



Another derivation of a sum rule for the two-dimensional two-component plasma

B. Jancovici^{a,*}, P. Kalinay^{b,1}, L. Šamaj^{b,1}

^aLaboratoire de Physique Théorique, Unité Mixte de Recherche no. 8627-CNRS, Université de Paris-Sud, Bâtiment 210, 91405 Orsay Cedex, France

^bInstitute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 842 28 Bratislava, Slovakia

Abstract

In a two-dimensional two-component plasma, the second moment of the *number density* correlation function has the simple value $\{12\pi[1-(\Gamma/4)]^2\}^{-1}$, where Γ is the dimensionless coupling constant. This result is derived directly by using diagrammatic methods. © 2000 Elsevier Science B.V. All rights reserved.

Dedicated to Joel Lebowitz on the occasion of his 70th birthday

1. Introduction

The system under consideration is the two-dimensional ($2d$) two-component plasma (TCP) (Coulomb gas), i.e., a system of positive and negative point-particles of charge $\pm q$, in a plane. Two particles at a distance r from each other interact through the $2d$ Coulomb interaction $\mp q^2 \ln(r/L)$, where L is some irrelevant length (set to unity, for simplicity). Classical equilibrium statistical mechanics is used. The dimensionless coupling constant is $\Gamma = \beta q^2$, where $\beta = 1/kT$ is the inverse temperature. The system is known to be stable against collapse when $\Gamma < 2$. Let $\langle \hat{n}(\mathbf{0})\hat{n}(\mathbf{r}) \rangle_T$ be the truncated density–density correlation function, where $\hat{n}(\mathbf{r})$ is the total microscopic number density at \mathbf{r} .

In a recent paper [1], an exact expression for the second moment of that density–density correlation function has been derived:

$$\int \langle \hat{n}(\mathbf{0})\hat{n}(\mathbf{r}) \rangle_T r^2 d^2\mathbf{r} = \frac{1}{12\pi(1-(\Gamma/4))^2}. \quad (1)$$

* Corresponding author.

E-mail addresses: bernard.jancovici@th.u-psud.fr (B. Jancovici), fyzipali@nic.savba.sk (P. Kalinay), fyzimaes@nic.savba.sk (L. Šamaj)

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However, the two alternative derivations which were given were rather indirect ones, and the Conclusion of the paper had the sentence “A more direct derivation is still wanted”. At about the same time, another paper [2] used a diagrammatic method for deriving an exact expression for the sixth moment of the pair correlation function of the $2d$ one-component plasma (OCP). The authors of both papers soon realized that the diagrammatic method of Ref. [2] could be easily adapted to the two-component case and used for providing a more direct derivation of (1), which is the main content of the present paper.

The paper is organized as follows. In Section 2, we generalize a renormalized Mayer expansion [2,3], to the case of a many-component fluid. The application of the formalism to the $2d$ TCP in Section 3 leads, with the aid of the results obtained in Ref. [2], to the sum rule (1) for the density correlation function. The charge correlation function is discussed in Section 4. Section 5 deals with consequences on finite-size effects for the sphere geometry, confirming predictions from conformal invariance [4,5].

2. Renormalized Mayer expansion for many-component fluids

We first consider a general classical multi-component fluid in thermodynamic equilibrium. The last system is composed of distinct species of particles $\{\sigma\}$ with the corresponding densities $\{n(\mathbf{r}, \sigma)\}$ at vector position \mathbf{r} of a d -dimensional space. The particles interact through the pair potential $v(\mathbf{r}_i, \sigma_i | \mathbf{r}_j, \sigma_j)$ which depends on the mutual distance of particles i, j as well as on their types σ_i, σ_j . Vector \mathbf{r}_i will be represented simply by i .

According to the Mayer diagrammatic formalism in density [6], the generalization from one-component to more-than-one component fluid consists in considering an additional particle-type label σ for each, field (black) or root (white), vertex. Simultaneously, besides the integration over spatial coordinate of a field circle, the summation over all σ -states at this vertex is assumed as well. The renormalized Mayer representation of the (excess) Helmholtz free energy [2], resulting from the expansion of each Mayer function in the inverse temperature and the consequent series elimination of two-coordinated field circles between every couple of three- or more-coordinated field circles (by coordination of a circle we mean its bond-ordination, i.e., the number of bonds meeting at this circle), can therefore be straightforwardly extended to the many-component case. The renormalized K -bonds are now given by

$$K_{1, \sigma_1 2, \sigma_2} = -\beta v_{1, \sigma_1 2, \sigma_2} + \text{diagram with 3 bonds} + \text{diagram with 4 bonds} + \dots$$

or, algebraically,

$$K(1, \sigma_1 | 2, \sigma_2) = [-\beta v(1, \sigma_1 | 2, \sigma_2) + \sum_{\sigma_3} \int [-\beta v(1, \sigma_1 | 3, \sigma_3)] n(3, \sigma_3) K(3, \sigma_3 | 2, \sigma_2) d3] \tag{2}$$

The procedure of the bond-renormalization transforms the ordinary graphical Mayer representation of the free energy into

$$\beta \bar{F}^{ex}[n] = \bullet \text{---} \bullet + D^{(0)}[n] + \sum_{s=1}^{\infty} D^{(s)}[n], \tag{3a}$$

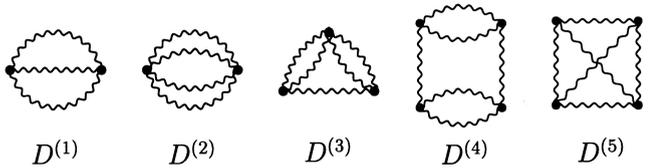
where \bar{F}^{ex} is minus the excess free energy,

$$D^{(0)} = \text{---} + \text{---} + \text{---} + \dots \tag{3b}$$

is the sum of all unrenormalized ring diagrams (which cannot undertake the renormalization procedure because of the absence of three- or more-coordinated field points) and

$$\sum_{s=1}^{\infty} D^{(s)} = \{ \text{all connected diagrams which consist of } N \geq 2 \text{ field } n(i, \sigma_i)\text{-circles of (bond) coordination } \geq 3 \text{ and multiple } K(i, \sigma_i | j, \sigma_j)\text{-bonds, and are free of connecting circles} \} \tag{3c}$$

represents the set of all remaining completely renormalized graphs. By multiple K -bonds we mean the possibility of an arbitrary number of K -bonds between a couple of field circles, with the topological factor $1/(\text{number of bonds})!$. The order of s -enumeration is irrelevant, let us say



$$D^{(1)} \quad D^{(2)} \quad D^{(3)} \quad D^{(4)} \quad D^{(5)}, \tag{4}$$

etc.

The truncated pair correlation

$$h(1, \sigma_1 | 2, \sigma_2) = \frac{n_2(1, \sigma_1 | 2, \sigma_2)}{n(1, \sigma_1)n(2, \sigma_2)} - 1 \tag{5}$$

is related to the pair direct correlation c via the Ornstein–Zernike (OZ) equation

$$h(1, \sigma_1 | 2, \sigma_2) = c(1, \sigma_1 | 2, \sigma_2) + \sum_{\sigma_3} \int c(1, \sigma_1 | 3, \sigma_3) n(3, \sigma_3) h(3, \sigma_3 | 2, \sigma_2) d3. \tag{6}$$

The free energy is the generating functional for c in the sense that

$$c(1, \sigma_1 | 2, \sigma_2) = \frac{\delta^2(\beta \bar{F}^{ex})}{\delta n(1, \sigma_1) \delta n(2, \sigma_2)}. \tag{7}$$

According to (3), the direct correlation is thus written as

$$c(1, \sigma_1 | 2, \sigma_2) = \text{diagram} + c^{(0)}(1, \sigma_1 | 2, \sigma_2) + \sum_{s=1}^{\infty} c^{(s)}(1, \sigma_1 | 2, \sigma_2), \tag{8a}$$

where $c^{(0)}(1, \sigma_1 | 2, \sigma_2) = \delta^2 D^{(0)} / \delta n(1, \sigma_1) \delta n(2, \sigma_2)$ can be readily shown to correspond to the renormalized Meeron graph

$$c^{(0)}(1, \sigma_1 | 2, \sigma_2) = \text{diagram} = \frac{1}{2!} K^2(1, \sigma_1 | 2, \sigma_2) \tag{8b}$$

and

$$c^{(s)}(1, \sigma_1 | 2, \sigma_2) = \frac{\delta^2 D^{(s)}}{\delta n(1, \sigma_1) \delta n(2, \sigma_2)} \tag{8c}$$

($s = 1, 2, \dots$) denotes the whole family of $(1, \sigma_1) | (2, \sigma_2)$ -rooted diagrams generated from $D^{(s)}$. To get explicitly a direct-correlation family, one has to take into account the functional dependence of the dressed K -bonds (2) on the density, too. It is straightforward to verify by variation of (2) that it holds

$$\frac{\delta K(1, \sigma_1 | 2, \sigma_2)}{\delta n(3, \sigma_3)} = K(1, \sigma_1 | 3, \sigma_3) K(3, \sigma_3 | 2, \sigma_2). \tag{9}$$

As a consequence, the functional derivative of $D^{(s)}$ with respect to the density generates root-circles, besides the field-circle positions, also on K -bonds, causing their “correct” K–K division. For example, in the case of the generator $D^{(1)}$ drawn in (4), we obtain

$$c^{(1)}(1, \sigma_1 | 2, \sigma_2) = \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \text{diagram 5} \tag{10}$$

3. Density correlations in the 2d TCP

Let us now concentrate on the neutral $2d$ TCP of positive ($\sigma = +$) and negative ($\sigma = -$) charges, with the Coulomb interaction energy given by

$$-\beta v(i, \sigma_i | j, \sigma_j) = \sigma_i \sigma_j \Gamma \ln |i - j|. \tag{11}$$

We consider the infinite-volume limit, characterized by homogeneous densities $n(1, \sigma) = n_\sigma$ and both isotropic and translationally invariant two-body correlations, $c(1, \sigma_1 | 2, \sigma_2) =$

$c_{\sigma_1\sigma_2}(|1 - 2|), h(1, \sigma_1|2, \sigma_2) = h_{\sigma_1\sigma_2}(|1 - 2|)$. The requirement of the charge neutrality, $n_+ = n_- = n/2$ (n is the total number density of particles), automatically implies the symmetry with respect to the $+ \leftrightarrow -$ interchange of the charge,

$$h_{++} = h_{--} \quad (=h_+), \quad h_{+-} = h_{-+} \quad (=h_-), \tag{12a}$$

$$c_{++} = c_{--} \quad (=c_+), \quad c_{+-} = c_{-+} \quad (=c_-). \tag{12b}$$

Thus, in Fourier space

$$f(\mathbf{r}) = \frac{1}{2\pi} \int \exp(i\mathbf{k} \cdot \mathbf{r}) \hat{f}(\mathbf{k}) d^2\mathbf{k}, \tag{13a}$$

$$\begin{aligned} \hat{f}(\mathbf{k}) &= \frac{1}{2\pi} \int \exp(-i\mathbf{k} \cdot \mathbf{r}) f(\mathbf{r}) d^2\mathbf{r} \\ &= \sum_{s=0}^{\infty} \frac{(-1)^s}{(s!)^2} \left(\frac{k^2}{4}\right)^s \frac{1}{2\pi} \int f(r) r^{2s} d^2\mathbf{r}, \end{aligned} \tag{13b}$$

the OZ equation (6) implies

$$\hat{h}_+(k) = \hat{c}_+(k)[1 + \pi n \hat{h}_+(k)] + \pi n \hat{c}_-(k) \hat{h}_-(k), \tag{14a}$$

$$\hat{h}_-(k) = \hat{c}_-(k)[1 + \pi n \hat{h}_+(k)] + \pi n \hat{c}_+(k) \hat{h}_-(k), \tag{14b}$$

where $k = |\mathbf{k}|$. Introducing

$$h = \frac{1}{4} \sum_{\sigma, \sigma'=\pm} h_{\sigma\sigma'} = \frac{1}{2}(h_+ + h_-), \tag{15a}$$

$$c = \frac{1}{4} \sum_{\sigma, \sigma'=\pm} c_{\sigma\sigma'} = \frac{1}{2}(c_+ + c_-), \tag{15b}$$

the summation of (14a) and (14b) yields

$$\hat{h}(k) = \hat{c}(k) + 2\pi n \hat{c}(k) \hat{h}(k). \tag{16}$$

In the renormalized format, due to the translational invariance of renormalized bonds $K(1, \sigma_1|2, \sigma_2) = K_{\sigma_1\sigma_2}(|1 - 2|)$, the Fourier transformation of relation (2) results in

$$\hat{K}_{\sigma\sigma'}(k) = [-\beta \hat{v}_{\sigma\sigma'}(k)] + 2\pi \sum_{\sigma''=\pm} [-\beta \hat{v}_{\sigma\sigma''}(k)] n_{\sigma''} \hat{K}_{\sigma''\sigma'}(k). \tag{17}$$

With regard to

$$-\beta \hat{v}_{\sigma\sigma'}(k) = -\sigma\sigma' \Gamma/k^2, \tag{18}$$

Eq. (17) yields

$$\hat{K}_{\sigma\sigma'}(k) = -\sigma\sigma' \frac{\Gamma}{k^2 + 2\pi\Gamma(n_+ + n_-)}, \tag{19a}$$

$$K_{\sigma\sigma'}(r) = -\sigma\sigma' \Gamma K_0[r\sqrt{2\pi\Gamma(n_+ + n_-)}] \tag{19b}$$

with K_0 being the modified Bessel function of second kind. The pair direct correlation (8) is expressible as

$$c_{\sigma_1\sigma_2}(|1-2|) = \sigma_1\sigma_2 \ln|1-2| + \frac{1}{2}[\Gamma K_0(|1-2|\sqrt{2\pi\Gamma n})]^2 + \sum_{s=1}^{\infty} c_{\sigma_1\sigma_2}^{(s)}(|1-2|). \tag{20}$$

c , Eq. (15b), is then given by

$$c(|1-2|) = \frac{1}{2}[\Gamma K_0(|1-2|\sqrt{2\pi\Gamma n})]^2 + \sum_{s=1}^{\infty} c^{(s)}(|1-2|), \tag{21a}$$

where

$$c^{(s)}(|1-2|) = \frac{1}{4} \sum_{\sigma_1, \sigma_2 = \pm} c_{\sigma_1\sigma_2}^{(s)}(|1-2|) \\ = \frac{1}{4} \sum_{\sigma_1, \sigma_2 = \pm} \left. \frac{\delta^2 D^{(s)}}{\delta n(1, \sigma_1) \delta n(2, \sigma_2)} \right|_{n(r, \sigma) = n/2}. \tag{21b}$$

As concerns the evaluation of $c^{(s)}$, because of the symmetry $K_{\sigma, \sigma} = -K_{\sigma, -\sigma}$, it is rather obvious that for $n_+ = n_-$ the summation on signs gives a non-vanishing $c^{(s)}$ only if all the vertices of the generator $D^{(s)}$ have an even bond-coordination [note that after the functional derivation (21b), with regard to (9), all the white circles will also have an even bond-coordination]. Furthermore the resulting $c^{(s)}$ is the same as in the case of the OCP with particle density $n_+ + n_- = n$. It was proven in Ref. [2] that the zeroth- and second-moments of such a $c^{(s)}$ vanish independently of the topology of $D^{(s)}$, so that

$$\hat{c}^{(s)}(k) = O(k^4). \tag{22}$$

To summarize, using formula [7]

$$\int_0^{\infty} K_0^2(x) x^{1+2s} dx = 2^{(2s-1)} \frac{(s!)^4}{(2s+1)!} \quad (s \geq 0), \tag{23}$$

in the Fourier representation (13b) of K_0^2 and regarding Eq. (22), the small- k expansion of the Fourier component of c (21) reads

$$\hat{c}(k) = \frac{\Gamma}{8\pi n} - \frac{k^2}{96(\pi n)^2} + O(k^4). \tag{24}$$

Inserting (24) into (16), we find

$$\hat{h}(k) = \frac{\Gamma}{8\pi n(1 - (\Gamma/4))} - \frac{k^2}{96(\pi n)^2(1 - (\Gamma/4))^2} + O(k^4). \tag{25}$$

The truncated density–density correlation is related to h [see definitions (5), (12a) and (15a)] via

$$\langle \hat{n}(\mathbf{0}) \hat{n}(\mathbf{r}) \rangle_T = n^2 h(r) + n \delta(\mathbf{r}). \tag{26}$$

With respect to (13b), we finally obtain

$$n \int h(\mathbf{r}) d^2\mathbf{r} = \frac{\Gamma}{4(1 - \Gamma/4)}, \quad (27a)$$

$$\int \langle \hat{n}(\mathbf{0}) \hat{n}(\mathbf{r}) \rangle_T r^2 d^2\mathbf{r} = \frac{1}{12\pi(1 - (\Gamma/4))^2}. \quad (27b)$$

The first formula (27a) is identical to the compressibility sum rule

$$n \int h(\mathbf{r}) d^2\mathbf{r} = \frac{\partial n}{\partial(\beta p)} - 1 \quad (28)$$

with the use of the exact equation of state $\beta p = n(1 - \Gamma/4)$, where p is the pressure. The second formula (27b) coincides with the new sum rule (1) suggested in Ref. [1].

4. Charge correlations in the 2d TCP

One might try to use the present formalism for studying the charge correlations. Unfortunately, one can only reproduce known results. Indeed, introducing the charge correlation and direct correlation functions

$$h' = \frac{1}{2}(h_+ - h_-), \quad c' = \frac{1}{2}(c_+ - c_-), \quad (29)$$

one now finds that the non-vanishing graphs contributing to c' are the ones which have their two root-vertices with an odd coordination and their field vertices still with an even coordination. For instance, only the first diagram in the $c^{(1)}$ family [see formula (10)] survives. The argument of Ref. [2] no longer applies, and the corresponding contribution to $c'(k)$ is $O(1)$ rather than $O(k^4)$. One finds

$$c'(k) = -\Gamma/k^2 + O(1) \quad (30)$$

and this leads only to the known Stillinger–Lovett sum rules for the zeroth and second moments of the charge correlation function h' .

5. Consequences

Cranking backwards the arguments in Ref. [1], it is now possible to derive conformal-invariance properties from the 2nd moment (27b). Indeed, within the scheme established in Ref. [1], the logarithm of the grand-canonical partition function of the 2d TCP, formulated on the surface of a $3d$ sphere of radius R , can be written as

$$\ln \Xi = 4\pi R^2 \beta p + f(R), \quad (31a)$$

where, in the limit $R \rightarrow \infty$,

$$\frac{\partial f(R)}{\partial R} = -\frac{1}{R} \left(1 - \frac{\Gamma}{4}\right)^2 4\pi \int \langle \hat{n}(\mathbf{0}) \hat{n}(\mathbf{r}) \rangle_T r^2 d^2\mathbf{r}. \quad (31b)$$

Assuming the sum rule (27b), one finds the behaviour, as $R \rightarrow \infty$,

$$f(R) \sim -\frac{1}{3} \ln R + \text{const}, \quad (32)$$

i.e., for an arbitrary coupling Γ , the finite-size correction to $\ln \Xi$ exhibits the universal form suggested by using predictions of the conformal-invariance theory [4,5], with the correct prefactor for the sphere geometry.

The mapping of the $2d$ TCP onto the massive Thirring model confirms the validity of a sum rule for the latter model (for details, see Section 4 of Ref. [1]).

6. Conclusion

Unlike previously known moments in Coulomb systems, the new sixth moment of the pair correlation function for the one-component plasma, and the new second moment of the density (not charge) correlation function for the two-component plasma have been exactly obtained only for two-dimensions and point-charges (no short-range interactions). A simple basic ingredient of the derivations is that these systems have only one length scale $n^{-1/2}$ provided by the density; the quantities of interest depend on the density only trivially through that length scale. Nevertheless, technically, showing that higher order graphs give to c contributions $O(k^4)$ (Ref. [2]) is somewhat lengthy. Whether a simpler derivation is possible is an open problem.

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