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A Generalization of the Stillinger–Lovett Sum Rules for the Two-Dimensional Jellium

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Abstract In the equilibrium statistical mechanics of classical Coulomb fluids, the long-range tail of the Coulomb potential gives rise to the Stillinger–Lovett sum rules for the charge correlation functions. For the jellium model of mobile particles of charge q immersed in a neutralizing background, the Stillinger–Lovett sum rules give the charge and second moment of the screening cloud around a particle of the jellium. In this paper, we generalize these sum rules to the screening cloud induced around a pointlike guest charge Zq immersed in the bulk interior of the 2D jellium with the coupling constant $\Gamma = \beta q^2$ (β is the inverse temperature), in the whole region of the thermodynamic stability of the guest charge amplitude $Z > -2/\Gamma$. The derivation is based on a mapping technique of the 2D jellium at the coupling $\Gamma =$ (even positive integer) onto a discrete 1D anticommuting-field theory; we assume that the final results remain valid for all real values of Γ corresponding to the fluid regime. The generalized sum rules reproduce for arbitrary coupling Γ the standard $Z = 1$ and the trivial $Z = 0$ results. They are also checked in the Debye–Hückel limit $\Gamma \to 0$ and at the free-fermion point $\Gamma = 2$. The generalized second-moment sum rule provides some exact information about possible sign oscillations of the induced charge density in space.

Keywords Coulomb systems · Jellium · Logarithmic interaction · Screening · Sum rules

1 Introduction

The present paper deals with the equilibrium statistical mechanics of a classical (i.e. non-quantum) jellium, sometimes called the one-component plasma, formulated in two spatial dimensions (2D).

The jellium model consists of mobile pointlike particles $j = 1, \ldots, N$ of charge q and position vectors $\mathbf{r}_j$, confined to a continuous domain Λ. The particles are embedded in

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a spatially uniform neutralizing background of charge density $-qn$. The bulk regime of interest corresponds to the limits $N \to \infty$ and $|\Lambda| \to \infty$ with the fixed particle density $n = N/|\Lambda|$.

According to the laws of 2D electrostatics, the particles can be thought of as infinitely long charged lines in the 3D space which are perpendicular to the confining 2D surface Λ. Thus, the electrostatic potential ϕ at a point $\mathbf{r} \in \Lambda$, induced by a unit charge at the origin $\mathbf{0}$, is given by the 2D Poisson equation

$$\Delta\phi(\mathbf{r}) = -2\pi\delta(\mathbf{r}). \tag{1.1}$$

For an infinite plane $\Lambda = R^2$, the solution of this equation, subject to the boundary condition $\nabla\phi(\mathbf{r}) \to 0$ as $|\mathbf{r}| \to \infty$, reads

$$\phi(\mathbf{r}) = -\ln\left(\frac{r}{r_0}\right), \tag{1.2}$$

where $r \equiv |\mathbf{r}|$ and the free length constant r_0 will be set for simplicity to unity. In the 2D Fourier space defined by

$$f(r) = \int \frac{\mathrm{d}^2 k}{2\pi} \hat{f}(k) \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}), \tag{1.3}$$

$$\begin{aligned} \hat{f}(k) &= \int \frac{\mathrm{d}^2 r}{2\pi} f(r) \exp(-\mathrm{i}\mathbf{k}\cdot\mathbf{r}) \\ &= \sum_{j=0}^{\infty} \frac{(-1)^j}{(j!)^2}\left(\frac{k^2}{4}\right)^j \frac{1}{2\pi}\int \mathrm{d}^2 r\, r^{2j} f(\mathbf{r}), \end{aligned} \tag{1.4}$$

the Coulomb potential (1.2) exhibits the form

$$\hat{\phi}(k) = \frac{1}{k^2} \tag{1.5}$$

with the characteristic singularity at $k = 0$. This maintain many generic properties of "real" 3D Coulomb fluids with the interaction potential $\phi(r) = 1/r$, $\mathbf{r} \in R^3$.

Because of the presence of the rigid background, the equilibrium statistics of the jellium is usually studied in the canonical ensemble under the condition of the overall charge neutrality. The 2D statistics depends on the coupling constant $\Gamma = \beta q^2$ with $\beta = 1/(k_B T)$ being the inverse temperature; the particle density n only scales appropriately the distance. Let the symbol $\langle \cdots \rangle_\beta$ denotes the canonical averaging. At the one-particle level, one introduces the average number density of particles

$$n(\mathbf{r}) = \left\langle \sum_j \delta(\mathbf{r} - \mathbf{r}_j) \right\rangle_\beta. \tag{1.6}$$

At the two-particle level, one introduces the two-body density

$$n^{(2)}(\mathbf{r}, \mathbf{r}') = \left\langle \sum_{j \neq k} \delta(\mathbf{r} - \mathbf{r}_j)\delta(\mathbf{r}' - \mathbf{r}_k) \right\rangle_\beta. \tag{1.7}$$

It is also useful to consider the pair correlation function

$$h(\mathbf{r}, \mathbf{r}') = \frac{n^{(2)}(\mathbf{r}, \mathbf{r}')}{n(\mathbf{r})n(\mathbf{r}')} - 1, \tag{1.8}$$

which tends to 0 at asymptotically large distances $|\mathbf{r}-\mathbf{r}'|\to\infty$.

The bulk jellium is in a fluid state for high enough temperatures, i.e. the density of particles is homogeneous, $n(\mathbf{r})=n$, and the two-body density is translation invariant, $n^{(2)}(\mathbf{r},\mathbf{r}')=n^{(2)}(|\mathbf{r}-\mathbf{r}'|)$. There were indications from numerical simulations [1] that around $\Gamma\sim 142$ the fluid system undergoes a phase transition to a 2D Wigner crystal; a recent study [2], based on Monte-Carlo simulations, cautions this conclusion. In any case, in what follows we shall restrict ourselves to the fluid jellium.

Through a simple scaling argument, the exact equation of state for the pressure P, $\beta P = n[1-(\Gamma/4)]$, has been known for long time [3]. The jellium is completely solvable, like any Coulomb system, in the high-temperature Debye–Hückel (DH) limit $\Gamma\to 0$ [4], characterized by a monotonic exponential decay of the pair correlation function $h(r)$ at asymptotically large distances $r\to\infty$. The systematic Γ-expansion of statistical quantities around the DH limit can be done within a bond-renormalized Mayer diagrammatic expansion [5]. The 2D jellium is mappable onto a system of free fermions at the special coupling $\Gamma=2$ [6]. This exactly solvable point is characterized by a pure Gaussian decay of the pair correlation. The evaluation of the leading term of the $(\Gamma-2)$ expansion for $h(r)$ indicates the change from the monotonic to oscillatory behavior just at $\Gamma=2$ [6].

The long-range tail of the Coulomb potential, which is reflected in the singular behavior of the Fourier component (1.5) around $k=0$, causes screening and thus gives rise to exact constraints (sum rules) for the charge correlation functions (see review [7]), like the zeroth- and second-moment Stillinger–Lovett conditions [8, 9]. Their derivation can be based on the exploration of the Ornstein–Zernicke (OZ) equation

$$h(\mathbf{r},\mathbf{r}') = c(\mathbf{r},\mathbf{r}') + \int \mathrm{d}^2 r''\, c(\mathbf{r},\mathbf{r}'') n(\mathbf{r}'') h(\mathbf{r}'',\mathbf{r}') \tag{1.9}$$

relating the pair correlation function h with the *direct* correlation function c. Within the diagrammatic scheme of the renormalized Mayer expansion [5], the direct correlation function of the bulk jellium is expressible as

$$c(r) = -\beta q^2 \phi(r) + c_{\mathrm{reg}}(r), \tag{1.10}$$

where c_{reg} denotes contributions of all completely renormalized Mayer diagrams. Since these contributions are short-ranged, the Fourier transform of c_{reg} has an analytic k-expansion around $k=0$. Consequently, as $k\to 0$,

$$\hat{c}(k) = -\frac{\Gamma}{k^2} + O(1). \tag{1.11}$$

Writing the OZ equation (1.9) in the 2D Fourier space

$$\hat{h}(k) = \hat{c}(k) + 2\pi n \hat{c}(k)\hat{h}(k), \tag{1.12}$$

the small-k expansion of $\hat{c}$ (1.11) fixes the zeroth and second moments of $h(r)$. In terms of the two-body density, these sum rules read

$$\int \mathrm{d}^2 r\, [n^{(2)}(\mathbf{r},\mathbf{0}) - n^2] = -n, \tag{1.13}$$

$$\int \mathrm{d}^2 r\, |\mathbf{r}|^2 [n^{(2)}(\mathbf{r},\mathbf{0}) - n^2] = -\frac{2}{\pi\Gamma}. \tag{1.14}$$

The two rules express the perfect screening property of the charge cloud around a particle of the jellium and an infinitesimal guest charge, respectively. It is clear from the derivation procedure that the consideration of a short-ranged, e.g. hard core, potential in addition to the Coulomb potential does not alter the results (1.13) and (1.14). We add for completeness that for the 2D jellium also the fourth-moment condition [10] (related to the availability of the exact equation of state) and the sixth-moment condition [11] (derived within a classification of renormalized Mayer diagrams) are known.

In this paper, we study a typical situation in the theory of colloidal mixtures [12, 13]: a "guest" particle with charge Zq is immersed into the bulk interior of a Coulomb system, in our case the jellium. Possible values of the parameter Z are restricted as follows. When q is the elementary charge e of an electron, Z is the valence of an atom and as such it should be an integer. In general, the jellium can be composed of multivalent charges ($q = \pm 2e, \pm 3e, \ldots$) and in that case Z can take rational values. In the considered case of the *pointlike* guest charge and two spatial dimensions, the value of Z is bounded from below by a collapse phenomenon. Namely, the Boltzmann factor of the guest charge Zq with a jellium charge q at distance r, $r^{\Gamma Z}$, is integrable at small 2D distances r if and only if

$$Z > -\frac{2}{\Gamma}. \tag{1.15}$$

This is the region of the thermodynamic stability for the jellium system plus the guest charge Zq.

The aim of the present paper is to extend the Stillinger–Lovett sum rules (1.13) and (1.14) to the presence of the guest charge Zq in the bulk jellium. For this purpose, we introduce "conditional" densities: let $n(\mathbf{r}|Zq, \mathbf{0})$ be the average density of jellium particles at point $\mathbf{r}$ induced by a pointlike charge Zq placed at the origin $\mathbf{0}$. The corresponding induced charge density will be denoted by $\rho(\mathbf{r}|Zq, \mathbf{0}) = q[n(\mathbf{r}|Zq, \mathbf{0}) - n]$. Evidently, if $Z = 1$, i.e. the fixed particle has the same charge as the species forming the jellium, it holds

$$n^{(2)}(\mathbf{r}, \mathbf{0}) = n(\mathbf{r}|q, \mathbf{0})n(\mathbf{0}). \tag{1.16}$$

The sum rules (1.13) and (1.14) can be thus rewritten in the form

$$\int \mathrm{d}^2 r\, \rho(\mathbf{r}|q, \mathbf{0}) = -q, \tag{1.17}$$

$$\int \mathrm{d}^2 r\, |\mathbf{r}|^2 \rho(\mathbf{r}|q, \mathbf{0}) = -\frac{2q}{\pi \Gamma n}. \tag{1.18}$$

The zeroth-moment condition (1.17) reflects a trivial fact that the charge q is screened by a cloud of the opposite charge $-q$. The condition (1.18) tells us that the second-moment of this charge cloud has a prescribed value. Our task is to generalize these exact constraints for the conditional charge density $\rho(\mathbf{r}|Zq, \mathbf{0})$, where the guest-charge parameter Z lies in the stability region (1.15). We notice that there exists one trivial case $Z = 0$, for which the obvious equality $n(\mathbf{r}|0, \mathbf{0}) = n$ implies that all charge moments vanish,

$$\int \mathrm{d}^2 r\, |\mathbf{r}|^{2j} \rho(\mathbf{r}|0, \mathbf{0}) = 0 \quad \text{for } j = 0, 1, 2, \ldots. \tag{1.19}$$

The generalization of the zeroth-moment relation (1.17) is straightforward:

$$\int \mathrm{d}^2 r\, \rho(\mathbf{r}|Zq, \mathbf{0}) = -Zq, \tag{1.20}$$

i.e., the guest charge Zq immersed in the jellium is screened by an excess cloud of jellium particles carrying exactly the opposite charge $-Zq$.

The generalization of the second-moment relation (1.18) is nontrivial. We would like to emphasize that the derivation of the sum rule (1.14), or its equivalent (1.18), using the OZ equation was based on the translation-invariance property of the bulk jellium. The introduction of the guest charge Zq with $Z \neq 1$ breaks the translation symmetry of the jellium and one has therefore to apply other more sophisticated approaches. Here, we use a mapping technique of the 2D jellium with the coupling constant $\Gamma =$ (even positive integer) onto a discrete 1D anticommuting-field (fermion) theory, introduced in [14] and developed further in [15–17]. The general formalism of the mapping technique is briefly recapitulated in Sect. 2.

The present application of the fermionic mapping to the thermodynamic limit of the jellium in the disc geometry, with the guest charge Zq fixed at the disc center, is the subject of Sect. 3. Within the fermion representation, a couple of constraints for fermionic correlators is derived by using specific transformations of anticommuting variables. Under the assumption of good screening properties of the jellium system, these fermionic constraints imply the electroneutrality sum rule (1.20) and the desired second-moment sum rule:

$$\int \mathrm{d}^2 r |\mathbf{r}|^2 \rho(\mathbf{r}|Zq, \mathbf{0}) = -\frac{1}{\pi \Gamma n} Zq \left[\left(2 - \frac{\Gamma}{2} \right) + \frac{\Gamma}{2} Z \right], \tag{1.21}$$

valid in the guest-charge stability region (1.15). Although this relation was obtained for the series of discrete values of the coupling constant $\Gamma = 2, 4, \ldots$, we assume its validity for all real values of Γ corresponding to the fluid regime. It is easy to verify that the formula (1.21) is consistent for $Z = 1$ with the result (1.18) and for $Z = 0$ with (1.19). In contrast to the zeroth-moment condition (1.20), the second-moment sum rule (1.21) provides some exact information about possible sign oscillations of the charge cloud screening the guest particle Zq and this topic is also discussed in Sect. 3.

The exact weak-coupling DH analysis of the studied guest-charge problem is presented in Sect. 4, with the final result

$$\int \mathrm{d}^2 r \, |\mathbf{r}|^2 \rho(\mathbf{r}|Zq, \mathbf{0}) = -\frac{2Zq}{\pi \Gamma n} \quad \text{as } \Gamma \to 0. \tag{1.22}$$

The crucial formula (1.21) evidently passes this test.

The exact treatment of the problem at the free fermion point $\Gamma = 2$, performed in Sect. 5, leads for stable $Z > -1$ to the result

$$\int \mathrm{d}^2 r \, |\mathbf{r}|^2 \rho(\mathbf{r}|Zq, \mathbf{0}) = -\frac{Zq(Z+1)}{2\pi n} \quad \text{at } \Gamma = 2. \tag{1.23}$$

The formula (1.21) passes also this test.

Some concluding remarks are given in Sect. 6.

2 General Formalism

Let us consider the jellium consisting of N mobile particles confined to a 2D domain Λ; the plain hard walls surrounding Λ do not produce image charges. In terms of the complex coordinates $(z, \bar{z})$, the potential energy of the particle-background system is given by

$$E = E_0 + q \sum_j \phi(z_j, \bar{z}_j) - q^2 \sum_{j<k} \ln |z_j - z_k|. \tag{2.1}$$

Here, $\phi(z,\bar{z})$ is the one-body potential induced by the background plus perhaps some additional fixed charges and E_0 is the (background–background, etc.) interaction constant which does not influence the statistical averages over particle positions and therefore will be omitted. The canonical partition function at the inverse temperature β reads

$$Z_N = \frac{1}{N!}\int_\Lambda \prod_{j=1}^{N}\left[\mathrm{d}^2 z_j\, w(z_j,\bar{z}_j)\right]\prod_{j<k}|z_j - z_k|^\Gamma, \tag{2.2}$$

where the one-body Boltzmann factor $w(z_j,\bar{z}_j) = \exp[-\beta q\phi(z_j,\bar{z}_j)]$. The particle density (1.6) can be obtained in the standard way

$$n(z,\bar{z}) = w(z,\bar{z})\frac{\delta \ln Z_N}{\delta w(z,\bar{z})}. \tag{2.3}$$

For the coupling constant $\Gamma = 2\gamma$ ($\gamma = 1, 2, \ldots$ an integer), it has been shown in [14] that the partition function (2.2) can be expressed as the integral over two sets of Grassmann variables $\{\xi_j^{(\alpha)}, \psi_j^{(\alpha)}\}$ each with γ components ($\alpha = 1, \ldots, \gamma$), defined on a discrete chain of N sites $j = 0, 1, \ldots, N-1$ and satisfying the ordinary anticommuting algebra [18], as follows:

$$Z_N = \int \mathcal{D}\psi\mathcal{D}\xi\, \exp[S(\xi,\psi)], \tag{2.4}$$

$$S(\xi,\psi) = \sum_{j,k=0}^{\gamma(N-1)} \Xi_j w_{jk} \Psi_k. \tag{2.5}$$

Here, $\mathcal{D}\psi\mathcal{D}\xi = \prod_{j=0}^{N-1} \mathrm{d}\psi_j^{(\gamma)}\cdots\mathrm{d}\psi_j^{(1)}\mathrm{d}\xi_j^{(\gamma)}\cdots\mathrm{d}\xi_j^{(1)}$ and the action S involves pair interactions of "composite" operators

$$\Xi_j = \sum_{\substack{j_1,\ldots,j_\gamma=0\\(j_1+\cdots+j_\gamma)=j}}^{N-1} \xi_{j_1}^{(1)}\cdots\xi_{j_\gamma}^{(\gamma)}, \qquad \Psi_k = \sum_{\substack{k_1,\ldots,k_\gamma=0\\(k_1+\cdots+k_\gamma)=k}}^{N-1} \psi_{k_1}^{(1)}\cdots\psi_{k_\gamma}^{(\gamma)}. \tag{2.6}$$

The interaction strength is given by

$$w_{jk} = \int_\Lambda \mathrm{d}^2 z\, w(z,\bar{z}) z^j \bar{z}^k, \qquad j,k = 0,1,\ldots,\gamma(N-1). \tag{2.7}$$

Using the notation $\langle\cdots\rangle = \int \mathcal{D}\psi\mathcal{D}\xi\,\mathrm{e}^S\cdots/Z_N$ for an averaging over the anticommuting variables with the action (2.5), the particle density (2.3) is expressible in the fermionic format as follows

$$n(z,\bar{z}) = w(z,\bar{z})\sum_{j,k=0}^{\gamma(N-1)} \langle \Xi_j \Psi_k\rangle z^j \bar{z}^k. \tag{2.8}$$

Specific constraints for the fermionic correlators $\langle \Xi_j \Psi_k\rangle$ follow from the fermionic representation of the partition function as the results of certain transformations of anticommuting variables which maintain the composite nature of the action (2.5).

Let us first rescale by a constant one of the field components, say

$$\xi_j^{(1)} \to \mu\xi_j^{(1)}, \qquad j = 0,1,\ldots,N-1. \tag{2.9}$$

Jacobian of this transformation equals to μ^N and the fermionic action S transforms to μS. Consequently,

$$Z_N = \mu^{-N} \int \mathcal{D}\psi \mathcal{D}\xi \exp\left(\mu \sum_{j,k=0}^{\gamma(N-1)} \Xi_j w_{jk} \Psi_k\right). \tag{2.10}$$

Z_N is independent of μ and so its derivative with respect to μ is equal to zero for any value of μ. In the special case $\mu = 1$, the equality $\partial_\mu \ln Z_N|_{\mu=1} = 0$ implies the constraint

$$\sum_{j,k=0}^{\gamma(N-1)} w_{jk} \langle \Xi_j \Psi_k \rangle = N. \tag{2.11}$$

Let us now consider another linear transformation of *all* ξ-field components

$$\xi_j^{(\alpha)} \to \lambda^j \xi_j^{(\alpha)}, \quad j = 0, 1, \dots, N-1, \ \alpha = 1, \dots, \gamma. \tag{2.12}$$

Jacobian of this transformation equals to $\lambda^{\gamma N(N-1)/2}$ and the fermionic action S transforms to $\sum_{j,k=0}^{\gamma(N-1)} \lambda^j \Xi_j w_{jk} \Psi_k$. Consequently,

$$Z_N = \lambda^{-\gamma N(N-1)/2} \int \mathcal{D}\psi \mathcal{D}\xi \exp\left(\sum_{j,k=0}^{\gamma(N-1)} \lambda^j \Xi_j w_{jk} \Psi_k\right). \tag{2.13}$$

The equality $\partial_\lambda \ln Z_N|_{\lambda=1} = 0$ implies the following constraint

$$\sum_{j,k=0}^{\gamma(N-1)} j w_{jk} \langle \Xi_j \Psi_k \rangle = \frac{1}{2}\gamma N(N-1). \tag{2.14}$$

The application of the transformation (2.12) to all ψ-field components leads to the complementary condition

$$\sum_{j,k=0}^{\gamma(N-1)} k w_{jk} \langle \Xi_j \Psi_k \rangle = \frac{1}{2}\gamma N(N-1). \tag{2.15}$$

3 Derivation of Sum Rules

We study the jellium model confined to the domain of disc geometry $\Lambda = \{\mathbf{r}, r < R\}$, with the guest charge Zq fixed at the origin $\mathbf{0}$. The guest charge Zq together with the total charge Nq of N mobile particles are compensated by the fixed background of charge density $-nq$ via the overall neutrality condition

$$Z + N = \pi R^2 n. \tag{3.1}$$

The potential induced by the homogeneous background is $q\pi n r^2/2$, the guest charge interacts with jellium particles logarithmically $-Zq \ln r$. The total one-body potential acting on each particle

$$\phi(\mathbf{r}) = q^2 \frac{\pi n r^2}{2} - Zq^2 \ln r \tag{3.2}$$

possesses the circular symmetry.

At the coupling $\Gamma = 2\gamma$ ($\gamma = 1, 2, \ldots$), the one-body Boltzmann factor $w(\mathbf{r}) = \exp[-\beta\phi(\mathbf{r})]$ reads

$$w(\mathbf{r}) = r^{2\gamma Z} \exp(-\gamma\pi n r^2). \tag{3.3}$$

Within the fermionic representation of the jellium (2.4–2.8), the interaction matrix (2.7) becomes diagonal

$$w_{jk} = \delta_{jk} w_j, \quad w_j = \int_\Lambda \mathrm{d}^2 r\, r^{2(\gamma Z + j)} \exp(-\gamma\pi n r^2). \tag{3.4}$$

The consequent diagonalization of the action (2.5) in composite operators, $S = \sum_{j=0}^{\gamma(N-1)} \Xi_j w_j \Psi_j$, implies that $\langle \Xi_j \Psi_k \rangle = \delta_{jk} \langle \Xi_j \Psi_j \rangle$ and the representation of the particle density (2.8) simplifies to

$$n(\mathbf{r}|Zq, \mathbf{0}) = \mathrm{e}^{-\gamma\pi n r^2} \sum_{j=0}^{\gamma(N-1)} \langle \Xi_j \Psi_j \rangle r^{2(\gamma Z + j)}. \tag{3.5}$$

The constraint (2.11) is expressible as

$$\sum_{j=0}^{\gamma(N-1)} w_j \langle \Xi_j \Psi_j \rangle = N \tag{3.6}$$

and the couple of complementary conditions (2.14) and (2.15) reduces to

$$\sum_{j=0}^{\gamma(N-1)} j w_j \langle \Xi_j \Psi_j \rangle = \frac{1}{2}\gamma N(N-1). \tag{3.7}$$

Using the definition of the interaction integrals (3.4), it is easy to show that the constraint (3.6) is equivalent to the relation

$$\int_\Lambda \mathrm{d}^2 r\, n(r|Zq, \mathbf{0}) = N, \tag{3.8}$$

which reflects a trivial fact: the total number of mobile particles in the disc domain Λ is equal to N. With regard to the electroneutrality condition (3.1), the relation (3.8) can be rewritten in the form

$$\int_\Lambda \mathrm{d}^2 r\, \rho(r|Zq, \mathbf{0}) = -Zq. \tag{3.9}$$

By a simple analysis we shall argue that this condition involves in fact two sum rules, the bulk one and the surface one. Let us divide the disc domain Λ onto its "bulk" part $\Lambda_b = \{\mathbf{r}, r < R/2\}$ and the "surface" part $\Lambda_s = \{\mathbf{r}, r = R - x \text{ with } 0 \le x < R/2\}$ (x denotes the distance from the disc boundary) and rewrite (3.9) as follows

$$\int_0^{R/2} 2\pi r\, \mathrm{d}r\, \rho(r|Zq, \mathbf{0}) + \int_0^{R/2} 2\pi(R - x)\, \mathrm{d}x\, \rho(x|Zq, \mathbf{0}) = -Zq. \tag{3.10}$$

Let us assume that the system of charges has good screening properties, i.e. the decay of particle correlations at large distances r is faster than any inverse power law, say exponential

$\propto \exp(-\kappa r)$ with κ being the inverse correlation length (like it is in the weak-coupling limit $\Gamma \to 0$) or even Gaussian $\propto \exp[-(\kappa r)^2]$ (like it is at the free-fermion point $\Gamma = 2$). In the $R \to \infty$ limit, the particle density differs from the constant n only: in the bulk region close to the disc center $\mathbf{0}$ (up to $r \sim \kappa^{-1}$) and in the surface region close to the $x = 0$ boundary (up to $x \sim \kappa^{-1}$). The charge profile close to the boundary $\rho(x|Zq, \mathbf{0})$ is influenced by the screened guest charge Zq (exponentially or even Gaussianly) weakly as $R \to \infty$. Forgetting these small terms, one can put

$$\rho(x|Zq, \mathbf{0}) \sim \rho(x|0, \mathbf{0}) = \rho(x) + \frac{1}{R} f_1(x) + \frac{1}{R^2} f_2(x) + \cdots, \tag{3.11}$$

where the long-ranged inverse-power-law terms $1/R, 1/R^2, \ldots$ are due to the nonzero curvature of the disc surface and the respective coefficients $f_1, f_2, \ldots$ are short-ranged functions of the dimensionless parameter κx. Thus, (3.10) splits in the limit $R \to \infty$ into the Z-dependent bulk electroneutrality condition of present interest

$$\int \mathrm{d}^2 r \, \rho(r|Zq, \mathbf{0}) = -Zq \tag{3.12}$$

and a series of Z-independent surface conditions

$$\int_0^\infty 2\pi(R - x) \, \mathrm{d}x \, \rho(x|0, \mathbf{0}) = 0, \tag{3.13}$$

the lowest one of which takes the form of the surface electroneutrality

$$\int_0^\infty \mathrm{d}x \, \rho(x) = 0. \tag{3.14}$$

To make use of the constraint (3.7), we first differentiate both sides of the density representation (3.5) with respect to r, then multiply the result by r and finally integrate over the disc domain, to obtain

$$\begin{aligned} &\int_\Lambda \mathrm{d}^2 r \, r \frac{\partial}{\partial r} n(r|Zq, \mathbf{0}) \\ &\quad = 2\gamma Z N - 2\gamma \pi n \int_\Lambda \mathrm{d}^2 r \, r^2 n(r|Zq, \mathbf{0}) + 2 \sum_{j=0}^{\gamma(N-1)} j w_j \langle \Xi_j \Psi_j \rangle. \end{aligned} \tag{3.15}$$

The lhs of this relation can be integrated by parts, the summation on the rhs is given by the constraint of interest (3.7). After simple algebra, the relation (3.15) is transformed to

$$\begin{aligned} &-2\pi\gamma n \int_\Lambda \mathrm{d}^2 r \, r^2 \rho(r|Zq, \mathbf{0}) \\ &\quad = (2 - \gamma) Z q + \gamma Z^2 q + 2\pi R^2 \left[\rho(R|Zq, \mathbf{0}) + \frac{\gamma}{2} q n \right]. \end{aligned} \tag{3.16}$$

Like in the previous analysis of (3.9), we divide the disc domain Λ onto its bulk and surface parts to express the integral in (3.16) as follows:

$$\int_0^{R/2} 2\pi r^3 \, \mathrm{d}r \, \rho(r|Zq, \mathbf{0}) + \int_0^{R/2} 2\pi (R - x)^3 \, \mathrm{d}x \, \rho(x|Zq, \mathbf{0}). \tag{3.17}$$

Under the assumption of good screening properties of the jellium, the bulk and surface regions are coupled weakly in the $R \to \infty$ limit and one can consider once more the expansion (3.11) for the boundary charge density. In this way, one gets from (3.16) the Z-dependent bulk condition

$$\int \mathrm{d}^2 r\, r^2 \rho(r|Zq, \mathbf{0}) = -\frac{1}{2\pi\gamma n} Zq[(2-\gamma) + \gamma Z], \tag{3.18}$$

which is equivalent after the substitution $\gamma = \Gamma/2$ to the one of primary importance (1.21), and a series of Z-independent surface conditions

$$-2\pi\gamma n \int_0^\infty 2\pi (R-x)^3\, \mathrm{d}x\, \rho(x|0, \mathbf{0}) = 2\pi R^2 \left[\rho(x=0|0, \mathbf{0}) + \frac{\gamma}{2} qn \right]. \tag{3.19}$$

The lowest-order surface condition can be obtained by summing (3.13), multiplied by $2\pi\gamma n R^2$, with (3.19). The final result reads

$$\rho(x=0) = -\frac{\gamma}{2} qn + 4\pi\gamma n \int_0^\infty \mathrm{d}x\, x\rho(x). \tag{3.20}$$

This relation is known as the contact theorem [19–21]. Although all relations were derived for $\gamma = \Gamma/2$ a positive integer, it is reasonable to extend their validity to all values of Γ corresponding to the fluid regime.

As was mentioned in the introduction, the generalized second-moment sum rule (1.21) is consistent with the available results (1.18) for $Z = 1$ and (1.19) for the trivial case $Z = 0$. In the next two sections, we test this sum rule also in the weak-coupling $\Gamma \to 0$ limit (Sect. 4) and at the free-fermion point $\Gamma = 2$ (Sect. 5).

In contrast to the zeroth-moment electroneutrality condition (3.12), the generalized second-moment sum rule (3.18), or equivalently (1.21), provides an exact information about possible sign oscillations of the induced charge density $\rho(r|Zq, \mathbf{0})$ in space. If $Z > 0$, the guest particle and jellium charges repeal each other and therefore $\rho(r|Zq, \mathbf{0}) \sim -qn$ as $r \to 0$. Provided that $\rho(r|Zq, \mathbf{0})$ does not change the sign when changing r from 0 to ∞ (where ρ vanishes), its second moment has the sign opposite to Zq. Similarly, if $Z < 0$, there is an attraction between the guest particle and jellium charges, so that $\rho(r|Zq, \mathbf{0})$ goes to infinity as $r \to 0$. Consequently, when $\rho(r|Zq, \mathbf{0})$ does not change the sign when going from $r = 0$ to $r \to \infty$, its second moment has again the sign opposite to Zq. The *sufficient* condition for sign oscillations of the charge density $\rho(r|Zq, \mathbf{0})$ in space is that its second-moment has the sign of Zq. In view of the result (1.21), the sufficient condition for oscillations is that the guest-charge parameter Z lies in the interval

$$-\frac{2}{\Gamma} < Z < 1 - \frac{4}{\Gamma}, \tag{3.21}$$

where the lower bound, see (1.15), ensures the thermodynamic stability of the pointlike guest charge Zq. The inequalities (3.21) have no solution for $\Gamma \le 2$. For $\Gamma > 4$, there exists also an interval of *positive* values of Z for which the induced charge density certainly exhibits sign oscillations.

4 Weak-Coupling Limit

The effective potential ϕ at distance r from the guest charge Zq, placed at the origin $\mathbf{0}$ and surrounded by mobile q-charges of the average density $n(\mathbf{r}|Zq, \mathbf{0})$ plus the neutralizing background of charge density $-qn$, is given by the 2D Poisson equation

$$\Delta\phi(\mathbf{r}) = -2\pi q\{Z\delta(\mathbf{r}) + [n(\mathbf{r}|Zq,\mathbf{0}) - n]\}. \tag{4.1}$$

The weak-coupling (high-temperature) region $\Gamma \to 0$ is described rigorously by the Debye–Hückel theory [4, 22]. Within this mean-field approach, the average particle density at a given point is approximated by replacing the potential of mean force by the average electrostatic potential at that point, $n(\mathbf{r}|Zq,\mathbf{0}) = n\exp[-\beta q\phi(\mathbf{r})]$. The mean-field Boltzmann factor can be linearized at high temperatures, $\exp[-\beta q\phi(\mathbf{r})] \sim 1 - \beta q\phi(\mathbf{r})$. The Poisson equation (4.1) then reads

$$(\Delta - \kappa^2)\phi(\mathbf{r}) = -2\pi Zq\delta(\mathbf{r}), \tag{4.2}$$

where $\kappa = \sqrt{2\pi\Gamma n}$ is the inverse Debye length.

Due to the circular symmetry of the problem, $\Delta = \partial_r^2 + (1/r)\partial_r$. Equation (4.2), subject to the condition of regularity at $r \to \infty$, thus implies

$$\phi(\mathbf{r}) = ZqK_0(\kappa r), \tag{4.3}$$

where K_0 is a modified Bessel function [23].

The induced charge density around the guest charge Zq is obtained in the form

$$\rho(\mathbf{r}|Zq,\mathbf{0}) = -Zqn\Gamma K_0(\kappa r). \tag{4.4}$$

Since the stability lower bound (1.15) is $Z > -\infty$ in the limit $\Gamma \to 0$, this result applies to all real values of Z. The charge density (4.4) is always a monotonic function of the distance r which keeps its plus ($Zq < 0$) or minus ($Zq > 0$) sign in the whole interval of $r \in (0,\infty)$. Its moments $I_j = \int_0^\infty 2\pi r\,\mathrm{d}r\, r^{2j}\rho(r|Zq,\mathbf{0})$ $(j = 0, 1, \ldots)$ are given by

$$I_j = -Zq\kappa^2\int_0^\infty \mathrm{d}r\, r^{2j+1}K_0(\kappa r) = -Zq\left(\frac{2}{\kappa}\right)^{2j}[\Gamma(1+j)]^2, \tag{4.5}$$

where $\Gamma(x)$ denotes the Gamma function. For $j = 0$, the electroneutrality condition (1.20) takes place. For $j = 1$, one arrives at the second-moment formula (1.22) which is in full agreement with the general result (1.21) taken in the weak-coupling limit $\Gamma \to 0$.

5 The Free-Fermion Point

The fermionic representation of the 2D jellium simplifies substantially for the coupling constant $\Gamma = 2$ ($\gamma = 1$), because the composite variables (2.6) become the ordinary anticommuting ones. Having the fermionic action of the form $S = \sum_{j=0}^{N-1}\xi_j w_j \psi_j$ it is easy to show that

$$Z_N = \prod_{j=0}^{N-1} w_j, \tag{5.1}$$

$$\langle \xi_j\psi_j\rangle = \frac{1}{w_j}, \quad j = 0, 1, \ldots, N-1. \tag{5.2}$$

In the limit of the infinite disc radius $R \to \infty$, the interaction strength (3.4) at $\gamma = 1$ is given by

$$w_j = \frac{1}{n} \frac{1}{(\pi n)^{Z+j}} \Gamma(Z + j + 1). \tag{5.3}$$

For an infinite number of jellium particles $N \to \infty$, the particle density (3.5) induced by the guest charge Zq reads

$$\frac{n(r|Zq, \mathbf{0})}{n} = f_Z(\pi n r^2), \quad f_Z(t) = \mathrm{e}^{-t} \sum_{j=0}^{\infty} \frac{t^{Z+j}}{\Gamma(Z + j + 1)}. \tag{5.4}$$

The same formula was derived previously by Jancovici [24]. The induced density (5.4) is well defined for $Z > -1$, and this is indeed the range of the guest-charge stability (1.15) for the coupling constant $\Gamma = 2$.

Let us first treat the region of $Z > 0$ ($q > 0$ will be considered for simplicity). We shall need the incomplete Gamma function which is defined as follows [23]:

$$\Gamma(Z, t) = \int_t^{\infty} \mathrm{d}s \, s^{Z-1} \mathrm{e}^{-s} = \Gamma(Z) - \int_0^t \mathrm{d}s \, s^{Z-1} \mathrm{e}^{-s}, \quad Z > 0. \tag{5.5}$$

It can be readily shown by applying a series of integrations by parts that

$$\Gamma(Z, t) = \Gamma(Z) - \Gamma(Z) \mathrm{e}^{-t} \sum_{j=0}^{\infty} \frac{t^{Z+j}}{\Gamma(Z + j + 1)}. \tag{5.6}$$

The function $f_Z(t)$, defined in (5.4), is therefore expressible as

$$f_Z(t) = 1 - \frac{\Gamma(Z, t)}{\Gamma(Z)} \tag{5.7}$$

and the induced charge density reads

$$\rho(r|Zq, \mathbf{0}) = -qn \frac{\Gamma(Z, \pi n r^2)}{\Gamma(Z)}, \quad Z > 0. \tag{5.8}$$

Since $\partial_t \Gamma(Z, t) = -t^{Z-1} \mathrm{e}^{-t}$, the derivative $\partial_r \rho(r|Zq, \mathbf{0})$ is positive for any value of r. Consequently, the induced charge density is the monotonically increasing function of r, going from $-qn$ at $r = 0$ to 0 at $r \to \infty$. The moments of the charge cloud around the guest particle $I_j = \int_0^{\infty} 2\pi r \, \mathrm{d}r \, r^{2j} \rho(r|Zq, \mathbf{0})$ ($j = 0, 1, \ldots$) are given by

$$I_j = -2\pi q n \int_0^{\infty} \mathrm{d}r \, r^{2j+1} \frac{\Gamma(Z, \pi n r^2)}{\Gamma(Z)} = -\frac{q}{(j+1)(\pi n)^j} \frac{\Gamma(Z + j + 1)}{\Gamma(Z)}, \tag{5.9}$$

where we have applied an integration by parts. For $j = 0$, one recovers the electroneutrality sum rule (1.20). For $j = 1$, one gets the result (1.23) which is in full agreement with the general result (1.21) taken at $\Gamma = 2$.

As concerns the stability region of negative Z-values $-1 < Z < 0$, we first write down a recursion relation for $f_Z(t)$ following from the definition (5.4):

$$f_Z(t) = \mathrm{e}^{-t} \frac{t^Z}{\Gamma(Z + 1)} + f_{Z+1}(t). \tag{5.10}$$

Thus,

$$\rho(r|Zq,\mathbf{0}) = qn\left[\mathrm{e}^{-\pi nr^2}\frac{(\pi nr^2)^Z}{\Gamma(Z+1)} - \frac{\Gamma(Z+1,\pi nr^2)}{\Gamma(Z+1)}\right], \quad Z > -1. \tag{5.11}$$

The induced charge density is now the monotonically decreasing function of r, going from ∞ at $r = 0$ to 0 at $r \to \infty$. It is easy to verify that the formula for its even moments coincides with the previous one (5.9). This fact permits one to extend the validity of the zeroth-moment (1.20) and second-moment (1.23) sum rules to the region of negative Z-values $-1 < Z < 0$.

6 Conclusion

In this paper, we have generalized the standard zeroth- and second-moment Stillinger–Lovett sum rules for the charge correlation functions to the presence of a guest charge immersed in the bulk interior of the 2D jellium. The derivation procedure was based on the fermionic technique which is associated specifically with the 2D jellium model.

The one-component jellium of mobile q-charges with a guest charge Zq may be seen as the limit of a "two-component" jellium with two types of charges q and Zq, where the number density of charges Zq tends to zero. Such model has been studied in [24] within the theory of solutions of McMillan and Mayer; the density of particles of charge Zq was considered to be small, and used as an expansion parameter for the free energy, the pair distribution functions, etc., of the mixture. There exists a second-moment partial sum rule for each component of the two-component jellium, see formula (5.4) in [25]. However, these sum rules hold only for specific densities of the two components which globally minimize the free energy; as an evidence of this fact, the sum rule contains the derivatives of the particle densities with respect to the background charge. This is why we were not able to accomplish in this way an alternative proof of the new sum rules for one guest charge in the jellium.

It is an open question whether the generalization of the standard sum rules can be accomplished also in higher dimensions or for many-component Coulomb fluids. The present results might inspire specialists to establish some new phenomenological arguments which go beyond the standard ones.

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