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Theory of quantum solids: Effect of lattice symmetry and anisotropy in the pair-correlation function

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The theory of quantum solids by Lowy and Woo employs a Hartree-Jastrow wave function in which the Hartree product, thus the wave function, is given its proper exchange symmetry. Coupled integral equations were derived for the one- and two-particle distribution functions, which enter into the energy expression. On account of mathematical and computational complications, the two-particle distribution function was not obtained from actually solving the integral equations. Instead, it was approximated by a product of two one-particle distribution functions with the pair-correlation function for the *liquid*. The latter lacks the proper lattice symmetry, and is not anisotropic. In this paper, we take into account the effects of both lattice symmetry and anisotropy on the pair-correlation function, solve the coupled integral equations to higher orders, and recalculate the energy curves. It is shown that lattice symmetry in the pair-correlation function lowers the liquid-to-solid transition density by about 2%, while anisotropy raises it by about 7%.

I. INTRODUCTION

The more successful treatments of the ground state of quantum crystals have all employed variational wave functions of the Hartree-Jastrow form, in which the Hartree product (of single-particle orbitals) is modified by a product of pair-correlating factors. Earlier variational calculations[1,2] had shared two common pitfalls. First, the single-particle orbitals had been taken as individually localized about lattice sites. As a consequence the Hartree product, and thus the wave function, failed to possess exchange symmetries which are appropriate for quantum crystals. Second, the energy expectation value had been evaluated with the help of cluster expansion procedures. In each case, mathematical complexities and computer limitations had required that the cluster series be truncated at a *very* low order. The mode of truncation was justified on the basis of physical insight which was less than reliable.

In 1976, we advanced a new variational method for treating the ground state of *Bose* solids.[3] In this theory, the single-particle orbitals have the prescribed lattice symmetry. Each is periodic and localized about *every* lattice site. Thus the Hartree-Jastrow wave function is symmetric with respect to particle exchange. Also, the energy expectation value is expressed in terms one- and two-particle distribution functions which are solutions of coupled integral equations. Thus the theory abstains from cluster expansions. It describes a procedure which sums the cluster series approximately to all orders.

In the actual solution of the coupled integral equations, a short cut was taken. The equation for the two-particle distribution function was solved only in the lowest order, rendering a liquidlike short-range pair correlation. The latter was then entered into the equation for the one-particle distribution function for an accurate solution of the density distribution. It was (and remains) our belief that for close-packed structures the short-range pair correlations are indeed liquidlike, and the approximation is highly reliable. However, some questions were raised[4] on the validity of such an approximation. In the desire that our theory, which has, we hope distinguished itself by the use of a properly symmetrized wave function and its abstention from cluster expansion procedures, not be marred by an approximation introduced purely for computational convenience, we conduct an investigation on the effects of the approximation. The equations for the one- and two-particle distribution function are solved to higher orders. The short-range pair-correlation function is first given its proper lattice symmetry in an isotropic approximation, and then proper anisotropy is introduced. We are able to demonstrate that at least for solid ^{4}He the corrections are not large.

II. GENERAL FORMALISM

For a system consisting of N molecules in volume Ω (such that the number density ρ equals N/Ω) governed by pairwise, central interactions, the Hamiltonian is given by

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

where $r_{ij}=|\vec{r}_i-\vec{r}_j|$. The Hartree-Jastrow wave function takes the form

$$\psi(\vec{r}_1,\ldots,\vec{r}_N)=\prod_{i=1}^{N}\phi(\vec{r}_i)\prod_{j<k,=1}^{N}e^{u(r_{jk})/2} \ . \tag{2}$$

$\phi(\vec{r})$ denotes a single-particle orbital, and $e^{u(r)/2}$ represents a pair-correlating factor which goes to zero when two strongly repulsive molecules overlap, and to unity when they move too far apart to interact. In Ref. 3, hereafter to be referred to as the Lowy-Woo theory, $\phi(\vec{r})$ is expanded in the reciprocal-lattice space

$$\phi(\vec{r})=\exp\left[\sum_{\vec{G}}t_{\vec{G}}e^{i\vec{G}\cdot\vec{r}}\right] \ , \tag{3}$$

where $\vec{G}$ denotes reciprocal-lattice vectors. The wave function ψ is thus symmetric with respect to particle exchange. Equation (2) is not of the most general form, but it is quite acceptable for describing a Bose solid which possesses strong short-range pair correlations. Where multiparticle correlations are important, Eq. (2) can be modified to include higher-order correlating factors.[5] A particular advantage of such a wave function is that it includes as a limiting case (when $t_{\vec{G}}=0$ for all $\vec{G}\neq 0$) a description of the liquid phase.

We define the n-particle distribution function as

$$p^{(n)}(1,\ldots,n)=\frac{N!}{(N-n)!}\frac{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_{n+1},\ldots,d\vec{r}_N}{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_1,\ldots,d\vec{r}_N} \ . \tag{4}$$

In particular, the one-particle distribution function

$$p^{(1)}(1)=N\frac{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_2,\ldots,d\vec{r}_N}{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_1,\ldots,d\vec{r}_N} \tag{5}$$

gives the density distribution. It describes long-range order in broken symmetry. The two-particle distribution function

$$p^{(2)}(1,2)=N(N-1)\frac{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_3,\ldots,d\vec{r}_N}{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_1,\ldots,d\vec{r}_N}\equiv p^{(1)}(1)p^{(1)}(2)g(1,2) \tag{6}$$

gives additional information on pair correlations. In liquid phase, $p^{(1)}(1)$ reduces to ρ, and $g(1,2)$ to the radial distribution function $g_0(r_{12})$. In this paper, we shall also need the three-particle distribution function

$$p^{(3)}(1,2,3)=N(N-1)(N-2)\frac{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_4,\ldots,d\vec{r}_N}{\int|\psi(\vec{r}_1,\ldots,\vec{r}_N)|^2d\vec{r}_1,\ldots,d\vec{r}_N}\equiv p^{(1)}(1)p^{(1)}(2)p^{(1)}(3)g_3(1,2,3) \ . \tag{7}$$

In the Kirkwood superposition approximation (KSA), $g_3(1,2,3)$ takes the form

$$g_3(1,2,3)\approx g(1,2)g(2,3)g(3,1) \ . \tag{8}$$

In terms of these distribution functions, the energy expectation value is given by

$$\begin{aligned}E&\equiv\langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle\\&=\frac{-\hbar^2}{4m}\int p^{(1)}(1)\nabla_1^2\ln\phi(\vec{r}_1)\,d\vec{r}_1\\&\quad+\frac{1}{2}\int p^{(2)}(1,2)\tilde{v}(r_{12})\,d\vec{r}_1d\vec{r}_2 \ ,\end{aligned} \tag{9}$$

where

$$\tilde{v}(\vec{r})=v(r)-(\hbar^2/4m)\nabla^2u(r) \ . \tag{10}$$

Let us employ the center-of-mass coordinate system and introduce the variables

$$\vec{s}=\tfrac{1}{2}(\vec{r}_1+\vec{r}_2) \ , \tag{11}$$

$$\vec{r}=\vec{r}_2-\vec{r}_1 \ . \tag{12}$$

First we expand the density in the reciprocal-lattice space, in *two* ways for later convenience:

$$p^{(1)}(1)=\rho\sum_{\vec{G}}p_{\vec{G}}e^{i\vec{G}\cdot\vec{r}_1} \tag{13}$$

and

$$p^{(1)}(1)=\frac{1}{\lambda}\exp\left[\sum_{\vec{G}}\Pi_{\vec{G}}e^{i\vec{G}\cdot\vec{r}_1}\right] \ , \tag{14}$$

where λ is a normalization constant. Next, we apply lattice symmetry to $p^{(n)}(1,\ldots,n)$:

$$p^{(n)}(1,\ldots,n)\equiv p^{(n)}(\vec{r}_1,\ldots,\vec{r}_n)=p^{(n)}(\vec{r}_1+\vec{R},\ldots,\vec{r}_n+\vec{R})\ , \tag{15}$$

where $\{\vec{R}\}$ denotes the set of lattice vectors, and realize that

$$g(1,2)\equiv g(\vec{r}_1,\vec{r}_2)=g(\vec{r}_1+\vec{R},\vec{r}_2+\vec{R}) \tag{16}$$

permits $g(1,2)$ to be expanded in the reciprocal-lattice space in the position coordinates $\vec{s}$ and $\vec{r}$:

$$g(1,2)=\sum_{\vec{G}} g_{\vec{G}}(\vec{r})e^{i\vec{G}\cdot\vec{s}}\ . \tag{17}$$

Again, with μ in the role of a normalization constant, we write for later convenience also the expansion

$$g(1,2)=\frac{1}{\mu}\exp\left[\sum_{\vec{G}}\gamma_{\vec{G}}(\vec{r})e^{i\vec{G}\cdot\vec{s}}\right]\ . \tag{18}$$

Finally we note that the KSA, Eq. (8), is consistent with the lattice symmetry condition (15).

We are now ready to derive equations for the distribution functions.

First, differentiate Eq. (5) with respect to $\vec{r}_1$ and introduce Eq. (6). We find

$$\nabla_1 p^{(1)}(1)=p^{(1)}(1)\nabla_1\ln\phi^2(\vec{r}_1)+\int p^{(2)}(1,2)\nabla_1 u(r_{12})\,d\vec{r}_2 \tag{19}$$

or

$$\nabla_1\ln p^{(1)}(1)=\nabla_1\ln\phi^2(\vec{r}_1)+\int p^{(1)}(\vec{r}_2)g(1,2)\nabla_1 u(r_{12})\,d\vec{r}_2\ . \tag{20}$$

With the help of Eqs. (3), (11)–(14), and (17), we reduce it to a relation between the quantities $\Pi_{\vec{G}}$, $p_{\vec{G}}$, and $g_{\vec{G}}(\vec{r})$, for given $t_{\vec{G}}$ and $u(r)$:

$$\Pi_{\vec{G}}-2t_{\vec{G}}=i\rho\sum_{\vec{G}'}p_{\vec{G}-\vec{G}'}\int\frac{\vec{G}\cdot\hat{r}}{G^2}u'(r)g_{\vec{G}'}(\vec{r})e^{i(\vec{G}-\vec{G}'/2)\cdot\vec{r}}\,d\vec{r}\ . \tag{21}$$

Next, differentiate Eq. (6) with respect to the relative coordinate $\vec{r}$ and introduce Eq. (7). We obtain

$$\nabla p^{(2)}(1,2)=p^{(2)}(1,2)[\nabla\ln\phi^2(\vec{r}_1)+\nabla\ln\phi^2(\vec{r}_2)+\nabla u(r_{12})]+\int p^{(3)}(1,2,3)[\nabla u(r_{13})+\nabla u(r_{23})]\,d\vec{r}_3\ . \tag{22}$$

In the KSA it reduces to

$$\begin{aligned}\nabla\ln p^{(1)}(1)+\nabla\ln p^{(1)}(2)+\nabla\ln g(1,2)=&\ \nabla\ln\phi^2(\vec{r}_1)+\nabla\ln\phi^2(\vec{r}_2)+\nabla u(r_{12})\\&+\int p^{(1)}(3)g(1,3)g(2,3)[\nabla u(r_{13})+\nabla u(r_{23})]\,d\vec{r}_3\ .\end{aligned} \tag{23}$$

With the help of Eqs. (3), (11)–(14), (17), and (18), we then find a second relation between the quantities $\Pi_{\vec{G}}$, $p_{\vec{G}}$, $\gamma_{\vec{G}}(\vec{r})$, and $g_{\vec{G}}(\vec{r})$ for given $t_{\vec{G}}$ and $u(r)$:

$$\begin{aligned}\nabla\gamma_{\vec{G}}(\vec{r})=&\ \hat{r}u'(r)\delta_{\vec{G},0}+\vec{G}(\Pi_{\vec{G}}-2t_{\vec{G}})\sin\tfrac{1}{2}\vec{G}\cdot\vec{r}\\&+\rho\sum_{\vec{G}',\vec{G}''}p_{\vec{G}-\vec{G}'-\vec{G}''}\int\hat{r}'u'(r')g_{\vec{G}'}(\vec{r}')g_{\vec{G}''}(\vec{r}-\vec{r}')\cos\left[\left(\vec{G}-\frac{\vec{G}'+\vec{G}''}{2}\right)\cdot\vec{r}'-\left(\frac{\vec{G}-\vec{G}''}{2}\right)\cdot\vec{r}\right]d\vec{r}'\ .\end{aligned} \tag{24}$$

In the case where only $\vec{G}=0$ components survive, this relation reduces to the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) equation for liquids, as expected.

Now, through the definitions (13) and (14) and (17) and (18), we have two more relations

$$p_{\vec{G}}=\frac{1}{N\lambda}\int\left[\exp\sum_{\vec{G}'}\Pi_{\vec{G}'}e^{i\vec{G}'\cdot\vec{r}}\right]e^{-i\vec{G}\cdot\vec{r}}\,d\vec{r} \tag{25}$$

and

$$g_{\vec{G}}(\vec{r})=\frac{1}{\Omega\mu}\int\left[\exp\sum_{\vec{G}'}\gamma_{\vec{G}'}(\vec{r})e^{i\vec{G}'\cdot\vec{r}}\right]e^{-i\vec{G}\cdot\vec{s}}\,d\vec{s}\ . \tag{26}$$

Equations (21) and (24)–(26) are to be solved simultaneously for $\Pi_{\vec{G}}$, $p_{\vec{G}}$, $\gamma_{\vec{G}}(\vec{r})$, and $g_{\vec{G}}(\vec{r})$, and in turn $p^{(1)}(1)$ and $g(1,2)$.

The energy expression (9) reduces to

$$E=N\sum_{\vec{G}}\left[\frac{\hbar^2}{4m}p_{\vec{G}}t_{\vec{G}}G^2+\tfrac{1}{2}\rho\sum_{\vec{G}'}p_{\vec{G}}p_{\vec{G}+\vec{G}'}\int\tilde{v}(r)g_{\vec{G}'}(\vec{r})e^{i(\vec{G}+\vec{G}'/2)\cdot\vec{r}}\,d\vec{r}\right]\ . \tag{27}$$

III. $g(1,2)$ WITH PROPER LATTICE SYMMETRY

In this section we would like to investigate the effect of imposing on $g(1,2)$ its proper spatial symmetry. We shall assume, however, that $g(1,2)$ is dominated by its isotropic part. In other words, we write

$$g(1,2)=g_I(1,2)+\delta g(1,2) \tag{28}$$

and assume $\delta g(1,2)$ small compared to $g_I(1,2)$, where[6]

$$g_I(1,2)=\sum_{\vec{G}} g_{\vec{G}}(r_{12})e^{i\vec{G}\cdot\vec{s}} \tag{29}$$

$$=\frac{1}{\mu}\exp\sum_{\vec{G}}\gamma_{\vec{G}}(r_{12})e^{i\vec{G}\cdot\vec{s}} \;. \tag{30}$$

The assumption is introduced to simplify the numerical work in Sec. IV. What we have now is a situation under which the short-range correlation between a pair of molecules depends on *where* the pair sits in the unit cell, but *not* on the *orientation* of the pair axis. In Sec. V we shall investigate the effect of introducing anisotropy into $g(1,2$

We might reexamine the equations for $p^{(1)}$ and $g(1,2)$. For $g(1,2)$ we could have started with a differentiation with respect to $\vec{r}_1$, as in Ref. 3. There, Eq. (20) gives

$$\nabla_1 p^{(2)}(1,2)=p^{(2)}(1,2)[\nabla_1\ln\phi^2(\vec{r}_1)+\nabla_1 u(r_{12})]+\int p^{(3)}(1,2,3)\nabla_1 u(r_{13})d\vec{r}_3 \tag{31}$$

or, as in Eq. (30) of Ref. 3, now with $g_I(1,2)$ replacing $g(1,2)$:

$$\nabla_1\ln g_I(1,2)=\nabla_1 u(r_{12})+\int p^{(1)}(3)g_I(1,3)[g_I(2,3)-1]\nabla_1 u(r_{13})\,d\vec{r}_3 \;. \tag{32}$$

In place of Eqs. (21) and (24) we now have

$$\Pi_{\vec{G}}-2t_{\vec{G}}=i\rho\sum_{\vec{G}'}p_{\vec{G}-\vec{G}'}\int\frac{\vec{G}\cdot\hat{r}}{G^2}u'(r)g_{\vec{G}'}(r)e^{i(\vec{G}-\vec{G}'/2)\cdot\vec{r}}\,d\vec{r} \tag{33}$$

and

$$\begin{aligned}-i(\vec{G}/2)\gamma_{\vec{G}}(r)+\hat{r}\gamma'_{\vec{G}}(r)-\hat{r}u'(r)\delta_{\vec{G},0}={}&i\vec{G}\,(\Pi_{\vec{G}}-2t_{\vec{G}})e^{-i\vec{G}/2\cdot\vec{r}}\\&+\rho\sum_{\vec{G}',\vec{G}''}p_{\vec{G}-\vec{G}'-\vec{G}''}e^{-i[(\vec{G}-\vec{G}'')/2]\cdot\vec{r}}\\&\times\int\hat{r}'u'(r')g_{\vec{G}'}(r')g_{\vec{G}''}(|\vec{r}-\vec{r}'|)e^{i[\vec{G}-(\vec{G}'+\vec{G}'')/2]\cdot\vec{r}'}\,d\vec{r}'\;.\end{aligned} \tag{34}$$

Our next task is to reduce them to manageable forms.

Equation (33) is easy to handle. The integral

$$I=\int\hat{G}\cdot\hat{r}u'(r)g_{\vec{G}'}(r)e^{i(\vec{G}-\vec{G}'/2)\cdot\vec{r}}\,d\vec{r}$$

reduces to

$$I=\frac{-4\pi i}{G_1^2}(\hat{G}\cdot\hat{G}_1)\int u'(r)g_{\vec{G}'}(r)(G_1r\cos G_1r-\sin G_1r)\,dr \;, \tag{35}$$

where

$$\vec{G}_1\equiv\vec{G}-\vec{G}'/2 \;. \tag{36}$$

This can be seen with the aid of Fig. 1. Thus, Eq. (33) becomes

$$\Pi_{\vec{G}}-2t_{\vec{G}}=4\pi\rho\sum_{\vec{G}'}p_{\vec{G}-\vec{G}'}\frac{1}{GG_1^3}\left(G-\frac{G'}{2}(\hat{G}\cdot\hat{G}')\right)\int u'(r)g_{\vec{G}'}(r)(G_1r\cos G_1r-\sin G_1r)\,dr \;. \tag{37}$$

Equation (34) requires more work. We take its inner product with $\hat{r}$ and integrate over the direction of $\hat{r}$, obtaining in the end

$$\gamma'_{\vec{G}}(r)=u'(r)\delta_{\vec{G},0}-\frac{4}{Gr^2}(\Pi_{\vec{G}}-2t_{\vec{G}})\left(\tfrac{1}{2}Gr\cos\tfrac{1}{2}Gr-\sin\tfrac{1}{2}Gr\right)+\frac{\rho}{4\pi}\sum_{\vec{G}',\vec{G}''}p_{\vec{G}-\vec{G}'-\vec{G}''}J \;, \tag{38}$$

with the integral J given by

$$\begin{aligned}J&=\int d\hat{r}\int d\vec{r}'(\hat{r}\cdot\hat{r}')u'(r')g_{\vec{G}'}(r')g_{\vec{G}''}(|\vec{r}-\vec{r}'|)e^{i[\vec{G}-(\vec{G}'+\vec{G}'')/2]\cdot\vec{r}'}e^{-i[(\vec{G}-\vec{G}'')/2]\cdot\vec{r}}\\&=\int d\vec{r}'u'(r')g_{\vec{G}'}(r')e^{i\vec{G}_2\cdot\vec{r}'}\int d\hat{r}(\hat{r}\cdot\hat{r}')g_{\vec{G}''}(|\vec{r}=\vec{r}'|)e^{-i\vec{G}_3\cdot\vec{r}} \;,\end{aligned} \tag{39}$$

where

$$\vec{G}_2 \equiv \vec{G} - (\vec{G}' + \vec{G}'')/2 \ , \tag{40}$$

$$\vec{G}_3 \equiv (\vec{G} - \vec{G}'')/2 \ . \tag{41}$$

In Appendix A, we show how J can be further simplified to yield

$$J = \frac{8\pi^2}{r^2} \sum_{l=0}^{\infty} (2l+1) j_l(G_3 r) \int H^l_{\vec{G}''}(r,r') u'(r') g_{\vec{G}'}(r') P_l(\hat{G}_2 \cdot \hat{G}_3) j_l(G_2 r')\, dr' \ , \tag{42}$$

where

$$H^l_{\vec{G}''}(r,r') = \tfrac{1}{2} \int_{|r-r'|}^{r+r'} P_l \left[\frac{r^2 + r'^2 - z^2}{2rr'} \right] g_{\vec{G}''}(z)(r^2 + r'^2 - z^2) z\, dz \ . \tag{43}$$

Consequently Eq. (38) reduces to the final form (for $\vec{G}=0$)

$$\begin{aligned}
-\int_{r_0}^{\infty} d\gamma_0(r) = {} & u(r_0) - \pi\rho \int_0^{\infty} ds\ u'(s) g_0(s) \int_{r_0-s}^{r_0+s} dt \frac{s^2-(t-r_0)^2}{r_0} t\,[g_0(|t|)-1] \\
& - \pi\rho \sum_{\{\vec{G}'\}}{}' w_{\vec{G}'} p_{\vec{G}'} \int_0^{\infty} ds\ u'(s) g_{\vec{G}'}(s) j_0\left[\frac{G's}{2}\right] \int_{r_0-s}^{r_0+s} dt \frac{s^2-(t-r_0)^2}{r_0} t g_0(|t|) \\
& - 2\pi\rho \sum_{\{\vec{G}'\}}{}' w_{\vec{G}'} p_{\vec{G}'} \sum_{l=0}^{\infty} (2l+1) \int_{r_0}^{\infty} dr \frac{j_l(G'r/2)}{r} \int_0^{\infty} dr' r' u'(r') j_l\left[\frac{G'r'}{2}\right] g_0(r') \\
& \times \int_{|r-r'|}^{r+r'} dz\ z \frac{r^2 + r'^2 - z^2}{2rr'} P_l \left[\frac{r^2 + r'^2 - z^2}{2rr'}\right] g_{\vec{G}'}(z) \ .
\end{aligned}$$

For $\vec{G} \neq 0$, (44)

$$\begin{aligned}
-\int_{r_0}^{\infty} d\gamma_{\vec{G}}(r) = {} & \frac{4}{G}(\Pi_{\vec{G}} - 2t_{\vec{G}}) \int_{r_0}^{\infty} dr \frac{1}{r^2} \left[\frac{Gr}{2} \cos\frac{Gr}{2} - \sin\frac{Gr}{2}\right] \\
& - 2\pi\rho p_{\vec{G}} \sum_{l=0}^{\infty} (2l+1) \int_{r_0}^{\infty} \frac{dr}{r} j_l\left[\frac{Gr}{2}\right] \int_0^{\infty} dr' r' u'(r') g_0(r') j_l(Gr') \\
& \times \int_{|r-r'|}^{r+r'} dz\ z \frac{r^2 + r'^2 - z^2}{2rr'} P_l \left[\frac{r^2 + r'^2 - z^2}{2rr'}\right] g_0(z) \\
& - 2\pi\rho \sum_{l=0}^{\infty} (2l+1) \sum_{\vec{G}'(\neq\vec{G})} p_{\vec{G}'} P_l \left[\frac{x+y}{(1+x^2+xy)^{1/2}}\right] \int_{r_0}^{\infty} \frac{dr}{r} j_l\left[\frac{G'r}{2}\right] \\
& \times \int_0^{\infty} dr' r' u'(r') g_0(r') j_l\left[\frac{Gr'}{2}(1+x^2+2xy)^{1/2}\right] \\
& \times \int_{|r-r'|}^{r+r'} dz\ z \frac{r^2 + r'^2 - z^2}{2rr'} P_l \left[\frac{r^2 + r'^2 - z^2}{2rr'}\right] g_{\vec{G}-\vec{G}'}(z) \\
& - 2\pi\rho \sum_{l=0}^{\infty} (2l+1) \sum_{\{\vec{G}'\}}{}' p_{\vec{G}-\vec{G}'} P_l \left[\frac{1-\frac{1}{2}xy}{(1+\frac{1}{4}x^2-xy)^{1/2}}\right] \\
& \times \int_{r_0}^{\infty} \frac{dr}{r} j_l\left[\frac{Gr}{2}\right] \int_0^{\infty} dr' r' u'(r') g_{\vec{G}}(r') j_l(Gr'(1+\tfrac{1}{4}x^2-xy)^{1/2}) \\
& \times \int_{|r-r'|}^{r+r'} dz\ z \frac{r^2 + r'^2 - z^2}{2rr'} P_l \left[\frac{r^2 + r'^2 - z^2}{2rr'}\right] g_0(z) \ ,
\end{aligned} \tag{45}$$

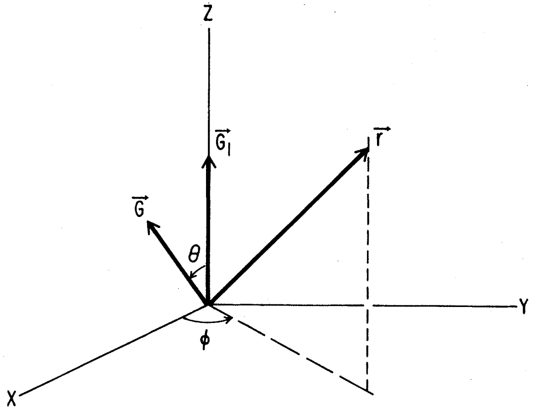

FIG. 1. Coordinate system for evaluating the integral I in Eq. (33).

where

$$x=G'/G \ , \tag{46}$$

$$y=\hat G\cdot\hat G' \ , \tag{47}$$

and the symbol $\sum'_{\{\vec G'\}}$ represents a summation over shells in the reciprocal space, each shell containing $w_{\vec G'}$ reciprocal-lattice points. The prime indicates the omission of $\vec G'=0$ from the sum. A four-dimensional integral form that appears repeatedly in the derivation has in the process been transformed into a simple two-dimensional integral, thus

$$\int_{r_0}^{\infty} dr \int d\vec r'(\hat r\cdot\hat r')U(r')V(|\vec r-\vec r'|) = \pi\int_0^\infty ds\; U(s)\int_{r_0-s}^{r_0+s} dt\; t\frac{s^2-(t-r_0)^2}{r_0}V(|t|) \ . \tag{48}$$

Note that a simplifying assumption has entered the derivation that leads to Eqs. (44) and (45). The assumption is that for all $\vec G\neq 0$ $g_{\vec G}(r)$ is very small compared to $g_0(r)$. This has enabled us to keep only terms which are linear in $g_{\vec G}(r)$, $\vec G\neq 0$. In writing out the double sum of Eq. (38), we omit terms which have simultaneously $\vec G'\neq 0$ and $\vec G''\neq 0$. Thus such terms do not appear in Eqs. (44) and (45). That such an assumption is valid must be demonstrated numerically. In the meantime, we wish to point out that the assumption is *not* related to our isotropic approximation. The isotropic approximation—which neglects $\delta g(1,2)$ in Eq. (28)—leaves $g(1,2)$ in the form of $g_l(1,2)$, which is isotropic but nevertheless varies with the center-of-mass position of the pair in the unit cell. The present assumption casts Eqs. (29) and (30) in the forms

$$g_l(1,2)=g_0(r_{12})+\sum_{\vec G\neq 0} g_{\vec G}(r_{12})e^{i\vec G\cdot\vec s} \ , \tag{49}$$

$$=\frac{1}{\mu}e^{\gamma_0(r_{12})}\exp\left[\sum_{\vec G\neq 0}\gamma_{\vec G}(r_{12})e^{i\vec G\cdot\vec s}\right] \ , \tag{50}$$

and declares $g_0(r_{12})$ dominant over the sum and $e^{\gamma_0(r_{12})}$ dominant over the product. It is tantamount to saying that an *isotropic, liquidlike* description of $g(1,2)$, not unlike that of Lowy and Woo, is basically sound, and will need only minor corrections. The validity of this statement, at least for solid ^{4}He, will be demonstrated numerically in the next section.

Developing the same thoughts further, we write from Eq. (49)

$$g_l(1,2)=g_0(r_{12})\left[1+\sum_{\vec G\neq 0}\frac{g_{\vec G}(r)}{g_0(r)}e^{i\vec G\cdot\vec s}\right] \tag{51}$$

and from Eq. (50)

$$g_l(1,2)\approx\frac{1}{\mu}e^{\gamma_0(r_{12})}\left[1+\sum_{\vec G\neq 0}\gamma_{\vec G}(r_{12})e^{i\vec G\cdot\vec s}\right] \ . \tag{52}$$

Equation (52) is consistent with keeping only linear $\vec G\neq 0$ terms. From Eqs. (51) and (52), we obtain $\ln g_0(r)=\gamma_0(r)-\ln\mu$ or

$$\frac{d}{dr}\ln g_0(r)=\frac{d}{dr}\gamma_0(r) \tag{53}$$

and

$$g_{\vec G}(r)/g_0(r)=\gamma_{\vec G}(r) \ . \tag{54}$$

Finally, in summary, we focus on Eqs. (13), (14), (37), (53), (54), (44), and (45) as a closed set of integral equations. Given a variational wave function, i.e., a set of $t_{\vec G}$ and $u(r)$, Eq. (37) is the first generalized BBGKY equation, which relates $\{\Pi_{\vec G}\}$ to $\{p_{\vec G}\}$. It requires information about $\{g_{\vec G}(r)\}$. Equations (44) and (45) form the second generalized BBGKY equation, which relates $\{\gamma_{\vec G}(r)\}$ to $\{g_{\vec G}(r)\}$. It in turn requires information about $\{\Pi_{\vec G}\}$ and $\{p_{\vec G}\}$. Equations (13) and (14) give us a defining relation between $\{\Pi_{\vec G}\}$ and $\{p_{\vec G}\}$, while Eqs. (53) and (54) give us defining relations between $\{\gamma_{\vec G}(r)\}$ and $\{g_{\vec G}(r)\}$. The solution of this set of coupled integral equations yields the one- and two-particle distribution functions: the density distribution and the short-range pair-correlation function. When the solution is substituted into Eq. (27), we obtain the energy expectation value $E(t_{\vec G},u(r))$. At every number density ρ, or specific volume $1/\rho$, E is to be minimized with respect to the variational parameters $t_{\vec G}$ and the parameters in $u(r)$.

IV. APPLICATION TO SOLID ^{4}He

In this section, we apply the isotropic approximation $g(1,2) \rightarrow g_l(1,2)$ to the ground-state calculation for solid ^{4}He. This represents a step beyond the Lowy-Woo theory, which employed a *liquid* approximation on $g(1,2)$, i.e.,

$$g(1,2) \rightarrow g_l(1,2) \rightarrow g_0(r_{12}) \rightarrow g_{\text{liquid}}(r_{12}) \ .$$

The model consists of a Lennard-Jones pairwise potential

$$v(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \ , \tag{55}$$

where $\epsilon = 10.22$ K and $\sigma = 2.556$ Å at zero temperature and number density $\rho = 0.030$ Å^{-3} (or $1/\rho = 33.3$ Å^3), the value identified as the solidification density in the Lowy-Woo calculation.[3] The variational wave function contains a one-parameter $u(r)$

$$u(r) = -(b\sigma/r)^5 \ , \tag{56}$$

where $b = 1.15$, again from Ref. 3. For $t_{\vec{G}}$, in keeping with the experience gained in Ref. 3, only two shells are taken; i.e., we retain only $t_{(1)}$ and $t_{(2)}$; and $t_{(2)}$, being insensitive in the actual numerical work, is fixed at the Ref. 3 value of 0.04. All this has been necessary since the solution of the set of coupled integral equations is an exceedingly expensive venture.

The ground state of solid ^{4}He is fcc, and thus the reciprocal lattice bcc. In all the reciprocal-lattice sums we keep just two shells: $G_{(1)} = 2.13$ Å^{-1} (half the body diagonal), and $G_{(2)} = 2.46$ Å^{-1} (edge of a unit cell). The corresponding weights are $w_{(1)} = 8$ and $w_{(2)} = 6$.

In Eq. (47), we realize that a combination of two $\vec{G}_{(1)}$'s can yield 0 or a $\vec{G}_{(2)}$, both of which we retain; it can also yield a $\vec{G}_{(3)}$, which we discard. Combinations of $\vec{G}_{(1)}$ and $\vec{G}_{(2)}$ or two $\vec{G}_{(2)}$'s, can lead to either 0 or other $\vec{G}_{(1)}$'s and $\vec{G}_{(2)}$'s, which we keep, as well as $\vec{G}_{(i)}$, $i \geqslant 3$, which we discard. In other words, we demand consistency in keeping only two shells in all the sums. Equation (44) now reads (for $\vec{G} = 0$)

$$\begin{aligned}
\ln g_0(r) = u(r) &- \pi\rho \int_0^\infty ds\ u'(s) g_0(s) \int_{r-s}^{r+s} dt \frac{s^2-(t-r)^2}{r} t[g_0(|t|)-1] \\
&- \pi\rho \int_0^\infty ds\ u'(s) \left[8p_{(1)} g_{(1)}(s) j_0\left(\frac{G_{(1)}s}{2}\right) + 6p_{(2)} g_{(2)}(s) j_0\left(\frac{G_{(2)}s}{2}\right)\right] \int_{r-s}^{r+s} dt \frac{s^2-(t-r)^2}{r} t g_0(|t|) \\
&- 2\pi\rho \sum_{l=0}^{\infty} (2l+1) \left[8P_{(1)} \int_r^\infty \frac{dr''}{r''} j_l\left(\frac{G_{(1)}r''}{2}\right) \int_0^\infty dr' r' u'(r') g_0(r') j_l\left(\frac{G_{(1)}r'}{2}\right)\right. \\
&\qquad \times \int_{|r''-r'|}^{r''+r'} dz\ z \frac{r''^2+r'^2-z^2}{2r'r''} P_l\left(\frac{r''^2+r'^2-z^2}{2r'r''}\right) g_{(1)}(z) \\
&\qquad + 6p_{(2)} \int_r^\infty \frac{dr''}{r''} j_l\left(\frac{G_{(2)}r''}{2}\right) \int_0^\infty dr' r' u'(r') g_0(r') j_l\left(\frac{G_{(2)}r'}{2}\right) \\
&\qquad \left. \times \int_{|r''-r'|}^{r''+r'} dz\ z \frac{r''+r'^2-z^2}{2r'r''} P_l\left(\frac{r''^2+r'^2-z^2}{2r'r''}\right) g_{(2)}(z)\right] \ .
\end{aligned} \tag{57}$$

For $\vec{G} \neq 0$, we note that another approximation should be made for the sake of consistency. By normalizing $p^{(1)}(1)$ in Eq. (13), we find $p_0 = 1$. All other $p_{\vec{G}}$'s are small compared to p_0. Hence it is reasonable to keep $p_{\vec{G}}$ only where there are no other $\vec{G} \neq 0$ factors. Thus Eq. (45) reduces to

$$\begin{aligned}
g_{\vec{G}}(r) = g_0(r) \Bigg\{ &\frac{4}{G}(\Pi_{\vec{G}} - 2t_{\vec{G}}) \int_r^\infty dr' \frac{1}{r'^2} \left(\frac{Gr'}{2} \cos\frac{Gr'}{2} - \sin\frac{Gr'}{2}\right) \\
&- \pi\rho \int_0^\infty ds\ u'(s) g_0(s) j_0\left(\frac{Gs}{2}\right) \int_{r-s}^{r+s} dt \frac{s^2-(t-r)^2}{r} t\ g_{\vec{G}}(|t|) \\
&- 2\pi\rho \sum_{l=0}^{\infty} (2l+1) \int_r^\infty \frac{dr''}{r''} j_l\left(\frac{Gr''}{2}\right) \int_0^\infty dr' r' u'(r') \left[g_{\vec{G}}(r') j_l\left(\frac{Gr'}{2}\right) + p_{\vec{G}} g_0(r') j_l(Gr')\right] \\
&\qquad \times \int_{|r''-r'|}^{r''+r'} dz\ z \frac{r''^2+r'^2-z^2}{2r'r''} P_l\left(\frac{r''^2+r'^2-z^2}{2r'r''}\right) g_0(z) \Bigg\} \ ,
\end{aligned}$$

with

$$\vec{G} = \vec{G}_{(1)}, \ \text{or} \ \vec{G}_{(2)} \ . \tag{58}$$

Note that in this mode $g_{(1)}(r)$ and $g_{(2)}(r)$ become decoupled.

If in Eq. (57) one considers only the first two terms on the right, $g_0(r)$ will reduce to $g_{\text{liquid}}(r)$ of Lowy and Woo. Equation (57) shows that there will actually be correction terms even for the isotropic, liquidlike part of $g(1,2)$.

Equation (37) now reads

$$\Pi_{\vec{G}} - 2t_{\vec{G}} = p_{\vec{G}}\alpha_{\vec{G}} + \beta_{\vec{G}}, \quad \vec{G} = \vec{G}_{(1)} \ \text{or} \ \vec{G}_{(2)} \ , \tag{59}$$

where

$$\alpha_{\vec{G}} = \frac{4\pi\rho}{G^3}\int_0^\infty dr\, u'(r)(Gr\cos Gr - \sin Gr)g_0(r) \tag{60}$$

and

$$\beta_{\vec{G}} = \frac{16\pi\rho}{G^3}\int_0^\infty dr\, u'(r)\left[\frac{Gr}{2}\cos\frac{Gr}{2} - \sin\frac{Gr}{2}\right]g_{\vec{G}}(r) \ . \tag{61}$$

The computational procedure begins with solving the liquid ^{4}He equation for $g_{\text{liquid}}(r)$. Using that as $g_0(r)$ and setting $g_{\vec{G}}(r)$ to zero for the moment, we solve Eqs. (59)–(61) with Eqs. (13) and (14) iteratively for $\Pi_{\vec{G}}$ and $p_{\vec{G}}$. Table I(a) shows how well the iteration procedure converges in a typical case. Using these $\Pi_{\vec{G}}$, $p_{\vec{G}}$, $g_0(r)$, and $g_{\vec{G}}(r)$ we next solve Eqs. (57) and (58) with Eqs. (53) and (54) for a new set of $g_0(r)$ and $g_{\vec{G}}(r)$. These are then entered in Eqs. (59)–(61) for a new iterative solution for $\Pi_{\vec{G}}$ and $p_{\vec{G}}$. Table I(b) shows intermediate results from this new round of calculations. This continues until convergence is attained.

TABLE I. Iterative procedure for $\rho = 0.030$ Å^{-3} at $t_{(1)} = 0.07$, $t_{(2)} = 0.04$, and $b = 1.15$.

Π(1)	Π(2)
First iterative calculation (a)	
0.192	0.111
0.218	0.124
0.232	0.131
0.240	0.134
0.245	0.136
Second iterative calculation (b)	
0.178	0.127
0.198	0.144
0.210	0.150
0.216	0.153
0.220	0.154
0.222	0.155

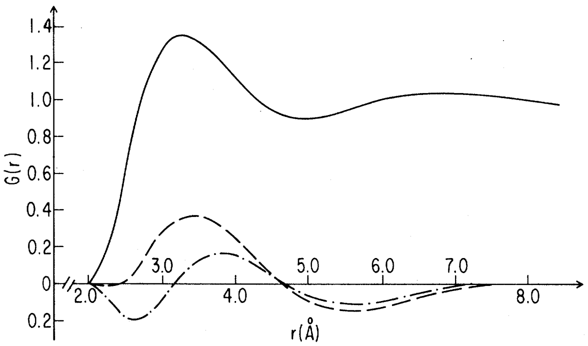

FIG. 2. $g_0(r)$ and $g_{\vec{G}}(r)$ for $\rho = 0.030$ Å^{-3} at $t_{(1)} = 0.07$, $t_{(2)} = 0.04$, and $b = 1.15$. ——$g_0(r)$; – – –$10 \times g_{(1)}(r)$; —·—·$10 \times g_{(2)}(r)$.

Figure 2 shows a typical set of $g_0(r)$, $g_{(1)}(r)$, and $g_{(2)}(r)$. Note that $g_{(1)}(r)$ and $g_{(2)}(r)$ are indeed small compared to $g_0(r)$. [In the figure, $g_{(1)}(r)$ and $g_{(2)}(r)$ have been *amplified by a factor of 10.*] Figure 3 shows the new density distribution at $\rho = 0.030$ Å^{-3}.

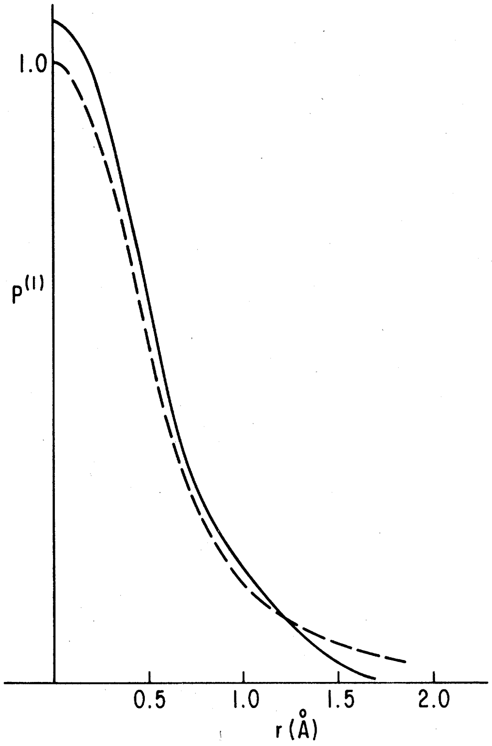

FIG. 3. Density distribution at $\rho = 0.030$ Å^{-3}. —— present calculation; – – – Lowy and Woo (Ref. 3).

It appears slightly more localized than that obtained by Lowy and Woo (LW).[3] Figure 4 shows the energy expectation value as $t_{(1)}$ varies from 0.0 to 0.09. We learn that the minimum remains at $t_{(1)}=0.07$, but the energy decreases by 0.16 K.

We were not in the position of carrying out numerical computation at more than one density. The new solidification density had to be estimated. In Ref. 3, the solidification density had been determined by a Maxwell construction. Figure 2 in Ref. 3 is too small to show an inflection at $1/\rho_c^{\mathrm{LW}} \equiv 33.3$ Å^{-3}, defined as the point at which $E_{\mathrm{solid}}=E_{\mathrm{liquid}}$. Let us exaggerate it in the plot of Fig. 5. Let the dashed curve labeled $E_{\mathrm{solid}}^{\mathrm{LW}}/N$ represent the Lowy-Woo solid energy, and the solid curve labeled E_{solid}/N the result of our present calculation, even though only one point—shown as the solid circle—has actually been calculated. Since E_{liquid} is unaffected by present work, the "solidification density" simply shifts from the intersection of $E_{\mathrm{solid}}^{\mathrm{LW}}$ with E_{liquid} to that of E_{solid} with E_{liquid}, i.e., from $1/\rho_c^{\mathrm{LW}}$ to $1/\rho_c$. Geometrical construction shows that BC equals AB times the slope of AC, or

$$\frac{1}{\rho_c}-\frac{1}{\rho_0^{\mathrm{LW}}} \approx \left|\frac{E_{\mathrm{solid}}^{\mathrm{LW}}}{N}-\frac{E_{\mathrm{solid}}}{N}\right| \Bigg/ \left|\frac{d}{d(1/\rho)}\left[\frac{E_{\mathrm{liquid}}}{N}\right]\right| . \tag{62}$$

We fitted $E_{\mathrm{liquid}}(1/\rho)$, as given in Table I of Ref. 3, to a cubic formula, and obtained

$$\frac{d}{d(1/\rho)}\left[E_{\mathrm{liquid}}/N\right] = -0.93+1.3\times10^{-2}\left[\frac{1}{\rho}\right]+2.5\times10^{-4}\left[\frac{1}{\rho}\right]^2 . \tag{63}$$

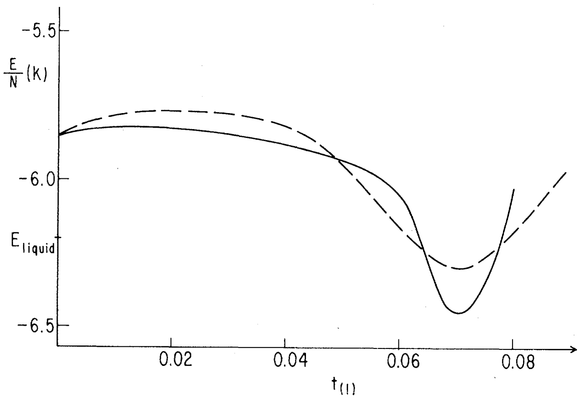

FIG. 4. Energy expectation value as function of the variational parameter $t_{(1)}$. $t_{(2)}=0.04$ and $b=1.15$. —— present calculation; – – – Lowy and Woo (Ref. 3).

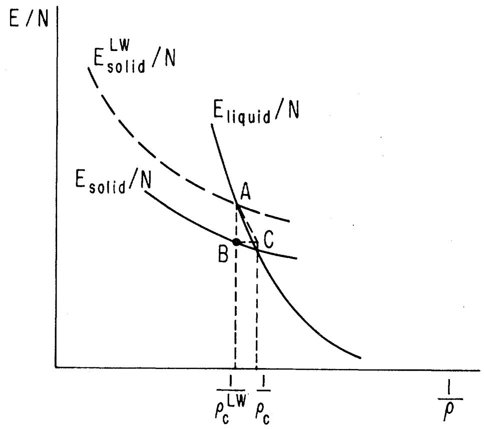

FIG. 5. Liquid to solid transition: an illustration.

The slope at 33.3 Å^3 is then -0.22 K Å^{-3}. Since $|E_{\mathrm{solid}}^{\mathrm{LW}}/N-E_{\mathrm{solid}}/N|=0.16$ K, $1/\rho_c \approx 1/\rho_c^{\mathrm{LW}}+0.73$ Å$^3=34.03$ Å^3. ρ_c, the new solidification density, equals 0.0294 Å^{-3}, a mere 2% below the Lowy-Woo value of 0.030 Å^{-3}.

V. ANISOTROPIC $g(1,2)$

In this section we investigate the effect of introducing anisotropy into the pair-correlation function.

Let us return to Eqs. (21) and (24)–(26) in Sec. II, which make a complete set of equations for $\Pi_{\vec{G}}$, $p_{\vec{G}}$, $\gamma_{\vec{G}}(\vec{r})$, and $g_{\vec{G}}(\vec{r})$. Along with the defining relations (17) and (18), Eq. (24) relates $\gamma_{\vec{G}}(\vec{r})$ to

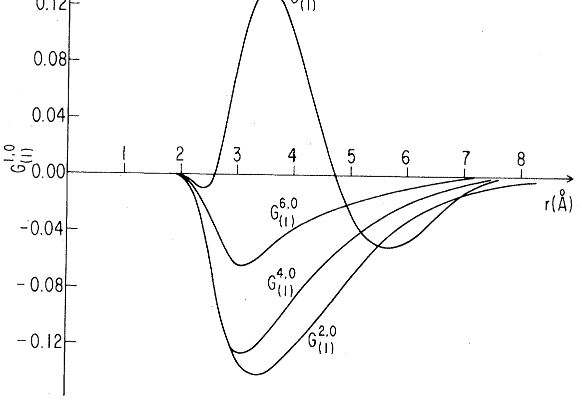

FIG. 6. $G_{(1)}^{l0}(r)$, obtained after one iteration for $\rho=0.030$ Å^{-3}.

$g_{\vec{G}}(\vec{r})$. We wish to solve these equations simultaneously, given $t_{\vec{G}}$, $u(r)$, $p_{\vec{G}}$, and $\Pi_{\vec{G}}$. The solutions are then entered into Eqs. (21) and (25) for a new set of $p_{\vec{G}}$ and $\Pi_{\vec{G}}$. The iterative process continues until self-consistency is achieved. This, of course, is the same program as pursued in Secs. III and IV. The only difference is that we now wish to consider $g(1,2)$ anisotropic. Accordingly, we expand $g(1,2)$ further, taking

$$g_{\vec{G}}(\vec{r}) = \sum_{l,m} G_{\vec{G}}^{lm}(r) Y_{lm}(\theta,\phi) \tag{64}$$

and

$$\gamma_{\vec{G}}(\vec{r}) = \sum_{l,m} \Gamma_{\vec{G}}^{lm}(r) Y_{lm}(\theta,\phi) \ . \tag{65}$$

Only even l need be retained on account of the inversion symmetry of $g_{\vec{G}}(\vec{r})$ and $\gamma_{\vec{G}}(\vec{r})$.

Substitution of Eqs. (64) and (65) into Eqs. (21) and (24) leads to

$$\Pi_{\vec{G}} - 2t_{\vec{G}} = i\rho \sum_{\vec{G}'} \sum_{lm} p_{\vec{G}-\vec{G}'} \int dr\ u'(r) G_{\vec{G}}^{lm}(r) \int d\hat{r} \frac{\vec{G}\cdot\hat{r}}{G^2} e^{i(\vec{G}-\vec{G}'/2)\cdot\vec{r}} Y_{lm}(\theta,\phi) \tag{66}$$

and

$$\begin{aligned}\frac{d}{dr}\Gamma_{\vec{G}}^{lm}(r) = {} & (4\pi)^{1/2} u'(r) \delta_{l,0} \delta_{\vec{G},0} + (\Pi_{\vec{G}} - 2t_{\vec{G}}) \int d\hat{r} (\vec{G}\cdot\vec{r}) \sin\frac{\vec{G}\cdot\vec{r}}{2} Y_{lm}^*(\theta,\phi) \\ & + \rho \sum_{\vec{G}',\vec{G}''} \sum_{l',m',l'',m''}{}' p_{\vec{G}-\vec{G}'-\vec{G}''} \int d\hat{r} Y_{lm}^*(\theta,\phi) \int d\vec{r}' \hat{r}\cdot\hat{r}' u'(r') G_{\vec{G}'}^{l'm'}(r') \\ & \times G_{\vec{G}''}^{l''m''}(|\vec{r} - \vec{r}'|) \cos\left[\left(\vec{G} - \frac{\vec{G}'+\vec{G}''}{2}\right)\cdot\vec{r}' - \left(\frac{\vec{G}-\vec{G}''}{2}\right)\cdot\vec{r}\right] \\ & \times Y_{l'm'}(\theta',\phi') Y_{l''m''}(\theta'',\phi'') \ ,\end{aligned} \tag{67}$$

where θ'' and ϕ'' denote the polar and azimuthal angles of $(\vec{r}' - \vec{r})$.

The iteration procedure reads as follows. We start with the liquid correlation function, i.e., all $G_{\vec{G}}^{lm}(r) = 0$ except $G_0^{00}(r) = g_0(r)$. Using Eqs. (66) and (25) we find $\Pi_{\vec{G}}$ and $p_{\vec{G}}$. Then Eq. (67) gives us $\Gamma_{\vec{G}}^{lm}(r)$, and Eq. (26) gives us $G_{\vec{G}}^{lm}(r)$. In this step Eq. (67) is simplified to read

$$\Gamma_{\vec{G}}^{lm}(r) = -2\pi[(2l+1)\pi]^{1/2} \rho p_{\vec{G}} \delta_{m,0} \sum_{l'} (2l'+1) \int_r^\infty K_{l,l'}(r') M_{l'}(r')\, dr' \ , \tag{68}$$

where

$$K_{l,l'}(r') = \int_{-1}^{1} dx P_l(x) P_{l'}(x) \operatorname{Re}(i^{l'} e^{-iGr'x/2}) \ , \tag{69}$$

$$M_{l'}(r') = \int_0^\infty dr'' u'(r'') j_{l'}(Gr'') g_0(r'') \int_{|r'-r''|}^{r'+r''} \frac{r'^2 + r''^2 - z^2}{2r'^2} P_{l'}\left(\frac{r'^2 + r''^2 - z^2}{2r'r''}\right) [g_0(z) - 1] z dz \ . \tag{70}$$

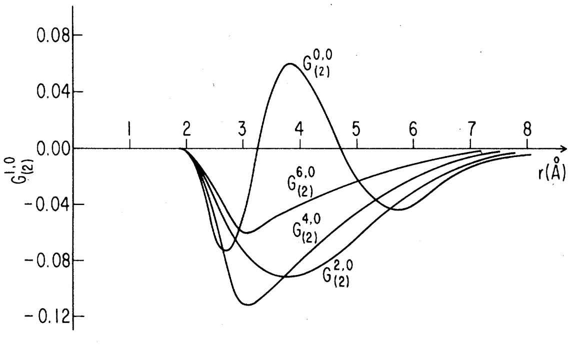

FIG. 7. $G_{(2)}^{l0}(r)$, obtained after one iteration for $\rho = 0.030$ Å^{-3}.

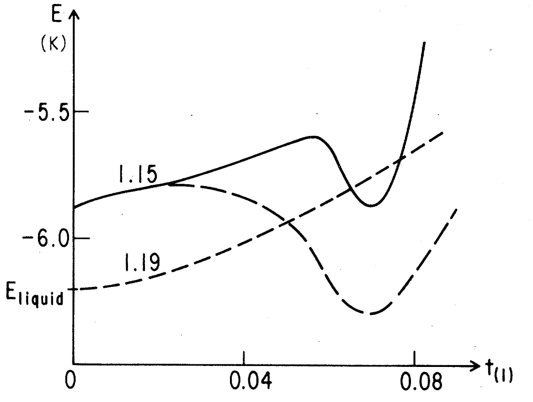

FIG. 8. Energy expectation values including anisotropic effects. —— present calculations; – – – Lowy and Woo (Ref. 3).

It can be seen that at this point only the $m=0$ components survive. In other words, we have only $G^{l0}_{\vec{G}}(r)$. Entering $G^{l0}_{\vec{G}}(r)$ into the right side of Eqs. (66) and (67) leads to a new set of $\Pi_{\vec{G}}$ and $G^{lm}_{\vec{G}}(r)$. This process will be repeated until convergence is reached. The approach to convergence is expected to be exceedingly rapid for solid ^{4}He since anisotropic effects are known to be small. In other words, we expect that for nonzero $\vec{G}$, l, and m, $G^{lm}_{\vec{G}}(r)$ be very small compared to $G^{00}_0(r)$.

Numerical results shown in Figs. 6 and 7 bear this out. $G^{l0}_{(1)}(r)$ at $\vec{G}_{(1)}$ and $G^{l0}_{(2)}(r)$ at $\vec{G}_{(2)}$ all turn out small. The amplitudes are all less than 0.15, while $G^{00}_0(r)$—the liquid correlation function, or $g_0(r)$ as shown in Fig. 2—reaches a peak of 1.3. Practicality does not permit us to go beyond one iteration. It is, however, easy to see that only minute changes are expected in the energy calculation even if we were to proceed further.

Figure 8 shows the variational energies obtained at density $\rho = 0.030$ Å^{-3}. We see that the effect of taking into consideration anisotropy in the two-particle distribution function is to shift the energy curve upward. Using the same method that determined the solidification density in Sec. IV, the transition density is found to have increased from 0.030 to 0.032 Å^{-3}. This is unfortunate since the experimental value lies *below* 0.030 Å^{-3}. Nevertheless, we have succeeded to show that the shift, at $< 7\%$, is not large, and that the approximation made on $g(1,2)$ in Ref. 3 is acceptable. The discrepancy with experiment can no doubt be made smaller by a more thorough search of the variational wave-function space. We intend to do it if and when demands on computer expenditure can be met.

ACKNOWLEDGMENTS

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APPENDIX A

Let the directional integral in Eq. (39) be denoted by τ:

$$\tau = \int d\hat{r}\,(\hat{r}\cdot\hat{r}')\,g_{\vec{G}''}(|\vec{r}-\vec{r}'|)\,e^{-i\vec{G}_3\cdot\vec{r}} \quad . \tag{A1}$$

Using the Rayleigh expansion formula:

$$e^{i\vec{a}_1\cdot\vec{a}_2} = 4\pi \sum_{l=0}^{\infty}\sum_{m=-l}^{l} (i)^l Y^*_{lm}(\hat{a}_1)\,Y_{lm}(\hat{a}_2)\,j_l(a_1a_2) \tag{A2}$$

and the coordinate system shown in Fig. 9, we find

$$\begin{aligned}\tau &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} 4\pi(i)^l j_l(G_3r)\int_0^{2\pi} d\phi \int_{-1}^{1} d\mu\,\mu\, g_{\vec{G}''}((r^2+r'^2-2rr'\mu)^{1/2})\,Y^*_{lm}(\hat{r}\cdot\hat{r}')\,Y_{lm}(-\vec{G}_3\cdot\hat{r}') \\ &= 8\pi^2\sum_{l=0}^{\infty}\left[\frac{2l+1}{4\pi}\right](i)^l j_l(G_3r)\,P_l(-\vec{G}_3\cdot\hat{r}')\int_{-1}^{1} d\mu\,\mu\, g_{\vec{G}''}((r^2+r'^2-2rr'\mu)^{1/2})\,P_l(\mu) \quad ,\end{aligned} \tag{A3}$$

where $\mu \equiv \cos\theta$.

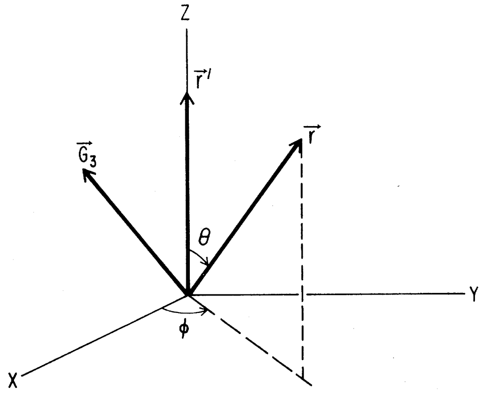

FIG. 9. Coordinate system for expansion, Eq. (A3).

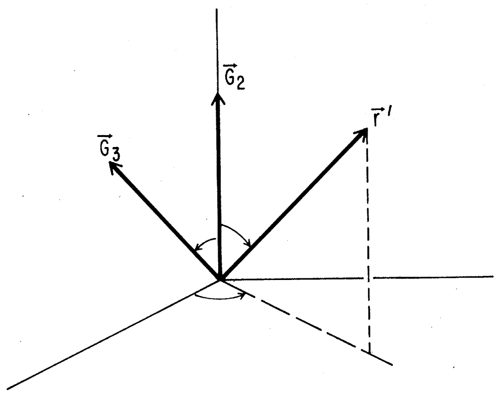

FIG. 10. Coordinate system for expansion, Eq. (A6).

Let

$$\frac{1}{r^2 r'^2} H^l_{\vec{G}''}(r,r') = \int_{-1}^{1} d\mu\, \mu\, g_{\vec{G}''}((r^2 + r'^2 - 2rr'\mu)^{1/2}) P_l(\mu) \ . \tag{A4}$$

[Same definition as in Eq. (43)] J becomes

$$J = 2\pi \sum_{l=0}^{\infty} (2l+1)(i)^l j_l(G_3 r) \frac{1}{r^2} \int dr'\, d\hat{r}'\, u'(r') g_{\vec{G}'}(r') e^{i\vec{G}_2\cdot\vec{r}'} H^l_{\vec{G}''}(r,r') P_l(-\hat{G}_3\cdot\hat{r}') \ . \tag{A5}$$

Now, with the help of Fig. 10

$$\begin{aligned}\int d\hat{r}'\, P_l(-\hat{G}_3\cdot\hat{r}') e^{i\hat{G}_2\cdot\hat{r}'} &= (-1)^l \int d\hat{r}'\, P_l(\hat{G}_3\cdot\hat{r}') e^{i\vec{G}_2\cdot\vec{r}'} = (-1)^l 2\pi P_l(\hat{G}_3\cdot\hat{G}_2) \int_{-1}^{1} d\mu\, e^{iG_2 r'\mu} P_l(\mu) \\ &= \frac{4\pi}{(i)^l} j_l(G_2 r') P_l(\hat{G}_3\cdot\hat{G}_2) \ . \end{aligned} \tag{A6}$$

We obtain finally

$$J = \frac{8\pi^2}{r^2} \sum_{l=0}^{\infty} (2l+1) j_l(G_3 r) \int dr'\, u'(r') g_{\vec{G}'}(r') P_l(\hat{G}_3\cdot\hat{G}_2) j_l(G_2 r') H^l_{\vec{G}''}(r,r') \ . \tag{A7}$$

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[1] See review by R. A. Guyer, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969), Vol. 23.

[2] See review by C. M. Varma and N. R. Werthamer, in *Physics of Liquid and Solid Helium*, edited by K. H. Bennemann and J. B. Ketterson (Interscience, New York, 1976), Vol. I.

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[4] M. D. Miller, W. J. Mullin, and R. A. Guyer, Phys. Rev. B 18, 3189 (1978).

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[6] Note that the "coefficients" are now functions of r_{12}, not $\vec{r}_{12}$. We keep the subscript as $\vec{G}$, however. Writing it as G would lead to the unfortunate implication that $g_{\vec{G}}(r) = g_{\vec{G}'}(r)$ and $\gamma_{\vec{G}}(r) = \gamma_{\vec{G}'}(r)$ as long as $G = G'$, even when $R\vec{G} \neq \vec{G}'$ (R being a rotational operator with the rotational symmetry of the reciprocal lattice).