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The Functional Derivative of the Radial Distribution Function for a Many-Particle Boson System

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Abstract

The functional derivative of the radial distribution function of a many-particle boson system, which was studied originally by Lee and Broyles, is considered. A new approximate expression for this functional derivative is obtained, which contains some additional terms. A discussion is given on the results obtained.

1. *Introduction*

The application of the variational principle to the energy functional of the ground state of a strongly interacting many-particle boson system described by a Bijl-Dingle-Jastrow wave function (Bijl, 1940; Dingle, 1949; Jastrow, 1955; Feenberg, 1969)

$$\Psi_N = \prod_{i<j} f(r_{ij}) \tag{1.1}$$

leads to a complicated Euler equation for $f(r)$ (Grypeos, 1974), in which the radial distribution function $G(r_{12}) = g(r_{12})/f^2(r_{12})$:

$$G(r_{12}) = \frac{N(N-1)}{\rho^2 f^2(r_{12})} \frac{\int \Pi_{i<j} f^2(r_{ij}) d\mathbf{r}_3 \cdots d\mathbf{r}_N}{\int \Pi_{i<j} f^2(r_{ij}) d\mathbf{r}_1 \cdots d\mathbf{r}_N} \tag{1.2}$$

and its functional derivative (Lee and Broyles, 1966)

$$\frac{\delta G(r_{12})}{\delta f(r)} = \frac{1}{\rho^2 f^2(r_{12}) f(r)} [4\rho^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1 + \mathbf{r}) + \int \rho^{(4)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_3 + \mathbf{r}) d\mathbf{r}_3$$
$$- \Omega \rho^{(2)}(r_{12}) \rho^{(2)}(r)] \tag{1.3}$$

appear.

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To simplify the situation, one first tries to approximate $\delta G(r_{12})/\delta f(r)$ by expressions that do not involve the three- and four-particle distribution functions $\rho^{(3)}$ and $\rho^{(4)}$. With this in mind, the following approximate form has been derived and used:

$$\frac{\delta G(r_{12})}{\delta f(r)} = 4\rho f(r)G(r_{12})G(r)[f^2(|\mathbf{r}-\mathbf{r}_{12}|)G(|\mathbf{r}-\mathbf{r}_{12}|)-1] \tag{1.4}$$

In the deduction of the above expression, the generalized Kirkwood superposition approximation (Jackson and Feenberg, 1961) has been employed for the three-, four-, and five-particle distribution functions.

In this paper, we present another approximate expression for $\delta G(r_{12})/\delta f(r)$ which is a generalization of (1.4) and might lead to improved results.

2. *Derivation of the Expression for $\delta G/\delta f$*

For the derivation of the generalized expression for $\delta G/\delta f$, use is made of the relation, which is known from the theory of classical fluids, between the K-distribution function $g^{(K)}$

$$g^{(K)} = \rho^{(K)}/\rho^K \tag{2.1}$$

and the potential of average force $W^{(K)}(K)$:

$$g^{(K)} = \exp\left[-\frac{1}{kT}W^{(K)}(K)\right] \tag{2.2}$$

as well as of the expansion of the latter in powers of the density.

This expansion has been derived (under quite general assumptions) by Meeron (1957), who generalized previous results on the series expansion of distribution functions, given by Mayer and Montroll (1941). The structure of the expansion is the following:

$$W^{(K)}(K) = U_{(K)} - kT\sum_{N\geqslant 1}\frac{\rho^N}{N!}\int Q(K,N)d(N) \tag{2.3}$$

where $U(K)$ is the direct interaction potential and $Q(K, N)$ is a sum of products of functions $h(ij) = \exp(-U_{(ij)}/kT) - 1$, which is obtained by means of certain rules. The various terms are represented by diagrams.

Expansion (2.3) is easily applicable to boson systems described by the trial function (1.1). In this case $h(ij)$ is substituted by $f^2(r_{ij}) - 1$.

The formula, which results by taking into account expansion (2.3) in the expression for $g^{(K)}$ in terms of $W^{(K)}$, may be rewritten in a way similar to that followed by Abe (Abe, 1959; Feenberg, 1969; Morita, 1959) in the case of $g^{(3)}$. We may therefore write for $g^{(K)}$

$$g^{(K)} = \left[\prod_{i<j=1}^{K} g(r_{ij})\right]e^{A(K)} \tag{2.4}$$

where $e^{A(K)}$ is the abbreviated form for an exponential function, the exponent of which is a sum of integral terms. In the case of $K = 3$, the expression for $e^{A(K)}$, if only the "leading term" is kept, is

$$e^{A(3)} = \exp\left[\rho \int h(11')h(21')h(31')d\mathbf{r}_1'\right] \tag{2.5}$$

It may be seen from expression (2.4) that the generalized Kirkwood superposition approximation for $g^{(K)}$ consists in taking only the first term, 1, in the series expansion of the exponential.

In order to derive the generalized approximate expression for $\delta G(r_{12})/\delta f(r)$, we first consider the second term in (1.3), which by means of (2.1) and (2.4) (with $K = 4$) becomes

$$\int \rho^{(4)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_3 + \mathbf{r})d\mathbf{r}_3 = \rho^4 \int g(r_{12})g(r_{13})g(|\mathbf{r}_1 - (\mathbf{r}_3 + \mathbf{r})|) \times g(r_{23})g(|\mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r})|)g(r)e^{A(4)}d\mathbf{r}_3 \tag{2.6}$$

This may also be written as follows:

$$\int \rho^{(4)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_3 + \mathbf{r})d\mathbf{r}_3 = \rho^4 g(r_{12})g(r)\Big[\int g(r_{13})g(r_{23}) \times g(|\mathbf{r}_1 - (\mathbf{r}_3 + \mathbf{r})|)g(|\mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r})|)d\mathbf{r}_3 + \int g(r_{13})g(r_{23})g(|\mathbf{r}_1 - (\mathbf{r}_3 + \mathbf{r})|) \times g(|\mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r})|)(e^{A(4)} - 1)d\mathbf{r}_3\Big] \tag{2.7}$$

We subsequently write the pair distribution function g in the form

$$g(r_{ij}) = 1 + \tilde{g}(r_{ij}) \tag{2.8}$$

Since $g(r_{ij})$ goes to 1 for $r_{ij} \to \infty$, it follows that $\tilde{g}(r_{ij})$ goes to zero for large values of its argument.

Among the terms which result after the above substitution, we shall not keep those that have products of more than two $\tilde{g}$ functions or more than one $\tilde{g}$ and one $(e^{A(K)} - 1)$. The effect of the neglected terms (the number of which is small), should not be important for a dilute system, in view also of some partial cancellation of successive terms.

The omission of the above-mentioned terms leads to the expression

$$\int \rho^{(4)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_3 + \mathbf{r})d\mathbf{r}_3 \approx \rho^4 g(r_{12})g(r)\Big\{\int d\mathbf{r}_3 + 4\int \tilde{g}(r_{13})d\mathbf{r}_{13} + \int \tilde{g}(r_{13})\tilde{g}(r_{23})d\mathbf{r}_3 + \int \tilde{g}(r_{13})\tilde{g}(|\mathbf{r}_1 - (\mathbf{r}_3 + \mathbf{r})|)d\mathbf{r}_3 + \int \tilde{g}(r_{23})\tilde{g}(|\mathbf{r}_1 - (\mathbf{r}_3 + \mathbf{r})|)d\mathbf{r}_3 + \int \tilde{g}(r_{13})\tilde{g}(|\mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r})|)d\mathbf{r}_3 + \int \tilde{g}(r_{23})\tilde{g}(|\mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r})|)d\mathbf{r}_3 + \int \tilde{g}(|\mathbf{r}_1 - (\mathbf{r}_3 + \mathbf{r})|)\tilde{g}(|\mathbf{r}_2 - (\mathbf{r}_3 + \mathbf{r})|)d\mathbf{r}_3 + \int (e^{A(4)} - 1)d\mathbf{r}_3$$

$$+\int \tilde{g}(r_{13})\,(e^{A(4)}-1)d\mathbf{r}_3+\int \tilde{g}(r_{23})\,(e^{A(4)}-1)d\mathbf{r}_3+\int \tilde{g}(|\mathbf{r}_1-(\mathbf{r}_3+\mathbf{r})|)\,(e^{A(4)}-1)d\mathbf{r}_3$$

$$+\int \tilde{g}(|\mathbf{r}_2-(\mathbf{r}_3+\mathbf{r})|)\,(e^{A(4)}-1)d\mathbf{r}_3\Big\} \tag{2.9}$$

If we also take into account the normalization condition

$$\rho\int [1-g(r)]\,d\mathbf{r}=1 \tag{2.10}$$

and formula (2.4) with $K = 3$, we arrive, after substitution into (1.3), at the following approximate expression of the functional derivative:

$$\frac{\delta G(r_{12})}{\delta f(r)}\approx\frac{\rho g(r_{12})g(r)}{f^2(r_{12})f(r)}\{4\tilde{g}(|\mathbf{r}_1-(\mathbf{r}_2+\mathbf{r})|)+4g(|\mathbf{r}_1-(\mathbf{r}_2+\mathbf{r})|)\,(e^{A(3)}-1)$$

$$+\rho\Big[\int \tilde{g}(r_{13})\tilde{g}(r_{23})d\mathbf{r}_3+\int \tilde{g}(r_{13})\tilde{g}(|\mathbf{r}_1-(\mathbf{r}_3+\mathbf{r})|)d\mathbf{r}_3+\int \tilde{g}(r_{23})\tilde{g}(|\mathbf{r}_1-(\mathbf{r}_3+\mathbf{r})|)d\mathbf{r}_3$$

$$+\int \tilde{g}(r_{13})\tilde{g}(|\mathbf{r}_2-(\mathbf{r}_3+\mathbf{r})|)d\mathbf{r}_3+\int \tilde{g}(r_{23})\tilde{g}(|\mathbf{r}_2-(\mathbf{r}_3+\mathbf{r})|)d\mathbf{r}_3$$

$$+\int \tilde{g}(|\mathbf{r}_1-(\mathbf{r}_3+\mathbf{r})|)\tilde{g}(|\mathbf{r}_2-(\mathbf{r}_3+\mathbf{r})|)d\mathbf{r}_3$$

$$+\int (e^{A(4)}-1)d\mathbf{r}_3+\int \tilde{g}(r_{13})\,(e^{A(4)}-1)d\mathbf{r}_3+\int \tilde{g}(r_{23})\,(e^{A(4)}-1)d\mathbf{r}_3$$

$$+\int \tilde{g}(|\mathbf{r}_1-(\mathbf{r}_3+\mathbf{r})|)\,(e^{A(4)}-1)d\mathbf{r}_3+\int \tilde{g}(|\mathbf{r}_2-(\mathbf{r}_3+\mathbf{r})|)\,(e^{A(4)}-1)d\mathbf{r}_3\Big]\Big\} \tag{2.11}$$

This expression will be discussed in the next section.

3. *Discussion*

It is interesting to make a few comments on the result obtained in the previous section.

Expression (2.11) for the functional derivative has the first term in common with expression (1.4), which follows from the corresponding expression for $\delta g(r_{12})/\delta u(r)$ of Lee and Broyles (1966). There are, however, two kinds of additional terms. First, there are terms that originate from the use of expression (2.4) instead of the generalized Kirkwood superposition approximation. Second, there are terms that originate from the use of this approximation for the distribution functions appearing in the "exact" expression for $\delta G(r_{12})/\delta f(r)$. The latter terms are absent in expression (1.4), because in its derivation the generalized Kirkwood approximation is also used for the distribution function $g^{(5)}$, while in the present approach that is not the case.

It is clear that if the Kirkwood superposition approximation is used for $K < 5$, the terms with the exponential in expression (2.11) do not appear.

It should be noted that there are indications that the usual superposition approximation is quite good for He^4 (Sim and Woo, 1969; Raveché and Mountain, 1974). Calculations for the test of the superposition approximation for higher distribution functions do not exist as far as we know.

The approximate expression for the functional derivative $\delta G(r_{12})/\delta f(r)$ that was obtained here or the corresponding one for $\delta g(r_{12})/\delta u(r)$ (which follows immediately because $g = f^2 G$ and $f = e^{u/2}$) may be used in solving, for example, the Euler equation for the correlation function $f(r)$ of Grypeos (1974) or the Euler equation for $g(r)$ of Lee and Broyles (1966). The numerical solution of these equations is quite a complicated task. This is mainly due to the fact that they are integrodifferential, as many other equations of many-body problems are (Grypeos and Mavrommatis, 1974; Wethamer, 1973; Becker, 1969; Pokrant and Stevens, 1973).

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