

racy of this number is of course subject to the same restrictions as discussed before in the case of platinum.

In conclusion, it has been shown that the effective coherence length of the normal metal should be calculated from the coefficient of normal electronic specific heat and the residual resistivity. If the data are then plotted in such a way as to exhibit all the temperature dependence in one term, one gets a linear plot of which the slope (k^{-1}) is very close to the calculated coherence length. Since the electron-electron interaction in both

Pt and Cu was found to be very close to zero, any more accuracy prediction for these metals will have to await much more precise film thickness control or measurements at even lower laboratory temperatures.

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Error Estimates in the Variational Many-Boson Calculation

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A simple test, recently suggested by Armstrong, is used to estimate the quality of the variational wave function first used by Aviles and Iwamoto in treating the ground state of the hard-sphere many-boson system. In this special case, Armstrong's method can be simplified by using a result obtained by Lieb in his recent work on the ground-state energy of the Bose gas. The wave function was previously used by the author to compute a first-order correction to the energy, due to a weak additional interaction outside the hard sphere. The errors in this computation are in good agreement with the estimates obtained by Armstrong's method.

A SIMPLE test, to be used in conjunction with a standard Rayleigh-Ritz variational method, to give some estimate of the accuracy of the trial function has recently been suggested by Armstrong.¹ He integrates the Schrödinger equation over all space, and obtains an expression for the energy

$$E_{NV} = \frac{\int dv H\psi}{\int dv \psi}, \quad (1)$$

provided the integral in the denominator is non-vanishing.² This is compared with the corresponding variational expression using the same trial function

$$E_V = \frac{\int dv \psi^* H\psi}{\int dv |\psi|^2}, \quad (2)$$

and the difference $E_V - E_{NV}$ between the two is a rough indicator of the quality of ψ .³ The original applications

¹ B. H. Armstrong, *Bull. Am. Phys. Soc.* **9**, 401 (1964), and private communication.

² If the denominator vanishes, it may be possible to rewrite Eq. (1). For example, if ψ has angular momentum different from zero, the Schrödinger equation in partial waves can be used to reformulate Eq. (1) in unambiguous form.

³ Certain special choices of ψ may accidentally give $E_V = E_{NV}$ without, in fact, corresponding to exact solutions. A notable case, observed by the author and Armstrong independently, is the trial function $\exp[-\alpha(r_1+r_2)]$ often used for the helium atom [E. Merzbacher, *Quantum Mechanics* (John Wiley & Sons, Inc., New York, 1961), pp. 430-436]. These special cases can be easily shown not to satisfy the eigenvalue equation.

of the method¹ were to standard one- and two-particle systems, including the ground state of helium.

It is the purpose of the present note to apply this procedure to a many-body system, previously extensively considered by several authors⁴⁻⁷ from a variational point of view. This system is the boson hard-sphere gas with⁷ or without⁴⁻⁶ an additional weak attraction or repulsion.

The variational method is very clearly described by Aviles.⁴ A product trial function

$$\psi(\mathbf{r}_1 \cdots \mathbf{r}_N) = \prod_{i<j}^N f(\mathbf{r}_i - \mathbf{r}_j) \quad (3)$$

is used to approximate the ground-state solution of the Hamiltonian

$$H = -(\hbar^2/2m) \sum_{i=1}^N \nabla_i^2 + \sum_{i<j}^N V(\mathbf{r}_i - \mathbf{r}_j). \quad (4)$$

The hard-sphere boundary condition requires that

$$f(\mathbf{r}) = 0, \quad \text{for } r \leq r_0, \quad (5)$$

while $V(\mathbf{r})$ is the additional weak interaction.⁷ The

⁴ J. B. Aviles, Jr., *Ann. Phys. (N.Y.)* **5**, 251 (1958).

⁵ F. Iwamoto, *Progr. Theoret. Phys. (Kyoto)* **19**, 597 (1958).

⁶ R. J. Drachman, *Phys. Rev.* **121**, 643 (1961).

⁷ R. J. Drachman, *Phys. Rev.* **131**, 1881 (1963).

variational energy takes the form⁴

$$E_V = \frac{\hbar^2}{2m} \frac{\rho r_0^3}{2} \int d^3x \left[\frac{\nabla f \cdot \nabla f - f \nabla^2 f}{f^2} + \frac{2m}{\hbar^2} V(x) \right] g(x), \quad (6)$$

where $\mathbf{x} = \mathbf{r}/r_0$, $\rho = N/\Omega$, and

$$g(\mathbf{r}_{12}) = \Omega^2 \int |\psi|^2 d\mathbf{r}_3 \cdots d\mathbf{r}_N / \int |\psi|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N$$

is the two-particle correlation function. Using the convenient trial function^{4,5}

$$f(x) = \begin{cases} 1 - x^{-1} e^{-\epsilon(x-1)}, & x \geq 1 \\ 0, & x \leq 1 \end{cases} \quad (7)$$

one can write the correlation function in the low-density limit⁴ as

$$g(x)/f^2(x) = 1 + (2/x)[e^{-\epsilon x} - e^{-2\epsilon x}] + (3\epsilon/16x) \times \{e^{-2\epsilon x}[(3\epsilon x - 13/2) \ln(4\gamma\epsilon x) - 3\epsilon x] + e^{2\epsilon x}(3\epsilon x + 13/2) \text{Ei}(-4\epsilon x)\}, \quad (8)$$

where γ is Euler's constant.

Consider first the pure hard-sphere gas, with $V=0$. Using Eqs. (6) and (8), one finds the minimum energy per particle [for $\epsilon^2 = \alpha/3$, $\alpha = 8\pi\rho r_0^3$] to be⁶

$$E_V/N = 4\pi\rho r_0(\hbar^2/2m)[1 + 5\alpha^{1/2}/3\sqrt{3} + \frac{3}{4}\alpha \ln\alpha + \cdots]. \quad (9)$$

Lieb⁸ has used Eq. (1) in another context in formulating a new method for the analysis of many-boson systems. For our purposes here, the important expression is his Eq. (3.7), which gives the result for the hard-sphere gas

$$\frac{E_{NV}}{N} = 4\pi\rho r_0 \frac{\hbar^2}{2m} \left[\frac{d}{dx} \bar{g}(x) \right]_{x=1}, \quad (10)$$

where

$$\bar{g}(\mathbf{r}_{12}) = \Omega^2 \int \psi d\mathbf{r}_3 \cdots d\mathbf{r}_N / \int \psi d\mathbf{r}_1 \cdots d\mathbf{r}_N$$

and is the appropriate two-body correlation function to use with the nonvariational Eq. (1).

We note that, due to the product form of ψ , \bar{g} is quite similar to g , and a similar analysis yields

$$\bar{g}(x) = f(x) \left(1 + (1/x) \{ e^{-\epsilon x} - \exp[-x(\epsilon^2 + \alpha/2)^{1/2}] \} \right). \quad (11)$$

There is, however, no term corresponding to the complicated expression in braces in Eq. (8), due to the

⁸ E. H. Lieb, Phys. Rev. **130**, 2518 (1963).

linearity in ψ of \bar{g} . This term has been shown⁶ to be responsible for the logarithmic term in Eq. (9).

One easily evaluates Eq. (10), inserting the value $\epsilon^2 = \alpha/3$ which minimizes E_V , and finds

$$E_{NV}/N = 4\pi\rho r_0(\hbar^2/2m)[1 + (\frac{5}{3}\alpha)^{1/2}]. \quad (12)$$

Defining $\Delta = [E_V - E_{NV}]N^{-1}$, one obtains

$$\Delta = 4\pi\rho r_0(\hbar^2/2m) \{ [(5\sqrt{2} - 3\sqrt{5})/3\sqrt{6}] \alpha^{1/2} + \frac{3}{4}\alpha \ln\alpha \} \quad (13)$$

as the difference between the variational and non-variational energies. Expressed in percentage, the errors are α^0 term-exact; $\alpha^{1/2}$ term-5%; $\alpha \ln\alpha$ term-100%.

One may therefore conclude that the part of ψ which yields the first term is exact, that yielding the second term is fairly good, while the third part is very poor, in spite of fairly good agreement between the exact and variational logarithmic terms in the energy.⁹

If one now uses ψ as an approximate solution of the pure hard-sphere ground state problem, one can add a perturbation:

$$V = \begin{cases} 0, & x < 1, \\ -V_0, & 1 < x < b, \\ 0, & x > b. \end{cases}$$

This is exactly the situation considered previously by the author.⁷ The first-order energy shift obtained is

$$\langle V \rangle_V/N = -4\pi\rho r_0(\hbar^2/2m)\delta[1 + (4/\sqrt{3})\alpha^{1/2} + \alpha \ln\alpha], \quad (14)$$

where $\delta = \pi r_0^2 V_0 (b-1)^3 / 3\hbar^2$. This is to be compared with the exact result⁹

$$\langle V \rangle/N = -4\pi\rho r_0(\hbar^2/2m)\delta[1 + (16\sqrt{2}/3\pi)\alpha^{1/2} + 4(\frac{4}{3} - \sqrt{3}/\pi)\alpha \ln\alpha]. \quad (15)$$

Defining $\Delta' = [\langle V \rangle_V - \langle V \rangle]N^{-1}$, one obtains

$$\Delta' = -4\pi\rho r_0(\hbar^2/2m)\delta[(4\pi\sqrt{3} - 16\sqrt{2})\alpha^{1/2} + (12\sqrt{3} - 13\pi)\alpha \ln\alpha]/3\pi \quad (16)$$

as the error in the first-order perturbation energy due to errors in the variational trial function ψ . Again, the α^0 term error vanishes, the $\alpha^{1/2}$ error is about 4%, while the error in the logarithmic term is about 70%. Thus, Δ' is clearly well correlated with Δ as expected, and hence the present calculation gives another indication of the usefulness of Armstrong's method.¹

⁹ In Ref. (6), where the logarithmic term in E_V was derived, it was noted that T. T. Wu [Phys. Rev. **115**, 1390 (1959)] had required three-particle correlations in the wave function to derive the exact coefficient $\frac{4}{3} - \sqrt{3}/\pi$. Since no such terms are contained in the present ψ , it is not surprising that Eq. (12) indicates a large error. Once again, one sees that excellence of a variational energy calculation tells very little about the accuracy of a trial function.