Debye thermodynamics for the two-dimensional one-component plasma

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The internal and free energies of a two-dimensional one-component plasma model, in the high-temperature Debye approximation, are reinvestigated, and a domain of validity for this model is discussed.

Recently[1-5] a great deal of attention has been paid to the canonical thermodynamics of the two-dimensional, two-component classical plasma interacting through a logarithmic Coulomb potential $\ln|r/L|$. This potential is a solution of the two-dimensional Poisson equation

$$\Delta\phi(\vec{r}) = -2\pi\delta(\vec{r}), \tag{1}$$

The distance L is a scaling length, which is arbitrarily set equal to unity.

Important to this theory is the parameter $T_c = e^2/2k_B$, which represents a critical temperature. This parameter has proved significant in a number of analyses of various two-dimensional systems.[2,3,6] The so-called one-component-plasma model (OCP) obtained by taking simultaneously the limits $N \to \infty$ and $e \to 0$ with $Ne < \infty$ and spreading out one of the components into a continuous and mechanically rigid background is also of a great interest.[4] The purpose of the present comment is to revisit the high-temperature domain of the two-dimensional OCP for two main reasons: First, to emphasize the special status of the Debye treatment for Coulomb systems when the space dimensionality is less than or equal to 2. This point is frequently overlooked in the current literature. The second is to correct several calculational mistakes[7] in Ref. 3.

Let us start from the definition of the potential energy $W(R)$ of N classical pointlike charges interacting through the logarithmic potential $\ln|r|$ in the presence of a neutralizing background.[1,3,4] After elementary algebra we obtain

$$W(R) \equiv W_{p\text{-}p} + W_{p\text{-}b} + W_{b\text{-}b}$$
$$= \tfrac{1}{2}e^2\sum_{i\neq j}^{N}\ln\left|\frac{r_{ij}}{R}\right| - \tfrac{1}{2}Ne^2\sum_{i=1}^{N}\left(\frac{r_i}{R}\right)^2$$
$$+ \tfrac{1}{4}N^2e^2\left(\frac{3}{2} + \ln\frac{1}{R^2}\right). \tag{2}$$

The volume of the system is πR^2.

The first term in $W(R)$ is the particle-particle contribution to the energy, while the second and the third terms represent the particle-background and background-background (self-energy) contributions, respectively. In contradistinction to OCP models with a spatial dimensionality greater than 2[4], $W_{p\text{-}p}$ and $W_{b\text{-}b}$ do not vanish when the average size R of the system becomes very large. This peculiarity shared by all OCP's with dimensionality smaller than 2[4] explains that the usual translation-invariant Debye-Hückel (mean-field)[1,3] treatment of the high-temperature thermodynamics (pertinent to the virial quantities of first order in $\epsilon = e^2/k_BT$) is only approximate. That is, beyond the neglect of ϵ^2 and higher-order terms, one finds that this analysis also neglects the symmetry-breaking term $W_{p\text{-}p}$ arising from the nonvanishing coupling with the background. At sufficiently low temperatures, this harmonic contribution $W_{p\text{-}b}$ may be responsible for the appearance of a long-range ordered crystalline phase. In this regard the ground state of the two-dimensional OCP defined through (2) has been shown to crystallize in a triangular lattice.[5] The corresponding potential energy of the Wigner-Seitz cell has also been computed.[5] This quantitative result may be understood quickly by the following semiquantitative argument. The potential energy of N charges interacting through the logarithmic potential is expected to be minimized when all the charges are located at the vertices of a regular N polygon.[8] Moreover, the Peierls argument requires that each site become a center of symmetry for the whole system which selects out the triangular lattice. However, it has not been determined if this triangular lattice persists at high temperature, as is the case for the OCP in one dimension.[9] We will investigate this problem in the so-called mean-field approximation. Within this approximation the

internal energy

$$\frac{E}{Nk_BT}=1+\frac{\rho 2\pi}{2k_BT}\int dr\, r[g_2(r)-1]\left(-e^2\ln\frac{|r|}{L}\right)$$

becomes

$$1+\frac{\rho\lambda_D^2e^2}{2k_BT}\int_0^\infty 2\pi\, dx\, x\left(\ln x+\ln\frac{\lambda_D}{L}\right)\epsilon K_0(|x|), \tag{3}$$

where

$$x=r/\lambda_D,\quad \lambda_D^2=k_BT/2\pi\rho e^2,\quad \rho=N/V.$$

In obtaining (3) the pair correlation function $g_2(r)$ has been approximated by $g_2(x)=1-\epsilon K_0(x)$. The function $K_n(x)$ denotes the modified Bessel function of the second kind

$$K_0(x)=\int_0^\infty du\exp(-x\cosh u), \tag{4}$$

together with the identities

$$\int_0^\infty du\frac{1}{(\cosh u)^2}=1 \tag{5a}$$

and

$$\int_0^\infty dx\, x\ln x\exp(-x\cosh u)=\frac{1-\gamma-\ln(\cosh u)}{(\cosh u)^2}, \tag{5b}$$

where $\gamma=0.5772$ is Euler's constant.

Recently, Calinon *et al.*[7] have remarked that the right-hand side of Eq. (8.6) in Ref. 3 is incomplete. This is because the factor 1 was omitted in the right-hand side of the integral

$$\int_0^\infty du\frac{\ln(\cosh u)}{(\cosh u)^2}=1-\ln 2. \tag{6}$$

When this is corrected, we obtain

$$E/Nk_BT=1+\tfrac{1}{2}\epsilon[\ln(2\lambda_D/L)-\gamma], \tag{7}$$

which differs by a constant from the result quoted in the last line of Ref. 3, Eq. (8.6).

The correct excess free energy then reads

$$\beta F^{\rm exc}=\int_0^\beta d\beta'\, E^{\rm exc}(\beta')$$

$$=\tfrac{1}{2}\epsilon[-\gamma+\tfrac{1}{2}+\ln(2\lambda_D/L)], \tag{8}$$

It is highly significant that (8) is in very good agreement with the only available exact result[6]

$$F^{\rm exc}\simeq -k_BT\ln[N^{1/2}(L/R)], \tag{9}$$

derived for $k_BT=\frac{1}{2}e^2$ from the canonical partition function ($Z_i=r_i/R$)

$$Q_N(\beta)=\int\cdots\int\frac{d^2\vec{r}_1\cdots d^2\vec{r}_N}{(\pi R^2)^N}e^{\beta W(r)}$$

$$=\exp[-\tfrac{1}{2}\beta e^2N\ln(R/L)]\exp(\tfrac{3}{8}\beta e^2N^2)$$

$$\times\int_0^1\cdots\int_0^1\frac{d^2Z_1\cdots d^2Z_N}{\pi^N}\prod_{1\le i<j\le N}^{N}|Z_i-Z_j|^{\beta e^2}$$

$$\times\exp\left(-\tfrac{1}{2}\beta e^2N\sum_{i=1}^{N}Z_i^2\right),$$

with the angular integration exactly performed, through[8]

$$\prod_{1\le i\le j\le N}|Z_i-Z_j|^2$$

$$=N!\begin{vmatrix} 1 & Z_1 & \cdots & Z_1^{N-1}\\ Z_2^* & Z_2^*Z_2 & \cdots & Z_2^*Z_2^{N-1}\\ \vdots & \vdots & & \vdots\\ Z_N^{*N-1} & Z_N^{*N-1}Z_N & \cdots & Z_N^{*N-1}Z_N^{N-1}\end{vmatrix}.$$

This agreement clearly demonstrates that the translation-invariant Debye approximation, relevant to the domain $\epsilon\ll 1$, may also be appropriate in the strong coupling limit ($\epsilon=2$ here).

The corresponding specific heat at constant volume

$$c_V=\left(\frac{\partial E}{\partial T}\right)_V=k_B(1+\tfrac{1}{4}\epsilon) \tag{10}$$

and the entropy per particle

$$s^{\rm exc}=\beta^2\frac{\partial F^{\rm exc}}{\partial\beta}=-\tfrac{1}{4}k_B\epsilon \tag{11}$$

appearing in Ref. 3 are left unchanged.

It is also worth mentioning that the extrapolation of E taken from Ref. 3, Eq. (8.6) (of which Chui[10] has made use) for the internal energy to a two-component plasma is not affected by the present modification if one allows the condition $\ln Ka\gg 1-\gamma$ to be extended to the equivalent $\ln Ka\gg 1-\gamma+\ln 2$, $K=\lambda_D^{-1}$. The length a is part of a wave-function normalization used in the one-dimensional Tomonaga model with imputities and electron-electron interaction.[10]

As a final remark, it is interesting to compare the present thermodynamics derived for the OCP model with the corresponding results obtained by Seiler[11] for the two-component Coulomb gas with

periodic boundary conditions, in the random-phase approximation. In this finite model, the logarithmic Coulomb law is replaced by the Ewald potential

$$-\sum_{\vec{k}} \frac{2\pi}{k^2 L^2} \exp[i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)] .$$

Both systems display the same equation of state, while their internal energy [cf. Eq. (22) in Ref. 11 with the present Eq. (7)] differ only by a constant in the $T \to \infty$ limit. However, the free energy and the entropy are markedly different (see Sec. III in Ref. 11).

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