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VARIATIONAL METHOD FOR THE GROUND STATE OF LIQUID He^4†

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(Received 13 May 1966)

A number of authors[1-6] have developed variational methods using the Bijl-Jastrow type of wave function to study the ground state of an interacting boson system. Recently, this procedure was applied to a realistic Hamiltonian for liquid He^4 by McMillan.[6] In his paper, the trial product-pair wave function was restricted to a certain parametric form and 32 Monte Carlo calculations were used to obtain a two-parameter fit. Without requiring this restriction, Hiroike[3] has obtained an integro-differential equation for the radial distribution function $g(r)$ by considering $\delta g(r)$ arbitrary. However, since this variational principle requires an arbitrary variation $\delta\Psi$ in the trial wave function rather than in $g(r)$, some doubt must remain as to the validity of Hiroike's method. Therefore, we present here a derivation of an equation for $g(r)$ by letting $\delta\Psi$ be arbitrary insofar as the product-pair form is maintained.

We consider the ground state of N spinless Bose particles of mass m confined in a volume Ω, interacting through the two-body potential $\varphi(r)$. With the trial wave function

$$\Psi = \exp[\tfrac{1}{2} \sum_{i<j} u(r_{ij})], \tag{1}$$

the expectation value of the Hamiltonian is given by

$$\frac{E}{N} = \frac{\hbar^2\rho}{8m}\int \nabla u(r)\nabla g(r) d\vec{r} + \frac{\rho}{2}\int \varphi(r) g(r) d\vec{r}, \tag{2}$$

where ρ is the density. The condition that Eq. (2) be stationary with respect to arbitrary variations of $u(r)$ is

$$\nabla^2 g(r) + \int \frac{\delta g(\vec{r}\,')}{\delta u(\vec{r})}\left[\nabla^2 u(r') - \frac{4m}{\hbar^2}\varphi(r')\right] d\vec{r}\,' = 0. \tag{3}$$

To determine the functional derivative $\delta g(\vec{r}\,')/\delta u(\vec{r})$, we notice that the variation of the two-particle distribution function

$$\rho^{(2)}(\vec{r}_1, \vec{r}_2) = N(N-1)\int \exp[\sum_{i<j} u(r_{ij})] d\vec{r}_3 \cdots d\vec{r}_N \Big/ \int \exp[\sum_{i<j} u(r_{ij})] d\vec{r}_1 \cdots d\vec{r}_N \tag{4}$$

is, with the aid of three-particle and four-particle distribution functions, expressed as

$$\begin{aligned}\delta\rho^{(2)}(\vec{r}_1, \vec{r}_2) = {} & \rho^{(2)}(\vec{r}_1, \vec{r}_2)\delta u(r_{12}) + \int \rho^{(3)}(\vec{r}_1, \vec{r}_2, \vec{r}_3)\delta u(r_{13}) d\vec{r}_3 \\ & + \int \rho^{(3)}(\vec{r}_1, \vec{r}_2, \vec{r}_3)\delta u(r_{23}) d\vec{r}_3 + \tfrac{1}{2}\iint \rho^{(4)}(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4)\delta u(r_{34}) d\vec{r}_3 d\vec{r}_4 \\ & - \frac{1}{\rho}\rho^{(2)}(\vec{r}_1, \vec{r}_2)[\int \rho^{(2)}(\vec{r}_1, \vec{r}_2)\delta u(r_{12}) d\vec{r}_2 + \tfrac{1}{2}\iint \rho^{(3)}(\vec{r}_1, \vec{r}_3, \vec{r}_4)\delta u(r_{34}) d\vec{r}_3 d\vec{r}_4].\end{aligned} \tag{5}$$

Putting each term in Eq. (5) into the form

$$\int [\quad] \delta u(r) d\vec{r},$$

we find that

$$\frac{\delta\rho^{(2)}(\vec{r}_1,\vec{r}_2)}{\delta u(\vec{r})}=\rho^{(2)}(\vec{r}_1,\vec{r}_2)\delta(\vec{r}_{12}-\vec{r})+2\rho^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_1+\vec{r})$$
$$-\tfrac{1}{2}\Omega\rho^{(2)}(\vec{r}_1,\vec{r}_2)\rho^{(2)}(\vec{r}_1,\vec{r}_1+\vec{r})+\tfrac{1}{2}\int\rho^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_3+\vec{r})dr_3. \quad (6)$$

At this point it is necessary to introduce the superposition approximation in order not to have a term in the equation with an integral of more than two dimensions. So within the superposition approximation, the last term T_4 of Eq. (6) works out to

$$T_4=\tfrac{1}{2}\int\rho^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_3+\vec{r})d\vec{r}_3\approx\tfrac{1}{2}\rho^4g(r_{12})g(r)\int g(r_{13})g(r_{23})g(|\vec{r}_3+\vec{r}-\vec{r}_1|)g(|\vec{r}_3+\vec{r}-\vec{r}_2|)d\vec{r}_3.$$

In order to clarify the next step, we introduce two new vectors, $\vec{r}_4$ and $\vec{r}_5$, which do not depend on the variable of integration. These are given by $\vec{r}_1-\vec{r}=\vec{r}_4$ and $\vec{r}_2-\vec{r}=\vec{r}_5$. We then obtain

$$T_4\approx\tfrac{1}{2}\rho^4g(r_{12})g(r)\int g(r_{13})g(r_{23})g(r_{43})g(r_{53})d\vec{r}_3\approx\tfrac{1}{2}\rho^3g(r_{12})g(r)\int\frac{\rho^{(5)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\vec{r}_5)}{\rho^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_4,\vec{r}_5)}d\vec{r}_3\approx\tfrac{1}{2}\rho^3(N-4)g(r_{12})g(r). \quad (7)$$

Note that the artificially introduced vectors, $\vec{r}_4$ and $\vec{r}_5$, no longer appear. Thus Eq. (6) becomes

$$\frac{\delta g(\vec{r}\,')}{\delta u(\vec{r})}\approx g(r)\delta(\vec{r}-\vec{r}\,')+2\rho g(r)g(r')[g(|\vec{r}-\vec{r}\,'|)-1]. \quad (8)$$

From the classical theory of fluids, the relation between $u(r)$ and $g(r)$ has been found to be[7]

$$u(r)=\ln g(r)-\frac{1}{(2\pi)^3\rho}\int\frac{[S(k)-1]^2}{S(k)}e^{i\vec{k}\cdot\vec{r}}d\vec{k}-B(r), \quad (9)$$

where $S(k)$ represents the structure factor and $B(r)$ the contribution from the bridge diagrams. Substituting Eqs. (8) and (9) into Eq. (3), we obtain an Euler-Lagrange equation

$$\frac{1}{g(r)}\nabla^2g(r)-\frac{1}{2}\left|\frac{\nabla g(r)}{g(r)}\right|^2-\frac{2m}{\hbar^2}\varphi(r)+\frac{1}{2(2\pi)^3\rho}\int\frac{[S(k)-1]^2}{S(k)}k^2e^{i\vec{k}\cdot\vec{r}}d\vec{k}$$
$$+2\pi\rho\int_0^\infty g(r')\left[\frac{\nabla^2g(r')}{g(r')}-\left|\frac{\nabla g(r')}{g(r')}\right|^2+\frac{1}{(2\pi)^3\rho}\int\frac{[S(k)-1]^2}{S(k)}k^2e^{i\vec{k}\cdot\vec{r}\,'}d\vec{k}-\frac{4m}{\hbar^2}\varphi(r')-\nabla^2B(r')\right]$$
$$\times\left[\frac{1}{rr'}\int_{|r-r'|}^{r+r'}g(\sigma)\sigma d\sigma-2\right]r'^2dr'-\tfrac{1}{2}\nabla^2B(r)=0. \quad (10)$$

This is similar to the result derived by Hiroike.[3] In his development, all constraints on $g(r)$ were dropped. However, it may be shown that $\delta g(r)$ is not arbitrary. For example, $\delta g(r)$ is limited by the relations

$$g(r)\geq 0, \quad (11a)$$

$$\rho\int[g(r)-1]d\vec{r}=-1. \quad (11b)$$

In order to compare with Hiroike's result we derive the variation of E/N due to the variation $\delta g(r)$ and then relate $\delta g(r)$ to $\delta u(r)$ through the functional derivative to obtain

$$\delta(E/N)=\iint J(r)\frac{\delta g(\vec{r})}{\delta u(\vec{r}\,'')}\delta u(r'')d\vec{r}\,''d\vec{r}, \quad (12)$$

where

$$J(r)=\frac{\hbar^2\rho}{8m}\left\{\left|\frac{\nabla g(r)}{g(r)}\right|^2-\frac{2\nabla^2g(r)}{g(r)}+\frac{4m}{\hbar^2}\varphi(r)-\frac{1}{(2\pi)^3\rho}\int\frac{[S(k)-1]^2[2S(k)+1]}{S^2(k)}e^{-i\vec{k}\cdot\vec{r}}k^2d\vec{k}\right.$$
$$\left.+\int\nabla^2g(r')\frac{\delta B(\vec{r}\,')}{\delta g(\vec{r})}d\vec{r}\,'+\nabla^2B(r)\right\}. \quad (13)$$

Substituting only the first term in Eq. (8) into Eq. (12) results in Hiroike's Eq. (H2-12). The neglected term is proportional to ρ, which explains his success in the study of the Bose fluid of hard spheres in the low-density limit. The density dependence of the neglected term also explains the agreement of his previous work in the limit of weak interactions since the interaction-dependent term in Eq. (H4-10) is also small for low density.

Including both terms of Eq. (8), we obtain a corrected equation

$$J(r)+2\rho\int J(r')g(r')[g(|\vec{r}-\vec{r}'|)-1]d\vec{r}'=0. \tag{14}$$

The difference between Eqs. (10) and (14) is due to the different positions of $\delta g(\vec{r}')/\delta u(\vec{r})$ in Eq. (12) and in the similar equation from which Eq. (3) was obtained. Thus the superposition approximation used in these derivations enters in different ways. It is uncertain whether Eq. (10) or Eq. (14) will be better, although Eq. (10) appears to depend less heavily on the superposition approximation.

A brief manipulation indicates that $\delta g(r)$ defined by Eq. (8) may not satisfy the condition

$$\int \delta g(r)d\vec{r}=0 \tag{15}$$

[as required by Eq. (11b)]. To remove this difficulty, we modify the functional derivative by writing

$$\frac{\delta\hat{g}(\vec{r}')}{\delta u(\vec{r})}=\frac{\delta g(\vec{r}')}{\delta u(\vec{r})}-\frac{1}{\Omega}\int\frac{\delta g(\vec{r}'')}{\delta u(\vec{r})}d\vec{r}'', \tag{16}$$

so that $\delta g(r)$ is altered to

$$\delta\hat{g}(r)=\delta g(r)-\frac{1}{\Omega}\int\delta g(r'')d\vec{r}''. \tag{17}$$

Substituting Eq. (8) into Eq. (16) shows that the corrections made to $\delta g(\vec{r}')/\delta u(\vec{r})$ and $\delta g(r)$ by this modification are of the order of Ω^{-1} compared to $\delta g(\vec{r}')/\delta u(\vec{r})$ and $\delta g(r)$, respectively. This correction will also add terms of Ω^{-1} to Eqs. (10) and (14). However, these additional terms will all be negligible in the limit as Ω goes to infinity. We notice that with this modification Eq. (11a) is still satisfied. Numerical calculations are in progress for liquid He^4 and for the charged-boson system. The results will be reported in a separate paper.

We are indebted to Professor C. F. Hooper, Jr., for several helpful discussions.

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†This research was supported in part by funds from the National Science Foundation and the National Aeronautics and Space Administration.

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