*Journal of Statistical Physics, Vol. 106, Nos. 5/6, March 2002 (© 2002)*

# Thermodynamic Properties of the Two-Dimensional Coulomb Gas in the Low-Density Limit

**P. Kalinay**[1] **and L. Šamaj**[1, 2]

*Received July 9, 2001; accepted October 17, 2001*

The model under consideration is the two-dimensional Coulomb gas of $\pm$ charged hard disks with diameter $\sigma$. For the case of pointlike charges ($\sigma = 0$), the system is stable against collapse of positive-negative pairs of charges in the range of inverse temperatures $0 \leqslant \beta < 2$, where its full exact thermodynamics was obtained recently. In the present work, we derive the leading correction to the exact thermodynamics of pointlike charges due to presence of the hard core $\sigma$ which enables us to extend the treatment beyond the collapse point $\beta = 2$. Our results, which are conjectured to be exact in the low-density limit in the interval $0 \leqslant \beta < 3$, reproduce correctly the singularities of thermodynamic quantities at the collapse point and agree well with Monte-Carlo simulations. The "subtraction" mechanism within the ansatz proposed by M. E. Fisher *et al.* [*J. Stat. Phys.* **79**:1 (1995)], which excludes the existence of intermediate phases between the collapse point $\beta = 2$ and the Kosterlitz–Thouless transition point $\beta_{\mathrm{KT}} = 4$, is confirmed, however, a different analytic structure of this ansatz is suggested.

**KEY WORDS:** Coulomb gas; thermodynamics; charge pairing; low-density limit, sum rule.

## 1. INTRODUCTION AND STRATEGY

The model under consideration is the two-dimensional Coulomb gas (2dCG), i.e., a neutral system of positive and negative unit charges $q_i = \pm 1$ in an infinite plane of points $\mathbf{r} \in R^2$, interacting through the pair potential

$$v(\mathbf{r}_i, \mathbf{r}_j) = \begin{cases} -q_i q_j \ln (|\mathbf{r}_i - \mathbf{r}_j|/L), & |\mathbf{r}_i - \mathbf{r}_j| > \sigma \\ \infty, & |\mathbf{r}_i - \mathbf{r}_j| \leqslant \sigma \end{cases} \tag{1.1}$$

[1] Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 842 28 Bratislava, Slovakia; E-mails: (P.K.) fyzipali@savba.sk, (L.Š.) fyzimaes@savba.sk

[2] Laboratoire de Physique Théorique, Université de Paris-Sud, Bâtiment 210, 91405 Orsay Cedex, France.

Here, the logarithmic Coulomb potential is the solution of the 2d Poisson equation $\Delta v(\mathbf{r}) = -2\pi\delta(\mathbf{r})$. The Coulomb potential is regularized at short distance by a hard-core potential of diameter $\sigma$ around each charge. The system is studied as the classical one and in thermodynamic equilibrium, via the grand canonical ensemble characterized by the (dimensionless) inverse temperature $\beta$ and the couple of equal particle fugacities $z_+ = z_- = z$. The fugacity $z$ has dimension $[\text{length}]^{-2}$. Within the grand canonical formalism, the length scale $L$ in (1.1) manifests itself as the rescaling of $z$, $z \to L^{\beta/2} z$. We shall set $L$ to unity for simplicity, keeping in mind that the true dimension of the rescaled $z$ is $[\text{length}]^{\beta/2-2}$. The corresponding particle number densities $n_+ = n_- = n/2$ ($n$ is the total particle density) enter into the formalism in the dimensionless combination $n\sigma^2$.

For small values of the dimensionless density $n\sigma^2$, the famous Kosterlitz–Thouless (KT) transition[1] of infinite order takes place at a specific density-dependent inverse temperature $\beta_{\mathrm{KT}}$.[2, 3] In the high-temperature conducting phase $\beta < \beta_{\mathrm{KT}}$, the effective potential between infinitesimal external charges decays exponentially due to perfect screening by the positive and negative charges of the Coulomb system. In the low-temperature dielectric phase $\beta > \beta_{\mathrm{KT}}$, the system charges form dipoles and no longer screen an external charge, so that the effective potential between infinitesimal external charges is proportional to the bare logarithmic potential. At high enough $n\sigma^2$, the KT critical line splits into a first order liquid-gas coexistence curve (for Monte-Carlo (MC) simulations, see refs. 4 and 5, for theoretical computation, see ref. 2).

In the low-density limit $n\sigma^2 \to 0$, which is of special interest in general and also in this paper, the thermodynamic behavior of the 2dCG as a function of $\beta$ undergoes fundamental changes at two points: $\beta_{\mathrm{c}} = 2$ (the collapse of pointlike particles) and $\beta_{\mathrm{KT}} = 4$ (the KT phase transition). The first (collapse) point reflects the fact that, for the case of strictly pointlike particles $\sigma = 0$, the singularity of the Coulomb potential $v(\mathbf{r})$ (1.1) at the origin prevents the thermodynamic stability against collapse of positive-negative pairs of charges (or, equivalently, the corresponding Boltzmann factor $r^{-\beta}$ is not integrable at short distances in 2d) for $\beta \geqslant 2$. Thus, for $0 \leqslant \beta < 2$, the system of pointlike particles is thermodynamically stable and the introduction of a hard core around particles is a marginal perturbation which does not change the thermodynamics substantially. On the other hand, for $2 \leqslant \beta < 4$, the introduction of a hard core is inevitable for avoiding the collapse: when one calculates thermodynamic quantities and at the end takes the limit $\sigma \to 0$ (with $z$ being fixed), while the density, the free energy and the internal energy per particle diverge due to collapse phenomenon, the specific heat and the truncated (Ursell) correlation functions are expected to remain finite.[6] In spite of the tendency to the collapse into neutral pairs of charges, there still exist free charges which are able to screen and the system remains in its conducting phase up to the KT phase transition at point $\beta_{\mathrm{KT}} = 4$. We would like to stress that, for a given fugacity $z$ and when $2 \leqslant \beta < 4$, although $n \to \infty$ as $\sigma \to 0$, the dimensionless density is supposed to go to the limit of interest, $n\sigma^2 \to 0$.

In what follows, we shall summarize in detail the known results in the two qualitatively different regimes $(0 \leqslant \beta < 2)$ and $(2 < \beta < 4)$, and at the collapse point $\beta_c = 2$.

In the stability range of inverse temperatures $0 \leqslant \beta < 2$, as has been already mentioned, the thermodynamics of the 2dCG is well defined even for the case of pointlike particles, $\sigma = 0$. The density derivatives of the Helmholtz free energy, like the pressure $p$, can be calculated exactly by using a simple scaling argument. For instance, the equation of state

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

has been known for a very long time.[7] The temperature derivatives of the Helmholtz free energy, like the internal energy $U$ or the constant volume (surface in 2d) specific heat $C_V$, are nontrivial quantities, the calculation of which can be based on an explicit density-fugacity relationship. This relationship was obtained only recently[8] via a mapping of the 2dCG onto a classical 2d sine-Gordon theory with a specific normalization of the cos-field, and then by using quite recent results about that integrable field theory.[9, 10] Explicitly one finds

$$\frac{n}{z^{4/(4-\beta)}} = \left(\frac{\pi\beta}{8}\right)^{\beta/(4-\beta)} \left[2\,\frac{\Gamma(1-\beta/4)}{\Gamma(1+\beta/4)}\right]^{4/(4-\beta)} \times \frac{\Gamma^2(1+\beta/[2(4-\beta)])}{(1/\pi)\,\Gamma^2(1/2+\beta/[2(4-\beta)])}\,\frac{\mathrm{tg}(\pi\beta/[2(4-\beta)])}{\pi\beta/[2(4-\beta)]} \tag{1.3}$$

where $\Gamma$ stands for the Gamma function The density-fugacity relationship (1.3) was checked on a few lower orders of its high-temperature $\beta$-expansion by using a renormalized Mayer expansion in *density*, valid just in the stability regime. For fixed $z$, the particle density exhibits the expected collapse singularity as $\beta \to 2^-$:

$$n \sim \frac{4\pi z^2}{2-\beta} \tag{1.4}$$

This behavior can be derived by using an independent-pair picture of the system around the collapse point,[6] which is another check of the exact results. Based on the density-fugacity relationship (1.3), the complete thermodynamics of the pointlike CG can be obtained by elementary means in the whole stability interval $0 \leqslant \beta < 2$.[8]

At the collapse point $\beta_c = 2$, by the continualization of Gaudin's lattice model,[11] which is expected to have the same properties as the 2dCG in the low-density limit, the truncated many-body densities (Ursell functions) were found in refs. 12 and 13. These densities have the remarkable property of going to well-defined limits as $n\sigma^2$ vanishes (as is believed, this property lasts up to the KT phase transition), identical to the densities of an equivalent Thirring model at the free-fermion point. The knowledge of all truncated many-body densities at $\beta_c = 2$ for $n\sigma^2 = 0$ permits one to extract the leading parts of thermodynamic quantities at $\beta = 2$ which, for a fixed fugacity $z$, do not vanish in the low-density limit $n\sigma^2 \to 0$.[12] Namely,

$$n = 4\pi z^2 \left[ \ln\left(\frac{1}{\sigma\pi z}\right) - C + O(1) \right] \tag{1.5a}$$

$$\beta p = 2\pi z^2 \left[ \ln\left(\frac{1}{\sigma\pi z}\right) - C + \frac{1}{2} + O(1) \right] \tag{1.5b}$$

$$u^{\text{ex}} = \frac{1}{4}\left[ \ln\left(\frac{\sigma}{\pi z}\right) - C + O(1) \right] \tag{1.5c}$$

$$\frac{c_V^{\text{ex}}}{k_B} = \frac{1}{6}\left[ \ln\left(\frac{1}{\sigma\pi z}\right) - C \right]^2 - \frac{1}{4}\left[ \ln\left(\frac{1}{\sigma\pi z}\right) - C \right] - \frac{1}{8} + O\left(\frac{1}{\ln(\sigma\pi z)}\right) \tag{1.5d}$$

Here, $u^{\text{ex}} = \langle E \rangle / N$ is the excess (over ideal) internal energy per particle, $c_V^{\text{ex}} = C_V^{\text{ex}}/N$ is the excess specific heat at constant volume per particle, and $C$ is the Euler constant.

The region of inverse temperatures $2 \leqslant \beta < 4$ is usually studied by using the Mayer series expansion of the specific grand potential in *fugacity*. It was proven that each term of the $z$-series converges in the insulator region $\beta > 4$.[14, 15] For $\beta \leqslant 4$, the existence of infinitely many thresholds at inverse temperatures

$$\beta_l = 4\left(1 - \frac{1}{2l}\right), \qquad l = 1, 2, \ldots \tag{1.6}$$

lying between $\beta_1 = \beta_c = 2$ and $\beta_\infty = \beta_{\text{KT}} = 4$, was observed by Gallavotti and Nicoló[14]: if $\beta > \beta_l$, only the Mayer series coefficients (cluster integrals) up to the order $2l$ are finite, and the cluster integrals of order $> 2l$ exhibit a large-distance divergence in the infinite-volume limit. Below the collapse point $\beta < 2$ (where the density format is appropriate) all cluster integrals diverge. The free energy is supposed to have at points $\{\beta_l\}_{l=1}^{\infty}$ a logarithmic dependence on the cut-off (in our case $n\sigma^2$).[16] Points $\{\beta_l\}_{l=1}^{\infty}$ were conjectured to correspond to a sequence of transitions from the pure multipole insulating phase ($\beta > 4$) to the conducting phase ($\beta < 2$) via an infinite number of intermediate phases.[14]

Such a conjecture was later denied by Fisher *et al.*[17] In the limit $n\sigma^2 \to 0$, they proposed the following ansatz for the equation of state in the fugacity format:[3]

$$\beta p = b_\psi(\beta)\, z^{2\psi(\beta)}[1 + e(z\sigma^{(4-\beta)/2}, \beta)] + \frac{1}{\sigma^2} \sum_{l=1}^{\infty} \bar{b}_{2l}(\beta)[z\sigma^{(4-\beta)/2}]^{2l} \tag{1.7}$$

where the temperature-dependent exponent is

$$2\psi(\beta) = \frac{4}{4-\beta} \tag{1.8}$$

The function $e$ vanishes as $n\sigma^2 \to 0$. At points $\beta_l$ [see relation (1.6)], $\psi(\beta_l) = l$. The coefficient $b_\psi(\beta)$ and the function $e(z\sigma^{(4-\beta)/2}, \beta)$ were suggested to be analytic in the whole conducting regime $0 \leqslant \beta < 4$. The coefficients $\{\bar{b}_{2l}(\beta)\}_{l=1}^{\infty}$ were suggested to be zero for $0 \leqslant \beta < 2$, and finite, analytic in $\beta$, for $2 \leqslant \beta < 4$. The divergence of the coefficients of an *analytic* expansion in $z^2$ was related to the appearance of the *anomalous* term $b_\psi z^{2\psi}$ in (1.7). Moreover, at $\beta_{\mathrm{KT}} = 4$, $\psi(\beta_{KT})$ becomes infinite and the anomalous term disappears from the ansatz, in agreement with the results of refs. 14 and 15.

The ansatz for the equation of state of the 2dCG (1.7) is consistent with the singular behavior of the fugacity series,[14] but does not imply the existence of low-density phase transitions between intermediate phases, which is in full agreement with the MC simulations.[4, 5] However, the supposed analytic behavior of the coefficients $b_\psi(\beta)$ and $\{\bar{b}_{2l}(\beta)\}_{l=1}^{\infty}$ is an ad-hoc assumption which must be tested on particular cases and in special limits. The test on the combined Debye–Hückel and Bjerrum theories,[17] which are essentially the mean-field ones, is not sufficient. Having at disposal the exact thermodynamics of the pointlike 2dCG in the stability region,[8] we now derive the exact form of the coefficient $b_\psi(\beta)$ in the stability region which does not exhibit the analytic structure proposed by Fisher *et al.*[17] In the stability region $0 \leqslant \beta < 2$, the presence of the hard

[3] We rescale $z$ by $\sigma^{(4-\beta)/2}$ in the ansatz in order to work with dimensionless quantities.

core $\sigma$ is a minor perturbation of the system of pointlike particles and one *can* consider the case of pointlike particles $n\sigma^2 = 0$ (or, equivalently, $z$ fixed and $\sigma = 0$) in the ansatz (1.7). The equation of state (1.2), when combined with the ansatz (1.7) with the function $e = 0$, yields

$$b_\psi(\beta) = \left(1 - \frac{\beta}{4}\right) \frac{n}{z^{4/(4-\beta)}} \tag{1.9}$$

Substituting $n/z^{4/(4-\beta)}$ by the rhs of (1.3), we get the exact $b_\psi(\beta)$ which behaves as follows

$$b_\psi(\beta) \propto \mathrm{tg}\left(\frac{\pi\beta}{2(4-\beta)}\right), \qquad 0 \leqslant \beta < 2 \tag{1.10}$$

Here, the proportionality factor is an analytic function of $\beta$ for $0 \leqslant \beta < 4$. The tg-function has the simple pole just at the collapse point $\beta_1 = \beta_c = 2$. This simple pole is nothing but a consequence of the collapse phenomenon: for a fixed finite $z$, $n \to \infty$ when approaching the collapse point $\beta_c = 2$. According to (1.5), the divergence of $n$ at $\beta_c = 2$ is logarithmic in the dimensionless $\sigma z$, so that the dimensionless density $n\sigma^2$ is still very small when $\sigma \to 0$ as is required in the ansatz proposal (1.7). It is interesting to notice that a "naive" analytic continuation of the exact $b_\psi(\beta)$ (1.10) from the stability region to the range of inverse temperatures $2 \leqslant \beta < 4$ has the singularities just at the thresholds $\{\beta_l\}_{l=1}^\infty$ given by (1.6). Indeed, the decomposition of the tg-function into simple fractions[18] gives

$$\frac{\mathrm{tg}(\pi\beta/[2(4-\beta)])}{\pi\beta/[2(4-\beta)]} = \frac{2}{\pi^2} \sum_{l=1}^{\infty} \frac{1}{(\beta_l - \beta)} \frac{(4-\beta)^2 (4-\beta_l)^2}{\beta(4-\beta_l) + \beta_l(4-\beta)} \tag{1.11}$$

The thresholds $\{\beta_l\}_{l=1}^\infty$ manifest themselves as simple poles at which $b_\psi$ exhibits the discontinuity from $\lim_{\beta \to \beta_l^-} b_\psi(\beta) \to \infty$ to $\lim_{\beta \to \beta_l^+} b_\psi(\beta) \to -\infty$.

The aim of this paper is to develop a technical basis for the ansatz (1.7) in order to understand its analytic structure discussed in the above two paragraphs. We do not enter the region of particular interest $2 \leqslant \beta < 4$ from the low-temperature KT side ($\beta > 4$) as is usual in the approaches based on the fugacity series expansions, but from the high-temperature stability side ($\beta < 2$). In this stability region, we derive the leading correction to the exact thermodynamics of pointlike charges[8] due to presence of the hard core of diameter $\sigma$. This is done by combining the zeroth-moment (electroneutrality) sum rule for the pair charge-charge correlation function[19] with the knowledge of the leading term of the short-distance expansion of that charge-charge correlation. Since both the electroneutrality sum rule and the leading short-distance expansion term remain valid up to the KT transition, we analytically extend our results from the stability region beyond the collapse point. The results, which are conjectured to be exact in the low-density limit $n\sigma^2 \to 0$ in the whole interval $0 \leqslant \beta < 3$, reproduce correctly the singularities of thermodynamic quantities at the collapse point $\beta_c = 2$ and agree well with the MC simulations.[4] In the leading order, we recover the ansatz (1.7) where the leading coefficient in the sum, $\bar{b}_2$, has the simple pole at the collapse point $\beta_1 = \beta_c = 2$ which exactly cancels the simple pole of $b_\psi$ at $\beta_c = 2$. Our results thus confirm the "subtraction" mechanism of Fisher *et al.*[17] which excludes the existence of intermediate phases proposed by Gallavotti and Nicoló,[14] however, the coefficients $\{\bar{b}_{2l}\}_{l=1}^{\infty}$ turn out to be nonzero in the whole interval $0 \leqslant \beta < 4$. They are suggested to exhibit simple poles at the corresponding points $\{\beta_l\}_{l=1}^{\infty}$ (1.6) which exactly cancel the corresponding simple poles of the anomaly coefficient $b_\psi(\beta)$ occurring at the same points.

The paper is organized as follows. The method is described in Section 2. The complete thermodynamics in the leading order in $\sigma$ is derived and then tested in various limits in Section 3. In Section 4, the comparison of our results is made with the MC simulations. In Section 5, a brief recapitulation is presented. A possible extension of our results to higher orders in $\sigma$ is also discussed and some concluding remarks are given.

## 2. METHOD

In the conducting phase of the two-component plasma with the Coulomb plus an arbitrary short-range pair interaction of particles, the zeroth and second moments of the charge-charge density are determined exclusively by the long-range tail of the Coulomb potential.[19] The starting point of our calculation is the zeroth-moment (electroneutrality) sum rule

$$n_q = \int [U_{q,-q}(\mathbf{r}) - U_{q,q}(\mathbf{r})]\, \mathrm{d}^2 r \tag{2.1}$$

Here, with the notation $\hat{n}_q(\mathbf{r}) = \sum_i \delta_{q,q_i} \delta(\mathbf{r} - \mathbf{r}_i)$ for the microscopic density of particles of charge $q = \pm 1$ at position $\mathbf{r}$, $n_q = \langle \hat{n}_q(\mathbf{r}) \rangle = n/2$ and the Ursell function $U_{q,q'}(\mathbf{r}, \mathbf{r}') = U_{q,q'}(|\mathbf{r} - \mathbf{r}'|)$ (denoted as $\rho^{(2)\mathrm{T}}_{q,q'}$ in refs. 12 and 13) is defined by

$$U_{q,q'}(\mathbf{r}, \mathbf{r}') = \langle \hat{n}_q(\mathbf{r})\, \hat{n}_{q'}(\mathbf{r}') \rangle - n_q \delta_{q,q'} \delta(\mathbf{r} - \mathbf{r}') - n_q n_{q'} \tag{2.2}$$

For the Coulomb system of interest (1.1), the difference $U_{q,-q} - U_{q,q}$ vanishes inside the hard core, and the total particle number density $n$ is given by

$$n(z, \sigma) = 2 \int_\sigma^\infty 2\pi r \, \mathrm{d}r [U_{q,-q}(r; z, \sigma) - U_{q,q}(r; z, \sigma)] \tag{2.3}$$

Hereinafter, we omit in the notation the dependence of quantities on $\beta$.

The dependence of the density $n$ on $\sigma$ in (2.3) comes from the cutoff in the integration over $r$ and from the $\sigma$-dependence of the Ursell functions themselves. These Ursell functions are supposed to be well defined and finite for the zero density, $n\sigma^2 = 0$, in the whole conducting regime $0 \leqslant \beta < 4$, including the collapse interval $2 \leqslant \beta < 4$. This belief is strongly supported by the finite values of the Ursell functions at the collapse point $\beta_c = 2$[12, 13]:

$$U_{q,-q}(r; z, 0) = \left( \frac{m^2}{2\pi} \right)^2 K_1^2(mr) \tag{2.4a}$$

$$U_{q,q}(r; z, 0) = -\left( \frac{m^2}{2\pi} \right)^2 K_0^2(mr) \tag{2.4b}$$

with fixed $m = 2\pi z$, $K_0$ and $K_1$ are modified Bessel functions. We can thus write

$$U_{q,q'}(r; z, \sigma) = U_{q,q'}(r; z, 0) + \Delta_{q,q'}(r; z, \sigma), \qquad r \geqslant \sigma \tag{2.5}$$

which defines $\Delta_{q,q'}(r; z, \sigma)$, vanishing when $\sigma \to 0$, as the change of $U_{q,q'}(r; z, 0)$ due to the introduction of the hard core $\sigma \leqslant r$ to pointlike particles. Subtracting Eq. (2.3) with $\sigma > 0$ and the same equation with $\sigma = 0$, one arrives at

$$\begin{aligned} n(z, \sigma) - n(z, 0) = & -2 \int_0^\sigma 2\pi r \, \mathrm{d}r [U_{q,-q}(r; z, 0) - U_{q,q}(r; z, 0)] \\ & + 2 \int_\sigma^\infty 2\pi r \, \mathrm{d}r [\Delta_{q,-q}(r; z, \sigma) - \Delta_{q,q}(r; z, \sigma)] \end{aligned} \tag{2.6}$$

Since $n(z, 0)$ is defined only in the stability regime $0 \leqslant \beta < 2$, for the time being we shall restrict ourselves to this range of $\beta$. We now make a heuristic assumption analogous to that made at the point $\beta_c = 2$ in refs. 12 and 13: in the low-density limit $n\sigma^2 \to 0$ and for $0 \leqslant \beta < 4$, one can neglect the quantities $\Delta_{q, \pm q}$ in Eq. (2.6). Consequently,

$$n(z, \sigma) = n(z, 0) - 2 \int_0^\sigma 2\pi r \, dr [U_{q,-q}(r; z, 0) - U_{q,q}(r; z, 0)] \tag{2.7}$$

Our assumption is equivalent to saying that in equation (2.6) only the contribution $\propto \int_0^\sigma r \, dr [U_{q,-q}(r; z, 0) - U_{q,q}(r; z, 0)]$ with $\sigma > 0$ is enough for removing, via a systematic short-distance expansions of $U_{q, \pm q}(r; z, 0)$, term by term the singularities of $n(z, 0)$ at points $\{\beta_l\}_{l=1}^{\infty}$ (see the Introduction). This scenario will be verified at the first singular point $\beta_1 = \beta_c = 2$.

The next step is to construct the short-distance expansions of $U_{q, \pm q}(r; z, 0)$ in the integral on the rhs of (2.7). For small enough $\beta$, the short-distance expansion of the Ursell functions is dominated by the Boltzmann factor of the corresponding pair Coulomb potential.[20, 21] In the case of oppositely charged particles, one has

$$U_{q,-q}(r; z, 0) \sim z^2 r^{-\beta} \qquad \text{as} \quad r \to 0 \tag{2.8}$$

valid in the whole interval $0 \leqslant \beta < 4$. Note that since $K_1(mr) \sim 1/(mr)$ for $r \to 0$, $U_{q,-q}(r; z, 0)$ at $\beta_c = 2$ [see relation (2.4a)] satisfies (2.8). In the case of the same charges, the leading term has a more complicated structure,

$$U_{q,q}(r; z, 0) \propto \begin{cases} r^\beta & \text{for} \quad 0 \leqslant \beta < 1 \\ r^{2-\beta} & \text{for} \quad 1 \leqslant \beta < 2 \end{cases} \qquad \text{as} \quad r \to 0 \tag{2.9}$$

The change of the power-law behavior is caused by the divergence of the prefactor to $r^\beta$ at $\beta = 1$.[21] Considering in (2.4b) that $K_0(mr) \sim -\ln r$ for $r \to 0$, the logarithmic behavior of $U_{q,q}(r; z, 0)$ at $\beta_c = 2$ can be understood as a limiting case of $r^{2-\beta}$ in (2.9). Within the sine-Gordon representation of the 2d pointlike CG, the formula corresponding to (2.8) is known as the conformal normalization of the cos-field. For such a theory, the short-distance expansion of correlation functions is available by using the Operator Product Expansion,[22] as was explicitly done in ref. 23. Although this method allows one to construct systematically the short-distance expansions of $U_{q, \pm q}(r; z, 0)$ with coefficients expressed in terms of Dotsenko–Fateev integrals,[24] it applies only to small values of $\beta$ and does not describe, e.g., the change of the behavior at $\beta = 1$ (2.9). In any case, in the interval $0 \leqslant \beta < 4$, the charge–charge combination of the Ursell functions is dominated at short distances by (2.8),

$$U_{q,-q}(r; z, 0) - U_{q,q}(r; z, 0) \sim z^2 r^{-\beta} \qquad \text{as} \quad r \to 0 \tag{2.10}$$

and we shall consider just this leading term.

Inserting (2.10) into (2.7), one obtains the basic formula

$$n(z, \sigma) = n(z, 0) - 4\pi z^2 \frac{\sigma^{2-\beta}}{2-\beta} \tag{2.11}$$

Although this result was derived in the region $0 \leqslant \beta < 2$ where $n(z, 0)$ is well defined by (1.3), it is reasonable to assume the continuation of (2.11) beyond the collapse point $\beta_c = 2$ because both the sum rule (2.3) and the leading short-distance expansion (2.10), which play the crucial role in the derivation of (2.11), remain valid up to the KT transition at $\beta_{\mathrm{KT}} = 4$. As will be shown in the subsequent section, the leading correction term in Eq. (2.11) removes the singularity of $n(z, 0)$ at $\beta_1 = \beta_c = 2$, and provides an adequate description of the 2dCG with $n\sigma^2$ small up to $\beta_2 = 3$ where another singularity of $n(z, 0)$ occurs. This singularity at $\beta_2 = 3$ should be removed by the next term of the short-distance expansion (2.10) inserted into (2.7), however, as was mentioned above, it is not simple to get the explicit form of that term for such a large value of $\beta$. In any case, for dimensional reasons, the next term in (2.11) must be proportional to $z^4 \sigma^{6-2\beta}$ (see the analysis in Section 5), and therefore it vanishes in the low-density limit for $\beta < \beta_2$.

## 3. THERMODYNAMICS

Based on the density-fugacity relationship (2.11), we derive in this section the thermodynamics of the 2dCG in the restricted region of interest $0 \leqslant \beta < 3$. Our findings will be compared with the known results and conjectures reviewed in the Introduction, namely with the exact formulae at $\beta_c = 2$ (1.5), with the predictions based on the independent-pair collapse picture for $\beta > 2$ and in the limit $\sigma \to 0$,[6] and with the proposal (1.7) for the equation of state. The stability regime $0 \leqslant \beta < 2$ will not be discussed in detail since there the introduction of the hard core to pointlike particles is a marginal perturbation.

We first express the relation (1.3) for the density of pointlike particles $n(z, 0)$ in a more convenient form,

$$n(z, 0) = \frac{4\pi \Phi(\beta)}{2-\beta} z^{4/(4-\beta)} \tag{3.1}$$

where we have introduced the function

$$\Phi(\beta) = \left(\frac{\pi\beta}{8}\right)^{\beta/(4-\beta)} \left[2\frac{\Gamma(1-\beta/4)}{\Gamma(1+\beta/4)}\right]^{4/(4-\beta)} \frac{2-\beta}{4\pi}$$
$$\times \frac{\Gamma^2(1+\beta/[2(4-\beta)])}{(1/\pi)\,\Gamma^2(1/2+\beta/[2(4-\beta)])} \frac{\mathrm{tg}(\pi\beta/[2(4-\beta)])}{\pi\beta/[2(4-\beta)]} \tag{3.2}$$

With regard to the collapse singularity (1.4), $\Phi$ was chosen such that $\Phi(\beta=2)=1$. The Taylor expansion of $\ln\Phi(\beta)$ around $\beta=2$ thus reads

$$\ln\Phi(\beta) = (\ln\pi + C)(\beta-2) + \frac{1}{2}(\ln\pi + C)(\beta-2)^2$$
$$+\frac{1}{4}\left[\ln\pi + C - \frac{17}{12}\zeta(3)\right](\beta-2)^3 + \cdots \tag{3.3}$$

The function $\Phi(\beta)$ is positive in the interval $0 \leqslant \beta < 8/3$, it crosses zero at point $\beta = 8/3$ (which is not exceptional from any point of view) and diverges to $-\infty$ as $\beta \to 3$. Using the representation (3.1) in Eq. (2.11), one gets for $n = n(z, \sigma)$

$$n = \frac{4\pi}{2-\beta} z^{4/(4-\beta)}[\Phi(\beta) - (\sigma z^{2/(4-\beta)})^{2-\beta}] \tag{3.4}$$

Notice that this relation is dimensionally correct—it is expressible in terms of dimensionless quantities

$$\xi = \sigma z^{2/(4-\beta)} \tag{3.5}$$

and $n\sigma^2$, or the packing fraction

$$\eta = \tfrac{1}{4}\pi n \sigma^2 \tag{3.6}$$

used in the MC simulations.[4] Taking into account the expansion (3.3) in Eq. (3.4) one sees that, for fixed $z$ and nonzero $\sigma$, the density $n$ is finite at $\beta_c = 2$; its value coincides with the expected result (1.5a). Formula (3.4) can be analytically continued to the region $2 < \beta < 3$. For $\beta > 2$ and small $\sigma$, the term $[\sigma z^{2/(4-\beta)}]^{2-\beta}$ becomes larger than $\Phi(\beta)$ and, when combined with the negative denominator $(2-\beta)$, it implies the positive sign of $n$ up to $\beta = 3$. When $\sigma \to 0$, this term and consequently $n$ diverge in the region $2 \leqslant \beta < 3$ as a consequence of the collapse phenomenon.

We proceed by the derivation of the equation of state. The grand canonical potential $\Omega$ is determined by the thermodynamic relation

$$n = z\,\frac{\partial(-\beta\Omega/V)}{\partial z} \tag{3.7}$$

where $V(\to\infty)$ is the volume (in 2d, the surface) of the homogeneous system. With respect to the boundary condition $(-\beta\Omega/V)|_{z=0} = 0$, the integration of (3.7), with $n$ substituted from Eq. (3.4), results in the equation of state for $\beta p = -\beta\Omega/V$,

$$\beta p = \frac{\pi(4-\beta)}{2-\beta}\,\Phi(\beta)\,z^{4/(4-\beta)} - \frac{2\pi}{\sigma^2(2-\beta)}\,(z\sigma^{(4-\beta)/2})^2 \tag{3.8}$$

Eq. (3.8) has the form of the ansatz (1.7) with

$$b_\psi = \frac{\pi(4-\beta)}{2-\beta}\,\Phi(\beta), \qquad \bar{b}_2 = -\frac{2\pi}{2-\beta} \tag{3.9}$$

In contrast to the conjecture made in ref. 17, these coefficients are not analytic functions of $\beta$ at $\beta = 2$. Let us now rewrite the equation of state (3.8) with the aid of the density-fugacity relationship (3.4) as follows

$$\frac{\beta p}{n} = \frac{1}{2} + \frac{(2-\beta)\,\Phi}{4(\Phi - \xi^{2-\beta})} \tag{3.10}$$

where $\xi$ is defined by (3.5). At $\beta_c = 2$ and for nonzero $\sigma$, (3.10) agrees with relations (1.5a) and (1.5b). In the limit of pointlike particles $\sigma \to 0$, our equation of state (3.10) reduces to the one obtained by Hauge and Hemmer[6]: in the stability regime $0 \leqslant \beta < 2$, the hard-core correction $\xi^{2-\beta}$ is negligible for small $\sigma$ and the $\sigma \to 0$ limit corresponds to (1.2), while for $2 < \beta < 3$ $\xi^{2-\beta}$ diverges when $\sigma \to 0$ and so $\beta p/n \to 1/2$, i.e., the pairs of $\pm 1$ charged particles collapse into neutral "free" particles of half density $n/2$.

Finally, the (excess) dimensionless specific free energy $f = \beta F^{\text{ex}}/N$ reads

$$\begin{aligned} f(n,\beta) &= \frac{\beta\Omega}{nV} + \ln z \\ &= -\frac{1}{2} - \frac{(2-\beta)\,\Phi}{4(\Phi - \xi^{2-\beta})} + \ln z \end{aligned} \tag{3.11}$$

where the implicit dependence of the fugacity $z(n, \beta)$ on the particle density $n$ is determined by Eq. (3.4). According to the elementary thermodynamics, the (excess) internal energy per particle $u^{\mathrm{ex}}$ is given by $u^{\mathrm{ex}} = \partial f(n, \beta)/\partial\beta$, explicitly

$$u^{\mathrm{ex}} = \frac{1}{2}\ln\sigma - \frac{1}{2(2-\beta)} - \frac{1}{2(\Phi-\xi^{2-\beta})}\left[\left(2-\frac{\beta}{2}\right)\Phi' + \Phi\ln\xi\right] \tag{3.12}$$

and the (excess) specific heat at constant volume per particle $c_V^{\mathrm{ex}}$ is given by $c_V^{\mathrm{ex}}/k_B = -\beta^2\partial^2 f(n, \beta)/\partial\beta^2$, explicitly

$$\begin{aligned}\frac{1}{\beta^2}\frac{c_V^{\mathrm{ex}}}{k_B} &= \frac{1}{2(2-\beta)^2} + \frac{(4-\beta)\,\Phi''}{4(\Phi-\xi^{2-\beta})}\\ &\quad - \frac{1}{2(2-\beta)(\Phi-\xi^{2-\beta})[\Phi-(2-\beta/2)\,\xi^{2-\beta}]}\\ &\quad \times\left\{(2-\beta)\,\Phi'\left[\Phi+\left(2-\frac{\beta}{2}\right)\Phi'\right] + (\Phi-\xi^{2-\beta})\,\frac{\Phi}{2}\right.\\ &\quad \left.+(2-\beta)\,\xi^{2-\beta}(\ln\xi)[(1+\ln\xi)\,\Phi+(4-\beta)\,\Phi']\right\}\end{aligned} \tag{3.13}$$

At $\beta_c = 2$ and for nonzero $\sigma$, $u^{\mathrm{ex}}$ is identical to (1.5c), while

$$\frac{c_V^{\mathrm{ex}}(\beta=2)}{k_B} = \frac{1}{3}\,\frac{[\ln(\pi z\sigma)+C]^3 + 2[\ln(\pi z\sigma)+C]^2}{1+2[\ln(\pi z\sigma)+C]} - \frac{17}{12}\,\zeta(3)\,\frac{1}{[\ln(\pi z\sigma)+C]} \tag{3.14}$$

The expansion of this expression into the Laurent series in $1/[\ln(\pi z\sigma)+C]$ reproduces the leading terms in (1.5d).

All formulae derived above involve all corrections to the thermodynamic quantities which come from the leading term of the short-distance expansion of the Ursell functions, see formula (2.8). As was discussed in the last paragraph of Section 2, the next terms of this short-distance expansion depend on higher powers of $r$ and they are vanishing in the limit $\sigma \to 0$ up to $\beta_2 = 3$. Consequently, at $\beta = 2$, the neglected corrections to $n,\ldots, c_V^{\mathrm{ex}}/k_B$ behave according to the power-law in $z\sigma$ which is a much quicker decay than $1/\ln(\pi z\sigma)$ in the limit $z\sigma \to 0$. In this sense we believe that our results are exact in the low-density limit at $\beta = 2$, and even for $\beta < 3$.

As a further test of our results, in the region $2 < \beta < 3$ and in the limit $\sigma \to 0$, $u^{\mathrm{ex}}$ diverges to $-\infty$ due to the term $(\ln\sigma)/2$ involving the energy of the collapsed pair of particles. $c_V^{\mathrm{ex}}$ behaves differently: $\xi^{2-\beta}$ becomes large for small $\sigma$ and kills all terms on the rhs of (3.13), except of the first one. The consequent finite result $c_V^{\mathrm{ex}}/k_B = \beta^2/[2(2-\beta)^2]$ coincides with the finding of ref. 6.

## 4. COMPARISON WITH MC SIMULATIONS

In the previous two sections, we have derived the thermodynamics of the 2dCG by adding the leading hard-core correction term to the exact density-fugacity relationship for the Coulomb system of pointlike particles. We have successfully tested various limits of our results. In this section, the comparison is made with the MC simulations of the 2dCG.[4]

Our result (3.14) for the heat capacity $c_V^{\mathrm{ex}}$ at the collapse point $\beta_c = 2$, as the function of the packing fraction $\eta$ (3.6), is represented in Fig. 1. by the solid line. The agreement with the MC simulations is much better than in the case of the previously derived formula (1.5d) (triangles), which involves the first three terms of the Laurent expansion of (3.14).

In Figs. 2 and 3, we represent by solid lines our plots of the internal energy $u^{\mathrm{ex}}$ (3.12) and the heat capacity $c_V^{\mathrm{ex}}$ (3.13), respectively, versus the inverse temperature $\beta$, for two values of the packing fraction $\eta = 5 \times 10^{-4}$ and $5 \times 10^{-3}$. The agreement with the MC data (circles) is very good for $u^{\mathrm{ex}}$ and less satisfactory for $c_V^{\mathrm{ex}}$. Our results are getting worse when increasing $\eta$,

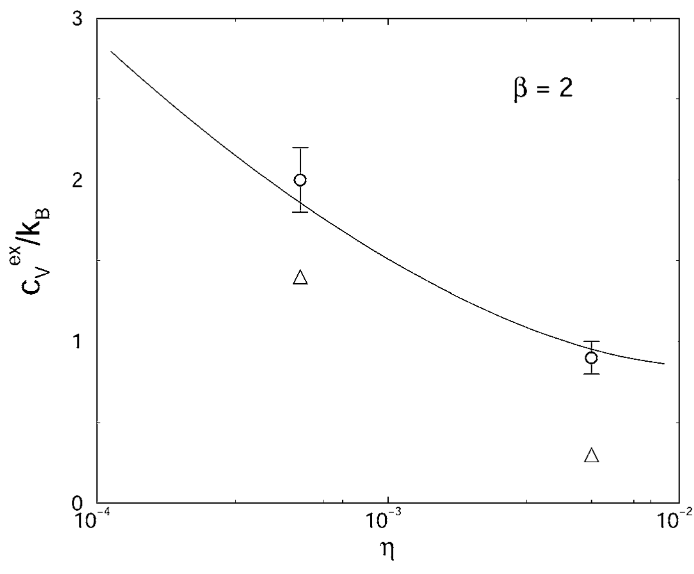


Fig. 1. The plot of $c_V^{\mathrm{ex}}/k_B$ vs. the packing fraction $\eta$ at $\beta_c = 2$: present result (3.14) (solid line), formula (1.5d) (triangles) and MC simulations (circles).

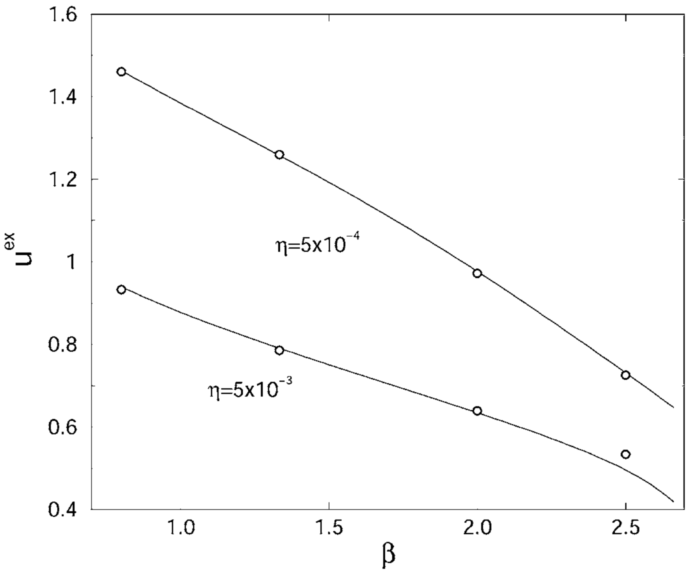


Fig. 2. The plot of $u^{ex}$ vs. the inverse temperature $\beta$ for $\eta = 5 \times 10^{-4}$ and $5 \times 10^{-3}$: present result (3.12) (solid lines) and MC simulations (circles).

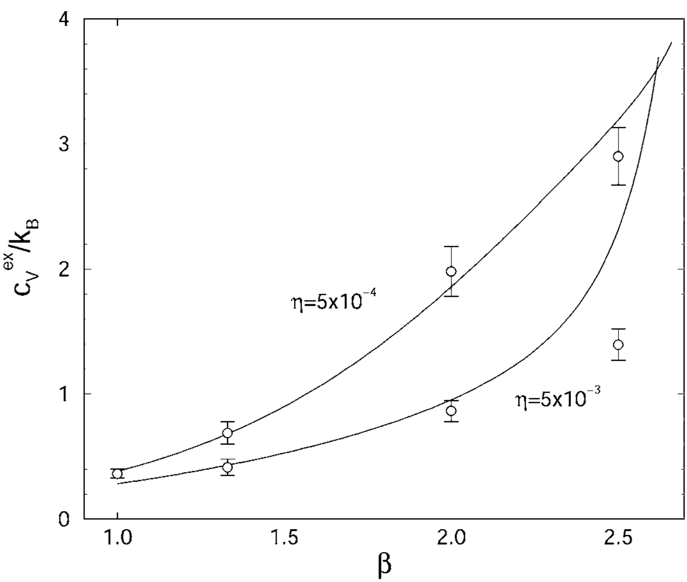


Fig. 3. The plot of $c_V^{ex}/k_B$ vs. the inverse temperature $\beta$ for $\eta = 5 \times 10^{-4}$ and $5 \times 10^{-3}$: present result (3.13) (solid lines) and MC simulations (circles).

what is obvious, and when approaching point $\beta = 3$: close to this point, the next (neglected) term of the hard-core corrections [which eliminates the next singularity of $n(z, 0)$ at $\beta_2 = 3$] starts to be important.

## 5. CONCLUSION

To recapitulate briefly the present paper, we have derived the leading correction to the exact thermodynamics of pointlike charges in the stability region $0 \leqslant \beta < 2$ of the 2dCG[8] due to presence of the hard core of diameter $\sigma$ around particles. The derivation was based on a combination of the electroneutrality sum rule (2.1) with the leading term of the short-distance expansion of Ursell functions in (2.10). The obtained basic formula (2.11) has an important feature: $n(z, \sigma)$ reduces to the exact $n(z, 0)$, given by (1.3), when $\sigma \to 0$. Since both the electroneutrality sum rule (2.1) and the leading term of the short-distance behavior (2.10) still apply beyond the collapse point $\beta_c = 2$, up to $\beta_{\mathrm{KT}} = 4$, we have proposed an analytic continuation of the relation (2.11) outside of the stability region. Although this is not a rigorously justified step [we do not know anything about the convergence properties of the complete series on the rhs of (2.11)], the extended formula (2.11) exhibits the expected behavior of the 2dCG when crossing the collapse point. Namely, for $\sigma > 0$, the leading correction term exactly cancels the singularity of $n(z, 0)$ at the collapse point $\beta_c = 2$ as it should be. As was argued at the end of Section 2, there are indications that formula (2.11) is exact in the low-density limit up to $\beta_2 = 3$ where another singularity of $n(z, 0)$ should be canceled by the next correction term proportional to $z^4 \sigma^{6-2\beta}$. In Section 3, we have derived the complete thermodynamics of the 2dCG implied by the relation (2.11), and tested in at the collapse point $\beta_c = 2$[12] and in the limit $\sigma \to 0$ for $2 \leqslant \beta < 3$.[6] The comparison with the MC simulations,[4] presented in Section 4, is satisfactory.

The extension of the thermodynamic treatment of the 2dCG around and beyond $\beta_2 = 3$, up to $\beta_{\mathrm{KT}} = 4$, requires to construct a systematic short-distance expansion of the Ursell functions in (2.3). This short-distance expansion, which leading term is presented in (2.10), can be done, in principle, systematically term by term. In basic formula (2.11), in analogy with the finding for the obtained leading "1" term, every new term of order "l" should remove the singularity of the pointlike $n(z, 0)$ at the threshold $\beta_l$ given by (1.6) in order to make the particle density $n(z, \sigma)$ finite and positive up to $\beta_{l+1}$. Thus, the density-fugacity relationship is expected in the form

$$n(z, \sigma) = n(z, 0) - \sum_{l=1}^{\infty} \frac{\bar{c}_{2l}(\beta)}{\beta_l - \beta} (z^2 \sigma^{\beta_l - \beta})^l \tag{5.1}$$

where the coefficient $\bar{c}_{2l}(\beta)$ $(l=1,2,...)$ is regular at $\beta=\beta_l$. According to our result (2.11), $\bar{c}_2(\beta)=4\pi$. Taking into account the formula (1.3) for $n(z,0)$, the exponent of $z$, $4/(4-\beta)$, is equal to $2l$ at the pole $\beta=\beta_l$ and the exponent of $\sigma$ in (5.1) is put by dimensional reasons. Note that since $n=z\partial(\beta p)/\partial z$, (5.1) automatically leads to the ansatz (1.7) with $e=0$ [because we have not taken into account in (2.6) "slight" hard-core changes of the correlation functions $\Delta_{q,\pm q}$ defined by (2.5)]. This confirms the "subtraction" mechanism of Fisher *et al.*,[17] indicating a total absence of phase transitions in the interval $2\leqslant\beta<4$ which were suggested in ref. 14. On the other hand, the coefficients $b_\psi$ and $\{\bar{b}_{2l}\}_{l=1}^{\infty}$ are *singular* functions of $\beta$, which is in contradiction to the analytic structure of the ansatz (1.7) proposed in ref. 17. The $l$th term in the sum on the rhs of (5.1) has the correct behavior in the limit $\sigma\to 0$: it goes to 0 when $\beta<\beta_l$ and removes the singularity of $n(z,0)$ at $\beta=\beta_l$ (and simultaneously gives rise to a logarithmic dependence on the hard core at this point). A systematic generation of the coefficients $\bar{c}_l(\beta)$ is our task for the future.

## ACKNOWLEDGMENTS

We are very indebted to B. Jancovici for valuable discussions, careful reading of the manuscript and useful comments. We thank also A. Alastuey and P. J. Forrester for stimulating discussions. Remarks of two unknown referees, which helped us to improve the presentation of our work, are very appreciated. The stay of L. Šamaj in LPT Orsay was supported by a NATO fellowship. The support by Grant VEGA 2/7174/20 is acknowledged.

## REFERENCES

1. J. M. Kosterlitz and D. J. Thouless, *J. Phys. C* **6**:1181 (1973).
2. Y. Levin, X. J. Li, and M. E. Fisher, *Phys. Rev. Lett.* **73**:2716 (1994).
3. A. Alastuey and F. Cornu, *J. Stat. Phys.* **89**:5 (1997).
4. J. M. Caillol and D. Levesque, *Phys. Rev. B* **33**:499 (1986).
5. G. Orkoulas and A. Z. Panagiotopoulos, *J. Chem. Phys.* **104**:7205 (1996).
6. E. H. Hauge and P. C. Hemmer, *Phys. Norvegica* **5**:209 (1971).
7. A. Salzberg and S. Prager, *J. Chem. Phys.* **38**:2587 (1963).
8. L. Šamaj and I. Travěnec, *J. Stat. Phys.* **101**:713 (2000).
9. C. Destri and H. de Vega, *Nucl. Phys. B* **358**:251 (1991).
10. Al. B. Zamolodchikov, *Int. J. Mod. Phys. A* **10**:1125 (1995).
11. M. Gaudin, *J. Phys. (France)* **46**:1027 (1985).
12. F. Cornu and B. Jancovici, *J. Stat. Phys.* **49**:33 (1987).
13. F. Cornu and B. Jancovici, *J. Chem. Phys.* **90**:2444 (1989).
14. G. Gallavotti and F. Nicoló, *J. Stat. Phys.* **39**:133 (1985).
15. E. Speer, *J. Stat. Phys.* **42**:895 (1986).

16. J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon, Oxford, 1989).
17. M. E. Fisher, X. J. Li, and Y. Levin, *J. Stat. Phys.* **79**:1 (1995).
18. I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products*, 5th edn. (Academic Press, London, 1994).
19. F. H. Stillinger and R. Lovett, *J. Chem. Phys.* **48**:3858 (1968); *J. Chem. Phys.* **49**:1991 (1968).
20. B. Jancovici, *J. Stat. Phys.* **17**:357 (1977).
21. J. P. Hansen and P. Viot, *J. Stat. Phys.* **38**:823 (1985).
22. K. Wilson, *Phys. Rev.* **179**:1499 (1969).
23. V. Fateev, D. Fradkin, S. Lukyanov, A. Zamolodchikov and Al. Zamolodchikov, *Nucl. Phys. B* **540**:587 (1999).
24. V. Dotsenko and V. Fateev, *Nucl. Phys. B* **240**:312 (1984); *Nucl. Phys. B* **251**:691 (1985).