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A Testbench for the Nested Dipole Hypothesis of Kosterlitz and Thouless

A. Alastuey[1] **and P. J. Forrester**[2]

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We consider the two-dimensional one-component plasma without a background and confined to a half-plane near a metal wall. The particles are also subjected to an external potential acting perpendicular to the wall with an inverse-power-law Boltzmann factor. The model has a known solvable isotherm which exhibits a Kosterlitz–Thouless-type transition from a conductive to an insulator phase as the power law is varied. This allows predictions of theoretical methods of analyzing the Kosterlitz–Thouless transition to be compared with the exact solution. In particular, we calculate the asymptotic density profile by resumming its low-fugacity expansion near the zero-density critical coupling in the insulator phase, and solving a mean-field equation deduced from the first BGY equation. Agreement with the exact solution is obtained. As the former calculation makes essential use of the nested dipole hypothesis of Kosterlitz and Thouless, the validity of this hypothesis is explicitly verified.

KEY WORDS: Kosterlitz–Thouless transition; Coulomb gas; renormalization equations; correlations; exact solution.

1. INTRODUCTION

The two-dimensional Coulomb gas refers to a neutral system of charged particles confined to a plane. The two species have opposite charge (magnitude q, say) and interact via the laws of two-dimensional electrostatics (logarithmic potential). To stop collapse between oppositely charged particles at low temperature, due to the singular behavior of the logarithmic potential at the origin, a hard-core or similar short-range regularization is

[1] Ecole Normale Supérieure de Lyon, Laboratoire de Physique, Unité de Recherche Associeé 1325 au Centre National de la Recherche Scientifique, 69364 Lyon Cedex 07, France. E-mail: alastuey@physique.ens-lyon.fr.

[2] Department of Mathematics, University of Melbourne, Parkville, Victoria 3052, Australia. E-mail: matpjf@maths.mu.oz.au.

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also required. For low densities and high temperature the two-dimensional Coulomb gas forms a conductive phase in which the positive and negative charges are dissociated and can screen a long-wavelength external charge density. In contrast, for low densities and low temperature, the system forms a dipole phase in which the positive and negative particles pair together. Perfect screening of a long-wavelength external charge will no longer occur.

Intricate structures of nested dipoles were hypothesized by Kosterlitz and Thouless[1] for the dominant configuration contributing to the polarization as the transition point is approached from the dipole phase. On the basis of this remarkable physical insight, an iterated mean-field theory was formulated and quantities of physical interest thereby calculated in the vicinity of the critical point. This so-called Kosterlitz–Thouless transition between the conductive and dielectric states occurs at the coupling $\Gamma = 4$ ($\Gamma := q^2/kT$) in the zero-density limit.

The nested dipole hypothesis and the iterated mean-field equations of Kosterlitz and Thouless were recently put on a firmer footing by Alastuey and Cornu,[2] who made a low-fugacity (ζ) analysis of the charge–charge correlation function and the dielectric constant ε for $\Gamma \to 4^+$. At order ζ^4 it was proved that the configurations giving the leading order contribution to $1/\varepsilon$ are the nested dipoles hypothesized by Kosterlitz and Thouless. Assuming this to be true at all orders, the low-fugacity series could be resummed, and the iterated mean-field equations of Kosterlitz and Thouless derived exactly.

The pairing transition from a conductive to a dielectric phase is not unique to the two-dimensional two-component Coulomb gas. One-component log-potential Coulomb gases also exhibit this transition, provided the neutralizing background consists of a lattice of oppositely charged particles[3] or there is no background and the system is in the vicinity of a conductive medium.[4] For the latter class of system a solvable model has been formulated which exhibits a pairing transition as a microscopic parameter is varied.[5] The model is the two-dimensional one-component plasma consisting of particles of positive charge only confined to a half-plane in the vicinity of a metal wall and subjected to a one-body external potential such that

$$e^{-\beta V(y)} = y^{-\alpha} \tag{1.1}$$

which acts in the direction perpendicular to the metal wall only. It is solvable at the special coupling $\Gamma = 2$, and exhibits a pairing transition as α is varied through one. It is our objective herein to use the exact solution as a testbench for the predictions of theoretical methods of analyzing the Kosterlitz–Thouless transition for this model.

We begin in Section 2 by considering the screening properties of the system with respect to an infinitesimal external dipole. In Section 3 the low-fugacity resummation technique of ref. 2 is applied to study the density profile in the dielectric phase near criticality, and the density profile is further analyzed using the first BGY equation. In Section 4 comparison of the theoretical predictions with the exact results is made. Concluding remarks are made in Section 5.

2. CHARACTERIZING THE PHASE

2.1. Definition of the Model

Consider a system of two-dimensional charges of strength q confined to a half-plane $y \geqslant d$ and suppose a perfect conductor occupies the half-plane $y \leqslant 0$. For each charge of strength q at position (x, y), say, in the system, the effect of the perfect conductor is to create an image charge of strength $-q$ at position $(x, -y)$. The electrostatic potential $\phi(\mathbf{r}, \mathbf{r}')$ experienced by a test particle of charge q at $\mathbf{r}' = (x', y')$ due to a particle of charge q at $\mathbf{r} = (x, y)$ is then

$$\phi(\mathbf{r}, \mathbf{r}') = q^2[v_c(|\mathbf{r} - \mathbf{r}'|) - v_c(|\mathbf{r} - \bar{\mathbf{r}}'|)] \tag{2.1a}$$

where

$$v_c(\mathbf{r} - \mathbf{r}') = -\log\{[(x - x')^2 + (y - y')^2]^{1/2}/L\} \quad \text{and} \quad \bar{\mathbf{r}} = (x, -y) \tag{2.1b}$$

For convenience the arbitrary length scale L henceforth will be set equal to unity. As well as interacting via the pair potential (2.1), the particles also experience a one-body potential with Boltzmann factor (1.1). Since the electrostatic potential $\phi(y)$ due to a background charge density $q\rho_b(y')$, $d \leqslant y' < \infty$, is given by

$$\phi(y) = -\pi q \int_d^\infty dy' \, [|y - y'| - (y + y')] \, \rho_b(y') \tag{2.2}$$

it is straightforward to check that the one-body potential given in (1.1) can be interpreted as being due to a background charge density

$$\rho_b(y') = \frac{\alpha}{2\pi\Gamma y'^2} \tag{2.3}$$

However, it is more convenient for our purposes below to interpret (1.1) as nonelectrical in origin, and making no contribution to the total charge density.

2.2. Response to an External Dipole

The conductor and dipole phases of the two-dimensional Coulomb gas can be distinguished by different screening properties of an infinitesimal external charge: the external charge is perfectly screened in the conductor phase, while only a fraction $1 - 1/\varepsilon$ is screened in the dipole phase. For Coulomb systems near a metal wall an external charge is automatically screened by its own image. We consider instead the screening of an infinitesimal dipole. The image of a dipole pointing perpendicular to a metal wall has the same magnitude and direction as the original dipole. A conductor phase should perfectly screen such an external dipole.

Let us use linear response theory to give a mathematical characterization of the screening of an external dipole. An external dipole at $\mathbf{r}_0 := (0, y_0)$ which is of strength p_0 and perpendicular to the metal wall adds to the Hamiltonian a term

$$H_{\text{ext}} = p_0 \left[\int_{\mathscr{D}} d\mathbf{r}' \frac{\partial}{\partial y_0} v_c(|\mathbf{r}' - \mathbf{r}_0|)\, Q(\mathbf{r}') + \int_{\mathscr{D}} d\mathbf{r}' \frac{\partial}{\partial \bar{y}_0} v_c(|\mathbf{r}' - \bar{\mathbf{r}}_0|)\, Q(\mathbf{r}') \right] \tag{2.4}$$

where $\bar{\mathbf{r}}_0 := (0, -y_0)$, $\bar{y}_0 := -y_0$, and $Q(\mathbf{r}')$ denotes the microscopic charge density at point $\mathbf{r}'$. The domain $\mathscr{D}$ is the half-plane $y \geqslant d$. According to linear response theory, the change in charge density at a point $\mathbf{r}$, $\delta q(\mathbf{r})$, say, due to the external dipole is given by

$$\delta q(\mathbf{r}) = -\beta[\langle H_{\text{ext}} Q \rangle - \langle H_{\text{ext}} \rangle \langle Q \rangle] \tag{2.5}$$

From (2.4) the r.h.s. of (2.5) can be written in terms of the charge–charge correlation

$$S(\mathbf{r}, \mathbf{r}') := \langle Q(\mathbf{r})\, Q(\mathbf{r}') \rangle - \langle Q(\mathbf{r}) \rangle \langle Q(\mathbf{r}') \rangle \tag{2.6}$$

as

$$\delta q(\mathbf{r}) = -\beta p_0 \int_{\mathscr{D}} d\mathbf{r}'\, S(\mathbf{r}, \mathbf{r}') \left\{ \frac{\partial}{\partial y_0} v_c(|\mathbf{r}' - \mathbf{r}_0|) + \frac{\partial}{\partial \bar{y}_0} v_c(|\mathbf{r}' - \bar{\mathbf{r}}_0|) \right\} \tag{2.7}$$

On the other hand, our characterization of the conductor phase as perfectly screening the dipole says

$$\int_{\mathscr{D}} d\mathbf{r}\; y\, \delta q(\mathbf{r}) = -p_0 \tag{2.8}$$

Substituting (2.7) in (2.8) gives the sum rule

$$\beta \int_{\mathscr{D}} d\mathbf{r}\, y \int_{\mathscr{D}} d\mathbf{r}'\, S(\mathbf{r}, \mathbf{r}') \left\{ \frac{\partial}{\partial y_0} v_c(|\mathbf{r}' - \mathbf{r}_0|) + \frac{\partial}{\partial \bar{y}_0} v_c(|\mathbf{r}' - \bar{\mathbf{r}}_0|) \right\} = 1 \tag{2.9}$$

to be obeyed by the system in the conductor phase.

The sum rule (2.9) can be further simplified. Now

$$\int_{\mathscr{D}} d\mathbf{r}\, y \int_{\mathscr{D}} d\mathbf{r}'\, S(\mathbf{r}, \mathbf{r}') \frac{\partial}{\partial y_0} v_c(|\mathbf{r}' - \mathbf{r}_0|) = \int_d^\infty dy\, y \frac{\partial}{\partial y_0} F(y_0, y) \tag{2.10a}$$

where

$$F(y_0, y) := \int_{-\infty}^\infty dx \int_{-\infty}^\infty dx' \int_d^\infty dy'\, S(y', y; x' - x) \times v_c(x' - x_0;\, y' - y_0) \tag{2.10b}$$

From the convolution formula for Fourier transforms we have

$$F(y_0, y) = \int_d^\infty dy'\, \tilde{S}(y', y; 0)\, \tilde{v}_c(0; y' - y_0) \tag{2.11}$$

In performing this step we are assuming that with y fixed, $S(x' - x;\, y', y)$ decays sufficiently as a function of y' and $x - x'$ for the integral in (2.10b) to be absolutely convergent and thus the order of integration to be unimportant. Next, it is a straightforward exercise to deduce from Poisson's equation

$$\nabla^2 v_c(|\mathbf{r}|) = -2\pi\delta(\mathbf{r}) \tag{2.12}$$

that

$$\tilde{v}_c(0; y' - y_0) = -\pi\, |y' - y_0| \tag{2.13}$$

Substituting (2.13) in (2.11) and then substituting the resulting expression in (2.10) and performing the differentiation gives

$$\int_{\mathscr{D}} d\mathbf{r}\, y \int_{\mathscr{D}} d\mathbf{r}'\, S(\mathbf{r}, \mathbf{r}') \frac{\partial}{\partial y_0} v_c(|\mathbf{r}' - \mathbf{r}_0|) = \pi \int_d^\infty dy\, y \int_d^\infty dy'\, \tilde{S}(y', y; 0)\, \mathrm{sgn}(y' - y_0) \tag{2.14}$$

Performing an analogous simplification on the second term on the l.h.s. of (2.9), we thus deduce that (2.9) is equivalent, subject to the clustering assumption for $S(x'-x;\, y', y)$ noted below (2.11), to the simpler sum rule

$$2\pi\beta \int_d^\infty dy\, y \int_{y_0}^\infty dy' \int_{-\infty}^\infty dx'\, S(y', y; x'-x) = 1 \tag{2.15}$$

This sum rule is to be satisfied in the conductive phase of any two-dimensional Coulomb system separated a distance d from a metal wall (when $y_0 = 0$ this result was obtained previously by Jancovici[6]).

A remarkable property of (2.15) is that it must hold for all positions $(0, y_0)$ of the external dipole. Differentiating with respect to y_0 and changing variables $x' \mapsto x' + x - x_0$, we thus have

$$\int_{\mathscr{D}} d\mathbf{r}\; yS(\mathbf{r}_0, \mathbf{r}) = 0 \tag{2.16}$$

Hence the perfect screening of an external dipole implies that the dipole moment of the internal screening cloud must vanish. For a phase which does not perfectly screen an external dipole, the sum rule (2.15) cannot hold. Rather, we would expect the l.h.s. to depend on y_0 and thus the dipole moment of the internal screening cloud will be nonzero.

2.3. Phase Transition and Potential Drop

In electrochemistry a fundamental quantity is the potential drop across the interface:

$$\Delta\phi = 2\pi q \int_d^\infty dy\; y\rho(y) \tag{2.17}$$

where $q\rho(y)$ denotes the total charge density at distance y from the interface. As previously noted,[5] the formula (2.17) exhibits a further interpretation of $\Delta\phi$: it is directly proportional to the mean distance between a particle and the metal wall, or equivalently the mean size of the particle–image pairs. Therefore, $\Delta\phi$ is expected to be finite in the insulator phase, while it should diverge in the conductor phase where the charges of the plasma are not paired by their own images. As seen from the integral expression (2.17), the finiteness of $\Delta\phi$ is closely related to the large-distance behavior of $\rho(y)$. In the insulator phase, $\rho(y)$ should decay as $1/y^{2+\varepsilon}$ $(\varepsilon > 0)$ when $y \to \infty$, while in the conductor phase $\rho(y)$ should decay typically as $1/y^2$ or slower. The relation between $\Delta\phi$ and the asymptotics of $\rho(y)$ will be studied in Section 3, by resumming the low-fugacity expansions.

The potential drop $\Delta\phi$, or the internal dipole moment

$$D(y_0) := 2\pi \int_{\mathscr{D}} d\mathbf{r}\; yS(\mathbf{r}_0, \mathbf{r}) \tag{2.18}$$

may be taken as equivalent indicators for characterizing the phase of the present model. A relation between both quantities can be obtained by starting with the compressibility sum rule

$$\zeta \frac{\partial \rho(y)}{\partial \zeta} = \frac{1}{q^2} \int_{-\infty}^{\infty} dx' \int_{d}^{\infty} dy'\; S(y, y'; x - x') \tag{2.19}$$

Taking the first moment of both sides gives

$$\zeta \int_{d}^{\infty} dy\; y \frac{\partial \rho(y)}{\partial \zeta} = \frac{1}{q^2} \int_{d}^{\infty} dy\; y \int_{-\infty}^{\infty} dx' \int_{d}^{\infty} dy'\; S(y, y'; x - x') \tag{2.20}$$

Next we want to interchange the order of the y and y' integrations on the r.h.s. and interchange the order of integration and differentiation on the l.h.s. From (2.17) and the explicit form of $S(y, y'; x - x')$ (see Section 4) we see that a necessary condition for the validity of both these operations is that $\Delta\phi$ be finite. Assuming this condition and the validity of the operations for the dipole phase, we obtain from (2.20), after using (2.17) and (2.18), the desired relationship:

$$\zeta \frac{\partial}{\partial \zeta} \Delta\phi = \frac{1}{q} \int_{d}^{\infty} dy'\; D(y') \tag{2.21}$$

This equation can only valid in the insulator phase, since in the conductor phase, the quantity on the r.h.s. of (2.20) is given by the universal value (2.15), so we have instead

$$\zeta \int_{d}^{\infty} dy\; y \frac{\partial \rho(y)}{\partial \zeta} = \frac{1}{2\pi\Gamma} \tag{2.22}$$

We stress that, in the conductor phase, the integrations over y and y' in the r.h.s. of (2.20) cannot be inverted. Otherwise, the corresponding integral, which also appears in the l.h.s. of (2.15), would vanish as a consequence of $D(y) = 0$. This non-absolute convergence is related to a slow decay of S for some configurations. At the same time, the differentiation with respect to ζ and the integration over y in the l.h.s. of (2.20) cannot be inverted either, because of a slow $1/y^2$ decay of $\rho(y)$ (see Section 3).

3. THE DENSITY PROFILE

A feature of the two-dimensional Coulomb gas is that all coefficients in the low-fugacity expansion of the pressure and correlation functions are convergent for $\Gamma \geqslant 4$.[7] This signals the transition from a conductive phase for $\Gamma < 4$ to an insulator phase for $\Gamma \geqslant 4$, in the zero-density limit. Similarly, by examining the second moment of the cluster integral for the density profile of a single particle, we expect that all the coefficients in the low-fugacity expansions for the model of Section 2.1 are convergent for $\Gamma + 2\alpha > 4$ and that this signals the transition from a conductive phase for $\Gamma + 2\alpha \leqslant 4$ to an insulator phase for $\Gamma + 2\alpha > 4$, in the zero-density limit. In this section the low-fugacity expansion for the density profile will be studied for $\Gamma + 2\alpha \to 4^+$, which is the limit of approaching the phase boundary from the dipole side, using the techniques introduced in ref. 2. More precisely, we will study the asymptotic density profile $\rho_{\Delta\phi}(y)$, which is defined as the portion of the low-fugacity expansion of $\rho(y)$ that gives the correct leading-order singular behavior of each term in the low-fugacity expansion of $\Delta\phi$, (2.17), in this limit.

Alastuey of Cornu[2] complemented their study of the low-fugacity expansions of the correlations in the dipole phase of the two-dimensional Coulomb gas by an analysis of the BGY equations. In Section 3.5 the first BGY equation is used to compute the leading asymptotic behavior of the density profile. Unlike the resummation of the low-fugacity expansion calculation, there is no underlying assumption that the phase of the model is near the critical point on the dipole side.

3.1. The Expansion at $O(\zeta^2)$

Suppose the model of Section 2.1 is generalized so that each particle is associated with a position-dependent fugacity $\zeta \mapsto \zeta(y)$ (or equivalently is subject to an extra one-body potential acting perpendicular to the interface). Denote the corresponding N-particle canonical partition function by Z_N and grand partition function by Ξ. Then from the formula

$$\rho(y) = \zeta \frac{\delta}{\delta\zeta(y)} \log \Xi \bigg|_{\zeta(y)=\zeta} \tag{3.1}$$

it is easy to show that

$$\rho(y) = \zeta \frac{\delta}{\delta\zeta(y)} Z_1 \bigg|_{\zeta(y)=\zeta} + \zeta^2 \left(2 \frac{\delta}{\delta\zeta(y)} Z_2 \bigg|_{\zeta(y)=\zeta} - Z_1 \frac{\delta}{\delta\zeta(y)} Z_1 \bigg|_{\zeta(y)=\zeta} \right) + O(\zeta^3) \tag{3.2}$$

Indeed (3.2) applies to any one-component system. Inserting the form of the partition functions for the model under consideration we have

$$\rho(y)=\frac{\zeta}{(2y)^{\Gamma/2}\,y^{\alpha}}+\frac{\zeta^2}{(2y)^{\Gamma/2}\,y^{\alpha}}\int_{-\infty}^{\infty}dx_1\int_{d}^{\infty}dy_1\,\frac{1}{(2y_1)^{\Gamma/2}\,y_1^{\alpha}}$$
$$\times\left\{\left(\frac{(x-x_1)^2+(y-y_1)^2}{(x-x_1)^2+(y+y_1)^2}\right)^{\Gamma/2}-1\right\}+O(\zeta^3) \tag{3.3}$$

Substituting the term of (3.3) proportional to ζ, $\rho^{(1)}(y)$, say, in (2.17), we find

$$\frac{\Delta\phi^{(1)}}{2\pi q}=\frac{\zeta 2^{-\Gamma/2}d^{-\Gamma/2-\alpha+2}}{\Gamma/2-\alpha+2} \tag{3.4}$$

(again, and below, we have used the superscript to indicate that only the term proportional to this power of ζ is being considered). Thus $\Delta\phi^{(1)}$ is singular in the limit $\Gamma+2\alpha\to 4^{+}$, and furthermore to leading order is independent of d. Both features are true of $\Delta\phi^{(n)}$ in general. The latter feature implies that only the large-y asymptotic portion of $\rho^{(n)}(y)$ contributes to the leading-order singular behavior of $\Delta\phi^{(n)}$, and thus $\rho^{(n)}_{\Delta\phi}(y)$ consists of terms in the asymptotic expansion of $\rho^{(n)}(y)$. With $n=1$, there is only one term, which is $\rho^{(1)}(y)$ itself, so trivially $\rho^{(1)}_{\Delta\phi}(y)=\rho^{(1)}(y)$.

Let us now determine the portion of the term of order ζ^2 in the low-density expansion of $\rho(y)$ which contributes to the leading-order singular behavior of $\Delta\phi$, and thus calculate $\rho^{(2)}_{\Delta\phi}(y)$. For this purpose we consider the double integral which is part of the coefficient of the ζ^2 term in (3.3) and analyze it for large y. We first break the integration over y_1 in the double integral in (3.3) into two intervals: $[d, y]$ and $[y, \infty]$. A change of variables $y_1\to yv_1$ shows that the latter interval of integration gives a contribution to the asymptotic expansion of $\rho^{(2)}(y)$ which is $O(y^{-\Gamma/2-\alpha-(\Gamma/2+\alpha-2)})$, and a corresponding contribution to $\Delta\phi^{(2)}$ which is $O(1/(\Gamma+2\alpha-4))$. For the interval $[d, y]$, use of the large-y expansion

$$\left(\frac{(x-x_1)^2+(y-y_1)^2}{(x-x_1)^2+(y+y_1)^2}\right)^{\Gamma/2}-1\sim-\frac{2\Gamma y_1 y}{x^2+y^2} \tag{3.5}$$

and integration over x gives a contribution to the asymptotic expansion of $\rho^{(2)}(y)$ of

$$\frac{\zeta^2}{(2y)^{\Gamma/2}\,y^{\alpha}}\int_{d}^{y}dy_1\,\mathscr{S}_y(y_1) \tag{3.6}$$

where

$$\mathscr{S}_y(y_1) := -\frac{2\pi\Gamma}{(2y_1)^{\Gamma/2}\, y_1^{\alpha-1}}, \qquad d \leqslant y_1 \leqslant y \tag{3.7}$$

Computing the integral, we find that (3.6) reads

$$-\frac{2\pi\Gamma\zeta^2}{2^\Gamma y^{\Gamma/2+\alpha}(\Gamma/2+\alpha-2)}\left(d^{-(\Gamma/2+\alpha-2)} - y^{-(\Gamma/2+\alpha-2)}\right) \tag{3.8}$$

Note that the first term in the last parentheses above is all that need be included for the leading-order asymptotic expansion of $\rho^{(2)}(y)$. However, both terms give a contribution to $\Delta\phi^{(2)}$ which is $O(1/(\Gamma+2\alpha-4)^2)$. Hence $\rho^{(2)}_{\Delta\phi}(y)$ is given by both terms in (3.8), or equivalently the integral formula (3.6). Following ref. 2, we can interpret the integral (3.6) as resulting from the partial screening of the fixed particle–image pair of separation $2y$ by the smaller pair of separation $2y_1$, via the operator (3.7).

3.2. Nested Dipole Hypothesis

Rather than attempt to calculate $\rho^{(n)}_{\Delta\phi}(y)$, $n \geqslant 3$, from the low-fugacity expansion (3.2), we make a nested dipole chain hypothesis, analogous in idea to that of Kosterlitz and Thouless[1] and technically to that of Alastuey and Cornu.[2] Technically we suppose all configurations contributing to $\rho^{(n)}_{\Delta\phi}(y)$ are nested chains of particle–image pairs, with the fixed particle–image pair the largest, and the screening operator acting between connected particles in the chain only. To specify the chains, we can ignore the images and consider the different ways of arranging the mobile particles into chains below the root particle at y. For example, at $O(\zeta^4)$ there are four distinct configurations, which are illustrated graphically in Fig. 1. The ordering $y \geqslant y_1 \geqslant y_2 \geqslant y_3 \geqslant d$ is equivalent to the nesting of the particle–image pairs so that each pair screens a pair of smaller size. The contributions to $\rho^{(4)}_{\Delta\phi}(y)$ from each graph are

$$\left[\int_d^y dy_1\, \mathscr{S}_y(y_1) \int_d^{y_1} dy_2\, \mathscr{S}_{y_1}(y_2)\right]\left[\int_d^y dy_1\, \mathscr{S}_y(y_1)\right]$$

$$\left[\int_d^y dy_1\, \mathscr{S}_y(y_1)\right]^3 .$$

$$\int_d^y dy_1\, \mathscr{S}_y(y_1)\left[\int_d^{y_1} dy_2\, \mathscr{S}_{y_1}(y_2)\right]^2$$

$$\int_d^y dy_1\, \mathscr{S}_y(y_1) \int_d^{y_1} dy_2\, \mathscr{S}_{y_1}(y_2) \int_d^{y_2} dy_3\, \mathscr{S}_{y_2}(y_3)$$

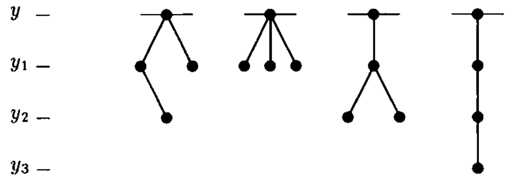

Fig. 1. Graphical representation of the four distinct chains at $O(\zeta^4)$.

respectively. Furthermore, the graphs need to be weighted by factors of 6, 1, 3, and 6, respectively, to account for relabeling degeneracy, and this linear combination then multiplied by an overall factor of $\zeta^4/[3!\,(2y)^{\Gamma/2}\,y^\alpha]$.

The nested structure allows the general terms of order n in ζ to be calculated by recurrence. As is shown in detail in ref. 2, Eqs. (4.26)–(4.28), we have

$$\rho_{\Delta\phi}^{(n)}(y)=\frac{\zeta}{(2y)^{\Gamma/2}\,y^\alpha}\,\frac{\zeta^{n-1}}{(n-1)!}\,S_{\Delta\phi}^{(n-1)}(y) \tag{3.9a}$$

where

$$S_{\Delta\phi}^{(n-1)}(y)=\sum_{p=1}^{n-1}\frac{(n-1)!}{p!\,(n-1-p)!}\times\sum_{\substack{q_\alpha\geqslant 0\\ q_1+\cdots+q_p=n-1-p}}\frac{(n-1-p)!}{q_1!\cdots q_p!}\,I_{q_1}(y)\cdots I_{q_p}(y) \tag{3.9b}$$

with

$$I_q(y)=\int_d^y dy'\,\mathscr{S}_y(y')\,S_{\Delta\phi}^{(q)}(y') \tag{3.9c}$$

Furthermore, it is shown in ref. 2 that $\rho_{\Delta\phi}^{(n-1)}(y)$ as given by this equation can be summed over n whatever the form of $\mathscr{S}_y(y')$, with the result

$$\rho_{\Delta\phi}(y)=\frac{\zeta}{(2y)^{\Gamma/2}\,y^\alpha}\exp\left[\int_d^y dy_1\,\mathscr{S}_y(y_1)(2y_1)^{\Gamma/2}\,y_1^\alpha\rho_{\Delta\phi}(y_1)\right] \tag{3.10}$$

Inserting the explicit form (3.7) gives the nonlinear integral equation

$$\rho_{\Delta\phi}(y)=\frac{\zeta}{(2y)^{\Gamma/2}\,y^\alpha}\exp\left[-2\pi\Gamma\int_d^y dy_1\,y_1\rho_{\Delta\phi}(y_1)\right] \tag{3.11}$$

which uniquely determines $\rho_{\Delta\phi}(y)$. Note that even though this equation was derived with the assumption $\Gamma + 2\alpha \to 4^+$ at each order in ζ, it is well defined for all values of $\Gamma + 2\alpha$.

3.3. Evaluation of $\rho_{\Delta\Phi}(y)$

By multiplying both sides of (3.11) by $y^{\Gamma/2+\alpha}$ and differentiating with respect to y we obtain the nonlinear differential equation

$$\frac{d}{dy} g(y) = -\frac{2\pi\Gamma}{y^{\Gamma/2+\alpha-1}} [g(y)]^2 \tag{3.12a}$$

where

$$g(y) := y^{\Gamma/2+\alpha} \rho_{\Delta\phi}(y) \tag{3.12b}$$

This is to be solved subject to the initial condition $\rho_{\Delta\phi}(d) = \zeta/[2d)^{\Gamma/2} d^{\alpha}]$, obtained by substituting $y = d$ in (3.11). Since the differential equation is first-order separable, the solution of the initial value problem is straightforward, and we find

$$\rho_{\Delta\phi}(y) = \frac{\zeta/(2y)^{\Gamma/2} y^{\alpha}}{1 + [2\pi\Gamma\zeta/2^{\Gamma/2}(\Gamma/2 + \alpha - 2)](d^{2-\Gamma/2-\alpha} - y^{2-\Gamma/2-\alpha})} \tag{3.13a}$$

provided $\Gamma + 2\alpha \neq 4$, while

$$\rho_{\Delta\phi}(y) = \frac{\zeta/(2y)^{\Gamma/2} y^{\alpha}}{1 + 2^{1-\Gamma/2}\pi\Gamma\zeta \log y} \tag{3.13b}$$

for $\Gamma + 2\alpha = 4$.

Inspection of (3.13a) shows that the exponents in the y-dependent terms of $\rho_{\Delta\phi}^{(n)}(y)$ depend on $\Gamma/2 + \alpha$ only. In particular there is no dependence on the fugacity ζ and consequently the phase transition will be independent of ζ. This behavior is to be contrasted with the two-dimensional Coulomb gas, in which the powers in the decay of the asymptotic charge–charge correlation at order $\zeta^{(2n)}$ [the quantity analogous to $\rho_{\Delta\phi}(y)$] are dependent on ζ and the phase transition is ζ dependent.

We can use the resummations (3.13) to calculate $\Delta\phi$ to all orders in ζ. First, from (2.17) we see that we require

$$\rho_{\Delta\phi}(y) = O\left(\frac{1}{y^{2+\varepsilon}}\right), \qquad \varepsilon > 0$$

for $\Delta\phi$ to be finite. Now from (3.13) we have

$$\rho_{\Delta\phi}(y) \sim \begin{cases} (2-\Gamma/2-\alpha)/2\pi\Gamma y^2, & \Gamma+2\alpha<4 \\ 1/(2\pi\Gamma y^2 \log y), & \Gamma+2\alpha=4 \\ c_{\zeta\Gamma\alpha}/y^{\Gamma/2+\alpha}, & \Gamma+2\alpha>4 \end{cases} \tag{3.14}$$

Hence $\Delta\phi$ is finite for $\Gamma+2\alpha>4$ (the dipole phase), and infinite for $\Gamma+2\alpha \leqslant 4$ (the conductor phase), independent of the fugacity ζ, as anticipated above.

The explicit value of $\Delta\phi$ in the insulator phase is given by computing the integral (2.17) with $\rho(y)$ replaced by (3.13a). We find

$$\frac{\Delta\phi}{2\pi q} = \frac{1}{2\pi\Gamma} \log\left[1 + \frac{2\pi\Gamma\zeta d^{2-\Gamma/2-\alpha}}{2^{\Gamma/2}(\Gamma/2+\alpha-2)}\right] \tag{3.15}$$

Again we emphasize that even though the intermediate steps leading to this result require $\Gamma+2\alpha \to 4^+$ at each order in ζ, (3.15) is well defined for all $\Gamma+2\alpha>4$.

3.4. Renormalization Flow Equation

In the two-dimensional Coulomb gas the renormalization flow equation relates the asymptotic charge–charge correlation to the space-dependent dielectric constant, with the space variable an implicit parameter. In the present model we can obtain a renormalization flow equation by relating $\rho_{\Delta\phi}(y)$ to

$$\Delta\phi(y) := 2\pi q \int_d^y dy_1\, y_1 \rho_{\Delta\phi}(y_1) \tag{3.16}$$

To do this we differentiate (3.16) and use the definition (3.12b) to obtain

$$\frac{d\Delta\phi(y)}{dy} = 2\pi q y^{1-\Gamma/2-\alpha} g(y) \tag{3.17}$$

Dividing (3.12a) and (3.17) then gives the desired equation

$$\frac{dg(y)}{d\Delta\phi(y)} = -\frac{\Gamma}{q} g(y) \tag{3.18}$$

This flow equation is subject to the initial condition $g(d) = 2^{-\Gamma/2}\zeta$ and $\Delta\phi(d) = 0$, and its exact solution is thus

$$g(y) = 2^{-\Gamma/2}\zeta e^{-\Gamma\Delta\phi(y)/q} \tag{3.19}$$

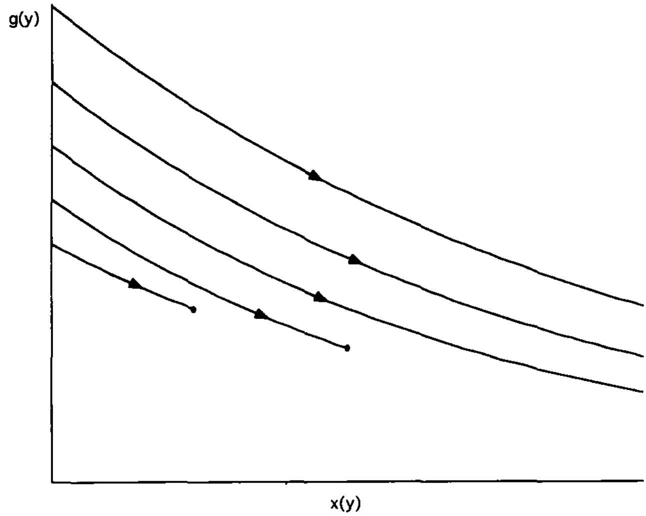

Fig. 2. The flow diagram, where we have written $x(y) := \Gamma\Delta(y)/q$. The different trajectories correspond to different values of $\Gamma + 2\alpha$. The trajectories terminate for $\Gamma + 2\alpha > 4$.

From (3.15), for $\Gamma + 2\alpha > 4$ the allowed values of $\Delta\phi(y)$ are in the finite interval $[0, \Delta\phi/2\pi q]$, while for $\Gamma + 2\alpha \leqslant 4$, $\Delta\phi(y)$ takes on all values in $[0, \infty[$. The flow diagram obtained from (3.19) thus has the appearance sketched in Fig. 2.

3.5. The First BGY Equation

In this subsection we will complement the above low-fugacity resummation study by an asymptotic analysis of the first BGY equation. Let us denote the force on a particle at $\mathbf{r}_1$ due to a particle at $\mathbf{r}_2$ by $\mathbf{F}_{21}$, so that

$$\mathbf{F}_{21} = -\nabla_1 \phi(\mathbf{r}_1, \mathbf{r}_2) \tag{3.20}$$

where $\phi(\mathbf{r}_1, \mathbf{r}_2)$ is given by (2.1a). Furthermore, denote the force on a particle at $\mathbf{r}_1$ due to the self-image particle and the one-body potential by $\mathbf{F}_1^{\text{im}}$ and $\mathbf{F}_1^{\text{ext}}$, respectively, so that

$$\mathbf{F}_1^{\text{im}} = -\frac{q^2}{2y_1}\mathbf{j} \qquad \text{and} \qquad \beta\mathbf{F}_1^{\text{ext}} = -\frac{\alpha}{y_1}\mathbf{j} \tag{3.21}$$

Then in terms of these forces the first BGY equation for the system is

$$\nabla_1 \rho(\mathbf{r}_1) = \beta\mathbf{F}_1^{\text{ext}}\rho(\mathbf{r}_1) + \beta\mathbf{F}_1^{\text{im}}\rho(\mathbf{r}_1) + \beta\int_{\mathscr{D}} d\mathbf{r}_2 \mathbf{F}_{21}\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \tag{3.22a}$$

Let us consider the y-components of this equation for $y_1 \to \infty$. We might expect that in this limit we can replace $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$ in the final term in (3.22a) by $\rho(\mathbf{r}_1)\,\rho(\mathbf{r}_2)$, which is equivalent to saying that if we write the final term in (3.22a) as

$$\beta \int_{\mathscr{D}} d\mathbf{r}_2 \mathbf{F}_{21} \rho(\mathbf{r}_1)\,\rho(\mathbf{r}_2) + \beta \int_{\mathscr{D}} d\mathbf{r}_2 \mathbf{F}_{21} \rho^{(2)T}(\mathbf{r}_1, \mathbf{r}_2) \tag{3.22b}$$

the term involving $\rho^{(2)T}(\mathbf{r}_1, \mathbf{r}_2)$ decays faster for large y_1 than the term involving $\rho(\mathbf{r}_1)\,\rho(\mathbf{r}_2)$ (which is a mean-field term), plus the one body forces on the r.h.s. of (3.22a). In the appendix this latter statement is proved subject to a mild clustering assumption. Thus, neglecting the second term in (3.22b), we are left with the mean-field-type equation

$$\frac{\partial}{\partial y_1} \rho(y_1) = \left[-\frac{\Gamma + 2\alpha}{2y_1} + \beta \int_{\mathscr{D}} d\mathbf{r}_2\, (F_{21})_y\, \rho(y_2) \right] \rho(y_1) \tag{3.23}$$

The integral over $\mathscr{D}$ in this equation can be simplified:

$$\begin{aligned}
&\int_{\mathscr{D}} d\mathbf{r}_2\, (F_{21})_y\, \rho(y_2) \\
&\quad = -q^2 \int_{-\infty}^{\infty} dx_2 \int_d^{\infty} dy_2 \left[\frac{\partial}{\partial y_1} v_c(|\mathbf{r}_1 - \mathbf{r}_2|) + \frac{\partial}{\partial \bar{y}_1} v_c(|\bar{\mathbf{r}}_1 - \mathbf{r}_2|) \right] \rho(y_2) \\
&\quad = -q^2 \int_d^{\infty} dy_2 \left[\frac{\partial}{\partial y_1} \tilde{v}_c(0;\, y_1 - y_2) - \frac{\partial}{\partial y_1} \tilde{v}_c(0;\, y_1 + y_2) \right] \rho(y_2) \\
&\quad = -2\pi q^2 \int_{y_1}^{\infty} dy_2\, \rho(y_2)
\end{aligned}$$

(this result can also be derived from Gauss's theorem in electrostatics). The mean-field equation now reads

$$\frac{\partial}{\partial y_1} \rho(y_1) = \left[-\frac{\Gamma + 2\alpha}{2y_1} - 2\pi\Gamma \int_{y_1}^{\infty} dy_2\, \rho(y_2) \right] \rho(y_1) \tag{3.24}$$

To solve this equation for large y_1 we seek a solution of the form

$$\rho(y_1) \sim \frac{c}{y_1^p} \tag{3.25}$$

Substituting this in (3.24) gives

$$-\frac{pc}{y_1^{p+1}} \sim -\frac{(\Gamma + 2\alpha)\,c}{2y_1^{p+1}} - \frac{2\pi\Gamma c^2}{(p-1)\, y_1^{2p-1}} \tag{3.26}$$

For $p > 2$ the second term on the right-hand side of (3.26) can be ignored and we obtain a solution provided

$$p = (\Gamma + 2\alpha)/2 \qquad (\text{and thus } \Gamma + 2\alpha > 4) \tag{3.27a}$$

For $p = 2$, (3.25) is an exact solution of (3.24) provided

$$c = \frac{4 - \Gamma - 2\alpha}{4\pi\Gamma} \qquad \text{and} \qquad \Gamma + 2\alpha < 4 \tag{3.27b}$$

For $\Gamma + 2\alpha = 4$ we find, after equating the first two orders on both sides of (3.24), that

$$\rho(y_1) \sim \frac{1}{2\pi\Gamma y_1^2 \log y_1} \tag{3.27c}$$

is an asymptotic solution.

We emphasize that the above analysis is asymptotically exact and nonperturbative: the asymptotic formulas obtained hold for all values of Γ, α, and ζ. As such, we can use these results to test the predictions (3.14) for the leading asymptotics of $\rho(y)$ as derived from $\rho_{\Delta\phi}(y)$. Surprisingly, the results obtained from $\rho_{\Delta\phi}(y)$ are in complete agreement with the nonperturbative exact results, even though it has been assumed in the derivation of $\rho_{\Delta\phi}(y)$ that the phase of the model is near the zero-fugacity critical point on the dipole side.

4. COMPARISON WITH THE SOLVABLE CASE

4.1. The Phase

When $\Gamma = 2$ the model of Section 2.2 is exactly solvable for all α.[5] The exact expressions for the density profile and truncated two-particle distribution function are

$$\rho(y) = 2\pi\zeta y^{-\alpha} \int_0^\infty dt \, \frac{e^{-4\pi y t}}{1 + 2\pi\zeta \int_d^\infty dY \, Y^{-\alpha} e^{-4\pi Y t}} \tag{4.1}$$

and

$$\rho^T(\mathbf{r}_1, \mathbf{r}_2) = -(2\pi\zeta)^2 (y_1 y_2)^{-\alpha} \left| \int_0^\infty dt \, \frac{e^{2\pi i x t} e^{-2\pi(y_1 + y_2)t}}{1 + 2\pi\zeta \int_d^\infty dY \, Y^{-\alpha} e^{-4\pi Y t}} \right|^2 \tag{4.2}$$

These expressions were used in ref. 5 to show that for $\alpha \leqslant 1$ the dipole moment of the internal screening cloud $D(y_0)$ as defined by (2.18) vanishes, while for $\alpha > 1$ it is nonzero. This behavior was interpreted as indicating that the system exhibits a conductive phase for $\alpha \leqslant 1$ and an insulator phase for $\alpha > 1$. In Section 2.2 we showed that the true indicator of a conductive phase is the sum rule (2.15), and the vanishing of $D(y_0)$ in a conductive phase is a corollary of this stronger requirement.

Noting that for a one-component system

$$S(y, y'; x-x') = q^2[\rho(y')\,\delta(x-x')\,\delta(y-y') + \rho^T(y, y'; x-x')] \tag{4.3}$$

and using the exact results (4.1) and (4.2), it is a straightforward exercise to show

$$2\pi\beta \int_d^\infty dy\, y \int_{y_0}^\infty dy' \int_{-\infty}^\infty dx'\, S(y, y'; x-x') = 1 - \frac{1 + 2\pi\zeta \int_d^{y_0} dY\, Y^{-\alpha}}{1 + 2\pi\zeta \int_d^\infty dY\, Y^{-\alpha}} \tag{4.4}$$

For $\alpha \leqslant 1$ the second term on the r.h.s. of (4.4) vanishes and the sum rule (2.15) holds, thus implying a conductive phase. For $\alpha > 1$, (2.15) is not obeyed, so the phase is an insulator. These conclusions are in agreement with those reached in ref. 5.

In Section 3.3 we have shown that the potential drop $\Delta\phi$ diverges for $\Gamma + 2\alpha \leqslant 4$ but is finite for $\Gamma + 2\alpha > 4$. In accordance with the interpretation of the formula (2.17) as saying $\Delta\phi$ is proportional to the mean distance of separation within the dipole formed by a particle and its image, we have taken this behavior to be an alternative phase indicator to the sum rule (2.15) for this system. For the solvable model we have the exact result[5]

$$\frac{\Delta\phi}{2\pi q} = \frac{1}{4\pi} \log\left(1 + 2\pi\zeta \frac{d^{1-\alpha}}{\alpha - 1}\right), \qquad \alpha > 1 \tag{4.5}$$

Remarkably, the expression for $\Delta\phi$, (3.15), with $\Gamma = 2$ deduced from the asymptotic density profile $\rho_{\Delta\phi}(y)$ is in precise agreement with this exact expression.

4.2. The Asymptotic Density $\rho_{\Delta\phi}(y)$

The asymptotic density $\rho_{\Delta\phi}(y)$ is defined as the portion of the asymptotic expansion of $\rho(y)$ that gives the correct singular behavior of $\Delta\phi$ as $\Gamma + 2\alpha \to 4^+$ at each order in ζ. From (4.1) we can calculate $\rho_{\Delta\phi}(y)$ exactly at $\Gamma = 2$.

Expanding (4.1) as a power series in ζ and then performing the integration over t gives

$$\rho(y)=\frac{\zeta}{2y^{\alpha+1}}\sum_{j=0}^{\infty}(-2\pi\zeta)^j\, y^{-j(\alpha+1)}$$
$$\times\int_{[d/y,\,\infty]^j}\frac{dY_1}{Y_1^\alpha}\cdots\frac{dY_j}{Y_j^\alpha}(Y_1+\cdots+Y_j+1)^{-1} \tag{4.6}$$

For large y the final factor in the integral can be approximated by 1 and we obtain

$$\rho(y)\sim\frac{\zeta}{2y^{\alpha+1}}\sum_{j=0}^{\infty}(-2\pi\zeta)^j\, y^{-j(\alpha+1)}\left\{\left(\frac{(y/d)^{\alpha-1}-1}{\alpha-1}\right)^j\right.$$
$$\left.+O\left([\alpha-1]^{-j+1}\left[\frac{y}{d}\right]^{j(\alpha-1)-1}\right)\right\} \tag{4.7}$$

The correction term in the asymptotic expansion above does not contribute to $\rho_{\Delta\phi}(y)$. Ignoring this term, we see that a geometric series remains, which after summation gives

$$\rho_{\Delta\phi}(y)=\frac{\zeta/2y^{\alpha+1}}{1+2\pi[\zeta/(\alpha-1)](d^{1-\alpha}-y^{1-\alpha})} \tag{4.8}$$

Comparison of this exact result at $\Gamma=2$ with the result (3.13a) obtained from the low-fugacity resummation using the nested dipole chain hypothesis shows that the resummation is exact at this coupling.

4.3. Leading Asymptotics of Density Profile

As noted in ref. 5, the leading large-y behavior of the density profile at $\Gamma=2$ is readily computed from (4.1). We find precise agreement with the behavior (3.14) at $\Gamma=2$, which is obtained from both the low-fugacity resummation and the mean-field equation.

It is interesting to note that since the asymptotic form of the density profile in the conductive phase is

$$\rho(y)\sim\frac{4-\Gamma-2\alpha}{4\pi\Gamma y^2} \tag{4.9}$$

The phase transition occurs when the $1/y^2$ tail vanishes.

5. CONCLUSION

The metal wall one-component plasma model of Section 2.1 exhibits both a conductive and an insulating phase. It has the special property of admitting an exact solution for the thermodynamics and all correlations along the line $(\Gamma, \alpha) = (2, \alpha)$ in parameter space.[5] This line intersects the transition line $\Gamma + 2\alpha = 4$. For general values of the parameters the transition can be analyzed in a similar way to the Kosterlitz–Thouless transition in the two-dimensional Coulomb gas.[2] In particular, by making a hypothesis that the dominant configurations are nested dipole chains [this is checked explicitly at $O(\zeta^2)$], we can resum the low-fugacity expansion of the asymptotic density $\rho_{\Delta\phi}(y)$ and calculate it explicitly as the solution of a nonlinear differential equation.

Comparison with exact solution verifies that the general expression for $\rho_{\Delta\phi}(y)$ is exact at $\Gamma = 2$. This provides compelling evidence for the correctness of the underlying nested dipole chain hypothesis. Since the nested dipole chain hypothesis also underlies the iterated mean-field equations of Kosterlitz and Thouless[1] (which are equivalent to the Kosterlitz renormalization equations[8]), we have also added further weight to the validity of these equations.

APPENDIX

In this appendix, we will prove that in the limit $y_1 \to \infty$ the second term in (3.22b),

$$\mathscr{F}_1^{(2)} := \beta \int_{\mathscr{S}} d\mathbf{r}_2 \, \mathbf{F}_{21} \rho_{(2)}^T(\mathbf{r}_1, \mathbf{r}_2) \tag{A1}$$

decays faster than the sum of the first term and the one-body terms on the r.h.s. of the BGY equation (3.22a), and therefore can be neglected in this limit. Our analysis is based on the simple assumption that for some $1 > \varepsilon > 0$

$$|\rho_{(2)}^T(\mathbf{r}_1, \mathbf{r}_2)| < \rho(\mathbf{r}_1)\, \rho(\mathbf{r}_2) \left(\frac{l}{|\mathbf{r}_1 - \mathbf{r}_2|} \right)^{\varepsilon} \tag{A2}$$

where l is a given length. We stress that the hypothesis (A2) is very reasonable since it merely asserts that the Ursell function $\rho_{(2)}^T(\mathbf{r}_1, \mathbf{r}_2)/[\rho(\mathbf{r}_1)\, \rho(\mathbf{r}_2)]$ decays for large separations $|\mathbf{r}_1 - \mathbf{r}_2|$ at least as fast as an inverse power. This weak clustering property surely holds in any homogeneous or inhomogeneous fluid phase.

Using (A2) and the inequality $|y_2 - y_1| \leqslant |\mathbf{r}_2 - \mathbf{r}_1|$, we find

$$|\mathscr{F}_1^{(2)}| < 2\Gamma\rho(y_1) \int_{\mathscr{D}} d\mathbf{r}_2\, \rho(y_2) \left(\frac{l}{|y_2 - y_1|}\right)^{\varepsilon} y_2 \\ \times \frac{1}{[(x_2-x_1)^2 + (y_2-y_1)^2]^{1/2}\, [(x_2-x_1)^2 + (y_2+y_1)^2]^{1/2}} \tag{A3}$$

In the integral on the r.h.s. of (A3), we can perform the integration over x_2 according to[9]

$$\int_{-\infty}^{\infty} dx_2 \frac{1}{[(x_2-x_1)^2 + (y_2-y_1)^2]^{1/2}\, [(x_2-x_1)^2 + (y_2+y_1)^2]^{1/2}} \\ = \frac{2}{(y_2+y_1)} K\left(\frac{2(y_2 y_1)^{1/2}}{y_2+y_1}\right) \tag{A4}$$

where $K(k)$ is the complete elliptic integral of the first kind

$$K(k) = \int_0^{\pi/2} \frac{d\phi}{(1-k^2\sin^2\phi)^{1/2}}$$

By splitting the domain of integration over y_2 into the intervals $[d, y_1/2]$ and $[y_1/2, \infty[$, we then find from (A3)

$$|\mathscr{F}_1^{(2)}| < 4\Gamma K\left(\frac{2\sqrt{2}}{3}\right)\left(\frac{2l}{y_1}\right)^{\varepsilon} \frac{\rho(y_1)}{y_1} \int_d^{y_1/2} dy_2\, y_2 \rho(y_2) \\ + 4\Gamma\rho(y_1) \int_{y_1/2}^{\infty} dy_2\, \rho(y_2) \left(\frac{l}{|y_2-y_1|}\right)^{\varepsilon} K\left(\frac{2(y_2 y_1)^{1/2}}{y_2+y_1}\right) \tag{A5}$$

[we have also used the monotonicity of $K(k)$].

For y_1 large, $\rho(y_1)$ is expected to decay as c/y_1^p, with $p \geqslant 2$ (this is shown explicitly in Section 3.5). The integral

$$\int_d^{y_1/2} dy_2\, y_2 \rho(y_2)$$

then remains bounded by some constant times $\log(y_1)$. Therefore the first term on the r.h.s. of (A5) decays at least as fast as $\log(y_1)/y_1^{p+1+\varepsilon}$, which is faster than the one-body self-image and external potential terms ($\sim 1/y_1^{p+1}$) appearing on the r.h.s. of the BGY equation (3.22a). Also, the integral

$$\int_{y_1/2}^{\infty} dy_2\, \rho(y_2) \left(\frac{l}{|y_2-y_1|}\right)^{\varepsilon} K\left(\frac{2(y_2 y_1)^{1/2}}{y_2+y_1}\right)$$

remains bounded by a constant times $1/y_1^{p-1+\varepsilon}$, as shown by the variable change $y_2 = \alpha y_1$. Indeed, the dimensionless integral

$$\int_{1/2}^{\infty} d\alpha \, \frac{1}{\alpha^p \, |\alpha - 1|^{\varepsilon}} \, K\left(\frac{2\alpha^{1/2}}{\alpha + 1}\right)$$

is finite because the singularity of $K(2\alpha^{1/2}/(\alpha + 1))$ at $\alpha = 1$ is only logarithmic:

$$K(2\alpha^{1/2}/(\alpha + 1)) \sim -\log |\alpha - 1|$$

when $\alpha \to 1$. Then, the second term on the r.h.s. of (A5) decays at least as fast as $1/y_1^{2p-1+\varepsilon}$, which is faster than the decay of the first term in (3.22b) ($\sim 1/y_1^{2p-1}$). Thus the whole two-body force (A1) can be neglected with respect to the other terms of the BGY equation (3.22a) in the limit $y_1 \to \infty$.

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