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Extension of the Variational Method for Hard-Sphere Bosons

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The coordinate-space variational treatment for the hard-sphere boson gas developed by Aviles and Iwamoto has been extended to include the first logarithmic term in the ground-state energy expansion. The result agrees, within four percent, with the exact results of Wu and others. The form of the variational wave function used is discussed and compared with that obtained using the pseudopotential method of Lee, Huang, and Yang.

1. INTRODUCTION

RECENT advances in the problem of the infinite volume, many-boson system have been due largely to the introduction of novel methods of calculation, often based on the formalism of field theory.[1] It has remained of interest, however, to attempt more straightforward solutions based on the conventional many-particle Schrödinger equation in coordinate space. Aviles[2] and Iwamoto[3] have independently developed a variational treatment, based on earlier incomplete work of Mott, Dingle,[4] and Jastrow,[5] and have succeeded in calculating the first two terms in a series solution for the ground-state energy of the boson hard-sphere system, which agrees well with the results of the exact methods. We have extended the investigation to include discussion of one more term in the series, which had been overlooked in the earlier exact calculations. This additional term was recently discovered by several authors,[6] and had been inherent in the variational method. We also discuss the relation between the variational wave function and that obtained using the pseudopotential method of Lee, Huang, and Yang.[7]

2. CALCULATION OF THE ENERGY

The variational method makes use of a trial function of the form

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\cdots\mathbf{r}_N)=\prod_{i<j} f(\mathbf{r}_i-\mathbf{r}_j). \tag{1}$$

Aviles[2] has shown that the ground-state energy per particle for a system of spinless, hard-sphere bosons of mass m, radius r_0 and of density ρ is given by:

$$E=\frac{\hbar^2}{2m}\frac{\rho r_0^3}{2}\int d^3x[(\nabla f(x))^2-f(x)\nabla^2 f(x)]G_0(x). \tag{2}$$

In this formula the two-particle correlation function is defined as

$$G_0(x)=1+\frac{1}{8\pi^3\rho r_0^3}\int d^3k\frac{\zeta^2}{1-\zeta}e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{3}$$

where

$$\zeta(k)=\rho r_0^3\int d^3x[f^2(x)-1]e^{-i\mathbf{k}\cdot\mathbf{x}},\quad x=r/r_0, \tag{4}$$

and only the "chain-connected" terms,[2] which are dominant at low density, have been included. For mathematical convenience, both Aviles[2] and Iwamoto[3] have chosen the variational two-particle function

$$\begin{aligned} f(x)&=1-x^{-1}e^{-\epsilon(x-1)},\quad x\geqq 1\\ &=0,\quad x\leqq 1. \end{aligned} \tag{5}$$

This form has the correct behavior near the hard-core boundary ($x=1$), and is short-ranged, (i.e., approaches unity rapidly as $x\rightarrow\infty$). A detailed discussion of the properties of this function will be given later. The parameter ϵ is left free to be varied after the integrations have been carried out, but it is important to bear in mind that consistency requires it to be proportional to $\rho^{\frac{1}{2}}$, as Aviles[2] has shown.

Using Eq. (5), $\zeta(k)$ can be evaluated from Eq. (4). For low density, the two leading terms are

$$\zeta=-\frac{\alpha}{\epsilon^2+k^2}+\frac{\alpha}{2k}\tan^{-1}\left(\frac{k}{2\epsilon}\right),\quad (\alpha=8\pi\rho r_0^3) \tag{6}$$

which will be referred to as ζ_0 and ζ_1, respectively. Aviles showed that ζ_0 contributes to lower order in the density than ζ_1, and he therefore consistently omitted the latter. To evaluate the next term in the expansion of the ground-state energy we must retain ζ_1.

We have not been able to evaluate the complete expression for G_0 with both of the above terms included in ζ. The main difficulty arises because of the presence of the transcendental function ζ_1 in the denominator of

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Eq. (3). We therefore have recourse to a Taylor's expansion about $\zeta=\zeta_0$, which yields the following expressions:

$$\frac{\zeta^2}{1-\zeta}=\sum_{n=0}^{\infty} Q_n(k)\zeta_1{}^n, \tag{7a}$$

$$Q_n(k)=\frac{1}{n!}\frac{d^n}{d\zeta_0{}^n}\left[\frac{\zeta_0{}^2}{1-\zeta_0}\right], \tag{7b}$$

$$G_0(x)=1+\frac{1}{\pi^2\alpha}\sum_{n=0}^{\infty}\int d^3k\, e^{-i\mathbf{k}\cdot\mathbf{x}}Q_n(k)\zeta_1{}^n. \tag{7c}$$

The $n=0$ term in Eq. (7c) has just the original form discussed by Aviles, since it corresponds to neglect of ζ_1. It consequently produces a term in G_0 of the form:

$$G_{00}(x)=1+\frac{2}{x}[e^{-\epsilon x}-e^{-\beta x}],\quad \beta=(\alpha+\epsilon^2)^{\frac{1}{2}}. \tag{8}$$

$Q_1(k)$ can be written in the simple form

$$Q_1(k)=[1-\zeta_0]^{-2}-1, \tag{9}$$

from which it follows immediately that, for $n>1$,

$$Q_n(k)=[1-\zeta_0]^{-n-1}. \tag{10}$$

We must now evaluate, in principle, all the higher terms G_{0n} in order to find the next term in the energy expansion. We can show (see Appendix), however, that only the terms $n=0$ and $n=1$ contribute, and will base our demonstration on the fact that the form of the higher terms [Eq. (10)] differs sharply from that of the first two.

To evaluate the term G_{01} we rewrite ζ_1 in the form

$$\zeta_1(k)=\frac{\alpha}{8\pi}\int d^3y\frac{e^{-2\epsilon y}}{y^2}e^{i\mathbf{k}\cdot\mathbf{y}}. \tag{11}$$

We substitute this result in Eq. (7c) and then reverse the order of integration and, after trivial angular integrations have been performed, obtain

$$G_{01}(x)=\frac{1}{2\pi^2}\int d^3y\frac{e^{-2\epsilon y}}{y^2}\int_0^{\infty}dk\, kQ_1(k)\frac{\sin k\omega}{\omega},$$

$$\omega=|\mathbf{y}-\mathbf{x}|. \tag{12}$$

The integration over k is easily done by contour integral methods and we have the expression

$$G_{01}(x)=\frac{\alpha}{2\pi}\int d^3y\frac{e^{-2\epsilon y}}{y^2}e^{-\beta\omega}\left[\frac{\alpha}{4\beta}-\frac{1}{\omega}\right]. \tag{13}$$

Some care must be exercised in evaluating this expression, and we obtain the final result

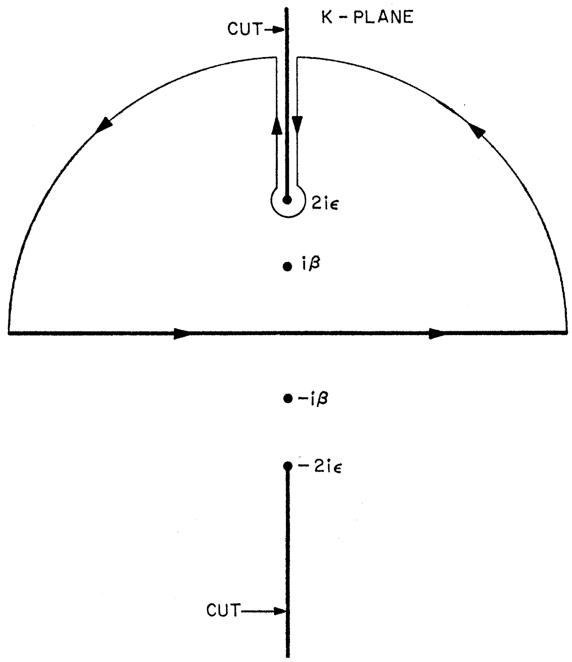

FIG. 1. Contour used to evaluate the two-particle correlation function $G_{01}(x)$.

$$G_{01}(x)=\frac{\alpha}{\beta x}\Bigg\{e^{-\beta x}\Bigg[\left(1-\frac{\alpha}{4\beta^2}-\frac{\alpha x}{4\beta}\right)$$

$$\times\left(\ln\left[\frac{2\epsilon-\beta}{2\epsilon+\beta}\right]-\mathrm{Ei}[-(2\epsilon-\beta)x]\right)$$

$$+\frac{\alpha}{4\beta}\left(\frac{e^{-[2\epsilon-\beta]x}-1}{2\epsilon-\beta}-\frac{1}{2\epsilon+\beta}\right)\Bigg]+\frac{\alpha}{4\beta(2\epsilon+\beta)}e^{-2\epsilon x}$$

$$+e^{\beta x}\left[1-\frac{\alpha}{4\beta^2}+\frac{\alpha x}{4\beta}\right]\mathrm{Ei}[-(2\epsilon+\beta)x]\Bigg\}, \tag{14}$$

where

$$\mathrm{Ei}(-y)\equiv-\int_y^{\infty}dx\frac{e^{-x}}{x}.$$

We have also been able to derive Eq. (14) by a more elegant method, involving contour integration of the expression

$$G_{01}(x)=\frac{1}{\pi x}\,\mathrm{Im}\int_{-\infty}^{\infty}dk\, e^{ikx}Q_1(k)\tan^{-1}\left(\frac{k}{2\epsilon}\right)$$

over the contour shown in Fig. 1. $Q_1(k)$ has second order poles at $k=\pm i\beta$, and branch points at $k=\pm 2i\epsilon$.

For the interesting special case $\epsilon^2=\alpha/3$, care must be taken with singularities in both ln and Ei functions, since then $\beta=2\epsilon$. Making the change of variables $z=\epsilon x$, we can then write the correlation function

$G_{00}+G_{01}$ as

$$G_0(z)=1+\frac{2\epsilon}{z}(e^{-z}-e^{-2z})+\frac{3\epsilon^2}{16z}\left\{e^{-2z}\left[\left(3z-\frac{13}{2}\right)\ln 4z-3z\right]+e^{2z}\left(3z+\frac{13}{2}\right)\mathrm{Ei}(-4z)\right\}. \quad (14a)$$

Still using the trial function defined in Eq. (5), we can write the final form for the energy as

$$E=2\pi\rho r_0\frac{\hbar^2}{2m}\int_\epsilon^\infty dz\, G_0(z)\times\left[ze^{-(z-\epsilon)}+\epsilon\left(\frac{2}{z}+\frac{1}{z^2}\right)e^{-2(z-\epsilon)}\right]. \quad (15)$$

Aviles has evaluated the terms which contribute to the energy to order $\alpha^{\frac{1}{2}}$, and we are interested here in the terms of order $\alpha \ln\alpha$, after the dimensional quantities $4\pi\rho r_0\hbar^2/2m$ have been removed. It is possible to evaluate (15) using the forms (8) and (14) for the two-particle correlation function, with the exact numerical value of ϵ unrestricted (although proportional to $\alpha^{\frac{1}{2}}$). If this is done, one derives a result for the logarithmic term in the energy which is independent of the value of ϵ. This calculation is long and straightforward, so we will illustrate the method by evaluating (15) letting $\epsilon^2=\alpha/3$ instead. This is the value of ϵ which was previously found[2] to minimize the lower terms in the energy. We break up the integral into parts,[8]

$$\int_\epsilon^\infty=\int_0^\infty-\int_0^\epsilon, \quad (16)$$

and observe that the first of these cannot contain a term of the desired form. Since ϵ is supposed small, we can expand all parts of the second integrand about $z=0$, and integrate term by term. Here we used the expansion of $\mathrm{Ei}(-4z)\cong \ln z+\sum C_nZ^n$. The only terms contributing to the desired order are the following:

$$E=-2\pi\rho r_0\frac{\hbar^2}{2m}\epsilon^2\int^\epsilon dz\left[\frac{3}{z}+6\epsilon\frac{\ln z}{z^2}\right]. \quad (17)$$

Thus it is easily seen that the logarithmic contribution to the energy is

$$E(\log)=4\pi\rho r_0(\hbar^2/2m)\times\tfrac{3}{4}\alpha\ln\alpha, \quad (18)$$

and as we stated before, this result is independent of the variational parameter.

Wu and others[6] give the value $(4/3)-(\sqrt{3}/\pi)$ for the exact coefficient of the $\alpha\ln\alpha$ term. This is equal to 0.782 and is to be compared with our approximate result of $\frac{3}{4}$. Note that the error is about 4%, and is in the right direction for a variational estimate, since for small α the entire term is negative. With $\epsilon^2=\alpha/3$ the ratio of the variational result, including all three terms, to the corresponding exact result becomes

$$R=(1+0.962\alpha^{\frac{1}{2}}+0.750\alpha\ln\alpha)/(1+0.960\alpha^{\frac{1}{2}}+0.782\alpha\ln\alpha). \quad (19)$$

DISCUSSION OF THE WAVE FUNCTION

To discuss the relationship between the variational method and the pseudopotential method,[7] we must consider the forms of both the general many-particle trial function, Eq. (1), and the specific form of the two-particle trial function, Eq. (5). It is clear that, for variational methods in general, good agreement of ground-state energy calculations does not necessarily indicate an accurate agreement between the assumed wave function and the correct wave function.

Lee, Huang, and Yang[7] have evaluated the coordinate space form of the wave function corresponding to their pseudopotential method for finding the energy. They point out that it consists of a part of the wave function of Eq. (1). That is, if we write

$$f(\mathbf{r}_{ij})=1+g(\mathbf{r}_{ij}), \quad (20)$$

then Eq. (1) can be expanded in a cluster series of the form

$$\Psi=1+\sum_{i<j}g(\mathbf{r}_{ij})+\sum_{\substack{i<j\\ i,j\neq k,l}}\sum_{k<l}g(\mathbf{r}_{ij})g(\mathbf{r}_{kl})+\cdots. \quad (21)$$

The result of the pseudopotential method selects from Eq. (21) only those terms in which each subscript appears no more than once. This truncated wave function obviously fails to satisfy the exact boundary condition that Ψ must vanish if any two particles approach closer than r_0, but the error in the energy thus introduced is of higher order than $\rho\alpha^{\frac{1}{2}}$.

Thus, we can now compare the form given by the pseudopotential method for the function $g(\mathbf{r}_{ij})$ with our trial function. The former is given indirectly as a Fourier integral,

$$g(\mathbf{x})=-\frac{1}{\pi^2\alpha^2}\int d^3k[k^2+\alpha-k(k^2+2\alpha)^{\frac{1}{2}}]e^{i\mathbf{k}\cdot\mathbf{x}}. \quad (22)$$

This function can be simplified by a contour integration process[9] as follows: After performing the angular part of the integration, we have

$$g(x)=-\frac{4}{\pi\alpha^2x}\,\mathrm{Im}\int_0^\infty dk[k^2+\alpha-k(k^2+2\alpha)^{\frac{1}{2}}]ke^{ikx}. \quad (23)$$

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[8] Both of these integrals diverge at the lower limit although their difference must be finite. One can formalize the procedure to be followed by replacing the lower limit by some small quantity a, which is smaller than, and independent of, ϵ.

[9] We are indebted to Dr. I. Harris for suggesting this procedure.

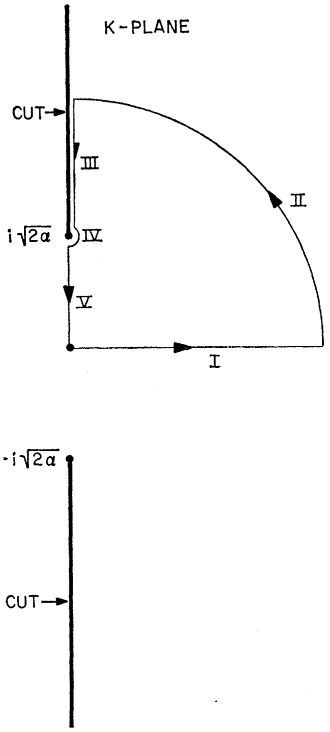

FIG. 2. Contour used to evaluate the coordinate-space function $f(x)$, given by the pseudopotential method.

Using the contour shown in Fig. 2, noting the presence of branch points at $\pm i(2\alpha)^{\frac{1}{2}}$, and the absence of singularities inside the contour, it is easily shown that the integral along contour I is equal to that along contour V. Hence, the function (22) can be rewritten as

$$f(x)=1+g(x)=1-\frac{16}{\pi x}\int_0^1 dz\, z^2(1-z^2)^{\frac{1}{2}} \times\exp[-(2\alpha)^{\frac{1}{2}}xz]. \quad (24)$$

Expansion of the exponential in Eq. (24) about $z=0$, combined with term-by-term integration, yields a series expression for $f(x)$ which satisfies the boundary condition at $x=1$ only approximately. This has been pointed out by Lee, Huang, and Yang,[7] who note that this inaccuracy does not affect the pseudopotential energy calculation except in higher order. Since our trial function satisfies the boundary condition exactly it is convenient, for comparison purposes, to replace x in the integrand of Eq. (24) by $x-1$, which insures the vanishing of $f(x)$ at $x=1$. The exponential can now be expanded about $z=0$ or $x=1$, and integration carried out term by term. The result is

$$f(x)=\left(1-\frac{1}{x}\right)\left(1+\frac{32(2\alpha)^{\frac{1}{2}}}{15\pi}-\frac{\alpha}{2}[x-1] +\frac{64(2\alpha)^{\frac{3}{2}}}{315\pi}[x-1]^2-\frac{5\alpha^2}{96}[x-1]^3+\cdots\right). \quad (25)$$

The corresponding expansion applied to Eq. (5) yields

$$f(x)=\left(1-\frac{1}{x}\right)\left(1+\epsilon-\frac{\epsilon^2}{2}[x-1] +\frac{\epsilon^3}{6}[x-1]^2-\frac{\epsilon^4}{24}[x-1]^3+\cdots\right). \quad (26)$$

Since our wave function is only approximate, it is not surprising that the value of ϵ which minimizes the energy gives poor agreement between Eqs. (25) and (26). However, a very close correspondence can be achieved if one chooses $\epsilon^2=\alpha$. With this value inserted in (26), we find that the ratios of the first few coefficients of (25) to those of (26) are

$$C_0=1,\quad C_1=0.96,\quad C_2=1,\quad C_3=1.10,\quad c_4=5/4. \quad (27)$$

Several points should be noted concerning these functions. First, when one uses the above value of ϵ in Aviles' expression for the energy [his formula (66)],

$$E=4\pi\rho r_0\frac{\hbar^2}{2m}\left[1+\epsilon\left(\left[1+\frac{\alpha}{\epsilon^2}\right]^{\frac{1}{2}}-\frac{1}{1+[1+\alpha/\epsilon^2]^{\frac{1}{2}}}\right)\right], \quad (28)$$

one finds that the ground-state energy is given by the first two terms of (26). This is also true for the pseudopotential method, where the first two terms of (25) give the exact energy value up to order $\rho\alpha^{\frac{1}{2}}$. This is the only choice of the variational parameter for which this relation is true. Second, with this value of the parameter the error in the logarithmic term is almost exactly the same as the error in the lower term. That is,

$$\frac{4}{3}\left[\frac{4}{3}-\frac{\sqrt{3}}{\pi}\right]\left[\frac{32\sqrt{2}}{15\pi}\right]=1.0009. \quad (29)$$

From the series results, Eq. (27), it appears that the two functions under consideration begin to differ widely for larger values of x. To examine this, we evaluate (24) for large x, and find that the exact function approaches unity as

$$f(x)\sim 1-Cx^{-4},\quad C=32\pi^{-1}(2\alpha)^{-\frac{3}{2}}. \quad (30)$$

This is a much longer-ranged behavior than the exponential fall-off of Eq. (5), and indicates that the trial function, although adequate for the ground-state energy, which depends mainly on behavior near the hard-sphere boundary, would not be good for an investigation of the low-lying excited states, whose phonon character requires longer-ranged correlations.

3. CONCLUSIONS

In the spirit of variational approximations, we have used a two-particle product wave function to calculate the first logarithmic term in the low-density series expression for the boson ground-state energy. It has been previously shown[7] that this product form is correct in the same approximation as is the pseudopotential method. However, Wu[6] has stated that a more complicated wave function is given by a higher order pseudopotential method, which also yields an exact result for the first logarithmic term in the energy. The good agreement between the results of the two methods, however, would seem to indicate continued usefulness for the variational technique, but probably only for ground-state energy calculations.

We have also studied the detailed behavior of the two-particle trial function assumed and have indicated that its success is due to its close accidental resemblance to the function derived by Lee, Huang, and Yang.[7] Mathematical difficulties have prevented us from applying this latter function directly to a variational calculation.

ACKNOWLEDGMENT

Many helpful discussions with Dr. J. B. Aviles, Jr. are most gratefully acknowledged.

APPENDIX

In order to show that terms in $G_0(x)$ higher than the second do not contribute to the logarithmic terms in the energy, we will now develop a method for obtaining the contribution from each of the terms in the sum given in Eq. (7). In this way, we can easily obtain the expression in Eq. (17) without completely calculating the expressions (8) and (14). Extending this procedure to $G_{0n}(x)$ for $n \geqq 2$, we show that no terms in the energy of order $\alpha \ln\alpha$ appear.

Making the substitutions $x = z/\epsilon$, $kx = y$, and choosing the special value $\alpha = 3\epsilon^2$ as before, we can use the energy expression (15) with

$$G_0(z) = 1 + \frac{4\epsilon}{3\pi z^3} \sum_{n=0}^{\infty} \int_0^{\infty} dy\, y \sin y Q_n \zeta_1^n, \qquad \text{(A1)}$$

where

$$\zeta_0 = -\frac{3}{1+(y/z)^2}; \quad \zeta_1 = \frac{3\epsilon z}{2y} \tan^{-1}\left(\frac{y}{2z}\right). \qquad \text{(A2)}$$

The integrals appearing in Eq. (A1) are broken into two parts, for $y \geqq 2z$ and $y \leqq 2z$, respectively. For $n=1$, the first of these integrals may be approximated by

$$-6\epsilon^2 \int_{2z}^{\infty} dy\, y^{-2} \sin y, \qquad \text{(A3)}$$

where the various parts of the integrand have been expanded in power series which converge for $y > 2z$. Integration by parts converts Eq. (A3) to one involving the cosine integral function,

$$-6\epsilon^2[(2z)^{-1} \sin(2z) - \mathrm{Ci}(2z)], \qquad \text{(A4)}$$

and for small z [which is the only region of importance; see Eq. (16)] this can be expanded to give the leading term:

$$6\epsilon^2 \ln z. \qquad \text{(A5)}$$

Inserting this expression in Eq. (15), we find exactly the result shown in Eq. (17). A similar expansion for $y < 2z$ is applied to the second part of the integral, and can be seen to give no additional terms of interest.

In the same way the higher terms can be shown not to contribute to the logarithmic term in the energy. For $y > 2z$, the leading term of Q_n is unity and this part of the integral for the correlation function $G_{0n}(z)$ becomes

$$\epsilon^{n+1} z^{n-3} (3\pi/4)^{n-1} \int_{2z}^{\infty} dy\, y^{1-n} \sin y. \qquad \text{(A6)}$$

For example, we can see that for $n=2$ the leading term is proportional to $\epsilon^3 z^{-1}$, while for $n=3$ it is proportional to $\epsilon^4 \ln z$. Neither of these terms contributes to the energy to the desired order, and similar arguments can be applied to the rest of the terms. Therefore, the result of Eq. (18) is the correct variational expression for the energy up to this order.