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Behavior at Small Distances and Low Temperatures of the Ion–Ion Distribution Function of the Two-Dimensional Coulomb Gas

Michel Lavaud[1]

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We compute upper and lower bounds for the canonical ion–ion distribution function $g_{11}^{(N)}(r)$ of the two-dimensional Coulomb gas for small r and $1 < \gamma < 2$, where γ is the plasma parameter. Both bounds are proportional to $r^{2-\gamma}/(\gamma-1)$, which proves that $g_{11}^{(N)}(r)$ behaves as $r^{2-\gamma}$, as conjectured by Hansen and Viot. We conjecture that, in the thermodynamic limit, $g_{11}(r) \sim 2(\gamma-1)^{-1}(r/a)^{2-\gamma}$, where $a=(\pi n)^{-1/2}$ is the mean interionic distance. We also compute the canonical one-body distribution function with one pair $(+,-)$ in a disk, for any r and any γ.

KEY WORDS: Two dimensions; Coulomb gas; point ions; point electrons; distribution function; small distances; low temperatures.

1. INTRODUCTION

Hansen and Viot[1] have shown, by studying the three-body problem and fitting the results of numerical simulations for systems with up to 196 ions and electrons, that the ion–ion distribution function of the two-dimensional Coulomb gas behaves as $r^{2-\gamma}$ as $r \to 0$ and $1 < \gamma < 2$, instead of r^{γ} as predicted by Widom's theorem,[2] where $\gamma = e^2/kT$ is the plasma parameter. The main aim of this paper is to prove this result for any N.

All computations are done on reduced quantities in the canonical ensemble. These quantities are defined in Section 2. In Section 3, we compute an upper bound for the reduced ion–ion distribution function with N pairs $(+,-)$, $\rho_{11}^{(N)}$, by means of the function with two pairs $\rho_{11}^{(2)}$. Sections 4–6 are devoted to computing the latter in the Hansen and Viot limit,

[1] Groupe de Recherche sur l'Énergétique des Milieux Ionisés (GREMI), UA 831, UFR Faculté des Sciences, 45067 Orleans, France.

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i.e., $r \to 0$ and $1 < \gamma < 2$. This gives an upper bound for $\rho_{11}^{(N)}$ proportional to $(\gamma-1)^{-1} r^{2-\gamma}$. In Section 7, we compute a lower bound for $\rho_{11}^{(N)}$ that has the same $(\gamma-1)^{-1} r^{2-\gamma}$ behavior. In Section 8, we study the behavior of the bounds in the thermodynamic limit. We show that the lower bound has a thermodynamic behavior, and we conjecture that it is the exact asymptotic behavior in the Hansen and Viot limit. A summary of the results is given in Section 9.

2. DEFINITIONS AND GENERAL PROPERTIES

We consider a two-dimensional system of N ions and N electrons with unit charge, included in a disk of radius R. The potential energy of the system is

$$U_{2N} = -\sum_{i<j}^{N} q_i q_j e^2 \ln(|\mathbf{r}_i - \mathbf{r}_j|/L) \tag{1}$$

where $\mathbf{r}_1,..., \mathbf{r}_N$ are the coordinates of the ions, $\mathbf{r}_{N+1},..., \mathbf{r}_{2N}$ the coordinates of the electrons, and $q_i e$ is the charge of the ith particle ($q_1 = \cdots = q_N = 1$; $q_{N+1} = \cdots = q_{2N} = -1$). L is an arbitrary length, which fixes the zero of energy.

The configuration integral and the unnormalized one-body and ion–ion distribution functions are defined, in the canonical ensemble, by

$$Q_N(R, L) = \int_{|\mathbf{r}_i| \leqslant R} e^{-\beta U_{2N}}\, d\mathbf{r}_1 \cdots d\mathbf{r}_{2N} \tag{2}$$

$$\rho_1^{(N)}(\mathbf{r}_1; R, L) = \int_{|\mathbf{r}_i| \leqslant R} e^{-\beta U_{2N}}\, d\mathbf{r}_2 \cdots d\mathbf{r}_{2N} \tag{3}$$

$$\rho_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R, L) = \int_{|\mathbf{r}_i| \leqslant R} e^{-\beta U_{2N}}\, d\mathbf{r}_3 \cdots d\mathbf{r}_{2N} \tag{4}$$

where $\beta = 1/kT$ is the inverse temperature.

The L and R dependences of these functions are

$$Q_N(R, L) = L^{N\gamma} R^{2(2N - N\gamma/2)} Q_N \tag{5}$$

$$\rho_1^{(N)}(\mathbf{r}_1; R, L) = L^{N\gamma} R^{2(2N-1-N\gamma/2)} \rho_1^{(N)}\left(\frac{\mathbf{r}_1}{R}\right) \tag{6}$$

$$\rho_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R, L) = L^{N\gamma} R^{2(2N-2-N\gamma/2)} \rho_{11}^{(N)}\left(\frac{\mathbf{r}_1}{R}, \frac{\mathbf{r}_2}{R}\right) \tag{7}$$

where $\gamma = \beta e^2$ is the plasma parameter, and we have defined the reduced functions

$$Q_N \equiv Q_N(1, 1) \tag{8}$$

$$\rho_1^{(N)}(\mathbf{x}_1) \equiv \rho_1^{(N)}(\mathbf{x}_1; 1, 1) \tag{9}$$

$$\rho_{11}^{(N)}(\mathbf{x}_1, \mathbf{x}_2) \equiv \rho_{11}^{(N)}(\mathbf{x}_1, \mathbf{x}_2; 1, 1) \tag{10}$$

From (5)–(7), the (normalized) canonical one-body and ion–ion distribution functions are independent of L:

$$g_1^{(N)}(\mathbf{r}_1; R) = \frac{N}{nQ_N(R, L)} \rho_1^{(N)}(\mathbf{r}_1; R, L) \tag{11}$$

$$g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R) = \frac{N(N-1)}{n^2 Q_N(R, L)} \rho_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R, L) \tag{12}$$

where $n = N/V$ ($V = \pi R^2$) is the ionic density.

They can be expressed in terms of the reduced functions (8)–(10):

$$g_1^{(N)}(\mathbf{r}_1; R) = \frac{\pi}{Q_N} \rho_1^{(N)} \left(\frac{\mathbf{r}_1}{R}\right) \tag{13}$$

$$g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R) = \left(1 - \frac{1}{N}\right) \frac{\pi^2}{Q_N} \rho_{11}^{(N)} \left(\frac{\mathbf{r}_1}{R}, \frac{\mathbf{r}_2}{R}\right) \tag{14}$$

The one-body and ion–ion distribution functions are defined in the thermodynamic limit by

$$g_1(\mathbf{r}_1) = \lim_{\substack{N, R \to \infty \\ n = \text{const}}} g_1^{(N)}(\mathbf{r}_1; R) \tag{15}$$

$$g_{11}(\mathbf{r}_1, \mathbf{r}_2) = \lim_{\substack{N, R \to \infty \\ n = \text{const}}} g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R) \tag{16}$$

3. UPPER BOUND OF THE REDUCED ION–ION DISTRIBUTION FUNCTION WITH *N* PAIRS BY MEANS OF THE DISTRIBUTION FUNCTION WITH TWO PAIRS

From now on, all computations will be done on the reduced quantities (8)–(10). The interpretation of the results can be done through formulas (13)–(16). Let us denote the reduced coordinates $\mathbf{r}_i/R$ ($i = 1,..., N$) of the ions by the complex numbers z_i, and the reduced coordinates $\mathbf{r}_i/R$

($i = N+1,\dots, 2N$) of the electrons by ξ_i. With these new variables, (8)–(10) take the form

$$Q_N = \int_{z_i,\xi_i \in D} |\Delta|^\gamma \, dz_1 \cdots dz_N \, d\xi_1 \cdots d\xi_N \tag{17}$$

$$\rho_1^{(N)}(z_1) = \int_{z_i,\xi_i \in D} |\Delta|^\gamma \, dz_2 \cdots dz_N \, d\xi_1 \cdots d\xi_N \tag{18}$$

$$\rho_{11}^{(N)}(z_1, z_2) = \int_{z_i,\xi_i \in D} |\Delta|^\gamma \, dz_3 \cdots dz_N \, d\xi_1 \cdots d\xi_N \tag{19}$$

where D is the disk of radius 1, and

$$\Delta = \frac{\prod_{i<j}^N (z_i - z_j) \prod_{i<j}^N (\xi_i - \xi_j)}{\prod_{i,j}^N (z_i - \xi_j)} \tag{20}$$

In (17)–(19), we have set $dz = dx\,dy$, where z is the complex number $x + iy$ (not to be confused with the usual notation $dz = dx + i\,dy$).

In the sequel, we make a repeated use of the following lemma.[3]

Lemma 1. Let $b_1,\dots, b_n$ be n nonnegative real numbers, and γ, real positive. We have

$$\left(\sum_{i=1}^n b_i\right)^\gamma \leqslant n^\chi \sum_{i=1}^n b_i^\gamma \tag{21}$$

with

$$\chi = \max(0, \gamma - 1) \tag{22}$$

This can be proved by using the inequality between weighted means (Ref. 4, p. 26, Theorem 16) for $\gamma > 1$ and Jensen's inequality (Ref. 4, p. 28, Theorem 19) for $0 < \gamma < 1$.

Canchy's formula reads[3]

$$\Delta = \det\left(\frac{1}{z_i - \xi_j}\right) \tag{23}$$

By developing the determinant Δ with respect to its first two lines by means of Laplace's theorem,[5] we find

$$\Delta = \sum_{i<j}^N (-1)^{i+j+1} a_{ij} A_{ij} \tag{24}$$

with

$$a_{ij} = \begin{vmatrix} 1/(z_1 - \xi_i) & 1/(z_1 - \xi_j) \\ 1/(z_2 - \xi_i) & 1/(z_2 - \xi_j) \end{vmatrix} \tag{25}$$

and A_{ij} is the minor obtained from Δ by deleting its first two lines and colums i and j.

Applying Lemma 1 to (24) with $b_i = |a_{ij}|\ |A_{ij}|$, $n = \frac{1}{2}N(N-1)$, we find

$$|\Delta|^\gamma \leqslant \left[\frac{1}{2}N(N-1)\right]^\chi \sum_{i<j}^{N} |a_{ij}|^\gamma\ |A_{ij}|^\gamma \tag{26}$$

Integrating (26) with respect to $z_3, ..., \xi_N$ gives

$$\rho_{11}^{(N)}(z_1, z_2) \leqslant \left[\frac{1}{2}N(N-1)\right]^{\chi+1} Q_{N-2}\rho_{11}^{(2)}(z_1, z_2) \tag{27}$$

This upper bound is valid for any z_1, z_2 and any γ.

4. UPPER BOUND OF THE REDUCED DISTRIBUTION FUNCTION WITH TWO PAIRS $\rho_{11}^{(2)}(z_1, z_2)$

From (19) and (20), we have

$$\rho_{11}^{(2)}(z_1, z_2) = |z_1 - z_2|^\gamma\ G(z_1, z_2) \tag{28}$$

with

$$G(z_1, z_2) = \int_{\xi_i \in D} \frac{|\xi_1 - \xi_2|^\gamma}{|z_1 - \xi_1|^\gamma\ |z_2 - \xi_1|^\gamma\ |z_1 - \xi_2|^\gamma\ |z_2 - \xi_2|^\gamma}\, d\xi_1\, d\xi_2 \tag{29}$$

By combining Lemma 1 with the triangular inequality, we find

$$|\xi_1 - \xi_2|^\gamma \leqslant 2^\chi(|z_1 - \xi_1|^\gamma + |z_1 - \xi_2|^\gamma) \tag{30}$$

Substituting (30) into (29) gives

$$G(z_1, z_2) \leqslant 2^{\chi+1} \int_D \frac{d\xi_1}{|z_2 - \xi_1|^\gamma} \int_D \frac{d\xi_2}{|z_1 - \xi_2|^\gamma\ |z_2 - \xi_2|^\gamma} \tag{31}$$

We have (see Appendix)

$$\int_D \frac{d\xi_1}{|z_2 - \xi_1|^\gamma} = \rho_1^{(1)}(|z_2|) = \frac{2\pi}{2-\gamma} F\left(\frac{\gamma}{2}, \frac{\gamma}{2} - 1; 1; |z_2|^2\right) \tag{32}$$

Further, the Riesz formula reads[6]

$$\int_{\mathbb{R}^d} \frac{d\xi_2}{|z_1-\xi_2|^{d-\alpha}\,|z_2-\xi_2|^{d-\beta}} = \frac{k_{\alpha,\beta}}{|z_1-z_2|^{d-(\alpha+\beta)}} \tag{33}$$

with

$$k_{\alpha,\beta} = \frac{\pi^{d/2}\Gamma(\alpha/2)\,\Gamma(\beta/2)\,\Gamma((d-\alpha-\beta)/2)}{\Gamma((d-\alpha)/2)\,\Gamma((d-\beta)/2)\,\Gamma((\alpha+\beta)/2)} \tag{34}$$

provided $0<\alpha<d$, $0<\beta<d$, $0<\alpha+\beta<d$.

Letting $\alpha=\beta=d-\gamma$, $d=2$, the Riesz formula is applicable provided $1<\gamma<2$, and the second integral in (31) is bounded by

$$C_\gamma/|z_1-z_2|^{2\gamma-2} \tag{35}$$

with

$$C_\gamma = k_{2-\gamma,2-\gamma} = \pi\,\frac{[\Gamma(1-\gamma/2)]^2\,\Gamma(\gamma-1)}{[\Gamma(\gamma)]^2\,\Gamma(2-\gamma)} \tag{36}$$

Applying the recurrence relation and the doubling formula for the gamma function (Ref. 7, Eq. 8.335.1, p. 938) we find

$$C_\gamma = \frac{C'_\gamma}{(2-\gamma)(\gamma-1)} \tag{37}$$

$$C'_\gamma = \frac{\pi^{3/2}2^\gamma\Gamma(2-\gamma/2)}{\Gamma(\gamma)\,\Gamma(3-\gamma)/2)} \tag{38}$$

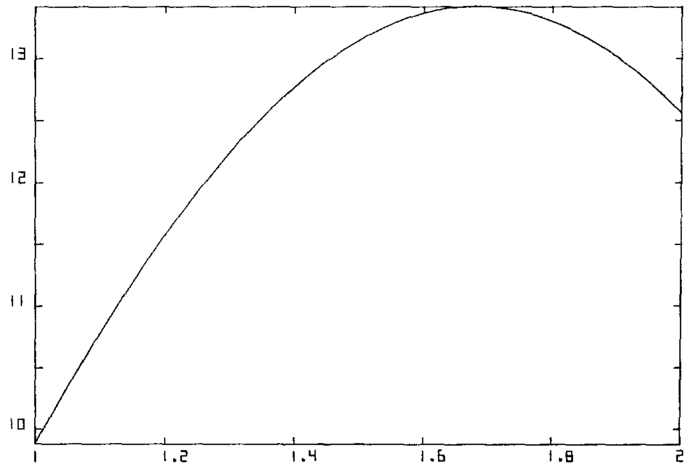

Fig. 1. Graph of the function C'_γ defined by Eq. (38).

The function C'_γ is drawn in Fig. 1 for $1 \leqslant \gamma \leqslant 2$. Regrouping (28)–(35), we obtain

$$\rho_{11}^{(2)}(z_1, z_2) \leqslant 2^{\chi+1} \rho_1^{(1)}(|z_2|)\, C_\gamma\, |z_1 - z_2|^{2-\gamma} \tag{39}$$

5. LOWER BOUND FOR $\rho_{11}^{(2)}(z_1, z_2)$

Let $|z_1 - z_2| = r$, $D_1 =$ disk centered at z_1 with radius $r^{1/2}$, and $D_2 =$ disk centered at z_1 with radius $r^{1/2} + r^{1/4}$. We assume that z_1 is not on the circle of radius 1, and we choose r sufficiently small so that $r^{1/2} + r^{1/4} < 1 - |z_1|$. We have thus (see Fig. 2)

$$D_1 \subset D_2 \subset D \tag{40}$$

Let Λ be any domain for the variables (ξ_1, ξ_2). We define

$$G(z_1, z_2; \Lambda) = \int_{(\xi_1,\xi_2)\in\Lambda} \frac{|\xi_1 - \xi_2|^\gamma}{|z_1 - \xi_2|^\gamma} \frac{d\xi_1\, d\xi_2}{|z_1 - \xi_1|^\gamma\, |z_2 - \xi_1|^\gamma\, |z_2 - \xi_2|^\gamma} \tag{41}$$

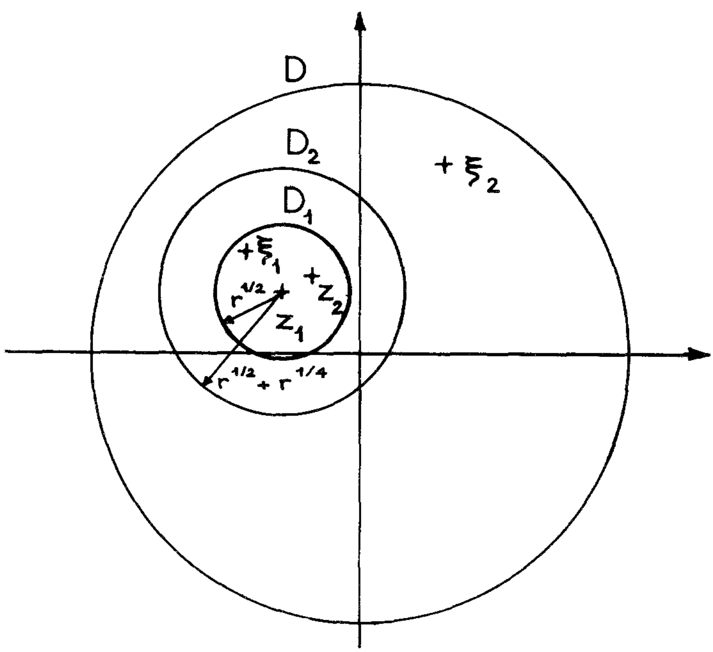

Fig. 2. Relative positions of the particles in the computation of the lower bound for the reduced ion–ion distribution function $\rho_{11}^{(2)}$.

Let $D - D_2$ denote the set of points that belong to D but not to D_2, and

$$\Lambda_1 = \{(\xi_1, \xi_2) \mid \xi_1 \in D_1, \xi_2 \in D - D_2\} \equiv D_1 \times (D - D_2) \tag{42}$$

In this domain, we have

$$\frac{|\xi_1 - \xi_2|}{|z_1 - \xi_2|} \geqslant 1 - \frac{|\xi_1 - z_1|}{|z_1 - \xi_2|} \geqslant 1 - r^{1/4} \tag{43}$$

By substituting (43) into (41), we find

$$G(z_1, z_2; \Lambda_1) \geqslant (1 - r^{1/4})^{\gamma} \int_{\xi_2 \in D - D_2} \frac{d\xi_2}{|z_2 - \xi_2|^{\gamma}} \times \int_{\xi_1 \in D_1} \frac{d\xi_1}{|z_1 - \xi_1|^{\gamma} \, |z_2 - \xi_1|^{\gamma}} \tag{44}$$

As $r \to 0$, the first integral goes to

$$\int_{\xi_2 \in D} \frac{d\xi_2}{|z_1 - \xi_2|^{\gamma}} = \rho_1^{(1)}(|z_1|) \tag{45}$$

By making the change of variable $\xi_1 - z_1 = r\zeta$, we find that the second one goes to

$$r^{2-2\gamma} \int_{\mathbb{R}^2} \frac{d\zeta}{|\zeta|^{\gamma} \, |1 - \zeta|^{\gamma}} = C_{\gamma} r^{2-2\gamma} \tag{46}$$

Regrouping (44)–(46), we find, for r sufficiently small,

$$G(z_1, z_2; \Lambda_1) \geqslant \rho_1^{(1)}(|z_1|) \, C_{\gamma} r^{2-2\gamma} \tag{47}$$

By noticing that $\Lambda_1 \cup \Lambda_2 \subset D^2$ and $\Lambda_1 \cap \Lambda_2 = \varnothing$, with $\Lambda_2 = (D - D_2) \times D_1$, we find

$$G(z_1, z_2) \geqslant G(z_1, z_2; \Lambda_1) + G(z_1, z_2; \Lambda_2) \tag{48}$$

Substituting (47)–(48) into (28) gives

$$\rho_{11}^{(2)}(z_1, z_2) \geqslant 2C_{\gamma} \rho_1^{(1)}(|z_1|) \, r^{2-\gamma} \tag{49}$$

for r sufficiently small and $1 < \gamma < 2$.

6. ASYMPTOTIC BEHAVIOR OF $\rho_{11}^{(2)}(z_1, z_2)$ AS $z_2 \to z_1$

We want to show that the lower bound (49) is exact in the limit $z_2 \to z_1$,

$$\rho_{11}^{(2)}(z_1, z_2) \underset{\substack{z_2 \to z_1, \\ 1 < \gamma < 2}}{\sim} 2C_{\gamma} \rho_1^{(1)}(|z_1|) \, r^{2-\gamma} \tag{50}$$

Let us multiply and divide the integrand of G by the quantity $|z_1-\xi_1|^\gamma+|z_1-\xi_2|^\gamma$:

$$G(z_1, z_2)=2\int \frac{|\xi_1-\xi_2|^\gamma}{|z_1-\xi_1|^\gamma+|z_1-\xi_2|^\gamma} \times \frac{d\xi_1}{|z_1-\xi_1|^\gamma\,|z_2-\xi_1|^\gamma}\,\frac{d\xi_2}{|z_2-\xi_2|^\gamma} \tag{51}$$

Let $\Lambda_1=D_1\times(D-D_2)$, $\Lambda_2=D_1\times D_2$, and $\Lambda_3=(D-D_1)\times D$. We have $D^2=\Lambda_1\cup\Lambda_2\cup\Lambda_3$ and $\Lambda_i\cap\Lambda_j=\varnothing$, so

$$G(z_1, z_2)=\sum_{i=1}^{3} G(z_1, z_2; \Lambda_i) \tag{52}$$

In Λ_1, we have the inequalities

$$|z_1-\xi_2|\geqslant r^{1/2}+r^{1/4} \tag{53}$$

$$|z_1-\xi_1|\leqslant r^{1/2} \tag{54}$$

$$|z_1-\xi_2|-|z_1-\xi_1|\leqslant|\xi_1-\xi_2|\leqslant|z_1-\xi_2|+|z_1-\xi_1| \tag{55}$$

The first term in the integrand of (51) can be reexpressed as

$$\left(\frac{|\xi_1-\xi_2|}{|z_1-\xi_2|}\right)^\gamma\left[1+\left(\frac{|z_1-\xi_1|}{|z_1-\xi_2|}\right)^\gamma\right]^{-1} \tag{56}$$

The first term of (56) is bounded by $(1-r^{1/4})^\gamma$ and $(1+r^{1/4})^\gamma$, and the second one by $(1+r^{\gamma/4})^{-1}$ and 1. Therefore, for r sufficiently small, we have

$$G(z_1, z_2; \Lambda_1)\sim 2\int_{\xi_1\in D_1}\frac{d\xi_1}{|z_1-\xi_1|^\gamma\,|z_2-\xi_1|^\gamma}\int_{\xi_2\in D-D_2}\frac{d\xi_2}{|z_2-\xi_2|^\gamma} \tag{57}$$

We have seen in the preceding section that the first integral goes to $C_\gamma r^{d-2\gamma}$ and the second one to $\rho_1^{(1)}(|z_1|)$

$$G(z_1, z_2; \Lambda_1)\underset{r\to 0}{\simeq} 2C_\gamma\rho_1^{(1)}(|z_1|)\,r^{2-2\gamma} \tag{58}$$

Because of (30), we have

$$G(z_1, z_2; \Lambda_i)\leqslant 2^{\chi+1}\int_{\Lambda_i}\frac{d\xi_1}{|z_1-\xi_1|^\gamma\,|z_2-\xi_1|^\gamma}\,\frac{d\xi_2}{|z_2-\xi_2|^\gamma} \tag{59}$$

In Λ_2, we have

$$|z_2-\xi_2|\leqslant|z_2-\xi_1|+|z_1-\xi_2|\leqslant r+r^{1/2}+r^{1/4}\leqslant 3r^{1/4}$$

This implies

$$\int_{D_2} \frac{d\xi_2}{|z_2-\xi_2|^\gamma} \leqslant \int_{|\xi| \leqslant 3r^{1/4}} |\xi|^{-\gamma}\, d\xi$$

and

$$G(z_1, z_2; \Lambda_2) \leqslant 2^{\chi+1} C_\gamma r^{2-2\gamma} \frac{3^{2-\gamma}}{2-\gamma} r^{(2-\gamma)/4} \tag{60}$$

In Λ_3, we have $|z_1 - \xi_1| \geqslant r^{1/2}$. By letting $\xi = z_1 - \xi_1$ in (59), we find

$$G(z_1, z_2; \Lambda_3) \leqslant 2^{\chi+1} \int_{r^{1/2} \leqslant |\xi| \leqslant 2} \frac{d\xi}{|\xi|^\gamma\, |r-\xi|^\gamma}\, \rho_1^{(1)}(|z_2|) \tag{61}$$

By taking $\xi = r\zeta$, the integral in (61) can be bounded by $r^{2-2\gamma}\,[2^{\gamma-1}/(\gamma-1)]\, r^{\gamma-1}$ provided $r < 1/4$. This gives

$$G(z_1, z_2; \Lambda_3) \leqslant r^{2-2\gamma} \frac{2^{\chi+\gamma}}{\gamma-1} \rho_1^{(1)}(|z_2|)\, r^{\gamma-1} \tag{62}$$

By comparing (60) and (62) to (58), we see that the contributions of Λ_2 and Λ_3 are negligible for r sufficiently small and $1 < \gamma < 2$, which proves (50).

7. LOWER BOUND FOR $\rho_{11}^{(N)}(z_1, z_2)$

Let

$$\Lambda_1 = \{(z_3,..., \xi_N) \mid \xi_1 \in D_1;\, z_3,..., z_N, \xi_2,..., \xi_N \in D - D_2\} \tag{63}$$

In this domain, we have [cf. (43)]

$$\frac{|\xi_1 - \xi_j|}{|z_1 - \xi_j|} \geqslant 1 - r^{1/4}, \qquad j = 2,..., N \tag{64}$$

$$\frac{|z_1 - z_j|}{|z_j - \xi_1|} \geqslant 1 - r^{1/4}, \qquad j = 3,..., N \tag{65}$$

Let us rewrite Δ in the form

$$\begin{aligned} |\Delta| = {} & |z_1 - z_2| \frac{1}{|z_1 - \xi_1|\, |z_2 - \xi_1|} \prod_{j=3}^{N} \frac{|z_1 - z_j|}{|z_j - \xi_1|} \\ & \times \prod_{j=2}^{N} \frac{|\xi_1 - \xi_j|}{|z_1 - \xi_j|} \frac{\prod_{2 \leqslant i < j}^{N} |z_i - z_j|\, |\xi_i - \xi_j|}{\prod_{i,j=2}^{N} |z_i - \xi_j|} \end{aligned} \tag{66}$$

By integrating (66) over $z_3 \cdots \xi_N$ and using (64)–(65), we see that the contribution of A_1 to $\rho_{11}^{(N)}(z_1, z_2)$ is larger than

$$|z_1 - z_2|^\gamma (1 - r^{1/4})^{2N-3} \int_{\xi_1 \in D_1} \frac{d\xi_1}{|z_1 - \xi_1|^\gamma |z_2 - \xi_1|^\gamma}$$

$$\times \int_{z_3 \cdots z_N; \xi_2 \cdots \xi_N \in D - D_2; z_2 \in D_1} |\Delta_{N-1}|^\gamma \, dz_3 \cdots dz_N \, d\xi_2 \cdots d\xi_N \qquad (67)$$

For r sufficiently small, the first integral goes to $C_\gamma r^{2-2\gamma}$ and the second one to $\rho_1^{(N-1)}(z_1)$. Since the domains A_i obtained from A_1 by exchanging ξ_1 and ξ_i are all disjoint and give a contribution bounded by the same quantity (67), we obtain, for z_2 sufficiently close to z_1, and $1 < \gamma < 2$,

$$\rho_{11}^{(N)}(z_1, z_2) \geqslant N C_\gamma \rho_1^{(N-1)}(z_1) \, |z_1 - z_2|^{2-\gamma} \qquad (68)$$

This is the generalization of (49) to the case of N pairs. In the case $N = 2$, we have proved that the lower bound is the exact asymptotic behavior in the limit $z_2 \to z_1$. Although we have not been able to prove it, it seems reasonable to expect that the same holds true for any N:

$$\rho_{11}^{(N)}(z_1, z_2) \underset{\substack{z_2 \to z_1 \\ 1 < \gamma < 2}}{\sim} N C_\gamma \rho_1^{(N-1)}(z_1) \, |z_1 - z_2|^{2-\gamma} \qquad (69)$$

8. BEHAVIOR OF THE BOUNDS IN THE THERMODYNAMIC LIMIT

Our upper and lower bounds are not accurate enough to give rigorous results in the thermodynamic limit. However, it is interesting to investigate their behavior if we assume that we can interchange the $r \to 0$ and the $N \to \infty$ limits.

With regard to the lower bound, this amounts to assuming that (68) is valid in the limit $N \to \infty$. Substituting (13)–(14) into (68) gives

$$g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R) \geqslant \left(1 - \frac{1}{N}\right) \pi C_\gamma \, g_1^{(N-1)}(\mathbf{r}_1; R) \left(\frac{r_{12}}{R}\right)^{2-\gamma} \frac{N Q_{N-1}}{Q_N} \qquad (70)$$

with $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. Using (37) and $R = a\sqrt{N}$, where $a = (\pi n)^{-1/2}$ is the mean interionic distance, we find

$$g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R) \geqslant \frac{N^{\gamma/2} Q_{N-1}}{(2-\gamma) Q_N} \left(1 - \frac{1}{N}\right) g_1^{(N-1)}(\mathbf{r}_1; R) \frac{\pi C'_\gamma}{\gamma - 1} \left(\frac{r_{12}}{a}\right)^{2-\gamma} \qquad (71)$$

Since the free energy per particle exists in the thermodynamic limit,[8,9] the ratio $Q_N(R, L)/Q_{N-1}(R, L)$ has a limit as $N \to \infty$. Using (5), we find that the first term on the rhs of (71) has a limit, too. Let us define

$$Q_N = \left(\frac{2\pi^2}{2-\gamma}\right)^N \frac{\Gamma(1+N\gamma/2)}{[\Gamma(2-\gamma/2)]^{2N}} R_N \tag{72}$$

and

$$f(\gamma) = \lim_{N \to \infty} R_N/R_{N-1} \tag{73}$$

The function $f(\gamma)$ exists, from the preceding argument and Stirling's formula, and satisfies $f(0) = f(2) = 1$ because $Q_N = \pi^{2N}$ for $\gamma = 0$ and $Q_N \sim N!\,(Q_1)^N$ for $\gamma \to 2$.[3]

Substituting (72)–(73) into (71) and using $g_1(\mathbf{r}_1) = 1$,[8,9] we find in the thermodynamic limit

$$g_{11}(\mathbf{r}_1) \geqslant f(\gamma) \frac{D_\gamma}{\gamma - 1} \left(\frac{r_{12}}{a}\right)^{2-\gamma} \tag{74}$$

with

$$D_\gamma = \frac{\sqrt{\pi}\, 2^{3\gamma/2-1} [\Gamma(2-\gamma/2)]^3}{\gamma^{\gamma/2} \Gamma(\gamma)\, \Gamma((3-\gamma)/2)} \tag{75}$$

The function D_γ is drawn in Fig. 3. It varies between 1.745 and 2.143. Our conjecture for Q_N can be written[10]

$$f(\gamma) \sim 1, \qquad \forall \gamma \in [0, 2] \tag{76}$$

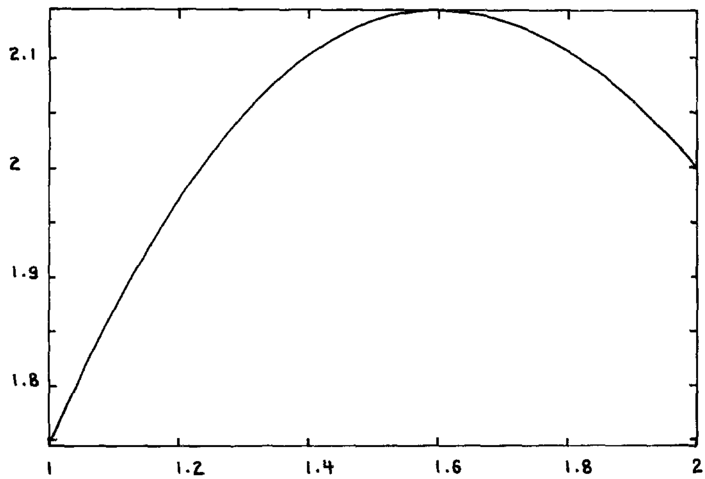

Fig. 3. Graph of the function D_γ defined by Eq. (76).

If we assume that this holds, together with conjecture (69), we obtain the following very simple approximation:

$$g_{11}(\mathbf{r}_1, \mathbf{r}_2) \underset{\substack{\mathbf{r}_2 \to \mathbf{r}_1 \\ 1<\gamma<2}}{\sim} \frac{2}{\gamma-1}\left(\frac{r_{12}}{a}\right)^{2-\gamma} \tag{77}$$

Our upper bound (27) is useless in the thermodynamic limit. Indeed, substituting (13), (14), and (50) into the upper bound (27), we find

$$g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R) \leqslant \left[\frac{N^{2(\chi+1)} Q_1 Q_{N-2}}{(2-\gamma)\, Q_N N^{1-\gamma/2}}\right] \frac{\pi C_\gamma'}{2^\chi(\gamma-1)}\, g_1^{(1)}(|\mathbf{r}_1|; R)\left(\frac{r_{12}}{a}\right)^{2-\gamma} \tag{78}$$

For $\gamma \sim 2$, the term in square brackets in (78) is approximately equal to $N^2/2\pi^2$. For other values of γ, (72) that shows it is proportional to $N^{3\gamma/2-1}$. Therefore it grows to infinity with N.

9. SUMMARY AND CONCLUSION

We have obtained lower and upper bounds, Eqs. (71) and (78), for the canonical ion–ion distribution function $g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R)$ for $\mathbf{r}_2$ sufficiently close to $\mathbf{r}_1$ and $1<\gamma<2$:

$$\frac{B_1(\gamma, N)}{\gamma-1}\, g_1^{(N-1)}(\mathbf{r}_1; R)\, r_{12}^{2-\gamma} \leqslant g_{11}^{(N)}(\mathbf{r}_1, \mathbf{r}_2; R) \leqslant \frac{B_2(\gamma, N)}{\gamma-1}\, r_{12}^{2-\gamma} \tag{79}$$

where B_1 and B_2 are bounded functions of γ for any N. This proves that $g_{11}^{(N)}$ behaves as $r^{2-\gamma}$ at small distances and low temperatures, as conjectured by Hansen and Viot. This shows further that $g_{11}^{(N)}$ behaves as $r/(\gamma-1)$ when one goes from the r^γ regime to the $r^{2-\gamma}$ regime, in the vicinity of $\gamma=1$ and r sufficiently small. For $N=2$, we prove that the lower bound in (79) is asymptotically exact, and we conjecture this is true for any N.

In the thermodynamic limit, we conjecture

$$f(\gamma)\frac{D_\gamma}{\gamma-1}\left(\frac{r_{12}}{a}\right)^{2-\gamma} \leqslant g_{11}(\mathbf{r}_1, \mathbf{r}_2) \tag{80}$$

where $f(\gamma)$ and D_γ are defined by Eqs. (72)–(73) and (75), and that (80) is asymptotically exact when $r_{12} \to 0$. Using further conjecture (76) for Q_N and $D_\gamma \approx 2$, we find

$$g_{11}(\mathbf{r}_1, \mathbf{r}_2) \sim \frac{2}{\gamma-1}\left(\frac{r_{12}}{a}\right)^{2-\gamma} \tag{81}$$

Finally, we compute the one-body distribution function with one pair for any γ and any r [cf. Eq. (A11)]:

$$g_1^{(1)}(\mathbf{r}; R) = \frac{\Gamma(3-\gamma/2)\,\Gamma(2-\gamma/2)}{\Gamma(3-\gamma)} F\left(\frac{\gamma}{2}, \frac{\gamma}{2} - 1; 1; \frac{r^2}{R^2}\right) \tag{82}$$

This gives back the result of Knorr for Q_1.

APPENDIX

We study the one-body distribution function with one pair:

$$g_1^{(1)}(z) = (\pi/Q_1)\,\rho_1(z) \tag{A1}$$

with

$$\rho_1(z) = \int_D \frac{d\xi}{|z-\xi|^\gamma} \tag{A2}$$

We use the simplified notation $\rho_1(z)$ instead of $\rho_1^{(1)}(z)$.

We want to prove

$$\rho_1(z) = \frac{2\pi}{2-\gamma} F\left(\frac{\gamma}{2}, \frac{\gamma}{2} - 1; 1; |z|^2\right) \tag{A3}$$

where $F(a, b; c; z)$ is the hypergeometric function[11]:

$$F(a, b; c; z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!} \tag{A4}$$

$$(a)_0 = 1, \qquad (a)_n = a(a+1)\cdots(a+n-1) \tag{A5}$$

Let $r = |z|$, $\tau = |z-\xi|$, $\zeta = e^{i\psi}$, and $l(r, \varphi) = |z-\zeta|$, where ζ is the point of intersection of the line $\xi - z$ with the circle of radius 1 (see Fig. 4). By taking the origin of coordinates at z, letting $\tau = lR$, and integrating over R, we find

$$\rho_1(z) = \frac{1}{2-\gamma} \int_0^{2\pi} l^{2-\gamma}\, d\varphi = \rho_1(r) \tag{A6}$$

Changing the variable of integration from φ to ψ, we get

$$\rho_1(z) = \frac{1}{2-\gamma} \operatorname{Re} \int_0^{2\pi} l^{2-\gamma} \left(1 - \frac{z}{\zeta}\right)^{-1} d\psi \tag{A7}$$

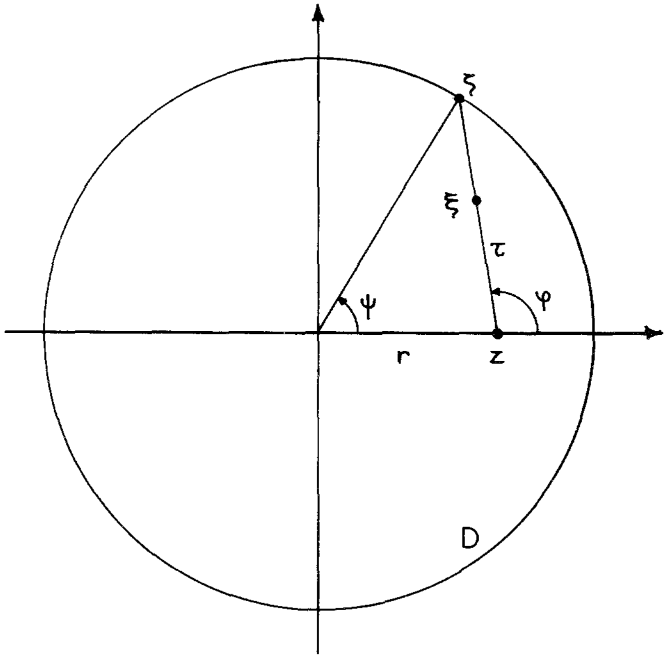

Fig. 4. Definition of the variables used in the computation of the one-body distribution with one pair, $g_1^{(1)}(r)$.

Then, we substitute

$$l^2 = |z-\zeta|^2 = (1 - z/\zeta)(1 - \bar{z}/\bar{\zeta})$$

into (A7). We can develop each term in a convergent binomial series, since $|z/\zeta| < 1$:

$$\rho_1(z) = \frac{1}{2-\gamma} \sum_{l,m=0}^{\infty} \frac{(\gamma/2)_l(\gamma/2-1)_m}{l!\, m!} r^{l+m} \int_0^{2\pi} e^{i(m-l)\psi}\, d\psi \tag{A8}$$

(A7) can be identified with (A3) with the aid of (A4)–(A5).

We check (A3) by integrating it with respect to z in the disk $|z| \leqslant 1$:

$$Q_1 = \frac{2\pi^2}{2-\gamma} \int_0^1 F\left(\frac{\gamma}{2}, \frac{\gamma}{2} - 1; 1; u\right) du \tag{A9}$$

Using a known integral for the hypergeometric function (Ref. 7, Eq. 7.512.4, p. 849), we find

$$Q_1 = \frac{2\pi^2}{2-\gamma} \frac{\Gamma(3-\gamma)}{\Gamma(3-\gamma/2)\, \Gamma(2-\gamma/2)} \tag{A10}$$

This can be identified to the value of Q_1 given by Knorr.[12]

Table I

r	0	1
$\frac{d}{dr}g_1^{(1)}(r)$	0	$\begin{cases} -\gamma(2-\gamma)(4-\gamma)/8(1-\gamma) & (0<\gamma<1) \\ -\infty & (1<\gamma<2) \end{cases}$
$g_1^{(1)}(r)$	$\frac{\Gamma(3-\gamma/2)\,\Gamma(2-\gamma/2)}{\Gamma(3-\gamma)}$	$1-\frac{\gamma}{4}$

From (A1), (A3), and (A10), we find

$$g_1^{(1)}(r)=\frac{\Gamma(3-\gamma/2)\,\Gamma(2-\gamma/2)}{\Gamma(3-\gamma)}F\left(\frac{\gamma}{2},\frac{\gamma}{2}-1;1;r^2\right) \tag{A11}$$

From the relation[13]

$$\frac{d}{dz}F(a,b;c;z)=\frac{ab}{c}F(a+1,b+1;c+1;z) \tag{A12}$$

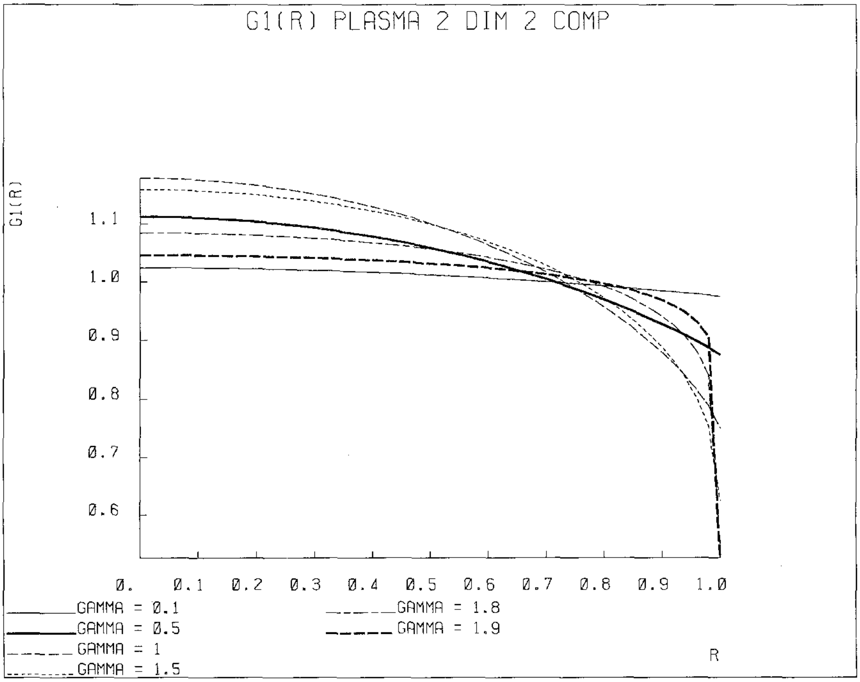

Fig. 5. Graph of $g_1^{(1)}(r)$ for $\gamma=0.1$, 0.5, 1.0, 1.5, 1.8, and 1.9. The solid line is for $\gamma=0.1$. The other curves are identified by their relative positions at $r=1$ from $g_1^{(1)}(1)=1-\gamma/4$.

and (A3)–(A4), we deduce that $g_1^{(1)}(r)$ is monotonically decreasing. Using further (Ref. 7, Eq. 9.122.1, p. 1042)

$$F(a, b; c; 1) = \frac{\Gamma(c)\,\Gamma(c-a-b)}{\Gamma(c-a)\,\Gamma(c-b)}, \qquad c > a+b \tag{A13}$$

and (Ref. 7, Eq. 9.102.1, p. 1040)

$$F(a, b; c; 1) = +\infty, \qquad c \leqslant a+b \tag{A14}$$

we can summarize the variations of $g_1^{(1)}(r)$ in Table I.

For $\gamma = 0$, we have $g_1^{(1)}(r) = 1$, $\forall r$. For $\gamma = 2$, we have

$$g_1^{(1)}(r) = 1, \qquad 0 \leqslant r < 1 \tag{A15}$$

$$g_1^{(1)}(1) = 1/2 \tag{A16}$$

We have drawn $g_1^{(1)}(r)$ in Fig. 5 for several other values of γ.

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