frohberg, Progr. Theoret. Phys. (Kyoto) Suppl., 383 (1965).
[3] J. Hansen and D. Levesque, Phys. Rev. **165**, 293 (1968).
[4] T. R. Koehler, Phys. Rev. Letters **18**, 654 (1967); H. Horner, Z. Physik **205**, 72 (1967).
[5] All indices on summations and products run from 1 to N unless otherwise stated.
[6] D. Rosenwald, Phys. Rev. **154**, 160 (1967).

where

$$V(r) = v(r) - (\hbar^2/2m)\nabla^2 \ln f(r).\qquad(4)$$

Let

$$W(\beta) = \left(\psi, \prod_{i<j} \exp[\beta V(r_{ij})]\psi\right)$$

$$= \int \phi^2(|r_1-R_1|)\phi^2(|r_2-R_2|)\cdots\phi^2(|r_N-R_N|)f^2(r_{12})f^2(r_{13})\cdots f^2(r_{N-1,N})\prod_{i<j} e^{\beta V(r_{ij})}dr_{12...N};\qquad(5)$$

then

$$E_V = \left[\frac{d}{d\beta}\ln W(\beta)\right]_{\beta=0}.\qquad(6)$$

The task left is to evaluate $W(\beta)$. In the Nosanow calculation[1] (NMH), an average quantity $\langle A(r_1,r_2,\cdots,r_k)\rangle$ is defined thus:

$$\langle A(r_1,r_2,\cdots,r_k)\rangle = \frac{\int \phi^2(|r_1-R_1|)\phi^2(|r_2-R_2|)\cdots\phi^2(|r_N-R_N|)A(r_1,r_2,\cdots,r_k)dr_{12...N}}{\int \phi^2(|r_1-R_1|)\phi^2(|r_2-R_2|)\cdots\phi^2(|r_N-R_N|)dr_{12...N}}$$

$$= \omega^{-k}\int \phi^2(|r_1-R_1|)\phi^2(|r_2-R_2|)\cdots\phi^2(|r_k-R_k|)A(r_1,r_2,\cdots,r_k)dr_{12...k},\qquad(7)$$

where

$$\omega = \int \phi^2(|r_i-R_i|)dr_i.$$

Thus,

$$W(\beta) = \omega^N \langle f^2(r_{12})f^2(r_{13})\cdots f^2(r_{N-1,N})\prod_{i<j} e^{\beta V(r_{ij})}\rangle.\qquad(8)$$

A cluster expansion[7] is then used to evaluate $W(\beta)$, resulting in

$$E_V = E_{2V} + E_{3V} + \cdots,$$

$$E_{2V} = \sum_{i<j} \frac{\int \phi^2(|r_1-R_1|)\phi^2(|r_2-R_2|)\cdots\phi^2(|r_N-R_N|)f^2(r_{ij})V(r_{ij})dr_{12...N}}{\int \phi^2(|r_1-R_1|)\phi^2(|r_2-R_2|)\cdots\phi^2(|r_N-R_N|)f^2(r_{ij})dr_{12...N}}$$

$$= \sum_{i<j} \frac{\int \phi^2(|r_i-R_i|)\phi^2(|r_j-R_j|)f^2(r_{ij})V(r_{ij})dr_i dr_j}{\int \phi^2(|r_i-R_i|)\phi^2(|r_j-R_j|)f^2(r_{ij})dr_i dr_j}\qquad(9)$$

$$= \sum_{i<j} \frac{\langle f^2(r_{ij})V(r_{ij})\rangle}{\langle f^2(r_{ij})\rangle},$$

$$E_{3V} = \frac{1}{2}\sum_{i,j,k}' \left\{\frac{\langle f^2(r_{ij})f^2(r_{jk})f^2(r_{ki})V(r_{ij})\rangle}{\langle f^2(r_{ij})f^2(r_{jk})f^2(r_{ki})\rangle} - \frac{\langle f^2(r_{ij})V(r_{ij})\rangle}{\langle f^2(r_{ij})\rangle}\right\},\text{ etc.}$$

E_{2V} in the first line gives the impression that it includes all interaction energies between two atoms, i and j, localized about sites R_i and R_j and correlated through $f(r_{ij})$, *in a medium formed by all the remaining $(N-2)$ atoms, each localized at a particular lattice site*. However, the second line shows that the medium is in fact uniform (vacuous). Since the potential $v(r)$ employed does not have a bound state, one concludes that no localization of the atoms can be expected if one truncates E_V at E_{2V} in an *unrestricted* variational calculation.[2] In other words, $E_T + E_{2V}$ does not exhibit an absolute minimum at a finite α. Upon the inclusion

of E_{3V}, it becomes physically possible to obtain localization. NMH have found that, by restricting their class of trial correlation functions $f(r)$ to those for which E_{3V} is small, they can truncate their E_V at E_{2V} and still obtain an energy minimum at a finite α, and that this minimum is not significantly altered by the inclusion of E_{3V}. However, if the restrictions on $f(r)$ are too severe, the localizing minimum may be very far from, and indeed quite unrelated to, the true absolute minimum. Our method of calculation will suggest the local nature of such a minimum and at the same time relax some of these restrictions.

We retain Eqs. (1) through (6). To evaluate $W(\beta)$, an average quantity $\langle A(r_1,r_2\cdots,r_k)\rangle$ is introduced, different

[7] N. G. Van Kampen, Physica **27**, 783 (1961).

from that of NMH:

$$\langle A(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_k)\rangle = \int \phi^2(|\mathbf{r}_1-\mathbf{R}_1|)\phi^2(|\mathbf{r}_2-\mathbf{R}_2|)\cdots\phi^2(|\mathbf{r}_k-\mathbf{R}_k|)\prod_{i<j} f^2(r_{ij})A(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_k)d\mathbf{r}_{12\ldots N}. \tag{10}$$

Then,

$$W(\beta)=\Big\langle \prod_{i<j} e^{\beta V(r_{ij})}\Big\rangle. \tag{11}$$

Let $q_{ij}\equiv e^{\beta V(r_{ij})}$ for convenience. $W(\beta)$ is then evaluated with the aid of the following cluster development:

$$W^{(2)}(\beta)=\prod_{i<j}\langle q_{ij}\rangle,$$

$$W^{(3)}(\beta)=W^{(2)}(\beta)\prod_{i<j<k}\frac{\langle q_{ij}q_{jk}q_{ki}\rangle}{W_{ijk}^{(2)}}, \tag{12}$$

$$W^{(N)}(\beta)=W^{(N-1)}(\beta)\prod_{i_1<i_2\cdots<i_N}\frac{\langle q_{i_1i_2}q_{i_1i_3}\cdots q_{i_{N-1}i_N}\rangle}{W_{i_1i_2\cdots i_N}^{(N-1)}}=W^{(N-1)}(\beta)\frac{\langle q_{12}q_{13}\cdots q_{N-1,N}\rangle}{W_{12\ldots N}^{(N-1)}}=\langle q_{12}q_{13}\cdots q_{N-1,N}\rangle\equiv W(\beta).$$

$W_{i_1i_2\cdots i_{n+1}}^{(n)}$ in the denominators denotes $W^{(n)}(\beta)$ for a system of $(n+1)$ atoms labeled i_1, i_2, $\cdots$, i_{n+1}. This cluster development is identical to that of NMH, except for the definition of $\langle\ \rangle$. The expansion is independent of the way in which $\langle\ \rangle$ is defined, and the rate of convergence in either case must be established numerically.

Correspondingly, our E_V is given by

$$E_V=E_V^{(2)}+E_V^{(3)}+\cdots,$$

$$E_V^{(2)}=\sum_{i<j}\frac{\int\phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-\mathbf{R}_j|)\{\prod_{k<l} f^2(r_{kl})\}V(r_{ij})d\mathbf{r}_{12\ldots N}}{\int\phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-\mathbf{R}_j|)\{\prod_{k<l} f^2(r_{kl})\}d\mathbf{r}_{12\ldots N}},$$

$$E_V^{(3)}=\frac{1}{2}\sum_{i,j,k}{}'\frac{\int\phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-\mathbf{R}_j|)\phi^2(|\mathbf{r}_k-\mathbf{R}_k|)\{\prod_{l<m} f^2(r_{lm})\}V(r_{ij})d\mathbf{r}_{12\ldots N}}{\int\phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-\mathbf{R}_j|)\phi^2(|\mathbf{r}_k-\mathbf{R}_k|)\{\prod_{l<m} f^2(r_{lm})\}d\mathbf{r}_{12\ldots N}}-(N-2)E_V^{(2)},\ \text{etc.}$$

$$\tag{13}$$

Comparing Eqs. (13) with Eqs. (9), we note that our $E_V^{(i)}$ differs from NMH's E_{iV} in that all particles are correlated in each order of the expansion. (All integrals appearing in our expressions are subsequently many-body integrals.) $E_V^{(2)}$ describes pairs of correlated atoms i and j moving in a medium formed by the remaining $(N-2)$ atoms, *correlated to each other and to atoms i and j.* Although in an unrestricted variational calculation the truncation of E_V at $E_V^{(2)}$ still fails to localize the atoms, such a truncation of E_V at any stage $E_V^{(i)}$ has included more physical information than a truncation of E_V at a corresponding stage of the NMH procedure. Better convergence of the expansion is therefore expected.

Next, we define some "liquid distribution functions," $P_n(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_n)$, in order to express Eqs. (13) in more useful forms. Let P_n be defined by

$$P_n(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_n)=N(N-1)\cdots(N-n+1)\frac{\int\{\prod_{i<j} f^2(r_{ij})\}d\mathbf{r}_{n+1,\ldots,N}}{\int\{\prod_{i<j} f^2(r_{ij})\}d\mathbf{r}_{12\ldots N}}. \tag{14}$$

In particular, we have

$$P_2(\mathbf{r}_1,\mathbf{r}_2)=N(N-1)\frac{\int\{\prod_{i<j} f^2(r_{ij})\}d\mathbf{r}_{34\ldots N}}{\int\{\prod_{i<j} f^2(r_{ij})\}d\mathbf{r}_{12\ldots N}}\equiv\rho^2 G(r_{12}), \tag{15}$$

and

$$P_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=N(N-1)(N-2)\frac{\int\{\prod_{i<j} f^2(r_{ij})\}d\mathbf{r}_{45\ldots N}}{\int\{\prod_{i<j} f^2(r_{ij})\}d\mathbf{r}_{12\ldots N}}. \tag{16}$$

The reason for naming these the "liquid distribution functions" is obvious: If one uses a Jastrow-type trial wave function $\prod_{i>j} f(r_{ij})$ to describe a liquid, these functions will be recognized as the distribution functions for the

liquid. The use of these functions greatly simplifies Eqs. (13), reducing the many-body integrals in $E_V^{(i)}$ to i-body integrals; thus

$$E_V^{(2)} = \sum_{i<j} \frac{\int \phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-\mathbf{R}_j|)V(r_{ij})G(r_{ij})d\mathbf{r}_i d\mathbf{r}_j}{\int \phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-\mathbf{R}_j|)G(r_{ij})d\mathbf{r}_i d\mathbf{r}_j},$$

$$E_V^{(3)} = \tfrac{1}{2}\sum_{i,j,k}' \frac{\int \phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-{}_j\mathbf{R}|)\phi^2(|\mathbf{r}_k-\mathbf{R}_k|)V(r_{ij})P_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k)d\mathbf{r}_i d\mathbf{r}_j d\mathbf{r}_k}{\int \phi^2(|\mathbf{r}_i-\mathbf{R}_i|)\phi^2(|\mathbf{r}_j-\mathbf{R}_j|)\phi^2(|\mathbf{r}_k-\mathbf{R}_k|)P_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k)d\mathbf{r}_i d\mathbf{r}_j d\mathbf{r}_k} - (N-2)E_V^{(2)}, \text{ etc.} \quad (17)$$

$E_V^{(2)}$ can be simplified further by the transformation of $\mathbf{r}_i$ and $\mathbf{r}_j$ to the center-of-mass coordinates $\mathbf{R}=\tfrac{1}{2}(\mathbf{r}_i+\mathbf{r}_j)$ and the relative coordinates $\mathbf{r}=\mathbf{r}_j-\mathbf{r}_i$, resulting in

$$\frac{E_V^{(2)}}{N} = \sum_d \tfrac{1}{2}n_d e^{(2)}(d;\alpha),$$

$$e^{(2)}(d;\alpha)$$

$$= \frac{\int_0^\infty rV(r)G(r)\sinh(\alpha^2 rd)e^{-1/2\alpha^2(r^2+d^2)}dr}{\int_0^\infty rG(r)\sinh(\alpha^2 rd)e^{-1/2\alpha^2(r^2+d^2)}dr}, \quad (18)$$

where the summation over d is performed over all shells about a fixed lattice site, d and n_d denoting the radius of the shell and the number of lattice sites in that shell.

Let us for the moment investigate the special case $\alpha=0$. Equations (1) and (2) reduce ψ to a Jastrow-type trial wave function appropriate for a boson liquid,

$$\psi_{\text{liq}}(1,2,\cdots,N) = \prod_{i<j} f(r_{ij}). \quad (19)$$

$G(r)$ becomes now the radial distribution function of the liquid described by ψ_{liq}. From Eqs. (4), (17), (15), and (13),

$$E_T = 0, \quad (20)$$

$$E_V^{(2)} = \sum_{i<j} \frac{\int V(r_{ij})G(r_{ij})d\mathbf{r}_i d\mathbf{r}_j}{\int G(r_{ij})d\mathbf{r}_i d\mathbf{r}_j}$$

$$= \tfrac{1}{2}N(N-1)\frac{\int V(r)G(r)d\mathbf{r}}{\int G(r)d\mathbf{r}}$$

$$= \tfrac{1}{2}N\rho \int V(r)G(r)d\mathbf{r}, \quad (21)$$

$$E_V^{(3)} = \tfrac{1}{2}\sum_{i,j,k}' \frac{\int\{\prod_{l<m} f^2(r_{lm})\}V(r_{ij})d\mathbf{r}_{12\ldots N}}{\int\{\prod_{l<m} f^2(r_{lm})\}d\mathbf{r}_{12\ldots N}}$$

$$- (N-2)E_V^{(2)} = 0. \quad (22)$$

Likewise, all higher orders in the E_V expansion yield zero exactly. Thus, for $\alpha=0$ our cluster expansion converges immediately and exactly, the energy expectation being given by

$$E_{\text{liq}} = E_T + E_V^{(2)} = \tfrac{1}{2}N\rho \int V(r)G(r)d\mathbf{r}, \quad (23)$$

which reduces to the more familiar form

$$E_{\text{liq}} = N\frac{\rho\hbar^2}{4m}\int \nabla \ln f(r)\cdot\nabla G(r)d\mathbf{r} + \tfrac{1}{2}N\rho\int v(r)G(r)d\mathbf{r}.$$

We now return to the more general case of finite α's. To evaluate $E_V^{(i)}$, we must possess the knowledge of $G(r)$, $P_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$, etc., corresponding to each choice of $f(r)$. (It must be emphasized here that these "liquid distribution functions" are not simply related to the distribution functions of the crystal: They have been introduced only for mathematical convenience.) Of several integral equations relating $f(r)$ to these distribution functions, we have chosen to use the BBGKY equation

$$\nabla_1 G(r_{12}) = G(r_{12})\nabla_1 \ln f^2(r_{12})$$

$$+ \rho G(r_{12})\int G(r_{23})G(r_{31})\nabla_1 \ln f^2(r_{13})d\mathbf{r}_3, \quad (24)$$

which embodies the Kirkwood superposition approximation (KSA) for $P_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$:

$$P_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \approx \rho^3 G(r_{12})G(r_{23})G(r_{31}). \quad (25)$$

Upon the substitution of Eq. (25) into Eq. (17), $E_V^{(3)}$ takes on a usable form. In fact, $E_V^{(2)}$ and $E_V^{(3)}$ are identical to NMH's E_{2V} and E_{3V}, with $f^2(r)$ replaced by $G(r)$. However, $f^2(r)$ still enters our energy formulas through $V(r)$.

III. RESULTS AND DISCUSSION

The simultaneous solution of Eqs. (24) and (25) starts with a parametrized $G(r)$. A complicated but efficient numerical procedure described in an earlier

paper[8] is then used to carry out an iterative solution for $f(r)$. The form of $f(r)$ is dictated by that of $G(r)$, given in Ref. 8, which involves five independent parameters and is consequently rather flexible. We have carried out an extensive investigation of the truncated energy

$$E^{(2)} = E_T + E_V^{(2)}. \tag{26}$$

In Fig. 1, we exhibit a set of $E^{(2)}(\alpha^2)$ curves for a family of η at the experimental density of the solid $\rho = 0.0244$ Å^{-3} (nearest-neighbor distance equal to 3.76 Å), η being one of the five parameters, the most important in that it determines the scale of the wave function. For each η, the curve shown corresponds to having the remaining four parameters optimized for the boson liquid, i.e., $E^{(2)}$ at $\alpha = 0$ is minimized. While varying these parameters independently over wide ranges, we have found that such a choice of these four parameters invariably gives the best energy minimum, even when the minimum is not at $\alpha = 0$. For small α (say, $\alpha < 1$), the energy curves become gradually inaccurate (indicated by broken lines), as the single-particle functions ϕ become more spread out, so that (1) the exchange effect is no longer negligible, (2) the summation over d in Eq. (18) needs to be extended far beyond the 38 shells that we have used for all our calculations, and more importantly (3) the truncated form of E_V becomes progressively inaccurate. The latter two sources of error are absent for $\alpha = 0$, for we have shown in Eq. (21) that all shells have been accounted for, and in Eq. (22) that $E_V^{(i)} = 0$, $i > 2$. However, these energies at $\alpha = 0$, indicated by circles in Fig. 1, must be corrected for the exchange effect. We have shown in a previous paper[9] how the effect of statistics may be incorporated in this approach for liquid He³. Using that method, the boson liquid energies have been adjusted to give energy expectation values for the corresponding fermion liquid. These values are shown as crosses in Fig. 1. Based on the all-important assumptions that the exchange energies are insignificant for large α^1, and that the cluster expansion converges well for large α (the latter to be discussed presently), we note then that in spite of the localizing minimum of approximately 5°K at $\alpha \approx 1$ ($\eta = 1.70$), the absolute minimum occurs at $\alpha = 0$. This shows that at $\rho = 0.0244$ Å^{-3} the liquid phase is preferred in our theory. It is, however, expected on physical grounds that an extension of this calculation to higher densities will yield absolute energy minima corresponding to solidlike wave functions.

NMH also obtain a localizing minimum of 4.8°K at $\alpha^2 = 1.30$. Furthermore, if the NMH calculation is extended beyond their restricted range (by letting their parameter σ become large), one finds that the $(E_T + E_{2V})$ versus α^2 envelope shows a similar behavior to Fig. 1;
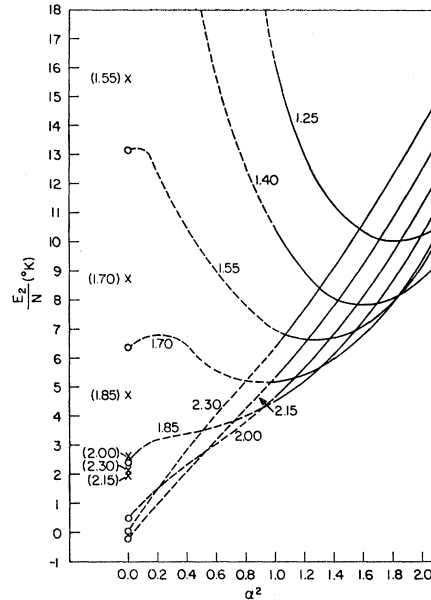
[8] W. E. Massey, Phys. Rev. **151**, 153 (1966).
[9] C. W. Woo, Phys. Rev. **151**, 138 (1966).

FIG. 1. $E^{(2)}(\alpha^2)$ versus α^2 for several values of the parameter η at $\rho = 0.0244$ Å^{-3}. Circles indicate mass-3 boson energies, crosses indicate liquid He³ energies.

in particular, as σ increases, the localizing minimum gradually disappears. The inaccuracies mentioned above for small α are likewise present in their expansion; these inaccuracies in fact persist at $\alpha = 0$. Therefore, a comparison between the liquid and solid minima is not possible. Since our classes of $f(r)$ do not include the NMH $f(r)$, we have not simulated their calculation within our theory. This, however, can be done by simply obtaining a $G(r)$ corresponding to NMH's $f(r)$ through an integral equation or a Monte Carlo type calculation.

Justification for the neglect of our $E_V^{(3)}$ (and higher-order terms) in our cluster expansion of the energy can of course come only from an exact evaluation. However, support for the assumption that $E_V^{(3)}$ is small within the range of functions studied here comes from the following analysis. In Ref. 1, NMH discussed
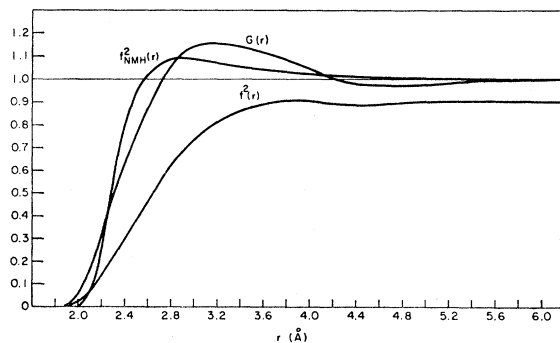

FIG. 2. The correlation function $f^2(r)$ and the distribution function $G(r)$ for $\eta = 1.70$. $f_{\text{NMH}}^2(r)$ is the optimum NMH correlation function.

TABLE I. Shell-by-shell contribution to $E_V{}^{(2)}$ and E_{2V} at $\alpha=1.2$, in °K.

Shell No.	Contribution to $E_V{}^{(2)}$	Contribution to NMH's E_{2V}
1	−3.8	−3.3
2	−4.3	−4.9
3	−1.6	−1.8
4	−1.4	−1.3
5	−0.3	−0.3
6	−0.1	−0.1

in detail the factors which affect the size of E_{3V} (and higher-order terms) in their expansion, the most important being that $f^2(r)$ be of short range and close to unity in the region where the single-particle Gaussians are large. This condition applies not to our $f^2(r)$ but to $G(r)$ as is evident from the structure of our energy formulas. In Fig. 2, we show an NMH $f^2(r)$ which satisfies this condition and for which the third-order energy E_{3V} has been calculated explicitly to be smaller than E_{V2} by two orders of magnitude. Also shown in Fig. 2 are our $f^2(r)$ and the corresponding $G(r)$ for $\eta=1.70$. The qualitative similarity between NMH's $f^2(r)$ and our $G(r)$ is evident. Quantitatively, this similarity is strengthened by the comparison of the shell-by-shell contributions to the energy in Table I. Thus $E_V{}^{(3)}$ is expected to be of the same order of magnitude as NMH's E_{3V}.

We have investigated a large class of $f(r)$, among which are those meeting NMH's criterion and those which obviously do not (e.g., Fig. 2). However, in our procedure each of these $f(r)$ generates a $G(r)$ that qualitatively satisfies the condition for quick convergence. Hence, as indicated earlier, our procedure permits a wider variation in $f(r)$.

Now a word about the application of the KSA. The magnitude of the error introduced by the use of this approximation can be estimated in the following manner. Note that the substitution of Eq. (24) in Eq. (4) allows $e^{(2)}(d;\alpha)$ in Eq. (18) to be written as a sum of two terms, denoted as $e_A{}^{(2)}$ and $e_B{}^{(2)}$. The KSA enters only through $e_B{}^{(2)}$, which for the classes of $f(r)$ considered is invariably smaller than $e_A{}^{(2)}$ by a factor of 5. Thus, an error of as much as 20% in $e_B{}^{(2)}$ due to the KSA will shift $E_V{}^{(2)}/N$ by only about 0.5°K.

We are continuing this investigation along the following lines: (1) the numerical evaluation of $E_V{}^{(3)}$, (2) a calculation of $G(r)$ for NMH's $f(r)$ and the subsequent application of the $G(r)$ to our energy formulas, and (3) an extension of this calculation to higher densities to observe the possible occurrence of the phase transition.

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