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THE FUNCTIONAL DERIVATIVE OF THE RADIAL DISTRIBUTION FUNCTION FOR A MANY PARTICLE BOSON SUSTEM

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Abstract : *The functional derivative of the radial distribution function of a many partiele boson system, which was studied originally by J.C. Lee and A. A. Broyles, is considcred. A new approximate expression for this functional derivative is obtained which contains some additional terms. Commcnts are also made on the obtained results and on the corresponding Euler equation for the correlation function f.*

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[1,2]

$$\Psi_N = \prod_{i<j} f(r_{ij}) \tag{1}$$

leads to a complicated Euler equation for f(r)[3], in which the radial distribution function $G(r_{12}) = \dfrac{g(r_{12})}{f^2(r_{12})}$:

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

and its functional derivative[4]

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

appear.

To simplify the situation, one first tries to approximate $\frac{\delta G(r_{12})}{\delta f(r)}$ by expressions which 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

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

In the deduction of the above expression, the generalized *Kirkwood* superposition approximation[5] has been employed for the three, four and five particle distribution functions.

In this paper, we present another approximate expression for $\frac{\delta G(r_{12})}{\delta f(r)}$ which is a generalization of (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 $g^{(K)}$

$$g^{(K)} = \frac{\rho^{(K)}}{\rho^K} \quad (5)$$

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

$$g^{(K)} = \exp(- W^{(K)}_{(K)}/kT) \quad (6)$$

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*[6], who generalized previous results on the series expansion of distribution functions, given by *Mayer and Montroll*[7]. The structure of the expansion is the following:

$$W^{(K)}_{(K)} = U_{(K)} - kT \sum_{N \geq 1} \rho^N / N! \int Q(K,N) d(N) \tag{7}$$

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

The formula, which results by taking into account expansion (7) in the expression for $g^{(K)}$ in terms of $W^{(K)}$, may be re-written in a way similar to that followed by Abe[2,8,9] in the case of $g^{(3)}$. We may therefore write for $g^{(K)}$:

$$g^{(K)} = \left[\prod_{i<j=1}^{K} g(r_{ij}) \right] \cdot e^{A(K)} \tag{8}$$

where $e^{A(K)}$ is 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:

$$e^{A(3)} = e^{\rho \int h(11') h(21') h(31') d\vec{r}\,'_1} \tag{9}$$

It may be seen from expression (8) that the generalized Kirkwood superposition approximation for $g^{(K)}$ consists in taking only the first term: 1, in the series expansion for the exponential.

In order to derive the generalized expression for $\frac{\delta G(r_{12})}{\delta f(r)}$, we first consider the second term in (3), which by means of (5) and (8) (with K = 4) becomes

$$\int \rho^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_3+\vec{r}) d\vec{r}_3 = \rho^4 \int g(r_{12}) g(r_{13}) g(|\vec{r}_1 - (\vec{r}_3+\vec{r})|) \cdot$$
$$\cdot\, g(r_{23}) g(|\vec{r}_2 - (\vec{r}_3+\vec{r})|) g(r) e^{A(4)} d\vec{r}_3 \tag{10}$$

This may also be written as follows:

$$\int \rho^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_3+\vec{r}) d\vec{r}_3 = \rho^4 g(r_{12}) g(r) \quad \{ \int g(r_{13}) g(r_{23}) \cdot$$
$$g(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|) g(|\vec{r}_2 - (\vec{r}_3+\vec{r})|) d\vec{r}_3 + \int g(r_{13}) g(r_{23}) g(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|) \cdot$$
$$g(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|) (e^{A(4)} - 1) d\vec{r}_3 \} \tag{11}$$

We write subsequently the pair distribution function g in the form

$$g(r_{ij}) = 1 + \tilde{g}(r_{ij}) \tag{12}$$

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 which have products of more than two $\tilde{g}$ functions or two $\tilde{g}$ 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:

$$\begin{aligned} &\int \rho^{(4)}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_3' + \vec{r})d\vec{r}_3 \approx \rho^4 g(r_{12})g(r) \ \{ \int d\vec{r}_3 + 4\int \tilde{g}(r_{13})d\vec{r}_{13} + \\ &\int \tilde{g}(r_{13})\tilde{g}(r_{23})d\vec{r}_3 + \int \tilde{g}(r_{13})\tilde{g}(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int \tilde{g}(r_{23})\tilde{g}(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|) \\ &d\vec{r}_3 + \int \tilde{g}(r_{13})\tilde{g}(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int \tilde{g}(r_{23})\tilde{g}(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \\ &\int \tilde{g}(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|)\tilde{g}(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int (e^{A(4)} - 1)d\vec{r}_3 + \int \tilde{g}(r_{13}) \\ &(e^{A(4)} - 1)d\vec{r}_3 + \int \tilde{g}(r_{23})\,(e^{A(4)} - 1)d\vec{r}_3 + \int \tilde{g}(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|)\,(e^{A(4)} - 1) \\ &d\vec{r}_3 + \int \tilde{g}(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|)\,(e^{A(4)} - 1)d\vec{r}_3\} \end{aligned} \tag{13}$$

If we take also into account the normalization condition

$$\rho \int (1 - g(r))d\vec{r} = 1 \tag{14}$$

and formula (8) with K = 3, we arrive, after substitution into (1) at the following approximate expression of the functional derivative

$$\begin{aligned} &\frac{\delta G(r_{12})}{\delta f(r)} \approx \frac{\rho g(r_{12})g(r)}{f^2(r_{12})f(r)}\{4\tilde{g}(|\vec{r}_1 - (\vec{r}_2 + \vec{r})|) + 4g(|\vec{r}_1 - (\vec{r}_2 + \vec{r})|) \\ &(e^{A(3)} - 1) + \rho[\int \tilde{g}(r_{13})\tilde{g}(r_{23})d\vec{r}_3 + \int \tilde{g}(r_{13})\tilde{g}(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int \tilde{g}(r_{23})\tilde{g} \\ &(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int \tilde{g}(r_{13})\tilde{g}(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int \tilde{g}(r_{23})\tilde{g}(|\vec{r}_2 - \\ &(\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int \tilde{g}(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|)\tilde{g}(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|)d\vec{r}_3 + \int (e^{A(4)} - 1) \\ &d\vec{r}_3 + \int \tilde{g}(r_{13})\,(e^{A(4)} - 1)d\vec{r}_3 + \int \tilde{g}(r_{23})\,(e^{A(4)} - 1)d\vec{r}_3 + \int \tilde{g}(|\vec{r}_1 - (\vec{r}_3 + \vec{r})|) \\ &(e^{A(4)} - 1)d\vec{r}_3 + \int \tilde{g}(|\vec{r}_2 - (\vec{r}_3 + \vec{r})|)\,(e^{A(4)} - 1)d\vec{r}_3]\} \end{aligned} \tag{15}$$

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.

The expression (15) for the functional derivative has the first term in common with the expression (4), which follows from the corresponding expression for $\frac{\delta g(r_{12})}{\delta u(r)}$ of J.C. Lee and A.A. Broyles[4]. There are, however two sorts of additional terms. First there are terms, which originate from the use of expression (8) instead of the generalized Kirkwood superposition approximation. Second, there are terms which originate from the use of this approximation for the distribution functions appearing in the «exact» expression for $\frac{\delta G(r_{12})}{\delta f(r)}$. The latter terms are absent in expression (4), because in its derivation the generalized Kirkwood superposition approximation is also used for the distrihution function $g^{(5)}$, while in the present derivation this 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 (15) do not appear.

It should be noted that there are indications that the usual superposition approximation is quite good[10,11] for liquid He^4. 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 $\frac{\delta G(r_{12})}{\delta f(r)}$ which was obtained here (or the corresponding one for $\frac{\delta g(r_{12})}{\delta u(r)}$, which follows immediatelly because $g = f^2 G$ and $f = e^{u/2}$) may be used in solving the Euler equation for g of ref. 4) or the Euler equation for the correlation function f(r):

$$G(r)\frac{d^2f(r)}{dr^2}+(\frac{2}{r}G\,(r)+\frac{dG(r)}{dr})\frac{df(r)}{dr}+[-\frac{m}{(h/2\pi)^2}(V(r)+\lambda_2)G(r)+$$

$$+\frac{1}{2r}\frac{dG(r)}{dr}+\frac{1}{4}\frac{d^2G(r)]}{dr^2}]f(r)-\frac{1}{4}\int d\vec{r}_{12}\,[(\frac{df(r_{12})}{dr_{12}})^2-f(r_{12})$$

$$\left(\frac{d^2f(r_{12})}{dr^2_{12}} + \frac{2}{r_{12}}\frac{df(r_{12})}{dr_{12}}\right) + \frac{2m}{(h/2\pi)^2} V(r_{12})f^2(r_{12}) + \frac{2m}{(h/2\pi)^2}\lambda_2 \left(f(r_{12}) - 1\right)^2]$$

$$\frac{\delta G(r_{12})}{\delta f(r)} + \frac{m}{(h/2\pi)^2}\lambda_2 G(r) = 0 \qquad (16)$$

The above equation is essentially the same with the equ. 18) of 3). The only difference is that the Lagrange multiplier λ_1, is zero and. appears the multiplier λ_2, due to the «healing condition»[12]. The choice $\lambda_1 = 0$ is necessary because the condition (21) of ref. 3) can not be satisfied, due to the explicit use of the normalization condition in the present case.

The numerical solution of equ. (16) is a rather complicated task This is mainly due to the fact that it is integrodifferential as many other equations of many-body problems are[13,14,15].

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ΠΕΡΙΛΗΨΙΣ

Η ΣΥΝΑΡΤΗΣΙΑΚΗ ΠΑΡΑΓΩΓΟΣ ΤΗΣ ΑΚΤΙΝΙΚΗΣ ΣΥΝΑΡΤΗΣΕΩΣ ΚΑΤΑΝΟΜΗΣ ΣΥΣΤΗΜΑΤΟΣ ΠΟΛΛΩΝ ΜΠΟΖΟΝΙΩΝ

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Εἰς τὴν ἐργασίαν αὐτὴν θεωροῦμεν τὴν συναρτησιακὴν παράγωγον τῆς ἀκτινικῆς συναρτήσεως κατανομῆς συστήματος πολλῶν μποζονίων, ἡ ὁποία ἐμελετήθη ἀρχικῶς ὑπὸ τῶν J.C. Lee καὶ A.A. Broyles. Δίδεται μία νέα προσεγγιστικὴ ἔκφρασις τῆς συναρτησιακῆς ταύτης παραγώγου, ἡ ὁποία περιέχει ὡρισμένους ἐπιπροσθέτους ὅρους. Διατυποῦνται ἐπίσης σχόλια ἐπὶ τοῦ ληφθέντος ἀποτελέσματος καὶ ἐπὶ τῆς ἀντιστοίχου ἐξισώσεως Euler διὰ τὴν συνάρτησιν ἀλληλοσυσχετίσεως f.