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PHYSICAL REVIEW VOLUME 188, NUMBER 1 5 DECEMBER 1969

Paired-Phonon Analysis for the Ground State and Low Excited States of Liquid Helium[†]

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(Received 1 July 1969)

The paired-phonon analysis operates in the function space generated by product functions compounded from (i) a starting trial function ψ of the Bijl-Dingle-Jastrow-type (BDJ) (a product of two-particle correlation factors $\exp[\frac{1}{2}U(r_{ij})]$; (ii) paired-phonon factors $\rho_{\vec{k}}^{*}\rho_{-\vec{k}}^{*}$ to all powers, (iii) multiple phonon factors $\rho_{\vec{k}}^{*}\cdots\rho_{\vec{l}}^{*}$ to all powers, with neglect of all matrix elements representing processes in which phonons coalesce, split, or scatter. Results in the present study include (i) a simpler and more general derivation of the fundamental relations; (ii) proof that the improved ground-state trial function $\hat{\psi}$ generated by the analysis is still in the BDJ function space [with $U(r)$ replaced by $U(r)+\delta U(r)$]; (iii) a formula expressing $\delta U(r)$ in terms of $S(k)$, the starting liquid-structure function, and $w(k)$, the residual interaction function; (iv) a convenient representation of the phonon factor $\rho_{\vec{k}}^{*}$ as a linear combination of phonon creation and annihilation operators; (v) explicit statement of the relation between the optimization condition $w(k)\equiv 0$ and the variational extremum property of the expectation value of H in the BDJ-type function space; (vi) usable approximate procedures for evaluating the residual interaction function $w(k)$ based on the hypernetted-chain (HNC) and Percus-Yevick (PY) relations; and (vii) numerical evaluation of $w(k)$, the energy shift δE, and the improved liquid-structure function $\hat{S}(k)$ using ψ's computed by Massey and Woo as starting functions. For ^{4}He at the equilibrium density, $(1/N)\delta E \sim -0.7\,^\circ$K; for the hypothetical boson-type ^{3}He system at $\rho = 0.0164\,\text{Å}^{-3}$, $(1/N)\delta E \sim -0.3\,^\circ$K (HNC) or $-0.5\,^\circ$K (PY). In the discussion, emphasis is placed on the practical possibility of accurate numerical evaluation of the interaction function $\omega(k)$ by the method of molecular dynamics applied to systems containing $10^2 - 10^3$ particles.

I. INTRODUCTION

Recent theoretical studies [1–5] of the ground state of liquid ^{4}He are based on the use of a Bijl-Dingle-Jastrow-type (BDJ) trial function in evaluating the expectation value of the Hamiltonian operator:

$$|0\rangle \equiv \Psi(1,2,\ldots,N) = \prod_{1\le i\le j\le N} e^{U(r_{ij})/2} \Big/ \left(\int \Pi e^{U} d\vec{r}_{1,2,\ldots,N}\right), \tag{1}$$

$$E_0 = \langle 0 | H | 0 \rangle \ . \tag{2}$$

Semiquantitative agreement is found between computed and experimental ground-state properties which include the equation of state (energy, pressure, and compressibility as functions of density) and the liquid-structure function as a function of density. It is clear however that the theory has not yet produced a close approach to the optimum BDJ trial function $\Psi = \Psi_{\text{opt}}$; firstly because the extremum property of the expectation value permits a poor trial function to give a fairly good result for the energy; and secondly because the number of parameters in the available parametrizations of the radial distribution function $g(r)$ or of the correlation function $U(r)$ are too small to generate much structure in either function. The problem of characterizing and computing the optimum BDJ-type trial function was solved in principle several years ago by Jackson and Feenberg[6] in a formal analysis of the paired-phonon space (although it was not recognized at that time that the improved description of the ground state remained within the BDJ function space). The analysis operates in the general function space

$$\Psi \prod_{\vec{k},\vec{l}} |\rho_{\vec{k}}|^{2n_{\vec{k}}} \rho_{\vec{l}}^{\,m_{\vec{l}}} , \qquad \begin{array}{l} n_{\vec{k}} = 0, 1, 2, \ldots \\ \\ m_{\vec{l}} = 0, 1, 2, \ldots \end{array} , \tag{3}$$

with neglect of processes in which phonons scatter, split, and coalesce. This neglect is justified ultimately by finding that the resulting optimum trial function for the ground state constructed from the building material of Eq. (3) is still a symmetrical product of two-particle factors [with a starting $U(r)$ replaced by a final $U(r) + \delta U(r)$].

The neglected processes generate components in the state function which do not occur in the BDJ-type function space. For example, the three-phonon component

$$|\vec{k}, \vec{l}, -\vec{k} - \vec{l}\rangle = \rho_{\vec{k}} \rho_{\vec{l}} \rho_{-\vec{k}-\vec{l}} |0\rangle / [N^3 S(k) S(l) S(|\vec{k} + \vec{l}\,|)]^{1/2} , \tag{4}$$

with $kl\,|\vec{k} + \vec{l}\,| \neq 0$, represents a process in which three phonons emerge from the substrate described by Ψ or three phonons are absorbed into the substrate. These processes make a substantial contribution to the ground-state energy.[7] Incidentally, the evaluation of this contribution to the energy is greatly simplified by the assumption that Ψ is actually the optimum BDJ-type function.

We are concerned with three problems in this study: (i) development of a simpler and more general analysis of the paired-phonon function space; (ii) description of practical methods of deriving semiquantitative results from the formal analysis; (iii) actual numerical evaluation of nearly optimum improvements in the correlation function, liquid-structure function, and energy.

Section II is devoted to the derivation of a general formula for matrix elements in the paired-phonon space [Eq. (17)]. In Ref. 6, these matrix elements were evaluated by the introduction of a generalized superposition approximation for the nth-order distribution function $p^{(n)}(1, 2, \ldots, n)$ generated by Ψ. Actually, the calculation involves only products of factors $h(r_{ij}) = g(r_{ij}) - 1$ which must occur in any correct representation of $p^{(n)}(1, 2, \ldots, n)$ as a sum of elementary clusters in $h(r_{ij})$ plus a remainder. For example,

$$\begin{aligned} p^{(4)}(1, 2, 3, 4) = \rho^4 [1 &+ h(r_{12}) + \cdots + h(r_{34}) + h(r_{12}) h(r_{23}) + \cdots + h(r_{24}) h(r_{43}) \\ &+ h(r_{12}) h(r_{34}) + \cdots + h(r_{13}) h(r_{24}) + \cdots + h(r_{12}) h(r_{23}) h(r_{34}) h(r_{41})] + \delta p^{(4)}(1, 2, 3, 4). \end{aligned} \tag{5}$$

The unknown remainder $\delta p^{(4)}(1, 2, 3, 4)$ is negligible unless all four points are within a sphere of radius not much greater than $\rho^{-1/3}$. In computing the expectation value of $|\rho_{\vec{k}}|^2 |\rho_{\vec{l}}|^2$, products of $h(r_{ij})$ factors more complicated than $h(r_{12}) h(r_{34})$ are not needed. Clusters containing additional $h(r_{ij})$ factors and also the unknown remainder $\delta p^{(4)}$ make contributions to the expectation value which are down by at least a factor of $1/N$. Thus, the matrix elements under discussion are free from the uncertainties and errors inherent in the superposition-type approximation for $p^{(n)}$. Nevertheless, it is useful to evaluate matrix elements in the paired function space by a simpler and more general procedure. This task is accomplished in Sec. II.

The results of the paired-phonon analysis are summarized in Sec. III. The section concludes with a brief discussion of the correspondence between these results and the Bogoliubov treatment of the weakly interacting boson system. In Sec. IV, the phonon factor $\rho_{\vec{k}}$ is expressed directly in terms of creation and destruction operators $A_{\vec{k}}^{\dagger}$ and $A_{\vec{k}}$. The improved liquid-structure function and excitation energies are shown to fit the Bijl-Feynman formula for the energy of an elementary excitation. This formula yields an improved value for the velocity of first sound. In Sec. V, the improved ground-state trial function $\hat{\Psi}$ is first determined as a combined infinite series and infinite product in the variables $|\rho_{\vec{k}}|^2$ multiplying the starting trial function Ψ. The series is summed to a final explicit exponential form giving a correction δU to the starting correlation function U. The optimization condition on Ψ is formulated in Sec. VI and shown to imply that Ψ satisfies the variational extremum condition on the expectation value of H. In precise explicit terms, this means that if the paired-phonon analysis generates no energy shift then small changes in Ψ (i.e., in U) produce no first-order change in the expectation value of H. Finally, methods of reducing the formal analysis to numerical terms are developed in Sec. VIII. Numerical results are exhibited in tabular and graphical forms in Secs. VII and VIII: Sec. VII for liquid ^{4}He at the equilibrium density $\rho = 0.0218\ \text{Å}^{-3}$, and Sec. VIII for the hypothetical boson-type ^{3}He system at $\rho = 0.0164\ \text{Å}^{-3}$.

Section IX supplements the rigorous statements in Sec. VI on the relation between optimization and extremum conditions by showing that the same statements hold when the evaluations are based on the HNC approximation for $U(r)$ as a functional in g and S.

II. MATRIX ELEMENTS IN THE PAIRED-FUNCTION SPACE

Our first concern is to evaluate the matrix element $\langle 0 | |\rho_{\vec{k}}|^{2n} | 0 \rangle$. We begin by introducing a generalized normalization integral

$$I(k|x) = \int \Psi^2 e^{-(x/N)|\rho_{\vec{k}}|^2} d\vec{r}_{12\cdots N}\ , \tag{6}$$

and a generalized liquid-structure function

$$S(k|x) = \frac{1}{NI(k|x)} \int \Psi^2 e^{-(x/N)|\rho_{\vec{k}}|^2} |\rho_{\vec{k}}|^2 d\vec{r}_{12\cdots N}$$

$$= -\frac{d}{dx} \ln I(k|x)\ . \tag{7}$$

Differentiation of $S(k|x)$ with respect to x yields

$$\frac{d}{dx} S(k|x) = S(k|x)^2$$

$$- \frac{1}{I(k|x)} \left\langle 0 \left| e^{-(x/N)|\rho_{\vec{k}}|^2} \left(\frac{1}{N} |\rho_{\vec{k}}|^2 \right)^2 \right| 0 \right\rangle . \tag{8}$$

References 6 and 8 give full details of the elementary proof that the expectation value of $[(1/N|\rho_{\vec{k}}|^2]^2$ is double the square of the expectation value of $(1/N)|\rho_{\vec{k}}|^2$. Entering Eq. (8) with this result, we get the differential equation

$$\frac{d}{dx} \frac{1}{S(k|x)} = 1\ , \tag{9}$$

and the solution[9]

$$S(k|x) = \frac{S(k)}{1 + xS(k)}\ . \tag{10}$$

Here $S(k) \equiv S(k|o)$, the liquid-structure function generated by Ψ. Equation (7) can be integrated with respect to x to yield[9]

$$I(k|x) = 1/[1 + xS(k)]\ . \tag{11}$$

Equations (6) and (11) imply a general explicit formula for the expectation value of $[(1/N)|\rho_{\vec{k}}|^2]^n$. To derive the formula suppose x so small that $xS(k) < 1$; then Eq. (6) generates one power series in x, and Eq. (11) another. The identity of the two series requires

$$\langle 0 | [(1/N)|\rho_{\vec{k}}|^2]^n | 0 \rangle = n!\,S(k)^n\ . \tag{12}$$

Equation (12) is a known result,[6] but the present derivation is strikingly simple compared to the original.

Next, consider generalized versions of Eqs. (6) and (7):

$$I(x) = I(x; \cdots c_{\vec{k}} \cdots)$$

$$= \int \Psi^2 \prod_{\vec{k},\, k_x > 0} e^{-(xc_{\vec{k}}/N)|\rho_{\vec{k}}|^2} d\vec{r}_{12\cdots N}, \tag{13}$$

$$S(k|x) = \frac{1}{NI(x)} \int \Psi^2 \prod_{\vec{h},\, \vec{h}_x > 0} e^{(xc_{\vec{h}}/N)|\rho\vec{h}|^2}$$

$$\times |\rho_{\vec{k}}|^2 d\vec{r}_{12\cdots N}$$

$$= (1/N) \langle |\rho_{\vec{k}}|^2 \rangle_x$$

$$= -(1/x)(d/dc_{\vec{k}}) \ln I(x)\ . \tag{14}$$

Equation (8) is replaced by

$$\frac{d}{dx} S(k|x) = -c_k S(k|x)^2$$

$$+ \sum_{\vec{l} \neq \vec{k},\, l_x > 0} c_{\vec{l}} \left(\langle \frac{1}{N} |\rho_{\vec{k}}|^2 \rangle_x \langle \frac{1}{N} |\rho_{\vec{l}}|^2 \rangle_x \right.$$

$$-\left\langle\frac{1}{N^2}|\rho_{\vec{k}}|^2|\rho_{\vec{l}}|^2\right\rangle_x\Bigg)\,, \tag{15}$$

where $\langle\ \rangle_x$ signifies the expectation value used in Eq. (14). We draw again on Ref. 8 for the result that the coefficient of $c_{\vec{l}}$ in Eq. (15) is of order $1/N$. The sum in Eq. (15) can be made negligible by limiting the number of nonzero summands to a sufficiently small number $p \ll N$. Under this restriction,

$$\begin{aligned} S(k\,|x) &\simeq S(k)/[1+xc_{\vec{k}}S(k)]\,, \\ I(x) &\simeq \prod_{\vec{k},\,k_x>0}\frac{1}{1+xc_{\vec{k}}S(k)}\,, \end{aligned} \tag{16}$$

and

$$\left\langle 0\left|\Pi_j\left(\frac{1}{N}|\rho_{\vec{k}_j}|^2\right)^{n_j}\right|0\right\rangle \simeq \Pi_j\left\langle 0\left|\left(\frac{1}{N}|\rho_{\vec{k}_j}|^2\right)^{n_j}\right|0\right\rangle$$

$$=\Pi_j(n_j)!S(k_j)^{n_j}\,,\quad \Sigma_j n_j \ll N\,. \tag{17}$$

Equation (16) exhibits the separability of the exponential factors in the integrand of the integral defining $I(x)$. Each exponential factor contributes to the integral as if the others were absent. Equation (17) includes all the matrix elements needed to obtain a representation of the Hamiltonian operator in the paired-function space.

III. REPRESENTATION OF THE HAMILTONIAN OPERATOR IN THE PAIRED-FUNCTION SPACE

Our objective here is to summarize the definitions and results of Ref. 6.

First Definitions

$$V^*(r)=v(r)-(\hbar^2/4m)\Delta U(r),$$

$$W(1,2,\ldots,N\,|\beta)=\prod_{i<j}e^{\beta V^*(r_{ij})}\,,\qquad \beta\leq 0,$$

$$I(\beta)=\langle 0\,|W|\,0\rangle,$$

$$\begin{aligned} p^{(2)}(r_{12}\,|\beta) &=\rho^2 g(r_{12}\,|\beta) \\ &=\frac{N(N-1)}{I(\beta)}\int\Psi^2W\,d\vec{r}_{34\cdots N}, \\ S(k\,|\beta) &=\frac{1}{NI(\beta)}\langle 0\,|\,|\rho_{\vec{k}}|^2W\,|0\rangle \\ &=1+\rho\int e^{i\vec{k}\cdot\vec{r}}[g(r\,|\beta)-g(\infty\,|\beta)]\,d\vec{r}, \end{aligned} \tag{18}$$

$$g(r)\equiv g(r\,|0),\qquad S(k)\equiv S(k\,|0),$$

$$I'(0)=\left(\frac{d}{d\beta}I(\beta)\right)_{\beta=0}=\langle 0|\sum_{i<j}V^*(r_{ij})|0\rangle=E_0,$$

$$\begin{aligned} S'(k) &=\left(\frac{d}{d\beta}S(k\,|\beta)\right)_{\beta=0} \\ &=\langle 0|\frac{1}{N}|\rho_k|^2[\sum_{i<j}V^*(r_{ij})-E_0]|0\rangle, \end{aligned}$$

$$g'(r)=\left(\frac{d}{d\beta}g(r\,|\beta)\right)_{\beta=0}.$$

Results

Normalized basis function in the $\rho_{\pm\vec{k}}$ function space:

$$|m,n\rangle=\rho_{\vec{k}}^{\ m}\rho_{\vec{k}}^{\ n}|0\rangle/[N^{m+n}S(k)^{m+n}]^{1/2}. \tag{19}$$

Matrix elements of W

$$\begin{aligned} \langle m',n'|W|m,n\rangle &=\delta_{m'+n-m-n'}[S(k\,|\beta)/S(k)]^{m'+n} \\ &\times[(m'+n)!\,I(\beta)]/[m+n)!\,(m'+n')!\,]^{1/2}. \end{aligned} \tag{20}$$

Matrix elements of H

$$\begin{aligned} \langle m',n'|H-E_0|m,n\rangle &=\langle m',n'|I|m,n\rangle \\ &\times\{[(mm'+nn')/(m+n')]e(k)+(m+n')w(k)\}, \end{aligned}$$

$$\begin{aligned} e(k) &=\hbar^2k^2/2mS(k)\,, \\ w(k) &=S'(k)/S(k)+(\hbar^2k^2/4m)(1-1/S(k). \end{aligned} \tag{21}$$

Here we have modified the notation of Ref. 6 by writing $e(k)$ for $\epsilon'(k)$ and $w(k)$ for $\epsilon''(k)$.

The functions $|m,n\rangle$ are normalized, but they do not form an orthogonal basis; and they do not describe states with definite numbers of phonons with momentum $\hbar\vec{k}$ and $-\hbar\vec{k}$. The special case $m=n=1$ illustrates these points since $|\rho_{\vec{k}}|^2\Psi$ is a linear combination of a no-phonon state and one with $\hbar\vec{k}$ and $-\hbar\vec{k}$ phonons. At this level, the first task is the construction of an orthonormal basis system describing states of independent "free" phonons. New functions $|e;s,p\rangle$ are generated by the real linear transformation

$$\begin{aligned} |e;s,p\rangle &=\sum_{l=0}^{p}a_{sp;l}|l+s,l\rangle\,, \\ a_{sp;l} &=0,\quad l>p;\quad s\geq -p,\quad p=0,1,2,\ldots, \end{aligned} \tag{22}$$

subject to the orthonormal property

$$\langle e; s, p \,|I|\, e; t, q\rangle = \delta_{p,q}\delta_{s,t} \,. \tag{23}$$

The factor $\delta_{s,t}$ simply expresses conservation of momentum since $|e; s, p\rangle$ is an eigenstate of the momentum operator with the eigenvalue $\hbar\vec{k}s$. The new basis functions describe a physical system containing $s+p$ "phonons" with momentum $\hbar\vec{k}$ and p "phonons" with momentum $-\hbar\vec{k}$. A state with momentum $-\hbar\vec{k}s$ is described by the complex-conjugate basis function ($|e; -s, s+p\rangle = |e; s, p\rangle^*$).

The explicit solution of the orthonormalization condition for $s=0$ is given in Ref. 6; the generalization to include $s \neq 0$ appears in Ref. 8. Here we simply state the solution:

$$a_{sp;l} = (-1)^{p+l} \frac{[(s+2l)!(s+p)!p!]^{1/2}}{l!(s+l)!(p-l)!} \,. \tag{24}$$

In the orthonormal representation the matrix of H reduces to the nearly diagonal form[8]

$$\begin{aligned}
&\langle e; s, p \,|H|\, e; s, p\rangle = E_0 + (s+2p)(e+w) \,,\\
&\langle e; s, p-1 \,|H|\, e; s, p\rangle = [p(p+s)]^{1/2} w \,, \qquad (25)\\
&\langle e; s, p+1 \,|H|\, e; s, p\rangle = [(p+1)(p+1+s)]^{1/2} w \,.
\end{aligned}$$

All other elements $\langle e; t, q \,|H|\, e; s, p\rangle$ vanish.

The quantum numbers and numerical coefficients in Eq. (25) can be identified with the corresponding quantities in the Bogoliubov treatment of the low density, weakly interacting system of bosons. This means that the matrix of H possesses an equivalent representation as a quadratic form in creation and annihilation operators. We define canonical creation and annihilation operators by the statements

$$\begin{aligned}
&a_{\vec{k}}^{\dagger}\,|e; s, p\rangle = (s+p+1)^{1/2}\,|e; s+1, p\rangle \,,\\
&a_{\vec{k}}\,|e; s, p\rangle = (s+p)^{1/2}\,|e; s-1, p\rangle \,, \qquad (26)\\
&a_{-\vec{k}}^{\dagger}\,|e; s, p\rangle = (p+1)^{1/2}\,|e; s-1, p+1\rangle \,,\\
&a_{-\vec{k}}\,|e; s, p\rangle = \sqrt{p}\,|e; s+1, p-1\rangle \,,
\end{aligned}$$

with the terminal condition $|e; -p-1, p\rangle \equiv 0$. The equivalent Hamiltonian operator in the occupation number space of the $\vec{k}$ and $-\vec{k}$ phonons is

$$\begin{aligned}
H_{\vec{k}} + H_{-\vec{k}} = {}&(a_{\vec{k}}^{\dagger} a_{\vec{k}} + a_{-\vec{k}}^{\dagger} a_{-\vec{k}})[e(k) + w(k)]\\
&+ (a_{\vec{k}} a_{-\vec{k}} + a_{\vec{k}}^{\dagger} a_{-\vec{k}}^{\dagger})\, w(\mathrm{k}) \,.
\end{aligned} \tag{27}$$

The transformation to diagonal form is accomplished by introducing new canonical creation and annihilation operators

$$\begin{aligned}
&A_{\pm\vec{k}} = \lambda a_{\pm\vec{k}} - \mu a_{\mp\vec{k}}^{\dagger} \,,\\
&A_{\pm\vec{k}}^{\dagger} = \lambda a_{\pm\vec{k}}^{\dagger} - \mu a_{\mp\vec{k}} \,,
\end{aligned} \tag{28}$$

subject to the condition $\lambda^2 - \mu^2 = 1$, or explicitly,

$$\begin{aligned}
&\lambda = 1/[1 - D(k)^2]^{1/2} \,,\\
&\mu = D(k)/[1 - D(k)^2]^{1/2} \,,\\
&D(k) = \frac{-w(k)}{e(k) + w(k) + [e(k)^2 + 2e(k)w(k)]^{1/2}} \,.
\end{aligned} \tag{29}$$

The condition $e(k) + 2w(k) \geq 0$ insures that $D(k)^2 \leq 1$, so that λ and μ are real quantities as implied by the notation of Eq. (28).

Up to this point only the wave vectors $\vec{k}$ and $-\vec{k}$ have occurred in the analysis. The necessary generalization to the product function space defined by

$$|\ldots, m_{\vec{k}}, n_{\vec{k}}, \ldots\rangle = \prod_{\vec{k}, k_x \geq 0} \rho_{\vec{k}}^{\,m_{\vec{k}}} \rho_{-\vec{k}}^{\,n_{\vec{k}}} |0\rangle \Big/ \Big(\prod_{\vec{k}, k_x > 0} N^{m_{\vec{k}} + n_{\vec{k}}} S(k)^{m_{\vec{k}} + n_{\vec{k}}} \Big)^{1/2} \tag{30}$$

introduces the matrix elements,

$$\begin{aligned}
&\langle \ldots, m'_{\vec{k}}, n'_{\vec{k}}, \ldots |I| \ldots, m_{\vec{k}}, n_{\vec{k}}, \ldots\rangle = \prod_{\vec{k}, k_x > 0} \langle m'_{\vec{k}}, n'_{\vec{k}} |I| m_{\vec{k}}, n_{\vec{k}}\rangle \,,\\
&\langle \ldots, m'_{\vec{k}}, n'_{\vec{k}}, \ldots |H - E_0| \ldots, m_{\vec{k}}, n_{\vec{k}}, \ldots\rangle = \sum_{l, l_x > 0} \langle m'_{\vec{l}}, n'_{\vec{l}} |H - E_0| m_{\vec{l}}, n_{\vec{l}}\rangle\\
&\qquad \times \prod_{k \neq l, k_x > 0} \langle m'_{\vec{k}}, n'_{\vec{k}} |I| m_{\vec{k}}, n_{\vec{k}}\rangle \,,
\end{aligned} \tag{31}$$

subject to the constraint $m'_{\vec{k}}+n_{\vec{k}}=m_{\vec{k}}+n'_{\vec{k}}$. The constraint eliminates all processes which can be interpreted as phonons coalescing, splitting, or scattering, and limits the range of trial functions to the paired-phonon space (for the description of the ground state).

Separability, as discussed in Sec. II, is assumed in writing the right-hand members of Eqs. (31). The assumption is justified if

$$\sum_{\vec{k},\, k_x>0} (m_{\vec{k}}+n'_{\vec{k}}) < \cdots < N . \tag{32}$$

It is now possible to generate a normalized orthogonal system of basis functions labeled with complete sets of quantum numbers s, p ranging over the wave vector space $\vec{k}, k_x>0$. Subject to the inequality of Eq. (32), the matrix representation of H in this function space is diagonal with the explicit form

$$H_D = E_0 + \tfrac{1}{2}\sum_{\vec{k}}[\hat{e}(k) - e(k) - w(k)] + \sum_k A_k{}^\dagger A_k \hat{e}(k), \tag{33}$$

in which
$$\hat{e}(k) = [e(k)^2 + 2e(k)w(k)]^{1/2} \le e(k) + w(k), \tag{34}$$

is the corrected excitation energy for a free phonon of momentum $\vec{k}$ and $A_{\vec{k}}{}^\dagger A_{\vec{k}}$ is an occupation-number operator with eigenvalues $0, 1, 2, \ldots$. The correction to the ground-state energy is negative or zero and vanishes only if $w(k)$ vanishes identically. If E_0 is the minimum expectation value attainable in the BDJ function space, the energy correction must vanish. Consequently $w(k)=0$ characterizes the optimum BDJ-type trial function. Some consequences of the optimization condition $w(k)=0$ are developed in Secs. VI and IX.

The preceding analysis establishes a parallelism between the theoretical terms and descriptions of two distinct computational procedures, one developed by Bogoliubov[10] for treating a boson system with weak interactions, the other emerging naturally out of the paired-phonon analysis for a boson system with strong and highly singular interactions at realistic liquid densities. The parallelism extends also to theories of the hard-core boson system at low density[11] and of the charged boson system at high density.[12] To avoid possible misunderstanding we state explicitly that the parallelism does not imply or suggest that an adequate treatment of liquid ^{4}He can emerge from the Bogoliubov formalism as a starting approximation. Basically, the problem for the theorist is to understand the emergence of mathematically equivalent connections at different and widely separated levels of approximation.

IV. OPERATOR REPRESENTATION OF $\rho_{\vec{k}}$

The general formula

$$\rho_{\vec{k}}|e; s, p\rangle = \sum_q |e; s+1, q\rangle\langle e; s+1, q|\rho_{\vec{k}}|e; s, p\rangle \tag{35}$$

defines a matrix representation of the function $\rho_{\vec{k}}$. Equations (20) and (22) are used to generate the expansion formulas:

$$\begin{aligned}\rho_{\vec{k}}|e; s, p\rangle &= \sum_{l=0}^{p} a_{s,p;l}[NS(k)(s+2l+1)]^{1/2}|s+l+1, l\rangle,\\ \langle e; s+1, q|\rho_{\vec{k}} &= \sum_{h=0}^{q} a_{s+1,q;h}[NS(k)(s+2h+2)]^{1/2}\langle s+h+1, h+1|,\end{aligned} \tag{36}$$

and these in turn yield formulas for the matrix elements of $\rho_{\vec{k}}$:

$$\begin{aligned}\langle e; s+1, q|\rho_{\vec{k}}|e; s, p\rangle &= \sum_{l=0}^{p} a_{s,p;l}[NS(k)(s+2l+1)]^{1/2}\langle e; s+1, q|I|s+l+1, l\rangle\\ &= \sum_{h=0}^{q} a_{s+1,q;h}[NS(k)(s+2h+2)]^{1/2}\langle s+h+1, h+1|I|e; s, p\rangle .\end{aligned} \tag{37}$$

The orthogonality relations

$$\begin{aligned} &\langle s+h+1, h+1 | I | e; s, p\rangle = 0, \quad h+1 < p; \\ &\langle e; s+1, q | I | s+l+1, l\rangle = 0, \quad l < q; \end{aligned} \tag{38}$$

are consequences of the orthonormal property defined by Eqs. (22) and (23) since, for example, $|s+l+1, l\rangle$ can be expressed as a linear combination of functions $|e; s+1, m\rangle$ with $m \leq l$. Nonvanishing elements occur in the right-hand members of Eq. (37) only for $p \leq h+1 \leq q+1$ and $q \leq l \leq p$ or, explicitly, only for $q = p$ and $q = p-1$. Consequently, Eq. (37) reduces to

$$\begin{aligned} \langle e; s+1, p | \rho_{\vec{k}} | e; s, p\rangle &= [NS(k)(s+2p+1)]^{1/2} a_{s,p;p}/a_{s+1,p;p} \\ &= [NS(k)]^{1/2} (s+p+1)^{1/2}, \\ \langle e; s+1, p-1 | \rho_{\vec{k}} | e; s, p\rangle &= [NS(k)(s+2p)]^{1/2} a_{s+1,p-1,p-1}/a_{s,p;p} \\ &= [NS(k)]^{1/2} \sqrt{p}\,. \end{aligned} \tag{39}$$

All other matrix elements of $\rho_{\vec{k}}$ vanish. Equations (26) and (39) imply the operator equivalence

$$\rho_{\vec{k}} = [NS(k)]^{1/2} (a_{\vec{k}}^{\dagger} + a_{-\vec{k}}). \tag{40}$$

Equations (28) and (29) yield

$$A_{\vec{k}}^{\dagger} + A_{-\vec{k}} = [\hat{e}(k)/e(k)]^{1/2} (a_{\vec{k}}^{\dagger} + a_{-\vec{k}})\,. \tag{41}$$

Consequently, $$\rho_{\vec{k}} = [NS(k)e(k)/\hat{e}(k)]^{1/2} (A_{\vec{k}}^{\dagger} + A_{-\vec{k}})\,. \tag{42}$$

Equation (40) tells us that the coefficient $S(k)e(k)/\hat{e}(k)$ in Eq. (42) must be interpreted as the liquid-structure function $\hat{S}(k)$ generated by the ground-state eigenfunction of H_D:

$$\hat{S}(k) = S(k)e(k)/\hat{e}(k) = \hbar^2 k^2/2m\hat{e}(k) = S(k)/[1+2w(k)/e(k)]^{1/2}\,. \tag{43}$$

Note that the third item of Eq. (43) is simply a statement of the Bijl-Feynman formula for the energy $\hat{e}(k)$ of an elementary excitation of momentum $\hbar\vec{k}$. Eq. (43) yields immediately

$$\hat{c}^2 = c^2 [1 + 2(w/e)_{k=0}]\,. \tag{44}$$

A second limiting form closely related to the preceding one can be derived from the definition of the interaction function $w(k)$ in Eq. (21):

$$[S'(k)/S^2(k)]_{k=0} = mc^2 [1 + 2(w/e)_{k=0}] = m\hat{c}^2\,. \tag{45}$$

V. GROUND-STATE EIGENFUNCTION OF H_D

The condition

$$A_{\vec{k}}^{\dagger} A_{\vec{k}} \hat{\Psi} = 0 \tag{46}$$

completely determines the ground-state eigenfunction of the operator H_D; Eq. (46) can be solved by writing $\hat{\Psi}$ in the product form:

$$\hat{\Psi} = \Big[\prod_{\vec{k}, k_x > 0} F_{\vec{k}}\Big] \Psi\,. \tag{47}$$

With $A_{\vec{k}}^{\dagger} A_{\vec{k}}$ expressed in terms of $a_{\pm\vec{k}}^{\dagger}$ and $a_{\pm\vec{k}}$, Eq. (46) reduces to an operator condition on $F_{\vec{k}}$:

$$\begin{aligned} \{[1 + D(k)^2](a_{\vec{k}}^{\dagger} a_{\vec{k}} + a_{-\vec{k}}^{\dagger} a_{-\vec{k}}) + 2D(k)^2 \\ - 2D(k)(a_{\vec{k}}^{\dagger} a_{-\vec{k}}^{\dagger} + a_{\vec{k}} a_{-\vec{k}})\} F_{\vec{k}} = 0\,. \end{aligned} \tag{48}$$

Equation (48) is solved by expressing $F_{\vec{k}}$ as a series in the functions $|e;o,p\rangle$:

$$F_{\vec{k}} = \sum_{0}^{\infty} C_p(k)|e;o,p\rangle/\Psi \,. \tag{49}$$

This form in Eq. (48), with help from Eq. (26) and the orthonormal property of $|e;o,p\rangle$, reduces it to a system of linear homogeneous difference equations for the coefficients $C_p(k)$:

$$[p(1+D^2)+D^2]C_p - pDC_{p-1} - (p+1)DC_{p+1} = 0. \tag{50}$$

The normalized solution of Eq. (50) is

$$C_p = D^p[1-D^2]^{1/2} \,. \tag{51}$$

Equations (19), (20), (24), and (51) now yield a completely explicit formula for $F_{\vec{k}}$ as a power series in $|\rho_{\vec{k}}|^2$:

$$F_{\vec{k}} = [1-D(k)^2]^{1/2} \sum_{q=0}^{\infty} \frac{1}{q!^2}\left(\frac{D(k)}{S(k)N}\,|\rho_{\vec{k}}|^2\right)^q \times \sum_{p=0}^{\infty} \frac{(p+q)!}{p!}[-D(k)]^p \,. \tag{52}$$

The closed form

$$\sum_{p=0}^{\infty} \frac{(p+q)!}{p}(-D)^p = \frac{q!}{(1+D)^{q+1}} \tag{53}$$

permits rewriting Eq. (52) as

$$F_{\vec{k}} = \left(\frac{1-D(k)}{1+D(k)}\right)^{1/2} \exp\left(\frac{D(k)}{NS(k)(1+D(k))}\,|\rho_{\vec{k}}|^2\right) \tag{54}$$

and Eq. (47) as

$$\Psi = \left(\prod_{\vec{k},\,k_x > 0} \frac{\hat{e}(k)}{e(k)}\right)^{1/2} \exp\left(\frac{1}{2N}\sum_{l}{}' \frac{e(l)-\hat{e}(l)}{2S(l)e(l)}\,|\rho_{\vec{l}}|^2\right)\Psi \tag{55}$$

The coefficients in Eqs. (55) are obtained from those in Eq. (54) by using Eq. (29) to show that

$$D/(1+D) = (e-\hat{e})/2e \;, \qquad (1-D)/(1+D) = \hat{e}/e \,. \tag{56}$$

Note that the summation over the complete wave-vector space (both $\vec{l}$ and $-\vec{l}$ excluding $\vec{l}=0$) is associated with a compensating factor of $\frac{1}{2}$.

The analysis is valid only within limits set by the separability condition of Eq. (32). In the present context, the equivalent condition is

$$\sum_{\vec{k}}(\hat{\Psi}, a_{\vec{k}}^{\dagger}a_{\vec{k}}\Psi) \ll N \,. \tag{57}$$

Equations (26), (47), and (49) can be used to convert the preceding inequality into

$$\sum_{\vec{k}} D(k)^2/[1-D(k)^2] \ll N \,. \tag{58}$$

To express Eq. (58) in a form suitable for numerical evaluation, we employ Eqs. (29) and (56) to show that

$$D^2/(1-D^2) = w^2/2\hat{e}(e+w+\hat{e}) \simeq (w/2\hat{e})^2 \;, \tag{59}$$

and obtain the working condition

$$\xi \equiv (2\pi^2\rho)^{-1}\int_0^{\infty} (w(k)/2\hat{e}(k))^2 k^2\,dk \ll 1 \;, \tag{60}$$

The theoretical description of the improved ground-state trial function $\hat{\Psi}$ is completed by computing the change δU in $U(r)$ defined by the ratio $\hat{\Psi}/\Psi$:

$$\begin{aligned}\delta U(r) &= N^{-1}\sum_{\vec{k}}\{[S(k)]^{-1} - [\hat{S}(k)]^{-1}\}e^{i\vec{k}\cdot\vec{r}} \\ &= [(2\pi)^3\rho]^{-1}\int\{[S(k)]^{-1} - [\hat{S}(k)]^{-1}\}e^{i\vec{k}\cdot\vec{r}}\,d\vec{k} \,. \end{aligned} \tag{61}$$

We observe that Eq. (61) can be derived directly from Eq. (16) without invoking the paired-phonon analysis which is needed here only to supply an independent computational formula for $\hat{S}(k)$.

VI. OPTIMIZATION AND VARIATIONAL EXTREMUM CONDITIONS

The condition $\delta E_0 \equiv \hat{E}_0 - E_0 = 0$ characterizes the optimum BDJ-type trial function. The equivalent statement $w(k)=0$ yields immediately

$$\begin{aligned} S'(k) &= (\hbar^2k^2/4m)[1-S(k)] \,, \\ g'(r) &= (\hbar^2/4m)\Delta g(r) = \int \frac{\delta g(\vec{r})}{\delta u(\vec{r}')} V^*(r')\,d\vec{r}'. \end{aligned} \tag{62}$$

Two parenthetical observations on the functional derivative appearing in Eq. (62) are interpolated here for the sake of clarity. First, note an explicit formula[13] in terms of the two, three, and four point distribution functions generated by the starting trial function Ψ:

$$\frac{\delta g(r)}{\delta u(r')} = g(r)\,\delta(\vec{r}' - \vec{r}) + \frac{2}{\rho^2}\,p^{(3)}(\vec{r},\vec{O},\vec{r}+\vec{r}') + \frac{1}{2\rho^2}\int[\,p^{(4)}(\vec{r},\vec{O},\vec{r}'+\vec{r}'',\vec{r}'')$$

$$-\rho^4 g(r) g(r')] d\vec{r}'' \ . \tag{63}$$

The second observation is the symmetry property: The functional derivative is a symmetrical function of $\vec{r}$ and $\vec{r}'$. The proof is based on a succession of coordinate changes, all leaving the right-hand member of Eq. (63) invariant. These are $\vec{r}$, $\vec{O}$, $\vec{r}+\vec{r}' \to -\vec{r}'$, $-\vec{r}-\vec{r}'$, $\vec{O}\to\vec{r}'$, $\vec{r}+\vec{r}'$, $\vec{O}\to\vec{r}'$, $\vec{O}$, $\vec{r}+\vec{r}'$ and $\vec{r}$, $\vec{O}$, $\vec{r}'+\vec{r}''$, $\vec{r}''\to-\vec{r}-\vec{r}''$, $-\vec{r}''$, $\vec{r}'$, $\vec{O}\to-\vec{r}+\vec{r}''$, $\vec{r}''$, $\vec{r}'$, $\vec{O}$, $\to\vec{r}'$, $\vec{O}$, $\vec{r}+\vec{r}''$, $\vec{r}''$.

What can be said about the variational extremum condition? The analysis starts from the formula

$$\int \Psi H \Psi \, d\vec{r}_{12\ldots N} = \frac{1}{2} N\rho \left(\frac{\hbar^2}{4m} \int \nabla g \cdot \nabla U \, d\vec{r} + \int g v \, d\vec{r} \right), \tag{64}$$

and the variational form

$$\delta \int \Psi H \Psi \, d\vec{r}_{12\cdots N} = \tfrac{1}{2} N\rho \int \delta U(r) \left(-\frac{\hbar^2}{4m} \Delta g(r) + \int \frac{\delta g(\vec{r}\,')}{\delta U(\vec{r})} V^*(r') \, d\vec{r}\,' \right) d\vec{r} \ . \tag{65}$$

Equation (65) states that the expectation value of H is stationary with respect to small changes in U if the optimization condition of Eq. (62) holds. The statement is exact since no approximations are made in passing from the BDJ-type trial function to Eqs. (62) and (65). In particular, the separability condition is trivially satisfied since $w(k) = 0$ implies $\hat{\Psi} = \Psi$.

VII. EVALUATION OF $S'(k)$ AND NUMERICAL RESULTS AT MASS 4(^{4}He)

The basic problem on which we now focus attention is the numerical evaluation of $S'(k)$ and $g'(r)$. We begin the discussion by representing $S'(k)$ as a linear functional in the two-, three-, and four-particle distribution functions generated by Ψ:

$$\begin{aligned} S'(k) &= (1/N) \int \Psi^2 |\rho_{\vec{k}}|^2 [V^*(12\cdots N) - \langle 0 | V^* | 0 \rangle] \, d\vec{r}_{12\cdots N} \\ &= V_k^* + (2/N) \int [p^{(3)}(123) - \rho^3 g(r_{12}) g(r_{13})] e^{i\vec{k}\cdot\vec{r}_{13}} V^*(r_{12}) \, d\vec{r}_{123} \\ &\quad + (1/2N) \int \{ p^{(4)}(1234) - \rho^4 g(r_{12}) g(r_{34}) [1 + 4h(r_{13})] \} e^{i\vec{k}\cdot\vec{r}_{34}} V^*(r_{12}) \, d\vec{r}_{1234} \ . \end{aligned} \tag{66}$$

Note that terms in $\rho^3 g(r_{12}) g(r_{13})$ and $\rho^4 g(r_{12}) g(r_{34}) \times h(r_{13})$ cancel against each other, but serve the useful purpose of reducing the three- and four-point integrals separately to the order of magnitude of N^0. The available symmetrical approximate forms for $p^{(3)}$ and $p^{(4)}$ are found to be inadequate in the evaluation of $S'(k)$. For example, the superposition and other simple approximate forms yield $S'(0) \neq 0$, implying $e(0+) \neq 0$. Therefore, we have turned to other procedures which do not employ the three- and four-particle distribution functions.

First, we wish to point out and stress that available practical techniques make possible the direct numerical evaluation of $g(r|\beta)$ for moderately large values of N.[14] The method of molecular dynamics has already been applied to evaluate $g(r)$ generated by BDJ-type trial function for a system of 864 particles.[4,15] The extension to compute $g(r|\beta)$ presents no additional problems or complications. Numerical results for two or three values of β in the range in which $g(r|\beta)$ is nearly linear in β would make possible the evaluation of $g'(r)$. From $g'(r)$ to $S'(k)$ is an easy step. We hope that this possibility of achieving a close approach to the optimum BDJ-type trial function will be realized in the near future. Until then, it is necessary to rely on less direct and accurate procedures to obtain some idea of how far presently available trial functions are from the optimum.

The methods to be discussed are based on approximate relations expressing $U(r)$ as a functional in g and S. These relations are (i) the hypernetted-chain (HNC)[16,17](Sec. VII A) and (ii) the Percus-Yevick (PY)[18] (Sec. VII B):

$$U_{\mathrm{HNC}}(r) + \beta V^*(r|\mathrm{HNC}) = \ln g(r|\beta) - P(r|S) , \tag{67a}$$

$$P(r|S) = \frac{1}{(2\pi)^3 \rho} \int e^{i\vec{k}\cdot\vec{r}} \frac{[S(k|\beta) - 1]^2}{S(k|\beta)} \, d\vec{k} , \tag{67b}$$

$$V^*(r|\mathrm{HNC}) = v(r) - (\hbar^2/4m) \Delta U_{\mathrm{HNC}}(r) ; \tag{67c}$$

$$U_{py}(r) + \beta V^*(r|py) = \ln g(r|\beta) - \ln[1 + P(r|S)] , \tag{68a}$$

$$V^*(r|py) = v(r) - (\hbar^2/4m) \Delta U_{\mathrm{PY}}(r) \ . \tag{68b}$$

The Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) relation can also be used to evaluate

$S'(k)$, but since no numerical results are available we do not develop the theory

A. HNC Relation: Method and Results

The operation of taking the derivative with respect to β evaluated at $\beta=0$ is applied to both left- and right-hand sides of Eq. (67a) with the result:

$$\rho g(r)\, V^*(r|\,\mathrm{HNC}) = \rho g'(r) + \frac{g(r)}{(2\pi)^3}\int e^{i\vec{k}\cdot\vec{r}}[1-S^2(k)]\,\frac{S'(k)}{S^2(k)}\,d\vec{k}\,. \tag{69}$$

Next, both members of Eq. (69) are converted into the associated Fourier transforms. With the notation

$$L(k) = \frac{S'(k)}{S^2(k)}\,,$$
$$V_k^* = \rho\int e^{i\vec{k}\cdot\vec{r}} g(r) V^*(r|\,\mathrm{HNC})\,d\vec{r}\,, \tag{70}$$

the resulting linear inhomogeneous integral equation for $L(k)$ is

$$L(h) = V_h^* + \frac{1}{(2\pi)^3\rho}\int[1-S(|\vec{k}+\vec{h}|)] \times [1-S^2(k)]\,L(k)\,d\vec{k}\,. \tag{71}$$

The question of uniqueness is considered briefly in Ref. 8, where an inequality is derived which proves that $L(k)$ is unique if $S(k) \leq 1$. In the actual physical situation $S(k)$ oscillates about the asymptotic value 1 and the argument developed in Ref. 8 does not prove uniqueness, but does make it highly plausible.

In the actual numerical evaluation the entering functions $U(r)$, $g(r)$, and $S(k)$ are taken from a recent theoretical determination by Massey and Woo. We have modified the given $S(k)$ slightly so that it conforms to the physical requirements at the origin $[S(k) \simeq \hbar k/2mc$,[19] $c = 238$ m/sec, the experimental velocity of first sound] while maintaining the correct normalization $[g(0)=0]$. The modification (confined to the region $k < 0.2\ \text{Å}^{-1}$) is simply a small vertical displacement so that the computed curve joins on smoothly to the straight line with correct slope passing through the origin. The slight change in normalization generated by the modification requires essentially invisible changes in $S(k)$ elsewhere.

Equation (71) can be solved by an iteration process using the function $\frac{1}{2}e(k)\{[S(k)]^{-1}-1\}$ as a starting approximation for $L(k)$ in the integral term [good if $S(k)$ is close to the optimum form]. Rapid convergence of the iterative process was induced by a simple geometric projection technique. The function V_k^* is obviously an extremely poor starting approximation since V_0^* is negative, while $L(0)$ must be positive to fit the physical relation $L(0) = m\hat{c}^2$ [Eq. (45)].

Numerical results for liquid ^{4}He at $\rho = 0.0218\ \text{Å}^{-3}$ are displayed in Figs. 1–3. Solid curves in Fig. 1 represent $L(k)$ and V_k^*. Experimental and theoretical results for the liquid-structure function appear in Fig. 2. Observe that the shoulder below $k = 1\ \text{Å}^{-1}$ in $S(k)$ is almost completely absent in $\hat{S}(k)$; also $\hat{S}(k)$ has a higher first maximum. The interaction function $w(k)$ is plotted as the solid curve in Fig. 3. One test of internal consistency is met at an adequate level; $\hat{c} = [(1/m)L(0)]^{1/2} = 219$ m/sec, not far from the experimental starting value of 238 m/sec. The energy shift $\delta E_0 = \hat{E}_0 - E_0$ [Eq. (33)] and the separation parameter ξ [Eq. (60)] have the values

$$N^{-1}\delta E_0 = 0.69\ {}^\circ\mathrm{K}\,,$$
$$\xi = 0.029\,. \tag{72}$$

The function $\hat{g}(r)$ can be computed as the Fourier transform of $\hat{S}(k)$. However, in practice, $\hat{S}(k)$ is not determined with sufficient accuracy for large values of k to produce sensible behavior of the Fourier transform for small values of $r\,[\hat{g}(r) > 0,\ \hat{g}(0) = 0]$. To overcome this difficulty we identify $\delta U(r)$ with

$$U_{\mathrm{HNC}}(r|\hat{g}_{\mathrm{HNC}}) - U_{\mathrm{HNC}}(r|g)\,,$$

and use the HNC relation directly to give

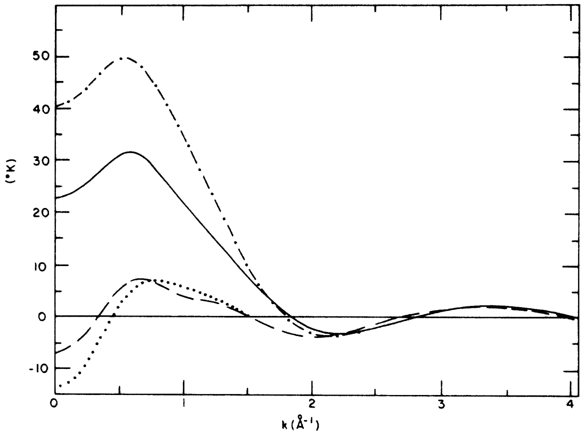

FIG. 1. HNC and PY approximations for $L(k)$ and V_k^*: solid line $L(k)$, HNC version [Eq. (71)]; dashed line V_k^*, HNC version [Eqs. (67c) and (70)]; dot-dashed line $L(k)$, PY version [Eq. (75)]; dotted line V_k^*, PY version [Eqs. (68b) and (70)].

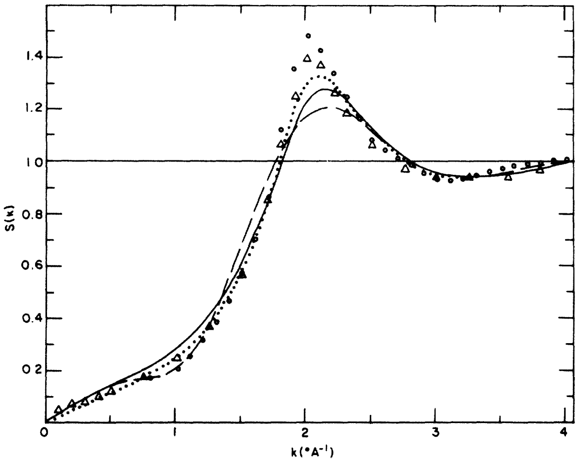

FIG. 2. Experimental and theoretical results for the liquid-structure function of liquid ^{4}He at $\rho = 0.021$ Å^{-3} ○ Neutron diffraction, 1.06 °K [D. G. Henshaw, Phys. Rev. 119, 9 (1960)]. △ x-ray diffraction, 1.4 °K [W. L. Gordon, C. H. Shaw, and J. G. Daunt, Phys. Chem. Solids 5, 117 (1958)]; dashed line Starting form (Ref. 5) $S(k)$, solid line HNC, $\hat{S}(k)$ [Eq. (43)], dotted line PY $\hat{S}(k)$ [Eq. (43)].

$$\hat{g}_{\mathrm{HNC}}(r) = g(r)\exp[\delta U(r) + P(r|\hat{S}) - P(r|S)] . \quad (73)$$

Deviations from the function defined by the Fourier transform of $\hat{S}(k)$ are negligible except in the region below $r = 2$ Å, where $g(r)$ is extremely small.

The entire calculation was repeated using $\hat{g}(r)$ as the starting function. In this second iteraction of the paired-phonon analysis all changes are almost negligible, indicating a close approach to an "optimum" trial function. The quotes call attention to the fact that the HNC relation is approximate. Numerical results for the new version of $w(k)$ are plotted as the dotted curve in Fig. 3. The optimization condition $w(k) = 0$ is very nearly satisfied by $\hat{g}(r)$, as is evident from comparing the first iteration and second iteration versions of

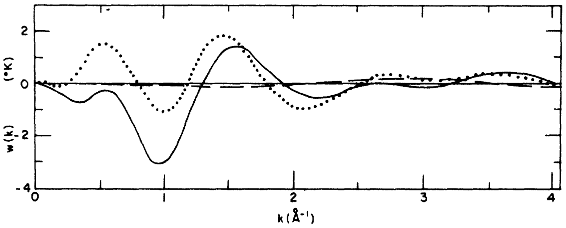

FIG. 3. Interaction function $w(k)$ in first and second iterations of the paired-phonon analysis: solid line HNC, 1st iteration; dashed line HNC, 2nd iteration; dotted line PY, 1st iteration.

$w(k)$. The second iteration yields an additional energy correction $N^{-1}\delta E_0 = -0.038$ °K and a separation parameter $\xi = 0.0005$. The total energy correction is $-0.69 - 0.04 = -0.73$, bringing the expectation value of $N^{-1}H$ down to -6.7 °K/atom (compare with the experimental value -7.2 °K/atom).

Because the HNC relation is an approximation, it is worthwhile to look at alternative procedures for estimating δE_0. Here, a suitable notation is helpful. Let

$$N^{-1}\langle \mathrm{KE}\rangle_{x,y} = (h^2/8m)\int \nabla g_x(r)\cdot\nabla U_y(r)\,d\vec{r} ,$$

and
$$N^{-1}\langle \mathrm{PE}\rangle_x = \tfrac{1}{2}\rho\int g_x(r)v(r)\,d\vec{r} . \quad (74)$$

Numerical results for several different sets of trial functions are listed in Table I.

In the first three lines, U in each line is computed from the given radial distribution function by solving the BBGKY equation with the Kirkwood superposition approximation for $p^{(3)}$. Line 2 shows a small energy shift in the wrong direction. Lines 4 and 5 involve only the HNC approximation and exhibit an energy shift of -0.64 °K/atom nearly identical with the shift generated by the first iteration of the paired-phonon analysis [Eq. (72)]. This last result can be associated with the identity of optimization and variational extremum

TABLE I. Estimated energy quantities[a] for ^{4}He at $\rho = 0.0218$ Å^{-3}.

Trial functions	$N^{-1}\langle\mathrm{KE}\rangle$	$N^{-1}\langle\mathrm{PE}\rangle$	$N^{-1}\langle H\rangle$
$g(r)$, $U(r\,|\,\mathrm{BBGKY,\ KSA})$	14.06	−20.03	−5.97
$\hat{g}_{\mathrm{HNC}}(r)$, $U(r\,|\,\mathrm{BBGKY,\ KSA})$	14.78	−20.69	−5.91
$\hat{g}_{\mathrm{PY}}(r)$, $U(r\,|\,\mathrm{BBGKY,\ KSA})$	14.36	−20.68	−6.32
$g(r)$, $U_{\mathrm{HNC}}(r\,|\,g)$	16.63	−20.03	−3.40
$\hat{g}_{\mathrm{HNC}}(r)$, $U_{\mathrm{HNC}}(r\,|\,\hat{g}_{\mathrm{HNC}})$	16.64	−20.69	−4.04
$g(r)$, $U_{\mathrm{PY}}(r\,|\,g)$	13.45	−20.03	−6.62
$\hat{g}_{\mathrm{PY}}(r)$, $U_{\mathrm{PY}}(r\,|\,\hat{g}_{\mathrm{PY}})$	13.94	−20.68	−6.74

[a] Unit is °K/atom.

conditions which is maintained when the exact $U(r|g)$ is replaced by $U_{\mathrm{HNC}}(r|g)$ in both the paired-phonon analysis and the formula for the expectation value of H[Eqs. (64) and (84)]. The proof that the substitution of U_{HNC} for U does not invalidate the identity of the two conditions is given in Sec. IX.

B. PY Relation: Method and Results

The operations which generate Eq. (71) for L from Eq. (67) are now applied to Eq. (68) with the result

$$L(h)=V_h^*+[(2\pi)^3\rho]^{-1}\int R(|\vec{\mathrm{k}}+\vec{\mathrm{h}}|)[1-S^2(k)]L(k)\,d\vec{\mathrm{k}},$$

$$R(k)=\rho\int e^{i\vec{\mathrm{k}}\cdot\vec{\mathrm{r}}}(1-e^{U_{\mathrm{PY}}(r)})\,d\vec{\mathrm{r}}\,. \tag{75}$$

Numerical results for ^{4}He at $\rho=0.0218\ \mathrm{Å}^{-3}$ are shown in Figs. 1–3. Dash-dot and dot curves in Fig. 1 represent $L(k)$ and V_k^*, respectively. The liquid-structure function $\hat{S}(k)$ is plotted as the dotted curve in Fig. 2. Here the PY version is a bit closer to the experimental points than is the HNC version. The interaction function $w(k)$ appears in Fig. 3 as the dotted curve. Here the two versions of $w(k)$ differ in detail, but are quite similar in magnitude and range of large values. The two versions of $L(k)$ in Fig. 1 differ substantially and the difference favors the HNC version. The difference is principally due to the fact that $\exp[U(r)]-1$ falls off more slowly for large r than $g(r)-1$. When the correlations generated by the zero-point fluctuations of the sound field[20] are included in U and Ψ, the function $\exp[U(r)]-1$ varies as r^{-2} for large r while $g(r)-1$ goes as r^{-4}. As a consequence $R(k)$ varies as k^{-1} for small k while $S(k)-1$ is a linear function of k.

Now the energy shift and the separation parameter have the values

$$N^{-1}\delta E_0=0.68\ {}^\circ\mathrm{K}\,,\qquad \xi=0.026\,, \tag{76}$$

both close to the corresponding HNC results.

To compute $\hat{g}_{\mathrm{PY}}(r)$ we identify $\delta U(r)$ with $U_{py}(r|\hat{g}_{py})-U_{\mathrm{PY}}(r|g)$ and use the PY relation to give

$$\hat{g}_{py}(r)=g(r)\{[1+P(r|\hat{S})]/[1+P(r|S)]\}e^{\delta U(r)}\,. \tag{77}$$

The remarks preceding and following Eq. (73) apply here.

The second iteration of the paired-phonon analysis now yields $N^{-1}\delta E_0=-0.036\ {}^\circ$K and $\xi=0.0011$. Again the agreement with the corresponding HNC results is close.

In Table I, the results for alternative methods of estimating $N^{-1}\delta E_0$ are consistently in the right direction, but small (– 0.35 °K from lines 1 and 3; – 0.12 °K from lines 6 and 7).

VIII. NUMERICAL RESULTS AT MASS 3 (^{3}He)

The ground-state boson-type solution of the Schrödinger equation for the N-particle ^{3}He system serves as the correlation function in recent studies of liquid ^{3}He by the method of correlated basis functions.[21–23] Variational calculations by Massey and Woo[5] and by Schiff and Verlet[4] give results for $U(r)$, $g(r)$, $S(k)$, and E_0 in the BDJ-type trial function space. We have applied the paired-phonon analysis to the ^{3}He system at the equilibrium density $\rho=0.0164\ \mathrm{Å}^{-3}$, taking the Massey-Woo determination of $g(r)$ and $S(k)$ as starting functions. The first iteration gives the results

$$\begin{aligned} N^{-1}\delta E_0&=-0.25\ {}^\circ\mathrm{K}\,, &&\\ \xi&=0.0060\,, && (\mathrm{HNC})\\ N^{-1}\delta E_0&=-0.50\ {}^\circ\mathrm{K}\,, &&\\ \xi&=0.019\,. && (\mathrm{PY}) \end{aligned} \tag{78}$$

The second iteration was carried through in the PY approximation with the results

$$N^{-1}\delta E_0=-0.049\ {}^\circ\mathrm{K}\,,\qquad \xi=0.0021\,, \qquad (\mathrm{PY}) \tag{79}$$

TABLE II. Estimated energy quantities[a] for ^{3}He at $\rho=0.0164\ \mathrm{Å}^{-3}$.

Trial functions	$N^{-1}\langle\mathrm{KE}\rangle$	$N^{-1}\langle\mathrm{PE}\rangle$	$N^{-1}\langle H\rangle$
$g(r)$, $U(r\|\mathrm{BBGKY, KSA})$	12.32	−14.41	−2.09
$\hat{g}_{\mathrm{PY}}(r)$, $U(r\|\mathrm{BBGKY, KSA})$	11.96	−14.56	−2.60
$g(r)$, $U_{\mathrm{HNC}}(r\|g)$	13.10	−14.41	−1.31
$g(r)$, $U_{\mathrm{PY}}(r\|g)$	11.88	−14.41	−2.53
$\hat{g}_{\mathrm{PY}}(r)$, $U_{\mathrm{PY}}(r\|\hat{g}_{\mathrm{PY}})$	11.39	−14.56	−3.17

[a] Energy unit is °K/atom.

with both numbers smaller by an order of magnitude than the corresponding numbers of the first iteration.

Results for energy quantities by alternative methods are listed in Table II. Lines 1 and 2 give an energy shift of − 0.51 °K/atom; lines 4 and 5 give − 0.64 °K/atom. These estimates are moderately close to the total shift of − 0.55 °K/atom generated by the paired-phonon analysis in the PY approximation.

We conclude this brief report on a formidable array of calculations by stating that the over-all similarity of the physical results generated by the HNC and PY relations encourages us to expect rather similar results from an accurate numerical evaluation of the $3(N-1)$ dimensional integral formula for $S'(k)$ by the method of molecular dynamics, or by any other suitable numerical technique.

IX. OPTIMIZATION AND VARIATIONAL EXTREMUM CONDITIONS IN THE HNC APPROXIMATION

We use Eqs. (62), (67), and (69) to derive a statement in which the two-particle correlation function U does not occur. First Eq. (67) generates

$$\Delta U_{\mathrm{HNC}}(r|g)=\Delta g(r)\left(\frac{1}{g(r)}-1\right)-\left(\frac{\nabla g(r)}{g(r)}\right)^2-\frac{1}{(2\pi)^3\rho}\int e^{i\vec{\mathrm{k}}\cdot\vec{\mathrm{r}}}\left(1-\frac{1}{S(k)}\right)k^2 d\vec{\mathrm{k}}\,. \tag{80}$$

Substitution from Eq. (62) into Eq. (69) produces the explicit statement

$$\frac{4m}{\hbar^2}v(r)-\Delta U_{\mathrm{HNC}}(r|g)=\Delta g(r)\left(\frac{1}{g(r)}-1\right)+\frac{1}{(2\pi)^3\rho}\int e^{i\vec{\mathrm{k}}\cdot\vec{\mathrm{r}}}\left(\frac{k}{S(k)}\right)^2[1-S(k)]\,d\vec{\mathrm{k}}\,. \tag{81}$$

Finally left- and right-hand sides of Eqs. (80) and (81) are summed to give the desired relation

$$\begin{gathered}2[g(r)-1]\Delta g(r)+\frac{1}{g(r)}\left(\frac{dg}{dr}\right)^2=\frac{4m}{\hbar^2}[\tilde{v}(r)-v(r)]\,,\\ \frac{4m}{\hbar^2}\tilde{v}(r)=\frac{1}{(2\pi)^3\rho}\int e^{i\vec{\mathrm{k}}\cdot\vec{\mathrm{r}}}\left(\frac{k}{S(k)}\right)^2[1-S^2(k)]\,d\vec{\mathrm{k}}=\Delta\frac{1}{(2\pi)^3\rho}\int e^{i\vec{\mathrm{k}}\cdot\vec{\mathrm{r}}}\left(1-\frac{1}{S(k)^2}\right)d\vec{\mathrm{k}}\;.\end{gathered} \tag{82}$$

Equation (82) is a highly nonlinear differential-integral condition on $g(r)$. We do not know that the equation possesses a solution or, if a solution exists, that it has sensible physical properties. In this context, something can be learned by using the experimental information on $g(r)$ and $S(k)$ to study the interrelations of the zeroes and stationary points of $g(r)-1$ and the zeroes of the right-hand side. Let $r_1, r_3, \ldots, r_{2n+1}, \ldots$ designate successive zeroes of $g(r)-1$ and $r_2, r_4, \ldots r_{2n}, \ldots$ successive positions at which $g(r)$ is stationary. Equation (82) requires

$$\begin{aligned}&\frac{dg}{dr}=(-1)^{n+1}\left(\frac{4m}{\hbar^2}(\tilde{v}(r)-v(r))\right)^{1/2}, \qquad r=r_{2n+1}\,;\\ &[1-g(r)]\frac{d^2g}{dr^2}=\frac{2m}{\hbar^2}[v(r)-\tilde{v}(r)], \qquad r=r_{2n}\\ &\qquad\qquad > 0\;.\end{aligned} \tag{83}$$

The sign factor in the first line of Eq. (83) fits the requirement that the slope at the first crossover $(r=r_1)$ is positive and also that it reverses sign at successive crossovers. The inequality in the second line of Eq. (83) involves the special (but highly plausible) assumption that $g(r)$ is stationary at only one point between successive zeroes of $g(r)-1$. These relations imply that $\tilde{v}-v$ has an odd number of zeroes between a crossover point $(r=r_{2n+1})$ and the following stationary point $[r=r_{2(n+1)}]$. We have estimated $\tilde{v}(r)$ from the observed liquid-structure function and check Eq. (83) at a semiquantitative level out to the second crossover ($r_3\sim 4.5$ Å). This modest success may be cited as evidence that Eq. (82) determines a function $g(r)$ with reasonable physical properties.

We are interested in the variational extremum properties of the right-hand side of Eq. (64) when the correlation function $U(r|g)$ is replaced by $U_{\mathrm{HNC}}(r|g)$:

$$\frac{2}{N\rho}\,\mathcal{E}(\rho|\mathrm{HNC}) \equiv \frac{\hbar^2}{4m}\int \nabla g\cdot\nabla U_{\mathrm{HNC}}(r|g)\,d\vec{r} + \int g v\,d\vec{r}$$

$$= \frac{\hbar^2}{4m}\int(\nabla g)^2\left(\frac{1}{g(r)}-1\right)d\vec{r} + \frac{\hbar^2}{4m}\,\frac{1}{(2\pi)^3\rho^2}\int k^2\,\frac{[S(k)-1]^2}{S(k)}\,d\vec{k} + \int g v\,d\vec{r}\ . \tag{84}$$

The variational form is

$$\frac{2}{N\rho}\,\delta\mathcal{E}(\rho|\mathrm{HNC}) = \frac{\hbar^2}{4m}\int\frac{\delta g(r)}{g(r)}\left(2[g(r)-1]\,\Delta g(r) + \frac{(\vec{\nabla}g)^2}{g} + \frac{4m}{\hbar^2}\,g(r)[v(r)-\tilde{v}(r)]\right)d\vec{r}\ , \tag{85}$$

and the right-hand integral is seen to vanish if the optimization condition of Eq. (82) holds. This verifies the statement made in Sec. VII in connection with the discussion of lines 4 and 5 in Table I. In summary, the HNC approximation maintains the direct connection between the optimization condition of the paired-phonon analysis and the variational extremum property of the expectation value of H. This connection is a special property of the HNC approximation; it does not hold for the PY form.

ACKNOWLEDGMENTS

We take pleasure in expressing our appreciation for the excellent facilities and to the cooperative staff at the Washington University Computing Center. The senior author is grateful to the Aspen Center for Physics for hospitality during the summer of 1968 and to the Physics Department of the State University of New York at Stony Brook for the opportunity to conduct a seminar on topics related to the material of this paper during the spring semester 1969.

[†] Supported in part by National Science Foundation Grant No. GP-8924.

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