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Equilibrium properties of two-dimensional Yukawa plasmas

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Abstract
Strongly coupled two-dimensional systems of dust particles are often observed in dusty plasma experiments. We analyse thermodynamic quantities of two-dimensional Yukawa plasmas and apply the results to structure formations in two-dimensional finite systems. We include the nonlocal effect which has been neglected in the previous analysis and give a relatively simple method to estimate important parameters in dusty plasmas.

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1. Introduction

The two-dimensional Yukawa system can be regarded as a model which covers both systems with long- and short-ranged interactions. Static and dynamic properties have been investigated including distribution functions, dynamic fluctuation spectra and dispersion relations of various modes of oscillations [1]. The results are of much interest by themselves and also help us estimate physical parameters in experiments [2–5].

Thermodynamics of a two-dimensional system is also essential in the shell model [6] which has been successfully applied in reproducing three-dimensional structure formations of Yukawa dust particles under the influence of a one-dimensional force field such as gravity [7] and in the isotropic environment [8, 9]. In this model, we assume that the system is composed of shells, their geometry reflecting the symmetry of the system, and optimize their number, positions and populations to minimize the total (free) energy. The negative intra-shell correlation (or cohesive) energy as a two-dimensional system keeps the optimized state from reduction to uniform distribution with infinite number of shells of infinitesimal surface density.

We here present thermodynamic properties of a two-dimensional Yukawa system and apply them to parameter estimation and theoretical understanding of structure formations of dust particles. We consider the system of particles with the surface density n and the temperature T interacting via the Yukawa potential

$$v(r) = \frac{e^2}{r}\exp(-r/\lambda), \tag{1}$$

where e is the charge on a particle, λ is the screening length and r is the mutual distance. We assume the existence of the inert uniform background charge of density $-ne$ which neutralizes the charge density of particles. This system is characterized by the parameters Γ and ξ given respectively by

$$\Gamma = \frac{e^2}{k_B T a} \qquad \text{and} \qquad \xi = \frac{a}{\lambda}, \tag{2}$$

where $a = 1/(\pi n)^{1/2}$ is the mean distance.

2. Thermodynamics of two-dimensional Yukawa plasmas

2.1. Expansion in coupling parameter and interpolation formula

We analyse here thermodynamics of two-dimensional Yukawa plasmas [10]. The two-dimensional nature of this system is clearly shown in the domain of weak coupling, especially when compared with the Coulombic case [11]. In the domain of intermediate or strong coupling, we have simple interpolations.

Let us first assume that the coupling is weak or $\Gamma \ll 1$. In this case, the many body screening effect is characterized by the two-dimensional Debye wave number K_D defined by $K_D = 2\pi n e^2/k_B T$ [11]. While K_D characterizes the screening by many body effects, λ denotes the inherent decay of interaction. When $1/K_D \ll \lambda$, the screening is controlled by $1/K_D$ and the result for the Coulombic case [11] is still valid. We thus assume, in contrast, that

$$e^2/k_B T \ll \lambda \ll 1/K_D. \tag{3}$$

In the random phase approximation (RPA) [12], the interaction (correlation or cohesive) energy per unit volume is given by

$$-\frac{n^2}{2k_B T}\int d\mathbf{r}\, v(r)u(r), \tag{4}$$

where

$$u(r) = \frac{1}{(2\pi)^2}\int d\mathbf{k}\frac{2\pi e^2}{(k^2 + 1/\lambda^2)^{1/2} + K_D}\exp(i\mathbf{k}\cdot\mathbf{r}), \tag{5}$$

indicating that the long-range divergence at $r \to \infty$ related to Coulomb-like interaction is cut off by the smaller of either λ or $1/K_D$. Due to reduced dimensionality, the RPA result is also logarithmically divergent for $r \to 0$ and we have to take the short-range correlation into account properly [11, 13]. The latter gives the effective cutoff around $r \sim e^2/k_B T$.

The Helmholtz free energy F is separated into the ideal gas part F^{ideal} and the interaction part ΔF as $F = F^{\text{ideal}} + \Delta F$, where $\Delta F = N k_B T f(\Gamma, \xi)$ and f is a dimensionless function of dimensionless quantities Γ and ξ. In the domain of weak coupling, we have

$$f(\Gamma, \xi) = -\frac{\Gamma^2}{2}\left[-\ln\left(2\frac{e^2/k_B T}{\lambda}\right) - 2\gamma + \frac{3}{2}\right] = -\frac{\Gamma^2}{2}\left[-\ln(2\Gamma\xi) - 2\gamma + \frac{3}{2}\right], \tag{6}$$

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

When $\Gamma \gg 1$, the internal energy U approaches to the value (Madelung energy) for the triangular lattice [14], similar to the case of Coulombic system [15], as

$$U'(\Gamma,\xi) = \frac{U}{Nk_BT} \to c(\xi)\Gamma \qquad \text{when} \quad \Gamma \to \infty. \tag{7}$$

Here, the normalized value $U' = U/Nk_BT$ is a dimensionless function of dimensionless parameters and $c(\xi)$ is a coefficient dependent on ξ [3, 14].

In the case where Γ is neither small nor large, we resort to the numerical simulation. We have obtained the value of U covering the domain of intermediate and strong coupling with $0.5 \leqslant \xi \leqslant 2$. We note that U reduces to the Madelung energy as (7) when $\Gamma \to \infty$ and analyse the behaviour of the normalized difference $[U'(\Gamma \to \infty, \xi) - U'(\Gamma, \xi)]/U'(\Gamma \to \infty, \xi)$ which decreases from unity to 0 with the increase of Γ from 0 to ∞. We finally have for $0.05 \leqslant \Gamma \leqslant 100$ and $0.5 \leqslant \xi \leqslant 2$ [10]

$$U'(\Gamma,\xi) = c(\xi)\Gamma - [c(\xi)\Gamma - U'(0.05,\xi)]\exp[-2.55(\Gamma^{0.18} - 0.05^{0.18})]. \tag{8}$$

This interpolation works with relative error less than 1% for $10 \leqslant \Gamma \leqslant 100$, less than 3% for $1 \leqslant \Gamma \leqslant 10$ and less than 10% for $0.05 \leqslant \Gamma \leqslant 1$. We obtain the nonideal part of the Helmholtz free energy $\Delta F = Nk_BTf(\Gamma,\xi)$ for $0.05 \leqslant \Gamma \leqslant 100$ and $0.5 \leqslant \xi \leqslant 2$ by [10]

$$f(\Gamma,\xi) = \left(\int_0^{\Gamma_1} + \int_{\Gamma_1}^{\Gamma}\right)\frac{\mathrm{d}\Gamma}{\Gamma}U'(\Gamma,\xi), \qquad \Gamma_1 = 0.05. \tag{9}$$

For $\Gamma \leqslant 0.05$, we apply the result in the weak coupling domain.

2.2. Remarks

At first sight, one may expect the existence of an additional internal energy (per particle) coming from the Yukawa repulsion

$$\frac{n}{2}\int \mathrm{d}\mathbf{r}\, v(r) = \frac{\Gamma}{\xi}k_BT \tag{10}$$

even in the case of no correlation between particles. We emphasize that this is *not* the case in our Yukawa plasmas: the neutralizing background is built-in and all contributions to thermodynamic quantities beyond the ideal gas values are due to correlation between particles. For example, the internal (correlation or cohesive) energy vanishes in randomly distributed or uniformly smeared-out cases. (In the Coulombic case, one is automatically reminded of the existence of neutralizing background by the fact that the integral (10) is divergent.)

When periodic boundary conditions are adopted and the area of the unit cell is kept constant in numerical simulations, the existence of the neutralizing background is automatically taken into account. In real systems, however, the background is missing or provided by real physical objects. In both cases, one has to be careful to take the situation properly into account.

3. Application: two-dimensional finite dust systems

3.1. Structure

We now apply the above results to the analysis of two-dimensional systems of dust particles observed in experiments where they are confined laterally by ring electrodes or other methods. Since the latter confinement is expressed by a parabolic potential in the system plane, the potential part of the Hamiltonian is written as

$$\frac{1}{2}\sum_{i\neq j}\frac{e^2}{r_{ij}}\exp(-r_{ij}/\lambda)+\frac{1}{2}\sum_i kr_i^2=\frac{k}{2}\lambda^2\left(\alpha\sum_{i\neq j}\frac{1}{r_{ij}/\lambda}\exp(-r_{ij}/\lambda)+\sum_i(r_i/\lambda)^2\right). \tag{11}$$

Here, $\alpha = e^2/k\lambda^3$ characterizes the strength of Yukawa interaction relative to lateral confinement. Note that the parabolic potential provides the effect similar to the neutralizing background which is *not* built-in in this system.

When the number of particles is not too small, we may express the structure by the radial density $\rho(r)$ and determine $\rho(r)$ so as to minimize the Helmholtz free energy as a functional of $\rho(r)$. When $\alpha \gg 1$, the system has a large lateral extension and we may further adopt the local expression for the Helmholtz free energy: the Helmholtz free energy is given by a spatial integral of the free energy density and the latter value is approximated by that of a uniform system with the number density at each point.

Some examples of results are shown in figures 1(*a*)–(*c*). In figures 1(*a*) and (*b*), we observe that, when $\alpha \geqslant 1$, numerical simulations are reproduced to a good accuracy [2, 3] and the effect of correlation (cohesion) plays an important role especially when $\alpha \gg 1$. We also note that the behaviour of the density on the periphery gives information on the temperature of the system [5].

In the Helmholtz free energy to be minimized, the term

$$\frac{e^2}{2}\iint \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'\frac{\exp(-|\mathbf{r}-\mathbf{r}'|/\lambda)}{|\mathbf{r}-\mathbf{r}'|}\rho(r)\rho(r') \tag{12}$$

leads to

$$e^2\delta\rho(r)\int \mathrm{d}\mathbf{r}'\frac{\exp(-|\mathbf{r}-\mathbf{r}'|/\lambda)}{|\mathbf{r}-\mathbf{r}'|}\rho(r'), \tag{13}$$

when the variation is taken with respect to $\rho(r)$. In the local approximation [2], the kernel of this integral has been replaced by $2\pi\lambda\delta(\mathbf{r}-\mathbf{r}')$. We include here the nonlocal effect evaluating the integral up to the next term as

$$2\pi\lambda\rho(r)+\pi\lambda^3\Delta\rho(r)=2\pi\lambda\rho(r)+\pi\lambda^3\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}r\frac{\mathrm{d}}{\mathrm{d}r}\rho(r). \tag{14}$$

We then have

$$2\pi e^2\lambda\rho(r)+\pi e^2\lambda^3\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}r\frac{\mathrm{d}}{\mathrm{d}r}\rho(r)=\mu-\frac{1}{2}kr^2, \tag{15}$$

μ being the Lagrange's multiplier, instead of (5.13) in [2]. This gives (corresponding to (5.17) and (5.18) in [2])

$$\lambda^2\rho(r)=\frac{1}{4\pi\alpha}\left[\left(\frac{r_1}{\lambda}\right)^2-\left(\frac{r}{\lambda}\right)^2\right]+\frac{2}{4\pi\alpha} \tag{16}$$

for $r \leqslant r_1$, where

$$\left(\frac{r_1}{\lambda}\right)^2=(8\alpha N+4)^{1/2}-2, \tag{17}$$

N being the total number of particles. An example of the result is shown in figure 1(*c*) and we observe that the discrepancy between simulation and theory is substantially improved

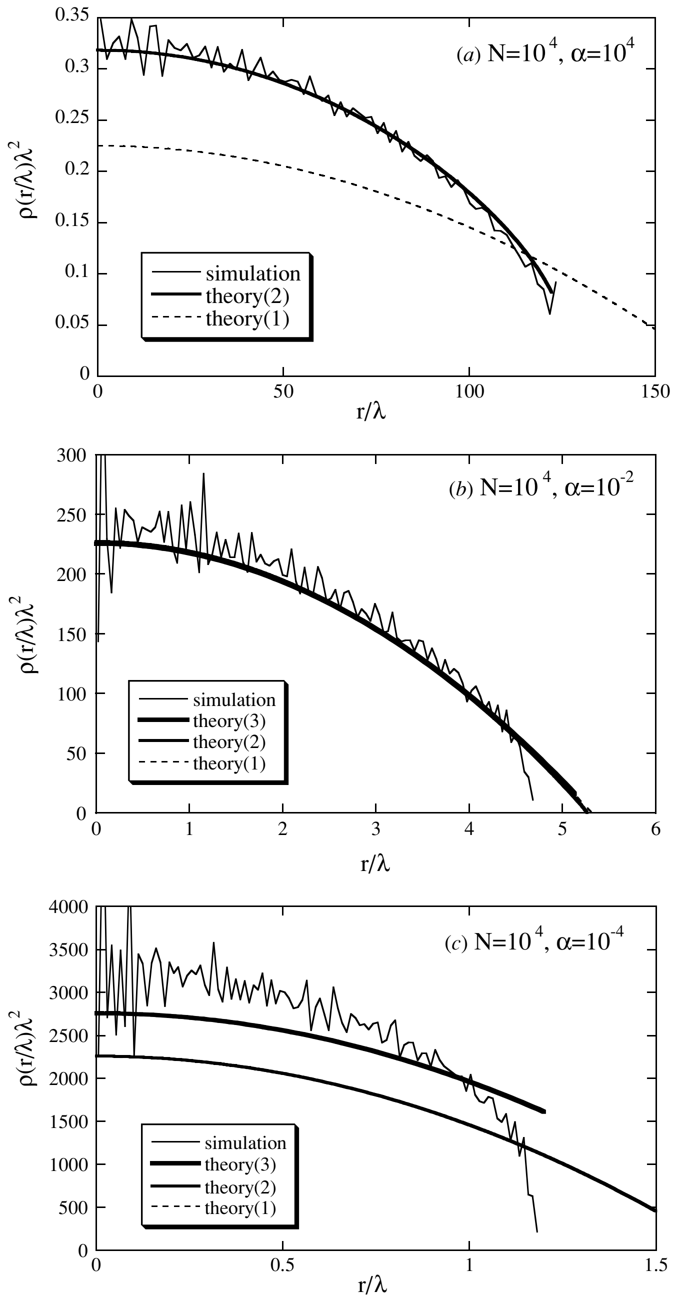

Figure 1. Radial distribution in the two-dimensional finite Yukawa system at low temperatures. Simulation (thin solid lines) are compared with theory: (1) (broken lines) local approximation without cohesive energy, (2) (solid line) local approximation with cohesive energy and (3) (thick solid line) with nonlocal effect. In (*b*), theories (1)–(3) are almost the same except for the discontinuity on the edge. In (*c*), (1) and (2) are almost the same.

compared with the previous result [2]. We also note that the effect of correlation energy is small when $\alpha \ll 1$.

3.2. Estimation of parameters

The charge on a dust particle e and the screening length λ are among the most important parameters in dusty plasmas. Theoretical results for the distribution of particles in two-dimensional finite systems can be applied to identify these parameters through direct observations of $\rho(r)$. Our theory includes α, the temperature and the number of particles as parameters and gives $\lambda^2\rho(r/\lambda)$ as a function of r/λ. Counting number of particles and noting that the dimensionless combination of the system radius r_m and the central density of particles $\rho(0)$, $\rho(0)r_m^2$, depends on α and the temperature, we can determine these two parameters from the observed value of $\rho(0)r_m^2$ and the density profile on the periphery. After α and the temperature are known, λ is obtained from the experimental value of r_m which is theoretically given in terms of λ.

In order to have the charge e from α and λ, however, the value of k is still to be identified and some trick has been needed. For example, the electrode giving vertical levitation is devised to specify the values of k by its radius of curvature [4].

We here note that, in the case of ring electrodes often used in experiments, k is related to the charge $Q_{\rm ring}$ of the ring electrode (with radius R_0) through [2]

$$k \sim \frac{1}{2}\frac{Q_{\rm ring}\exp(-R_0/\lambda)}{R_0}\left(1+\frac{R_0}{\lambda}+\frac{R_0^2}{\lambda^2}\right). \tag{18}$$

Therefore, we have

$$k \sim \frac{1}{2}C_{\rm ring}V_{\rm ring}\frac{\exp(-R_0/\lambda)}{R_0}\left(1+\frac{R_0}{\lambda}+\frac{R_0^2}{\lambda^2}\right). \tag{19}$$

Here $V_{\rm ring}$ and $C_{\rm ring}$ are the electrostatic potential and the capacitance of the ring electrode, respectively, both of which can be measured experimentally. Combined with the determination of α and λ, this gives a new relatively simple method to estimate e and λ in dusty plasmas compared with those hitherto reported [4] or those including observation of dynamics.

4. Conclusions

We have obtained thermodynamic quantities of two-dimensional Yukawa plasmas and expressed results in the form of simple interpolation formulae. Results are applied to analyses of structure formations of dust particles with inclusion of the nonlocal effect. It is shown that the results are useful in estimating dust charge and other parameters.

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