Thermodynamics of a two-dimensional Yukawa fluid

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Thermodynamic quantities of a two-dimensional Yukawa system, a model for various systems including single-layered dust particles observed in dusty plasmas, are obtained and expressed by simple interpolation formulas. In the domain of weak coupling, the analytical method based on the cluster expansion is applied and, in the domain of intermediate and strong coupling, numerical simulations are performed. Due to reduced dimensionality, the treatment based on the mean field fails at the short range and exact behavior of the binary correlation is to be taken into account even in the case of weak coupling.

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I. INTRODUCTION

The two-dimensional Yukawa system has been investigated as a typical example and model system in two dimensions which covers systems with both the long- and short-ranged interactions by adjusting a single parameter. On the other hand, the formation of horizontal layers composed of dust particles has been observed in recent dusty plasma experiments and it has been shown that the number of layers is determined by the competition between mutual repulsion and strength of vertical confinement [1]. When the latter is strong enough, we have the single-layered state as the ground state of the layered system. Those dust particles can be regarded as interacting via the Yukawa potential and we have a two-dimensional Yukawa system in reality. They have provided us with a unique example of a two-dimensional finite system whose microscopic characteristics can be easily observed by charge coupled device cameras and even by the naked eye. Both static and dynamic properties have been investigated including distribution functions, dynamic fluctuation spectra, and dispersion relations of various modes of oscillations [2]. The results are of much interest by themselves and also help us to estimate physical parameters of ambient plasmas in experiments [3–5].

In this paper, we give the thermodynamic quantities of a two-dimensional Yukawa system. Thermodynamic quantities are of fundamental importance and play an essential role, for example, to determine the equilibrium of a system in external potential. We employ both analytical methods based on the cluster expansion and numerical simulations. In principle, we are able to obtain these quantities by numerical simulations. In the domain of weak coupling, however, thermal fluctuations usually make it difficult to obtain accurate values in simulations and analyses based on the expansion with respect to the coupling parameter becomes useful.

Yukawa systems in dusty plasmas are often in the state of strong coupling due to large charge on dust particles and both two- and three-dimensional lattices have been observed. As well as two-dimensional dust crystals in the domain of strong coupling, the two-dimensional Yukawa system in the weak coupling domain is also interesting. It has been known that [6,7], in the domain of weak coupling, thermodynamic quantities of a two-dimensional system of charges have different behavior from that of a three-dimensional one due to reduced dimensionality. In three dimensions, the mean field theory (the random phase approximation) works in the domain of weak coupling, correctly describing the major many-body effect, the screening of the long-range interaction. In two dimensions, however, the consideration of the short-range (two-body) correlation is needed with the same weight as the long-range screening even in the domain of weak coupling. The leading terms in thermodynamic quantities of the two-dimensional Coulomb system have been obtained by one of the authors by properly taking the short-range correlation into account [6,7]. We here extend those results to a two-dimensional Yukawa system.

We consider the system of particles with the surface density n and the temperature T interacting via the Yukawa potential

$$v(r) = \frac{e^2}{r}\exp(-r/\lambda), \tag{1.1}$$

where e is the charge on a particle 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

$$\Gamma = \frac{e^2}{k_B T a} \tag{1.2}$$

and

$$\xi = \frac{a}{\lambda}, \tag{1.3}$$

where a is the mean distance defined by

$$a = \frac{1}{(\pi n)^{1/2}}. \tag{1.4}$$

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II. WEAK COUPLING

We here assume that the coupling is weak or

$$\Gamma \ll 1. \tag{2.1}$$

As is shown shortly below, the many body screening effect is characterized by the two-dimensional Debye wave number K_D defined by

$$K_D = \frac{2\pi n e^2}{k_B T}. \tag{2.2}$$

Another definition of the coupling parameter which we denote by ε is the ratio between the Landau length $e^2/k_B T$ and the Debye length $1/K_D$ and is related to Γ as below and is also small:

$$\varepsilon = \frac{e^2/k_B T}{1/K_D} = 2\Gamma^2 \ll 1. \tag{2.3}$$

In the Coulombic case ($\lambda \to \infty$), the pressure P is calculated as [6,7]

$$\frac{P}{nk_B T} - 1 = \frac{\varepsilon}{4}[\ln(2\varepsilon) - 1 + 2\gamma] \quad \text{for} \quad \varepsilon \ll 1 \quad (\lambda \to \infty), \tag{2.4}$$

where γ=0.5772… is the Euler's constant. This is to be compared with the three-dimensional (3D) Debye-Hückel result for the pressure p which is regular as an expansion with respect to the coupling parameter ε,

$$\frac{p}{nk_B T} - 1 = -\frac{\varepsilon}{6} \quad \text{for} \quad \varepsilon \ll 1 \quad (3\text{D}, \lambda \to \infty). \tag{2.5}$$

Here the three-dimensional Debye wave number and the coupling parameter are defined, respectively by $k_D^2 = 4\pi n e^2/(k_B T)$ and $\varepsilon = (e^2/k_B T)/(1/k_D)$. The nonanalytic nature of the expansion appears in the next order [8].

The Debye wave number K_D characterizes the screening by many body effects whereas λ denotes the inherent decay of interaction. When $1/K_D \ll \lambda$, the screening is controlled by $1/K_D$ and the result (2.4) is still valid. We thus assume, on the contrary, that

$$e^2/k_B T \ll \lambda \ll 1/K_D. \tag{2.6}$$

We note that this condition is rewritten as

$$K_D a = 2\Gamma \ll \xi = \frac{a}{\lambda} \ll \frac{a}{(e^2/k_B T)} = \frac{1}{\Gamma} \tag{2.7}$$

and ξ can be of the order of unity when $\Gamma \ll 1$.

A. Random phase approximation

We first note that the Fourier transform of the Yukawa potential in two dimensions is given by

$$v(r) = \frac{1}{(2\pi)^2} \int d\mathbf{k} v(k) \exp(i\mathbf{k} \cdot \mathbf{r}), \tag{2.8}$$

$$v(k) = \frac{2\pi e^2}{(k^2 + 1/\lambda^2)^{1/2}}. \tag{2.9}$$

Following the standard procedure [7,9], we obtain the conductivity $\sigma(\mathbf{k},\omega)$ and the dielectric response function $\varepsilon(\mathbf{k},\omega)$ in the random phase approximation as

$$\sigma(\mathbf{k},\omega) = -i \frac{ne^2\omega}{k_B T k^2} \mathcal{W}\left\{ \frac{\omega}{k} \left(\frac{m}{k_B T} \right)^{1/2} \right\}, \tag{2.10}$$

$$\varepsilon(\mathbf{k},\omega) = 1 + \frac{K_D}{(k^2 + 1/\lambda^2)^{1/2}} \mathcal{W}\left\{ \frac{\omega}{k} \left(\frac{m}{k_B T} \right)^{1/2} \right\}. \tag{2.11}$$

Here m is the mass, K_D is the Debye wave number given by Eq. (2.2), and $\mathcal{W}(z)$ is defined by

$$\mathcal{W}(z) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dx \frac{x \exp(-x^2/2)}{x - z - i0}. \tag{2.12}$$

From the fluctuation-dissipation theorem [7,9], the static form factor $S(k)$ and the pair correlation function $h(r)$ in the random phase approximation are given, respectively, by

$$S(k) = \frac{(k^2 + 1/\lambda^2)^{1/2}}{(k^2 + 1/\lambda^2)^{1/2} + K_D} \tag{2.13}$$

and

$$h(r) = -\frac{u(r)}{k_B T}, \tag{2.14}$$

$$u(r) = \frac{1}{(2\pi)^2} \int d\mathbf{k} u(k) \exp(i\mathbf{k} \cdot \mathbf{r}), \tag{2.15}$$

$$u(k) = \frac{2\pi e^2}{(k^2 + 1/\lambda^2)^{1/2} + K_D}. \tag{2.16}$$

The interaction (correlation or cohesive) energy per unit volume given by

$$\frac{n^2}{2} \int d\mathbf{r} v(r) h(r) \tag{2.17}$$

is logarithmically divergent for $r \to 0$ indicating that the short-range correlation is not taken into account properly in this approximation.

B. Thermodynamic quantities by cluster expansion

To obtain correct thermodynamic quantities, it is necessary to start from the cluster expansion. The pressure P is given by Mayer's giant cluster expansion as [8,10]

$$\frac{P}{nk_B T} - 1 = -n \frac{\partial W}{\partial n}, \tag{2.18}$$

where W is the sum of contributions from the ring diagrams W_0 and the prototype graphs W_p. In the prototype graphs, the interaction potential is replaced by the screened one $u(r)$ defined by Eq. (2.15) as shown in Fig. 1. In the Coulombic case ($\lambda \to \infty$), the interaction is screened into the form [6,7]

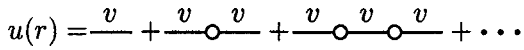

FIG. 1. Screened interaction $u(r)$. The lines connecting the dots represent the bare interaction $v(r)$ and integrals are taken over positions of dots.

$$u(r) = \frac{e^2}{r}\int_0^\infty dx \frac{x}{x + K_D r} J_0(x), \tag{2.19}$$

where $J_0(x)$ is the Bessel function.

The contribution of the ring diagrams W_0 is calculated as

$$W_0 = \frac{1}{2n}\frac{1}{(2\pi)^2}\int d\mathbf{k}[-\ln\{1 + n\beta v(k)\} + n\beta v(k)], \tag{2.20}$$

where $\beta = 1/k_B T$ and $n\beta v(k) = K_D/(k^2 + 1/\lambda^2)^{1/2}$. The leading contribution from the prototype graphs is given by the one with two junctions

$$W_p^{(2)} = \frac{n}{2}\int d\mathbf{r}\left[\exp\{-\beta u(r)\} - 1 + \beta u(r) - \frac{1}{2}\{\beta u(r)\}^2\right]. \tag{2.21}$$

As is pointed out by one of the authors [6,7], both of the contributions from W_0 and W_p^2 are divergent in the short range ($r \to 0$ or $k \to \infty$) and cannot be evaluated independently. We introduce

$$W' = \frac{n\beta^2}{4}\int d\mathbf{r} u(r) v(r) = \frac{n\beta^2}{4}\frac{1}{(2\pi)^2}\int d\mathbf{k} u(k) v(k) \tag{2.22}$$

and evaluate $W_0 - W'$ and $W_p^{(2)} + W'$ separately as in Refs. [6,7].

The value of $W_0 - W'$ is evaluated as

$$W_0 - W' = \frac{\varepsilon}{8}\left[\frac{2}{(K_D\lambda)^2}\ln(1 + K_D\lambda) - \frac{2}{K_D\lambda} + \frac{1}{1 + (K_D\lambda)^2}\frac{K_D\lambda}{1 + K_D\lambda}\right] \tag{2.23}$$

and, when $K_D\lambda \ll 1$, we have

$$W_0 - W' \sim \frac{5}{24}\varepsilon K_D\lambda \ll \varepsilon. \tag{2.24}$$

In evaluating $W_p^{(2)} + W'$, we divide the integral over r into $0 < r < r_0$ (I_1) and $r_0 < r < \infty$ (I_2), taking r_0 such that $\beta e^2 \ll r_0 \ll \lambda \ll 1/K_D$. Using this condition, we have

$$I_1 \sim \frac{\varepsilon}{4}\left[-\ln\left(\frac{\beta e^2}{r_0}\right) - \gamma + \frac{3}{2}\right], \tag{2.25}$$

$$I_2 \sim \frac{\varepsilon}{4}\left[-\ln\left(2\frac{r_0}{\lambda}\right) - \gamma\right], \tag{2.26}$$

and therefore

$$W_p^{(2)} + W' \sim \frac{\varepsilon}{4}\left[-\ln\left(2\frac{\beta e^2}{\lambda}\right) - 2\gamma + \frac{3}{2}\right], \tag{2.27}$$

when $\beta e^2 \ll \lambda \ll 1/K_D$ (see the Appendix).

Finally we have

$$W_0 + W_p^{(2)} \sim \frac{\varepsilon}{4}\left[-\ln\left(2\frac{\beta e^2}{\lambda}\right) - 2\gamma + \frac{3}{2}\right] \tag{2.28}$$

and the pressure is calculated as

$$\frac{P}{nk_BT} - 1 \sim -\frac{\varepsilon}{4}\left[-\ln\left(2\frac{\beta e^2}{\lambda}\right) - 2\gamma + \frac{3}{2}\right]. \tag{2.29}$$

The argument of the logarithm expresses that the integral over r, which is logarithmically divergent for both $r \to 0$ and $r \to \infty$, is cutoff at βe^2 and λ, respectively.

In the case of Coulomb interaction ($\lambda \to \infty$), we have [6,7]

$$W_0 - W' = \frac{1}{8}\varepsilon \quad (\lambda \to \infty), \tag{2.30}$$

$$W_0 + W_p^{(2)} \sim \frac{\varepsilon}{4}\left[-\ln(2\varepsilon) - 2\gamma + \frac{3}{2}\right] = \frac{\varepsilon}{4}\left[-\ln\left(2\frac{\beta e^2}{1/K_D}\right) - 2\gamma + \frac{3}{2}\right] \quad (\lambda \to \infty), \tag{2.31}$$

and

$$\frac{P}{nk_BT} - 1 = \frac{\varepsilon}{4}[\ln(2\varepsilon) - 1 + 2\gamma] = \frac{\varepsilon}{4}\left[\ln\left(2\frac{\beta e^2}{1/K_D}\right) - 1 + 2\gamma\right] \quad (\lambda \to \infty). \tag{2.32}$$

When the result for the Yukawa system (2.28) is compared with the Coulombic case (2.31), we see that the long-range cutoff at $1/K_D$ is replaced by λ. This result may be naturally expected from the condition (2.6). In order to determine the constant such as $-\ln 2 - 2\gamma + 3/2$, however, we need the analyses in Refs. [6,7] and the present paper. Similar analyses on the pair correlation function have been done based on the cluster expansion for the Coulombic case [11].

The Helmholtz free energy F is separated into the ideal gas part F^{ideal} and the interaction part ΔF as

$$F = F^{\text{ideal}} + \Delta F, \tag{2.33}$$

where

$$\Delta F = Nk_BTf(\Gamma, \xi) \tag{2.34}$$

and f is a dimensionless function of dimensionless quantities Γ and ξ. Since

$$P/nk_BT - 1 = -V(\partial/\partial V)_{T,N,\lambda} f(\Gamma, \xi) = n(\partial/\partial n)_{T,\lambda} f(\Gamma, \xi), \tag{2.35}$$

we have

TABLE I. Cohesive energy of 2D Yukawa particles obtained by molecular dynamics simulation with the results of the Coulombic system [13].

Γ	$U/\Gamma N k_B T$	Γ	$U/\Gamma N k_B T$	Γ	$U/\Gamma N k_B T$	Γ	$U/\Gamma N k_B T$
			$\xi=0.0$				
0.158	−0.430	0.224	−0.528	0.500	−0.640	0.707	−0.735
1.00	−0.780	1.23	−0.817	1.41	−0.842	1.58	−0.848
1.73	−0.872	1.87	−0.882	2.00	−0.890	2.12	−0.896
2.24	−0.908	2.35	−0.904	2.74	−0.924	5.00	−0.986
7.07	−1.01	15.8	−1.05	22.4	−1.07	50.0	−1.08
			$\xi=0.5$				
0.277	−0.383	0.397	−0.424	0.500	−0.466	0.501	−0.456
0.526	−0.480	0.659	−0.504	1.99	−0.671	3.25	−0.722
3.39	−0.732	6.62	−0.783	10.1	−0.809	13.0	−0.819
13.5	−0.822	19.5	−0.836	33.5	−0.850	49.8	−0.859
52.0	−0.860	69.7	−0.864	96.5	−0.868	102.	−0.869
			$\xi=1.0$				
0.133	−0.225	0.198	−0.261	0.202	−0.268	0.332	−0.320
0.346	−0.328	0.393	−0.339	0.528	−0.372	0.661	−0.393
0.667	−0.398	1.32	−0.487	1.60	−0.495	1.78	−0.504
2.71	−0.544	3.05	−0.552	3.06	−0.553	3.20	−0.560
4.14	−0.582	4.44	−0.590	4.96	−0.599	5.65	−0.605
6.03	−0.610	6.56	−0.616	7.22	−0.619	9.91	−0.637
10.1	−0.635	17.3	−0.659	20.3	−0.662	24.4	−0.666
26.6	−0.670	29.4	−0.672	29.9	−0.672	36.3	−0.676
36.6	−0.676	39.9	−0.678	51.6	−0.682	54.8	−0.683
68.0	−0.687	71.8	−0.687	78.0	−0.689	97.8	−0.690
			$\xi=1.5$				
3.19	−0.454	5.42	−0.481	9.62	−0.508	16.2	−0.524
24.9	−0.534	28.4	−0.537	37.1	−0.543	52.8	−0.548
			$\xi=2.0$				
0.264	−0.201	0.267	−0.203	0.331	−0.221	0.337	−0.229
0.661	−0.272	0.662	−0.272	0.663	−0.274	1.32	−0.321
2.68	−0.363	3.21	−0.372	3.27	−0.373	3.38	−0.377
6.68	−0.402	6.78	−0.401	9.80	−0.415	10.1	−0.418
13.0	−0.424	19.2	−0.432	20.0	−0.433	25.1	−0.437
27.4	−0.439	31.2	−0.441	32.9	−0.442	35.7	−0.442
38.7	−0.443	56.2	−0.448	57.3	−0.449	65.9	−0.450
66.2	−0.450	73.3	−0.451	76.3	−0.451	82.6	−0.453

$$f(\Gamma,\xi) = -\frac{\varepsilon}{4}\left[-\ln\left(2\frac{\beta e^2}{\lambda}\right) - 2\gamma + \frac{3}{2}\right] = -\frac{\Gamma^2}{2}\left[-\ln(2\Gamma\xi) - 2\gamma + \frac{3}{2}\right]. \tag{2.36}$$

The nonideal part of the entropy ΔS and the internal (correlation or cohesive) energy U given, respectively, by

$$\Delta S = -\left(\frac{\partial \Delta F}{\partial T}\right)_{N,V} \tag{2.37}$$

and

$$U = \Delta F + T\Delta S \tag{2.38}$$

are calculated as

$$\Delta S = N k_B \frac{\varepsilon}{4}\left[\ln\left(2\frac{\beta e^2}{\lambda}\right) + 2\gamma - \frac{1}{2}\right] = N k_B \frac{\Gamma^2}{2}\left[\ln(2\Gamma\xi) + 2\gamma - \frac{1}{2}\right], \tag{2.39}$$

and

$$U = Nk_BT\frac{\varepsilon}{2}\left[\ln\left(2\frac{\beta e^2}{\lambda}\right) + 2\gamma - 1\right]$$
$$= Nk_BT\,\Gamma^2[\ln(2\Gamma\xi) + 2\gamma - 1]. \qquad (2.40)$$

We note that these results are derived with the condition (2.7) or $2\Gamma \ll \xi \ll 1/\Gamma$.

In the case of Coulomb interaction ($\lambda \to \infty$), they are given by

$$f(\Gamma, \xi = 0) = -\frac{\varepsilon}{4}[-\ln(2\varepsilon) - 2\gamma + 2] = -\Gamma^2[-\ln(2\Gamma) - \gamma + 1], \qquad (2.41)$$

$$\Delta S(\lambda \to \infty) = Nk_B\frac{\varepsilon}{4}[\ln(2\varepsilon) + 2\gamma] = Nk_B\Gamma^2[\ln(2\Gamma) + \gamma], \qquad (2.42)$$

and

$$U(\lambda \to \infty) = \Delta F + T\Delta S = Nk_BT\frac{\varepsilon}{2}[\ln(2\varepsilon) + 2\gamma - 1]$$
$$= Nk_BT\Gamma^2[2\ \ln(2\Gamma) + 2\gamma - 1]. \qquad (2.43)$$

III. INTERMEDIATE AND STRONG COUPLING

In the case where Γ is not small, the expansion with respect to coupling cannot be applied and we resort to the numerical simulation. We apply the molecular dynamics to the system of 256 Yukawa particles. The periodic boundary condition with the deformable parallelogram unit cell is adopted. In order to analyze the strongly coupled domain near possible lattice formation, it may be necessary to take the deformation of the periodicity into account [1,12]. In this paper, however, we restrict the coupling parameter within the domain of fluid where such deformation is expected to have no serious effect.

By numerical simulations for combinations of Γ and ξ, we have obtained the value of U covering the domain of intermediate and strong coupling with $0.5 \leqslant \xi \leqslant 2$. The results are summarized in Table I and shown in Figs. 2(a)–2(c) in the form of $U/\Gamma Nk_BT$. As in the case of the Coulombic system [11], we observe that, when Γ increases, U approaches the value (Madelung energy) for triangular lattice [12] as

$$U'(\Gamma, \xi) = \frac{U}{Nk_BT} \to c(\xi)\Gamma \quad \text{when} \quad \Gamma \to \infty, \qquad (3.1)$$

where the normalized value $U' = U/Nk_BT$ is a function of dimensionless parameters and $c(\xi)$ is a coefficient dependent on ξ [12] and is approximately expressed as [4]

$$\pi^{1/2}c(\xi) = -1.9605 + 0.8930\xi - 0.1959\xi^2 + 0.01715\xi^3. \qquad (3.2)$$

IV. INTERPOLATION FORMULAS

We present here simple interpolation formulas for thermodynamic quantities of a two-dimensional Yukawa system. We

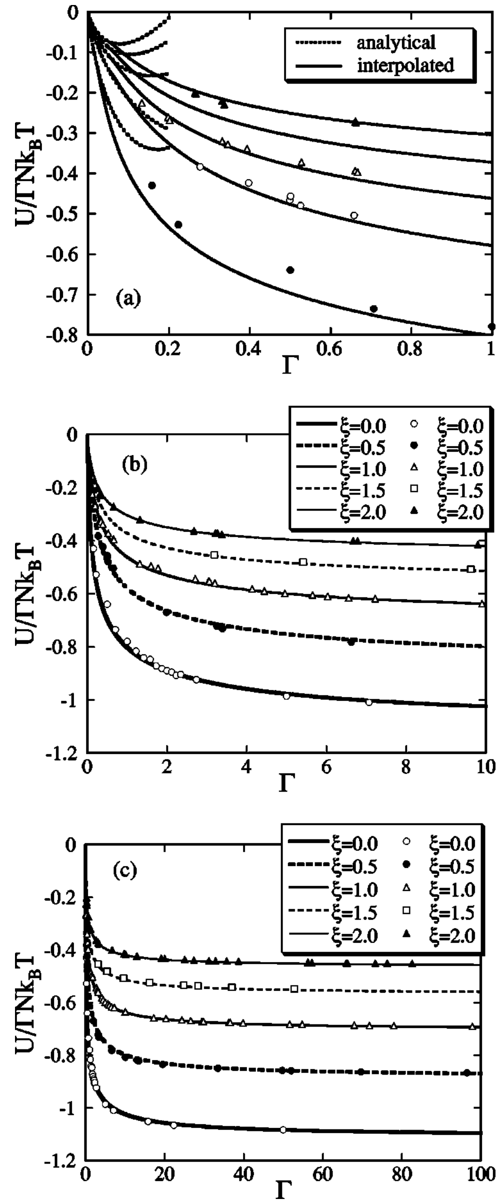

FIG. 2. Interaction (correlation or cohesive) energy divided by Γ vs Γ. In (a), marks are the results of numerical simulations, the solid lines are interpolated values and the broken lines are analytical results. In (b) and (c), marks are the results of numerical simulations and the lines are interpolated values.

first consider the values of U; since the relations (2.33)–(2.35), (2.37), and (2.38) hold irrespective of the strength of coupling, other thermodynamic quantities are derived from the value of U.

As for the expansion with respect to the coupling parameter, we apply the result (2.40) in the weak coupling domain $\Gamma \leqslant 0.05 \ll 1$:

$$U'(\Gamma, \xi) = \Gamma^2[\ln(2\Gamma\xi) + 2\gamma - 1], \quad \Gamma \leqslant 0.05. \qquad (4.1)$$

We note that U reduces to the Madelung energy for the triangular lattice [12] as Eq. (3.1) when the coupling is strong enough, and analyze the behavior of the normalized difference from those values,

$$\frac{U'(\Gamma \to \infty, \xi) - U'(\Gamma, \xi)}{U'(\Gamma \to \infty, \xi)}, \tag{4.2}$$

which decreases from unity to 0 with the increase of Γ from 0 to ∞. As a result, we find that the decrease can be expressed by a simple functional form of $\sim \exp(-x\Gamma^y)$ with a coefficient $x=2.55$ and the power $y=0.18$ which are independent of ξ for $0.5 \leqslant \xi \leqslant 2$. Based on this observation, we finally have for $0.05 \leqslant \Gamma \leqslant 100$ and $0.5 \leqslant \xi \leqslant 2$

$$U'(\Gamma,\xi) = c(\xi)\Gamma - [c(\xi)\Gamma - U'(0.05,\xi)] \times \exp[-2.55(\Gamma^{0.18} - 0.05^{0.18})]. \tag{4.3}$$

We plot the values given by this interpolation in Figs. 2(a)–2(c). We confirm that 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 $0.05 \leqslant \Gamma \leqslant 1$.

For the Coulombic case, we apply the weak coupling result (2.43) to the weak coupling domain $\Gamma \leqslant 0.02$

$$U'(\Gamma,\xi=0) = \Gamma^2[2\ln(2\Gamma) + 2\gamma - 1]. \tag{4.4}$$

In the case of intermediate and strong coupling, we use the values previously given by one of the authors [13]. After similar analysis, we have

$$U'(\Gamma,\xi=0) = c(\xi=0)\Gamma - [c(\xi=0)\Gamma - U'(0.02,\xi=0)] \times \exp[-2.55(\Gamma^{0.18} - 0.05^{0.18})] \tag{4.5}$$

for $0.02 \leqslant \Gamma \leqslant 100$. The result is also plotted in Figs. 2(a)–2(c). Relative error is less than 1% for $2 \leqslant \Gamma \leqslant 100$, less than 3% for $1 \leqslant \Gamma \leqslant 2$, and less than 15% for $0.02 \leqslant \Gamma \leqslant 1$.

Since we have assumed Eq. (2.7) or $2\Gamma \ll \xi$ in deriving Eq. (4.1) for the domain of weak coupling, we cannot decrease ξ in Eq. (4.1) to values comparable with Γ. In this sense, the analytical result for $\Gamma \sim \xi \ll 1$ is left unresolved. In connecting the weak coupling expressions to that in the intermediate and strong coupling domain, we have chosen $\Gamma = 0.05$ for $0.5 \leqslant \xi \leqslant 2$ and $\Gamma = 0.02$ for $\xi = 0$ as the limit of applicability of analytical results observing the overall behavior of the error. The analysis in the range $0 < \xi < 0.5$ is similarly left unresolved in this paper.

Based on the relations (2.33)–(2.35), (2.37), and (2.38), we obtain the nonideal part of the Hemholtz free energy $\Delta F = Nk_BTf(\Gamma,\xi)$ for $0.05 \leqslant \Gamma \leqslant 100$ and $0.5 \leqslant \xi \leqslant 2$ as

$$f(\Gamma,\xi) = \left(\int_0^{\Gamma_1} + \int_{\Gamma_1}^{\Gamma}\right)\frac{d\Gamma}{\Gamma}U'(\Gamma,\xi) = \frac{\Gamma_1^2}{2}\left[\ln(2\Gamma_1\xi) + 2\gamma - \frac{3}{2}\right] + c(\xi)(\Gamma - \Gamma_1) - c(\xi)\frac{\exp(x\Gamma_1^y)}{yx^{1/y}}\left[\gamma\left(\frac{1}{y},x\Gamma^y\right) - \gamma\left(\frac{1}{y},x\Gamma_1^y\right)\right] + \frac{\exp(x\Gamma_1^y)}{y}U'(\Gamma_1,\xi)[\mathrm{Ei}(-x\Gamma^y) - \mathrm{Ei}(-x\Gamma_1^y)], \tag{4.6}$$

where $\Gamma_1 = 0.05$, $x=2.55$, $y=0.18$, and $\gamma(z,p)$ and $\mathrm{Ei}(-z)$ are the incomplete gamma function and the exponential integral function, respectively:

$$\gamma(z,p) = \int_0^p dt\, \exp(-t)t^{z-1}, \tag{4.7}$$

$$\mathrm{Ei}(-z) = -\int_z^\infty dt\frac{\exp(-t)}{t}. \tag{4.8}$$

The pressure is given by

$$\frac{P}{nk_BT} - 1 = n\left(\frac{\partial f(\Gamma,\xi)}{\partial n}\right)_{T,\lambda} = \frac{1}{2}U'(\Gamma,\xi) - \frac{\Gamma_1^2}{4} - \frac{1}{2}\xi\frac{dc(\xi)}{d\xi}(\Gamma - \Gamma_1) + \frac{1}{2}\xi\frac{dc(\xi)}{d\xi}\frac{\exp(x\Gamma_1^y)}{yx^{1/y}}\left[\gamma\left(\frac{1}{y},x\Gamma_1^y\right) - \gamma\left(\frac{1}{y},x\Gamma^y\right)\right] - \frac{1}{2}\Gamma_1^2\frac{\exp(x\Gamma_1^y)}{y}[\mathrm{Ei}(-x\Gamma^y) - \mathrm{Ei}(-x\Gamma_1^y)]. \tag{4.9}$$

The entropy is given by

$$\frac{\Delta S}{Nk_B} = U'(\Gamma,\xi) - f(\Gamma,\xi). \tag{4.10}$$

It should be noted that, since the entropy is given as the difference between $U'(\Gamma,\xi)$ and $f(\Gamma,\xi)$, the relative error is largely enhanced even when both $U'(\Gamma,\xi)$ and $f(\Gamma,\xi)$ have small relative errors. The values of $f(\Gamma,\xi) = \Delta F/Nk_BT$, $P/nk_BT - 1$ and $\Delta S/Nk_B$ are shown in Figs. 3–5.

In the Coulombic case with $0.02 \leqslant \Gamma \leqslant 100$, we have

$$f(\Gamma,\xi=0) = \Gamma_1^2[\ln(2\Gamma_1) + \gamma - 1] + c(\xi=0)(\Gamma - \Gamma_1) - c(\xi=0)\frac{\exp(x\Gamma_1^y)}{yx^{1/y}}[\gamma(1/y,x\Gamma^y) - \gamma(1/y,x\Gamma_1^y)] + \frac{\exp(x\Gamma_1^y)}{y}U'(\Gamma_1,\xi=0)[\mathrm{Ei}(-x\Gamma^y) - \mathrm{Ei}(-x\Gamma_1^y)], \tag{4.11}$$

$$\frac{P}{nk_BT} - 1 = \frac{1}{2}U'(\Gamma,\xi=0), \tag{4.12}$$

and

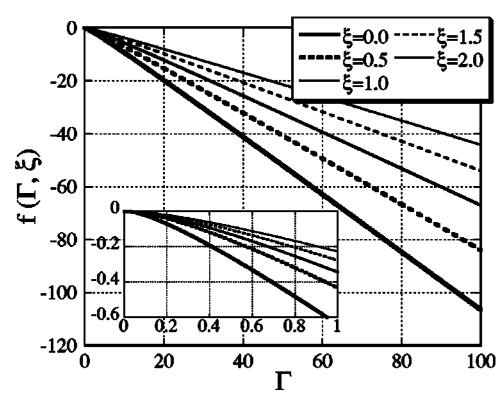

FIG. 3. Normalized values of the nonideal part of Helmholz free energy $f = \Delta F/Nk_BT$ vs Γ for $\xi = 0, 0.5, 1, 1.5$, and 2.

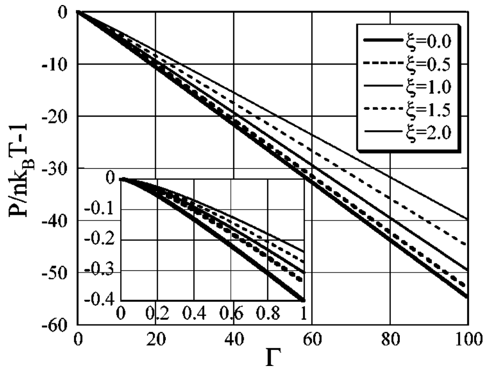

FIG. 4. Normalized values of the nonideal part of pressure $P/nk_{\mathrm{B}}T-1$ vs Γ for $\xi=0,\ 0.5,\ 1,\ 1.5$, and 2.

$$\frac{\Delta S}{Nk_B} = U'(\Gamma,\xi=0) - f(\Gamma,\xi=0), \tag{4.13}$$

where $\Gamma_1=0.02$, $x=2.55$, and $y=0.18$. The results are also plotted in Figs. 3–5.

V. CONCLUSION

We have obtained thermodynamic quantities of a two-dimensional Yukawa system. In the domain of weak coupling, the analytical results are derived based on the giant cluster expansion and the effect of reduced dimensionality is explicitly shown. In the domain of intermediate and strong coupling, molecular dynamics have been applied and the results are expressed as the simple interpolation formulas. These results will be useful in investigating two-dimensional systems including the single-layered dust particles in dusty plasmas.

APPENDIX

In evaluating I_1, we may put $u(r)\sim v(r)$ and $\exp[-\beta\times v(r)]\sim\exp[-(\beta e^2/r)(1-r/\lambda+r^2/2\lambda^2)]$. We thus have

$$\pi n\int_0^{r_0} drr\left[\exp\left\{-\frac{\beta e^2}{r}\exp(-r/\lambda)\right\}-1+\frac{\beta e^2}{r}\exp(-r/\lambda)\right]$$
$$\sim\frac{\varepsilon}{4}\left[-\ln\left(\frac{\beta e^2}{r_0}\right)-\gamma+\frac{3}{2}\right]. \tag{A1}$$

The integral

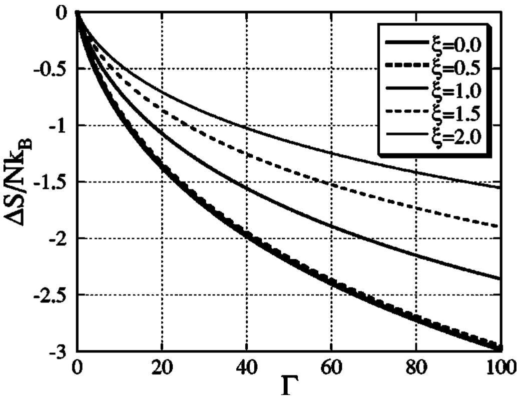

FIG. 5. Normalized values of the nonideal part of entropy $\Delta S/Nk_{\mathrm{B}}$ vs Γ for $\xi=0,\ 0.5,\ 1,\ 1.5$, and 2.

$$\frac{n}{2}\int_0^{r_0} d\mathbf{r}\beta^2 u(v-u)\sim\frac{n}{2}\int_0^{r_0} d\mathbf{r}\beta^2 v(v-u) \tag{A2}$$

is estimated to be of higher order.

In integral I_2, we may evaluate as

$$\pi n\int_{r_0}^{\infty} drr[\exp(-\beta u)-1+\beta u-\beta^2u^2/2]$$
$$\sim-\pi n\int_{r_0}^{\infty} drr\beta^3u^3/3!\sim-\pi n\int_{r_0}^{\infty} drr\beta^3v^3/3!. \tag{A3}$$

Here we note that, since $\lambda\ll 1/K_D$, the integrand becomes small enough before the many body screening becomes effective and we estimate its value to be of the order of $\varepsilon(\beta e^2/\lambda)|\ln(\beta e^2/\lambda)|\ll\varepsilon$. The remaining integral is similarly estimated as

$$\frac{\pi n}{2}\int_{r_0}^{\infty} drr\beta^2uv\sim\frac{\pi n}{2}\int_{r_0}^{\infty} drr\beta^2v^2\sim\frac{\varepsilon}{4}\left[-\ln\left(2\frac{r_0}{\lambda}\right)-\gamma\right]. \tag{A4}$$

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