New Variational Wave Function for Bose Liquids*

Chia-Wei Woo†

Department of Physics, Northwestern University, Evanston, Illinois 60201

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A new variational wave function is proposed for the ground state of Bose liquids. It consists of the optimized Jastrow function multiplied to exponentials of three-particle functions. The form of the latter is determined variationally in a formal analysis carried out for the weakly interacting Bose gas. Its appearance implies the summation of a new class of diagrams beginning with fourth-order terms in the interaction strength. Several calculations for realistic systems are proposed.

For a Bose liquid characterized by the Hamiltonian

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

the Jastrow wave function

$$\psi_J(1, 2, \cdots, N) = \prod_{i<j} \exp[\tfrac{1}{2} u(r_{ij})] = \exp[\tfrac{1}{2} \sum_{i<j} u(r_{ij})]$$ (2)

provides a generally adequate description of the ground state. Such a wave function has been used extensively for liquid helium[1] and the charged Bose gas.[2] In a recent analysis[3] we carried out energy calculations for a weakly interacting Bose gas, using the approximate, Jastrow method on the one hand, and the exact, Hugenholtz-Pines prescription on the other. The pairwise potential $v(r)$ was assumed to have a Fourier transform, represented by $\lambda v(k)$, where λ measures the strength of the interaction. The energies obtained in both calculations were displayed as power series in λ, thus permitting order-by-order comparison and a diagrammatic analysis. Results of the analysis suggested that the use of an optimized Jastrow function effectively sums all terms exactly to $O(\lambda^3)$ and selects terms to higher orders. The terms which are most susceptible to the summation correspond to one-ring diagrams and ladder diagrams. This probably accounts for the success of the Jastrow method.

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 applies density-fluctuation or free-phonon operators to the ground-state wave function, thus obtaining a set of basis functions, and then computes matrix elements between these states. Thereafter, a standard perturbation expansion may be carried out, with the nondiagonal part of the Hamiltonian matrix serving as the perturbation. In particular, Campbell and Feenberg[4] found that when an optimized Jastrow function $\hat{\psi}_J$ is used to represent the ground state, the matrix element connecting the ground state and a two-phonon state vanishes. Hence the leading perturbation correction ΔE to the Jastrow energy

$$\hat{E}_J = \langle \hat{\psi}_J | H | \hat{\psi}_J \rangle / \langle \hat{\psi}_J | \hat{\psi}_J \rangle$$ (3)

is a second-order term propagated by three phonons. For liquid helium, Davidson and Feenberg[5] found ΔE to be about $- 0.76°K$ per particle, which when added to $\hat{E}_J$ (about $- 6.7°K$) led to reasonable agreement with the experimental value, $- 7.14°K$. In a sequel[6] to Ref. 3 we showed that $\hat{E}_J + \Delta E$ is exact to $O(\lambda^4)$ for a weakly interacting Bose gas. Thus the simplest perturbation correction in the representation of CBF completes the energy series to $O(\lambda^4)$ and gathers for summation yet a new class of diagrams.

There are practical difficulties in going beyond the Davidson-Feenberg correction. First of all, with each higher order, either in the perturbation expansion or in the vertex, comes an additional threefold integration. Secondly, the orthogonalization of the basis becomes increasingly prohibitive. In complement to the CBF procedure, and as a practical alternative, we wish to present here yet another method which reaches beyond the range of the Jastrow theory.

The idea is very simple. A natural extension of Jastrow's method calls for the inclusion of three-particle factors in the variational wave function; thus,

$$\psi(1, 2, \cdots, N) = \exp[\tfrac{1}{2} \sum_{i<j} u(ij)] \exp[\tfrac{1}{2} \sum_{i<j<k} w(ijk)] = \psi_J \prod_{i<j<k} \exp[\tfrac{1}{2} w(ijk)].$$ (4)

For liquids,

$$u(ij) = u(r_{ij}) = \sum_{\vec{k}}' u(k) \exp(-i\vec{k} \cdot \vec{r}_{ij}), \tag{5}$$

$$w(ijk) = w(r_{ij}, r_{jk}, r_{ki}) = \sum_{kl}' w(\vec{k}, \vec{l}, -\vec{k} - \vec{l}) \exp[i\vec{k} \cdot \vec{r}_i + i\vec{l} \cdot \vec{r}_j - i(\vec{k} + \vec{l}) \cdot \vec{r}_k], \tag{6}$$

where the prime on the summation denotes the exclusion of terms with vanishing $\vec{k}$, $\vec{l}$, or $\vec{k} + \vec{l}$. Obvious as it may seem, to our knowledge such a wave function has never been tried. The reason, we believe, is as follows. In the Jastrow theory, one has *some* idea as to what $u(r)$ should look like. For instance, it must cause the wave function to vanish rapidly whenever the hard cores of two particles overlap. At long range it must approach a constant. Also, the radial distribution function $g(r)$ or the liquid structure function $S(k)$ defined in terms of $\hat{\psi}_J$ must be consistent with experimental (neutron and x-ray scattering) data. In choosing an appropriate form for ψ_J, the latter condition is often leaned upon for guidance.[7] On the other hand, little is known about the properties of the three-particle function $w(ijk)$. 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: Neither the experimental nor the Jastrow $g(r)$ is sufficinetly accurate to assure precise determination of their difference. The question thus remains open as to what would constitute a reasonable form for $w(ijk)$.

At this point, our view of the variational approach takes on a change in direction. In the past, the Jastrow function was varied in search of good numerical results. Formal analyses were carried out only *afterwards*, to explain why and how the method works. Armed with the experience of the diagrammatic analysis in Refs. 3 and 6, we now find it possible, and indeed much more efficient, to first determine what kind of a $w(ijk)$ is needed—in order to include a new class of important diagrams—before attempting serious numerical calculations for realistic systems.

Let the exact energy per unit volume be written as follows:

$$E/\Omega = \sum_m \lambda^m E_m/\Omega. \tag{7}$$

In Ref. 3 we found that the optimization of ψ_J reproduces E/Ω correctly to $O(\lambda^3)$. In $O(\lambda^4)$, however,

$$E_4/\Omega = \hat{\epsilon}_4/\Omega + \Delta\epsilon_4/\Omega, \tag{8}$$

and only $\hat{\epsilon}_4/\Omega$ is included. In our present work, it is clear that a sensible choice of $w(ijk)$ must be capable of accounting for $\Delta\epsilon_4/\Omega$, which is given by Eq. (36) of Ref. 6:

$$\frac{\Delta\epsilon_4}{\Omega} = n^3 \sum_{kl} \frac{v^2(k)v^2(l)}{k^4 l^2} - 2n^3 \sum_{kl} \frac{v^2(k)v^2(l)}{k^4[k^2 + l^2 + (\vec{k} + \vec{l})^2]} - 2n^3 \sum_{kl} \frac{v^2(k)v^2(l)}{k^2 l^2[k^2 + l^2 + (\vec{k} + \vec{l})^2]}$$

$$- \frac{n^3}{2} \sum_{kl} \frac{v^2(k)v(l)v(\vec{k} + \vec{l})}{k^2 l^2(\vec{k} + \vec{l})^2} + n^3 \sum_{kl} \frac{v^2(k)v(l)v(\vec{k} + \vec{l})}{k^4 l^2} - 2n^3 \sum_{kl} \frac{v^2(k)v(l)v(\vec{k} + \vec{l})}{k^4[k^2 + l^2 + (\vec{k} + \vec{l})^2]}, \tag{9}$$

when n stands for the number density, and Ω, $\hbar$, and m have been set equal to 1.

Now, the expectation value of H with respect to ψ is given by

$$\epsilon/\Omega = \tfrac{1}{2} n^2 \int \tilde{v}(ij)g(ij) \, d^3r_i d^3r_j - \tfrac{1}{16} n^3 \int g(ijk)\nabla_i^2 w(ijk) \, d^3r_i \, d^3r_j \, d^3r_k, \tag{10}$$

where

$$\tilde{v}(ij) = \lambda v(r_{ij}) - \tfrac{1}{4}\nabla_i^2 u(ij), \tag{11}$$

and the l-particle distribution function $g(12\cdots l)$ is defined by

$$g(1, 2\cdots l) = \frac{1}{n^l} \frac{N!}{(N-l)!} \frac{\int \psi^2 d^3 r_{l+1} \cdots d^2 r_N}{\int \psi^2 d^3 r_1 \cdots d^3 r_N}. \tag{12}$$

Note that $g(12\cdots l)$ depends on both $u(ij)$ and $w(ijk)$. Coupled Bogoliubov-Born-Green-Kirkwood-Yvon equations can be derived from Eq. (12), resulting in the following relations between u, w, $g(12)$, $g(123)$,

etc.:

$$\nabla_1 g(12) = g(12)\nabla_1 u(12) + n\int g(123)\nabla_1 u(13)\, d^3 r_3 + n\int g(123)\nabla_1 w(123)\, d^3 r_3$$
$$+ \tfrac{1}{2} n^2 \int g(1234)\nabla_1 w(134)\, d^3 r_3 d^3 r_4, \tag{13}$$

$$\nabla_1 g(123) = g(123)[\nabla_1 u(12) + \nabla_1 u(13) + \nabla_1 w(123)] + n\int g(1234)[\nabla_1 u(14) + \nabla_1 w(124) + \nabla_1 w(134)]\, d^3 r_4$$
$$+ \tfrac{1}{2} n^2 \int g(12\,345)\nabla_1 w(145) d^3 r_4 d^3 r_5, \tag{14}$$

etc. By expressing u, w, $g(12)$, $g(123)$, etc. all in momentum space and as power series in λ, one finds

$$u(k) = \int u(r)e^{-i\vec{k}\cdot\vec{r}}\, d^3 r = \sum_m \lambda^m u_m(k), \tag{15}$$

etc.; we can solve these equations for $g(12\cdots l)$ in terms of u and w, and substitute the results into Eq. (10). Taking $u(k)$ to be that which optimizes the Jastrow function, as given in Ref. 3, we obtain

$$\epsilon/\Omega = \sum_m \lambda^m \epsilon_m/\Omega, \tag{16}$$

$$\epsilon_1/\Omega = \tfrac{1}{2} n^2 v(0) = \hat{\epsilon}_1/\Omega = E_1/\Omega, \tag{17}$$

$$\epsilon_2/\Omega = -\tfrac{1}{2} n^2 \sum_{\vec{k}} v^2(k)/k^2 = \hat{\epsilon}_2/\Omega = E_2/\Omega, \tag{18}$$

$$\frac{\epsilon_3}{\Omega} = n^3 \sum_k \frac{v^3(k)}{k^4} + \frac{n^2}{2}\sum_{kl}\frac{v(k)v(l)v(\vec{k}+\vec{l})}{k^2 l^2} = \frac{\hat{\epsilon}_3}{\Omega} = \frac{E_3}{\Omega}, \tag{19}$$

$$\frac{\epsilon_4}{\Omega} = \frac{-5n^4}{2}\sum_k \frac{v^4(k)}{k^6} - \frac{3n^3}{2}\sum_{kl}\frac{v^2(k)v(l)v(\vec{k}+\vec{l})}{k^2 l^2(\vec{k}+\vec{l})^2} - 3n^3\sum_{kl}\frac{v^2(k)v(l)v(\vec{k}+\vec{l})}{k^4 l^2}$$
$$- \frac{n^2}{2}\sum_{klp}\frac{v(l)v(p)v(\vec{k}+\vec{l})v(\vec{k}+\vec{p})}{k^2 l^2 p^2} + \frac{\epsilon_4^W}{\Omega} = \frac{\hat{\epsilon}_4}{\Omega} + \frac{\epsilon_4^W}{\Omega}, \tag{20}$$

where ϵ_4^W/Ω represents the only terms that depend on $w(ijk)$,

$$\frac{\epsilon_4^W}{\Omega} = \frac{-n^3}{4}\sum_{kl} k^2 u_1(k)u_1(l)w_2(\vec{k},\vec{l},-\vec{k}-\vec{l}) + \frac{n^3}{16}\sum_{kl} k^2 w_2(\vec{k},\vec{l},-\vec{k}-\vec{l})w_2(-\vec{k},-\vec{l},\vec{k}+\vec{l})$$
$$+ \frac{n^3}{16}\sum_{kl} k^2[u_1(k)u_1(l) + u_1(k)u_1(\vec{k}+\vec{l}) + u_1(l)u_1(\vec{k}+\vec{l})]w_2(\vec{k},\vec{l},-\vec{k}-\vec{l}). \tag{21}$$

Minimizing ϵ_4^W/Ω with respect to $w_2(\vec{k},\vec{l},-\vec{k}-\vec{l})$, we find

$$w_2(\vec{k},\vec{l},-\vec{k}-\vec{l}) = -\frac{\vec{k}\cdot\vec{l}\,u_1(k)u_1(l) + \vec{k}\cdot(-\vec{k}-\vec{l})u_1(k)u_1(\vec{k}+\vec{l}) + \vec{l}\cdot(-\vec{k}-\vec{l})u_1(l)u_1(\vec{k}+\vec{l})}{k^2 + l^2 + (\vec{k}+\vec{l})^2}, \tag{22}$$

$$\epsilon_4^W/\Omega = \Delta\epsilon_4/\Omega \tag{23}$$

of Eq. (9). The condition on $w(ijk)$ is thus satisfied. The steps involved in this calculation are rather lengthy. We had to demonstrate, for example, that $w(ijk)$ is $O(\lambda^2)$; that the Kirkwood superposition approximation fails to hold beyond $O(\lambda)$, now that the quantum analogy of three-body forces is included; and that $g(1234)$ must also be evaluated; etc. These will be reported in detail elsewhere. We shall also discuss there the connection of this approach to Davison and Feenberg's perturbation procedure, as well as the types of new diagrams now included. The remaining space in this note will be devoted to suggesting a few applications of our present finding.

First of all, we propose that the trial wave function defined by Eqs. (4), (6), and (22) be used for studying the ground state of liquid helium in a Monte Carlo or molecular-dynamics calculation. In Eq. (22) each u_1 should be replaced by the full u; and for u the optimum Jastrow function should be used. We expect the resulting energy to agree with that reported by Davison and Feenberg, but here we have an upper bound.

Next we propose that the same trial wave function be used for the charged Bose gas. For $r_s \ll 1$, this will lead to two exact terms as expected.[8] For intermediate densities, this will improve the variational results previously obtained[9] using the Jastrow function. This in turn will improve the metallic-density electron-gas calculation using the CBF theory.[10]

Thirdly, one might attempt to use the new trial wave function to improve the agreement between experimental and theoretical values of the liquid structure function in helium, in particular in the region about the first peak. Preliminary results indicate that four-particle functions may be needed in the case of a weakly interacting Bose gas, if exact agreement is to be achieved for $S(k)$ up to $O(\lambda^2)$. This observation, however, need not be relevant in the case of helium.[11]

Finally we wish to remark that, in view of possible improvements yet to be made on helium calculations, the statements which have recently been appearing in literature[12] concerning He-He potentials based on Jastrow-type calculations are in our opinion premature.

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[10]F. Y. Wu, private communication.

[11]For helium in two dimensions, H.-W. Lai, A. Rahman, and C.-W. Woo have sought to improve $S(k)$ using three-particle functions. Indications are that there is indeed an improvement of the right magnitude, but the results are not yet conclusive.

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Higher-Order Corrections due to the Order Parameter to the Flux-Flow Conductivity of Dirty, Type-II Superconductors

Hajime Takayama

Department of Physics, University of Tokyo, Tokyo, Japan

and

Kazumi Maki

Department of Physics, Tohoku University, Sendai, Japan

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We study theoretically the higher-order corrections in $\Delta(\vec{r})$, the superconducting order parameter, to the flux-flow conductivity of dirty, type-II superconductors. It is shown that the Thompson term (i.e., the anomalous term) in the flux-flow conductivity is extremely sensitive to the higher-order corrections and decreases rapidly in the vortex state, while the Caroli-Maki term is affected only slightly by the higher-order corrections.

The flux-flow conductivity of type-II superconductors in the vortex state is of particular interest, since this involves the time-dependent variation of the superconducting order parameter. An early theory proposed by Caroli and Maki (CM)[1] appeared to describe the flux-flow resistivity of dirty, type-II superconductors rather well. Recently, however, Thompson[2] and Takayama and Ebisawa[3] have shown that in the calculation of CM some diagrams were neglected which describe the additional dissipation due to the presence of the order parameter. Since this correction term is of the same order of magnitude as the CM term, in the vicinity of the transition temperature[2,3] at least, the inclusion of this new term certainly destroys the good agreement so