

Statics and Thermodynamics of Strongly Coupled Multicomponent Plasmas

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A description of strongly coupled plasmas, in which the direct correlation functions, $c_{ij}(\mathbf{r})$, are obtained by simple scaling from a universal function, is derived and found to be in full agreement with available computer simulation data, which it thus extends for arbitrary mixtures. It is thermodynamically consistent with the "ion-sphere" charge-averaging prediction for the enhancement factors for nuclear reaction rates, the results for which confirm the universality of the bridge functions for mixtures.

This Letter is devoted to an analysis of a basic and extensively studied model of charged fluids, namely the classical one-component plasma (OCP) and its extension to mixtures.¹ I show that a description of strongly coupled plasmas, in which the direct correlation functions (DCF's), $c_{ij}(\mathbf{r})$, are obtained by simple scaling from a universal function, is highly accurate and thermodynamically consistent. The predictions of the model agree to about 1% with the available computer simulation data for one- and two-component plasmas in two and three dimensions. The scaling enables us to extend OCP data to arbitrary mixtures, while its specific form is very important for calculating enhancement factors for nuclear reaction rates.

Consider a q -component system of point ions of charges $Z_i e$, concentrations X_i , total number density $\rho = N/V$, at a given temperature $T = (\beta k_B)^{-1}$, imbedded in a uniform neutralizing background, and interacting via the Coulomb potential $\beta u_{ij}(\mathbf{r}) = Z_i Z_j \Gamma / r$. $\Gamma = \beta e^2 / a$ is the coupling parameter, and distances are measured in units of the D -dimensional Wigner-Seitz ("ion-sphere") radius, $a \sim \rho^{-1/D}$. We focus our attention on strongly coupled plasmas, characterized by negative compressibility, $\beta(\partial P / \partial \rho)_{T, \mathbf{x}} \lesssim 0$, corresponding to, say, $\Gamma \gtrsim 1$ for the OCP.

Computer simulation data revealed^{2,3} that the DCF's decay rather rapidly to their rigorous large-distance behavior, $c_{ij}(\mathbf{r}) = -Z_i Z_j \Gamma / r$ for $r \gtrsim 1$, while the pair functions are hard-core-like, $g_{ij}(\mathbf{r}) = 0$ for $r \lesssim 1$. Incorporating these observations in the Ornstein-Zernicke relations, by ignoring the quantity

$$\rho \sum_{ij} X_i X_j \int g_{ij}(\mathbf{r}) [c_{ij}(\mathbf{r}) + \beta u_{ij}(\mathbf{r})] d\mathbf{r},$$

we arrive^{3,4} at the following key approximation:

$$\beta U / N = \frac{1}{2} [\beta(\partial P / \partial \rho)_{T, \mathbf{x}} + \sum_i X_i c_{ii}(0)]. \quad (1)$$

Equation (1) is exact in the mean-spherical approximation (MSA), and agrees to about 1% with the Monte Carlo (MC) and hypernetted-chain

(HNC) results^{3,5} for the OCP. I have studied mixtures⁶ with quite disparate interparticle potentials by means of the modified HNC approach³ and my results extend the concept of "universality of the bridge functions"^{3,7} to mixtures. In particular, I obtained thermodynamically consistent results for the DCF's that reproduce the available computer data for both equation of state and $g_{ij}(\mathbf{r})$. With the help of these results I have confirmed the validity of Eq. (1) for plasma mixtures, and obtained direct predictions for the screening function at small separations, $\lim_{r \rightarrow 0} H_{ij}(\mathbf{r})$, where

$$H_{ij}(\mathbf{r}) = \ln \{ g_{ij}(\mathbf{r}) \exp[\beta u_{ij}(\mathbf{r})] \}.$$

$H_{ij}(0)$ is the key for calculating the enhancement factors of nuclear reaction rates,⁸ at the same time providing a direct diagrammatic check of the accuracy of the universality of the bridge functions.³

Equation (1) being a very accurate statement, together with the exact thermodynamic relation

$$\beta \left(\frac{\partial P}{\partial \rho} \right)_{T, \mathbf{x}} = \frac{1}{D} \left[\left(\frac{\beta U}{N} \right) + \frac{1}{D} \Gamma \frac{d}{d\Gamma} \left(\frac{\beta U}{N} \right) \right], \quad (2)$$

provides a model by which we check the accuracy of global statements concerning the DCF's $c_{ij}(\mathbf{r})$.

We start with the OCP. Let $r_0(\Gamma)$ be the characteristic decay length of $c(\mathbf{r})$ to its asymptotic $1/r$ behavior, and write

$$c(\mathbf{r}) = \frac{-\Gamma}{r_0(\Gamma)} Q[r/r_0(\Gamma)], \quad (3)$$

where $Q(\mathbf{r}) \sim 1/r$ for $r \gg 1$. Let us further assume that Q depends on Γ only through r_0 , and write $c(0) = -B\Gamma/r_0(\Gamma)$, $\beta(\partial P / \partial \rho)_{T, \mathbf{x}} = 1 - A r_0^{D-1}(\Gamma)\Gamma$, where $B = Q(0)$, $A = \rho \int [Q(x) - 1/x] d\mathbf{x}$ are constants. Using (1) and (2) we write the differential equation for $r_0(\Gamma)$ that turns out to have the physically expected saturation property: $\lim_{\Gamma \rightarrow \infty} r_0(\Gamma)$

$=R,$

$$\lim_{\Gamma \rightarrow \infty} \left[-\frac{\beta U/N}{\Gamma} \right] = \alpha_M$$

(= fluid "Madelung" constant),

$$R^D = \frac{D+1}{(2D+1)(D-1)} \frac{B}{A}, \quad (4)$$

$$\alpha_M = \frac{D^2}{(2D+1)(D-1)} \frac{B}{R}. \quad (5)$$

$$F^D(y) = \frac{(2D+1)(D-1)}{D+1} \frac{(D+1)U_0 + y^2 d(U_0/y)/dy - D^2}{(2D+1)(D-1)U_0 - y^2 d(U_0/y)/dy}. \quad (7)$$

The accuracy of assumption (3) can best be judged by considering a least favorable case, namely when $\beta(\partial P/\partial \rho)_T = 0$. For that point the solution of the model equations (6) and (7) gives the following constants:

$$y^0 \cong D^2/(D+1) + D/(2D+1),$$

$$U_0(y^0) \cong -D^2/(D+1) + 1/(2D+3),$$

and

$$F(y^0) \cong 1 - (D+1)/[D(D-1)(2D+3)],$$

in very good agreement with the predictions of the MC equation of state.¹ $F(\Gamma)$ is a slowly varying function in agreement with direct observation of the decay rate of $c(r)$.

A "one-fluid" equation of state for plasma mixtures is known to be accurate.¹ My model predicts a "one-fluid" equation of state $(\beta U/N)_{\text{mixture}} = U_0(Z_{\text{eff}}^2 \Gamma)$, provided (i) that

$$c_{ij}(r)/\Gamma = (-Z_i Z_j / r^{ij}) Q_{X,Z}(r/r_0^{ij}),$$

with $Q_{X,Z}$ a Γ -independent function that may depend on charges and concentrations, and (ii) that a decoupling of the Γ -dependence of r_0^{ij} is assumed: $r_0^{ij} = t_{ij}(\{X, Z\}) r_0(\Gamma)$. Under these assumptions, Eqs. (1) and (2) lead to (4)–(7), provided we modify the constants, $A \rightarrow A'$ and $B \rightarrow B'$, according to

$$B' = (\sum_i X_i Z_i^2 / t_{ii}) B_{X,Z}, \quad (8)$$

$$A' = (\sum_{i,j} X_i X_j Z_i Z_j t_{ij}^{D-1}) A_{X,Z}. \quad (9)$$

In the limit $\Gamma \rightarrow \infty$ we expect only one physical scale, and thus make the further assumption that R is independent of charges and concentrations. In view of the relations (4), (5), (8), and (9), this leads to the following identity:

$$\sum_i X_i Z_i^2 / t_{ii} = \sum_{i,j} X_i X_j Z_i Z_j t_{ij}^{D-1}. \quad (10)$$

Expressing A and B in terms of the physical quantities R and α_M and writing $y = \alpha_M \Gamma$, we finally obtain (i) a universal differential equation for the ratio $F(y) = r_0(\Gamma)/R$,

$$\left[1 - \frac{D+1}{2D+1} F^D \right] \frac{y}{F} \frac{dF}{dy} = (D+1)(1-F^D) - \frac{D^3}{(2D+1)(D-1)} \frac{F}{y}, \quad (6)$$

and (ii) a universal expression for the potential energy $\beta U/N = U_0(y)$, obeying the relation

The solution to this identity equation for t_{ij} is

$$t_{ij} = \frac{1}{2} (Z_i^{1/D} + Z_j^{1/D}) / \langle Z \rangle^{1/D} \quad (11)$$

giving the "ion-sphere" charge averaging

$$Z_{\text{eff}}^2 = \sum_i X_i Z_i^2 / t_{ii} = \langle Z \rangle^{1/D} \langle Z^{2-1/D} \rangle \quad (12)$$

(the notation is $\langle Z^p \rangle = \sum_i X_i Z_i^p$).

We have thus derived a universal scaling form for the DCF's:

$$c_{ij}(r) = \frac{-Z_i Z_j \Gamma}{t_{ij} F(Z_{\text{eff}}^2 \Gamma)} Q \left[\frac{r}{t_{ij} F(Z_{\text{eff}}^2 \Gamma)} \right], \quad (13)$$

where $Q(r) = \lim_{\Gamma \rightarrow \infty} [-c_{\text{OCP}}(r)/\Gamma]$ is a given function. This form is thermodynamically consistent provided (i) t_{ij} and Z_{eff}^2 are given by (11) and (12), respectively, (ii) F is a universal function given in terms of the OCP energy $U_0(\Gamma)$ by Eq. (7), and (iii) the equation of state for the mixture is given by the "one-fluid" model with the "ion-sphere" charge averaging. This description agrees to about 1% with all available data for the OCP and binary mixtures in the strong-coupling regime.⁷ These results are formally valid for any dimensionality D and for arbitrary mixtures.

Exactly the same analysis leading to (11)–(13) within the HNC and MSA models can be performed by use of⁴ [instead of Eq. (2)]

$$\Gamma \frac{d}{d\Gamma} \left\{ \frac{1}{2} \left[\beta \left(\frac{\partial P}{\partial \rho} \right)_{T,X} - 1 \right] + \left(1 - \frac{1}{D} \right) \left(\frac{\beta U}{N} \right) \right\} = \frac{\beta U}{N}. \quad (14)$$

This leads to universal functions $F_{\text{HNC}}(y) \cong F(y)$ and $U_{\text{HNC}}(y) \cong U_0(y)$ that are very similar to those obtained via Eq. (2). The fact that $(\alpha_M)_{\text{HNC}} \cong \alpha_M$ is consistent with the identity $Q_{\text{HNC}} = Q$ provided that $R_{\text{HNC}}^D = [(2D+1)/(D+1)] R^D$. Indeed, we find by direct comparison of HNC and MC data in

three dimensions that

$$Q_{\text{HNC}}(r) = \left[\frac{D+1}{2D+1} \right]^{1/D} Q \left[\left(\frac{D+1}{2D+1} \right)^{1/D} r \right],$$

to an accuracy of about 1%. The analytic solution of the MSA and the numerical HNC results, in three dimensions, give $R_{\text{HNC}}=2$. Thus we find $R=1.66$, in agreement with direct observation of the DCF's $c_{ij}(r)$.

By a straightforward extension of the analysis for the OCP⁸ it can be rigorously shown⁷ that the short-distance behavior of $H_{ij}(r)$ is given by

$$H_{ij}(r) = (\bar{\mu}_{z_i} + \bar{\mu}_{z_j} - \bar{\mu}_{z_i+z_j}) + \Gamma/4 \langle Z^2 \rangle r^2 + \dots, \quad (15)$$

$$H_{ij}(0) = f_0 \langle \Gamma \langle Z \rangle^{1/3} Z_i^{5/3} \rangle + f_0 \langle \Gamma \langle Z \rangle^{1/3} Z_j^{5/3} \rangle - f_0 \langle \Gamma \langle Z \rangle^{1/3} (Z_i + Z_j)^{5/3} \rangle,$$

$$H_{ij}(0) = U_0 \langle \Gamma \langle Z \rangle^{1/3} \langle Z^{5/3} \rangle \rangle [Z_i^{5/3} + Z_j^{5/3} - (Z_i + Z_j)^{5/3}] / \langle Z^{5/3} \rangle,$$

and

$$H_{ij}(0) = -0.9 \Gamma \langle Z \rangle^{1/3} [Z_i^{5/3} + Z_j^{5/3} - (Z_i + Z_j)^{5/3}],$$

respectively. For $\Gamma \gg 1$, these three approximations yield nearly identical results for $H_{ij}(0)$, that are in about 1% agreement with the predictions of the universality of the bridge functions.⁷ All these results for $H_{ij}(0)$ are concentration independent for a given total charge density. The results of Itoh *et al.*⁹ scale like our $c_{ij}(0)$, and are clearly thermodynamically inconsistent, predicting about 10% too high values for $H_{ij}(0)$ —enormous error for the enhancement factors.

¹See, e.g., *Strongly Coupled Plasmas*, edited by G. Kalman and P. Carini (Plenum, New York, 1978). A review article by M. Baus and J. P. Hansen is to be

where

$$\bar{\mu}_{z_i} = \frac{\partial}{\partial X_i} \left(\beta \frac{\mathcal{F}}{N} \right) \Big|_{\Gamma \langle Z \rangle^{1/D}}$$

is the chemical potential for a charge Z_i at a given total charge density and temperature, and \mathcal{F} is the excess free energy for the mixture [$\beta \mathcal{F}/N = f_0(\Gamma)$ for the OCP]. For example, in the linear,

$$\beta \frac{\mathcal{F}}{N} = \sum_i X_i f_0(\Gamma \langle Z \rangle^{1/3} Z_i^{5/3}),$$

“one-fluid,” $\beta \mathcal{F}/N = f_0(\Gamma \langle Z \rangle^{1/3} \langle Z^{5/3} \rangle)$, and “ion-sphere,” $\beta \mathcal{F}/N = -0.9 \Gamma \langle Z \rangle^{1/3} \langle Z^{5/3} \rangle$, approximations, one thus obtains

published.

²J. P. Hansen, *Phys. Rev. A* **8**, 3096 (1973); J. P. Hansen, G. M. Torrie, and P. Vieillefosse, *Phys. Rev. A* **16**, 2153 (1977).

³Y. Rosenfeld and N. W. Ashcroft, *Phys. Rev. A* **20**, 1208 (1979).

⁴Y. Rosenfeld and N. W. Ashcroft, *Phys. Rev. A* **20**, 2162 (1979).

⁵K. C. Ng, *J. Chem. Phys.* **61**, 2680 (1974).

⁶Y. Rosenfeld, in *Proceedings of the Centre National de la Recherche Scientifique International Colloquium on Physics of Dense Matter*, Paris, France, 17–22 September 1979 (to be published). Details of the calculations and comparisons will be published separately.

⁷Y. Rosenfeld and N. W. Ashcroft, *Phys. Lett.* **73A**, 31 (1979).

⁸See, e.g., B. Jancovici, *J. Stat. Phys.* **17**, 357 (1977).

⁹N. Itoh, H. Totsuji, S. Ichimaru, and H. E. DeWitt, to be published.

Spectral Cascade Processes in Interchange-Mode Turbulence

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The spectral cascade processes in interchange-mode turbulence have been studied in the limit $k_{\parallel}=0$. For positive-energy waves we find a cascade process towards smaller and larger k_{\perp} . We also obtain possibilities for up conversion. The conservation relations of the system are discussed.

The spectral cascade process for mode coupling of drift waves has recently been discussed.^{1,2} It was found that the spectrum cascades towards

larger and smaller wave number perpendicular to the external magnetic field. This does, however, not allow an excitation of a mode with high-