

Analytic form for the one-component plasma structure factor

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By giving the direct correlation function a form consistent with features of the one-component plasma (OCP), a simple analytic expression for the static structure factor $S(k)$ of the OCP is derived. This expression yields results, for dense plasma, that compare well with the numerical solutions of the modified hypernetted-chain equation as well as with computer-simulation data.

In liquid alkali metals, where the electron-ion interaction is known to be extremely weak, the Coulomb interaction between the positive ions is a dominant feature in determining the static structure. Therefore, to describe the structure factor of such charged particles, the model of the one-component plasma (OCP) has received special attention.¹ The OCP reference system is an idealized system of pointlike charges moving in a neutralizing uniform background of opposite charges. An equilibrium state of the OCP system with the number density ρ and the temperature T may be characterized by a dimensionless plasma parameter $\Gamma = (Ze)^2 / (ak_B T)$, where Ze is the charge of an ion and $a = [3 / (4\pi\rho)]^{1/3}$ represents the ion-sphere radius.

Determination of the structure factor and the thermodynamics for the OCP system has been largely accomplished by Monte Carlo (MC) calculations.^{2,3} Nevertheless, it is of interest that there is an approximate theory which can be carried out analytically for such a system. Analytic expressions for the excess internal energy as well as for specific heat and for isothermal compressibility have already been found by fitting MC numerical data.^{3,4} It has also been possible to describe the OCP structure factor on the basis of the numerical solutions of the hypernetted-chain (HNC) and modified HNC (MHNC) integral equations.⁵⁻⁷

In the spirit of studying model systems, we have derived a simple analytic expression for the OCP static structure factor, consistent with the form of the direct correlation function $c(r)$ of the OCP system. For this purpose, we assume that $c(r)$ may be adequately described by

$$c(x) = \begin{cases} -\Gamma(C - Dx^2), & 0 < x < a_1, \\ -\Gamma(A - Bx), & a_1 < x < a_2, \\ -\Gamma/x, & a_2 < x, \end{cases} \quad (1)$$

for a suitable choice of the constants. The direct correlation function goes to zero as $x (=r/a)$ approaches to infinity, and it behaves reasonably well for small x ,⁸ but the salient feature of this formulation lies in the fact that $c(x)$ is written as a linear relation, at intermediate range. This characteristic has already been observed in the MC data.⁹

In order to reduce the number of constants we have adjusted them until the logarithmic derivatives of $c(x)$ match at a_1 and a_2 . Thus, we can express four of them by

the following relations

$$\begin{aligned} A &= 2/a_2, \quad B = 1/a_2^2, \\ C &= (4a_2 - a_1)/2a_2^2, \quad D = 1/2a_1a_2. \end{aligned} \quad (2)$$

By using the Fourier transform of Eq. (1), we obtain the static structure factor under the simple analytical form

$$S(k) = \left[1 - \frac{3\Gamma}{(k^4 a^4 a_2^2)} [\cos(kaa_1) + 2\cos(kaa_2) - 3\sin(kaa_1)/(kaa_1)] \right]^{-1}, \quad (3)$$

and we can observe that $S(k)$ satisfies the perfect screening condition, which is a typical OCP feature, i.e.,

$$S(k) = (ka)^2 / (3\Gamma) \text{ as } k \rightarrow 0. \quad (4)$$

Relation (3) was fitted to the MHNC data of the OCP structure factor, tabulated by Rogers, Young, Dewitt, and Ross⁷ because MHNC is the most accurate description of the OCP static structure properties presently available, when compared with MC results.

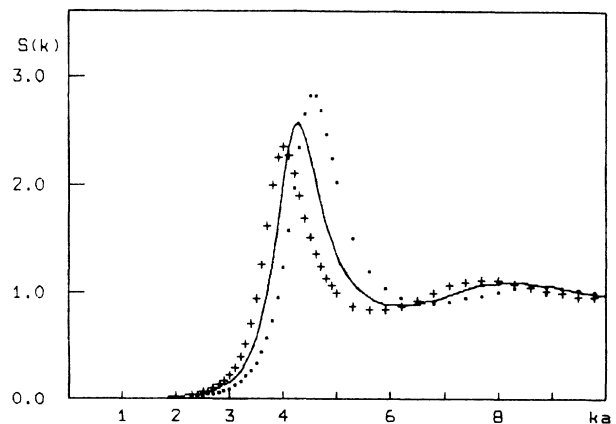


FIG. 1. Effect of the parameter α_2 on the structure factor. [$\alpha_2 = 1.35$ (●); 1.45 (—); 1.55 (+) and $\alpha_1 = 0.7828$, for $\Gamma = 120$.]

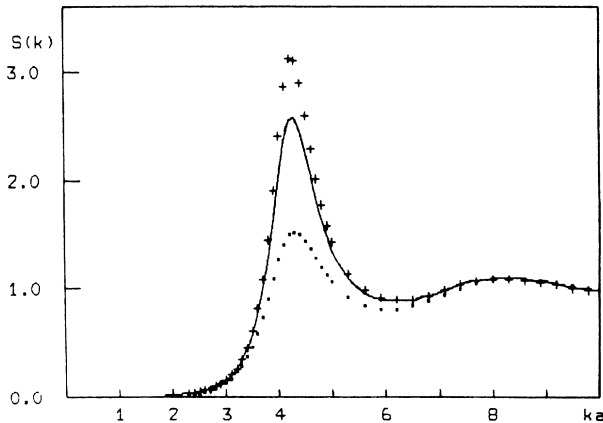


FIG. 2. Effect of the parameter a_1 on the structure factor. [$a_1=0.6528$ (●); 0.7828 (—); 0.8128 (+) and $a_2=1.45$, for $\Gamma=120$.]

Results for the behavior of the structure factor relative to variations of a_1 and a_2 are presented in Figs. 1, 2, and 3. Examining Figs. 1 and 2 shows that the parameter a_1 is mainly related to the height of the first peak of $S(k)$, whereas a_2 is related to the location of the successive peaks. It follows from the great stability of the main peak position of $S(k)$ that the best value of a_2 is 1.45. As far as the parameter a_1 is concerned, it may be seen that the magnitude of the main peak increases as a_1 increases. In order to obtain a_1 , expression (3) was adjusted to the first peak structure factor tabulated by Rogers *et al.*,⁷ in the range of Γ between 100 and 160 where the liquid metal comes into existence. The parameter was found to be

$$a_1 = -0.1455 \times 10^{-2} \Gamma + 0.9574. \quad (5)$$

Figure 2 shows the role played by the purely parabolic portion of the direct correlation function since the hyperbolic branch as well as the linear part are not modified, when a_2 is a constant. Thus, it is the variation of $c(r)$ at very small distances, correlative to the variation of a_1 , which induces a change of the first peak height of $S(k)$. We can also see the effect of the short range of $c(r)$ on the structure factor, in Fig. 3, where both a_1 and a_2 are brought to vary, while $c(0) (= -\Gamma C)$ is kept constant to preserve Eq. (2). It clearly appears that, when a_1 and a_2 are drawn closer together, the first peak of $S(k)$ increases and moves towards the large q . If a_1 is equal to a_2 , we ob-

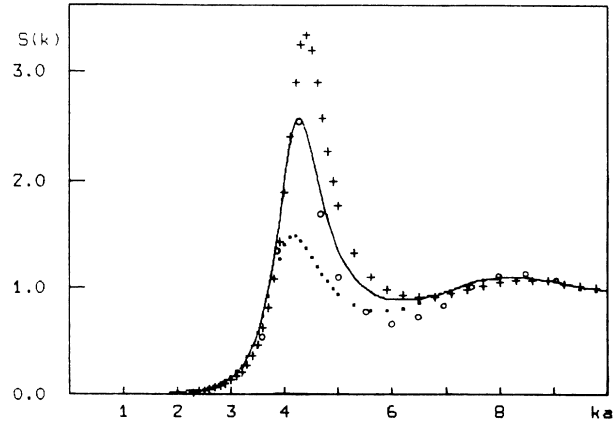


FIG. 3. Influence of the linear part of $c(r)$ on the structure factor. [a_1 and a_2 are, respectively, 0.6528 and 1.50 (●); 0.7828 and 1.45 (—); 0.8128 and 1.40 (+), for $\Gamma=120$. ○ represents the results of Ref. 7.]

serve a divergence of the main peak, for the range under consideration, which is not the signature of a phase transition but which is only related to the unphysical description of the short-range correlation.

On the other hand, a good value of $c(0)$ can be obtained from the exact relation¹⁰

$$c(0) = 2\beta \frac{U}{N} - \beta \left[\frac{\partial p}{\partial \rho} \right]_T - \frac{\rho}{2} \int d^3r g(r) [c(r) + \beta u(r)], \quad (6)$$

where we recognize the standard relations for internal energy, compressibility, pair correlation function, effective pair potential and $\beta=1/(k_B T)$. From this relation, one finds that $c(0) = -122$, with HNC equation, for $\Gamma=100$ while our model gives $c(0) = -118.5$.

The model predictions provide a knowledge of the crudest features of the structure which could be useful in the refined theories. Besides, as expected, the model reproduces the first peak of the Rogers *et al.*⁷ structure factor with an optimum agreement and, in the low- q region, the corresponding values of $S(k)$ are very close to each other. Even if beyond the main peak of $S(k)$ the difference still remains significant, our expression for $S(k)$ is convenient to perform calculations, on liquid metals, which require the integration of $S(k)$.

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