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Three-particle distribution function in liquid ^{4}He

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Several approximate forms of the three-particle distribution function are studied using error functions introduced to estimate the accuracy with which they satisfy the sequential relation connecting the two- and three-particle distribution functions. The procedure is based on modification and extension of the formal density-cluster expansion developed by Abe in the context of the classical statistical mechanics of an imperfect gas. Numerical evaluation of the error functions are carried out by expanding functions of the complicated multidimensional cluster integrals in terms of the associated Legendre functions. The results obtained numerically in the first three lowest-order approximations for the ground state of liquid ^{4}He at equilibrium density show that the overall magnitude of the error function decreases significantly as the order of approximation increases to the next higher order.

I. INTRODUCTION

Description of the structure of a fluid in terms of the distribution functions $p^{(n)}(1,2,\ldots,n)$ is relatively simple and convenient.[1–4] In particular, many recent studies on the structure of classical and quantum fluids are centered upon the radial-distribution function $g(r_{12})=\rho^{-2}p^{(2)}(1,2)$, which is also known as the pair-correlation function. The importance of the function $g(r)$ follows from the fact that in a fluid the pair correlation is far more significant than the simultaneous correlation of three, or of more particles and hence the $g(r)$ can determine many important properties associated with the structure of the fluid. In addition, the liquid structure function $S(k)$, which is the Fourier transform of $g(r)$, can be obtained from neutron or x-ray scattering and thus the function $g(r)$ can be determined experimentally.

The radial-distribution function, however, does not give full description of the structure present in fluids at equilibrium and any improvement must include the contribution of the simultaneous correlations of triples, quadruples, etc., of particles. That is, the distribution functions $p^{(n)}(1,2,\ldots,n)$ for $n=3,4,\ldots,$ as well as $n=2$ must be incorporated for a more accurate and complete discussion of macroscopic equilibrium properties. The improvement over results based on consideration of the $g(r)$ alone is generally quite difficult. The first step in this direction should be concerned with the study of the three-particle distribution function $p^{(3)}(1,2,3)$.

Although one can consider experimental determination of $p^{(3)}(1,2,3)$ from triple elastic scattering similar to that of $g(r)$, no success has yet been made to date. On the other hand, if the potential energy function is known, $p^{(3)}(1,2,3)$ can be evaluated directly and exactly from the computer simulation using the Monte Carlo or molecular-dynamics techniques.[5–7] In many cases, however, it is necessary to express $p^{(3)}(1,2,3)$ as an explicit functional in $g(r)$, but no such expressions which are exact and useful are available. Some approximate forms giving $p^{(3)}(1,2,3)$ as a functional in $g(r)$ are studied in this paper and error functions are introduced to test their accuracies. Numerical evaluation is carried out for the case of liquid ^{4}He.

II. BASIC FORMULATION

Many important properties of an extended uniform system of N interacting bosons confined in a box of volume Ω can be discussed in terms of the n-particle distribution functions defined by

$$p^{(n)}(1,2,\ldots,n) = N(N-1)\cdots(N-n+1) \times \int |\psi_0(1,2,\ldots,N)|^2\, d\vec{r}_{n+1,n+2,\ldots,N} \ , \qquad (1)$$

where $\psi_0(1,2,\ldots,N)$ is the normalized ground-state wave function generated by the Schrödinger equation. For the two lowest members, we obtain the particle number density ρ and the radial distribution function $g(r)$:

$$p^{(1)}(1)=\rho=N/\Omega \ , \qquad (2)$$

$$p^{(2)}(1,2)=\rho^2 g(r_{12}) \ . \qquad (3)$$

Equation (1) implies that the two successive distribution functions are connected by the sequential relation

$$p^{(n-1)}(1,2,\ldots,n-1) = \frac{1}{N-n+1} \int p^{(n)}(1,2,\ldots,n)\, d\vec{r}_n \ . \quad (4)$$

In particular, for $n=2$, Eq. (4) yields the normalization condition

$$\rho \int [g(r)-1]\, d\vec{r} = -1 \ , \quad (5)$$

and for $n=3$, the sequential relation

$$\rho^2 g(r_{12}) = \frac{1}{N-2} \int p^{(3)}(1,2,3)\, d\vec{r}_3 \quad (6)$$

is a linear inhomogeneous integral equation for the symmetric positive-valued function $p^{(3)}(1,2,3)$.

It is convenient to define two functions $h(r)$ and $\delta p(1,2,3)$ by[8]

$$h(r) = g(r) - 1 \ , \quad (7)$$

$$\begin{aligned} p^{(3)}(1,2,3) = \rho^3[1 &+ h(r_{12}) + h(r_{23}) + h(r_{31}) \\ &+ h(r_{12})h(r_{23}) + h(r_{23})h(r_{31}) \\ &+ h(r_{31})h(r_{12})] + \delta p(1,2,3) \ . \end{aligned} \quad (8)$$

Equation (6) then reduces to

$$\int \delta p(1,2,3)\, d\vec{r}_3 = -\rho^3 \int h(r_{13})h(r_{23})\, d\vec{r}_3 \ . \quad (9)$$

The remainder term $\delta p(1,2,3)$ is small when all three particles are well separated or when any two are close and far from the third. It is large only when all three particles are close. We introduce here the usual assumption of strong repulsive forces between pairs of particles when they approach closely, thus requiring $g(0)=0$ or $h(0)=-1$. Then, for $\vec{r}_1 = \vec{r}_2$, Eq. (8) becomes

$$\delta p(1,1,3) = -\rho^3 h^2(r_{13}) \ . \quad (10)$$

Two of the common approximations for $p^{(3)}(1,2,3)$ are the convolution approximation $p_c^{(3)}(1,2,3)$ given by

$$\delta p_c(1,2,3) = \rho^4 \int h(r_{14})h(r_{24})h(r_{34})\, d\vec{r}_4 \ , \quad (11)$$

and the Kirkwood superposition approximation

$$p_K^{(3)}(1,2,3) = \rho^3 g(r_{12})g(r_{23})g(r_{31}) \ , \quad (12)$$

which is equivalent to

$$\delta p_K(1,2,3) = \rho^3 h(r_{12})h(r_{23})h(r_{31}) \ . \quad (13)$$

The convolution approximation satisfies the sequential relation (9), but fails to meet the requirement Eq. (10) and $p_c^{(3)}(1,2,3)$ is not necessarily positive valued. Nevertheless, it simplifies the calculation of many quantities such as multiphonon states, many-particle structure functions, and interaction matrix elements. On the other hand, the Kirkwood superposition approximation satisfies Eq. (10) but fails in Eq. (4). Because of the symmetric nature and simplicity, this form has been extensively used in solving the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of equations as a convenient closure.

A form of $p^{(3)}(1,2,3)$ more accurate and more complicated than those of the convolution and Kirkwood superposition approximations was derived by Abe[9] using the standard cluster-expansion technique as in the classical statistical mechanics of an imperfect gas. His result is

$$p^{(3)}(1,2,3) = p_K^{(3)}(1,2,3)\exp[A(1,2,3)] \ , \quad (14)$$

where

$$\begin{aligned} A(1,2,3) = \rho &\int h(r_{14})h(r_{24})h(r_{34})\, d\vec{r}_4 \\ &+ \rho^2 \int \Big[h(r_{24})h(r_{45})h(r_{35})[h(r_{14})h(r_{15}) + h(r_{14})h(r_{25}) + h(r_{15})h(r_{34})] \\ &\qquad + h(r_{14})h(r_{24})h(r_{34})h(r_{15})h(r_{25})h(r_{35})h(r_{45}) \left(\frac{1}{2} + \sum_{i=1}^{3} \frac{1}{h(r_{i4})} \right) \Big]\, d\vec{r}_4 d\vec{r}_5 + O(\rho^3) \ . \end{aligned} \quad (15)$$

Since $h(r)$ is a function of ρ, Eq. (15) is not a genuine power series of $A(1,2,3)$ in ρ. In order to overcome this difficulty in the problem of many-boson systems in the uniform limit, a new expansion parameter

$$\alpha = 1 - g(0) \ , \quad (16)$$

is used in Refs. 8 and 10–12 for the series expansion of $A(1,2,3)$:

$$\begin{aligned} A(1,2,3) = A_2(1,2,3) &+ A_3(1,2,3) \\ &+ A_4(1,2,3) + O(\alpha^5) \ . \end{aligned} \quad (17)$$

Explicit results for $A_n(1,2,3)$ have been derived through $n=4$ and their expressions are given diagrammatically in Fig. 1, where each line represents an

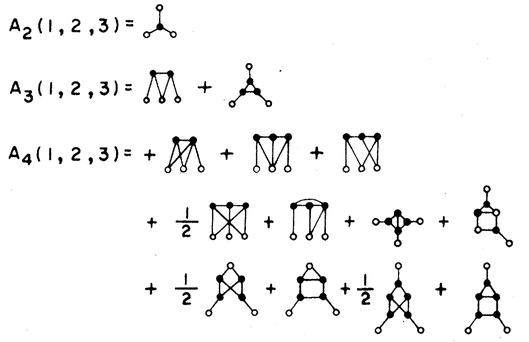

FIG. 1. Diagrammatic representations of $A_n(1,2,3)$ for $n=2$, 3, and 4.

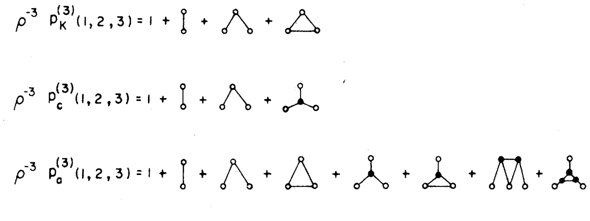

FIG. 2. Diagrammatic representations of approximate forms for $\rho^{-3}p^{(3)}(1,2,3)$ given by Eqs. (11), (12), and (18).

h factor and a solid circle is used for a factor of ρ and volume integrations over Ω and open circles for the points $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$ in all possible distinct arrangements of the labels 1, 2, and 3 on the open circles.

In Eq. (17) $A_n(1,2,3)$ is of $O(\alpha^n)$ and this fact becomes explicit only when a suitable change of variable is made for r. The α-expansion formalism is particularly useful in the uniform limit and/or weak-coupling limit.[12] A major defect of this approach is that in a realistic problem of the liquid ^{4}He, $\alpha \equiv 1 - g(0) = 1$ and it is not clear if the expansion is still valid. The term $A_3(1,2,3)$, which is absent in Eq. (15), is necessary to obtain the extended Abe form accurate through $O(\alpha^3)$

$$\begin{aligned}p_A^{(3)}(1,2,3) = {} & \rho^3[1+h(r_{12})+h(r_{23})+h(r_{31})+h(r_{12})h(r_{23})\\ & +h(r_{23})h(r_{31})+h(r_{31})h(r_{12})+h(r_{12})h(r_{23})h(r_{31})]\\ & +[1+h(r_{12})+h(r_{23})+h(r_{31})]\rho^4\int h(r_{14})h(r_{24})h(r_{34})\,d\vec{r}_4\\ & +\rho^5\int h(r_{14})h(r_{25})h(r_{45})[h(r_{34})h(r_{35})+h(r_{24})h(r_{35})+h(r_{34})h(r_{15})]\,d\vec{r}_4 d\vec{r}_5\\ & +\rho^6\int h(r_{14})h(r_{25})h(r_{36})h(r_{45})h(r_{56})h(r_{64})\,d\vec{r}_4 d\vec{r}_5 d\vec{r}_6 \ . \qquad (18)\end{aligned}$$

The diagrammatic representations of $\rho^{-3}p^{(3)}(1,2,3)$ are shown in Fig. 2 for three approximations given by Eqs. (11), (12), and (18).

III. APPROXIMATIONS AND ERROR FUNCTIONS

In this section, we study approximate forms of $p^{(3)}(1,2,3)$ defined by

$$p_m^{(3)}(1,2,3) = p_K^{(3)}(1,2,3)\prod_{n=2}^{m}\exp[A_n(1,2,3)], \quad m \geq 2 \ . \qquad (19)$$

Noting that the exact $p^{(3)}(1,2,3)$ satisfies the sequential relation (6)

$$\int p^{(3)}(1,2,3)\,d\vec{r}_3 = \rho^2 g(r_{12})(N-2) \ , \qquad (20)$$

we introduce error functions $\eta_K(r)$ and $\eta_m(r)$ by

$$\int p_K^{(3)}(1,2,3)\,d\vec{r}_3 = \rho^2 g(r_{12})[N-2+\eta_K(r_{12})] \ , \qquad (21)$$

$$\int p_m^{(3)}(1,2,3)\,d\vec{r}_3 = \rho^2 g(r_{12})[N-2+\eta_m(r_{12})] \ . \qquad (22)$$

Then one obtains

$$\begin{aligned}\eta_K(r_{12}) &= \rho\int h(r_{13})h(r_{23})\,d\vec{r}_3\\ &= -\rho^{-2}\int \delta p(1,2,3)\,d\vec{r}_3 \ , \qquad (23)\end{aligned}$$

$$\eta_m(r) = \eta_K(r) + \Delta_m(r) \ , \qquad (24)$$

where

$$\Delta_m(r_{12}) = \rho\int g(r_{13})g(r_{23}) \times \left[\prod_{n=2}^{m}\exp[A_n(1,2,3)] - 1\right] d\vec{r}_3 \ . \qquad (25)$$

These error functions are expected to be significantly different from zero only near the origin $r=0$.

The numerical evaluation of $\Delta_m(r)$ is somewhat involved, since there are many h factors connected to each other in complicated ways, in particular, for $m \geq 3$. To simplify the numerical procedure, we choose, without loss of generality, a Cartesian coordinate system such that $\vec{r}_1 = 0$ and $\vec{r}_2$ is along the z axis. The integration variables $\vec{r}_3$, $\vec{r}_4$, . . . , are general vectors. Expanding the h factors in Legendre functions, we find, after somewhat lengthy algebra, that in terms of

$$\mu_{ij}=(r_i^2+r_j^2-r_{ij}^2)/(2r_ir_j)\ , \tag{26}$$

$$H_l(i,j)=\int_{-1}^{1} h(r_{ij})P_l(\mu_{ij})\,d\mu_{ij}\ , \tag{27}$$

Equations (23) and (25) become

$$\eta_K(r_{12})=2\pi\rho\int_0^\infty r_3^2h(r_3)H_0(2,3)\,dr_3\ , \tag{28}$$

$$\Delta_m(r_{12})=2\pi\rho\int_0^\infty dr_3\,r_3^2g(r_3)\int_{-1}^{1}d\mu_{23}\,g(r_{23})\left[\prod_{n=2}^{m}\exp[A_n(1,2,3)]-1\right]\ , \tag{29}$$

where

$$A_2(1,2,3)=\pi\rho\sum_{l=0}^{\infty}(2l+1)P_l(\mu_{23})\int_0^\infty dr_4r_4^2h(r_4)H_l(2,4)H_l(3,4)\ , \tag{30}$$

$$A_3(1,2,3)=A_{3a}(1,2,3)+A_{3b}(1,2,3)+A_{3c}(1,2,3)+A_{3d}(1,2,3)\ , \tag{31}$$

$$\begin{aligned}A_{3a}(1,2,3)={}&(\pi\rho)^2\sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{l_3=0}^{\infty}(2l_1+1)(2l_2+1)(2l_3+1)\begin{pmatrix}l_1&l_2&l_3\\0&0&0\end{pmatrix}P_{l_3}(\mu_{23})\\&\times\int_0^\infty dr_4\,r_4^2h(r_4)H_{l_1}(2,4)\int_0^\infty dr_5\,r_5^2H_{l_1}(4,5)H_{l_2}(2,5)H_{l_3}(3,5)\ ,\end{aligned} \tag{32}$$

$$A_{3b}(1,2,3)=2(\pi\rho)^2\sum_{l=0}^{\infty}(2l+1)P_l(\mu_{23})\int_0^\infty dr_4\,r_4^2h(r_4)H_l(3,4)\int_0^\infty dr_5\,r_5^2h(r_5)H_l(2,5)H_l(4,5)\ , \tag{33}$$

$$\begin{aligned}A_{3c}(1,2,3)={}&(\pi\rho)^2\sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{l_3=0}^{\infty}(2l_1+1)(2l_2+1)(2l_3+1)\begin{pmatrix}l_1&l_2&l_3\\0&0&0\end{pmatrix}\\&\times\int_0^\infty dr_4\,r_4^2H_{l_1}(2,4)H_{l_2}(3,4)\\&\times\int_0^\infty dr_5\,r_5^2h(r_5)H_{l_3}(3,5)H_{l_3}(4,5)\\&\times\left[P_{l_2}(\mu_{23})P_{l_3}(\mu_{23})\begin{pmatrix}l_1&l_2&l_3\\0&0&0\end{pmatrix}+2\sum_{m=1}^{l_{23}}(-1)^m\left[\frac{(l_2-m)!(l_3-m)!}{(l_2+m)!(l_3+m)!}\right]^{1/2}\right.\\&\left.\times P_{l_2}^m(\mu_{23})P_{l_3}^m(\mu_{23})\begin{pmatrix}l_1&l_2&l_3\\0&0&0\end{pmatrix}\right]\ ,\end{aligned} \tag{34}$$

$$\begin{aligned}A_{3d}(1,2,3)={}&2(\pi\rho)^3\sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{l_3=0}^{\infty}\sum_{l_4=0}^{\infty}\prod_{i=1}^{4}(2l_i+1)\begin{pmatrix}l_1&l_3&l_4\\0&0&0\end{pmatrix}\begin{pmatrix}l_2&l_3&l_4\\0&0&0\end{pmatrix}P_{l_2}(\mu_{23})\\&\times\left[\begin{pmatrix}l_1&l_3&l_4\\0&0&0\end{pmatrix}\begin{pmatrix}l_2&l_3&l_4\\0&0&0\end{pmatrix}+2\sum_{m=1}^{l_{34}}\begin{pmatrix}l_1&l_3&l_4\\0&m&-m\end{pmatrix}\begin{pmatrix}l_2&l_3&l_4\\0&m&-m\end{pmatrix}\right]\\&\times\int_0^\infty dr_4\,r_4^2h(r_4)\int_0^\infty dr_5\,r_5^2H_{l_1}(2,5)H_{l_3}(4,5)\\&\times\int_0^\infty dr_6\,r_6^2H_{l_2}(3,6)H_{l_3}(4,6)H_{l_4}(5,6)\ .\end{aligned} \tag{35}$$

In Eqs. (27)–(35), $P_l(\mu)$, and $P_l^m(\mu)$ are the Legendre functions and associated Legendre functions, respectively, and $l_{ij}=\min(l_i,l_j)$. The values of the Wigner 3-j symbol are given by[13]

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} = (-1)^{j_1-j_2+m_3}(2j_3+1)^{-1/2}(j_1m_1j_2m_2|j_3m_3) \quad , \tag{36}$$

$$(j_1m_1j_2m_2|j_3m_3)=\delta_{m_1+m_2,m_3}\left[\frac{(2j_3+1)(j_1+j_2-j_3)!(j_1-m_1)!(j_2-m_2)!(j_3+m_3)!(j_3-m_3)!}{(j_1+j_2+j_3+1)!(j_1-j_2+j_3)!(j_2+j_3-j_1)!(j_1+m_1)!(j_2+m_2)!}\right]^{1/2}$$

$$\times \sum_{s>0}(-1)^{s+j_1-m_1}\frac{(j_1+m_1+s)!(j_2+j_3-m_1-s)!}{s!(j_1-m_1-s)!(j_3-m_3-s)!(j_2-j_3+m_1+s)!} \quad , \tag{37}$$

in which the summation is over all positive integer values of s such that the arguments of the factorials in the denominator are non-negative.

To evaluate the error functions η_K, η_2, and η_3 for the case of liquid ^{4}He at equilibrium density, we used the liquid structure function $S(k)$ obtained in the paired-phonon analysis by Campbell and Feenberg[14] under the hypernetted-chain approximation. The h function defined by Eq. (7) is obtained by the Fourier transform of $S(k)-1$:

$$h(r)=\frac{1}{(2\pi)^3\rho}\int[S(k)-1]e^{i\vec{k}\cdot\vec{r}}d\vec{k} \quad , \tag{38}$$

with $\rho=0.0218$ Å^{-3}. Since the Campbell-Feenberg data of $S(k)$ are given as a function of a dimensionless variable Dk ($D=2.45934$ Å), we also use the dimensionless variable $Q=r/D$. The numerical results for the radial distribution function $g(r)$ obtained from Eq. (38) do not exactly satisfy the normalization condition given by Eq. (5) and hence we have normalized $g(r)$ for r values up to $r_{\max}=10D$, where $g(r)$ practically reaches its asymptotic value unity after several oscillations. The summations $\sum_{l_i=0}^{\infty}$ in Eqs. (30)–(35) are replaced by finite summations of the form $\sum_{l_i=0}^{l_{\max}}$. In order to determine the values of $l_{\max}$ for Δ_2 and Δ_3, we have evaluated Δ_2 for $l_{\max}=0,1,2,\ldots,7$ and Δ_3 for $l_{\max}=0,1,2,3,4$ at $Q=0.2,0.4,0.6,\ldots,3.2$. The numerical results are given in Tables I and II. The most important domain of the η and Δ functions is near the origin and there $l_{\max}=7$ for Δ_2 and $l_{\max}=4$ for Δ_3 seem quite adequate.

Our final numerical results for η_K, η_2, and η_3 are tabulated in Table III and also plotted in Fig. 3 as functions of $Q=r/D$. It is clear that our results for the error functions indicate the overall inequalities

$$|\eta_K(r)|>|\eta_2(r)|>|\eta_3(r)| \quad , \tag{39}$$

TABLE I. Numerical values of Δ_2.

Q \ $l_{\max}$	0	1	2	3	4	5	6	7
0.2	−0.7310	−0.7217	−0.7232	−0.7232	−0.7232	−0.7232	−0.7232	−0.7232
0.4	−0.4406	−0.3987	−0.4107	−0.4123	−0.4123	−0.4123	−0.4123	−0.4123
0.6	−0.1946	−0.1144	−0.1333	−0.1430	−0.1430	−0.1426	−0.1426	−0.1426
0.8	−0.0604	0.0253	0.0246	0.0042	0.0018	0.0031	0.0035	0.0035
1.0	−0.0165	0.0406	0.0648	0.0455	0.0393	0.0403	0.0416	0.0419
1.2	−0.0163	0.0074	0.0370	0.0289	0.0230	0.0229	0.0246	0.0253
1.4	−0.0170	−0.0146	0.0031	0.0032	0.0044	0.0007	0.0025	0.0026
1.6	0.0003	−0.0061	−0.0036	−0.0022	−0.0039	−0.0028	−0.0012	0.0003
1.8	0.0251	0.0190	0.0130	0.0119	0.0101	0.0108	0.0117	0.0127
2.0	0.0334	0.0316	0.0271	0.0245	0.0234	0.0240	0.0245	0.0246
2.2	0.0142	0.0151	0.0158	0.0153	0.0152	0.0159	−0.0169	0.0169
2.4	−0.0135	−0.0127	−0.0113	−0.0099	−0.0091	−0.0085	−0.0078	−0.0075
2.6	−0.0243	−0.0242	−0.0242	−0.0237	−0.0230	−0.0224	−0.0221	−0.0218
2.8	−0.0142	−0.0144	−0.0149	−0.0154	−0.0156	−0.0154	−0.0151	−0.0149
3.0	0.0023	0.0020	0.0017	0.0012	0.0008	0.0006	0.0006	0.0007
3.2	0.0107	0.0105	0.0104	0.0103	0.0102	0.0100	0.0099	0.0099

TABLE II. Numerical values of Δ_3.

Q \ $l_{\max}$	0	1	2	3	4
0.2	−1.0473	−0.9583	−0.9483	−0.9394	−0.9366
0.4	−0.7259	−0.6229	−0.6161	−0.6108	−0.6126
0.6	−0.4282	−0.3033	−0.2991	−0.3033	−0.3025
0.8	−0.2361	−0.1322	−0.1128	−0.1268	−0.1232
1.0	−0.1197	−0.0648	−0.0313	−0.0456	−0.0517
1.2	−0.0538	−0.0396	−0.0125	−0.0202	−0.0221
1.4	−0.0136	−0.0149	−0.0060	−0.0103	−0.0130
1.6	0.0179	0.0190	0.0136	0.0095	0.0085
1.8	0.0371	0.0455	0.0366	0.0319	0.0300
2.0	0.0372	0.0472	0.0441	0.0399	0.0388
2.2	0.0132	0.0174	0.0207	0.0202	0.0197
2.4	−0.0170	−0.0187	−0.0160	−0.0136	−0.0130
2.6	−0.0256	−0.0284	−0.0286	−0.0273	−0.0265
2.8	−0.0127	−0.0136	−0.0141	−0.0145	−0.0143
3.0	0.0036	0.0044	0.0044	0.0036	0.0035
3.2	0.0111	0.0122	0.0124	0.0118	0.0120

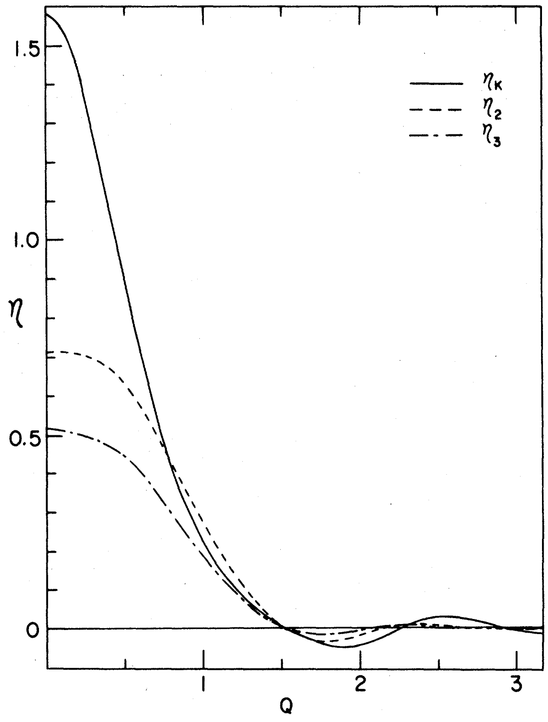

FIG. 3. Error functions as function of $Q = r/D$ ($D = 2.45\,934$ Å).

and hence a higher-order approximation for the exponent in the Abe form of Eq. (14) is more accurate at least in the sense that the magnitude of the error function $\eta_m(r)$ is smaller, or equivalently, the sequential relation is more accurately satisfied. This also suggests that the α-ordering scheme originally introduced in the uniform limit could be useful in more realistic problems such as liquid ^{4}He.

TABLE III. Numerical values of the error functions.

Q	η_K	η_2	η_3
0.0	1.5840	0.7122	0.5161
0.2	1.4334	0.7102	0.4968
0.4	1.0853	0.6730	0.4727
0.6	0.7132	0.5706	0.4107
0.8	0.4202	0.4237	0.2970
1.0	0.2278	0.2697	0.1761
1.2	0.1116	0.1369	0.0895
1.4	0.0375	0.0401	0.0245
1.6	−0.0142	−0.0139	−0.0057
1.8	−0.0438	−0.0311	−0.0138
2.0	−0.0420	−0.0174	−0.0032
2.2	−0.0115	0.0054	0.0082
2.4	0.0201	0.0126	0.0071
2.6	0.0282	0.0064	0.0017
2.8	0.0142	−0.0007	−0.0000
3.0	−0.0040	−0.0033	−0.0005
3.2	−0.0120	−0.0021	−0.0000
3.4	−0.0079	0.0000	0.0004
3.6	0.0010	0.0011	0.0000

IV. CONCLUDING REMARKS

Here we present several remarks concerning the approximations for $p^{(3)}(1,2,3)$ and their relationships to other works in closely related areas.

(i) Smallness of the magnitude of the error function $\eta_m(r)$ is only a necessary condition for a good approximation of $p^{(3)}(1,2,3)$, and certainly not a sufficient requirement. A best example to illustrate this point is the convolution approximation $p_c^{(3)}(1,2,3)$ given by Eq. (11). It satisfies the sequential relation exactly and hence its error function vanishes identically, but it fails to meet the condition given by Eq. (10), and also according to Berdahl's analysis[15] of the ground state of a boson gas it gives an incorrect description even to lowest nontrivial order in a perturbation theory.

(ii) The importance of the two diagrams of $A_3(1,2,3)$ given in Fig. 1 was demonstrated by Pokrant,[16] who included the two diagrams in his evaluation of the liquid structure function and the ground-state energy, leading to good agreement with experimental values. It has also been demonstrated that use of the same liquid structure function in a perturbation calculation of the energy yields an even better agreement.[17] Thus, our numerical result on the error function $\eta_3(r)$ is consistent with these observations on the ground-state-energy calculation.

(iii) Important computer simulation studies of $p^{(3)}(1,2,3)$ have been made by Raveché and Mountain.[5,7] In particular, they have introduced a useful quantity defined by

$$F(r_{12}|p^{(3)}) = \int d\vec{r}_3\, g(r_{13})g(r_{23}) \times \left[\frac{p^{(3)}(1,2,3)}{p_K^{(3)}(1,2,3)} - 1 \right] . \qquad (40)$$

Here we do not give the details of their studies involving $F(r|p^{(3)})$, but we simply point out that if the approximation of Eq. (19) is made in Eq. (40), the function $\Delta_m(r)$ defined by Eq. (25) is obtained:

$$\Delta_m(r) = \rho F(r|p_m^{(3)}) \ . \qquad (41)$$

(iv) Derivations of the several forms for the three-particle distribution function $p^{(3)}(1,2,3)$ given by Eqs. (14), (15), and (17)–(19) are all based on the assumption that the ground state of the many-particle boson system is described by the Jastrow wave function

$$\psi_J = \prod_{i<j}^{N} \exp[\tfrac{1}{2} u(r_{ij})] \ , \qquad (42)$$

where $u(r)$ is the pair correlation function determined usually by variational procedures.[3,10–12,14,16,18] The problem of expanding the trial function space beyond the Jastrow function space has been considered by many authors,[18–22] using the trial function of the form

$$\psi_0 = \psi_J \prod_{i<j<k}^{N} \exp[\tfrac{1}{2} u_3(\vec{r}_i, \vec{r}_j, \vec{r}_k)] \ , \qquad (43)$$

where $u_3(\vec{r}_i, \vec{r}_j, \vec{r}_k)$ is the three-particle factor. In particular, the importance of this factor is demonstrated in recent studies by Chang and Campbell[21] and Pandharipande,[22] who show that the contribution from the three-particle factor to the ground-state energy significantly improves agreement with experimental observations. Chang and Campbell[20] also find in their study of the roton spectrum that $u_3(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ produces an improved density dependence over the pure Jastrow trial function and that the amount of the improvement is sensitive to the approximation for $p^{(3)}(1,2,3)$, or more precisely, its Fourier transform $S^{(3)}(\vec{k}_1, \vec{k}_2, \vec{k}_3)$. While the evidence of the importance of the three-particle factor in the ground-state wave function is abundant, very little study has been made on the approximation for $p^{(3)}(1,2,3)$ based on such an expanded Jastrow form.

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