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A. G. Khrapak and S. A. Khrapak

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On the internal energy of the classical two-dimensional one-component-plasma

A. G. Khrapak[1] and S. A. Khrapak[2,a]
[1]*Joint Institute for High Temperatures, Russian Academy of Sciences, 125412 Moscow, Russia*
[2]*Aix-Marseille-Université, CNRS, Laboratoire PIIM, UMR 7345,*
13397 Marseille cedex 20, France

We describe a new semi-phenomenological approach to estimate the internal energy of the classical one-component-plasma in two dimensions. This approach reproduces the Debye-Hückel asymptote in the limit of weak coupling, the ion disc asymptote in the limit of strong coupling, and provides reasonable interpolation between these two limits. The present analytic results are compared with those from other approximations as well as with existing data from numerical simulations. © *2015 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License.* [http://dx.doi.org/10.1063/1.4929778]

I. INTRODUCTION

The one-component-plasma (OCP) is an idealized system of identical point-like particles of charge e immersed in a uniform neutralizing background of opposite charge.[1–3] This model is of considerable interest from the fundamental point of view and has wide interdisciplinary applications, including ionized matter in white dwarfs, interiors of heavy planets, alkali metals, colloidal suspensions, and complex (dusty) plasmas.[3–5] Although thermodynamic properties of the OCP have been extensively studied over decades, simple physically motivated approaches are still of considerable interest.[4,6,7] The purpose of this paper is to discuss a simple approach to estimate the internal energy of two dimensional (2D) classical OCP in a wide parameter regime.

In two dimensions, two different systems are actually referred to as the OCP. The first is characterized by the conventional 3D Coulomb interaction potential ($\propto r^{-1}$), but the particle motion is restricted to a 2D surface. This system has been used as a first approximation for the description of electron layers bound to the surface of liquid dielectrics and of inversion layers in semi-conductor physics.[2] It is also relevant to colloidal and complex (dusty) plasma mono-layers in the regime of week screening.[3,5,8] In the second system, the interaction potential is defined via the 2D Poisson equation and scales logarithmically with distance ($\propto -\ln(r)$). The experimental realizations of such system are less obvious, but nevertheless it received significant attention because of various field theoretical models[2] and existence of exact analytic solutions for some special cases. Our present paper is restricted to this latter case of logarithmic interaction in 2D. Note that both OCP systems (with Coulomb and logarithmic interactions), represent a very important limiting case of particle systems with extremely soft repulsive interactions, and share some common thermodynamic properties (for a recent example see Ref. 9).

The system studied is characterized by the particle density n, and the temperature T (in the following temperature is measured in energy units, i.e., $k_B = 1$). The interaction potential between two particles at a distance r from one another follows from the solution of the 2D Poisson equation around a central test particle and is logarithmic,

$$V(r) = -e^2 \ln(r/L), \tag{1}$$

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[a]Also with Forschungsgruppe Komplexe Plasmen, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Oberpfaffenhofen, Germany

where L is an arbitrary scaling length. It is common[10] to set $L = a$, where $a = (\pi n)^{-1/2}$ is the 2D Wigner-Seitz radius. The strength of the interparticle interactions is measured by the coupling parameter, $\Gamma = e^2/T$, and does not depend on the particle density (separation) in the considered case (as already mentioned we do not consider here the 2D systems of particles interacting via the conventional 3D Coulomb potential, which have also been extensively studied in the literature[11,12]). As Γ increases, the OCP shows a transition from a weakly coupled gaseous regime ($\Gamma \ll 1$) to a strongly coupled fluid regime ($\Gamma \gg 1$) and crystallizes into the triangular lattice near $\Gamma \simeq 135 - 140$.[10,13] We show below that a unified hybrid approach can be constructed that allows to estimate the internal energy of the 2D OCP across these coupling regimes.

II. LINEAR DEBYE-HÜCKEL (DH) APPROXIMATION

The solution of the linear Poisson-Boltzmann equation, $\Delta\phi = k_{\mathrm{D}}^2\phi$, in 2D is

$$\phi(r) = eK_0(rk_{\mathrm{D}}), \tag{2}$$

where $K_0(x)$ is the zero-order modified Bessel function of the second kind and $k_{\mathrm{D}} = \sqrt{2\pi ne^2/T}$ is the inverse screening length. Note the relation $ak_{\mathrm{D}} = \sqrt{2\Gamma}$. The reduced excess (that over non-charged particles) energy of the systems can be evaluated from

$$u_{\mathrm{ex}} \equiv \frac{U_{\mathrm{ex}}}{NT} = \frac{[e\phi(r) - V(r)]_{r\to 0}}{2T}, \tag{3}$$

where N is the number of particles ($N \to \infty$ in the thermodynamic limit). This corresponds to the Debye-Hückel (DH) approximation for the weakly coupled ($\Gamma \ll 1$) limit. With the help of the expansion $K_0(x) \simeq -\gamma + \ln 2 - \ln x + O(x^2)$ for $x \ll 1$ we easily obtain

$$u_{\mathrm{DH}}(\Gamma) = -\frac{\Gamma}{4}\left(\ln\frac{\Gamma}{2} + 2\gamma\right), \tag{4}$$

where $\gamma \simeq 0.57721$ is the Euler's constant. This is the well known DH result,[10,14] which provides accurate description only in the limit of extremely weak coupling.

III. DEBYE-HÜCKEL PLUS HOLE (DHH) APPROXIMATION

To extend the applicability of the DH approach to the moderately coupled OCP in 3D, the simple phenomenological "Debye-Hückel plus hole" (DHH) approximation was proposed.[6,15] The main idea behind the DHH approximation is that the exponential particle density must be truncated close to a test particle in order to avoid density to be negative upon linearization. The DHH approach has been recently applied to Yukawa systems in 3D.[16] Here we demonstrate how it can be implemented for the 2D OCP.

The potential inside the hole (disk in 2D case) of radius h satisfies

$$\Delta\phi = 2\pi en - 2\pi e\delta(\mathbf{r}). \tag{5}$$

The solution can be written as

$$\phi_{\mathrm{in}}(r) = -e\ln(r/a) + \mathcal{A}_0 + \mathcal{A}_2 r^2, \tag{6}$$

where $\mathcal{A}_2 = (e/2a^2)$. Outside the hole, the potential satisfies the linearized Poisson-Boltzmann equation, so that

$$\phi_{\mathrm{out}}(r) = \mathcal{B}K_0(rk_{\mathrm{D}}). \tag{7}$$

The two solutions should be matched at $r = h$, requiring $\phi_{\mathrm{in}}(h) = \phi_{\mathrm{out}}(h) = T/e$ (the last condition ensures that particle density vanishes at the hole boundary in the linear approximation) and $\phi'_{\mathrm{in}}(h) = \phi'_{\mathrm{out}}(h)$. Using the identity $K_0'(x) = -K_1(x)$ we get the following transcendent equation for $z = (h/a)$
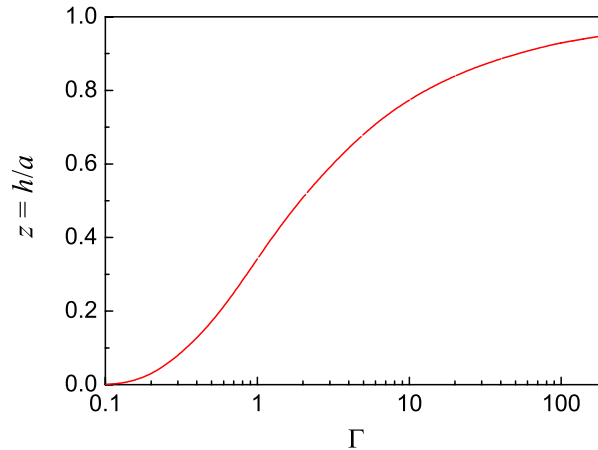
FIG. 1. Reduced radius of the hole, $z = h/a$, around the test particle as a function of the coupling parameter Γ in the 2D OCP.

$$z^2 + z\sqrt{\frac{2}{\Gamma}}\frac{K_1(\sqrt{2\Gamma}z)}{K_0(\sqrt{2\Gamma}z)} - 1 = 0. \tag{8}$$

Unlike the 3D case, where the analytical solution exists, in the 2D case numerical solution is required. The numerical solution for $z(\Gamma)$ is shown in FIG. 1. The reduced excess energy can be evaluated using equation (3), which yields $u_{\text{DHH}} = (e\mathcal{A}_0/2T)$. Thus, the DHH approximation in 2D yields

$$u_{\text{DHH}}(\Gamma) = \frac{1}{2} + \frac{\Gamma}{2}\ln z - \frac{\Gamma}{4}z^2. \tag{9}$$

In the limit $\Gamma \ll 1$, Eq. (9) reduces to the DH result of Eq. (4), but it remains adequate at much higher Γ than the DH approach does. For example, in the special case $\Gamma = 2$, exact results can be obtained analytically.[17,18] The exact excess energy at this point is $u_{\text{exact}}(2) = -\gamma/2 \simeq -0.28861$.[17] The DHH value is very close to that, $u_{\text{DHH}}(2) \simeq -0.29324$, while the DH value is considerably below the exact one, $u_{\text{DH}}(2) \simeq -0.57721$. In the strongly coupled regime $\Gamma \gg 1$, the DHH approximation yields the correct scaling $u_{\text{ex}} \propto \Gamma$, but the coefficient of proportionality is incorrect ($-1/4$ instead of $\simeq -3/8$). In Figure 2 we compare the energies obtained using the DHH approach with those obtained using Monte Carlo (MC)[10] and molecular dynamics (MD)[13] computer simulations.
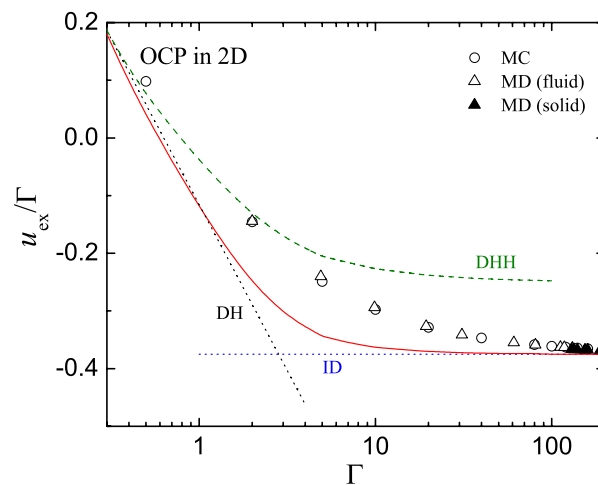

FIG. 2. Reduced excess energy u_{ex}/Γ versus the coupling parameter Γ for the 2D OCP. Symbols are the results from MC[10] and MD[13] simulations. Various dashed curves correspond to the DH, DHH, and ID approximations, as indicated in the figure. The (red) solid curve shows the result of the hybrid DHH + ID approaximation of Eq. (16).

IV. ION DISC MODEL (IDM)

The ion disc model (IDM) in 2D OCP is an analog of the ion sphere model (ISM) in 3D OCP[2,19] (which can be also generalized to Yukawa systems[20]). The main idea of this approximation is that in the regime of strong coupling, the particles repel each other and form a regular structure with the interparticle spacing of order a. Each particle can be considered as restricted to the cell (disc in 2D) of radius a, filled with the neutralizing background. The cells are charge neutral and do not overlap, and hence the potential energy of the system is just the sum of potential energy of each cell. The latter is readily calculated from the pure electrostatic consideration.[7] The result is

$$u_{\mathrm{IDM}} = -\frac{3}{8}\Gamma = -0.375\Gamma. \tag{10}$$

The result is very close to the static component of the actual excess energy of the 2D OCP in both strongly coupled fluid and solid phases. For instance, the Madelung constant of the 2D OCP forming the triangular lattice is $M = -0.37438\Gamma$. The thermal component of the excess energy, which is close to 1.0 (in reduced units) at strong coupling, can also be added.[7,21] It was proven mathematically that Eq. (10) provides the lower bounds of the excess internal energy in the thermodynamic limit.[22] The IDM asymptote is also shown in FIG. 2.

V. HYBRID DHH + IDM APPROXIMATION

This construction is analogous to that of the DHH + ISM approach for the 3D OCP that we have recently proposed.[23] We consider a test particle along with the piece of the neutralizing charge (disc of radius h) as a new compound particle. The internal energy of such a compound particle consists of two parts: energy of a uniformly charged disk of radius h and charge $q = -e(h/a)^2$ and the energy of a charge e placed in the center of such a disk. Solving the Poisson equation inside and outside the disc and matching the solutions we can get for the energy of the uniformly charged disc

$$u_{\mathrm{d}} = \frac{q^2}{T}\left(\frac{1}{8} - \frac{1}{2}\ln\frac{h}{a}\right). \tag{11}$$

The energy of a charge e placed in the center of such a disc is

$$u_{\mathrm{p}} = \frac{eq}{T}\left(\frac{1}{2} - \ln\frac{h}{a}\right). \tag{12}$$

The energy of the compound particle is then

$$u_{\mathrm{cp}}(\Gamma) = \Gamma z^2\left(\ln z - \frac{1}{2}\right) + \Gamma z^4\left(\frac{1}{8} - \frac{1}{2}\ln z\right). \tag{13}$$

In the limit of strong coupling, the effective charge of the compound particle tends to zero and, therefore, its internal energy should be an adequate measure of the excess energy of the whole system (per particle). We get in this limit $z \to 1$ and $u_{\mathrm{cp}} \simeq -\frac{3}{8}\Gamma$, which coincides with the static IDM result.

The energy associated with the remaining interaction between the compound particles (they are not charge neutral since $z \le 1$) can be estimated from the 2D energy equation

$$u_{\mathrm{pp}} = (\pi n/T)\int_h^\infty r V_{\mathrm{eff}}(r)[g(r) - 1]dr, \tag{14}$$

where $V_{\mathrm{eff}}(r) = -e_{\mathrm{eff}}^2 \ln(r/a)$ is the effective interaction potential with $e_{\mathrm{eff}} = e + q = e[1 - z^2]$ and $g(r)$ is the radial distribution function. Since the effective charge e_{eff} is considerably reduced compared to the actual charge e, especially in the strong coupling regime, it is not very unreasonable to use an expression originates from the linearized Boltzmann relation, $g(r) \simeq 1 - e_{\mathrm{eff}}\phi_{\mathrm{out}}(r)/T$,

where ϕ_{out} is given by Eq. (7) in the DHH approximation. This yields

$$u_{\text{pp}}(\Gamma) = \frac{\Gamma(1-z^2)^3}{K_0(\sqrt{2\Gamma}z)} \int_z^{\infty} x \ln x K_0(\sqrt{2\Gamma}x) dx. \qquad (15)$$

Numerical integration is generally required in (15), but it can be shown to reduce to the DH result in the weakly coupled limit ($\Gamma \ll 1$).

Our estimate for the OCP excess energy within the hybrid DHH + IDM approximation is then simply

$$u_{\text{hyb}}(\Gamma) = u_{\text{cp}}(\Gamma) + u_{\text{pp}}(\Gamma). \qquad (16)$$

This is the main result of the present paper. Eq. (16) reduces to the DH and IDM asymptotes in respective limits of weak and strong coupling. The quality of the interpolation between these two limits is illustrated in FIG. 2 (red solid curve). The approach clearly somewhat underestimates the excess energy, especially in the transitional regime between weak and strong coupling. Nevertheless, the agreement with the accurate numerical data from MC and MD simulations is reasonable, especially taking into account the simplicity of the approach.

ACKNOWLEDGMENTS

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