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A Mean Spherical Model with Coulomb Interactions. II. Correlations at a Free Surface

E. R. Smith[1]

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Studies of the mean spherical model with Coulomb interactions are continued, by considering a system on a d-dimensional lattice which is periodic in $d-1$ dimensions and has a free surface in the remaining dimension. It is shown explicitly that correlations along the free surface decay as y^{-d} in d dimensions and show that the surface properties of this model are those expected for a charged system in its plasma phase.

KEY WORDS: Spherical model; Coulombic systems; correlation function decay; surface properties.

1. INTRODUCTION

While many new results have been obtained recently about the structure of correlation functions in the plasma phase of charged systems, there are few examples which can be worked out explicitly. The recent review of Martin[1] summarizes many of these global sum rules and provides a comprehensive list of references, including many papers on the two-dimensional, one-component plasma. This model has provided exact results which illustrate the general theory. Other examples which illustrate some of the properties of Coulombic systems are one dimensional,[2-7] and are flawed as examples of the general theory of plasma states because the two-component, one-dimensional Coulombic system has no plasma phase.[3,4,7]

In the first paper of this series[8] (hereafter referred to as I), I introduced a mean spherical model on a lattice with Coulombic interactions. I considered a d-dimensional lattice

$$\Lambda = [-M, M]^{\otimes(d-1)} \otimes [1, N]$$

[1] Mathematics Department, La Trobe University, Bundoora, Victoria, Australia 3083.

with a real-valued charge $q(\mathbf{n})$ at each lattice site $\mathbf{n}$. The electric potential $\Phi(\mathbf{n}, \mathbf{n}'; X)$ at a site $\mathbf{n}$ on the lattice due to a unit charge at $\mathbf{n}'$ in boundary conditions X is the solution of the d-dimensional Poisson equation

$$D_{\mathbf{n}}^2 \Phi(\mathbf{n}, \mathbf{n}'; X) = -\omega_d \delta_{\mathbf{n},\mathbf{n}'} \tag{1}$$

on the lattice Λ with boundary conditions X applied. In Eq. (1), ω_d is the surface area of a d-dimensional sphere of unit radius. The energy of a configuration $\{q(\mathbf{n}), \mathbf{n} \in \Lambda\}$ is then

$$W(\{q(\mathbf{n})\}) = \frac{1}{2} \sum_{\mathbf{n} \in \Lambda} \sum_{\mathbf{n}' \in \Lambda} q(\mathbf{n})\, \Phi(\mathbf{n}, \mathbf{n}'; X) \tag{2}$$

The charge variables $q(\mathbf{n})$ are real numbers and the partition function is evaluated subject to the mean spherical constraint

$$\left\langle \sum_{\mathbf{n} \in \Lambda} q^2(\mathbf{n}) \right\rangle = \|\Lambda\|\, Q^2 \tag{3}$$

where Q is an elementary charge magnitude and $\|\Lambda\|$ is the number of lattice sites in Λ.

In I, this model was solved exactly for two cases:

1. $2M + 1 = N$ and X a Neumann boundary condition on Λ.
2. Boundary conditions X periodic in each of the directions in which Λ spans $2M + 1$ sites, and a Dirichlet condition at either end of the lattice in the other direction.

To summarize the results of I, one may consider bulk and surface (or finite system) results.

1.2. Bulk Results

1. The bulk interior of the system is in a plasma phase at small enough coupling $\Gamma = \beta Q^2$. For $d \geqslant 3$ there is a critical coupling $\Gamma = \Gamma_c$. For $\Gamma > \Gamma_c$ the system is in a nonplasma phase in which charges oscillate in sign across the lattice. The critical behavior of the transition at $\Gamma = \Gamma_c$ is typical of a mean spherical model.

2. In the plasma bulk phase, charges are screened. There is a critical coupling $\Gamma = \Gamma_0(d) = 2d/\omega_d$. For $\Gamma < \Gamma_0(d)$, the two-charge correlation function decays monotonically with a correlation length which decreases as Γ increases. When $\Gamma = \Gamma_0(d)$ the two-charge correlation function has range of exactly one lattice spacing. For $\Gamma > \Gamma_0(d)$ the two-charge correlation function oscillates in sign while decaying with an exponential envelope, the

correlation length increasing with increasing Γ. The Stillinger–Lovett sum rules for the thermodynamic limit of the correlation functions hold. There is no thermodynamic singularity at $\Gamma = \Gamma_0(d)$.

Thus, the bulk of the system behaves as a Coulombic system may be expected to behave.

1.2. Surface and Finite System Results

1. The mean square dipole moment of the finite system obeys the expected altered forms in the different boundary conditions of the second Stillinger–Lovett sum rule.

2. The mean square charge on a site close to a surface of the system is not Q^2. In an applied field the value of $\langle q(\mathbf{n}) \rangle$ relaxes to zero exponentially fast as $\mathbf{n}$ moves into the bulk of the system and the decay length for this relaxation is the correlation length of the bulk phase [but see the note in this paper after Eq. (37b)].

3. Correlations along the Neumann or Dirichlet condition surfaces of the system decay exponentially fast.

These results are to be expected, but the large values of $\langle q(\mathbf{n}) \rangle$ and $\langle q^2(\mathbf{n}) \rangle$ which may be obtained for $\mathbf{n}$ close to a surface force one to consider whether the mean spherical constraint interferes significantly with the Coulombic nature of the system.

This paper considers a mean spherical model with a free surface and shows that correlation functions along the surface can decay as y^{-d}, where y is the projection onto the surface of the displacement between the two correlating charges. This finally establishes the charged mean spherical model as a proper Coulombic system, so that one may assume that much of the qualitative information one can find about it generalizes to other Coulombic systems.

In the next section I introduce the lattice with a free surface, solve for Φ in the boundary conditions used, and calculate the partition function, constraint equation, and correlation functions for the system in its plasma phase. In Section 3 I analyze charge–charge correlations along the free surface, and conclude with a discussion of these results in Section 4.

2. THE MODEL AND ITS EXACT SOLUTION

Consider a lattice $\Lambda_d = [0, N] \otimes [-M, M]^{\otimes d-1}$. Impose the boundary condition on $\Phi(\mathbf{n}, \mathbf{n}'; DF)$ that at $\mathbf{n} = (n, \mathbf{v})$, with $n = 0$, $\Phi((0, \mathbf{v}), \mathbf{n}'; DF) = 0$, that is, a Dirichlet condition. We have a free space condition for $n > N$. The potential is periodic with period $(2M+1)$ in each of the components of $\mathbf{v}$ and $\mathbf{v}'$. The potential is then

$$\Phi(\mathbf{n}, \mathbf{n}'; DF) = \frac{\omega_d}{2\pi} \sum_{\mathbf{K} \in L_d} (2M+1)^{-(d-1)} \exp \frac{2\pi i \mathbf{K} \cdot (\mathbf{v} - \mathbf{v}')}{2M+1} \times \int_{-\pi}^{\pi} dk \frac{\exp[ik(n-n')] - \exp[ik(n+n')]}{2(\cosh \omega(\mathbf{K}) - \cos k)} \tag{4}$$

Here L_d is the $(d-1)$-dimensional lattice $[-M, M]$, and $\omega(\mathbf{K})$ is given by

$$\cosh \omega(\mathbf{K}) = 1 + \sum_{\alpha=2}^{d} \left(1 - \cos \frac{2\pi K_\alpha}{2M+1}\right) \tag{5}$$

Note that $\omega(\mathbf{K}) \to 0$ as $\mathbf{K} \to \mathbf{0}$ and that for small $\mathbf{K}$, $\omega(\mathbf{K}) = 2\pi |\mathbf{K}|/(2M+1) + O(\mathbf{K}^2)$. This potential is periodic with period $2M+1$ in each of the components of $\mathbf{v}$ and $\mathbf{v}'$ and solves Eq. (1). Further, it is zero by inspection when $n = 0$, and as $n \to \infty$ this potential behaves as $\omega_d n'/(2M+1)^{d-1} + O(n^{-1})$, which is appropriate for such a potential. The partition function for the system is then, with $\Gamma = \beta Q^2$,

$$Z(\Gamma, \Lambda_d) = \left\{ \prod_{\mathbf{n} \in \Lambda_d} \int_{-\infty}^{\infty} dq(\mathbf{n}) \right\} \times \exp \left\{ -\frac{1}{2} \beta \sum_{\mathbf{n} \in \Lambda_d} \sum_{\mathbf{n}' \in \Lambda_d} q(\mathbf{n})\, \Phi(\mathbf{n}, \mathbf{n}'; DF)\, q(\mathbf{n}') - \beta\lambda \left[\sum_{\mathbf{n} \in \Lambda_d} q^2(\mathbf{n}) - Q^2 \|\Lambda_d\| \right] \right\} \tag{6}$$

where $\|\Lambda_d\| = (2M+1)^{d-1} N$. The matrix $\Phi(\mathbf{n}, \mathbf{n}'; DF)$ is Hermitian. Its eigenvalue equation can be written in the form

$$\sum_{\mathbf{n}' \in \Lambda_d} \Phi(\mathbf{n}, \mathbf{n}'; DF)\, \Psi(\mathbf{n}'; \mathbf{K}, l) = \mu(\mathbf{K}, l)\, \Psi(\mathbf{n}; \mathbf{K}, l) \tag{7}$$

with

$$\Psi(\mathbf{n}; \mathbf{K}, l) = (2M+1)^{-(d-1)/2} \exp[2\pi i \mathbf{K} \cdot \mathbf{v}/(2M+1)]\, \psi(n; \mathbf{K}, l) \tag{8}$$

The $\psi(n; \mathbf{K}, l)$ are then the normalized eigenfunctions of

$$\frac{\omega_d}{2\pi} \sum_{n'=0}^{N} \int_{-\pi}^{\pi} dk \frac{e^{ik(n-n')} - e^{ik(n+n')}}{2(\cosh \omega(\mathbf{K}) - \cos k)} \psi(n'; \mathbf{K}, l) = \mu(\mathbf{K}, l)\, \psi(n; \mathbf{K}, l) \tag{9}$$

Some manipulation then gives

$$\psi(n+1; \mathbf{K}, l) - 2\left\{\cosh[\omega(\mathbf{K})] - \frac{\omega_d}{2\mu(\mathbf{K}, l)}\right\} \psi(n; \mathbf{K}, l) + \psi(n-1; \mathbf{K}, l) \quad (10)$$

on $1 \leqslant n \leqslant N-1$ with $\psi(0; \mathbf{K}, l) = 0$ and Eq. (9) with $n = N$ as the eigenvalue equation. The solutions to (10) are of the form

$$\psi(n; \mathbf{K}, l) = A(\mathbf{K}, l) \sin[n\theta(\mathbf{K}, l)] \quad (11)$$

with

$$\mu(\mathbf{K}, l) = \tfrac{1}{2}\omega_d[\cosh \omega(\mathbf{K}) - \cos \theta(\mathbf{K}, l)]^{-1} \quad (12)$$

and the $\vartheta(\mathbf{K}, l)$ $(1 \leqslant l \leqslant N)$ are the N solutions on $(0, \pi)$ of

$$F_N(\theta) = \cot(N\theta) - \frac{e^{\omega(\mathbf{K})} - \cos \theta}{\sin \theta} = 0 \quad (13)$$

This gives precisely the correct number of eigenvalues. The normalization constants $A(\mathbf{K}, l)$ are given by

$$\sum_{l=1}^{N} \psi^2(n; \mathbf{K}, l) = 1 \quad (14)$$

This normalization is fairly messy, but I note here that if one works it out it gives

$$F'_N[\theta(\mathbf{K}, l)]\, \psi(n; \mathbf{K}, l)\, \psi(n'; \mathbf{K}, l) = \frac{-2 \sin[n\theta(\mathbf{K}, l)] \sin[n'\theta(\mathbf{K}, l)]}{\sin^2[N\theta(\mathbf{K}, l)]} \quad (15)$$

a result that will be useful below.

A unitary transformation of the $q(\mathbf{n})$ to

$$\hat{q}(\mathbf{K}, l) = \sum_{\mathbf{K} \in L_d} \sum_{n=1}^{N} q(\mathbf{n})\, \Psi^*(\mathbf{n}; \mathbf{K}, l) \quad (16)$$

then allows the integrals in the partition function and the correlation functions to be performed simply as Gaussian integrals. We obtain

$$Z(\Gamma, \Lambda_d) = e^{\lambda\Gamma \|\Lambda_d\|} \prod_{\mathbf{K} \in L_d} \prod_{l=1}^{N} \left[\frac{\pi}{\beta[\lambda + \frac{1}{2}\mu(\mathbf{K}, l)]}\right]^{1/2} \quad (17)$$

and

$$\frac{\langle q(\mathbf{n})\, q(\mathbf{n}')\rangle}{Q^2} = \frac{1}{2\Gamma} \sum_{\mathbf{K} \in L_d} \sum_{l=1}^{N} \frac{\Psi(\mathbf{n}; \mathbf{K}, l)\, \Psi^*(\mathbf{n}'; \mathbf{K}, l)}{\lambda + \frac{1}{2}\mu(\mathbf{K}, l)} \quad (18)$$

The mean spherical constraint then gives, by differentiating $\log Z$ with respect to λ,

$$2\Gamma = \sum_{\mathbf{K}\in L_d} \sum_{l=1}^{N} \frac{1}{\lambda + \frac{1}{2}\mu(\mathbf{K}, l)} \|\Lambda_d\|^{-1} \tag{19}$$

The existence of the partition function requires $\lambda > -\frac{1}{2}\mu(\mathbf{K}, l)$, $\forall \mathbf{K} \in L_d$, and $1 \leqslant l \leqslant N$, so that we require $\lambda > -\omega_d/8d$. The value $\Gamma_c(d)$ of Γ which gives the solution $\lambda = -\omega_d/8d$ to Eq. (19) then gives the critical point of the transition for $d \geqslant 3$. There is no such solution for $d = 1, 2$. Note that the value $\lambda = 0$ is allowed. This gives $\Gamma_0(d) = 2d/\omega_d$. At $\Gamma = \Gamma_0(d)$ the bulk correlations have a range of exactly one lattice spacing, $\langle q(\mathbf{n})\, q(\mathbf{n}')\rangle$ being zero in the bulk interior of the system if $\mathbf{n} \neq \mathbf{n}'$ and $\mathbf{n}$ and $\mathbf{n}'$ are not nearest neighbors on the lattice. The correlation functions in the bulk interior of the system are the same as those found with other boundary conditions in I.

We may write the sum over l in (19) as a contour integral using the nernel $F_N'(\theta)/F_N(\theta)$. The contour must exclude the poles of this kernel at $\theta = \theta_k = k\pi/N$, where the residue of this kernel is -1. The resulting contour integrals and sums may then be written using the contour shift $C_1 \to C_2$ described in I. There are two cases:

(i) $\lambda > 0$: we define $y_0(\mathbf{K})$ by

$$y_0(\mathbf{K}) = \frac{\omega_d}{4\lambda} + \cosh \omega(\mathbf{K})$$

(ii) $\lambda < 0$: we define $Y_0(\mathbf{K})$ by

$$\cosh Y_0(\mathbf{K}) = -\frac{\omega_d}{4\lambda} - \cosh \omega(\mathbf{K})$$

We obtain, for $\lambda > 0$,

$$2\Gamma = \frac{1}{\lambda} - \frac{\omega_d}{4\lambda^2}(2M+1)^{-(d-1)} \times \sum_{\mathbf{K}\in L_d} \left[\frac{1}{\sinh y_0(\mathbf{K})}\left(1 + \frac{2e^{-2Ny_0(\mathbf{K})}}{1 - e^{-2Ny_0(\mathbf{K})}}\right) - \frac{1}{N} g_+(\mathbf{K})\right] \tag{20a}$$

and for $\lambda < 0$,

$$2\Gamma = \frac{1}{\lambda} + \frac{\omega_d}{4\lambda^2}(2M+1)^{-(d-1)} \times \sum_{\mathbf{K}\in L_d} \frac{1}{\sinh Y_0(\mathbf{K})}\left(1 + \frac{2e^{-2NY_0(\mathbf{K})}}{1 - e^{-2NY_0(\mathbf{K})}}\right) + \frac{1}{N} g_-(\mathbf{K}) \tag{20b}$$

where

$$g_+(\mathbf{K})=\frac{e^{-\omega(\mathbf{K})}\cosh y_0(\mathbf{K})+1+N\sinh^2[y_0(\mathbf{K})]/\sinh^2[Ny_0(\mathbf{K})]}{\sinh^2 y_0(\mathbf{K})\{e^{-\omega(\mathbf{K})}+\cosh y_0(\mathbf{K})+\sinh y_0(\mathbf{K})\coth[Ny_0(\mathbf{K})]\}} \tag{21}$$

where $g_-(\mathbf{K})$ is the same as $g_+(\mathbf{K})$ but with $Y_0(\mathbf{K})$ replacing $y_0(\mathbf{K})$. As $N\to\infty$ and then $M\to\infty$, we find, for $\lambda>0$,

$$2\Gamma=\frac{1}{\lambda}-\frac{\omega_d}{4\lambda^2}(2\pi)^{-(d-1)}\int_{[-\pi,\pi]^{d-1}} d^{d-1}\mathbf{K}\,\frac{1}{\sinh y_0(\mathbf{K})} \tag{22a}$$

and for $\lambda<0$,

$$2\Gamma=\frac{1}{\lambda}+\frac{\omega_d}{4\lambda^2}(2\pi)^{-(d-1)}\int_{[-\pi,\pi]^{d-1}} d^{d-1}\mathbf{K}\,\frac{1}{\sinh Y_0(\mathbf{K})} \tag{22b}$$

where

$$\cosh y_0(\mathbf{K})=\frac{\omega_d}{4\lambda}+1+\sum_{\alpha=2}^{d}(1-\cos K_\alpha) \tag{23a}$$

and

$$\cosh Y_0(\mathbf{K})=\frac{\omega_d}{4\,|\lambda|}+1+\sum_{\alpha=2}^{d}(1-\cos K_\alpha) \tag{23b}$$

We may take the limit $\lambda\to 0+$ of (22a) or $\lambda\to 0-$ of (22b) and in both cases find $\Gamma_0(d)=2d/\omega_d$ for $\lambda=0$, a result known from I.

3. CHARGE–CHARGE CORRELATION FUNCTIONS

We consider here the charge–charge correlation function $P(n,n';\mathbf{v})$ given by

$$P(n,n';\mathbf{v})=\langle q(n,\mathbf{0})\,q(n',\mathbf{v})\rangle/Q^2 \tag{24}$$

which may be written using Eq. (12) in (18),

$$P(n,n';\mathbf{v})=\frac{1}{2\Gamma\lambda}\delta_{n,n'}\delta_{\mathbf{v},\mathbf{0}}-\frac{\omega_d}{8\Gamma\lambda^2}(2M+1)^{-(d-1)} \times\sum_{\mathbf{K}\in L_d} e^{2\pi i\mathbf{v}\cdot\mathbf{K}/(2M+1)}G(n,n';\mathbf{K}) \tag{25}$$

where

$$G(n, n'; \mathbf{K}) = \sum_{l=1}^{N} \frac{\psi(n; \mathbf{K}, l)\,\psi(n'; \mathbf{K}, l)}{\omega_d/4\lambda + \cosh\omega(\mathbf{K}) - \cos\theta(\mathbf{K}, l)} \tag{26}$$

In fact, we want

$$p(n, n'; \mathbf{v}) = \lim_{N\to\infty}\lim_{M\to\infty} P(N-n, N-n'; \mathbf{v}) \tag{27}$$

We want to study p for n, n' large, to give the correlation functions in the bulk interior of the system, and for n, n' finite, to give surface correlations.

First, we must evaluate G. We may use Eq. (15) to write

$$\begin{aligned} G(n, n'; \mathbf{K}) = &-\frac{1}{2\pi i}\oint_{C_1} \frac{\sin(n\theta)\sin(n'\theta)}{F_N(\theta)\sin^2(N\theta)[\omega_d/4\lambda + \cosh\omega(\mathbf{K}) - \cos\theta]}\,d\theta \\ &+ \frac{1}{2\pi i}\sum_{k=-(N-1)}^{N} \\ &\times \oint_{C_\varepsilon(k)} \frac{\sin(n\theta)\sin(n'\theta)}{F_N(\theta)\sin^2(N\theta)[\omega_d/4\lambda + \cosh\omega(\mathbf{K}) - \cos\theta]}\,d\theta \end{aligned} \tag{28}$$

where $C_\varepsilon(k)$ is a small anticlockwise contour of radius ε about $\theta_k = k\pi/N$, the radius ε being chosen small enough that no other singularity of the integrand than that at θ_k occurs within the contour. The contour C_1 is that defined in I. The sum over integrals round the $C_\varepsilon(k)$ may be evaluated fairly simply to give

$$\begin{aligned} J(\mathbf{K}) &= \frac{1}{2\pi i}\sum_{k=-(N-1)}^{N}\oint_{C_\varepsilon(k)} \frac{\sin(n\theta)\sin(n'\theta)}{F_N(\theta)\sin^2 N\theta[\omega_d/4\lambda + \cosh\omega(\mathbf{K}) - \cos\theta]}\,d\theta \\ &= H(\mathbf{K}, n-n') + H(\mathbf{K}, n'-n) - H(\mathbf{K}, n+n') - H(\mathbf{K}, -n-n') \end{aligned} \tag{29}$$

where

$$H(\mathbf{K}, n) = \frac{1}{4N}\sum_{k=-(N-1)}^{N} \frac{e^{in\theta_k}}{\omega_d/4\lambda + \cosh\omega(\mathbf{K}) - \cos\theta_k} \tag{30}$$

We may write this sum as a contour integral round C_1 using the kernal $G_{N+}(\theta) = 2iN/(e^{2iN\theta} - 1)$ if $0 \leqslant n \leqslant 2N$ and $G_{N-}(\theta) = -2iN/(e^{-2iN\theta} - 1)$ if $-2N \leqslant n \leqslant 0$. We may then transform the contour C_1 to C_2, also given in I, and evaluate $H(\mathbf{K}, n)$ in terms of poles at $\cos\theta = \omega_d/4\lambda + \cosh\omega(\mathbf{K})$.

We obtain, for $\lambda > 0$,

$$H(\mathbf{K}, n) = \frac{1}{2\sinh y_0(\mathbf{K})}\,\frac{e^{-|n|\,y_0(\mathbf{K})} + e^{-(2N-|n|)\,y_0(\mathbf{K})}}{1 - e^{-2Ny_0(\mathbf{K})}} \tag{31a}$$

and for $\lambda < 0$,

$$H(\mathbf{K}, n) = -\frac{(-1)^n}{2\sinh Y_0(\mathbf{K})} \frac{e^{-|n|\,Y_0(\mathbf{K})} + e^{-(2N-|n|)\,Y_0(\mathbf{K})}}{1 - e^{-2NY_0(\mathbf{K})}} \tag{31b}$$

The integral in Eq. (28) may be written as

$$K(n-n') + K(n'-n) - K(n'+n) - K(-n-n')$$

where

$$K(n) = -\frac{1}{8\pi i} \oint_{C_1} \frac{e^{in\theta}}{F_N(\theta)\sin^2(N\theta)[\omega_d/4\lambda + \cosh\omega(\mathbf{K}) - \cos\theta]}\, d\theta \tag{32}$$

This expression for $K(n)$ may be written using the contour C_2 and then evaluated. The results are, for $\lambda > 0$,

$$K(n) = -\frac{e^{-(2N-n)\,y_0(\mathbf{K})} + e^{-(2N+n)\,y_0(\mathbf{K})}}{e^{y_0(\mathbf{K})} - e^{-\omega(\mathbf{K})}} (1 + A_+(N, y_0(\mathbf{K}), \omega(\mathbf{K}))) \tag{33a}$$

and for $\lambda < 0$,

$$K(n) = (-1)^n \frac{e^{-(2N-n)\,Y_0(\mathbf{K})} + e^{-(2N+n)\,Y_0(\mathbf{K})}}{e^{Y_0(\mathbf{K})} + e^{-\omega(\mathbf{K})}} (1 + A_-(N, Y_0(\mathbf{K}), \omega(\mathbf{K}))) \tag{33b}$$

Here

$$A_+(N, y, \omega) = \left(1 + \frac{2\sinh(y)\, e^{-2Ny}}{(e^y - e^{-\omega})(1 - e^{-2Ny})}\right)(1 - e^{-2Ny})^2 - 1 \tag{34a}$$

and

$$A_-(N, Y, \omega) = \left(1 + \frac{2\sinh Y_0 e^{-2NY}}{(e^Y + e^{-\omega})(1 - e^{-2NY})}\right)(1 - e^{-2NY})^2 - 1 \tag{34b}$$

We are now able to construct $G(N-n, N-n'; \mathbf{K})$ in the limit $n \to \infty$ to obtain $p(n, n'; \mathbf{v})$. When we put all the terms together we obtain, for $\lambda > 0$,

$$\begin{aligned} p(n, n'; \mathbf{v}) = {} & \frac{1}{2\Gamma\lambda}\delta_{n,n'}\delta_{\mathbf{v},\mathbf{0}} - \frac{\omega_d}{8\Gamma\lambda^2}(2M+1)^{-(d-1)} \\ & \times \sum_{\mathbf{K}\in L_d} e^{2\pi i\mathbf{v}\cdot\mathbf{K}/(2M+1)} \frac{e^{-|n-n'|\,y_0(\mathbf{K})}}{\sinh y_0(\mathbf{K})} \\ & - \frac{\omega_d}{4\Gamma\lambda^2}(2M+1)^{-(d-1)} \sum_{\mathbf{K}\in L_d} e^{2\pi i\mathbf{v}\cdot\mathbf{K}/(2M+1)} e^{-(n+n')\,y_0(\mathbf{K})} \\ & \times \left[\frac{1}{e^{y_0(\mathbf{K})} - e^{\omega(\mathbf{K})}} - \frac{1}{2\sinh y_0(\mathbf{K})}\right] \end{aligned} \tag{35a}$$

and for $\lambda < 0$,

$$\cdot p(n, n'; \mathbf{v}) = \frac{1}{2\Gamma\lambda} \delta_{n,n'} \delta_{\mathbf{v},\mathbf{0}} + \frac{\omega_d(-1)^{n-n'}}{8\Gamma\lambda^2} (2M+1)^{-(d-1)}$$

$$\times \sum_{\mathbf{K} \in L_d} e^{2\pi i \mathbf{v} \cdot \mathbf{K}/(2M+1)} \frac{e^{-|n-n'| Y_0(\mathbf{K})}}{\sinh Y_0(\mathbf{K})} + \frac{\omega_d}{4\Gamma\lambda^2} (2M+1)^{-(d-1)}$$

$$\times \sum_{\mathbf{K} \in L_d} e^{2\pi i \mathbf{v} \cdot \mathbf{K}/(2M+1)} (-1)^{n+n'} e^{-(n+n') Y_0(\mathbf{K})}$$

$$\times \left(\frac{1}{e^{Y_0(\mathbf{K})} + e^{-\omega(\mathbf{K})}} - \frac{1}{2 \sinh Y_0(\mathbf{K})} \right) \tag{35b}$$

We may note that then two expressions separate neatly into a bulk correlation function

$$p_B(n, n'; \mathbf{v}) = \lim_{\substack{n \to \infty, n' \to \infty \\ n - n' \text{ fixed}}} p(n, n'; \mathbf{v})$$

and a surface correlation function

$$p_s(n, n'; \mathbf{v}) = p(n, n'; \mathbf{v}) - p_B(n, n'; \mathbf{v}) \tag{36}$$

Thus, in the limit $M \to \infty$ we have, for $\lambda > 0$,

$$p_B(n, n'; \mathbf{v}) = \frac{1}{2\Gamma\lambda} \delta_{n,n'} \delta_{\mathbf{v},\mathbf{0}} - \frac{\omega_d}{8\Gamma\lambda^2} (2\pi)^{-(d-1)}$$

$$\times \int_{R_d} d^{d-1}\mathbf{K} \frac{e^{i\mathbf{K} \cdot \mathbf{v} - |n-n'| y_0(\mathbf{K})}}{\sinh y_0(\mathbf{K})} \tag{37a}$$

and for $\lambda < 0$,

$$p_B(n, n'; \mathbf{v}) = \frac{1}{2\Gamma\lambda} \delta_{n,n'} \delta_{\mathbf{v},\mathbf{0}} + \frac{\omega_d}{8\Gamma\lambda^2} (2\pi)^{-(d-1)}$$

$$\times \int_{R_d} d^{d-1}\mathbf{K} \frac{e^{i\mathbf{k} \cdot \mathbf{v}} (-1)^{n-n'} e^{-|n-n'| Y_0(\mathbf{K})}}{\sinh Y_0(\mathbf{K})} \tag{37b}$$

where

$$\cosh \omega(\mathbf{K}) = 1 + \sum_{\alpha=2}^{d} (1 - \cos K_\alpha)$$

and for $\lambda > 0$, $\cosh y_0(\mathbf{k}) = \omega_d/4\lambda + \cosh \omega(\mathbf{K})$, while for $\lambda < 0$, $\cosh Y_0(\mathbf{K}) = -\omega_d/4\lambda - \cosh \omega(\mathbf{K})$. The region R_d is $[-\pi, \pi]^{d-1}$. These bulk correlation functions are exactly the same as the bulk correlation functions found in I, a result to be expected. The bulk correlation length is $1/y_0(\mathbf{0})$ for $\lambda > 0$ and $1/Y_0(\mathbf{0})$ for $\lambda < 0$, not the results given after Eqs. (103) and (104) in I. Those results in I are valid only in the limit as $\lambda \to 0$. (I thank the referee of the present paper for pointing out the error in I.)

The surface correlation functions are a diffeent matter. They may be written, for $\lambda > 0$,

$$p_s(n, n'; \mathbf{v}) = -\frac{\omega_d}{4\Gamma\lambda^2}\frac{1}{(2\pi)^{d-1}}\int_{R_d} d^{d-1}\mathbf{K}\, e^{i\mathbf{K}\cdot\mathbf{v}} e^{-(n+n')\, y_0(\mathbf{K})} \times\left[(e^{y_0(\mathbf{K})} - e^{-\omega(\mathbf{K})})^{-1} - \frac{1}{2\sinh y_0(\mathbf{K})}\right] \tag{38a}$$

and for $\lambda < 0$,

$$p_s(n, n'; \mathbf{v}) = +\frac{\omega_d}{4\Gamma\lambda^2}\frac{1}{(2\pi)^{d-1}}\int_{R_d} d^{d-1}\mathbf{K}\, e^{i\mathbf{k}\cdot\mathbf{v}}(-1)^{n+n'} e^{-(n+n')\, Y_0(\mathbf{K})} \times\left[(e^{Y_0(\mathbf{K})} + e^{-\omega(\mathbf{K})})^{-1} - \frac{1}{2\sinh Y_0(\mathbf{K})}\right] \tag{38b}$$

The functions $y_0(\mathbf{K})$ and $Y_0(\mathbf{K})$ are analytic in the K_α^2, the K_α being the components of $\mathbf{K}$, but $\omega(\mathbf{K})$ is not analytic at $\mathbf{K} = \mathbf{0}$; for small $\mathbf{K}$, $\omega(\mathbf{K}) \simeq |\mathbf{K}|$.

Note that the inverse two-dimensional transform of $|\mathbf{K}|$ is $-1/(2\pi\, |\mathbf{r}|^3)$ and the inverse one-dimensional transform of $|K|$ is $-1/(2\pi\, |\mathbf{r}|^2)$.

Thus, for $\lambda > 0$, the long-range part of the surface correlation function is

$$p_s(n, n'; \mathbf{v}) = -\frac{e^{-(n'+n+1)\, y_0(\mathbf{0})}}{4\pi\Gamma\lambda}|\mathbf{v}|^{-3} \quad \text{for} \quad d = 3 \tag{39a}$$

$$p_s(n, n'; \mathbf{v}) = -\frac{e^{-(n'+n+1)\, y_0(\mathbf{0})}}{2\pi\Gamma\lambda}|\mathbf{v}|^{-2} \quad \text{for} \quad d = 2 \tag{39b}$$

while for $\lambda < 0$,

$$p_s(n, n'; \mathbf{v}) = \frac{(-1)^{n+n'} e^{-(n+n'+1)\, Y_0(\mathbf{0})}}{4\pi\Gamma\lambda}|\mathbf{v}|^{-d} \quad \text{for} \quad d = 3 \tag{39c}$$

$$p_s(n, n'; \mathbf{v}) = \frac{(-1)^{n+n'} e^{-(n+n'+1)\, Y_0(\mathbf{0})}}{2\pi\Gamma\lambda}|\mathbf{v}|^{-2} \quad \text{for} \quad d = 2 \tag{39d}$$

We may now define

$$M_s(\mathbf{v}) = \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty} p_s(n, n'; \mathbf{v}) \tag{40}$$

and evaluate it quite simply. We obtain

$$M_s(\mathbf{v}) = -(8\pi^2\Gamma)^{-1} \qquad \text{for} \quad d=3 \tag{41a}$$

$$M_s(\mathbf{v}) = -(2\pi^2\Gamma)^{-1} \qquad \text{for} \quad d=2 \tag{41b}$$

4. DISCUSSION

The main results of this paper are Eqs. (39) and (41). They show that while the system is in a high-temperature phase the surface correlation functions decay algebraically, not exponentially as the correlations do in the bulk of the system. Equations (41a), (41b) show that the correlation functions obey the sum rule discussed by Martin[1] and first introduced by Jancovici.[9,10] They obey this sum rule at all couplings which allow the system to be in its high-temperature phase, whether the bulk correlations are decaying monotonically or alternating in sign. There is no alteration of sign with $|\mathbf{v}|$ in this long-range part of the surface correlation function even when $\Gamma > \Gamma_0\,|d|$.

The correlation functions in the bulk may be evaluated by an asymptotic expansion in large $|\mathbf{n}|$. This gives a bulk charge–charge correlation function at large $|\mathbf{n}|$. For $\lambda > 0$ this is composed of an algebraically decaying factor times $\exp(-|\mathbf{n}|/L)$, where $L = 1/y_0(\mathbf{0})$ is the correlation length for the system. For $\lambda < 0$ the situation is similar but the asymptotic expansion for $p_B(\mathbf{n}, \mathbf{n}')$ contains an extra factor

$$\prod_{\alpha=1}^{d} (-1)^{(n_\alpha - n'_\alpha)}$$

and the correlation length is $L = 1/Y_0(\mathbf{0})$.

The surface correlation functions have quite different long-range behavior. The amplitude of the $|\mathbf{v}|^{-d}$ factor decays exponentially fast as the sampling distances n, n' from the surface increase. The correlation function for this decay is $1/y_0(\mathbf{0})$ [or $1/Y_0(\mathbf{0})$] and the sign of this amplitude oscillates as $(-1)^{n+n'}$. This surface layer correlation length L is the same as the bulk correlation length. For $\lambda > 0$ we have

$$L_+ = \frac{1}{y_0(\mathbf{0})} = \left(\log\left\{\frac{\omega_d}{4\lambda} + 1 + \left[\left(\frac{\omega_d}{4\,|\lambda|} + 1\right)^2 - 1\right]^{1/2}\right\}\right)^{-1} \tag{42a}$$

and for $\lambda < 0$ we have

$$L_- = \frac{1}{Y_0(\mathbf{0})} = \left(\log\left\{\frac{\omega_d}{4\,|\lambda|} - 1 + \left[\left(\frac{\omega_d}{4\,|\lambda|} - 1\right)^2 - 1\right]^{1/2}\right\}\right)^{-1} \tag{42b}$$

For $\lambda > 0$ the surface correlations do not oscillate in sign ith increasing components of $\mathbf{v}$, so that for $\Gamma > \Gamma_0(d)$ the nature of the decay of the charge–charge correlation functions with $\mathbf{v}$ is roughly similar to that for $\Gamma < \Gamma_0(d)$.

At $\Gamma = \Gamma_0(d)$, where the bulk charge–charge correlation function is nonzero only if $\mathbf{n} = \mathbf{n}'$ or if $\mathbf{n}$ and $\mathbf{n}'$ are nearest neighbors, the surface correlation function is zero if n and n' are not both zero. In this case the long-range part of the surface correlation function is restricted to the surface layer $n = n' = 0$ only. This reflects the behavior of the surface correlation functions in the two-dimensional, one-component plasma at $\Gamma = 2$. In that system the long-range surface correlations are damped with a Gaussian decay as the sample points move into the bulk, which reflects the Gaussian decay of the bulk correlation functions at $\Gamma = 2$. In this mean spherical model the Gaussian decay is replaced by a decay to zero over one lattice spacing, both in the bulk correlation functions and in the decay of the surface correlation amplitude as the sample points move into the bulk.

At $\Gamma = \Gamma_0(d)$, the long-range part of the surface correlation function is

$$p_s(0, 0, \mathbf{v}) = \begin{cases} -(1/12\pi)\,|\mathbf{v}|^{-3} & \text{for} \quad d = 3 \\ -(1/4\pi)\,|\mathbf{v}|^{-2} & \text{for} \quad d = 2 \end{cases} \tag{43}$$

The fact that the long-range part of the charge–charge correlation function obeys the standard Coulombic sum rules means that this charged mean spherical model really does behave as a Coulombic system. The mean spherical constraint does not play much of a role near the surface, since one knows, from I, that very large fluctuations are possible at the surface.

One may then place some reliance on the properties of such a system at a surface bounded by a dielectric. I shall turn to that problem in a later paper.

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