



Universal free energy correction for the two-dimensional one-component plasma

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Abstract

The universal finite-size correction to the free energy of a Coulomb system is checked in the special case of a two-dimensional one-component plasma on a sphere. The correction is related to the known second moment of the short-range part of the direct correlation function for a planar system. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Two-dimensional Coulomb systems are models which have attracted some attention. On a two-dimensional manifold, a Coulomb system is a system made of particles interacting through the corresponding Coulomb potential plus perhaps some short-range interaction. In a plane, the Coulomb interaction energy of two particles of charges q and q' , separated by a distance r , is defined as $-qq' \ln(r/L)$, where L is some (irrelevant) length.

Some time ago, it has been shown that the free energy of such systems has a universal finite-size correction [1] very similar (except for its sign) to the one which occurs in a system with short-range forces at a critical point [2]: for a finite Coulomb system of characteristic size R , the free energy F has the large- R behaviour

$$\beta F = AR^2 + BR + \frac{\chi}{6} \ln R + \dots, \quad (1)$$

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where β is the inverse temperature. A and B are non-universal constants describing the bulk and boundary contributions, respectively. $(\chi/6)\ln R$ is the universal correction, depending only on the Euler number χ which describes the topology of the manifold on which the system lives. However, the general derivation [1] of (1) had some heuristic features. The purpose of the present paper is to check (1) in the special case of a one-component plasma on the surface of a sphere, by a different method.

The one-component plasma is a system made of one species of point-particles of charge q in a uniform neutralizing background. On a sphere of radius R , the interaction between two particles can be chosen [3,4] as $-q^2 \ln[(2R/L)\sin(\psi/2)]$, where ψ is the angular distance (seen from the sphere centre) between the two particles. There are also particle–background and background–background interactions. A dimensionless coupling constant is $\Gamma = \beta q^2$.

A sphere has no boundaries and its Euler number is $\chi = 2$. Furthermore, for a given particle density, R^2 is proportional to the number of particles N . Thus, expansion (1) becomes

$$\beta F = CN + \frac{1}{6} \ln N + \dots, \quad (2)$$

where C is a constant. The model is exactly solvable [3] when $\Gamma = 2$ and it can be checked [1] that (2) is obeyed in that case. Also, exact calculations [5] for finite values of N at $\Gamma = 4$ and $\Gamma = 6$ are well fitted by (2).

The present derivation of (2) relies on a recent result [6] about the direct correlation function $c(r)$ of the plane one-component plasma. By a diagrammatic analysis, it has been shown in Ref. [6] that the second moment of the short-range part $c_{SR}(r)$ has the simple value

$$n^2 \int c_{SR}(r) r^2 d^2\mathbf{r} = \frac{1}{12\pi}. \quad (3)$$

A remarkable feature of (3) is its universality, in the sense that it is independent of the coupling constant Γ . It will now be shown how (3) leads to (2). More specifically, we show how (3) implies the finite-size correction to the chemical potential $\mu = \partial F / \partial N$:

$$\beta\mu = \beta\mu_\infty + \frac{1}{6N} + \dots. \quad (4)$$

This derivation bears some similarity with another one about the two-component plasma [7,8].

2. Density functional theory approach

We consider the OCP of average density n_s on the sphere of radius R (with a corresponding number of particles $N = 4\pi R^2 n_s$). Introducing the stereographic projection of the sphere onto the plane \mathcal{P} tangent to its south pole (see Fig. 1), we map the homogeneous OCP on the sphere onto a modified inhomogeneous plasma on the plane,

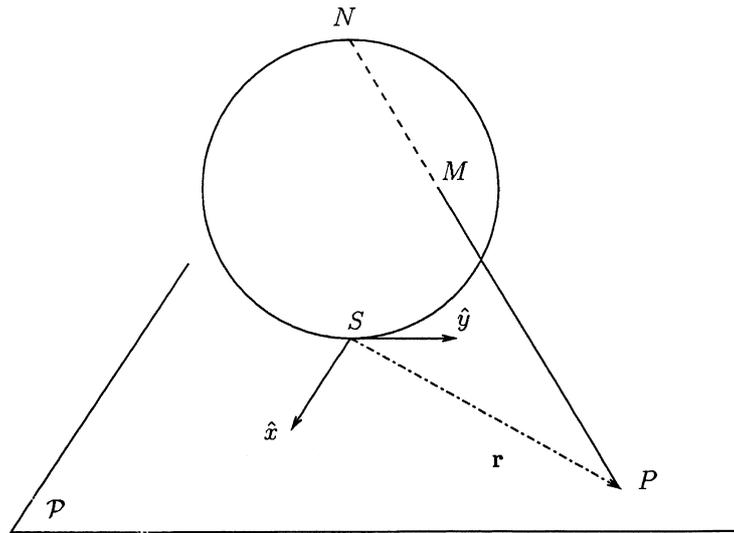


Fig. 1. Stereographic projection from the North pole onto the plane \mathcal{P} . A point M on the sphere is projected onto P , with Cartesian coordinates \mathbf{r} ($\mathbf{r} = \mathbf{0}$ at the South pole S).

with local particle density

$$n(\mathbf{r}) = n_s \left(1 + \frac{r^2}{4R^2} \right)^{-2} . \tag{5}$$

In terms of planar coordinates \mathbf{r}_1 and \mathbf{r}_2 , the interaction potential between the two particles on the sphere with angular distance ψ_{12} can be written as the sum of the planar two-dimensional Coulomb potential $v_p(\mathbf{r}, \mathbf{r}') = -q^2 \ln[|\mathbf{r} - \mathbf{r}'|/L]$ and one-body terms since:

$$-\ln \left[\frac{2R}{L} \sin \left(\frac{\psi_{12}}{2} \right) \right] = -\ln \left[\frac{|\mathbf{r}_1 - \mathbf{r}_2|}{L} \right] + \frac{1}{2} \ln \left(1 + \frac{r_1^2}{4R^2} \right) + \frac{1}{2} \ln \left(1 + \frac{r_2^2}{4R^2} \right) . \tag{6}$$

The two one-body terms appearing on the right-hand side of Eq. (6), as well as the metric, create a central potential and we can consider the projected planar system as a OCP interacting through the standard pair potential v_p , in an external one-body central potential $V_R^N(r)$. The latter acts as a confining mechanism ensuring the proper density given by Eq. (5), and its detailed form need not be precised. Without background, the free energy \mathcal{F}' for the set of particles with pair potential v_p can be formally expanded in a Mayer diagrammatic representation [6], with a leading term $(\frac{1}{2}) \int n(\mathbf{r}) v_p(\mathbf{r}, \mathbf{r}') n(\mathbf{r}') d^2\mathbf{r} d^2\mathbf{r}'$ for the excess (over ideal) part of \mathcal{F}' . The presence of a neutralizing background cancels this mean-field electrostatic term and the intrinsic free energy functional of the inhomogeneous OCP becomes

$$\mathcal{F}[n(\mathbf{r})] = \mathcal{F}'[n(\mathbf{r})] - \frac{1}{2} \int n(\mathbf{r}) v_p(\mathbf{r}, \mathbf{r}') n(\mathbf{r}') d^2\mathbf{r} d^2\mathbf{r}' . \tag{7}$$

The local chemical potential reads

$$\mu(\mathbf{r}) = \frac{\delta \mathcal{F}[n]}{\delta n(\mathbf{r})} = \frac{\delta \mathcal{F}'[n]}{\delta n(\mathbf{r})} - \int v_p(\mathbf{r}, \mathbf{r}') n(\mathbf{r}') d^2 \mathbf{r}' \quad (8)$$

and the second functional derivative of \mathcal{F} yields:

$$\beta \frac{\delta \mu(\mathbf{r})}{\delta n(\mathbf{r}')} = \frac{\delta^2 \beta \mathcal{F}'[n]}{\delta n(\mathbf{r}) \delta n(\mathbf{r}')} - \beta v_p(\mathbf{r}, \mathbf{r}') \quad (9)$$

$$= -c(\mathbf{r}, \mathbf{r}') + \frac{\delta(\mathbf{r} - \mathbf{r}')}{n(\mathbf{r})} - \beta v_p(\mathbf{r}, \mathbf{r}') \quad (10)$$

$$= -c_{SR}(\mathbf{r}, \mathbf{r}') + \frac{\delta(\mathbf{r} - \mathbf{r}')}{n(\mathbf{r})}, \quad (11)$$

where the variations of the excess contribution to \mathcal{F}' give rise to the usual direct correlation function [9], having a short-range part given by

$$c_{SR}(\mathbf{r}, \mathbf{r}') = c(\mathbf{r}, \mathbf{r}') + \beta v_p(\mathbf{r}, \mathbf{r}'). \quad (12)$$

Note that the chemical potential of the OCP on the sphere coincides with $\mu(0)$ for the optimum density profile (5).

Eq. (11) emphasizes the short-range dependence of the chemical potential on a density perturbation. Consequently, $\mu(0)$ is the same in a finite N -particle OCP in the central potential $V_R^N(r)$ and in the limit $N \rightarrow \infty$ with an external potential $V_R^\infty(r)$ ensuring the same density variation around the origin as expression (5), namely:

$$n(\mathbf{r}) = n_s \left(1 - \frac{r^2}{2R^2} \right) + \dots \quad (13)$$

For the purpose of the present analysis, it is sufficient to truncate (5) after second order in r , as it becomes clear below. The knowledge of the finite-size correction to the chemical potential for the OCP on the sphere then amounts to computing the shift $\delta\mu(0)$ induced by switching $V_R^\infty(r)$ starting from the infinite homogeneous planar OCP with density n_s (corresponding to the stereographic projection of the “spherical” plasma in the thermodynamic limit $R \rightarrow \infty$). The density variation caused by the addition of $V_R^\infty(r)$ reads $\delta n(\mathbf{r}) \simeq -n_s r^2 / (2R^2)$ and induces the shift

$$\beta \delta\mu(0) = \int \left[-c_{SR}(\mathbf{r}) + \frac{\delta(\mathbf{r})}{n(\mathbf{r})} \right] \delta n(\mathbf{r}) d^2 \mathbf{r} \quad (14)$$

$$= \frac{n_s}{2R^2} \int c_{SR}(r) r^2 d^2 \mathbf{r}, \quad (15)$$

where the direct correlation function to be considered is that of the homogeneous reference planar OCP. From sum rule (3), we finally obtain

$$\beta \delta\mu(0) = \frac{1}{24\pi n_s R^2} = \frac{1}{6N}, \quad (16)$$

and Eq. (4) is recovered.

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