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One-component plasma structure factor in tabular form

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The one-component plasma structure factor $S(q,\Gamma)$ has been computed with a hypernetted-chain equation modified by the hard-sphere bridge function. The structure factor is tabulated for reduced wave number $0.1 \le q \le 25.0$ and Coulomb coupling parameter $0.1 \le \Gamma \le 180$. The hypernetted-chain results are in excellent agreement with Monte Carlo calculations. This table should be useful for calculations on dense plasmas and liquid metals.

I. INTRODUCTION

A real plasma is a two-component system of charges of opposite sign, i.e., electrons and ions, with a Hamiltonian of the form

$$\begin{aligned} H &= K_i + K_e + U_{ii} + U_{ei} + U_{ee} \\ &= \sum_{i=1}^{N_i} \frac{P_i^2}{2M_i} + \sum_{\alpha=1}^{N_e} \frac{P_\alpha^2}{2m_e} + \sum_{\substack{i<j \\ i,j=1}}^{N_i} \frac{(Ze)^2}{r_{ij}} \\ &\quad - \sum_{i=1}^{N_i} \sum_{\alpha=1}^{N_e} \frac{Ze^2}{r_{i\alpha}} + \sum_{\substack{\alpha<\beta \\ \alpha,\beta=1}}^{N_e} \frac{e^2}{r_{\alpha\beta}} \end{aligned} \tag{1}$$

for ions of mass M_i and charge Ze. Charge neutrality requires $N_e = ZN_i$. Obviously this two-component system requires a quantum-mechanical treatment to prevent a collapse that would occur in classical mechanics. At high density, Fermi statistics for the electrons cause a degeneracy and an effective decoupling of the electrons from the ions. At sufficiently high degeneracy the internal energy of the system can be written as

$$\begin{aligned} E &= \langle H \rangle = \langle K_i \rangle + \langle K_e \rangle + \langle U_{ee} \rangle + \langle U_{ii} + U_{ei} \rangle \\ &= \tfrac{3}{2} N_i kT + N_e(\tfrac{3}{5}\epsilon_F + \epsilon_{\text{ex}} + \epsilon_{\text{corr}}) + U \ , \end{aligned} \tag{2}$$

where the angular brackets indicate an ensemble average, and U is the internal energy of the ion-ion Coulomb interaction in the present of the electron fluid. The electron term above includes the kinetic energy $3\epsilon_F/5$, exchange energy ϵ_{ex}, and correlation energy ϵ_{corr}. In the limit of very high density the Fermi energy is sufficiently large that the electrons approach a uniform background distribution of charge. This limit is the one-component classical plasma (or OCP). The Coulomb energy becomes

$$\begin{aligned} U &= \left\langle \left[\sum_{\substack{i<j \\ i,j=1}}^{N_i} \frac{(Ze)^2}{r_{ij}} + \cdots \right] \right\rangle \\ &= kT \left\langle \left[\sum_{\substack{i<j \\ i,j=1}}^{N_i} \frac{\Gamma}{|\vec{x}_i - \vec{x}_j|} + \cdots \right] \right\rangle \\ &= N_i kT f(\Gamma) \ , \end{aligned} \tag{3}$$

where the ellipsis stands for unspecified background terms and $\Gamma = (Ze)^2/kTa$, $x = r/a$, and $a = (4\pi N_i/3V)^{-1/3}$. Because the OCP represents the high-density limit of real plasma, it has become very useful as a reference system for thermodynamic perturbation theories, and the OCP thermodynamic properties and distribution functions have been computed to high accuracy.[1,2]

II. CALCULATIONS AND RESULTS

Recent Monte Carlo (MC) simulations have given very accurate results, i.e., five figures, for the OCP internal energy as a function of Γ, and this can be expressed as an analytic function[3] of Γ. Monte Carlo simulations also give the OCP pair distribution function $g(x,\Gamma)$ directly out to a distance of $x = N^{1/3}/2$, where N is the number of particles used in the simulation. The OCP structure factor is defined as

$$S(k,\Gamma) = 1 + \rho \int d^3r\, e^{i\vec{k}\cdot\vec{r}} [g(r,\Gamma) - 1] \tag{4}$$

or, in reduced units,

$$S(q,\Gamma) = 1 + 3 \int_0^\infty x^2 dx \frac{\sin(qx)}{qx} h(x,\Gamma) \ , \tag{5}$$

where $q = ka$ and $h(x,\Gamma) = g(x,\Gamma) - 1$. The recent MC results do not give $S(q,\Gamma)$ directly. It can be obtained in practice from the MC $g(x,\Gamma)$ data where these data are extended to $x = \infty$ with a hypernetted-chain tail.[4]

The formal theory of liquids is now sufficiently well developed that the thermodynamic properties of any liquid can be calculated accurately if the interparticle potential $\varphi(r)$ is known. A widely used approximation is the fluid variational theory. In this theory the configurational Helmholtz free energy may be approximated using the Gibbs-Bogolyubov inequality[5,6]

$$A \le A_0 + \langle U - U_0 \rangle_0 \ . \tag{6}$$

This states that the free energy of the actual system (A) is bounded above by the free energy of the reference (A_0) plus the difference in the potential energy between the actual system and the reference system averaged over all reference configurations. Calculations have been made using hard spheres[7] and the OCP[4,8] as reference systems. By employing hard spheres, molecules are approximated as "billiard balls" with an infinite repulsion for separations less than or equal to the hard-sphere diameter d, but with an interaction $\varphi(r)$ for $r > d$. The value of d is chosen as the one that minimizes A. A convenient feature of the hard-sphere system is that both the reference free energy and pair distribution function (or structure factor) can be expressed analytically. Thermodynamic properties are computed numerically by taking the appropriate derivatives of the free energy. In general, the use of hard spheres introduces repulsions that tend to be too large. This can be overcome by using inverse power or "soft-sphere" reference fluids. The "softest" of these is the OCP. It has been found useful for calculations on dense plasmas and liquid metals where the principal forces are Coulombic.[4,8,9]

It has not yet been possible to describe the OCP structure factors and pair distribution functions in an analytic form that is as convenient for calculations as for hard spheres. In an earlier paper we demonstrated the usefulness of the OCP as a reference system for liquid-metal calculations and made comparisons with MC simulations.[8] For these calculations we used a tabular form of Hansen's OCP MC $S(q,\Gamma)$ results.[4] Tosi and co-workers[10] have attempted to fit Hansen's data but their analytic expressions are less accurate and are computationally much slower than our table look-up scheme.

Recently, we found that our tables occasionally produced irregularities in the pressure and energy and more frequently in their derivatives. Calculations of $(\partial P/\partial T)_s$ showed an unrealistic scatter. We subsequently determined that these were the result of statistical fluctuations in the MC $S(q,\Gamma)$ data. It was for this reason that we decided to recompute the $S(q,\Gamma)$ table using a new modification of the hypernetted-chain equation.

The pair distribution function for a liquid is given by

$$g(r)=\exp[-\beta\varphi(r)+h(r)-c(r)+B(r)] , \tag{7}$$

where $h(r)$ is the total correlation function, $c(r)$ is the direct correlation function, and $B(r)$ is the bridge function. The total and direct correlation functions are related through the Ornstein-Zernicke equation according to

$$\tilde{h}(k)=\tilde{c}(k)+\rho\tilde{h}(k)\tilde{c}(k) , \tag{8}$$

where the tilde indicates the Fourier transform. Due to the complexity of calculating $B(r)$ it is frequently set equal to zero and an iterative solution to Eqs. (7) and (8) is carried out. This is referred to as the hypernetted-chain (HNC) approximation.

Rosenfeld and Ashcroft[11] have produced a simple method for including $B(r)$ in an augmented HNC equation. They argue that the $B(r)$ for monotonic repulsive potentials form a universal set and propose using the hard-sphere bridge functions to represent $B(r)$. They further note that the Percus-Yevick hard-sphere bridge function has the same analytic form as the true hard-sphere bridge function and suggest that it be used in actual calculations. $B(r,\eta)$ is a rather complex algebraic function of r and the hard-sphere packing fraction η, and is described in Ref. 11. In order to select the $B(r,\eta)$ that should be used in a particular situation, the Rosenfeld-Ashcroft procedure requires the compressibility obtained by differentiating the pressure equation to match the corresponding result from the compressibility equation. This is accomplished by iterating on η until this condition is satisfied. We used 2048 points and a grid size $\Delta x=0.025$ in each solution of the HNC equation. Once the hard-sphere diameter was located within an uncertainty $\pm\Delta x/4$, the accepted value η_Γ was obtained by quadratic interpolation. The tabulated values of $S(q,\Gamma)$ were then obtained from a similar interpolation to obtain $S(q,\Gamma)$ at η_Γ. Lado[12] has recently proposed an alternative procedure in which the free energy is minimized. In the present work we have followed the Rosenfeld-Ashcroft procedure. Our HNC computer code produces both $g(x,\Gamma)$ and $S(q,\Gamma)$. Table I compares the results of the current work with the most accurate Monte Carlo internal energy calculations.[3] The agreement is very good. Figure 1 is a comparison of $g(x,170)$ obtained in the present calculation with the MC result. Very close agreement is observed with small differences occurring at the peaks and valleys.

The tabulated values of $S(q,\Gamma)$ for $0.1 \le g \le 25.0$ and $0.1 \le \Gamma \le 180$ are given elsewhere.[13] Note that $S(0,\Gamma)=0$. For $\Gamma \le 1$, we used the unmodified HNC equation because it is very accurate in this range. We terminated the table at $\Gamma=180$ because of the large amount of computer time required [5 min of Cray-1 CPU (central processing unit) time for $S(q,180)$] and because the OCP freezes to a solid phase[3] at $\Gamma \approx 178$.

For liquid-metal calculations we compute the right-hand side of Eq. (6) using the tabular $S(q,\Gamma)$. The exact expressions are to be found in Ref. 8. An interpolation

TABLE I. Comparison of reduced internal energies from unmodified HNC, Monte Carlo calculations, and the modified HNC equation. Values of the hard-sphere packing fraction used in the bridge functions are also given.

		U/NkT		
Γ	HNC	MC	HNC bridge	η
2	-1.315	-1.320 ± 0.000	-1.323	0.095
5	-3.732	-3.757 ± 0.000	-3.762	0.158
10	-7.935	-7.998 ± 0.001	-8.004	0.215
20	-16.538	-16.673 ± 0.001	-16.677	0.278
50	-42.788	-43.102 ± 0.001	-43.103	0.364
100	-86.974	-87.522 ± 0.001	-87.525	0.435
150	-131.364	-132.110 ± 0.002	-132.106	0.466
170	-149.152	-149.970 ± 0.001	-149.975	0.480

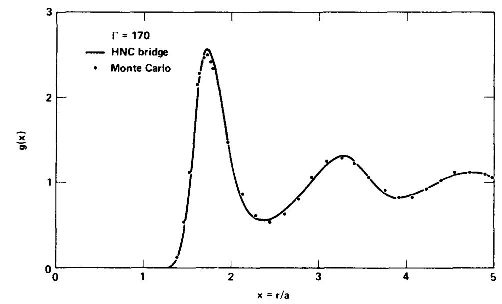

FIG. 1. Comparison of Monte Carlo and modified HNC OCP $g(x,\Gamma)$ for $\Gamma=170$.

scheme is used to find the Γ corresponding to the minimum value of the expression. This value is then taken to be the configurational Helmholtz free energy. With the new tabular $S(q,\Gamma)$, the problem of smoothness in the computed thermodynamic functions has been solved, and the results are in excellent agreement with Monte Carlo calculations[8] on ions interacting through pseudopotentials.

We have found in comparing calculations on liquid alkali metals[9] with experiments that the Γ values span a range almost as large as the table itself. Thus the liquid near the melting curve reaches $\Gamma=180$ at moderate pressures, and on the shock Hugoniot near 1 Mbar pressure; the temperature is so high that $\Gamma\approx 1$.

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[13] See AIP document No. PAPS-PLRAA-28-2990-15 for 15 pages of tabulated values of $S(q,\Gamma)$ for $0.1\leq q\leq 25.0$ and $0.1\leq\Gamma\leq 180$. Order by PAPS number and journal reference from American Institute of Physics, Phyics Auxiliary Publication Service, 335 East 45th Street, New York, N.Y. 10017. The price is \$1.50 for each microfiche (98 pages) or \$5.00 for photocopies of up to 30 pages, and \$0.15 for each additional page over 30 pages. Airmail additional. Make checks payable to the American Institute of Physics.