Three-Particle Variational Wave Function for Bose Liquids[*]

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A new variational wave function is proposed for the ground state of Bose liquids. It consists of a Jastrow function multiplied by exponentials of three-particle functions. The form of the wave function is deduced from a formal analysis carried out for the weakly interacting Bose gas characterized by a strength parameter λ. By using the wave function proposed here, the energy obtained is exact to $O(\lambda^4)$. Several useful and straightforward applications of the new method to liquid helium and Coulomb gases are suggested.

I. JASTROW THEORY FOR BOSE LIQUIDS

Systems of strongly correlated bosons are known as Bose liquids. These strong correlations may be in the form of short-ranged repulsive cores, as in the case of liquid He^4, or in the form of long-ranged interactions, as in the case of the charged Bose gas. One of the most powerful tools for studying the ground state and the low-lying excited states of Bose liquids has been the Jastrow theory. Over the last decade, the application of Jastrow's theory has led to certain quantitative as well as qualitative success[1] for both liquid He^4 and the charged Bose gas.

I assume a pairwise central potential and consider a Bose liquid made up of N particles in a normalizing volume Ω and characterized by the Hamiltonian

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

The wave functions must be symmetrical with respect to exchange. For a noninteracting system, appropriate wave functions can be formed by symmetrizing products of plane waves. In the more realistic case, where the potential $v(r)$ is not identically zero, it is convenient to consider one particle at a time, moving in an effective single-particle field provided collectively by its peers. A self-consistent scheme may then be set up, resulting in the Hartree products

$$\psi_{n_1, n_2, \ldots, n_N}(1, 2, \ldots, N) = S \prod_{i=1}^{N} \varphi_{n_i}(\vec{r}_i) , \tag{2}$$

where S stands for the symmetrization operator and $\{n_i\}$ denote complete sets of quantum numbers. For translationally invariant systems, $\{n_i\}$ are the $3N$ wave vectors $\vec{k}_1, \vec{k}_2, \ldots, \vec{k}_N$, and the single-particle orbitals remain plane waves. The ground-state wave function then reduces to unity. More generally, I let $n_i = 0$ represent the lowest orbital, and express the Hartree ground-state wave function as

$$\psi_H(1, 2, \ldots, N) = \prod_{i=1}^{N} \varphi_0(\vec{r}_i) . \tag{3}$$

This is the first step toward describing a many-particle system. It forms what is known as the independent-particle picture.

The ordinary perturbation theory based on an independent-particle model fails in the case of strongly correlated systems. For liquid helium, $v(r)$ contains a strong repulsive core and leads to divergent matrix elements. For Coulomb systems, while the matrix elements converge, certain classes of important terms in the perturbative expansion diverge in the limit of small momentum transfers. These difficulties stem from the inability of single-particle products to account for strong interparticle correlations. While the more sophisticated and widely accepted approach toward repairing the damage relies on the employment of summation techniques borrowed from quantum field theory, a more direct and practical method is definitely that due to Bijl,[2] Dingle,[3] and Jastrow,[4] who sought to circumvent the difficulties by laboriously avoiding divergences. In what shall be referred to as the Jastrow model, interparticle correlations are taken into account in the least costly manner: by incorporating two-particle functions from the outset into the basis,

$$\psi^J_{n_1, n_2, \ldots, n_N}(1, 2, \ldots, N)$$

$$= S \prod_{i=1}^{N} \varphi_{n_i}(\vec{r}_i) \prod_{1 \leq j < k \leq N} f(\vec{r}_j, \vec{r}_k) . \tag{4}$$

For the ground state,

$$\psi^J_{0,0,\ldots,0}(1, 2, \ldots, N) = \prod_{i=1}^{N} \varphi_0(\vec{r}_i) \prod_{1 \leq j < k \leq N} f(\vec{r}_j, \vec{r}_k)$$

$$= \psi_H(1, 2, \ldots, N) \prod_{1 \leq j < k \leq N} f(\vec{r}_j, \vec{r}_k) . \tag{5}$$

In the case of translationally invariant systems such as liquids,

$$f(\vec{r}_i, \vec{r}_j) = f(r_{ij}) , \tag{6}$$

and Ψ_H reduces to 1, giving rise to the well-known Jastrow function

$$\psi_J(1, 2, \ldots, N) = \psi_H \prod_{1 \leq j < k \leq N} f(r_{jk}) = \prod_{i<j} f(r_{ij}) . \tag{7}$$

Writing

$$\ln f^2(r) = u(r) , \tag{8}$$

the more convenient form of the function is obtained,

$$\psi_J(1, 2, \ldots, N) = \prod_{i<j} \exp[\tfrac{1}{2} u(r_{ij})] = \exp\!\left(\tfrac{1}{2} \sum_{i<j} u(r_{ij})\right) , \tag{9}$$

which by now appears regularly in the literature[1] on variational calculations for Bose liquids.

In a recent analysis,[5] we carried out energy calculations for a weakly interacting Bose gas in an effort to unearth the ingredients for the success of Jastrow's theory. Using a Fourier transformable but otherwise general pairwise potential $\lambda v(r)$,

$$\lambda v(k) = \int d\vec{r} \, \lambda v(r) e^{-\vec{k}\cdot\vec{r}} , \tag{10}$$

where λ measures the strength of the interaction, we first calculated the exact ground-state energy E using a prescription due to Hugenholtz and Pines,[6] and expressed it as a power series in λ. Replacing $\hbar$ and m by 1 and defining the number density n by

$$n = N/\Omega , \tag{11}$$

We found that

$$E = \sum_m \lambda^m E_m , \tag{12}$$

with

$$E_0 = 0 = \hat{\epsilon}_0 , \tag{13}$$

$$E_1 = \tfrac{1}{2} n^2 v(0) = \hat{\epsilon}_1 , \tag{14}$$

$$E_2 = -\tfrac{1}{2} n^2 \sum_{\vec{k}} \frac{v^2(k)}{k^2} = \hat{\epsilon}_2 , \tag{15}$$

$$E_3 = n^3 \sum_{\vec{k}} \frac{v^3(k)}{k^4} + \tfrac{1}{2} n^2 \sum_{\vec{k}\vec{l}} \frac{v(k) v(l) v(\vec{k}+\vec{l})}{k^2 l^2} = \hat{\epsilon}_3 , \tag{16}$$

$$E_4 = \hat{\epsilon}_4 + \Delta\epsilon_4 , \tag{17}$$

etc., where

$$\hat{\epsilon}_4 = \frac{-5n^4}{2} \sum_{\vec{k}} \frac{v^4(k)}{k^6} - \frac{3n^3}{2} \sum_{\vec{k}\vec{l}} \frac{v^2(k) v(l) v(\vec{k}+\vec{l})}{k^2 l^2 (\vec{k}+\vec{l})^2}$$

$$- 3n^3 \sum_{\vec{k}\vec{l}} \frac{v^2(k) v(l) v(\vec{k}+\vec{l})}{k^4 l^2}$$

$$- \frac{n^2}{2} \sum_{\vec{k}\vec{l}\vec{p}} \frac{v(l) v(p) v(\vec{k}+\vec{l}) v(\vec{k}+\vec{p})}{k^2 l^2 p^2} \tag{18}$$

and

$$\Delta\epsilon_4 = \frac{-n^3}{2} \sum_{\vec{k}\vec{l}} \frac{v^2(k) v(l) v(\vec{k}+\vec{l})}{k^2 l^2 (\vec{k}+\vec{l})^2}$$

$$+ n^3 \sum_{\vec{k}\vec{l}} \frac{v^2(k) v(l) v(\vec{k}+\vec{l})}{k^4 l^2} + n^3 \sum_{\vec{k}\vec{l}} \frac{v^2(k) v^2(l)}{k^4 l^2}$$

$$- 2n^3 \sum_{\vec{k}\vec{l}} \frac{v^2(k) v(l)}{k^2[k^2 + l^2 + (\vec{k}+\vec{l})^2]}\left(\frac{v(l)}{k^2} + \frac{v(l)}{l^2} + \frac{v(\vec{k}+\vec{l})}{k^2}\right) . \tag{19}$$

In the above equations, a new set of energy notations $\hat{\epsilon}_m$ have been defined for convenience of later identification.

Next the ground-state energy was calculated by means of the Jastrow theory. The expectation value ϵ_J of the Hamiltonian defined by Eqs. (1) and (10) taken with respect to the Jastrow function of Eq. (9) yielded

$$\epsilon_J/\Omega = \tfrac{1}{8} n^2 \int g'(r) u'(r) \, d\vec{r} + \tfrac{1}{2} n^2 \int g(r) v(r) \, d\vec{r} , \tag{20}$$

where $g(r_{12})$ or $g(12)$, the radial distribution function, equals the two-particle distribution function $P(12)$ apart from a constant factor n^2, with the latter defined by the general formula

$$P(12\ldots\nu) \equiv n^\nu g(12\ldots\nu) = \frac{N!}{(N-\nu)!} \frac{\int \psi_J^2 d\vec{r}_{\nu+1}\ldots d\vec{r}_N}{\int \psi_J^2 d\vec{r}_1 \ldots d\vec{r}_N} \tag{21}$$

for the ν-particle distribution function $P(12\ldots\nu)$. Introducing Fourier transforms

$$g_m(k) = \int d\vec{r} \, g_m(r) e^{-i\vec{k}\cdot\vec{r}} , \tag{22}$$

$$u_m(k) = \int d\vec{r} \, u_m(r) e^{-i\vec{k}\cdot\vec{r}} , \tag{23}$$

while expanding g and u in power series of λ,

$$g(r_{12}) \equiv g(12) = \sum_m \lambda^m g_m(12) , \tag{24}$$

$$u(r_{12}) \equiv u(12) = \sum_m \lambda^m u_m(12) , \tag{25}$$

the Fourier coefficients u_m and g_m were related through the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) equation[1]

$$\nabla_1 g(12) = g(12) \nabla_1 u(12) + n \int g(123) \nabla_1 u(13) \, d\vec{r}_3 , \tag{26}$$

where

$$g(123) = g(12) g(23) g(31) e^{A(1,2,3)} , \tag{27}$$

$$A(1, 2, 3) = n \int [g(14) - 1][g(24) - 1]$$

$$\times [g(34) - 1] d\vec{r}_4 + \cdots . \tag{28}$$

This enabled the expression of ϵ_J/Ω as a functional of $g_m(k)$. A minimization procedure invented by Jackson, Feenberg, and Campbell[7] known as the paired-phonon analysis then led to an optimized set of $g_m(k)$:

$$\hat{g}_0(k) = 1 , \tag{29}$$

$$\hat{g}_1(k) = -2v(k)/k^2 , \tag{30}$$

$$\hat{g}_2(k) = \frac{6nv^2(k)}{k^4} + 2\sum_{\vec{l}} \frac{v(l)v(\vec{k}+\vec{l})}{k^2 l^2} + \sum_{\vec{l}} \frac{v(l)v(\vec{k}+\vec{l})}{l^2(\vec{k}+\vec{l})^2} , \tag{31}$$

etc., along with the corresponding energy upper bound

$$\hat{\epsilon}_J = \sum_m \lambda^m \hat{\epsilon}_m , \tag{32}$$

where $\hat{\epsilon}_m$ have already been given in Eqs. (13)–(16) and (18) for $m = 1$–4. Note that $\hat{\epsilon}_J$ is exact through $O(\lambda^3)$. In higher orders of λ, Jastrow's theory fails to take into account all contributions. However, term-by-term comparison of $\hat{\epsilon}_J$ with the energy series E obtained by means of the Hugenholtz–Pines perturbation procedure suggests that Jastrow's model effectively sums one-ring and ladder diagrams. This single fact is probably sufficient to account for the success of the Jastrow theory.

For the sake of completeness as well as for later use, I quote from Ref. 5 the optimum Jastrow function:

$$\hat{\psi}_J(1, 2, \dots, N) = \exp\left(\tfrac{1}{2}\sum_{i<j} \hat{u}(ij)]\right), \tag{33}$$

with $\hat{u}(ij)$ defined through its Fourier coefficients,

$$\hat{u}_0(k) = 0 , \tag{34}$$

$$\hat{u}_1(k) = \hat{g}_1(k) , \tag{35}$$

$$\hat{u}_2(k) = \hat{g}_2(k) - \tfrac{1}{2}\sum_{\vec{l}} \hat{g}_1(l)\hat{g}_1(\vec{k}+\vec{l}) - n\hat{g}_1^2(k) , \tag{36}$$

$$\hat{u}_3(k) = \hat{g}_3(k) - \sum_{\vec{k}} \hat{g}_1(l)\hat{g}_2(\vec{k}+\vec{l})$$
$$+ \tfrac{1}{3}\sum_{\vec{l}\vec{p}} \hat{g}_1(l)\hat{g}_1(p)\hat{g}_1(\vec{k}+\vec{l}+\vec{p})$$
$$- 2n\hat{g}_1(k)\hat{g}_2(k) + n^2\hat{g}_1^3(k) , \tag{37}$$

etc. Also, it should be remarked that up to order λ^2, $\hat{g}(k)$ agrees with the exact $g(k)$—denoted by $g^e(k)$—obtained via the Hugenholtz–Pines procedure. [8]

II. BEYOND THE JASTROW THEORY

To go beyond the Jastrow theory, there is the perturbation procedure developed by Feenberg and co-workers, [1] known as the method of correlated basis functions (CBF). In this method, one begins with an approximate ground-state wave function ψ_0, such as the optimum Jastrow function $\hat{\psi}_J$ of Eq. (33), and applies on it density-fluctuation or free-phonon operators $\rho_{\vec{k}}$:

$$\rho_{\vec{K}} = \sum_{i=1}^{N} e^{i\vec{K}\cdot\vec{r}_i} . \tag{38}$$

A set of basis functions is then obtained:

$$|0\rangle = \psi_0 , \tag{39}$$

$$|\vec{K}\rangle = \rho_{\vec{K}}\psi_0 , \tag{40}$$

$$|\vec{K}, \vec{L}\rangle = \rho_{\vec{K}}\rho_{\vec{L}}\psi_0 , \tag{41}$$

$$|\vec{K}, \vec{L}, \vec{P}\rangle = \rho_{\vec{K}}\rho_{\vec{L}}\rho_{\vec{P}}\psi_0 , \tag{42}$$

etc., using which one can compute the matrix elements of 1 and H. Thereafter, the 1 matrix and the Hamiltonian matrix may be simultaneously diagonalized via standard perturbation techniques. The matrix element connecting $|0\rangle$ and $|\vec{K}\rangle$ vanishes for nonzero $\vec{K}$ on account of momentum conservation. Thus contributions to the ground-state energy correction arise from diagrams whose initial and final vertices are matrix elements connecting $|\vec{K}, \vec{L}\rangle$, $|\vec{K}, \vec{L}, \vec{P}\rangle$, $\dots$, etc., to $|0\rangle$. In second order, the terms contributing toward energy correction are represented by the diagrams in Fig. 1.

In the special case where ψ_0 is chosen to be of the Jastrow form, it is noted that the set of correlated basis functions generated by this method becomes precisely the two-particle basis of Eq. (4). As pointed out in a recent letter, [9] since other forms of the ψ_0 are readily available, Feenberg's CBF theory should not be considered an extension of Jastrow's theory. Also, Eq. (40) states that Feynman's phonon spectrum in liquid helium emerges from the CBF as a zeroth-order approximation.

Campbell and Feenberg[7] showed that when the *optimized* Jastrow function $\hat{\psi}_J$ is employed to represent the ground state, the matrix element connecting the ground state $|0\rangle$ to every two-phonon state $|\vec{K}, \vec{L}\rangle$ vanishes. Hence the diagram shown in Fig. 1(a) does not contribute toward perturbative corrections. The leading correction is given by the three-phonon diagram Fig. 1(b). For liquid helium, Davison and Feenberg[10] evaluated Fig. 1(b) to yield $-0.76\,°K/N$, which when added to the unperturbed energy

$$\hat{\epsilon}_J \equiv \langle \hat{\psi}_J | H | \hat{\psi}_J \rangle / \langle \hat{\psi}_J | \hat{\psi}_J \rangle = -6.70\,°K/N$$

led to reasonable agreement with the experimental value of $-7.14\,°K/N$. In order to understand the implications of perturbative calculations in the CBF, we evaluated diagram 1(b) for the weakly in-
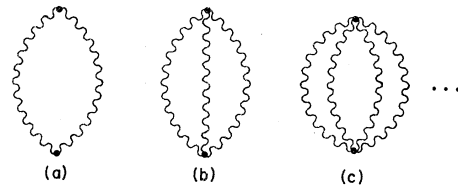

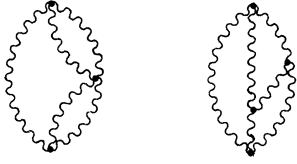FIG. 1. Second-order perturbative corrections in the CBF representation.

FIG. 2. Examples of higher-order contributions.

teracting Bose gas, and found[11] that its leading term is of order λ^4 and equals $\Delta\epsilon_4$ of Eq. (19). Thus one sees that the simplest perturbative correction in the representation of CBF completes the energy series to $O(\lambda^4)$ and gathers for summation yet a new class of diagrams in the independent-particle picture.

There are practical difficulties in going beyond the Davison–Feenberg correction. First of all, with each higher order, either in the perturbation expansion (e. g., Fig. 2) or in the vertex [e. g., Fig. 1(c)], comes an additional internal phonon line, thus another threefold integration over momentum. Second, the orthogonalization of the basis becomes increasingly prohibitive: It is not only necessary to orthogonalize all states to $|0\rangle$, but also with respect to one another. As a complement to the CBF theory, and as a practical alternative, another method is presented here that reaches beyond the range of the Jastrow theory.

The idea is extremely simple, and indeed obvious. A natural extension of Jastrow's theory calls for the inclusion of three-particle functions in the basis. Following the pattern established by Eqs. (4)–(9), I construct for the ground state of a Bose liquid the variational wave function

$$\psi(1, 2, \ldots, N) = \prod_{1 \leq i < j \leq N} f(r_{ij}) \prod_{1 \leq i < j < k \leq N} h(r_{ij}, r_{jk}, r_{ki})$$

$$\equiv \prod_{i<j} e^{u(ij)/2} \prod_{i<j<k} e^{w(ijk)/2}$$

$$= \psi_J(1, 2, \ldots, N) \exp\left(\frac{1}{2} \sum_{i<j<k} w(ijk)\right) . \tag{43}$$

To obtain an energy upper bound, the proper variational procedure requires the minimization of the energy expectation value

$$\epsilon \equiv \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$$

$$\equiv \sum_m \lambda^m \epsilon_m , \tag{44}$$

with respect to $u(ij)$ and $w(ijk)$. It is found to be possible to derive and solve coupled Euler–Lagrange equations and determine the optimum $u(ij)$ and $w(ijk)$ at least to $O(\lambda^4)$. (For realistic systems it is clear from Ref. 7 and from the work of Broyles and co-workers[12] that the solution of a highly nonlinear Euler–Lagrange equation is by no means straightforward, even in the case of a Jastrow calculation.) The choice of ψ is expected to

at least account for the Davison–Feenberg correction. In other words, ϵ of Eq. (44) upon minimization must reproduce the exact energy series of Eqs. (12)–(19) to at least $O(\lambda^4)$. Also, an improved $g(k)$ is expected.

III. GENERALIZED BBGKY EQUATIONS AND ENERGY MINIMIZATION

Since the use of the optimized Jastrow function corresponds to summing a large class of important diagrams in the independent-particle picture, it is probably a reasonably good starting point for the present work. Instead of determining $u(ij)$ freely along with $w(ijk)$, the optimized form $\hat{u}(ij)$ is chosen for $u(ij)$ as defined by Eqs. (33)–(37) and (29)–(31). Clearly this cannot be rigorous: While it is perfectly general to express the true ground-state eigenfunction as a product of factors involving ever increasing numbers of particles, thus

$$\psi_G(1, 2, \ldots, N) = \prod_i \varphi_0(i) \prod_{i<j} f(ij) \prod_{i<j<k} h(ijk)$$

$$\times \prod_{i<j<k<l} q(ijkl) \ldots , \tag{45}$$

it is far from obvious that each factor should be optimized when taken alone. However, to $O(\lambda^4)$ it can be shown easily that simultaneous solution of the Euler–Lagrange equations for $u(ij)$ and $w(ijk)$ does give rise to $\hat{u}(ij)$. In anticipation of this result, one begins with $u(ij) = \hat{u}(ij)$ and varies $w(ijk)$ alone in the minimization of ϵ.

The evaluation of ϵ makes use of the Jackson–Feenberg transformation[7]—an integration by parts valid for real ψ:

$$\int \psi \nabla_i^2 \psi \, d\vec{r}_1 \ldots d\vec{r}_N = \frac{1}{2} \int \psi^2 \nabla_i^2 \ln\psi \, d\vec{r}_1 \ldots d\vec{r}_N . \tag{46}$$

The result is given by

$$\epsilon/\Omega = \frac{1}{2} n^2 \int \tilde{v}(ij) g(ij) \, d\vec{r}_i \, d\vec{r}_j$$

$$- \frac{1}{18} n^3 \int g(ijk) \nabla_i^2 w(ijk) \, d\vec{r}_i \, d\vec{r}_j \, d\vec{r}_k , \tag{47}$$

where

$$\tilde{v}(ij) = \lambda v(r_{ij}) - \frac{1}{4} \nabla_i^2 \hat{u}(ij) , \tag{48}$$

and the ν-particle distribution function $g(12 \ldots \nu)$ is defined by Eq. (21), with ψ_J replaced now by ψ. Note that $g(12 \ldots \nu)$ depends on both $\hat{u}(ij)$ and $w(ijk)$. They are quite different from the optimum $g(12 \ldots \nu)$ determined earlier in the Jastrow theory. In order to express ϵ/Ω in a usable form, explicit relations between $g(12 \ldots \nu)$, the known functions $\hat{u}(ij)$ or $\hat{g}(ij)$, and the unknown function $w(ijk)$ first must be obtained; then these relations substituted into Eq. (47). This is accomplished by generalizing the BBGKY equation (26).

Equation (26) was obtained by applying the operator ∇_1 to the definition of $g(12)$, Eq. (21). The replacement of ψ_J by ψ in Eq. (21) now leads to a somewhat more complicated version:

$$\nabla_1 g(12) = g(12)\nabla_1 \hat{u}(12) + n \int g(123)\nabla_1 \hat{u}(13)\, d\vec{r}_3$$

$$+ n \int g(123)\nabla_1 w(123)\, d\vec{r}_3$$

$$+ \tfrac{1}{2} n^2 \int g(1234)\nabla_1 w(134)\, d\vec{r}_3\, d\vec{r}_4 \ . \qquad (49)$$

This equation alone is not sufficient for determining the relations between g, $\hat{u}$, and w to the order desired. Applying ∇_1 on the three- and four-particle distribution functions $g(123)$ and $g(1234)$, it is found that

$$\nabla_1 g(123) = g(123)\left[\nabla_1 \hat{u}(12) + \nabla_1 \hat{u}(13) + \nabla_1 w(123)\right]$$

$$+ n \int g(1234)\left[\nabla_1 \hat{u}(14) + \nabla_1 w(124) + \nabla_1 w(134)\right] d\vec{r}_4 + \tfrac{1}{2} n^2 \int g(12345)\nabla_1 w(145)\, d\vec{r}_4\, d\vec{r}_5 \qquad (50)$$

and

$$\nabla_1 g(1234) = g(1234)\left[\nabla_1 \hat{u}(12) + \nabla_1 \hat{u}(13) + \nabla_1 \hat{u}(14) + \nabla_1 w(123) + \nabla_1 w(124) + \nabla_1 w(134)\right]$$

$$+ n \int g(12345)\left[\nabla_1 \hat{u}(15) + \nabla_1 w(125) + \nabla_1 w(135) + \nabla_1 w(145)\right] d\vec{r}_5 + \tfrac{1}{2} n^2 \int g(123456)\nabla_1 w(156)\, d\vec{r}_5\, d\vec{r}_6 \ .$$

$$(51)$$

Also, I define the functions $x(123)$ and $y(1234)$ for convenience:

$$g(123) \equiv g(12)g(23)g(31)\left[1 + x(123)\right] \qquad (52)$$

and

$$g(1234) \equiv g(12)g(13)g(14)g(23)g(24)g(34)\left[1 + y(1234)\right] \ . \qquad (53)$$

Note that $x(123)$ is no longer given by Abe's correction

$$x(123) = n \int \left[g(14) - 1\right]\left[g(24) - 1\right]$$

$$\times \left[g(34) - 1\right] d\vec{r}_4 + \cdots \ , \qquad (54)$$

which is well known in classical theory of liquids. The introduction of three-particle factors in the trial wave function corresponds to taking into consideration three-particle interactions between molecules of a classical liquid. In the same way that a cluster expansion of $g(12)$ leads off with $e^{u(12)}$, $x(123)$ is expected to lead off with $w(123)$: a fact which I shall presently verify. Likewise, e, $y(1234)$ is expected to be a functional of $g(ij)$ and $g(ijk)$.

It is more convenient to work in the momentum space. One thus Fourier transforms $\hat{u}$, w, the g's, x, and y and expresses them as power series in λ:

$$\hat{u}(ij) = \sideset{}{'}\sum_{\vec{k}} \hat{u}(k)\, e^{i\vec{k}\cdot\vec{r}_{ij}} = \sum_m \lambda^m \hat{u}_m(ij) = \sum_m \lambda^m \sideset{}{'}\sum_{\vec{k}} \hat{u}_m(k) e^{i\vec{k}\cdot\vec{r}_{ij}} \ , \qquad (55)$$

$$w(ijk) = \sum_{\vec{k}\vec{l}} w(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) \exp[i\vec{k}\cdot\vec{r}_i + i\vec{l}\cdot\vec{r}_j - i(\vec{k}+\vec{l})\cdot\vec{r}_k]$$

$$= \sum_m \lambda^m w_m(ijk) = \sum_m \lambda^m \sideset{}{'}\sum_{\vec{k}\vec{l}} w_m(\vec{k}, \vec{l}, -\vec{k}-\vec{l})\exp[i\vec{k}\cdot\vec{r}_i + i\vec{l}\cdot\vec{r}_j - i(\vec{k}+\vec{l})\cdot\vec{r}_k] \ , \qquad (56)$$

$$g(ij) = \sideset{}{'}\sum_{\vec{k}} g(k)e^{i\vec{k}\cdot\vec{r}_{ij}} = \sum_m \lambda^m g_m(ij) = \sum_m \lambda^m \sideset{}{'}\sum_{\vec{k}} g_m(k) e^{i\vec{k}\cdot\vec{r}_{ij}} \ , \qquad (57)$$

etc. The primes on the summation signs denote the exclusion of terms with vanishing $\vec{k}$, $\vec{l}$, or $\vec{k}+\vec{l}$. Substituting these expansions into Eq. (49) and using the earlier results in Eqs. (34)–(37), the following are obtained:

$$g_0(k) = 1 \ , \qquad (58)$$

$$g_1(k) = \hat{u}_1(k) = \hat{g}_1(k) \ , \qquad (59)$$

$$g_2(k) = \hat{u}_2(k) + \tfrac{1}{2}\sideset{}{'}\sum_{\vec{l}} g_1(l)g_1(\vec{k}+\vec{l}) + ng_1^2(k) = \hat{g}_2(k) \ , \qquad (60)$$

$$g_3(k) = \hat{u}_3(k) + ng_1(k)\hat{u}_2(k) + ng_2(k)\hat{u}_1(k)$$

$$- \sideset{}{'}\sum_{\vec{l}} \frac{\vec{k}\cdot\vec{l}}{k^2}\left[g_1(\vec{k}+\vec{l})\hat{u}_2(l) + g_2(\vec{k}+\vec{l})\hat{u}_1(l) + ng_1(l)g_1(\vec{k}+\vec{l})\hat{u}_1(l) + ng_1(k)g_1(\vec{k}+\vec{l})\hat{u}_1(l) + ng_1(k)g_1(l)\hat{u}_1(l)\right]$$

$$+ n\sideset{}{'}\sum_{\vec{l}} \left(g_1(\vec{k}+\vec{l})w_2(\vec{k},\vec{l},-\vec{k}-\vec{l}) - \frac{\vec{k}\cdot\vec{l}}{k^2}\left[g_1(\vec{k}+\vec{l})w_2(-\vec{k},-\vec{l},\vec{k}+\vec{l}) + \hat{u}_1(l)x_2(-\vec{k},-\vec{l},\vec{k}+\vec{l})\right]\right)$$

$$- \frac{n^2}{2}\sideset{}{'}\sum_{\vec{l}\vec{p}} \frac{\vec{k}\cdot\vec{l}}{k^2}\, y_1(\vec{k}+\vec{l},\, -\vec{k},\vec{p},\, -\vec{l}-\vec{p})w_2(-\vec{l},-\vec{p},\vec{l}+\vec{p}) \ , \qquad (61)$$

etc. In the above, I had to make use of Eq. (63) below and the anticipated result

$$w_1(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) = 0 , \tag{62}$$

which is required in order that the energy series up to $O(\lambda^3)$ be unaltered by the introduction of w into the wave function. Note that $g(k)$ is also unaltered up to $O(\lambda^2)$; however, $g_3(k)$ differs from $\hat{g}_3(k)$.

Substituting the expansion formulas such as Eqs. (55)–(57) into Eq. (50), further relations between w, x, and y are obtained as follows:

$$x_0(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) = w_0(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) = 0 , \tag{63}$$

$$x_1(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) = w_1(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) , \tag{64}$$

$$x_2(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) = w_2(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) - n \sum_{\vec{p}}{}' \frac{\vec{k}\cdot\vec{p}}{k^2}$$
$$\times g_1(p) y_1(\vec{l}, -\vec{p}, -\vec{k}-\vec{l}, \vec{k}+\vec{p}) , \tag{65}$$

etc. Finally, doing the same to Eq. (51) leads to

$$y_0(\vec{k}, \vec{l}, \vec{p}, -\vec{k}-\vec{l}-\vec{p}) = 0 , \tag{66}$$

$$y_1(\vec{k}, \vec{l}, \vec{p}, -\vec{k}-\vec{l}-\vec{p}) = 0 , \tag{67}$$

etc.

Armed with these relations, I now return to eval-

uate the energy expectation value ϵ. It is found, after some lengthy algebra, that

$$\epsilon = \sum_{m>0} \lambda^m \epsilon_m , \tag{68}$$

$$\epsilon_1 = \hat{\epsilon}_1, \tag{69}$$

$$\epsilon_2 = \hat{\epsilon}_2 , \tag{70}$$

$$\epsilon_3 = \hat{\epsilon}_3 , \tag{71}$$

$$\epsilon_4 = \hat{\epsilon}_4 + \delta\epsilon_4 , \tag{72}$$

etc., where

$$\delta\epsilon_4 = -\tfrac{1}{4} n^3 \sum_{\vec{k}\vec{l}} k^2 g_1(k) g_1(l) w_2(\vec{k}, \vec{l}, -\vec{k}-\vec{l})$$

$$+ \tfrac{1}{16} n^3 \sum_{\vec{k}\vec{l}} k^2 w_2(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) w_2(-\vec{k}, -\vec{l}, \vec{k}+\vec{l})$$

$$+ \tfrac{1}{16} n^3 \sum_{\vec{k}\vec{l}} k^2 [g_1(k) g_1(l) + g_1(k) g_1(\vec{k}+\vec{l})$$

$$+ g_1(l) g_1(\vec{k}+\vec{l})] w_2(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) . \tag{73}$$

To $O(\lambda^4)$, this expression is what one wishes to minimize with respect to w_2. The solution of the Euler–Lagrange equation

$$\delta\epsilon[w_2]/\delta w_2 = 0 \tag{74}$$

is straightforward, yielding

$$w_2(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) = -\frac{\vec{k}\cdot\vec{l} g_1(k) g_1(l) + \vec{k}\cdot(-\vec{k}-\vec{l}) g_1(k) g_1(\vec{k}+\vec{l}) + \vec{l}\cdot(-\vec{k}-\vec{l}) g_1(l) g_1(\vec{k}+\vec{l})}{k^2 + l^2 + (\vec{k}+\vec{l})^2} . \tag{75}$$

The corresponding energy is given by Eqs. (68)–(72), with

$$\delta\epsilon_4 = \Delta\epsilon_4 \tag{76}$$

of Eq. (19), as expected.

At least to this order, the same results are obtained when one frees $u(ij)$ from the choice $\hat{u}(ij)$ and varies it along with $w(ijk)$.

IV. DISCUSSION

To the author's knowledge, a wave function that includes three-particle factors in the form of Eq. (44) has never been tried in variational calculations for quantum liquids. The reason is believed to be the following. In the Jastrow theory, one has *some* idea as to what $u(r)$ should look like. For instance, it must make the wave function vanish rapidly whenever the hard cores of two particles overlap. In other words, $u(r) \to 0$ as $r \to 0$. Furthermore, it can be shown easily that for a Lennard-Jones 6-12 potential, $u(r)$ goes as r^{-5} at small r. At long range, $u(r)$ must approach a constant. Asymptotically, $u(r) \to r^{-2}$. Also, the radial distribution function $g(r)$ or the liquid-structure function $S(k)$ is known quite well from neutron- and x-ray-scattering experiments. The variational

calculation must be able to reproduce detailed features of these functions. In choosing an appropriate form for $u(r)$, the latter condition is often leaned upon for guidance. In fact in certain reasonably successful calculations,[13] the energy expectation value ϵ_J is first expressed as a functional of $g(r)$ via the solution of integral equations relating $u(r)$ to $g(r)$—such as the BBGKY equation (26), or the Percus-Yevick equation, or the hypernetted chain—and then minimized with respect to $g(r)$. This procedure allows one to choose a form for $g(r)$ which contains all the essential features of the experimental data. On the other hand, little is known about the properties of the three-particle factor $w(ijk)$. Presumably whatever discrepancy remains between the experimental $g(r)$ and the $g(r)$ determined by optimizing ψ_J must be accountable to $w(ijk)$ and higher-order correlations. But such information is unreliable. One is dealing with small differences between large numbers. Neither the Jastrow $g(r)$ nor the experimental data are sufficiently accurate to assure a precise determination of their difference. The question thus remains open as to what would constitute a reasonable form for $w(ijk)$.

In this work, the view of the variational approach

took on a change of direction. Instead of blindly varying $w(ijk)$ in search of good numerical results, a formal analysis was carried out for a system which possesses an exact solution, namely, the weakly interacting Bose gas. The form of the leading term of $w(ijk)$ was determined, and it was shown that it managed to pick up, to $O(\lambda^4)$, precisely what the Jastrow theory has missed. Such

a three-particle factor enables the variational theory to include a totally new class of diagrams in the independent-particle picture. In $O(\lambda^4)$, they are identically the diagrams evaluated by Davison and Feenberg[10,11] in their CBF perturbation theory.

It is proposed that in place of Eq. (75) which defines the optimum w_2, the following form of w be used in any actual calculation:

$$w(\vec{k}, \vec{l}, -\vec{k}-\vec{l}) = -\frac{\vec{k}\cdot\vec{l}\,h(k)h(l) + \vec{k}\cdot(-\vec{k}-\vec{l})h(k)h(\vec{k}+\vec{l}) + \vec{l}\cdot(-\vec{k}-\vec{l})h(l)h(\vec{k}+\vec{l})}{k^2 + l^2 + (\vec{k}+\vec{l})^2} , \quad (77)$$

where

$$h(k) \equiv g(k) - 1 . \quad (78)$$

Expanding Eq. (77) in powers of λ, it is clear that the leading term reduces to Eq. (75). This ensures that the matrix elements connecting ψ to three-phonon states $\rho_{\vec{k}}\rho_{\vec{l}}\rho_{-\vec{k}-\vec{l}}\psi$ must vanish in $O(\lambda^2)$. My belief is that in higher orders they also vanish, or are much reduced in magnitude when compared to the matrix elements connecting $\hat{\psi}_J$ to $\rho_{\vec{k}}\rho_{\vec{l}}\rho_{-\vec{k}-\vec{l}}\hat{\psi}_J$. A proof of this statement requires a generalization of the paired-phonon analysis[7] of Jackson and Feenberg, which as yet does not exist.

To conclude this report, I wish to propose several applications of the present analysis to familar Bose liquids.

(i) The trial wave function defined by Eqs. (44), (56), and (77) should be applied to study the ground state of liquid helium. On account of the many folds of integrations involved, a Monte Carlo or molecular-dynamics technique is desirable. Note that Eq. (77) differs in form from its counterpart proposed by the author in an earlier letter.[14] To the leading order they are actually identical. The present form is preferred because $u(r)$ is frequently unintegrable and consequently $u(k)$ cannot be defined, whereas $h(k)$ in Eq. (77) is well defined.

The resulting energy change is expected to be roughly of the same magnitude as the perturbative correction found by Davison and Feenberg. However, what one obtains here will be a variational upper bound. There is an apparent inconsistency: The total energy obtained by Davison and Feenberg is actually *lower* than the experimental energy. If this result persists, it must be concluded that the Lennard-Jones potential with parameters determined by de Boer and Michels[15] must be inaccurate. Even though the claim may seem to be similar to certain statements in recent literature,[16] the conclusion is based on the mere requirement that the variational energy be higher than the true energy—a consistency condition which is not so optimistic as to imply the exact agreement between

these two values.

Incidentally, the form in which w is given is particularly convenient for calculations that make use of a Fourier-transformable He-He potential, such as that of Mihara and Puff[17] and of Sposito.[18]

(ii) In a recent Monte Carlo calculation to be reported elsewhere, a convenient two-parameter form for $w(ijk)$ was employed,

$$w(ijk) = A/(r_{ij}^2 + r_{jk}^2 + r_{ki}^2)^m , \quad (79)$$

in an attempt to improve the liquid-structure function in helium. We found significant improvement in the agreement between the calculated result and experiment, especially in the regions about the first maximum and the first minimum. In the present analysis of a weakly interacting Bose gas, it was noted that $g(k)$ agrees with $g^e(k)$ to $O(\lambda^2)$.[8] The finding that the newly obtained $g(k)$ is unaltered from $\hat{g}(k)$ up to $O(\lambda^2)$ is consistent with this fact. In $O(\lambda^3)$, however, $g(k)$ and $\hat{g}(k)$ disagree. This suggests that $\hat{g}_3(k)$ is inaccurate, and that the inclusion of three-particle factors into the wave function results in an improved $g_3(k)$. A calculation of $g_3^e(k)$ via the Hugenholtz–Pines procedure is highly desirable for verifying this statement and for measuring the extent of the improvement. It may also show us why a three-particle function of the form Eq. (79) works.

(iii) The same trial wave function should be attempted for the charged Bose gas. For $r_s \ll 1$, this will lead to two exact terms as expected[19] and estimates for higher-order terms yet undetermined by other methods. For intermediate densities, this will improve the variational results previously obtained[20] using the Jastrow theory. This in turn will improve the metallic-density electron-gas calculation based on the CBF theory.[21] It is interesting, and indeed of practical importance, to find out whether an improved wave function such as that proposed here would give rise to positive-definite $g(r)$ at small r.

(iv) To $O(\lambda^4)$, the optimum choice of ψ requires that the Jastrow factor ψ_J be the one which is op-

timized while taken alone. Will this result remain valid to all orders? While a formal analysis proves to be rather difficult, a numerical test is possible for both liquid He^4 and the charged Bose gas. One could first carry out a paired-phonon analysis using the Jastrow function alone, and then study the effect of including three-particle factors

such as that in Eq. (79). The energy thus obtained is expected to be *lower* than that obtained in (ii).

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Ion Velocity Distribution of a Weakly Ionized Gas in a Uniform Electric Field of Arbitrary Strength*

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The velocity-distribution function of ions in a neutral gas is studied. A uniform electric field of arbitrary strength is assumed and only binary-ion–neutral-particle collisions are considered. Under these conditions part of the Boltzmann-equation collision operator is replaced by a kinetic model which enables the ion velocity distribution to be found in compact analytical form if the mean free time between ions and neutrals is independent of velocity. This velocity distribution exhibits the expected properties of drift, elevated ion temperature (as compared to the neutral gas), and skewness in the field direction. In addition, the velocity distribution obtained agrees with the known distributions in the extreme cases of (a) low fields and arbitrary masses and (b) arbitrary fields but extremely disparate ion and gas masses. Other tests are made for this distribution with satisfactory agreement.

I. INTRODUCTION

Previous research on the effect of an applied electric field on the motion of charged particles colliding elastically with a neutral gas has proceeded along several lines,[1-5] none of which establishes analytically the ion velocity distribution for arbitrary fields and ion-neutral mass ratios. The

analytical results thus far obtained for elastic collisions are only applicable for extreme ion-neutral mass ratios.[1-4] Most experiments studying weakly ionized gaseous systems in uniform electric fields are done when the extreme conditions previously mentioned are not applicable.

We shall use the BGK[6] or kinetic-model method which has not apparently been exploited for this