Radial Distribution Function of Dense Quantum Fluids II

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Quantum effects for the two-particle distribution in the dense hard sphere system are considered tentatively by the approximation scheme proposed in the previous paper. Even in the crude approximation the effect of the quantum statistics appear clearly.

1. Introduction

In the previous paper[1], we proposed a formalism for the theoretical calculation of the radial distribution function of the quantum system, basing on the cluster expansion and its resummation technique. The two-particle distribution function, or more precisely, the two-particle reduced density matrix ρ_2 of the system can be cast in a form*,

$$\rho_2 = e^{-\beta H_2} e^{\beta H_2^{(0)}} \exp\left(\sum_{\lambda=1} \beta_\lambda^{(2)}\right) \rho_2^{(0)} \qquad (1.1)$$

Here $\rho_2^{(0)}$ is the two-particle reduced density matrix of the reference ideal system in which the interaction between particles is cut off. H_2 is the true Hamiltonian of the two particle system and $H_2^{(0)}$ is that of same system in which the inter-particle interaction is cut off. $\beta_\lambda^{(2)}$ are the cluster operators which appear in our formalsm[1]. It is to be remarked here that the effects of the quantum mechanics are taken into consideration through the non commutability of these operators (I_2, $H_2^{(0)}$, $\beta_\lambda^{(2)}$, $\rho_2^{(0)}$). The effect of the quantum statistics, on the other hand, comes into our formula through the reduced density matrix $\rho_2^{(0)}$··

Starting from our general formula (1. 1) , we can contrive various approximation scheme. If we neglect all the quantum effects, we have the well known formula for the classical fluids.[2]

$$\rho_2(1,2) = \exp(-\beta\phi(1,2) + S(1,2) + B(1,2))\rho^2 \qquad (1.2)^{**}$$

where $\phi(1,2)$ is the interaction potential between the particle 1 and the particle 2. $S(1, 2)$ and $B(1,2)$ give the effects of the correlation with the other particles in the system. ρ is the particle number density of the system. Our general formula (1. 1) may be regarded as the straight-forward extention of this classical formula to the quantal case. By the inspection of the process of the extension to the quantum system which has been introduced by the present auther[4], we can see that the effect of the quantum statistics comes into our form-alism through the separate route from that of the dynamical effects, that is, it comes into the formula through the reduced density matrix of the ideal quantum system which we introduce and call it the reference ideal system for this purpose.

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* This is to be interpreted as the relation between operatos.

** We use the notations 1 and 2 inplace of the particle coordinates, r_1, r_2. Similar abbreviations will be used throughout this paper.

Fig. 1 $g_2^{P.-Y.6)}$ $\rho a^3=0.573$

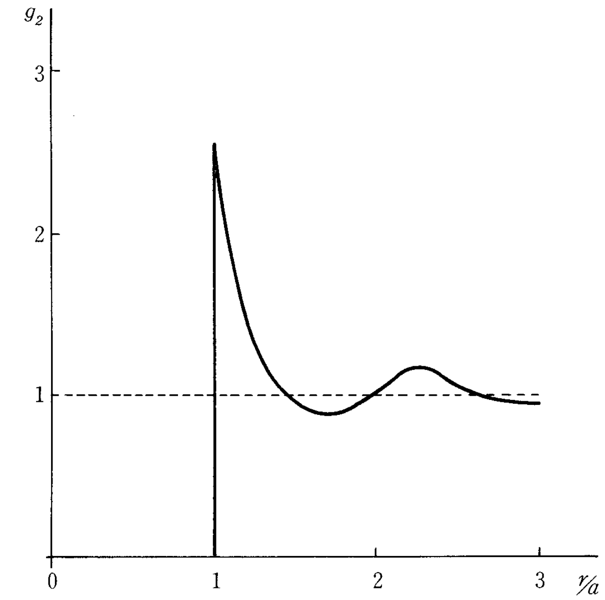
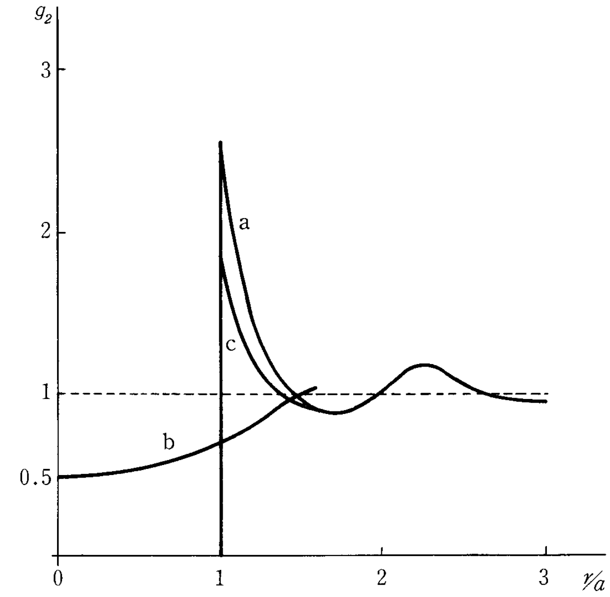


Fig. 2 a : $g_2^{P.-Y.}$ **b** : $g_2^{(0)}$ (Fermi) **c** : g_2



As the second step we want to test the following approximation scheme

$$\rho_2(1,2)=g_{2,c}(r)g_2^{(0)}(r), \quad r=|\boldsymbol{r}_1-\boldsymbol{r}_2| \qquad (1.3)$$

$$g_{2,c}(r)=\exp(-\beta\phi(1,2)+S(1,2)+B(1,2))$$

$$g_2^{(0)}(r)=\rho_2^{(0)}(1,2)/\rho^2 \qquad (1.4)$$

where $g_2^{(0)}$ is the radial distribution function of the reference ideal system.

2. Quantum hard sphere system

The approximation scheme (1. 3) proposed above, may be said to be somewhat arbitrary. The effects of the quantum dynamics and the cross effects of quantum dynamics and the quantum statistics are all neglected. However, in the light of the modified cluster method which has been introduced by the auther[4], this form may be regarded as the natural first step of the introduction of the effect of the quantum statistics.

One of the important points to be mentioned here is the fact that this formalism can be applied to the dense systems. For instanse, when we consider the hard sphere system, we can take as $g_{2,c}$ the formula of the Percus -Yevick approximation which has been introduced by these authers in the treatment of the classical fluids and now its relation to the cluster expansion method is shown in detail[2]. Fig.1 gives $g_2^{P.-Y.}$, that is, the radial distribution of the classical hard sphere fluids calculated by this P.-Y. approximation. Fig.2 is the results of our approximation (1. 3) .

3. Discussions

The results given here are based on the very crude approximations. We can see, however, the effects of the quantum statistics very clearly, especially in the case of the Fermi statistics.

Further investigations based on the detailed numerical calculations are now in progress together with the improvements of the approximation scheme.

To extend the general formulation proposed in the previous paper[1] to the theoretical calculation of the other physical quantities will be quite interesting. We desire to take up these problem in the near future.

References

1) H. Ichimura ; The Academic Reports, Fac. Eng. Tokyo Institute of polytechnics. Vol. 12, No. 1 (1989)

2) B. J. Berne ; Modern Theoretical Chemistry Vol5. Plenum Press New York (1976)

3) H, Ichimura ; Prog. Theor. Phys. 37 ; 484 (1967)

4) H. Ichimura ; Prog. Theor. Phys. 31 ; 538 (1964)

5) J. K. Percus & G. J. Yevick ; Phys. Rev. 110 ; 1 (1958)

6) L. Verlet & D. Levesque ; Physica 36 ; 254 (1967)