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Equation of State in the Fugacity Format for the Two-Dimensional Coulomb Gas

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We derive the general form of the equation of state, in the fugacity format, for the two-dimensional Coulomb gas. Our results are valid in the conducting phase of the Coulomb gas, for temperatures above the Kosterlitz–Thouless transition. The derivation of the equation of state is based on the knowledge of the general form of the short-distance expansion of the correlation functions of the Coulomb gas. We explicitly compute the expansion up to order $O(\zeta^6)$ in the activity ζ. Our results are in very good agreement with Monte Carlo simulations at very low density.

KEY WORDS: Coulomb gas; equation of state; sine-Gordon model; exact results

1. INTRODUCTION AND SUMMARY OF RESULTS

The system under consideration is a classical two component Coulomb gas composed of positive and negative particles with charges $+1$ and -1. The particles live in a two dimensional plane and they are small impenetrable disks of diameter σ. The interaction between two charges q and q' at a distance r from each other is

$$v(r) = \begin{cases} -qq' \ln \frac{r}{L} & r > \sigma \\ +\infty & r \leq \sigma \end{cases} \tag{1.1}$$

where L is an arbitrary length scale fixing the zero of the potential. This is the two dimensional version of the restricted primitive model for electrolytes. We shall work using the grand canonical formalism with fugacity λ (dimensions $length^{-2}$) and inverse reduced temperature (coulombic coupling) β. The arbitrary length scale L can be absorbed in the fugacity by defining the rescaled fugacity $z = \lambda L^{\beta/2}$ which has dimensions $length^{(\beta-4)/2}$. A dimensionless activity which will prove

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useful later can be defined as $\zeta = z\sigma^{(4-\beta)/2} = \lambda\sigma^2(L/\sigma)^{\beta/2}$. Notice that if L is chosen as $L = \sigma$, $\zeta = \lambda\sigma^2$ does not depend on β for fixed fugacity λ. We consider only neutral configurations in the thermodynamic limit. Let $n_+ = n_-$ be the density of positive (negative) particles. The total number density is $n = n_+ + n_- = 2n_+$.

In the low density limit $n\sigma^2 \to 0$, there are two values of the coupling β of special interest. At $\beta = \beta_{\text{KT}} = 4$ the system undergoes the Kosterlitz–Thouless transition of infinite order.[1] In the high temperature phase $\beta < \beta_{\text{KT}}$, the system is in a conducting phase with free ions that can screen external charges. The correlations have an exponential decay and they satisfy several screening sum rules, for instance the Stillinger-Lovett sum rule.[2] In the low temperature phase, for $\beta > \beta_{\text{KT}}$, the gas is in a dielectric phase where all charges are bound forming dipolar pairs. The perfect screening sum rule is no longer satisfied.

The other value for β of interest is $\beta = 2$. For $\beta < 2$ the thermodynamic quantities and correlation functions of the system have a finite value in the limit of point particles $\sigma = 0$, while for $2 \leq \beta < 4$ at fixed fugacity z, the density, the free energy and internal energy of the system diverge when $\sigma \to 0$. This is due to the collapse of pairs of point particles of opposite sign. On the other hand, it is believed[3] that the truncated density correlation functions remain finite in the limit $\sigma \to 0$ when $2 \leq \beta < 4$.

For $\beta < 2$ and $\sigma = 0$, the equation of state for the pressure p of the plasma has been known for a long time.[4] A simple scaling argument gives the volume dependence of the free energy which leads to the pressure

$$\beta p = \left(1 - \frac{\beta}{4}\right) n. \tag{1.2}$$

On the other hand the temperature dependence of the free energy is highly non trivial. Only recently, exact results for the full thermodynamics of the two-dimensional Coulomb gas, in the region $\beta < 2$ and $\sigma = 0$, have been obtained by Šamaj and Travěnec.[5] These results have been obtained using the equivalence between the classical Coulomb gas and the quantum sine-Gordon model. In two dimensions this model is integrable, the free energy is known in terms of the soliton mass,[6] and the relation between the soliton mass and the coupling of the sine-Gordon model (i.e. the fugacity of the Coulomb gas) in the conformal normalization has been found.[7] This gives the exact density–fugacity relationship for the Coulomb gas, which allows one to find all the thermodynamic quantities of the system.[5]

In the region $2 \leq \beta < 4$, since the density diverges in the limit $n\sigma^2 \to 0$ for fixed fugacity, it is more appropriate to study the fugacity expansion of the pressure, rather than its density expansion. In Ref. 8, Gallavotti and Nicoló considered a version of the Coulomb gas with a soft short-distance cutoff. They proved that a Mayer series expansion of the pressure in integer powers of the fugacity have well defined coefficients up to order $2l$ for $\beta > \beta_l$, where

$$\beta_l = 4\left(1 - \frac{1}{2l}\right) \qquad l = 1, 2, 3, \ldots \tag{1.3}$$

whereas higher order Mayer coefficients diverge. For $\beta > 4$ all Mayer coefficients are finite, while for $\beta < 2$ all Mayer coefficients diverge.

Their findings lead them to conjecture that the plasma undergoes a series of intermediate phase transitions at $\beta = \beta_l$ from the conducting phase at $\beta = \beta_1 = 2$ up to the dielectric phase at $\beta = \beta_\infty = \beta_{\mathrm{KT}} = 4$, as opposed to the traditional Kosterlitz–Thouless scenario where the conducting-dielectric phase transition takes place at $\beta = 4$.

Fisher *et al.*[9] denied this conjecture. They proposed an ansatz for the pressure, which, in our notations ($\zeta = z\sigma^{(4-\beta)/2}$), reads

$$\beta p = b_\psi(\beta) z^{4/(4-\beta)} \left[1 + e(\beta, \zeta)\right] + \frac{1}{\sigma^2} \sum_{l=1}^{\infty} \bar{b}_{2l}(\beta) \zeta^{2l}. \tag{1.4}$$

In this ansatz, they conjectured that $b_\psi(\beta)$ and $\bar{b}_{2l}(\beta)$ are analytic for $\beta < 4$ and that $e(\beta, \zeta)$ is an analytic function of β for $\beta < 4$ and is also analytic in ζ for $\zeta > 0$. Furthermore, for $n\sigma^2 \to 0$, at fixed z, $e(\beta, z\sigma^{(4-\beta)/2}) \to 0$.

While the ansatz (1.4) is fully compatible with Gallavotti and Nicoló findings, these later conditions on $b_\psi(\beta)$, $\bar{b}_{2l}(\beta)$, and $e(\beta, \zeta)$ imply that the pressure exhibits no singularities up to $\beta = 4$, thus there are no intermediate phase transitions.

Using the exacts results for $\beta < 2$ and $\sigma = 0$,[5] Kalinay and Šamaj[3] devised a method to obtain results for the thermodynamic properties of the Coulomb gas in the low density limit $n\sigma^2 \ll 1$ up to $\beta < 3$. Their findings confirm the form (1.4) of the ansatz proposed by Fisher *et al.* but the analytic structure of the coefficients $b_\psi(\beta)$ and $\bar{b}_{2l}(\beta)$ is different. They have simple poles at $\beta = \beta_l$ but they conjectured that a cancellation occurs. At $\beta = \beta_l$, the exponent of the fugacity in the nonanalytic part of βp is integer: $4/(4 - \beta_l) = 2l$. Then it turns out that residues of $\bar{b}_{2l}(\beta)$ and $b_\psi(\beta)$ at $\beta = \beta_l$ are opposite, thus giving no singularities for the pressure at $\beta = \beta_l$, confirming the absence of intermediate phase transitions.

The cancellation of singularities was verified in Ref. 3 at the first threshold $\beta = \beta_1 = 2$, and conjectured for the other thresholds. The aim of this work is to extend further the analysis of Ref. 3. One important ingredient in the analysis of Ref. 3 is the knowledge of the short-distance expansion of the density correlations functions of the Coulomb gas, $n^{(2)}_{+-}(r)$ and $n^{(2)}_{++}(r)$. The cancellation at $\beta = 2$ was obtained in Ref. 3 using the fact that, at the lowest order when $r \to 0$, $n^{(2)}_{+-}(r) - n^{(2)}_{++}(r) \sim z^2 r^{-\beta}$.

In a recent work,[10] we presented the general framework to obtain higher order terms of this expansion and explicitly computed the two next order terms of the short-distance expansion of the correlation functions. Based on this previous analysis,[10] we will show that the function $e(\beta, \zeta)$ in the ansatz (1.4) is nonanalytic in ζ. Actually, we will show that the ansatz (1.4) should be generalized to

$$\beta p = \frac{1}{\sigma^2}\sum_{l=1}^{\infty} \bar{b}_{2l}(\beta)\zeta^{2l} + b_{\psi}(\beta) z^{\frac{4}{4-\beta}}[1 + e_{1,0}(\beta, \zeta)] + \frac{1}{\sigma^2}\sum_{m=0}^{\infty}\sum_{n}^{*} \zeta^{\frac{4m+\beta n^2}{4-\beta}} \tilde{e}_{n,m}(\beta, \zeta). \tag{1.5}$$

The sum $\sum_n^*$ is for $n \geq 2$ when $m = 0$ and for $n \geq 0$ for $m \geq 1$. For $m = 1$ the function $e_{n,1}(\beta, \zeta) = 0$. The functions $\tilde{e}_{n,m}$ and $e_{1,0}$ admit an expansion in integer powers of ζ and $\ln \zeta$,

$$\tilde{e}_{n,m}(\beta, \zeta) = \sum_{k=0}^{\infty} \tilde{e}_{n,m,k}(\beta, \ln \zeta)\, \zeta^{2k^* + n} \tag{1.6}$$

$$e_{1,0}(\beta, \zeta) = \sum_{k=0}^{\infty} e_{1,0,k}(\beta, \ln \zeta)\, \zeta^{2k+2} \tag{1.7}$$

where $k^* = k + 1$ for $n = 0, 1$ and $k^* = k$ for $n \geq 2$. Notice that the lowest order in this expansion is at least ζ^2. Thus, in the limit $n\sigma^2 \to 0$, fixed z, and $\beta < 4$, these terms are irrelevant in the sense that $\tilde{e}_{n,m}(\beta, z\sigma^{(4-\beta)/2}) \to 0$.

The explicit calculation of $b_{\psi}(\beta)$ and $\bar{b}_2(\beta)$ was done in Ref. 3. Here we will compute explicitly $\bar{b}_4(\beta)$ and $e_{1,0,0}(\beta, \ln \zeta)$. We will show that the cancellation mechanism between $b_{\psi}(\beta)$ and $\bar{b}_{2l}(\beta)$ conjectured in Ref. 3 indeed takes place for $l = 2$ at $\beta = \beta_2 = 3$.

The outline of this paper is the following. In Section 2, we will recall some basic facts about the exact results[5] for $\beta < 2$ and $\sigma = 0$ and about the general strategy proposed by Šamaj and Kalinay[3] to obtain the thermodynamics of the Coulomb gas for $\beta > 2$ in the low density limit. In Section 3, we prove that the equation of state in the fugacity format has the form proposed in Eq. (1.5). In Section 4, we compute explicitly the coefficients $\bar{b}_4(\beta)$ and $e_{1,0,0}(\beta, \ln \zeta)$ and verify the cancellation mechanism between $b_{\psi}(\beta)$ and $\bar{b}_4(\beta)$ at $\beta = \beta_2 = 3$. In Section 5, from our analytical results for the equation of state, we compute the internal energy and the specific heat of the two-dimensional Coulomb gas and we compare our results with the ones obtained from Monte Carlo simulations.[11]

2. PREVIOUS RESULTS AND GENERAL STRATEGY

2.1. The Coulomb Gas of Point Charges for $\beta < 2$

For point particles, $\sigma = 0$ and $\beta < 2$, the classical Coulomb gas can be mapped into the Euclidean quantum sine-Gordon model by carrying out a Hubbard–Stratonovich transformation. The grand canonical partition function Ξ

of the Coulomb gas can be written as

$$\Xi = \frac{\int \mathcal{D}\phi \exp[-S(z)]}{\int \mathcal{D}\phi \exp[-S(0)]} \tag{2.1}$$

with the sine-Gordon action

$$S(z) = -\int d^2\mathbf{r} \left[\frac{1}{16\pi} \phi(\mathbf{r}) \Delta \phi(\mathbf{r}) + 2z \cos(b\phi(\mathbf{r})) \right] \tag{2.2}$$

where we defined

$$b^2 = \beta/4. \tag{2.3}$$

Under this mapping, the bulk density and two-body densities of charges $q = \pm 1$ and $q' = \pm 1$ are given by[5,12]

$$n_q = z \langle e^{ibq\phi} \rangle \tag{2.4}$$

and

$$n^{(2)}_{qq'}(|\mathbf{r} - \mathbf{r}'|) = z^2 \left\langle e^{ibq\phi(\mathbf{r})} e^{ibq'\phi(\mathbf{r}')} \right\rangle \tag{2.5}$$

where the averages are taken with respect to the sine-Gordon action (2.2).

The complete mapping between the classical Coulomb gas and the sine-Gordon model requires[5,13] to use the conformal normalization,[7] where, when $z \to 0$, the free fields are normalized according to $\langle e^{ib\phi(0)} e^{-ib\phi(\mathbf{r})} \rangle_{z=0} = r^{-\beta}$. Under this conformal normalization, the expectation value of exponential fields is known[14,15]

$$\langle e^{ibQ\phi} \rangle = \left(\frac{\pi z}{\gamma(\beta/4)} \right)^{\frac{\beta Q^2}{4-\beta}} \exp[I_b(Q)] \tag{2.6}$$

with $\gamma(x) = \Gamma(x)/\Gamma(1-x)$ where $\Gamma(x)$ is the Euler Gamma function, and

$$I_b(Q) = \int_0^\infty \frac{dt}{t} \left[\frac{\sinh^2(2Qb^2t)}{2\sinh(b^2t)\sinh(t)\cosh[(1-b^2)t]} - 2Q^2b^2e^{-2t} \right]. \tag{2.7}$$

This expression is valid for $\beta|Q| < 2$, otherwise the integral $I_b(Q)$ diverges, but it is possible to do an analytic continuation[16] of this formula for other values of βQ using a reflection formula satisfied by $\langle e^{ibQ\phi} \rangle$ presented in Ref. 15. For $Q = \pm 1$, the integral (2.7) can be computed explicitly and

$$\langle e^{ib\phi} \rangle = \langle e^{-ib\phi} \rangle = 2 \left(\frac{\pi z}{\gamma(\beta/4)} \right)^{\frac{\beta}{4-\beta}} \left(\frac{\Gamma(\xi/2)}{\Gamma(\frac{1+\xi}{2})} \right)^2 \frac{\tan(\pi\xi/2)}{(4-\beta)\gamma(\beta/4)} \tag{2.8}$$

where $\xi = \beta/(4-\beta)$.

Equation (2.4) combined with (2.8) gives the exact density–fugacity relationship[5]

$$n = n[z,0] = z^{4/(4-\beta)} \frac{4}{4-\beta} b_{\psi}(\beta) \tag{2.9}$$

with

$$b_{\psi}(\beta) = \frac{\pi^{\frac{\beta}{4-\beta}}}{(\gamma(\beta/4))^{\frac{4}{4-\beta}}} \left(\frac{\Gamma(\xi/2)}{\Gamma\left(\frac{1+\xi}{2}\right)} \right)^2 \tan(\pi\xi/2). \tag{2.10}$$

We introduced the notation $n[z,\sigma]$ to indicate that the density is a function of z and the hard core diameter σ. Here $\sigma = 0$, but we shall use that notation later on.

Equation (2.9) together with the thermodynamic relation $n = z\partial(\beta p)/\partial z$ leads to

$$\beta p = b_{\psi}(\beta) z^{\frac{4}{4-\beta}}. \tag{2.11}$$

This is the exact pressure–fugacity relationship for point-like particles when $\beta < 2$. Notice that both (1.4) and (1.5) are compatible with (2.11) when $\sigma = 0$ and $\beta < 2$.

At $\beta = 2$, the density diverges, as expected, due to the collapse phenomenon. As already noticed in Ref. 3, a naive analytic continuation of (2.9) for $\beta \geq 2$ does not give the correct density–fugacity relationship beyond the collapse: the function $n[z,0]$ diverges at the thresholds $\beta = \beta_l$ and can become negative, it cannot represent the density in the region $2 \leq \beta < 4$.

2.2. The Coulomb Gas beyond $\beta = 2$ in the Low Density Limit

The method[3] to study the properties of the Coulomb gas for $\beta > 2$ and $\sigma \neq 0$ when $n^2\sigma \ll 1$ is based on the electroneutrality sum rule

$$n_+ = \int_{\mathbb{R}^2} \left[n_{+-}^{(2)}(r) - n_{++}^{(2)}(r) \right] d\mathbf{r} \tag{2.12}$$

It is believed that the truncated correlation functions $n_{qq'}^{(2)T}(r; z, \sigma)$ are well defined for $\sigma = 0$ up to $\beta < 4$. Assuming that the difference $n_{qq'}^{(2)T}(r; z, \sigma) - n_{qq'}^{(2)T}(r; z, 0)$ is negligible for $r > \sigma$, and using the electroneutrality sum rule (2.12), Kalinay and Šamaj[3] proposed that the density $n[z,\sigma]$ for the Coulomb gas with hard core σ is given by

$$n[z,\sigma] = n[z,0] - 4\pi \int_0^{\sigma} \left[n_{+-}^{(2)}(r; z, 0) - n_{++}^{(2)}(r; z, 0) \right] r\, dr \tag{2.13}$$

in the limit $n\sigma^2 \ll 1$.

Using the dominant order term in the small-r expansion of the correlation functions, $n_{+-}^{(2)}(r) - n_{++}^{(2)}(r) \sim z^2 r^{-\beta}$, Kalinay and Šamaj [3] obtained the first correction

$$n[z,\sigma] = n[z,0] - 4\pi z^2 \frac{\sigma^{2-\beta}}{2-\beta} \tag{2.14}$$

and they showed that it cancels the pole at $\beta = 2$ from $n[z,0]$.

3. THE EQUATION OF STATE IN THE FUGACITY FORMAT

3.1. The Short Distance Expansion of Correlation Functions and the Operator Product Expansion

To proceed further with the program proposed by Kalinay and Šamaj, [3] we need to compute the higher order terms of the short-distance expansion of the correlation functions. In a previous work, [10] we showed how the operator product expansion for the exponential fields in the sine-Gordon model can be used to obtain the short distance expansion of the correlation functions of the Coulomb gas. Let us recall and extend some of the results from Ref. 10.

The operator product expansion for the exponential fields of the sine-Gordon models reads [17]

$$\langle e^{ibQ_1\phi(0)} e^{ibQ_2\phi(\mathbf{r})}\rangle = \sum_{n=-\infty}^{n=+\infty} \Big[C_{Q_1Q_2}^{n,0}(r) \langle e^{ib(Q_1+Q_2+n)\phi}\rangle + C_{Q_1Q_2}^{n,2}(r) \big\langle (\partial\phi)^2 (\bar\partial\phi)^2 e^{ib(Q_1+Q_2+n)\phi} \big\rangle + \cdots \Big] \tag{3.1}$$

where the dots denote subdominant contributions from higher order descendant fields $\prod_i \partial^{m_i}\phi \prod_j \bar\partial^{n_j}\phi \; e^{ib(Q_1+Q_2+n)\phi}$, where only the fields with $\sum_i m_i = \sum_j n_j = m$ have non vanishing expectation value. The level $m = 1$ field has zero expectation value because it is a total derivative. [17]

The functions $C_{Q_1Q_2}^{n,m}(r)$ of the operator product expansion have the following form [17]

$$C_{Q_1Q_2}^{n,m}(r) = z^{|n|} r^{m+\beta Q_1 Q_2 + n\beta(Q_1+Q_2) + 2|n|(1-\frac{\beta}{4}) + n^2\beta/2} f_{Q_1Q_2}^{n,m}(z^2 r^{4-\beta}) \tag{3.2}$$

where each $f_{Q_1Q_2}^{n,m}$ admit a power series expansion of the form

$$f_{Q_1Q_2}^{n,m}(x) = \sum_{k=0}^{\infty} f_k^{n,m}(Q_1, Q_2) x^k. \tag{3.3}$$

The connexion of the operator product expansion with the Coulomb gas is clear by noticing that $\langle e^{ib(Q_1+Q_2+n)\phi}\rangle$ is closely related to the excess chemical potential of an external charge $Q_1 + Q_2 + n$ introduced in the plasma.[18] Also, the coefficients $f_k^{n,0}(Q_1, Q_2)$ are expressible in terms $(n + 2k)$-fold Coulomb type integrals: they are the partition functions of a system with two fixed point charges Q_1 and Q_2 separated by a distance 1 and with n (positive for $n > 0$, negative for $n < 0$) point particles and k pairs of positive and negative point particles approaching the fixed particles. For explicit expressions of some of these coefficients see Refs. 10, 17.

A few technical details, explained in greater detail in Ref. 10, should be kept in mind when using the expansion (3.1) to compute the correlation functions of the Coulomb gas. First, the $(n + 2k)$-fold Coulomb type integrals in the coefficients $f_k^{n,m}(Q_1, Q_2)$ are defined for a certain range of values of Q_1, Q_2 and β since we are dealing with point particles, in order to avoid the collapse. Beyond those ranges an analytic continuation should be used.

Second, for certain values of Q_1, Q_2 and β different terms in the expansion (3.1) can become of the same order. When this occurs the coefficient of each term usually has a pole, but adding all contributions of the same power in r and taking the appropriate limit gives a finite result and logarithmic terms $\ln(zr^{(4-\beta)/2})$ appear. One important case where this happens is in the computation of $n_{+-}^{(2)}$. As clearly seen from Eq. (3.1), when $Q_1 = -Q_2 = 1$, the terms for n and $-n$ are of the same order in r. One consequence is the appearance of $\ln(zr^{(4-\beta)/2})$ terms in the expansion of $n_{+-}^{(2)}(r)$ coming from the contributions of terms $|n| \geq 1$ in (3.1). However, for $n = 0$, the corresponding terms in Eq. (3.1) do not have a logarithmic correction. For details see Ref. 10. This last remark is important for the following analysis, and, as we shall see, it is the reason why the first term of the equation of state (1.5) is an analytic series in the fugacity.

Using (2.5) and the operator product expansion (3.1), including the contributions of all descendant fields, we find that the general form of the short-distance expansion of the correlation functions is

$$n_{++}^{(2)}(r) = \sum_{n=-\infty}^{n=+\infty} \sum_{m=0}^{+\infty} \sum_{k=0}^{+\infty} n_{n,m,k}^{++} \frac{1}{r^4} \left(zr^{\frac{4-\beta}{2}}\right)^{\frac{\beta(2+n)^2+4m}{4-\beta}} \left(zr^{\frac{4-\beta}{2}}\right)^{2k+2+|n|} \tag{3.4}$$

$$n_{+-}^{(2)}(r) = \sum_{n=-\infty}^{n=+\infty} \sum_{m=0}^{+\infty} \sum_{k=0}^{+\infty} n_{n,m,k}^{+-} \frac{1}{r^4} \left(zr^{\frac{4-\beta}{2}}\right)^{\frac{\beta n^2+4m}{4-\beta}} \left(zr^{\frac{4-\beta}{2}}\right)^{2k+2+|n|} \tag{3.5}$$

The indexes used are m for the order of the descendant field (remember that the term for $m = 1$ is zero), n for the number of particles of sign $\text{sgn}(n)$ added and k for the number of pair of positive and negative particles added. The coefficients $n_{n,m,k}^{+-}$ and $n_{n,m,k}^{++}$ depend on β and eventually on $\ln(zr^{(4-\beta)/2})$, except those for neutral configurations $n_{0,0,k}^{+-}$ and $n_{-2,0,k}^{++}$ which depend only on β as explained above.

3.2. The Fugacity Expansions of the Density and the Pressure

Substituting (3.4) and (3.5) into (2.13) leads to the following form for the density

$$n[z,\sigma] = n[z,0] + \sum_{n=-\infty}^{+\infty}\sum_{m=0}^{+\infty}\sum_{k=0}^{+\infty}\frac{1}{\sigma^2}\left[c^{+-}_{n,m,k}\zeta^{\frac{4m+\beta n^2}{4-\beta}} + c^{++}_{n,m,k}\zeta^{\frac{4m+\beta(n+2)^2}{4-\beta}}\right]\zeta^{2k+2+|n|} \tag{3.6}$$

with $n[z,0]$ given by Eqs. (2.9) and (2.10) and $\zeta = z\sigma^{(4-\beta)/2}$. Finally, using $n = z\partial(\beta p)/\partial z$, the fugacity expansion of pressure is of the form

$$\begin{aligned}\beta p &= b_\psi(\beta)z^{4/(4-\beta)}\\ &+ \sum_{n=-\infty}^{\infty}\sum_{m=0}^{+\infty}\sum_{k=0}^{+\infty}\frac{1}{\sigma^2}\zeta^{\frac{4m+\beta n^2}{4-\beta}}\left[p^{+-}_{n,m,k}\zeta^{2k+2+|n|} + p^{++}_{n-2,m,k}\zeta^{2k+2+|n-2|}\right]\end{aligned} \tag{3.7}$$

Notice that the terms corresponding to $m = 0$ and $n = 0$ are analytic in z. These, together with the terms $m = 0$ and $n = 1$, reproduce the ansatz (1.4) from Fisher *et al.*[9] Writing these terms apart in (3.7) the pressure–fugacity relationship can finally be written as announced in the introduction

$$\beta p = \frac{1}{\sigma^2}\sum_{l=1}^{\infty}\bar{b}_{2l}(\beta)\zeta^{2l} + b_\psi(\beta)z^{\frac{4}{4-\beta}}[1+e_{1,0}(\beta,\zeta)] + \frac{1}{\sigma^2}\sum_{m=0}^{\infty}\sum\nolimits_n^{*}\zeta^{\frac{4m+\beta n^2}{4-\beta}}\tilde{e}_{n,m}(\beta,\zeta). \tag{3.8}$$

The sum $\sum_n^*$ does not contains the terms $m = 0$ and $n = 0, 1$ since they are explicitly written apart: the sum is for $n \geq 2$ when $m = 0$ and for $n \geq 0$ for $m \geq 1$.

The functions $\tilde{e}_{n,m}(\beta,\zeta)$ and $e_{1,0}(\beta,\zeta)$ admit a power series expansion in terms of ζ and $\ln\zeta$ given in Eqs. (1.6) and (1.7). They are at least of order $\zeta^2 = z^2\sigma^{(4-\beta)}$, so they vanish in the limit $n\sigma^2 \to 0$ for fixed z and $\beta < 4$: they are irrelevant. On the other hand, in the analytic part of βp as a series in ζ (first sum in (3.8)), the l-th term becomes relevant for $\beta > \beta_l = 4[1 - (1/(2l))]$, i.e. it diverges in the limit $n\sigma^2 \to 0$.

At $\beta = \beta_l$, the term $z^{4/(4-\beta)}b_\psi(\beta)$ has a pole, as seen from (2.10), but it is expected that the coefficient $\sigma^{-2}\bar{b}_{2l}(\beta)\zeta^{2l}$, which becomes relevant at that point, also has a pole and cancels the divergence from $z^{4/(4-\beta)}b_\psi(\beta)$. This was checked at $\beta = \beta_1 = 2$ for the first term $l = 1$ in Ref. 3. In the next section we check that this cancellation also takes place at $\beta = \beta_2 = 3$.

4. EXPLICIT CALCULATIONS

4.1. The Equation of State in the Fugacity Format

In Ref. 10 we computed explicitly the short-distance expansion of the correlation functions (3.4) and (3.5) up to order $r^{8-3\beta}$, that is, we computed the terms corresponding to $(n,m,k)=(-2,0,0)$ and $(n,m,k)=(-1,0,0)$ for $n^{(2)}_{++}$, and $(n,m,k)=(0,0,0)$, $(n,m,k)=(0,0,1)$ and $(n,m,k)=(\pm 1,0,0)$ for $n^{(2)}_{+-}$. The neutral configurations: for $n^{(2)}_{++}$, $(n,m,k)=(-2,0,0)$ gives the order $r^{4-2\beta}$, and for $n^{(2)}_{+-}$, $(n,m,k)=(0,0,0)$ gives the order $r^{-\beta}$, and $(n,m,k)=(0,0,1)$ the order $r^{4-2\beta}$. The configurations with at most one charge ± 1 give the order $r^{2-\beta}$ [$(n,m,k)=(-1,0,0)$ for $n^{(2)}_{++}$ and $(n,m,k)=(\pm 1,0,0)$ for $n^{(2)}_{+-}$]. Explicitly,

$$n^{(2)}_{+-}(r) = z^2 r^{-\beta} + z^3\langle e^{ib\phi}\rangle r^{2-\beta}\left(\tilde{n}_3^{+-} - \pi\beta^2 \ln\left[\left(\frac{\pi z}{\gamma(\beta/4)}\right)^{\frac{2}{4-\beta}} r\right]\right) + z^4 r^{4-2\beta}\tilde{n}_4^{+-} + O(r^4, r^{8-3\beta}, r^{6-2\beta}) \tag{4.1}$$

$$n^{(2)}_{++}(r) = z^3\langle e^{ib\phi}\rangle r^{2-\beta}\tilde{n}_3^{++} + z^4 r^{4-2\beta}\tilde{n}_4^{++} + O(r^4, r^{8-3\beta}, r^{6-2\beta}) \tag{4.2}$$

with $\langle e^{ib\phi}\rangle$ given by Eq. (2.8), and

$$\tilde{n}_3^{+-} = -\frac{\pi\beta^2}{4}\left[\frac{4}{\beta} I_b'(1) - 4 + 4C + \psi\left(\frac{\beta}{2}\right) + \psi\left(-\frac{\beta}{2}\right) + \psi\left(1-\frac{\beta}{2}\right) + \psi\left(1+\frac{\beta}{2}\right)\right] \tag{4.3}$$

$$\tilde{n}_4^{+-} = J(\beta, -\beta, \beta) \tag{4.4}$$

$$\tilde{n}_3^{++} = \pi\gamma\left(1-\frac{\beta}{2}\right)^2 \gamma(\beta-1) \tag{4.5}$$

$$\tilde{n}_4^{++} = -\frac{4\pi^2}{(2-\beta)^2}\gamma\left(1-\frac{\beta}{4}\right)^3 \gamma\left(-1+\frac{3\beta}{4}\right) \tag{4.6}$$

where $\psi(x) = d\ln\Gamma(x)/dx$ is the digamma function and $C=-\psi(1)$ is the Euler constant. The definition and some properties of the functions $I_b'(1) = \partial I_b(Q)/\partial Q|_{Q=1}$ and $J(\beta,-\beta,\beta)$ are presented in the appendix.

The use of (2.13) leads to the density

$$n[z,\sigma] = z\langle e^{ib\phi}\rangle\left\{2 - \frac{4\pi z^2\sigma^{4-\beta}}{4-\beta}\left(\tilde{n}_3^{+-} - \tilde{n}_3^{++} - \frac{\pi\beta^2}{4-\beta}\left[\ln\left[\left(\frac{\pi z}{\gamma(\beta/4)}\right)^2 \sigma^{4-\beta}\right] - 1\right]\right)\right\} - \frac{4\pi z^2\sigma^{2-\beta}}{2-\beta} - \frac{2\pi z^4\sigma^{2(3-\beta)}}{3-\beta}(\tilde{n}_4^{+-} - \tilde{n}_4^{++}) + O(\sigma^6, \sigma^{10-3\beta}, \sigma^{8-2\beta}) \tag{4.7}$$

Integrating the thermodynamic relation $n = z\partial(\beta p)/\partial z$, we find the equation of state in the fugacity format

$$\beta p = b_\psi(\beta) z^{4/(4-\beta)}\,[1 + e(\beta,\zeta)] + \frac{1}{\sigma^2}\left[\frac{-2\pi}{2-\beta}\zeta^2 + \bar{b}_4(\beta)\zeta^4 + O(\zeta^6)\right] \quad (4.8)$$

with

$$\bar{b}_4(\beta) = -\frac{\pi}{2(3-\beta)}\left[J(\beta,-\beta,\beta) + \frac{4\pi^2}{(2-\beta)^2}\gamma\left(1-\frac{\beta}{4}\right)^3\gamma\left(-1+\frac{3\beta}{4}\right)\right] \quad (4.9)$$

and

$$\begin{aligned} e(\beta,\zeta) = -\frac{4\pi\zeta^2}{(4-\beta)^2(6-\beta)}\Bigg\{&(4-\beta)\left(\frac{-\pi\beta^2}{4}\left[\frac{4}{\beta}I_b'(1) - 4 + 4C + \psi\left(\frac{\beta}{2}\right)\right.\right.\\ &\left.\left.+\psi\left(-\frac{\beta}{2}\right) + \psi\left(1-\frac{\beta}{2}\right) + \psi\left(1+\frac{\beta}{2}\right)\right] - \pi\gamma\left(1-\frac{\beta}{2}\right)^2\gamma(\beta-1)\right)\\ &-\pi\beta^2\left[\frac{2(\beta-5)}{6-\beta} + \ln\left(\frac{\pi\zeta}{\gamma(\beta/4)}\right)^2\right]\Bigg\} + o(\zeta^2) \end{aligned} \quad (4.10)$$

We have verified that the function $e(\beta, z\sigma^{(4-\beta)/2}) \to 0$ when $n\sigma^2 \to 0$ at fixed z.

4.2. Cancellations at $\beta = 3$ for the Relevant Terms

Near $\beta = 3$, the contribution to βp from $n[z,0]$ is

$$b_\psi(\beta) z^{4/(4-\beta)} \underset{\beta\to 3}{\sim} \frac{\pi^3}{8}\gamma(1/4)^4 z^4 \frac{1}{\beta-3} \quad (4.11)$$

On the other hand, in the appendix it is shown that

$$\bar{b}_4(\beta) \underset{\beta\to 3}{\sim} -\frac{\pi^3}{8}\gamma(1/4)^4\frac{1}{\beta-3}. \quad (4.12)$$

Thus the divergences of each term at $\beta = 3$ cancel each other yielding a finite result for the pressure. The cancellation mechanism conjectured in Ref. 3, indeed take place at $\beta = 3$.

4.3. Cancellations at $\beta = 2$ for Irrelevant Terms

Actually a more complex mechanism of cancellations of divergences appears to take place, at $\beta = \beta_l$, when the generically nonanalytic contributions in $z^{4/(4-\beta)}$ become analytic z^{2l}, also with the irrelevant terms (terms that vanish when $n\sigma^2 \to 0$). To illustrate this, notice that at $\beta = 2$, $\bar{b}_4(\beta)\zeta^4/\sigma^2$ has a pole, but so does the term $b_\psi(\beta)z^{4/(4-\beta)}e(\beta, \zeta)$ which is also of order ζ^4 at $\beta = 2$. The finiteness of the correlation functions in the region up to $\beta < 4$ (in particular at $\beta = 2$ for the present case) ensures that both divergent contributions cancel each other.

The calculations of the short distance expansion of the correlation functions at $\beta = 2$ has been done in Ref. 10. Using the results from Ref. 10, in particular the results from Appendices A and B of Ref. 10, it is easy to check that the contribution of terms of order ζ^4 in the pressure are finite:

$$\begin{aligned}\beta p \underset{\beta=2}{=} & -\pi z^2 [-1 + 2C + 2\ln(\pi z\sigma)] \\ & - \frac{\pi^3 z^4 \sigma^2}{4}\{-3 - 4(C + \ln\pi)[1 + 2(C + \ln\pi)] \\ & + 4[-1 + 2\ln(z\sigma) + 4(\ln\pi + C)]\ln(z\sigma)\} + o(z^4\sigma^2) \end{aligned} \tag{4.13}$$

We have also written the relevant contribution (nonvanishing when $\sigma \to 0$) which was computed in Ref. 3.

If the conjecture that the truncated correlation functions are finite up to $\beta = 4$ is true, this cancellation mechanism of irrelevant terms should take place at other values of β where the coefficients in Eq. (3.8) diverge. For instance, in (4.8) the product $b_\psi(\beta)e(\beta, \zeta)$ has a pole at $\beta = 3$. At this value of β, the nonanalytic contribution to the pressure $b_\psi(\beta)e(\beta, \zeta)z^{4/(4-\beta)}$ becomes analytic of order ζ^6. The pole at $\beta = 3$ of $b_\psi(\beta)e(\beta, \zeta)$ should be canceled with a similar diverging term from $\bar{b}_6(\beta)\zeta^6/\sigma^2$, which we have not computed here.

5. COMPARISON WITH MONTE CARLO SIMULATIONS

In the canonical format, the excess dimensionless free energy per particle is given by

$$f(n, \beta) = \frac{-\beta p}{n} + \ln\zeta \tag{5.1}$$

where ζ should be expressed in terms of the density n by inverting the relation (3.6). The excess internal energy per particle u^{exc} and the excess specific heat at constant volume per particle c_V^{exc} can be obtained as

$$u^{\text{exc}} = \frac{\partial f(n, \beta)}{\partial\beta} \tag{5.2}$$

and

$$c_V^{\text{exc}} = -\beta^2 \frac{\partial^2 f(n, \beta)}{\partial\beta^2}. \tag{5.3}$$

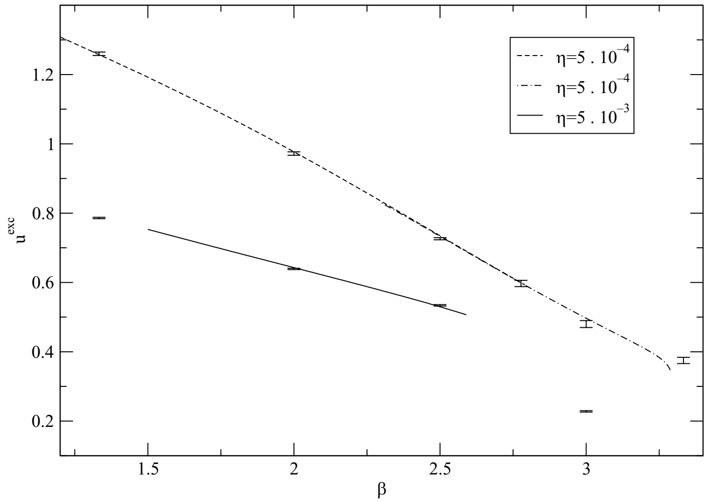

Fig. 1. The internal energy u^{exc} as a function of β. The lines are our analytical results and the bars are the Monte Carlo simulation results. For $\eta = 5 \cdot 10^{-4}$ the dashed line shows the results obtained with the full expression (4.8), while the dash-dot line shows the results obtained from (5.4).

Using the expressions (4.7) and (4.8) for the density and the pressure, accurate to order $O(\zeta^6)$, obtained in the previous section, we numerically inverted the density–fugacity relationship (4.7) and computed the internal energy and specific heat for two low density packing fractions $\eta = \pi n \sigma^2/4$, $\eta = 5 \cdot 10^{-4}$ and $\eta = 5 \cdot 10^{-3}$. In Ref. 11, Monte Carlo simulations of the two-dimensional Coulomb gas were performed for these two packing fraction values.

Our analytical results are compared to the Monte Carlo simulation ones in Figs. 1 and 2. In Fig. 1, we plot the internal energy u^{exc} as a function of the inverse temperature β. For $\eta = 5 \cdot 10^{-4}$, we show two curves. The dashed line corresponds to the results obtained from Eq. (4.8). As it was discussed in the preceding section, the term $b_\psi(\beta)e(\beta, \zeta)$ from Eq. (4.8) has a pole at $\beta = 3$, which should be canceled with the next order term $\bar{b}_6(\beta)\zeta^6/\sigma^2$ which has not been computed. For this reason, the comparison with Monte Carlo results can only be done for $\beta < 3$. However, since $b_\psi(\beta)e(\beta, \zeta)$ vanishes when $\eta \to 0$, we decided to compare the Monte Carlo results with those obtained from our analytical formulas by omitting this "irrelevant" term. This is shown in Fig. 1 with the dot-dash line. Explicitly, this last curve is obtained by approximating the pressure by

$$\beta p = b_\psi(\beta) z^{4/(4-\beta)} + \frac{1}{\sigma^2}\left[\frac{-2\pi}{2-\beta}\zeta^2 + \bar{b}_4(\beta)\zeta^4\right] \tag{5.4}$$

instead of using Equation (4.8). Eq. (5.4) can be used up to the next pole at $\beta = \beta_3 = 10/3$. For very low volume fractions, $\eta = 5 \cdot 10^{-4}$, the agreement

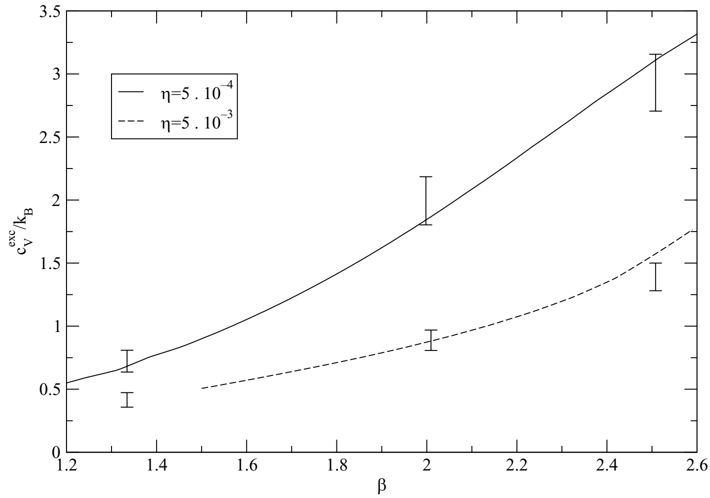

Fig. 2. The specific heat c_V^{exc} as a function of β. The lines are our analytical results and the bars are the Monte Carlo simulation results.

with Monte Carlo simulations is very good, both using the correct formula (4.8), for $\beta < 3$, or the "truncated" one (5.4), for $2 < \beta < 10/3$. For higher volume fractions, $\eta = 5 \cdot 10^{-3}$, the agreement is still very good when using the complete formula (4.8). On the other hand, the "truncated" formula Eq. (5.4), does not give a good agreement (curve not shown) as it can expected because the omitted term becomes important at high volume fractions.

In Fig. 2, we plot the specific heat c_V^{exc} as a function of β. The agreement with Monte Carlo simulations is fairly good, even at the relatively high volume fraction $\eta = 5 \cdot 10^{-3}$. In any case, the agreement with the simulations is much better than the one obtained with only the first order term $\bar{b}_2(\beta)\zeta^2/\sigma^2$ in the pressure, shown in Fig. 3 of Ref. 3, as expected.

6. CONCLUSION

Using the exact results for the thermodynamics of the two-dimensional Coulomb gas of point particles for $\beta < 2$,[(5)] the short-distance expansion of the density correlations functions,[(10)] and the program proposed by Kalinay and Šamaj,[(3)] we have derived the general form of the equation of state in the fugacity format (1.5), for the two-dimensional Coulomb gas composed of small core diameter σ particles and for $\beta < 4$. We explicitly computed the second corrections due to the hard core, up to terms $O(\zeta^6)$ in the activity ζ, the first corrections (order ζ^2) were computed in Ref. 3.

The general form of the equation of state (1.5) is compatible with the fact that an analytic expansion of the pressure in powers of the fugacity have finite Mayer coefficients up to order $2l$ for $\beta > \beta_l$, confirming the findings of Gallavotti and Nicoló.[(8)] However, the explicit calculations we performed show that the pressure does not have any singularities at $\beta = \beta_1 = 2$ nor at $\beta = \beta_2 = 3$, contrary to the conjecture of a series of intermediate phase transitions proposed by Gallavotti and Nicoló,[(8)] and supporting the arguments of Fisher *et al.*[(9)] against this conjecture. But the general form for the equation of state (1.5) we found is more complex than the ansatz (1.4) proposed by Fisher *et al.*.[(9)] Finally, we compared our results against Monte Carlo simulations results and we found good agreement.

APPENDIX A: TECHNICAL DETAILS

The function $I_b'(1)$ appearing in Eq. (4.3) is defined as $I_b'(1) = \partial I_b(Q)/\partial Q|_{Q=1}$ with $I_b(Q)$ given by Eq (2.7). Explicitly,

$$I_b'(1) = \frac{\beta}{4}\int_0^\infty \frac{dt}{t}\left[-4e^{-2t} + \frac{t\sinh(\beta t)}{\sinh t\cosh[\left(1-\frac{\beta}{4}\right)t]\sinh(\beta t/4)}\right]. \tag{A.1}$$

This expression converges only for $\beta < 2$. To use it beyond $\beta > 2$ it is useful to write it as

$$\frac{4}{\beta}I_b'(1) = \mathcal{I}_1(\beta) + \mathcal{I}_2(\beta) \tag{A.2}$$

where

$$\mathcal{I}_1(\beta) = 2\int_0^\infty \left(-\frac{e^{-2t}}{t} + \frac{\cosh(\beta t/4)}{\sinh t\cosh[\left(1-\frac{\beta}{4}\right)t]}\right)dt \tag{A.3}$$

$$\mathcal{I}_2(\beta) = 2\int_0^\infty \left(-\frac{e^{-2t}}{t} + \frac{\cosh(3\beta t/4)}{\sinh t\cosh[\left(1-\frac{\beta}{4}\right)t]}\right)dt \tag{A.4}$$

The first integral, $\mathcal{I}_1(\beta)$, is well defined for $\beta < 4$. The second one, $\mathcal{I}_2(\beta)$, is defined for $\beta < 2$, but it can be analytically continued up to $\beta < 10/3$, by writing it as

$$\mathcal{I}_2(\beta) = \frac{4}{2-\beta} + \frac{8}{3\beta-8} + \frac{2}{3-\beta} + \frac{8}{5\beta-16} + 2\int_0^\infty \left[-\frac{e^{-2t}}{t} + 2\frac{e^{-t(4+\beta)/2} - e^{-3t(4-\beta)} + e^{-t(4-\beta)} + e^{-t(10-3\beta)}}{(1-e^{-2t})\left(1+e^{-2t(1-\frac{\beta}{4})}\right)}\right]dt. \tag{A.5}$$

The function $J(\beta, -\beta, \beta)$ appearing in Eq. (4.4) is a special case of the integral

$$J(\beta Q, -\beta Q, \beta) = \int d^2x\, d^2y\, \frac{|x|^{\beta Q}|1-y|^{\beta Q}}{|y|^{\beta Q}|1-x|^{\beta Q}|x-y|^{\beta}}. \tag{A.6}$$

for $Q = 1$. Using the results from Ref. 19, in the appendix B of Ref. 10 we showed that

$$J(\beta, -\beta, \beta) = \left[s(\beta/2)J_1^+ + s(\beta)J_2^+\right]^2 + \left[s(\beta/2)J_2^+\right]^2 \tag{A.7}$$

with

$$J_1^+ = \frac{\Gamma\left(1-\frac{\beta}{2}\right)^3\Gamma\left(2-\frac{\beta}{2}\right)}{\Gamma(2-\beta)\Gamma(3-\beta)}\, {}_3F_2\left(1-\frac{\beta}{2}, 2-\frac{\beta}{2}, -\frac{\beta}{2}; 2-\beta, 3-\beta; 1\right) \tag{A.8}$$

$$J_2^+ = \frac{\Gamma\left(1-\frac{\beta}{2}\right)\Gamma\left(2-\frac{\beta}{2}\right)\Gamma\left(1+\frac{\beta}{2}\right)^2}{2}\, {}_3F_2\left(2-\frac{\beta}{2}, 1+\frac{\beta}{2}, \frac{\beta}{2}; 2, 3; 1\right). \tag{A.9}$$

where we used the notation $s(x) = \sin(\pi x)$ and where ${}_3F_2(a_1, a_2, a_3; b_1, b_2; z) = \sum_{k=0}^{\infty} \frac{(a_1)_k(a_2)_k(a_3)_k}{(b_1)_k(b_2)_k k!} z^k$ is a generalized hypergeometric function, and $(a)_k = \Gamma(a+k)/\Gamma(a)$ is the Pochhammer symbol.

In the appendix B of Ref. 10 we proved that near $\beta = 2$,

$$J(\beta, -\beta, \beta) \underset{\beta \to 2}{=} (2\pi)^2 \left[\frac{1}{(\beta-2)^2} + \frac{1}{\beta-2} + 1\right] + O(\beta-2). \tag{A.10}$$

In order to verify the cancellation mechanism at $\beta = 3$ presented in Section 4.2, we need the value of $J(\beta, -\beta, \beta)$ at $\beta = 3$.

For this purpose, it is convenient to write J_1^+ as

$$J_1^+ = \frac{\Gamma\left(1-\frac{\beta}{2}\right)^3\Gamma\left(2-\frac{\beta}{2}\right)}{\Gamma(4-\beta)^2}\Big[(2-\beta)(3-\beta)^2 + \left(1-\frac{\beta}{2}\right)\left(2-\frac{\beta}{2}\right)(-\beta/2)(3-\beta) + S(\beta)\Big] \tag{A.11}$$

where

$$S(\beta) = \sum_{k=2}^{+\infty} \frac{\left(1-\frac{\beta}{2}\right)_k\left(2-\frac{\beta}{2}\right)_k(-\beta/2)_k}{(4-\beta)_{k-1}(4-\beta)_{k-2}k!}. \tag{A.12}$$

At $\beta = 3$, we have $S(3) = -\gamma(1/4)^2/(16\pi)$. Then at $\beta = 3$,

$$J_1^+ \underset{\beta = 3}{=} \frac{\pi}{2}\gamma(1/4)^2. \tag{A.13}$$

On the other hand J_2^+ can be evaluated directly at $\beta = 3$, using[20]

$$ {}_3F_2(1/2, 5/2, 3/2; 2, 3; 1) = \frac{8}{9\pi}\gamma(1/4)^2. \tag{A.14}$$

We find that $J_2^+ = -J_1^+$ at $\beta = 3$. This yields

$$ J(3, -3, 3) = \frac{\pi^2}{2}\gamma(1/4)^4. \tag{A.15}$$

This result, combined with the explicit expression (4.9) for $\bar{b}_4(\beta)$, gives the behavior (4.12) for $\bar{b}_4(\beta)$ near $\beta = 3$.

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