PHYSICAL REVIEW E VOLUME 49, NUMBER 6 JUNE 1994

Two-dimensional one-component plasma at coupling $\Gamma=4$: Numerical study of pair correlations

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(Received 24 January 1994)

We consider a classical two-dimensional one-component plasma of charged particles in a circularly symmetric neutralizing background, at a coupling constant of $\Gamma=e^2/k_BT=4$. The numerical results, based technically on a successive increase of the number of particles and on a Van der Monde determinantal representation of Boltzmann factors, strongly indicate a Gaussian-type falloff of the truncated bulk charge-charge correlations, similarly as in the exactly solvable $\Gamma=2$ case.

PACS number(s): 52.25.Kn, 61.20.Gy, 05.90.+m

The classical one-component plasma, or jellium, is a system of identical pointlike particles of charge e embedded in a spatially uniform neutralizing background. In two dimensions, the Coulomb interaction energy between two particles at a distance r reads $-e^2\ln(r/L)$, where a length scale L fixes the zero of energy. For the system at temperature T, the only dimensionless coupling constant is $\Gamma=e^2/k_BT$. The availability of exact results for the thermodynamic and correlation functions at coupling $\Gamma=2$ [1], even in the case of an inhomogeneous background [2,3], provides density profiles for a variety of electrostatic boundary conditions, including simple models of electrodes [4,5] (see recent review [6]).

Of special interest is the Γ dependence of the decay of the bulk two-particle distribution functions in two-dimensional (2D) jellium. At the high temperature (weak coupling $\Gamma\to 0$) limit, truncated distribution functions display exactly the Debye-Hückel screening of exponential type, as has been shown generally using the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) integral equation hierarchy [7] and the field-theoretic approach [8]. At the special coupling $\Gamma=2$, the decay is of the pure Gaussian form $\exp(-\pi\rho r^2)$ with ρ the particle density. A temperature expansion around $\Gamma=2$ [1] suggests that the monotonic decay of the two-body density for $\Gamma<2$ changes to an oscillating one in the region $\Gamma>2$. For $\Gamma>142$, the plasma system becomes a 2D Wigner crystal [9]. An attempt to estimate the character of the correlation decay for intervalues of Γ has been made within the mean spherical model of the discrete lattice version of plasma [10]. For this system there exists an intermediate coupling constant Γ_0, identified intuitively as a counterpart of $\Gamma=2$, which characterizes the decay of truncated charge-charge distribution functions as follows: for $\Gamma<\Gamma_0$ the screening is exponential and monotonic with a correlation length decreasing with increasing Γ; at $\Gamma=\Gamma_0$ the pair correlation has a range of one lattice spacing; at $\Gamma>\Gamma_0$ the decay is exponentially fast with oscillations and a correlation length that increases with increasing Γ. Although the spherical constraint introduces an extra-long-range interaction, the zeroth and second moment Stillinger-Lovett sum rules [11] hold (indicating a dominant role of the tail of Coulomb interaction at asymptotically large distance [12]). On the other hand, because the charge variables are continuous the mean-spherical constraint interferes significantly with the Coulomb nature of the lattice plasma in the description of correlations at a free surface [13] and does not provide a Kosterlitz-Thouless transition for a two-component Coulomb system [10]. An approximate evaluation of the pair distribution [14], based on a closure of the BGY hierarchy at the level of the three-particle correlation function which is exact for both the Debye-Hückel $\Gamma\to 0$ limit and the $\Gamma=2$ case and simultaneously satisfies the sum rules for arbitrary Γ, predicts a transition from the region of monotonically vanishing correlations ($\Gamma<2$) to one of oscillating correlations with powerlike falloff ($\Gamma>2$). It has been proven in Ref. [15] that if the correlations of a charged system are integrable and monotonic at infinity, they decay faster than any inverse power.

The present paper aims to clarify to a certain extent whether the Gaussian decay of correlations is a peculiar property of the $\Gamma=2$ coupling. This key question is investigated via the example of jellium at coupling $\Gamma=4$, characterized by the phenomenon of vanishing pressure, which is, after $\Gamma=2$, the simplest case with an integral power Van der Monde determinantal representation of the Coulomb Boltzmann factor. Although jellium at $\Gamma=4$ is not equivalent to a system of independent fermions (and so cannot be solved in a standard way as in the $\Gamma=2$ case), the Van der Monde determinantal formalism is a powerful means for developing simple, efficient, and quickly converging series expansions. As a model system, we consider a fluid of N particles in a disk and, taking advantage of the circular symmetry, calculate numerically the short-distance expansion of the truncated particle-particle correlation around the disk center for successively increasing N. Then we propose a simple Gaussian-type form of the bulk two-body density which satisfies the charged-fluid sum rules [11] and fits very well the asymptotic $N\to\infty$ tendency of numerical data. A comparison with Monte Carlo (MC) simulations [16] shows the adequacy of the suggested form of pair correlations in the region of large particle-particle distance as well.

Let N particles $j=0,1,\ldots,N-1$ of charge e and with position vectors $\mathbf{r}_j$ be confined to a disk of radius R whose center is taken as the origin $\mathbf{0}$. The disk is filled uniformly by a neutralizing background of charge density $-e\rho$; $\rho=N/\pi R^2$ stands for the number density. The total potential energy Φ of the background particle system follows from elementary electrostatics [6],

$$\Phi=\frac{N^2e^2}{2}\left[\ln R-\frac{3}{4}\right]-\frac{Ne^2}{2}\ln L+\frac{e^2\pi\rho}{2}\sum_j r_j^2-e^2\sum_{j<k}\ln r_{jk}\ , \tag{1}$$

where $r_j=|\mathbf{r}_j|$ and $r_{jk}=|\mathbf{r}_j-\mathbf{r}_k|$. For $\Gamma=4$, the Boltzmann factor is written as

$$\exp\left[-\frac{\Phi}{k_BT}\right]=C\prod_j e^{-2\pi\rho r_j^2}\prod_{j<k}r_{jk}^4\ , \tag{2}$$

and the partition function reads

$$Z_N=\frac{1}{N!}\int_{r_0<R}d^2\mathbf{r}_0\cdots\int_{r_{N-1}<R}d^2\mathbf{r}_{N-1}\prod_j w(r_j)\prod_{j<k}r_{jk}^4 \tag{3a}$$

with an irrelevant constant dropped, and

$$w(r)=e^{-2\pi\rho r^2}\ . \tag{3b}$$

The statistical quantities of interest are the particle density

$$\rho(\mathbf{r})=\rho(r)=\left\langle\sum_j\delta(\mathbf{r}_j-\mathbf{r})\right\rangle \tag{4}$$

and the two-body density of particles localized at the origin and at distance r from the center of the disk,

$$\rho^{(2)}(\mathbf{0},\mathbf{r})=\rho^{(2)}(r)=\left\langle\sum_{j\neq k}\delta(\mathbf{r}_j)\delta(\mathbf{r}_k-\mathbf{r})\right\rangle\ . \tag{5}$$

The correlations will be considered in the truncated form

$$h(\mathbf{0},\mathbf{r})=h(r)=\frac{\rho^{(2)}(r)-\rho(0)\rho(r)}{\rho(0)\rho(r)}\ . \tag{6}$$

Due to the circular symmetry of $w(r)$ in (3), the logarithm of Z_N is the generating functional in the sense that

$$\rho(r)=\frac{w(r)}{2\pi r}\frac{\delta\ln Z_N}{\delta w(r)}\ , \tag{7}$$

$$\rho^{(2)}(r)-\rho(0)\rho(r)=\lim_{\bar r\to 0}\frac{w(\bar r)w(r)}{(2\pi\bar r)(2\pi r)}\frac{\delta^2\ln Z_N}{\delta w(\bar r)\delta w(r)}\ , \tag{8}$$

as one can show after some algebra. Of course, the partition function with angle-independent $w(r)$ cannot generate correlations between two points, neither of which are at the origin.

To obtain a convenient formula for Z_N, (3), we use the Van der Monde determinantal representation

$$\prod_{j<k}r_{jk}^4=|\det(r_je^{i\theta_j})^k|_{j,k=0,\ldots,N-1}|^4\ , \tag{9}$$

where (r_j,θ_j) are the polar coordinates of $\mathbf{r}_j$, and write

$$Z_N=\frac{1}{N!}\int_{r_0<R}d^2\mathbf{r}_0\cdots\int_{r_{N-1}<R}d^2\mathbf{r}_{N-1}\prod_j w(r_j)K(\{\mathbf{r}\})K^*(\{\mathbf{r}\}) \tag{10a}$$

with

$$K(\{\mathbf{r}\})=\det(r_je^{i\theta_j})^k\det(r_je^{i\theta_j})^k\ . \tag{10b}$$

Due to the orthogonality relation

$$\int_0^{2\pi}d\theta\, e^{i(j-k)\theta}=2\pi\delta_{jk}\ , \tag{11}$$

it is sufficient to analyze the two-determinant product K. It can be expressed as

$$\begin{aligned}K(\{\mathbf{r}\})&=\sum_{P,P'}(-1)^{P+P'}\prod_j(r_je^{i\theta_j})^{P(j)}(r_je^{i\theta_j})^{P'(j)}\\&=\sum_{P,P'}(-1)^{P'}\prod_j(r_je^{i\theta_j})^{P(j)+P'P(j)}\\&=\sum_{P,P'}(-1)^{P'}\prod_j[r_{P(j)}e^{i\theta_{P(j)}}]^{j+P'(j)}\ .\end{aligned} \tag{12}$$

The terms generated by the summation over P' for two different P's differ from each other only by a permutation of particle indices. Let us consider the summation over P' for a specific permutation P, say $P=I$, and represent each term in the sum solely by the set of powers that appear, i.e., α_k denotes the number of values of j for which $j+P'(j)=k$. Doing so, the sum over P' appears as

$$\sum_\alpha C_\alpha\{\alpha_0,\ldots,\alpha_{2(N-1)}\}\ . \tag{13}$$

More explicitly, coefficients C_α are generated by

$$\sum_{P'}(-1)^{P'}\prod_j x_{j+P'(j)}=\sum_\alpha C_\alpha x_0^{\alpha_0}x_1^{\alpha_1}\cdots x_{2(N-1)}^{\alpha_{2(N-1)}}\ . \tag{14}$$

Now when $K^*(\{\mathbf{r}\})$ is appended and the integration performed, the orthogonality (11) shows that only terms in $K^*(\{\mathbf{r}\})$ with the same $\{\alpha_0,\ldots,\alpha_{2(N-1)}\}$ can couple to a term in (13). Under the permutations P in $K^*(\{\mathbf{r}\})$, they will occur in $\alpha_0!\alpha_1!\cdots\alpha_{2(N-1)}!$ different ways. Since the same result is obtained for any P in (12), the $1/N!$ in (10a) is canceled, and we have

$$Z_N=\sum_{\{\alpha\}}C_\alpha^2\prod_{j=0}^{2(N-1)}(\alpha_j!w_{2j}^{\alpha_j})\ , \tag{15}$$

where

$$w_{2j}=\int_0^R dr\, 2\pi r r^{2j} w(r) \ . \tag{16}$$

After performing all necessary functional derivatives of $\ln Z_N$ with respect to the $w(r)$, $w(r)$ will appear only in the special form (3b), and hence w_{2j} will be expressed in terms of the incomplete Γ function

$$w_{2j}=\frac{\pi}{(2\pi\rho)^{j+1}}\int_0^{2N} dt\, t^j e^{-t} \ . \tag{16'}$$

According to (14), the explicit evaluation of Z_N requires algebraic manipulations with $N!$ permutations. For small particle number, we have

$$Z_2=w_0w_4+2w_2^2 \ , \tag{17a}$$

$$Z_3=w_0w_4w_8+2w_0w_6^2+2w_2^2w_8+4w_2w_4w_6+6w_4^3 \ , \tag{17b}$$

$$Z_4=w_0w_4w_8w_{12}+2w_0w_4w_{10}^2+2w_0w_6^2w_{12}+2w_2^2w_8w_{12}+4w_0w_6w_8w_{10}+4w_2w_4w_6w_{12}+4w_2w_4w_8w_{10}+4w_2^2w_{10}^2$$
$$+4w_4^2w_8^2+6w_0w_8^3+6w_4^3w_{12}+8w_2w_6w_8^2+8w_2w_6^2w_{10}+8w_4^2w_6w_{10}+18w_4w_6^2w_8+24w_6^4 \ , \tag{17c}$$

and so on.

We were able to perform the numerical calculations up to $N=12$ particles. The density ratio $\rho(r)/\rho(0)$ is expanded in the dimensionless variable

$$x^2=2\pi\rho r^2 \tag{18}$$

as follows:

$$\frac{\rho(r)}{\rho(0)}=1+\sum_1^\infty \rho_n x^{2n} \ . \tag{19}$$

The plots of the coefficients $\{\rho_n\}_1^{10}$ as functions of $1/N$ ($N=2,\ldots,12$) are pictured in Fig. 1. Since $\rho_n\to 0$ in the limit $N\to\infty$, they indicate the level of the bulk regime in the neighborhood of the disk center for a given particle number N. It is seen that the convergence of $\{\rho_n\}$ to zero is very quick. The numerical results for $h(r)$ at given N are represented by the coefficients $\{h_n\}_1^{10}$, defined by the short-distance expansion of $h(r)$ around the origin

$$h(r)=-1+\sum_1^\infty h_n x^{2n} \ , \tag{20}$$

in Table I. The value of $h(0)=-1$ is fixed by the equality $\rho^{(2)}(0)=0$ (two particles of the same charge have infinite electrostatic energy at zero distance). For every N, $h_1=0$ in accordance with the expectation of the leading bare-potential term r^Γ suggested by a temperature series expansion around $\Gamma=2$ [1]. There exists another exact result concerning the short-distance expansion of $h(r)$ [17] which relates coefficients h_2 and h_3. Adapted from the original derivation for three dimensions to 2D jellium, at $\Gamma=4$, it gives

$$h_2/h_3=-2 \ . \tag{21}$$

As is evident from Table I, this relation is satisfied with good accuracy for larger numbers of particles N. The dependences of coefficients $\{h_n\}_2^{10}$ on $1/N$ are also presented in a transparent graphical form in Fig. 2—here, only coefficients with "stabilized" signs are included. In spite of relative oscillations of data, the convergence rapidity of the coefficients towards their asymptotic $N\to\infty$ values in satisfactory.

Before proposing a realistic $N\to\infty$ form of the bulk correlation $h(r)$, we summarize all necessary and suggested requirements put on $h(r)$ for our special choice of the coupling constant $\Gamma=4$.

(1) Around $r=0$, $h(r)\sim -1+h_2r^4+h_3r^6$ with $h_2/h_3=-2$.

(2) The behavior of $h(r)$ is not monotonic and in the limit $r\to\infty$ it tends to zero.

(3) The bulk $h(r)$ satisfies the charged-fluid sum rules: (i) the zeroth moment condition (electroneutrality)

$$\rho\int d^2\mathbf{r}\, h(r)=-1 \ , \tag{22}$$

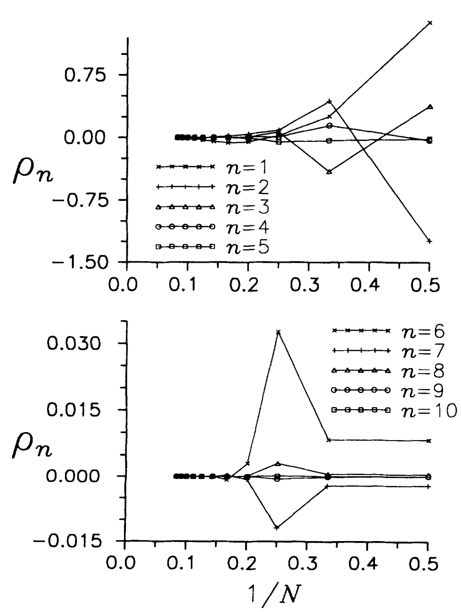

FIG. 1. Plots of the coefficients $\{\rho_n\}$ of the density ratio expansion (19) versus the inverse of the particle number $1/N$.

TABLE I. Numerical results for the coefficients of the short-distance expansion of the truncated correlation $h(r)$ (20) at given particle number N; data in the last $N \to \infty$ rows correspond to the conjectured bulk $h(r)$ (see the text).

N	h_1	h_2	h_3	h_4	h_5
2	0.0	+1.355 046	−3.231 287	+6.832 461	−14.21 119
3	0.0	+0.471 452	−0.032 860	−0.470 709	+0.475 605
4	0.0	+0.328 143	−0.115 455	+0.124 426	−0.151 631
5	0.0	+0.291 305	−0.116 573	+0.025 883	−0.000 247
6	0.0	+0.289 171	−0.127 002	+0.031 100	−0.005 368
7	0.0	+0.299 528	−0.141 810	+0.038 722	−0.008 044
8	0.0	+0.311 935	−0.155 258	+0.045 271	−0.010 184
9	0.0	+0.321 550	−0.164 106	+0.048 979	−0.011 156
10	0.0	+0.327 146	−0.168 077	+0.049 919	−0.011 065
11	0.0	+0.329 409	−0.168 628	+0.049 222	−0.010 486
12	0.0	+0.329 583	−0.167 470	+0.047 991	−0.009 889
∞	0.0	+0.331 160	−0.165 580	+0.045 710	−0.008 925

N	h_6	$10^4 h_7$	$10^5 h_8$	$10^6 h_9$	$10^7 h_{10}$
2	+29.486 75	−611 596.7	$+1.26\times10^7$	-2.63×10^8	$+5.45\times10^9$
3	−0.045 628	−3546.110	+36 486.51	−41 198.07	-2.65×10^6
4	+0.064 880	−6.381 514	−773.3779	+10 019.14	−140 541.0
5	−0.007 913	+63.088 66	−266.0815	+735.0464	−743.9691
6	+0.001 142	−9.376 899	+65.739 34	−287.8598	+883.6680
7	+0.001 461	−2.113 369	−3.417 962	+51.976 21	−265.9129
8	+0.001 992	−3.586 906	+6.420 553	−15.852 18	+62.123 59
9	+0.002 164	−3.773 724	+6.106 815	−9.153 277	+9.919 973
10	+0.002 019	−3.163 457	+4.299 950	−4.964 303	+4.552 500
11	+0.001 781	−2.480 785	+2.777 045	−2.219 653	+0.476 262
12	+0.001 597	−2.078 634	+2.151 043	−1.633 722	+0.637 621
∞	+0.001 365	−1.729 902	+1.882 054	−1.800 560	+1.540 933

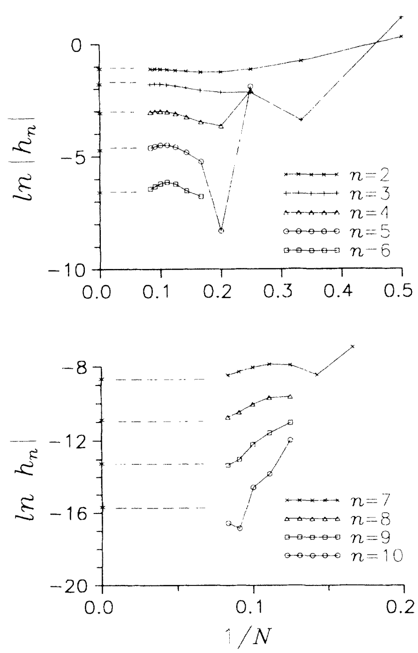

FIG. 2. Logarithmic plots of the absolute values of coefficients $\{h_n\}$, defined by the short-distance expansion of $h(r)$ around the origin (20), versus 1/(particle number N); horizontal dashed lines reflect the analytical estimates given by (25) with coefficients fixed by requirements (1)–(3).

(ii) the second moment condition (Stillinger-Lovett) [18,19]

$$\rho^2 \int d^2\mathbf{r}\, r^2 h(r) = -\frac{1}{2\pi} , \tag{23}$$

(iii) the fourth moment condition (compressibility) [20]

$$\int d^2\mathbf{r}\, r^4 h(r) = 0 . \tag{24}$$

Our proposal for the truncated particle-particle correlation is a superposition of two functions of Gaussian type

$$h_{\text{trial}}(r) = -(a_1 + b_1 x^2 + c_1 x^4) e^{-\nu_1 x^2} - a_2 e^{-\nu_2 x^2} , \tag{25}$$

where the parameters are determined by the requirements (1)–(3) as follows: $\nu_1=0.397$, $\nu_2=0.849$, $a_1=3.886$, $b_1=-0.909$, $c_1=0.043$, $a_2=-2.886$. The consequent short-distance expansion of h_{trial} around $\mathbf{r}=\mathbf{0}$ results in coefficients $\{h_n\}$ tabulated in the last $N\to\infty$ rows in Table I and represented by horizontal dashed lines in Fig. 2. It is seen that the predicted coefficients fit very well the asymptotic tendency of numerical data. Although slight oscillations of data points prevent application of a $1/N$ polynomial extrapolation, even data for $N=12$ confirm a strong evidence for the Gaussian nature of the correlation decay at $\Gamma=4$, in full agreement with the rigorous results of Ref. [15]. When compared to the Gaussian decay of the truncated correlation at $\Gamma=2$, transcribed in terms of dimensionless distance x as $-\exp(-x^2/2)$, the asymptotic correlations for $\Gamma=2$, since $\nu_1<1/2$, are weaker than those for the $\Gamma=4$ coupling, which agrees with the expected minimum of correlation effects at $\Gamma=2$. The special role of the function (25) is supported by our experience that when one requires the fulfillment of the sum rules in other simple superpositions of two Gaussian-type functions or a single Gaussian function, the real $h(r)$ either does not exist or the coefficients of its short-distance expansion around the origin differ from the corresponding numerical estimates by a few orders of magnitude.

The MC results [16] for the truncated correlation at $\Gamma=4$, presented together with the plot of $h_{\text{trial}}(r)$ in Fig. 3, confirm the applicability of the suggested h_{trial} in the region of large particle-particle distance as well. The striking coincidence between the model-analytical results, based on the supposition of the Gaussian decay of $h(r)$, and the MC simulations is surprising in view of the contemporary status of the topic summarized briefly in the introductory part of this work.

In conclusion, it is not clear whether the correlations in the coupling range $2<\Gamma<4$ also possess a Gaussian nature, i.e., whether or not the Gaussian falloff is a consequence of the Van der Monde representation "symmetry" of Boltzmann factors. The framework of the procedure outlined remains unchanged for higher $\Gamma=6,8,\ldots$, but much more numerical work has to be done for obtaining reliable data.

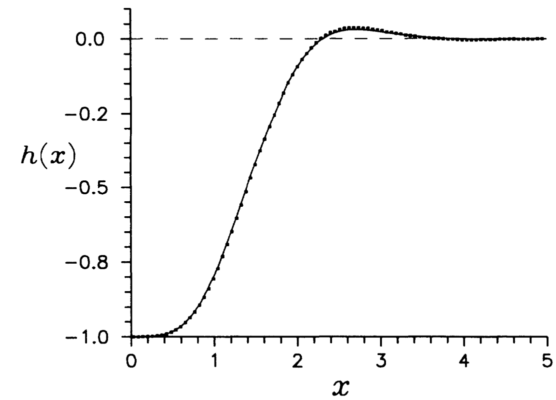

FIG. 3. Truncated pair correlation $h(r)$ versus dimensionless particle-particle distance $x=(2\pi\rho)^{1/2}r$. Solid line, the form suggested in the present work (25); squares, the MC data deduced from a system of 256 particles [16].

We are grateful to Bernard Jancovici for very useful comments, which enabled us to improve our presentation. We thank Dominique Levesque for sending us the MC data for pair correlations of 2D jellium at special coupling $\Gamma=4$, referred to in Ref. [16]. This work was supported by a grant from the National Science Foundation.

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