Amplitude Function of Asymptotic Correlations Along Charged Wall in Coulomb Fluids

Abstract In classical semi-infinite Coulomb fluids, two-point correlation functions exhibit a slow inverse-power law decay along a uniformly charged wall. In this work, we concentrate on the corresponding amplitude function which depends on the distances of the two points from the wall. Recently [L. Šamaj, J. Stat. Phys. 161, 227 (2015)], applying a technique of anticommuting variables to a 2D system of charged rectilinear wall with “counter-ions only”, we derived a relation between the amplitude function and the density profile which holds for any temperature. In this paper, using the M"obius conformal transformation of particle coordinates in a disc, a new relation between the amplitude function and the density profile is found for that model. This enables us to prove, at any temperature, the factorization property of the amplitude function in point distances from the wall and to express it in terms of the density profile. Presupposing the factorization property of the amplitude function and using specific sum rules for semi-infinite geometries, a relation between the amplitude function of the charge-charge structure function and the charge profile is derived for many-component Coulomb fluids in any dimension.

Keywords Coulomb fluid · Counter-ions · Free-fermion point · Sum rules

1 Introduction

The topic of interest in this paper is the equilibrium statistical mechanics of classical Coulomb fluids which consist in mobile charges and perhaps fixed surface or volume charge densities, the system as a whole being electroneutral. The charged entities interact by the Coulomb potential whose
form depends on the manifold in which the system is formulated. For an infinite $d$-dimensional Euclidean space, the electrostatic potential $v$ at a point $r \in \mathbb{R}^d$, induced by a unit charge at the origin $0$, is the solution of the Poisson equation

$$\Delta v(r) = -s_d \delta(r),$$

where $s_d$ is the surface area of the unit sphere in $d$ dimensions: $s_2 = 2\pi$, $s_3 = 4\pi$, etc. This $d$-dimensional definition of the Coulomb potential maintains generic properties of “real” 3D Coulomb systems with $v(r) = 1/r$, $r = |r|$. In 2D, the solution of (1.1), subject to the boundary condition $\nabla v(r) \to 0$ as $r \to \infty$, reads as $v(r) = -\ln(r/L)$ where the scale $L$ is free. For $d \geq 3$, we have $v(r) = 1/r^{d-2}$.

In standard “dense” Coulomb fluids like the one-component plasma (jellium with a neutralizing bulk background) and the two-component plasma (Coulomb gas of ± charges), the number of mobile charges is proportional to the volume of the confining domain. Such systems exhibit good screening properties and their bulk two-point correlations have a short-ranged decay. There exist many exact sum rules which relate the particle one-body and two-body densities, in the bulk, semi-infinite and finite geometries, see review [20].

In “sparse” Coulomb systems of charged macromolecule surfaces, the number of identical mobile charges (coined as counter-ions) is proportional to the charged surface boundary from which they are released [3,10,21]. The high-temperature (weak-coupling) limit is described by the Poisson-Boltzmann (PB) theory [1] and by its systematic improvement via the loop expansion [2,22,23]. The low-temperature (strong-coupling) limit is more controversial, the single-particle picture of counter-ions in the linear surface-charge potential appears in the leading strong-coupling order, see e.g. [5,18,19,23,29]. In spite of the fact that sparse Coulomb fluids have poor screening properties, the standard sum rules hold in semi-infinite and finite geometries [31,32,33].

In semi-infinite geometry of an electric double layer, the screening cloud around a particle sitting near hard wall is asymmetric and therefore two-point correlations decay slowly as an inverse-power law along the wall [11,12,35]. The corresponding amplitude function, which depends on the distances of the two points from the wall, satisfies a sum rule [12,15,28]. A relation between the amplitude function and the dipole moment was found in Ref. [16]. The contribution of the long-ranged charge-charge correlations along a domain boundary, together with a bulk contribution, explains the dependence of the dielectric susceptibility tensor on the shape of the confining domain, in the thermodynamic limit, as required by macroscopic electrostatics [6,7,8]. Interestingly, in all exactly solvable cases the amplitude function factorizes itself in the two point distances from the wall.

In a recent paper about 2D charged rectilinear wall with counter-ions only [33], we used a technique of anticommuting variables [25] to derive a relation between the amplitude function and the density profile which holds for any coupling (temperature) of the fluid regime. Moreover, using the Möbius conformal transformation of particle coordinates in the partition function for a disc geometry, an exact formula for the dielectric susceptibility tensor was
derived. Since this tensor contains also long-ranged correlations along the wall, it is likely that a more detailed exploration of the Möbius conformal transformation might reveal another relation between the amplitude function and the density profile which is complementary to the one derived in Ref. [33].

In this paper, using the formalism of anticommuting variables, we repeat the Möbius conformal transformation of particle coordinates on the level of the partition function and one-body density (Sect. 2). In this way, we derive a new relation between the amplitude function and the density profile (Sect. 3). This enables us to prove the factorization property of the amplitude function for any temperature, at least for the simplified 2D model of the charged line with counter-ions only. The amplitude function is subsequently expressed locally in terms of the density profile. In Sect. 4, a relation of our result to the sum rule obtained by Blum et al. [4] enables us to extend the analysis to one-component jellium. The generalization of the formalism to charge-charge structure function of many-component Coulomb fluids in any dimension is presented in Sect. 5. Here, presupposing the factorization property of the amplitude function, its explicit relation to the charge density profile is established. A short recapitulation and conclusions are drawn in Sect. 6.

2 2D charged rectilinear wall with counter-ions only

We consider a system of \(N\) identical pointlike particles of elementary charge \(-e\) confined to a 2D domain \(D\) of points \(r = (x, y)\). The system is studied within the canonical ensemble at the inverse temperature \(\beta = 1/(k_B T)\). The particle interaction part of the energy reads \(-e^2 \sum_{i<j}^{N} \ln |r_i - r_j|\), where the free length scale \(L\) is set to unity. The one-body Boltzmann factor \(w(r) = \exp[-\beta u(r)]\) involves all external potentials (e.g. due to a neutralizing bulk or surface background) acting on particles. Introducing the coupling constant \(\Gamma = 2\gamma = \beta e^2\), the partition function is given by

\[
Z_N(\gamma) = \frac{1}{N!} \int_D \prod_{i=1}^{N} \left( d^2r_i \right) w(r_i) \prod_{(i<j)}^{N} |r_i - r_j|^{2\gamma},
\]  

(2.1)

where we omit irrelevant constant prefactors.

The one-body density of particles at point \(r \in D\) is defined by

\[
n(r) = \langle \hat{n}(r) \rangle, \quad \hat{n}(r) = \sum_{i=1}^{N} \delta(r - r_i),
\]  

(2.2)

where \(\hat{n}(r)\) is the microscopic density of particles and \(\langle \cdots \rangle\) denotes the statistical average over canonical ensemble. The corresponding averaged charge density is simply \(\rho(r) = -en(r)\). At two-particle level, one introduces the two-body densities

\[
n_2(r, r') = \left\langle \sum_{(i \neq j)=1}^{N} \delta(r - r_i)\delta(r' - r_j) \right\rangle.
\]  

(2.3)
The one-body and two-body densities can be obtained from the partition function (2.1) in the standard way as the functional derivatives:

\[ n(r) = w(r) \frac{1}{Z_N} \frac{\delta Z_N}{\delta w(r)}, \quad (2.4) \]

\[ n_2(r, r') = w(r)w(r') \frac{1}{Z_N} \frac{\delta^2 Z_N}{\delta w(r) \delta w(r')}, \quad (2.5) \]

The two-body densities \( n_2(r, r') \) decouple to the product of densities \( n(r) \) and \( n(r') \) at asymptotically large distances \(|r - r'| \to \infty\). Therefore it is useful to introduce the (truncated) Ursell functions

\[ U(r, r') = n_2(r, r') - n(r)n(r') \quad (2.6) \]

which vanish at \(|r - r'| \to \infty\). For one-component systems of particles of charge \(-e\), the charge-charge structure function is defined as

\[ S(r, r') = e^2 \left[ \langle \hat{n}(r)\hat{n}(r') \rangle - n(r)n(r') \right] = e^2 \left[ U(r, r') + n(r)\delta(r - r') \right]. \quad (2.7) \]

The structure and Ursell functions differ from one another by a term which is nonzero only if the two points merge, i.e.

\[ U(r, r') = \frac{S(r, r')}{e^2} \quad \text{if } r \neq r'. \quad (2.8) \]

For any finite or infinite domain \( D \), the structure function satisfies the zeroth-moment sum rule [20]

\[ \int_D d^2r \, S(r, r') = \int_D d^2r' \, S(r, r') = 0. \quad (2.9) \]

2.1 Formalism of anticommuting variables

The formalism of anticommuting variables for 2D one-component plasmas has been introduced in Ref. [25] and developed further in Refs. [26,27,30,31,32]. For \( \gamma \) a positive integer, the partition function (2.1) can be expressed in terms of two sets of anticommuting variables \( \{\xi_i^{(\alpha)}, \psi_i^{(\alpha)}\} \) each with \( \gamma \) components \((\alpha = 1, \ldots, \gamma)\), defined on a discrete chain of \( N \) sites \( i = 0, 1, \ldots, N - 1 \), as follows

\[ Z_N(\gamma) = \int \mathcal{D}\psi\mathcal{D}\xi \, e^{S(\xi, \psi)}, \quad S(\xi, \psi) = \sum_{\iota, j=0}^{\gamma(N-1)} \Xi_{i_\iota j} \psi_j. \quad (2.10) \]

Here, \( \mathcal{D}\psi\mathcal{D}\xi \equiv \prod_{i=0}^{N-1} d\psi_i^{(\gamma)} \cdots d\psi_i^{(1)} d\xi_i^{(\gamma)} \cdots d\xi_i^{(1)} \) and the action \( S(\xi, \psi) \) involves pair interactions of composite operators

\[ \Xi_1 = \sum_{i_1, \ldots, i_\gamma \geq 0 \atop (i_1 + \cdots + i_\gamma = 1)} \xi_i^{(1)} \cdots \xi_i^{(\gamma)}, \quad \psi_1 = \sum_{i_1, \ldots, i_\gamma \geq 0 \atop (i_1 + \cdots + i_\gamma = 1)} \psi_i^{(1)} \cdots \psi_i^{(\gamma)}. \quad (2.11) \]
i.e. the products of \( \gamma \) anticommuting variables with the fixed sum of site indices. Using complex variables \( z = x + iy \) and \( \bar{z} = x - iy \), the interaction matrix is given by

\[
    w_{ij} = \int_D d^2z \, z^i \bar{z}^j w(z, \bar{z}), \quad i, j = 0, 1, \ldots, \gamma(N - 1).
\]

The one-body and two-body densities are expressible explicitly as

\[
    n(r) = w(z, \bar{z}) \sum_{i, j=0}^{\gamma(N-1)} \langle \Xi_i \Psi_j \rangle z^i \bar{z}^j, \quad (2.13)
\]

\[
    n_2(r_1, r_2) = w(z_1, \bar{z}_1)w(z_2, \bar{z}_2) \sum_{i_1, j_1, i_2, j_2=0}^{\gamma(N-1)} \langle \Xi_{i_1} \Psi_{j_1} \Xi_{i_2} \Psi_{j_2} \rangle z_1^{i_1} \bar{z}_1^{j_1} z_2^{i_2} \bar{z}_2^{j_2}, \quad (2.14)
\]

where \( \langle \cdots \rangle \equiv \int D\psi D\xi e^{-S}/Z_N(\gamma) \) denotes averaging over the anticommuting variables.

Next we consider the disc domain \( D = \{ r, |r| \leq R \} \) with a constant line charge density \( \sigma_e \) on the disc circumference \( r = R \). The requirement of the electroneutrality fixes the number of counter-ions with charge \( -e \) to \( N = 2\pi R \sigma \). For this model, we have \( w(z, \bar{z}) \equiv w(r) = 1 \) [33] and

\[
    w_{ij} = w_i \delta_{ij}, \quad w_i = 2\pi \int_0^R dr \, r^{2i+1} = \frac{\pi}{i+1} R^{2(i+1)}. \quad (2.15)
\]

The diagonalization of the action in composite operators

\[
    S(\xi, \psi) = \sum_{i=0}^{\gamma(N-1)} \Xi_i w_i \Psi_i \quad \text{(2.16)}
\]

implies that \( \langle \Xi_i \Psi_j \rangle = \delta_{ij} \langle \Xi_i \Psi_i \rangle \), \( \langle \Xi_{i_1} \Psi_{j_1} \Xi_{i_2} \Psi_{j_2} \rangle \neq 0 \) only if \( i_1 + j_1 = i_2 + j_2 \), etc. This fact simplifies the series representations of the one-body and two-body densities:

\[
    n(r) = \sum_{i=0}^{\gamma(N-1)} \langle \Xi_i \Psi_i \rangle r^{2i}, \quad (2.17)
\]

\[
    n_2(r_1, r_2) = \sum_{i_1+j_1, i_2+j_2=0}^{\gamma(N-1)} \langle \Xi_{i_1} \Psi_{j_1} \Xi_{i_2} \Psi_{j_2} \rangle z_1^{i_1} \bar{z}_1^{j_1} z_2^{i_2} \bar{z}_2^{j_2}. \quad (2.18)
\]

2.2 Conformal transformation

We consider the particles with complex coordinates \( (z, \bar{z}) \) inside the disc domain \( D = \{ (z, \bar{z}), z\bar{z} \leq R^2 \} \). The Möbius conformal transformation

\[
    z' = \frac{z + Ra}{1 + R^2}, \quad \bar{z}' = \frac{\bar{z} - Ra}{1 - R^2}. \quad (2.19)
\]
(with a free complex parameter \(a\) such that \(a\overline{a} \neq 1\)) transforms the particle coordinates in the disc domain \(D\) to another domain \(D'\) defined by the inequality
\[
(R^2 - z'z')(1 - a\overline{a}) \geq 0.
\]
(2.20)

If \(a\) is chosen such that \(a\overline{a} < 1\), the original disc domain \(D\) is mapped onto itself, \(D' = D\). Note that \(a = 0\) corresponds to the identity transformation.

2.2.1 Partition function

Let us study the effect of the M"{o}bius transformation of all particle coordinates on the partition function
\[
Z_N(\gamma) = \frac{1}{N!} \int_D \prod_{i=1}^{N} dz_i d\overline{z}_i \prod_{i<j=1}^{N} |z_i - z_j|^{2\gamma}.
\]
(2.21)

Under the conformal transformation (2.19), each surface element \(d\overline{z} \overline{d}z\) transforms as
\[
d\overline{z} \overline{d}z = \frac{(1 - a\overline{a})^2}{(1 - \frac{z_a^2}{R})^2 (1 - \frac{\overline{z}_a^2}{R})^2} d\overline{z}' d\overline{z}'.
\]
(2.22)

and each square of the distance between two particles transforms as
\[
|z_i - z_j|^2 = \frac{(1 - a\overline{a})^2}{(1 - \frac{z_i^2}{R}) (1 - \frac{z_j^2}{R}) (1 - \frac{\overline{z}_i^2}{R}) (1 - \frac{\overline{z}_j^2}{R})} |z_i' - z_j'|^2.
\]
(2.23)

The partition function (2.21) can be written in terms of the transformed coordinates as follows
\[
Z^a_N(\gamma) = \frac{1}{N!} \int_D \prod_{i=1}^{N} d\overline{z}_i' d\overline{z}_j' \left[ \frac{(1 - a\overline{a})}{(1 - \frac{z_i^2}{R}) (1 - \frac{\overline{z}_i^2}{R})} \right]^\nu \prod_{i<j=1}^{N} |z_i' - z_j'|^{2\gamma},
\]
(2.24)

where we use the notation \(\nu \equiv \gamma(N - 1) + 2\). The transformed variables \(z'\) and \(\overline{z}'\) under integration can be replaced by the original ones \(z\) and \(\overline{z}\). We see that the effect of the conformal transformation consists in changing the circular one-body Boltzmann factor \(w(r) = 1\) to the non-circular one
\[
w^a(z, \overline{z}) = \left[ \frac{(1 - a\overline{a})}{(1 - \frac{z}{R}) (1 - \frac{\overline{z}}{R})} \right]^\nu.
\]
(2.25)

The diagonal \(S\)-action (2.16) transforms itself into the non-diagonal one
\[
S^a(\xi, \psi) = \sum_{i,j=0}^{\gamma(N-1)} \Xi_i w^a_{ij} \psi_j,
\]
(2.26)
where

\[ w_{ij}^a = \int_D d^2z \left[ \frac{(1 - a\bar{a})}{(1 - \frac{z}{R})} \frac{1}{(1 - \frac{\bar{z}}{R})} \right]^{\nu} z^i \bar{z}^j, \quad i, j = 0, 1, \ldots, \gamma(N - 1). \tag{2.27} \]

The equivalence of the original partition function \( Z_N(\gamma; \{w_i\}) \) with the transformed one \( Z_N^a(\gamma; \{w_{ij}^a\}) \),

\[ Z_N(\gamma) = Z_N^a(\gamma), \tag{2.28} \]

can be expressed in terms of the integrals over anticommuting variables as

\[ \int D\psi D\xi \exp [S(\xi, \psi)] = \int D\psi D\xi \exp [S^a(\xi, \psi)]. \tag{2.29} \]

### 2.2.2 Particle density

Under the conformal transformation (2.19), the density \( n(z, \bar{z}; \{w_i\}) \equiv n(r) \) transforms itself to \( n^a(z', \bar{z}'; \{w_{ij}^a\}) \) according to

\[ n(z, \bar{z})d\bar{z} = n^a(z', \bar{z}')d\bar{z}'. \tag{2.30} \]

Note that this relation, when integrated over the disk domain \( D \), ensures the conservation of the total number of particles under the conformal transformation. Equivalently,

\[ n(z, \bar{z}) = \left[ \frac{(1 - \frac{z}{R})}{(1 - \frac{\bar{z}}{R})} \frac{1}{(1 - a\bar{a})} \right]^2 n^a(z', \bar{z'}). \tag{2.31} \]

Within the formalism of anticommuting variables, the transformed particle density is expressible as

\[ n^a(z', \bar{z}') = w^a(z', \bar{z}')^{\gamma(N-1)} \sum_{i,j=0}^{\gamma(N-1)} \langle \Xi_i \Psi_j \rangle^a(z')^i(\bar{z}')^j, \tag{2.32} \]

where the symbol \( \langle \cdots \rangle^a \) means the averaging with the \( S^a \)-action (2.26). We conclude that

\[ n(r) = \left[ \frac{(1 - a\bar{a})}{(1 - \frac{z}{R})} \frac{1}{(1 - \frac{\bar{z}}{R})} \right]^{\gamma(N-1)} \sum_{i,j=0}^{\gamma(N-1)} \langle \Xi_i \Psi_j \rangle^a(z')^i(\bar{z}')^j. \tag{2.33} \]

### 3 Derivation of sum rules

In this part, we use the above exact relations between the original and transformed partition functions and particle densities to derive certain sum rules.
3.1 Partition function

We start with the equality of the original and transformed partition functions, see Eqs. (2.28) and (2.29). First we expand the transformed interaction matrix (2.27) in linear $a$, $\bar{a}$ and quadratic $a\bar{a}$ terms:

$$w_{ij}^a = \delta_{ij}w_i + \frac{\nu a}{R} \delta_{i,j+1}w_i + \frac{\nu \bar{a}}{R} \delta_{i+1,j}w_{i+1} + a\bar{a}\delta_{ij} \left( \frac{\nu^2}{R^2}w_{i+1} - \nu w_i \right) + \cdots,$$

(3.1)

where $w_i$ are the original interaction strengths (2.15). The corresponding expansion of the transformed action (2.26) around the original action (2.16) reads as

$$S^a = S + \frac{\nu a}{R} \sum_i \Xi_{i+1}w_{i+1}\Psi_i + \frac{\nu \bar{a}}{R} \sum_i \Xi_i w_{i+1}\Psi_{i+1}$$

$$+ a\bar{a} \sum_i \Xi_i \left( \frac{\nu^2}{R^2}w_{i+1} - \nu w_i \right) \Psi_i + \cdots.$$  

(3.2)

Inserting this expansion into Eq. (2.29) and expanding the exponential in $a$, $\bar{a}$ and $a\bar{a}$ terms, we obtain

$$Z_N(\gamma) = Z_N(\gamma) \left[ 1 + a\bar{a} \sum_i \langle \Xi_i \Psi_i \rangle \left( \frac{\nu^2}{R^2}w_{i+1} - \nu w_i \right) \right.$$

$$\left. + a\bar{a} \sum_{i,j} \Xi_i \Xi_j \langle \Psi_{i+1} \Psi_{j+1} \rangle + \cdots \right].$$  

(3.3)

The term proportional to $a\bar{a}$ must vanish. Simultaneously, there holds

$$\sum_i w_i \langle \Xi_i \Psi_i \rangle = \int_D d^2r \, n(r) = N$$  

(3.4)

and

$$\sum_i w_{i+1} \langle \Xi_i \Psi_i \rangle = \int_D d^2r \, r^2 n(r).$$  

(3.5)

From the representation (2.18) we get

$$\sum_{i,j} w_{j+1} \langle \Xi_i \Psi_{i+1} \Xi_j \Psi_j \rangle r^{2(i+1)} = \int_D d^2r' \, r \cdot r' n_2(r, r'),$$  

(3.6)

where $r \cdot r' = (z z' + \bar{z} \bar{z}')/2$ denotes the scalar product of vectors $r$ and $r'$. Consequently, we end up with the sum rule

$$\int_D d^2r \int_D d^2r' r \cdot r' \langle \hat{n}(r) \hat{n}(r') \rangle = \frac{R^2 N}{\gamma(N-1) + 2}.$$  

(3.7)
This sum rule has already been derived in connection with the calculation of the dielectric susceptibility tensor, see Eq. (6.10) of Ref. [33]. The same equality holds for the truncated correlator \( \langle \hat{n}(r)\hat{n}(r') \rangle - n(r)n(r') \) since
\[
\int_D d^2r \int_D d^2r' r \cdot r' n(r)n(r') = 0 \tag{3.8}
\]
after the integration of \( \cos(\varphi - \varphi') \) over the angle \( \varphi - \varphi' \) from 0 to \( 2\pi \).

### 3.2 Particle density

In the density relation [233], we expand up to terms linear in \( \alpha \) and \( \alpha \) the transformed coordinates
\[
z' = z + Ra - \frac{z^2}{R} \hat{a} + \cdots, \quad \tilde{z'} = \tilde{z} + R\tilde{a} - \frac{\tilde{z}^2}{R} a + \cdots \tag{3.9}
\]
and, with the aid of the \( S^a \)-expansion [32], the transformed correlators
\[
\langle \Xi \psi_j \rangle_a = \delta_{ij} \langle \Xi \psi_i \rangle + \delta_{i+1,j} \frac{\nu a}{R} \sum_k w_{k+1} \langle \Xi \psi_{i+1} \Xi_{k+1} \psi_k \rangle + \delta_{i,j+1} \frac{\nu a}{R} \sum_k w_{k+1} \langle \Xi_{i+1} \psi_i \Xi_{j+1} \psi_j \rangle + \cdots. \tag{3.10}
\]
Thus we obtain
\[
0 = \frac{\gamma(N-1)}{R} (\tilde{z} a + \tilde{z} a)n(r) + \frac{\nu a}{R} \sum_{ij} w_{j+1} \langle \Xi_i \psi_{i+1} \Xi_j \psi_j \rangle z^i \tilde{z}^{j+1}
\]
\[
+ \frac{\nu a}{R} \sum_{ij} w_{j+1} \langle \Xi_i \psi_i \Xi_j \psi_{j+1} \rangle \tilde{z}^{i+1} z^j
\]
\[
+ (\tilde{z} a + \tilde{z} a) \sum_i \langle \Xi_i \psi_i \rangle (z\tilde{z})^i \left( \frac{R}{z^2} - \frac{1}{R} \right). \tag{3.11}
\]
After simple algebra, this result leads to the equality
\[
[\gamma(N-1) + 2] \int_D d^2r' r \cdot r' \langle \hat{n}(r)\hat{n}(r') \rangle = 2r^2 n(r) - \frac{1}{2} r(R^2 - r^2) \frac{\partial}{\partial r} n(r). \tag{3.12}
\]
Applying the integration \( \int_D d^2r \) to this relation, it reduces to the previous sum rule [34], but the present sum rule is more informative.

Let the vector \( \mathbf{r} \) be taken along the \( x \)-axis, \( \mathbf{r} = (r, 0) \), so that \( \mathbf{r} \cdot \mathbf{r'} = r r' \cos \varphi' \). Substituting the correlator in [3.12] by its truncation \( \langle \hat{n}(r)\hat{n}(r') \rangle - n(r)n(r') \equiv S(\mathbf{r}, \mathbf{r'})/e^2 \) and using the zeroth-moment sum rule [2.9], we obtain
\[
[\gamma(N-1) + 2] \left[ \int_0^{2\pi} d\varphi' \int_0^R dr' (r')^2 (1 - \cos \varphi') \frac{S(\mathbf{r}, \mathbf{r'})}{e^2} \right]
\]
\[
+ \int_D d^2r' \frac{S(\mathbf{r}, \mathbf{r'})}{e^2} = -2r n(r) + \frac{1}{2} (R-r)(R+r) \frac{\partial}{\partial r} n(r). \tag{3.13}
\]
To go from the disc to the semi-infinite rectilinear geometry in the limit $R \to \infty$, we switch to the variables $x = R - r$ and $x' = R - r'$. Eq. (3.13) then becomes

$$
\frac{\gamma(N-1) + 2}{R} \left[ \frac{1}{2} \int_{-\pi}^{\pi} \frac{d\varphi}{\pi} \int_0^\infty dx' \left( \frac{2R \sin(\varphi/2)}{2} \right)^2 \frac{S(x, x'; \varphi)}{e^2} \right] + \int_{-\pi}^{\pi} d(R\varphi) \int_0^\infty dx' \frac{S(x, x'; \varphi)}{e^2} = - \left[ x \frac{\partial}{\partial x} n(x) + 2n(x) \right]. \quad (3.14)
$$

For the disc geometry it was shown [17] that, as the radius $R \to \infty$, the Ursell function of two particles at finite distances $x$ and $x'$ from the disc boundary and with the angle $\varphi \neq 0$ between them behaves as

$$
U(x, x'; \varphi) = \frac{S(x, x'; \varphi)}{e^2} \approx \frac{f(x, x')}{2R \sin(\varphi/2)^2}, \quad \varphi \neq 0. \quad (3.15)
$$

Since $(x' - x)\delta(x - x') = 0$, we can also write

$$
\int_0^\infty dx' x' \frac{S(x, x'; \varphi)}{e^2} = \int_0^\infty dx' (x' - x) \frac{S(x, x'; \varphi)}{e^2} = \int_0^\infty dx' (x' - x) U(x, x'; \varphi). \quad (3.16)
$$

Introducing the lateral distance $y = R\varphi$ for the rectilinear geometry, Eq. (3.14) becomes

$$
2\pi\gamma\sigma \left[ \pi \int_0^\infty dx' f(x, x') + \int_{-\infty}^0 dy \int_0^\infty dx' (x' - x) U(x, x'; y) \right] = - \left[ x \frac{\partial}{\partial x} n(x) + 2n(x) \right]. \quad (3.17)
$$

There exists a 2D relation between asymptotic behavior and dipole moment seen from a fixed point with coordinate $x$ [16]:

$$
\int_{-\infty}^\infty dy \int_0^\infty dx' (x' - x) U(x, x'; y) = \pi \int_0^\infty dx' f(x, x'). \quad (3.18)
$$

Consequently, Eq. (3.17) implies that

$$
\int_0^\infty dx' f(x, x') = - \frac{1}{2\pi^2 \Gamma \sigma} \left[ x \frac{\partial}{\partial x} n(x) + 2n(x) \right]. \quad (3.19)
$$

In the previous paper [33], we found that

$$
\pi f(x, 0) = - \left[ x \frac{\partial}{\partial x} n(x) + 2n(x) \right]. \quad (3.20)
$$

Combining the last two equations, we finally arrive at the relation

$$
\int_0^\infty dx' f(x, x') = \frac{1}{2\pi \Gamma \sigma} f(x, 0) \quad (3.21)
$$
containing only the function of interest \( f(x, x') \).

This equation can be checked on two exactly solvable 2D cases of the present counter-ion system \([33]\). The PB \( \Gamma \to 0 \) limit yields \( f(x, x') \) of the long-range form \([31]\)

\[
f(x, x') = -\frac{2}{\pi^2 \Gamma} \frac{b^4}{(x + b)^4(x' + b)^4}, \quad b = \frac{1}{\pi \Gamma \sigma}.
\] (3.22)

At \( \Gamma = 2 \), we have \( f(x, x') \) of the short-range form \([13, 31]\)

\[
f(x, x') = -4\sigma^2 e^{-4\pi \sigma x} e^{-4\pi \sigma x'}.
\] (3.23)

It is easy to verify that both exact solutions fulfill our Eq. (3.21).

3.3 Properties of the amplitude \( f \)-function

Now we aim at showing fundamental properties of the \( f \)-functions following from Eq. (3.21).

It is known that in 2D the function \( f(x, x') \) obeys the sum rule \([12, 15, 28]\)

\[
\int_0^\infty dx \int_0^\infty dx' f(x, x') = -\frac{1}{2\pi^2 \Gamma}.
\] (3.24)

Applying the integration operation \( \int_0^\infty dx \) to Eq. (3.21), we get

\[
\int_0^\infty dx f(x, 0) = -\frac{\sigma}{\pi}.
\] (3.25)

Taking \( x = 0 \) in (3.21) and using the symmetry \( f(x, x') = f(x', x) \), the \( f \)-function with both points at the \( x = x' = 0 \) boundary is given by

\[
f(0, 0) = -2\Gamma \sigma^2.
\] (3.26)

As a check, the exactly solvable \( \Gamma \to 0 \) limit (3.22) and \( \Gamma = 2 \) case (3.23) satisfy this relation.

The function \( f(x, x') \) is assumed to be an analytic holomorphic function of its arguments. Therefore, when deriving both sides of the relation (3.21) with respect to \( x \), one can interchange the integration and derivation \([34]\) to obtain

\[
\int_0^\infty dx' \frac{\partial f(x, x')}{\partial x} = \frac{1}{2\pi \Gamma \sigma} \frac{\partial f(x, 0)}{\partial x}.
\] (3.27)

The two Eqs. (3.21) and (3.27) can be fulfilled simultaneously only if

\[
\frac{\partial f(x, x')}{\partial x} = h(x) f(x, x')
\] (3.28)

with some unknown function \( h(x) \). Equivalently,

\[
\frac{\partial}{\partial x} \ln [-f(x, x')] = h(x).
\] (3.29)
Taking into account the symmetry relation $f(x, x') = f(x', x)$, this PDE has the unique solution

$$\ln [-f(x, x')] = \int dx \, h(x) + \int dx' \, h(x').$$

(3.30)

Consequently, the function $f(x, x')$ factorizes as follows

$$f(x, x') = -g(x)g(x'), \quad g(x) = \exp \left[ \int dx \, h(x) \right].$$

(3.31)

The factorization property of $f(x, x')$, seen in the $\Gamma \to 0$ limit (3.22) and at $\Gamma = 2$ (3.23), thus extends to any value of $\Gamma$.

Due to the factorization property, the density profile $n(x)$ determines the function $f(x, x')$ as follows

$$f(x, x') = -\frac{1}{2\pi^2 \Gamma \sigma^2} \left[ x \frac{\partial n(x)}{\partial x} + 2n(x) \right] \left[ x' \frac{\partial n(x')}{\partial x'} + 2n(x') \right] .$$

(3.32)

The prefactor is fixed by the sum rule (3.24) together with the equality

$$\int_0^\infty dx \left[ x \frac{\partial n(x)}{\partial x} + 2n(x) \right] = \int_0^\infty dx \, n(x) = \sigma ,$$

(3.33)

where we used the integration by parts for $x\partial n(x)/\partial x$, the known fact that $n(x)$ goes to 0 faster than $1/x$ as $x \to \infty$ and the electroneutrality condition.

4 Another approach to one-component systems

4.1 Counter-ions only

There exists an alternative way how to derive in the 2D case with counter-ions only the important relation (3.19). In 2D, the coupling constant $\Gamma = \beta e^2$ is dimensionless. The particle density $n$ has dimension $[\text{length}]^{-2}$ and the surface charge density $\sigma$ has dimension $[\text{length}]^{-1}$, so one can write

$$n(x; \sigma) = \sigma^2 t(\sigma x) ,$$

(4.1)

where $t$ is an unknown function. For this scaling form of the density profile, we obtain the equality

$$\sigma \frac{\partial n(x)}{\partial \sigma} = 2\sigma^2 t(\sigma x) + \sigma^3 x t'(\sigma x) = 2n(x) + x \frac{\partial n(x)}{\partial x} .$$

(4.2)

Blum et al. [4] derived a sum rule which relates the variation of the particle density $n(x)$ with respect to the surface charge density to the dipole moment seen by a fixed particle. In 2D, the sum rule reads as

$$\frac{\partial n(x)}{\partial \sigma} = -2\pi \Gamma \int_{-\infty}^{\infty} dy \int_0^{\infty} dx' \, (x' - x)U(x, x'; y)$$

(4.3)
With the aid of the relations (3.18) and (4.2), we recover Eq. (3.19).
We can go to higher dimensions \(d\) within the present approach. The \(d\)-dimensional Blum counterpart of the 2D sum rule (4.3) is

\[
\frac{\partial n(x)}{\partial \sigma} = -s_d \beta e^2 \int_{-\infty}^{\infty} dy \int_{0}^{\infty} dx' (x' - x) U(x, x'; y). \tag{4.4}
\]

The 2D relation between asymptotic behavior and dipole moment (3.18) takes in \(d\) dimensions the form \([16]\)

\[
\int_{-\infty}^{\infty} dy \int_{0}^{\infty} dx' (x' - x) U(x, x'; y) = \frac{s_d}{2} \int_{0}^{\infty} dx' f(x, x'). \tag{4.5}
\]

so that

\[
\frac{\partial n(x)}{\partial \sigma} = -\frac{s_d^2}{2} \beta e^2 \int_{0}^{\infty} dx' f(x, x'). \tag{4.6}
\]

This formula can be readily checked on the exactly solvable PB limit \(\Gamma \to 0\) in any dimension \(d\) \([31,33]\):

\[
n(x) = \frac{ab}{(x + b)^2}, \quad f(x, x') = -\frac{8}{\beta e^2 s_d^2 (x + b)^3 (x' + b)^3}, \tag{4.7}
\]

where

\[
b = \frac{2}{(\beta e^2 \sigma s_d)} \text{ is the Gouy-Chapmann length.}
\]

We cannot prove in general the factorization property (3.31) of the function \(f(x, x')\) in dimensions \(d \geq 3\) since we miss a relation like the 2D one (3.20) derived for any temperature in Ref. \([33]\). Let us suppose that the factorization property takes place, i.e. \(f(x, x') = -g(x)g(x')\), and apply the present formalism to obtain \(g(x)\). The generalization of the 2D sum rule (3.24) to any dimension \(d\) reads as

\[
\int_{0}^{\infty} dx \int_{0}^{\infty} dx' f(x, x') = -\frac{2}{\beta e^2 s_d^2}. \tag{4.8}
\]

Inserting the factorization assumption into this equation implies

\[
\int_{0}^{\infty} dx g(x) = \sqrt{\frac{2}{\beta e^2 s_d^2}}. \tag{4.9}
\]

Then, considering \(f(x, x') = -g(x)g(x')\) in Eq. (4.6) leads to

\[
g(x) = \sqrt{\frac{2}{\beta e^2 s_d^2}} \frac{\partial n(x)}{\partial \sigma}, \tag{4.10}
\]

i.e. for every distance \(x\) from the wall the function \(g(x)\) is expressible locally in terms of the density profile. Note that the relations (4.9) and (4.10) are fully consistent since the integration of Eq. (4.10) over \(x\) from 0 to \(\infty\) reduces to (4.9) due to the electroneutrality condition \(\int_{0}^{\infty} dx n(x) = \sigma\). The factorized \(d\)-dimensional PB solution (4.7) with

\[
g(x) = \sqrt{\frac{8}{\beta e^2 s_d^2 (x + b)^3}} \tag{4.11}
\]

evidently fulfills Eq. (4.10).
4.2 Jellium model

The relation (4.10) in fact holds for an arbitrary one-component system whose $f(x,x')$-function factorizes into $-g(x)g(x')$. Here, we present the jellium model of mobile pointlike particles with charge $-e$ immersed in a homogeneous (bulk) background of density $n_0$ and charge density $en_0$. The system is constrained to the $d$-dimensional Euclidean half-space of points $\mathbf{r} = (x,y)$ with $y = (y_1,\ldots,y_{d-1})$, the coordinates $y_i \in (-\infty, \infty)$ and $x \geq 0$. There is a plane charged by a constant surface charge density $\sigma e$ at $x = 0$. The density profile $n(x)$ and the function $f(x,x')$ were calculated exactly in two cases.

The high-temperature Debye-Hückel (linearized PB) theory in $d$ dimensions \[\text{[11]}\] yields the density profile

$$n(x,\sigma) = n(x,\sigma = 0) + \sigma e^{-\kappa x}, \quad (4.12)$$

where $\kappa = \sqrt{s_d/\beta e^2 n_0}$ is the inverse Debye length. The asymptotic $|y| = y \to \infty$ decay of the Ursell function along the wall was found in the form

$$U(x,x';y) \simeq \frac{2n_0}{s_d} e^{-\kappa x} e^{-\kappa x'} \frac{1}{y^d}, \quad (4.13)$$
i.e.

$$g(x) = \sqrt{\frac{2n_0}{s_d}} e^{-\kappa x}. \quad (4.14)$$

With regard to the equality $\partial n(x)/\partial \sigma = \kappa e^{-\kappa x}$, it is easy to verify that this $g$-function satisfies Eq. (4.10).

The other exactly solvable case is the 2D jellium at coupling $\Gamma = 2$. The free-fermion method \[\text{[11]}\] yields the density profile

$$n(x,\sigma) = \frac{n_0}{\sqrt{\pi}} \int_{-\pi \sigma \sqrt{2}}^{\infty} dt \frac{1}{1+\phi(t)} e^{-(t-x\sqrt{2})^2}, \quad (4.15)$$

where $\phi$ denotes the error function

$$\phi(t) = \frac{2}{\sqrt{\pi}} \int_{0}^{t} du e^{-u^2}. \quad (4.16)$$

The asymptotic decay of the Ursell function along the wall

$$U(x,x';y) \simeq \frac{2n_0}{\pi} \exp \left\{ -2 \left[ x^2 + x'^2 + 2\pi \sigma (x + x') + 2\pi^2 \sigma^2 \right] \right\} \frac{1}{1+\phi(-\pi \sigma \sqrt{2})} \frac{1}{y^2}, \quad (4.17)$$

implies the $g$-function of the form

$$g(x) = n_0 \sqrt{\frac{2}{\pi}} \frac{e^{-2(x+\pi \sigma)^2}}{1+\phi(-\pi \sigma \sqrt{2})}. \quad (4.18)$$

After simple algebra it can be shown that

$$g(x) = \frac{1}{2\pi} \frac{\partial n(x)}{\partial \sigma} \quad (4.19)$$

which is in agreement with our result (4.10).
5 A generalization to many-component Coulomb systems

Now let us consider a general Coulomb system which consists of \(s\) species of particles \(\alpha = 1, \ldots, s\) with the corresponding charges \(q_n e\) (\(q_n\) is the valence and \(e\) the elementary charge), plus perhaps a fixed background of density \(n_0\) and charge density \(\rho_0 = e n_0\). As before, the particles are constrained to the \(d\)-dimensional Euclidean half-space of points \(r = (x, y)\) with \(x \geq 0\). There is a plane charged by a constant surface charge density \(\sigma e\) at \(x = 0\). The microscopic density of particles of species \(\alpha\) is given by \(\hat{n}_\alpha (r) = \sum_i \delta_{\alpha, \alpha_i} \delta (r - r_i)\), where \(i\) indexes the charged particles. The total microscopic charge density reads as \(\hat{\rho} (r) = \rho_0 + \sum \alpha q_\alpha e \hat{n}_\alpha (r)\). For the present geometry, the averaged charge density depends only on the \(x\)-coordinate, \(\rho (x) = \langle \hat{\rho} (r) \rangle\).

The charge-charge structure function, defined by

\[
S(r, r') \equiv \langle \hat{\rho} (r) \hat{\rho} (r') \rangle - \langle \hat{\rho} (r) \rangle \langle \hat{\rho} (r') \rangle,
\]

depends on coordinates \(x, x'\) and on the lateral distance \(y = |y - r'|\), \(S(x, x'; y)\). The asymptotic large-\(y\) behavior is of the form

\[
S(x, x'; y) \sim \frac{F (x, x')}{{y^{d/2}}},
\]

(5.2)

For the previous one-component system of particles with charge \(-e\), \(F (x, x')\) is related to \(f (x, x')\) by \(F (x, x') = e^2 f (x, x')\). The counterpart of the one-component sum rule (4.8) is

\[
\int_{-\infty}^{\infty} dy \int_{0}^{\infty} dx' F (x, x') = -\frac{2}{\beta s_d^2}.
\]

(5.3)

According to Blume et al. [4], the many-component generalization of Eq. (4.4) reads as

\[
\frac{\partial \rho (x)}{\partial (e \sigma)} = -s_d \beta \int_{-\infty}^{\infty} dy \int_{0}^{\infty} dx' (x' - x) S(x, x'; y).
\]

(5.4)

The many-component generalization of the relation (4.5) reads [16]

\[
\int_{-\infty}^{\infty} dy \int_{0}^{\infty} dx' (x' - x) S(x, x'; y) = \frac{s_d}{2} \int_{0}^{\infty} dx' F (x, x'),
\]

(5.5)

so that

\[
\frac{\partial \rho (x)}{\partial (e \sigma)} = -\frac{s_d^2 \beta}{2} \int_{0}^{\infty} dx' F (x, x').
\]

(5.6)

Let us presuppose that the \(F\)-function factorizes as

\[
F (x, x') = -G (x) G (x').
\]

(5.7)

Taking into account the sum rule (5.3) and Eq. (5.6), we find the direct local relation between the \(G\)-function and the charge profile:

\[
G (x) = \frac{1}{\beta} \frac{1}{s_d} \frac{1}{\left| \frac{\partial \rho (x)}{\partial (e \sigma)} \right|}.
\]

(5.8)

Note that \(G (x)\) is determined up to an irrelevant sign; for simplicity, we have chosen \(G (x) > 0\).
5.1 Exactly solvable cases

In the Debye-Hückel high-temperature limit [11], the charge density profile takes the form

\[ \rho(x, \sigma) = \rho(x, \sigma = 0) - e \sigma \kappa e^{-\kappa x}, \]  
(5.9)

where \( \kappa = \sqrt{s_d \beta e^2 \sum \alpha q^2 n^\alpha} \) is the multi-component inverse Debye length.

The asymptotic amplitude function \( F(x, x') \) was found in the form

\[ F(x, x') = -\frac{2 \kappa^2}{\beta s_d} e^{-\kappa (x + x')}, \]  
(5.10)

implying

\[ G(x) = \sqrt{\frac{2 \kappa}{\beta s_d}} e^{-\kappa x}. \]  
(5.11)

Since \( \partial \rho(x) / \partial (e \sigma) = -\kappa e^{-\kappa x} \), it is trivial to verify that this \( G \)-function satisfies Eq. (5.8).

Another exactly solvable case is the 2D two-component plasma (Coulomb gas) of \( \pm e \) charges at coupling \( \Gamma = 2 \) [9][14]. The density profiles of \( \pm e \) particles read as

\[ n_\pm(x, \sigma) = n_\pm(x, \sigma = 0) + \frac{m^2}{2\pi} \int_0^{2\pi \sigma} \frac{dt}{\sqrt{m^2 + t^2}} e^{-2\sqrt{m^2 + t^2}x}, \]  
(5.12)

where \( m \) is a rescaled fugacity which has dimension of an inverse length. Since \( n_+(x, \sigma = 0) = n_-(x, \sigma = 0) \), the charge density \( \rho(x) = e [n_+(x) - n_-(x)] \) results in

\[ \rho(x) = -\frac{e}{\pi} \int_0^{2\pi \sigma} \sqrt{m^2 + t^2} e^{-2\sqrt{m^2 + t^2}x}. \]  
(5.13)

Introducing the variable \( k_0 = \sqrt{m^2 + (2\pi \sigma)^2} \), we obtain that

\[ \frac{\partial \rho(x)}{\partial (e \sigma)} = -2k_0 e^{-2k_0 x}. \]  
(5.14)

Simultaneously, it holds [1]

\[ F(x, x') = -\frac{k_0^2 e^2}{\pi^2} e^{-2k_0 (x + x')}, \quad G(x) = -\frac{k_0 e}{\pi} e^{-2k_0 x}. \]  
(5.15)

Taking \( \beta e^2 = 2 \), Eq. (5.8) is readily shown to be satisfied.
6 Conclusion

This paper was motivated by the previous one [33] where, using the technique of anticommuting variables for a 2D model of the charged wall with counterions only, a new relation was found between the amplitude function \( f(x, x') \) (with \( x' = 0 \)) of the asymptotic decay of two-body densities along the wall and the particle density profile \( n(x) \), see Eq. (3.20). Here in Sect. 2, using the Möbius conformal transformation of particle coordinates on the level of one-body density for the same model, the complementary relation (3.19) was derived. The combination of the two exact relations enabled us to prove the factorization property \( f(x, x') = -g(x)g(x') \) and to express \( g(x) \) in terms of the density profile.

For more-complicated many-component Coulomb fluids in any dimension, it is necessary to concentrate on the charge-charge structure function (5.1) with the asymptotic behavior (5.2) and to look on the relation between the amplitude function \( F(x, x') \) and the charge density profile \( \rho(x) \). In all exactly solvable cases which are available in the high-temperature limit and at the 2D free-fermion coupling, the amplitude function \( F(x, x') \) factorizes. There is no proof of the factorization property of the amplitude function at any temperature. In general, the statistical independence of two particles at asymptotically large distances is reflected by the nullity of the truncated correlation functions. In our semi-infinite problem, the distance between two particles goes to infinity along the wall, \( y \to \infty \), but the distances of the particles from the wall \( x, x' \) are finite. One can intuitively argue that the limit \( y \to \infty \) automatically decouples the subspaces \( x \) and \( x' \) which is behind the factorization property of the amplitude function. Presupposing \( F(x, x') = -G(x)G(x') \) for any Coulomb fluid, the combination of two sum rules (5.4) and (5.5) permits us to express \( G(x) \) in terms of the charge density profile \( \rho(x) \), see Eq. (5.8).

As concerns future perspective, it would be desirable to find simplified models or new methods to prove the factorization property of the amplitude function for more general Coulomb fluids. A better comprehension of the form of the amplitude function might clarify the form of the dielectric susceptibility tensor for an arbitrarily shaped domain.

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