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A Mean Spherical Model with Coulomb Interactions

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We consider simple cubic lattice systems Λ in d dimensions with a continuous real charge variable $q(\mathbf{n})$ at each lattice site $\mathbf{n}$. These variables are subject to a mean spherical constraint forcing $\langle \sum_{\mathbf{n} \in \Lambda} q^2(\mathbf{n}) \rangle = \|\Lambda\| Q^2$, where $\|\Lambda\|$ is the number of lattice sites in Λ and Q is an elementary charge. The energy of the charges comes from interactions with an electrostatic potential, which is the solution of a symmetric second-difference Poisson equation on the lattice. Two cases are considered, both of which allow the inclusion of the effects of a fixed, constant, external electric field. On the lattice $\Lambda_1 = [1, N]^{\otimes d}$, a Neumann condition is imposed at the surface of the lattice. The lattice $\Lambda_2 = [1, N] \otimes [-M, M]^{\otimes (d-1)}$ is periodic in each direction ranging over $[-M, M]$ and has a Dirichlet condition imposed at the other two surfaces. On Λ_2 a finite electric field may be applied, while on Λ_2 a finite potential difference may be applied across the lattice. The models are exactly solvable. We study the distribution functions on each system and show that they satisfy appropriate forms of the first two Stillinger–Lovett moment conditions. The two charge distribution functions show screening behavior at high temperature and extreme short range at an intermediate temperature $T_0(d)$, and oscillate as they decay to zero for $T < T_0(d)$. Because of the continuous nature of the charge variables, there is no Kosterlitz–Thouless transition in two dimensions. In three dimensions the change in the decay behavior of the distribution functions at $T < T_0(d)$ is precursor to a phase transition to a charge ordered state.

KEY WORDS: Spherical model; Coulombic systems; correlation function decay; Stillinger–Lovett relations.

1. INTRODUCTION

Understanding of the statistical mechanics of Coulombic systems has been markedly advanced in recent years by using specific information from the properties of the two-dimensional, one-component plasma at coupling

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$\Gamma = Q^2/kT = 2$. This plasma system is useful because its thermodynamics and distribution functions may be calculated exactly at $\Gamma = 2$ in a variety of electrostatic boundary conditions.[1-7] General theory, based on an assumption of the BBGKY integral equation hierarchy[8] and, alternatively, based on field-theoretic descriptions of statistical mechanics[9,10] showed that in the bulk of a general Coulombic system at high temperature (weak coupling), distribution functions display exact screening. That is, the Debye–Hückel picture of the correlation functions in a weakly coupled disordered Coulombic system is qualitatively correct. In the bulk of the two-dimensional, one-component plasma at $\Gamma = 2$, the distribution functions certainly obey all these screening sum rules. However, the exact results showed a variety of decay of distribution functions with distance along surfaces.[4-6] These exact results then led to a rigorous analysis of distribution functions along surfaces in Coulombic systems. Integral equation analysis[11,12] and field-theoretic techniques[13] then showed that algebraic decay of distribution functions along surfaces is a very general property of weakly coupled Coulombic systems.

The power of this single, exactly solvable Coulombic system to generate new understanding of Coulombic systems has been quite remarkable. Two questions arise. One is whether results on the two-dimensional, one-component plasma at $\Gamma = 2$ other than screening and slow decay at surfaces generalize to other Coulombic systems. The other is whether other exactly solvable Coulombic systems can be found to generate further general understanding. We report calculations on just such a model in this paper. One particular property of the one-component, two-dimensional plasma that we examine closely is the decay of the two-particle distribution functions. At weak coupling, this is known to be exponential on general grounds.[8,10] At coupling $\Gamma = 2$ the decay is of the form $\exp(-\pi\rho\mathbf{r}^2)$ with ρ the particle density. At coupling $\Gamma > 2$, Jancovici's original solution suggested that a thermodynamic perturbation theory for the distribution functions shows that they will oscillate as they decay. The correlation length has a minimum at $\Gamma = 2$. The oscillations at $\Gamma > 2$ seem to reflect the behavior in the two-component plasma at strong coupling and high density, where computer simulations suggest the presence of a charge ordered state.[14,15]

In this paper we introduce a lattice system with Coulombic interactions. It is exactly solvable. In each dimension d there is an intermediate temperature $T_0(d)$ which characterizes the decay of truncated charge–charge distribution functions. For $T > T_0(d)$ the decay is monotone and exponential with a correlation length decreasing with decreasing temperature. At $T = T_0(d)$ the distribution functions have a range of exactly one lattice spacing, which represents a correlation length minimum. At

$T < T_0(d)$ the distribution functions decay with oscillations and a correlation length that increases with decreasing temperature. This is exactly what is seen in the two-dimensional, one-component plasma and suggests that this behavior may be fairly general in Coulombic systems. Unfortunately, the price of having the system exactly solvable is the introduction of a mean spherical constraint on the mean square charge magnitudes. While this does make the mean square charges equal to Q^2, it introduces an extra long-range interaction. Whether the resulting system behaves as a "Coulombic" one is important in attempts to generalize the properties of the system. The general notion of a spherical model was first introduced by Berlin and Kac[16] in an attempt to understand phase transitions in Ising-like magnetic models. Their success was remarkable and such models have served as very useful examples ever since. We introduce our charged spherical model in the same spirit.

In the general picture of the study of Coulombic systems, charged lattice systems have come to play an important role. One example of this is seen in studies of the discrete Gaussian model in two dimensions. Up to a factor of a nonsingular spin wave partition function, this system has the same partition function as a discrete lattice Coulombic system in two dimensions.[17,18] The roughening transition in the discrete Gaussian model is exactly the Kosterlitz–Thouless transition from a screening plasma to a dielectric phase in the discrete Coulomb system.

Another example is the work of Fröhlich *et al.*,[19] who showed that a three-dimensional Coulomb lattice gas could have a transition to a charge ordered state at strong coupling. The exactly solvable systems introduced here allow us to illustrate many of these phenomena. The Kosterlitz–Thouless transition is unfortunately beyond the capacity of the model because of the continuous nature of the charge variables introduced.

Two lattice systems are introduced. The first is $\Lambda_1 = [1, N]^{\otimes d}$, with a charge $q(\mathbf{n}) \in \mathbb{R}$ at each $\mathbf{n} \in \Lambda_1$. The second is $\Lambda_2 = [1, N] \otimes [-M, M]^{\otimes (d-1)}$, also with a charge $q(\mathbf{n}) \in \mathbb{R}$ at each $\mathbf{n} \in \Lambda_2$. On the lattice there are d unit spacing vectors $\{\mathbf{e}_\alpha,\ 1 \leqslant \alpha \leqslant d\}$ corresponding to a translation of one lattice spacing in each possible direction. For a given configuration of charges $\{q(\mathbf{n}),\ \mathbf{n} \in \Lambda\}$, the electrostatic potential $\Psi_0(\mathbf{n})$ obeys the Poisson equation

$$D_{\mathbf{n}}^2 \Psi_0(\mathbf{n}) = -\omega_d q(\mathbf{n}); \qquad \mathbf{n} \in \Lambda \tag{1}$$

where ω_d is the surface area of the unit sphere in d dimensions. The operator $D_{\mathbf{n}}^2$ is given by

$$D_{\mathbf{n}}^2 F(\mathbf{n}) = \sum_{\alpha=1}^{d} [F(\mathbf{n} + \mathbf{e}_\alpha) - 2F(\mathbf{n}) + F(\mathbf{n} - \mathbf{e}_\alpha)] \tag{2}$$

The boundary condition on Λ_1 is given as follows. Let $\mathbf{n} \in \Lambda_1$ be a lattice vector such that $\mathbf{n}+\mathbf{e}_\alpha$ (or $\mathbf{n}-\mathbf{e}_\alpha) \notin \Lambda_1$. Then $\Psi_0(\mathbf{n})$ is defined for these points, too, so that $\Psi_0(\mathbf{n}+\mathbf{e}_\alpha) = \Psi_0(\mathbf{n})$ [or $\Psi_0(\mathbf{n}-\mathbf{e}_\alpha) = \Psi_0(\mathbf{n})$]. This completes the list of values of $\Psi_0(\mathbf{n})$ required in Eq. (1) and means that the electric field has zero normal component at the edge of Λ_1. This is a Neumann boundary condition on Λ_1. A Neumann boundary condition allows a fixed external electric field to be applied to the system.[20] This field is assumed to be of the form $\mathbf{E} = E\mathbf{e}_1$ for convenience and so arises from an electrostatic potential

$$\Psi_1(\mathbf{n}) = [\tfrac{1}{2}(N+1) - (\mathbf{n}\cdot\mathbf{e}_1)]\, E \tag{3}$$

The constant term is included to give zero average potential across the lattice.

On lattice Λ_2 the potential $\Psi_0(\mathbf{n})$ is periodic with period $2M+1$ in each direction $\mathbf{e}_\alpha$, $2 \leqslant \alpha \leqslant d$. In the $\mathbf{e}_1$ direction a Dirichlet condition

$$\Psi_0(\mathbf{n}) = 0 \qquad \text{if} \quad \mathbf{n}\cdot\mathbf{e}_1 = 0 \quad \text{or} \quad N+1 \tag{4}$$

applies. The two separated surfaces at $\mathbf{n}\cdot\mathbf{e}_1 = 0$ and $\mathbf{n}\cdot\mathbf{e}_1 = N+1$ may be set at different potentials $\pm\frac{1}{2}V$ so that an extra potential

$$\Psi_1(\mathbf{n}) = \frac{1}{2}\, V\left(1 - \frac{2(\mathbf{n}\cdot\mathbf{e}_1)}{N+1}\right) \tag{5}$$

applies to the system, and gives rise to a constant external electric field $(V/N+1)$.

The Hamiltonians for the system take the form

$$\begin{aligned} H_N(\Lambda) = {} & \frac{1}{2} \sum_{\mathbf{n}\in\Lambda} [q(\mathbf{n})\, \Psi_0(\mathbf{n}) + 2q(\mathbf{n})\, \Psi_1(\mathbf{n})] \\ & + \lambda \left\{ \sum_{\mathbf{n}\in\Lambda} q^2(\mathbf{n}) - Q^2\, \|\Lambda\| \right\} \end{aligned} \tag{6}$$

where $\|\Lambda\|$ is the number of lattice sites. Thus, $\|\Lambda_1\| = N^d$, $\|\Lambda_2\| = (2M+1)^{d-1} N$.

The fixed elementary charge magnitude for the system is Q, and λ is a parameter whose value is the one that forces the constraint condition

$$\left\langle \sum_{\mathbf{n}} q^2(\mathbf{n}) \right\rangle = Q^2\, \|\Lambda\| \tag{7}$$

to hold. These two mean spherical models are analyzed in Section 2, where general sum forms for the partition functions, constraint equations, one-and two-charge distribution functions, and the mean square dipole moment fluctuation tensor are derived. In Section 3 the constraint parameter equations are studied. In particular, it is shown that the value $\lambda = 0$ does occur, and that for $d \geqslant 3$ there is a critical coupling beyond which the solution λ for the constraint parameter behaves in a singular way. In Section 4 global sum rules are studied. These are the net charge on the system Λ_2, the polarization of the system, and the global first and second Stillinger–Lovett sum rules. These sum rules are seen to apply in an appropriate way on both lattices. Section 5 studies the one- and two-charge distribution functions. The existence of a correlation length minimum is demonstrated. This occurs at a particular temperature $T_0(d)$ corresponding to $\lambda = 0$. Above this temperature charges are screened with monotonic exponential decay of the two-particle distribution function in the bulk. Below this temperature the decay is similar, but is modulated by a sign alternation across the lattice. It is shown that in the bulk of the lattice, far from the surface, the normal plasma result for the second Stillinger–Lovett sum rule holds, as long as the coupling is weak enough to ensure that the system has not undergone a phase transition. In Section 6 it is shown that for $d = 3$ there is a transition to a charge ordered state and some of its properties are studied. Section 7 concludes with a discussion of the results.

2. THE SYSTEM AND ITS PROPERTIES

On Λ_1 the operator $D_{\mathbf{n}}^2$ has eigenfunctions of the form

$$F(\mathbf{k}, \mathbf{n}) = \prod_{\alpha=1}^{d} f(k_\alpha, n_\alpha) \tag{8}$$

for $\mathbf{k} \in R_1 = [0, N-1]^{\otimes d}$. The $f(k, n)$ are given by

$$f(k, n) = (2/N)^{1/2} \cos[\pi k(n - \tfrac{1}{2})/N], \qquad 1 \leqslant n \leqslant N \tag{9}$$

if $k \neq 0$, while $f(0, n) = N^{-1/2}$, $1 \leqslant n \leqslant N$. The corresponding eigenvalues are $-2\xi(\mathbf{k})$, with

$$\xi(\mathbf{k}) = \sum_{\alpha=1}^{d} \left[1 - \cos\left(\frac{\pi k_\alpha}{N}\right)\right] \tag{10}$$

It is useful below to have $\xi^*(k) = \xi(k\mathbf{e}_1) = 1 - \cos(\pi k/N)$. On Λ_2 the operator $D_{\mathbf{n}}^2$ has eigenfunctions of the form

$$G(\mathbf{k}, \mathbf{n}) = (2M+1)^{-(d-1)/2} \left(\frac{2}{N}\right)^{1/2} \sin\left(\frac{\pi k_1 n_1}{N+1}\right) \prod_{\alpha=2}^{d} \exp \frac{2\pi i k_\alpha n_\alpha}{2M+1} \tag{11}$$

for $\mathbf{k} \in R_2 = [1, N] \otimes [-M, M]^{\otimes d-1}$. The corresponding eigenvalues are $-2\eta(\mathbf{k})$, with

$$\eta(\mathbf{k}) = 1 - \cos\left(\frac{\pi k_1}{N+1}\right) + \sum_{\alpha=2}^{d} \left[1 - \cos\left(\frac{2\pi k_\alpha}{2M+1}\right)\right] \tag{12}$$

It is also useful below to have $\eta^*(k) = \eta(k\mathbf{e}_1) = 1 - \cos(\pi k/N+1)$. Note that on Λ_1, one of the eigenvalues is zero $[\xi(\mathbf{0}) = 0]$. None of the eigenvalues on Λ_2 is zero. As will be seen from the explicit solutions, this means that (1) on Λ_2 has a solution for all configurations $\{q(\mathbf{n}), \mathbf{n} \in \Lambda_2\}$. On the other hand, Eq. (1) on Λ_1 has a solution for a given configuration $\{q(\mathbf{n}), \mathbf{n} \in \Lambda_1\}$ if and only if the charge neutrality constraint

$$\sum_{\mathbf{n} \in \Lambda_1} q(\mathbf{n}) = 0 \tag{13}$$

holds. These solutions may be found by using the unitary transformations:

$$\text{on } \Lambda_1\text{:} \quad \hat{q}(\mathbf{k}) = \sum_{\mathbf{n} \in \Lambda_1} q(\mathbf{n}) \, F(\mathbf{k}, \mathbf{n}); \qquad q(\mathbf{n}) = \sum_{\mathbf{k} \in R_1} \hat{q}(\mathbf{k}) \, F(\mathbf{k}, \mathbf{n}) \tag{14a}$$

and

$$\text{on } \Lambda_2\text{:} \quad \hat{q}(\mathbf{k}) = \sum_{\mathbf{n} \in \Lambda_2} q(\mathbf{n}) \, G^*(\mathbf{k}, \mathbf{n}); \qquad q(\mathbf{n}) = \sum_{\mathbf{k} \in R_2} \hat{q}(\mathbf{k}) \, G(\mathbf{k}, \mathbf{n}) \tag{14b}$$

On Λ_1 the charge neutrality constraint (13) becomes

$$N^{d/2} \hat{q}(\mathbf{0}) = 0 \tag{15}$$

On Λ_1 the potential $\Psi_0(\mathbf{n})$ may be expanded in terms of the $F(\mathbf{k}, \mathbf{n})$ and their properties as eigenvectors of $D_{\mathbf{n}}^2$ used to give

$$\Psi_0(\mathbf{n}) = \sum_{\substack{\mathbf{k} \in R_1 \\ \mathbf{k} \neq \mathbf{0}}} \frac{\omega_d}{2\xi(\mathbf{k})} \hat{q}(\mathbf{k}) \, F(\mathbf{k}, \mathbf{n}) \tag{16}$$

Here the need for the charge neutrality constraint (15) is obvious, since $\xi(\mathbf{0}) = 0$. The charge–charge interaction contribution to the Hamiltonian is then

$$\frac{1}{2} \sum_{\mathbf{n} \in \Lambda_1} q(\mathbf{n}) \, \Psi_0(\mathbf{n}) = \sum_{\substack{\mathbf{k} \in R_1 \\ \mathbf{k} \neq \mathbf{0}}} \frac{\omega_d}{4\xi(\mathbf{k})} q^2(\mathbf{k}) \tag{17}$$

The potential $\Psi_0(\mathbf{n})$ on Λ_2 may be explicitly constructed as

$$\Psi_0(\mathbf{n}) = \sum_{\mathbf{k} \in R_2} \frac{\omega_d}{2\eta(\mathbf{k})} \hat{q}(\mathbf{k}) \, G^*(\mathbf{k}, \mathbf{n}) \tag{18}$$

This object exists for all configurations $\{q(\mathbf{n}), \mathbf{n} \in \Lambda_2\}$, since the sums are finite, so that all the $\hat{q}(k)$ always exist, and none of the $\eta(\mathbf{k})$ are zero. On Λ_2, then, the charge–charge interaction energy is

$$\frac{1}{2} \sum_{\mathbf{n} \in \Lambda_2} q(\mathbf{n})\, \Psi_0(\mathbf{n}) = \sum_{\mathbf{k} \in R_2} \frac{\omega_d}{4\eta(\mathbf{k})} \hat{q}^2(\mathbf{k}) \tag{19}$$

The interaction of the charges with the external field is, on Λ_1,

$$\sum_{\mathbf{n} \in \Lambda_1} q(\mathbf{n})\, \Psi_1(\mathbf{n}) = N^{d/2-1} E \cdot 2^{1/2} \sum_{k=1}^{N-1} \hat{q}(k\mathbf{e}_1)\, a(k) \tag{20}$$

where

$$a(k) = \sum_{n=1}^{N} \left(\frac{N+1}{2} - n\right) \cos\left[\frac{\pi k}{N}\left(n - \frac{1}{2}\right)\right] = \frac{\frac{1}{2}[1-(-1)^k] \cos(\pi k/2N)}{1-\cos(\pi k/N)} \tag{21}$$

On Λ_2 this interaction energy is

$$\sum_{\mathbf{n} \in \Lambda_2} q(\mathbf{n})\, \Psi_1(\mathbf{n}) = (2M+1)^{(d-1)/2} (N+1)^{-1/2}\, V \cdot 2^{1/2} \sum_{k=1}^{N} q(k\mathbf{e}_1)\, b(k) \tag{22}$$

where

$$b(k) = \sum_{n=1}^{N} \left(\frac{1}{2} - \frac{n}{N+1}\right) \sin\left(\frac{\pi k n}{N+1}\right) = \frac{1}{4}[1+(-1)^k] \cot\left(\frac{\pi k}{2(N+1)}\right) \tag{23}$$

The Hamiltonians for the two systems may be written as

$$H(\Lambda_1) = \sum_{\substack{\mathbf{k} \in R_1 \\ \mathbf{k} \neq \mathbf{0}}} \left\{\left[\lambda + \frac{\omega_d}{4\xi(\mathbf{k})}\right] \hat{q}^2(\mathbf{k}) + 2^{1/2} \frac{E}{N} \|\Lambda_1\|^{1/2} \hat{q}(\mathbf{k})\, A(\mathbf{k})\right\} - \lambda Q^2 \|\Lambda_1\| \tag{24}$$

and

$$H(\Lambda_2) = \sum_{\mathbf{k} \in R_2} \left\{\left[\lambda + \frac{\omega_d}{4\eta(\mathbf{k})}\right] q^2(\mathbf{k}) + 2^{1/2} V \frac{\|\Lambda_2\|^{1/2}}{[N(N+1)]^{1/2}} q(\mathbf{k})\, B(\mathbf{k})\right\} - \lambda Q^2 \|\Lambda_2\| \tag{25}$$

where $A(\mathbf{k}) = a(\mathbf{k})$ if $\mathbf{k} = k\mathbf{e}_1$ with $1 \leqslant k \leqslant N-1$ and otherwise $A(\mathbf{k}) = 0$, and $B(\mathbf{k}) = b(\mathbf{k})$ if $\mathbf{k} = k\mathbf{e}_1$ with $1 \leqslant k \leqslant N$ and otherwise $B(\mathbf{k}) = 0$. On Λ_1

the electric field is E, but on Λ_2 the electric field is $V/(N+1)$, which tends to zero in the thermodynamic limit. This is a natural consequence of the different boundary conditions. These two Hamiltonians contain a term $\lambda[\sum_{\mathbf{n}\in\Lambda} q^2(\mathbf{n}) - Q^2 \|\Lambda\|]$ to constrain the mean square charges according to Eq. (7).

On Λ_1 the partition function is

$$Z(\Lambda_1) = \left[\prod_{\mathbf{n}\in\Lambda_1} \int_{-\infty}^{\infty} dq(\mathbf{n})\right] \delta\left(\sum_{\mathbf{n}\in\Lambda_1} q(n)\right) \exp[-\beta H(\Lambda_1)] \tag{26}$$

and on Λ_2 the partition function is

$$Z(\Lambda_2) = \left[\prod_{\mathbf{n}\in\Lambda_2} \int_{-\infty}^{\infty} dq(\mathbf{n})\right] \exp[-\beta H(\Lambda_2)] \tag{27}$$

The transformation $\{q(\mathbf{n}),\ \mathbf{n}\in\Lambda_j\} \to \{\hat{q}(\mathbf{k}),\ \mathbf{k}\in R_j\}$ is unitary in each case, so that its Jacobian is one. The partition functions may thus be evaluated immediately, provided that

$$\lambda > -\omega_d/4\xi(\mathbf{k}) \qquad \forall \mathbf{k}\in R_1\backslash\{\mathbf{0}\} \quad \text{on } \Lambda_1$$

$$\lambda > -\omega_d/4\eta(\mathbf{k}) \qquad \forall \mathbf{k}\in R_2 \quad \text{on } \Lambda_2$$

These bounds are

$$\text{on } \Lambda_1\text{:} \quad \lambda > -\omega_d\left[8d\cos^2\left(\frac{\pi}{2N}\right)\right]^{-1} \tag{28}$$

$$\text{on } \Lambda_2\text{:} \quad \lambda > -\omega_d\left\{8\left[(d-1)\cos^2\left(\frac{\pi}{2(2M+1)}\right) + \cos^2\left(\frac{\pi}{N+1}\right)\right]\right\}^{-1} \tag{29}$$

The constraint equations are $\partial[\log Z(\Lambda)]/\partial\lambda = 0$. The partition functions are

$$Z(\Lambda_1) = N^{-d/2}\left(\frac{\pi}{\beta}\right)^{(\|\Lambda_1\|-1)/2} \prod_{\substack{\mathbf{k}\in R_1 \\ \mathbf{k}\neq \mathbf{0}}} \left[\lambda + \frac{\omega_d}{4\xi(\mathbf{k})}\right]^{-1/2} \times \exp\left\{\left[\lambda\Gamma + \frac{1}{2}\beta E^2 J_1(\lambda)\right] \|\Lambda_1\|\right\} \tag{30}$$

where $\Gamma = \beta Q^2$ and

$$Z(\Lambda_2) = \left(\frac{\pi}{\beta}\right)^{\|\Lambda_2\|/2} \prod_{\mathbf{k} \in R_2} \left[\lambda + \frac{\omega_d}{4\eta(\mathbf{k})}\right]^{-1/2} \times \exp\left\{\left[\lambda\Gamma + \frac{1}{2}\beta V^2 J_2(\lambda)\right] \|\Lambda_2\|\right\} \tag{31}$$

where

$$J_1(\lambda) = \frac{1}{N^2} \sum_{k=1}^{N-1} \frac{a^2(k)}{\lambda + \omega_d/[4\xi^*(k)]} \tag{32}$$

$$J_2(\lambda) = \frac{1}{N(N+1)} \sum_{k=1}^{N} \frac{b^2(k)}{\lambda + \omega_d/[4\eta^*(k)]} \tag{33}$$

The constraint equations become: on Λ_1,

$$2\Gamma = \sum_{\substack{\mathbf{k} \in R_1 \\ \mathbf{k} \neq \mathbf{0}}} \left(\lambda + \frac{\omega_d}{4\xi(\mathbf{k})}\right)^{-1} \|\Lambda_1\|^{-1} - \beta E^2 \frac{\partial J_1(\lambda)}{\partial \lambda} \tag{34}$$

and on Λ_2,

$$2\Gamma = \sum_{\mathbf{k} \in R_2} \left(\lambda + \frac{\omega_d}{4\eta(\mathbf{k})}\right)^{-1} \|\Lambda_2\|^{-1} - \beta V^2 \frac{\partial J_2(\lambda)}{\partial \lambda} \tag{35}$$

The one-charge distribution function $\langle q(\mathbf{n})\rangle$ depends only on $n = \mathbf{n} \cdot \mathbf{e}_1$ in both cases. The results (and most of those below) are obtained by changing $q(\mathbf{n})$ to a sum over $\hat{q}(\mathbf{k})$ and then performing the resulting Gaussian integrals. The results are

$$\langle q(\mathbf{n})\rangle = -\frac{E}{N} \sum_{k=1}^{N-1} \frac{a(k) \cos[(\pi k/N)(n - \frac{1}{2})]}{\lambda + \omega_d/[4\xi^*(k)]} \tag{36a}$$

on Λ_1 and

$$\langle q(\mathbf{n})\rangle = -\frac{V}{N+1} \sum_{k=1}^{N} \frac{b(k) \sin[\pi k n/(N+1)]}{\lambda + \omega_d/[4\eta^*(k)]} \tag{36b}$$

on Λ_2.

The component of the mean dipole of the system in the direction of the applied constant external field is, on Λ_1,

$$M_1 = N^{d-1} \sum_{n=1}^{N} n \langle q(\mathbf{n})\rangle = \frac{E}{N^2} \sum_{k=1}^{N} \frac{a^2(k)}{\lambda + \omega_d/[4\xi^*(k)]} N^d \tag{37}$$

and, on Λ_2,

$$M_2 = (2M+1)^{d-1} \sum_{n=1}^{N} n\langle q(\mathbf{n})\rangle$$

$$= -V \sum_{k=1}^{N} \frac{b(k)\, c(k)}{\lambda + \omega_d/[4\eta^*(k)]} (2M+1)^{d-1} \tag{38}$$

where

$$c(k) = \frac{1}{N+1} \sum_{n=1}^{N} \sin\left(\frac{\pi k n}{N+1}\right) = -\frac{1}{2}(-1)^k \cot\left(\frac{\pi k}{2(N+1)}\right) \tag{39}$$

Equation (37) shows M_1 to be linear in E and (38) shows M_2 to be linear in V, in the thermodynamic limit, since, as will be seen in Section 3, the equations for λ become independent of $E(V)$ in the thermodynamic limit.

The truncated two-charge distribution function is

$$P_{(2)}(\mathbf{m}, \mathbf{n}) = \{\langle q(\mathbf{m})\, q(\mathbf{n})\rangle - \langle q(\mathbf{m})\rangle\langle q(\mathbf{n})\rangle\}/Q^2 \tag{40}$$

The results for $P_{(2)}(\mathbf{m}, \mathbf{n})$ do not depend on E (or V), since the parameter λ does not depend on E (or V) as just stated.

On Λ_1 this is given by

$$P_{(2)}(\mathbf{m}, \mathbf{n}) = \frac{1}{2\Gamma} \sum_{\substack{\mathbf{k}\in R_1 \\ \mathbf{k}\neq \mathbf{0}}} \frac{F(\mathbf{k}, \mathbf{m})\, F(\mathbf{k}, \mathbf{n})}{\lambda + \omega_d/[4\xi(\mathbf{k})]} \tag{41}$$

and on Λ_2 it is given by

$$P_{(2)}(m, n) = \frac{1}{2\Gamma} \sum_{\mathbf{k}\in R_2} \frac{G(\mathbf{k}, \mathbf{m})\, G^*(\mathbf{k}, \mathbf{n})}{\lambda + \omega_d/[4\eta(\mathbf{k})]} \tag{42}$$

The total dipole moment fluctuation tensor is defined by

$$G_{(2)}(\Gamma) = \frac{1}{\|\Lambda\|} \sum_{\mathbf{n}\in\Lambda} \sum_{\mathbf{m}\in\Lambda} (\mathbf{nm})\, P_{(2)}(\mathbf{m}, \mathbf{n}) \tag{43}$$

Some of the diagonal elements simplify. On Λ_1

$$G_{(2)}(\Gamma)_{\alpha\alpha} = \frac{1}{\Gamma N^2} \sum_{k=1}^{N-1} \frac{a^2(k)}{\lambda + \omega_d/[4\xi^*(k)]} \tag{44}$$

which is independent of α. Notice from Eq. (37) that $G_{(2)}(\Gamma)_{\alpha\alpha}$ on Λ_1 is precisely $M_1/(\Gamma E N^d)$. On Λ_2, only the (11) element simplifies this much. On Λ_2, then,

$$G_{(2)}(\Gamma)_{1,1} = \frac{N+1}{\Gamma N} \sum_{k=1}^{N} \frac{c^2(k)}{\lambda + \omega_d/[4\eta^*(k)]} \tag{45}$$

A final interesting property to study is the average charge on system Λ_2. This is

$$U(\Gamma) = \left\langle \sum_{\mathbf{n} \in \Lambda_2} q(\mathbf{n}) \right\rangle$$
$$= -(2M+1)^{(d-1)/2} \frac{V}{2(N+1)}$$
$$\times \sum_{k=1}^{N} \frac{b(k)[1-(-1)^k] \cot[\pi k/2(N+1)]}{\lambda + \omega_d/[4\eta^*(k)]} \tag{46}$$

3. THE CONSTRAINT EQUATIONS

The constraint equations (34) and (35) show that for small Γ, λ is large and positive in each case, while for large Γ, λ approaches its lower bound, which is negative. In this section it will be assumed that $\lambda > -\omega_d/8d$. The problem of λ less than this value arises at the phase transition in $d=3$. The parameter

$$v = 1 + \omega_d/4\lambda \tag{47}$$

is of fundamental importance in the work reported below. If $\lambda > 0$, then $v > 1$ and we may define y_0 by

$$\cosh(y_0) = v \tag{48}$$

If $-\omega_d/8d < \lambda < 0$, then $v < 1 - 2d$, so that $v < -1$ and thus we may define Y_0 by

$$\cosh(Y_0) = -v \tag{49}$$

We notice that only in the case $d=1$, which is not very interesting, can we have

$$-1 < v < 0$$

Next we must evaluate the functions $J_1(\lambda)$ and $J_2(\lambda)$. From Eqs. (32) and (21) we obtain

$$J_1(\lambda) = \frac{1}{8\lambda N^2} \sum_{\substack{k=-(N-1) \\ k \neq 0}}^{N} \frac{[1-(-1)^k][1+\cos(\pi k/N)]}{[v-\cos(\pi k/N)][1-\cos(\pi k/N)]} \tag{50}$$

This form has been obtained by summing the even summand over

$-(N-1)\leqslant k\leqslant N-1$, dividing by two and then including the $k=N$ term, which is zero. A similar manipulation gives

$$J_2(\lambda)=\frac{1}{8N(N+1)\,\lambda}\sum_{k=-N}^{N+1}\frac{[1+(-1)^k]\{1+\cos[\pi k/(N+1)]\}}{v-\cos[\pi k/(N+1)]} \tag{51}$$

The function $p_+(\zeta, N)=[\exp(iN\zeta)+1]^{-1}$ has simple poles of residue (i/N) at $\zeta=\pi k/N$ for k odd and is analytic elsewhere in the complex ζ plane. We may use this fact to write $J_1(\lambda)$ as an integral around the contour C_1 shown in Fig. 1. Using C_1 includes a contribution from a pole of the integrand at $\zeta=0$ and this must be subtracted out. The procedure gives

$$J_1(\lambda)=\frac{1}{\omega_d}-\frac{1}{8\pi N\lambda}\oint_{C_1}\frac{p_+(\zeta, N)[1+\cos(\zeta)]}{[v-\cos(\zeta)][1-\cos(\zeta)]}\,d\zeta \tag{52}$$

The function $p_-(\zeta, N)=[\exp(iN\zeta)-1]^{-1}$ has simple poles of residue $(-i/N)$ at $\zeta=\pi k/N$ for k even and is analytic elsewhere in the complex ζ plane. This may be used to give, in the same way,

$$J_2(\lambda)=\frac{v+1}{8\pi N\lambda}\oint_{C_1}\frac{p_-(\zeta, N+1)}{v-\cos(\zeta)}\,d\zeta-\frac{1}{4N\lambda} \tag{53}$$

In both cases the contour C_1 may now be shifted to C_2, which is illustrated in Fig. 2 for the two cases $v>1$ and $v<-1$. The parts of C_2 with $\zeta=\pm\pi+iy$ cancel each other (except for the poles at $\zeta=\pm\pi\pm iY_0$ when $v<-1$) because the integrand is periodic in ζ with period 2π. The parts of C_2 with $\mathrm{im}(\zeta)=L$ include an integrand which is $O(e^{-L})$ and the parts of C_2 with $\mathrm{im}(\zeta)=-L$ include an integrand which is $O(e^{-(N+1)L})$ for $J_1(\lambda)$

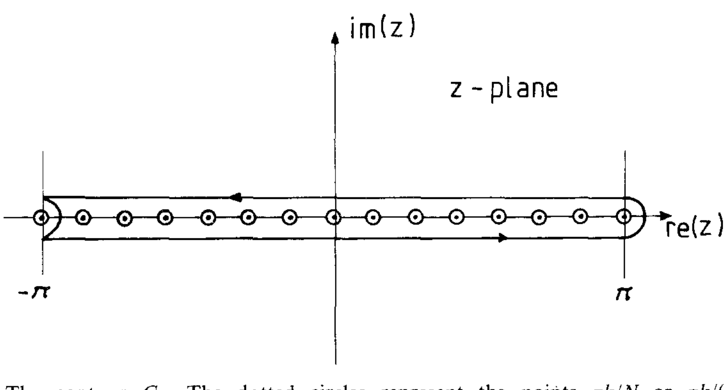

Fig. 1. The contour C_1. The dotted circles represent the points $\pi k/N$ or $\pi k/(N+1)$, depending on whether system 1 or 2 is being treated. These points are where the sum terms come from.

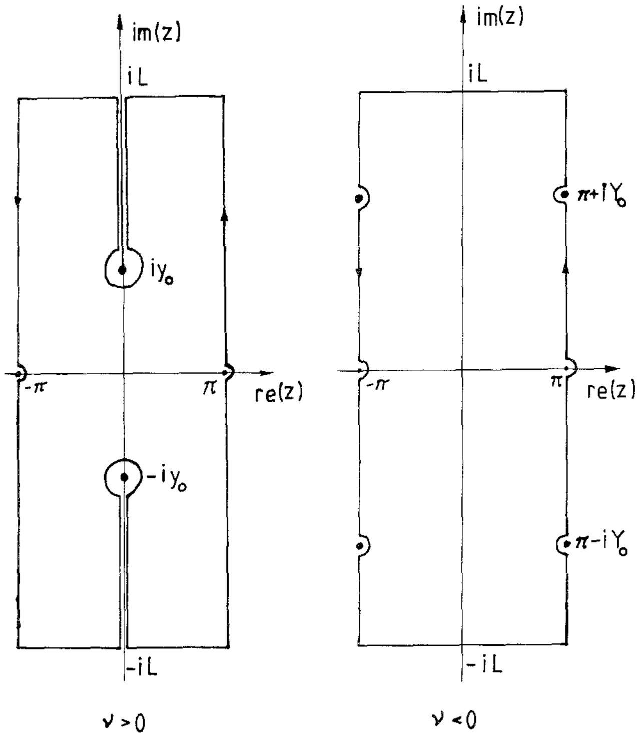

Fig. 2. The contour C_2 for $\nu > 1$ and for $\nu < -1$. Simple poles are represented by heavy dots. The poles along the real axis are omitted.

and $O(e^{-(N+2)L})$ for $J_2(\lambda)$. These contributions tend to zero as $L \to \infty$. Thus, in both cases the integral around C_2 consists entirely of the contributions of the poles at $\cos(\zeta) = \nu$. These may be evaluated fairly simply and give

$$J_1(\lambda) = \frac{1}{\omega_d}\left[1 - \frac{1}{N}\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} \tanh\left(\frac{N}{2} y_0\right)\right], \qquad \lambda > 0 \tag{54}$$

$$J_2(\lambda) = \frac{1}{4N\lambda}\left[\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} \coth\left(\frac{N+1}{2} y_0\right) - 1\right], \qquad \lambda > 0 \tag{55}$$

$$J_1(\lambda) = \frac{1}{\omega_d}\left[1 - \frac{1}{N}\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} R_N\left(\frac{NY_0}{2}\right)\right], \qquad \lambda < 0 \tag{56}$$

$$J_2(\lambda) = \frac{1}{4N\lambda}\left[\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} R_N\left(\frac{N+1}{2} Y_0\right) - 1\right], \qquad \lambda < 0 \tag{57}$$

Here $R_N(x) = \tanh(x)$ if N even and $R_N(x) = \coth(x)$ if N odd. In both cases the function $J(\lambda)$ is continuously differentiable at $\lambda = 0$. Hence we see that the term $\partial J_j(\lambda)/\partial \lambda$ in the constraint equations is $O(1/N)$. The constraint equations are thus

$$2\Gamma = \sum_{\substack{\mathbf{k} \in R_l \\ \mathbf{k} \neq \mathbf{0}}} \frac{1}{\lambda + \omega_d/[4\xi(k)]} \frac{1}{N^d} + O\left(\frac{\beta E^2}{N}\right) \tag{58}$$

for Λ_1 and

$$2\Gamma = \sum_{\mathbf{k} \in R_2} \frac{1}{\lambda + \omega_d/[4\eta(\mathbf{k})]} \frac{1}{N(2M+1)^{d-1}} + O\left(\frac{\beta V^2}{N}\right) \tag{59}$$

on Λ_2. These results indicate that the external electric field does not affect the value of λ in the limit of a large system. We shall see below that this is because surface effects screen the electric field from the center of the system.

We may now study the case $\lambda = 0$. The sums on $\mathbf{k}$ are then simple and give

$$\Gamma = \Gamma_0(d) = \frac{2d}{\omega_d} + O\left(\frac{1}{N}\right) \qquad \text{when} \quad \lambda = 0 \tag{60}$$

As we shall see below, this is an important intermediate coupling, corresponding to coupling $\Gamma = 2$ in the two-dimensional, one-component plasma. For $\lambda > -\omega_d/8d$, the function $\lambda(\Gamma)$ is an analytic function of λ with $\lambda = O(1/\Gamma)$ at small Γ and $\lambda(2d/\omega_d) = 0$. For $d = 1$ or 2, $\lambda(\Gamma) \to -\omega_d/8d$ as $\Gamma \to \infty$. For $d \geqslant 3$ the situation is more complicated. In the sum on $\mathbf{k}$ for the constraint equation on Λ_1, each sum on $0 \leqslant k_\alpha \leqslant N-1$ may be written as a sum on $l_\alpha = N - k_\alpha$, so that the sum on $\mathbf{k} \in R_1$ with $\mathbf{k} \neq \mathbf{0}$ becomes a sum on $\boldsymbol{l} \in R_3 = [1, N]^{\otimes 3}$ with $\boldsymbol{l} \neq \mathbf{N}_0 = (N, N, N)$. For $\lambda < 0$, the constraint equation may then be written as

$$2\Gamma = \frac{\omega_d}{4\lambda^2 N^d} \sum_{\substack{\boldsymbol{l} \in R_3 \\ \boldsymbol{l} \neq \mathbf{N}_0}} \left[\left(\frac{\omega_d}{4|\lambda|} - d\right) - \sum_{\alpha=1}^{d} \cos\left(\frac{\pi l_\alpha}{N}\right)\right]^{-1} - |\lambda|^{-1} + O\left(\frac{1}{N}\right) \tag{61}$$

This sum may be written as an integral when $N \to \infty$, and for $\lambda > \lambda_c = -\omega_d/8d$ an analytic function $\lambda(\Gamma)$ results. At $\lambda = \lambda_c$, $\omega_d/4|\lambda| = 2d$ and so $\Gamma = \Gamma_c$ with

$$2\Gamma_c(d) = \frac{8d}{\omega_d}\left[\frac{2d}{(2\pi)^d}\int_{[-\pi,\pi]^d} d^d\mathbf{k} \left(d + \sum_{\alpha=1}^{d} \cos k_\alpha\right)^{-1} - 1\right] \tag{62}$$

For $\Gamma > \Gamma_c(d)$ the situation is further complicated. Here we must expand carefully in powers of N. We have

$$\lambda = \frac{-\omega_d}{8d\cos^2(\pi/2N)} + zN^{-d}$$

This then gives

$$z = \frac{1}{2[\Gamma - \Gamma_c(d)]} \tag{63a}$$

On Λ_2 a similar construction for λ is needed. It gives

$$\lambda = -\frac{\omega_d}{8}\left[\cos^2\left(\frac{\pi}{2(N+1)}\right) + (d-1)\cos^2\left(\frac{\pi}{2M+1}\right)\right]^{-1} + \frac{z}{\|\Lambda_2\|}$$

with

$$z = 2/[\Gamma - \Gamma_c(d)] \tag{63b}$$

4. GLOBAL SUM RULES

The first global average we examine is the average total charge on Λ_2, given by Eq. (46). The summand here contains a factor $b(k)[1-(-1)^k]$, and $b(k)$ [see Eq. (23)] contains a factor $1+(-1)^k$, so that the summand is zero for all k. Thus, on Λ_2

$$U(\Gamma) = 0 \tag{64}$$

The Dirichlet system carries zero charge on average. One can view this result as a consequence of the fact that on Λ_2, $\Psi_1(\mathbf{n}) = \frac{1}{2}V[1 - 2n/(N+1)]$ has zero average across the lattice.

The next object of interest is the mean dipole moment component parallel to the applied field. On Λ_1, this is, from Eqs. (37) and (21),

$$M_1 = EN^d \frac{1}{8N^2\lambda} \sum_{\substack{k=-(N-1) \\ k\neq 0}}^{N} \frac{[1-(-1)^k][1+\cos(\pi k/N)]}{[\nu - \cos(\pi k/N)][1-\cos(\pi k/N)]} \tag{65}$$

This sum may be written as a contour integral using $p_+(\zeta, N)$ as with $J_1(\lambda)$ in Section 3. If the contour C_1 is used, then there is a contribution from the pole at $\zeta = 0$, which must be subtracted out. The result is

$$M_1 = E\,\|\Lambda_1\| \left[\frac{1}{\omega_d} - \frac{1}{8\pi N\lambda}\oint_{C_1} \frac{p_+(\zeta, N)}{\nu - \cos\zeta}\,\frac{1+\cos\zeta}{1-\cos\zeta}\,d\zeta\right] \tag{66}$$

The integral in Eq. (66) may now be evaluated by distorting the contour C_1 into the contour C_2. This gives

$$M_1 = \frac{E\,\|A_1\|}{\omega_d}\left[1 - \frac{1}{N}\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} \tanh\left(\frac{N}{2}\,y_0\right)\right] \qquad \text{for} \quad \lambda > 0 \tag{67}$$

$$M_1 = \frac{E\,\|A_1\|}{\omega_d}\left[1 - \frac{1}{N}\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} R_N\left(\frac{NY_0}{2}\right)\right] \qquad \text{for} \quad \lambda < 0 \tag{68}$$

From Eqs. (38), (39), and (23), M_2 on A_2 may be written

$$M_2 = \frac{V\,\|A_2\|}{16N\lambda}\left\{(1+v)\sum_{k=-N}^{N+1} \frac{1+(-1)^k}{v - \cos[\pi k/(N+1)]} - 2N - 2\,\frac{v+1}{v-1}\right\} \tag{69}$$

This may be written as a contour integral around C_1, using the function $p_-(\zeta, N+1)$. The contour may be distorted into C_2 and then evaluated. The procedure gives

$$M_2 = \frac{N+1}{8N\lambda}\,V\,\|A_2\|\left[\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} \coth\left(\frac{N+1}{2}\,y_0\right) - 1 - \frac{2v}{(N+1)(v-1)}\right] \tag{70}$$

for $\lambda > 0$ and

$$M_2 = \frac{N+1}{8N\lambda}\,V\,\|A_2\|\left[\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} R_N\left(\frac{N+1}{2}\,Y_0\right) - 1 - \frac{2v}{(N+1)(v-1)}\right] \tag{71}$$

for $\lambda < 0$.

The next global property is the first Stillinger–Lovett sum rule, which evaluates

$$G_1(\Gamma, \mathbf{m}) = \sum_{\substack{\mathbf{n} \in A \\ \mathbf{n} \neq \mathbf{m}}} \langle q(\mathbf{n})\, q(\mathbf{m}) \rangle \tag{72}$$

We may write this as

$$G_1(\Gamma, \mathbf{m}) = Q^2 \sum_{\mathbf{n} \in A} P_{(2)}(m, n) - \langle q^2(\mathbf{m}) \rangle + \langle q(\mathbf{m}) \rangle \left\langle \sum_{\mathbf{n} \in A} q(\mathbf{n}) \right\rangle \tag{73}$$

Now the last term in Eq. (73) is zero on A_1 by the charge neutrality constraint [Eq. (13)] and zero on A_2 by the result for $U(\Gamma)$ [Eq. (64)].

The sum over $P_{(2)}(\mathbf{m}, \mathbf{n})$ in Eq. (73) may be evaluated from Eq. (41) or (42). On Λ_1, $\sum_{\mathbf{n} \in \Lambda_1} F(\mathbf{k}, \mathbf{n}) = 0$ if $\mathbf{k} \neq \mathbf{0}$ by the orthogonality conditions on the $F(\mathbf{k}, \mathbf{n})$, and thus, on Λ_1,

$$G_1(\Gamma, \mathbf{m}) = -\langle q^2(\mathbf{m})\rangle \tag{74}$$

which is an almost trivial result on Λ_1. On Λ_2 a similar manipulation gives

$$\begin{aligned} G_1(\Gamma, \mathbf{m}) = & -\langle q^2(\mathbf{m})\rangle + \frac{Q^2}{8\Gamma(N+1)\lambda} \\ & \times \sum_{k=-N}^{N+1} \frac{1-(-1)^k}{\nu - \cos[\pi k/(N+1)]} \\ & \times \left\{ \exp\left[\frac{i\pi k}{N+1}(m-1)\right] - \exp\left[\frac{i\pi k}{N+1}(m+1)\right]\right\} \end{aligned} \tag{75}$$

The sum here may be written as a contour integral around C_1 using $p_-(\zeta, N+1)$. Thus,

$$G_1(\Gamma, \mathbf{m}) = -\langle q^2(\mathbf{m})\rangle - \frac{Q^2}{8\pi\Gamma\lambda} \oint_{C_1} \frac{p_-(\zeta, N+1)}{\nu - \cos(\zeta)} \left(e^{i(m-1)\zeta} - e^{i(m+1)\zeta}\right) d\zeta \tag{76}$$

This contour integral may then be distorted to C_2 and calculated, giving

$$G_1(\Gamma, m) = -\langle q^2(m)\rangle - \frac{Q^2}{2\lambda\Gamma} \frac{\sinh\{[(N+1)/2 - m]\, y_0\}}{\sinh[\frac{1}{2}(N+1)\, y_0]} \quad \text{for } \lambda > 0 \tag{77}$$

and

$$G_1(\Gamma, \mathbf{m}) = -\langle q^2(\mathbf{m})\rangle - \frac{Q^2}{2\lambda\Gamma}(-1)^m S(N, m, Y_0) \qquad \text{for} \quad \lambda < 0 \tag{78}$$

where

$$S(N, m, Y_0) = \begin{cases} \cosh\left[\left(\dfrac{N+1}{2} - m\right) Y_0\right] \Big/ \cosh\left(\dfrac{N+1}{2} Y_0\right) & \text{for } N \text{ even} \\ \sinh\left[\left(\dfrac{N+1}{2} - m\right) Y_0\right] \Big/ \sinh\left(\dfrac{N+1}{2} Y_0\right) & \text{for } N \text{ odd} \end{cases} \tag{79}$$

for N large and m close to the center of the system, this gives $G_1(\Gamma, \mathbf{m}) = -\langle q^2(\mathbf{m})\rangle$. For m finite, in the limit $N \to \infty$ we obtain

$$G_1(\Gamma, \mathbf{m}) = \begin{cases} -\langle q^2(m)\rangle - \dfrac{Q^2}{2\Gamma\lambda} e^{-my_0} & \lambda > 0 \\ -\langle q^2(m)\rangle - \dfrac{Q^2}{2\Gamma\lambda}(-1)^m e^{-mY_0} & \lambda < 0 \end{cases} \tag{80}$$

For $N+1-m=m'$ finite in the limit $N\to\infty$ we obtain similar results, namely

$$G_1(\Gamma, \mathbf{m}) = \begin{cases} -\langle q^2(m)\rangle + \dfrac{Q^2}{2\Gamma\lambda} e^{-m'y_0} & \lambda > 0 \\ -\langle q^2(m)\rangle + (-1)^{m'} \dfrac{Q^2}{2\Gamma\lambda} e^{-m'Y_0} & \lambda < 0 \end{cases} \tag{81}$$

These results show quite explicitly that while deviation from the strict neutrality of the counter charge cloud about a given charge is possible, it does not occur in the bulk of the system, but is confined to the surfaces. The screening length is $1/y_0$ or $1/Y_0$, depending on whether $\lambda \gtrless 0$.

The remaining sum rule we consider is the second Stillinger–Lovett sum rule, which gives a value to $g_{(2)}(\Gamma) = \operatorname{trace} G_{(2)}(\Gamma)$ on Λ_1 and to $G_{(2)}(\Gamma)_{11}$ on Λ_2. On Λ_2, $G_{(2)}(\Gamma)_{\alpha\alpha}$ may be identified as $M_1/(\Gamma E \|\Lambda_1\|)$, which is evaluated in Eq. (68). Thus, on Λ_1

$$g_{(2)}(\Gamma) = \frac{d}{\Gamma\omega_d}\left[1 - \frac{1}{N}\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} \tanh\left(\frac{N}{2} y_0\right)\right] \tag{82}$$

for $\lambda > 0$, and for $\lambda < 0$ the same form applies, but with $R_N(NY_0/2)$ replacing $\tanh(\frac{1}{2}Ny_0)$. In the limit $N\to\infty$ this gives $g_{(2)}(\Gamma) = d/\Gamma\omega_d$, which is the correct value for a plasma system with Neumann boundary conditions.

On Λ_2, Eqs. (39) and (45) give

$$G_{(2)}(\Gamma)_{11} = \frac{N+1}{8\Gamma N\lambda} \sum_{K+-N}^{N+1} \frac{1+\cos[\pi k/(N+1)]}{v\cos[\pi k/(N+1)]} - \frac{N+1}{\Gamma N\omega_d} \tag{83}$$

The function $r(\zeta, N+1) = \{\exp[2i(N+1)\zeta] - 1\}^{-1}$ has simple poles of residue $-i/2(N+1)$ at $\zeta = \pi k/N+1$. Hence Eq. (83) may be written as

$$G_{(2)}(\Gamma)_{11} = \frac{(N+1)^2}{4\Gamma N\lambda}\left[\frac{v+1}{2\pi}\oint_{C_1} \frac{r(\zeta, N+1)}{v-\cos\zeta} d\zeta - 1\right] - \frac{N+1}{N\Gamma\omega_d} \tag{84}$$

The integral here may be evaluated by distorting C_1 into C_2. The result is

$$G_{(2)}(\Gamma)_{11} = \frac{(N+1)^2}{4\Gamma N\lambda}\left\{\left(1 + \frac{8\lambda}{\omega_d}\right)^{1/2} \coth[(N+1)\, y_0] - 1\right\} - \frac{N+1}{N\Gamma\omega_d} \tag{85}$$

for $\lambda > 0$, while for $\lambda < 0$ this is unchanged except for Y_0 replacing y_0. This means that $G_{(2)}(\Gamma)_{11}$ does not exist on Λ_2 in the thermodynamic limit and this, too, is to be expected in a system with a Dirichlet boundary condition.

5. DISTRIBUTION FUNCTIONS

5.1. One-Charge Distribution Functions

On Λ_1, Eqs. (35) and (21) give the one-charge distribution function as

$$\langle q(\mathbf{n})\rangle = -\frac{E}{8N\lambda}\sum_{k=-(N-1)}^{N}\frac{1-(-1)^k}{\nu-\cos(\pi k/N)} \times\left\{\exp\left(\frac{i\pi k}{N}n\right)+\exp\left[\frac{i\pi k}{N}(n-1)\right]\right\} \tag{86}$$

where $n=\mathbf{e}_1\cdot\mathbf{n}$. This may be written as an integral using $p_-(\zeta, N)$ around C_1. The contour may then be distorted to C_2 and evaluated. Thus

$$\langle q(\mathbf{n})\rangle = -\frac{E}{4\lambda}\frac{\sinh\{[(N+1)/2-n]\,y_0\}}{\sinh(\frac{1}{2}y_0)\cosh(\frac{1}{2}Ny_0)} \quad \text{for} \quad \lambda>0 \tag{87}$$

$$\langle q(\mathbf{n})\rangle = \frac{-E(-1)^n}{4\lambda\cosh(\frac{1}{2}Y_0)}\,T_N(N, n, Y_0) \quad \text{for} \quad \lambda<0 \tag{88}$$

with

$$T_N(N, n, Y_0)=\begin{cases}\cosh\left[\left(\dfrac{N+1}{2}-n\right)Y_0\right]\Big/\cosh\left(\dfrac{N}{2}Y_0\right) & \text{for } N \text{ even}\\ \sinh\left[\left(\dfrac{N+1}{2}-n\right)Y_0\right]\Big/\sinh\left(\dfrac{N}{2}Y_0\right) & \text{for } N \text{ odd}\end{cases} \tag{89}$$

In the limit $N\to\infty$ with n finite, we obtain

$$\langle q(n)\rangle = \begin{cases} -\dfrac{E}{2\lambda}e^{-ny_0} & \text{for} \quad \lambda>0\\ -\dfrac{E}{2\lambda}(-1)^n e^{-nY_0} & \text{for} \quad \lambda<0\end{cases} \tag{90}$$

and for $n'=N+1-n$ finite we find

$$\langle q(N+1-n)\rangle = \begin{cases} \dfrac{E}{2\lambda}e^{-n'y_0} & \text{for} \quad \lambda>0\\ \dfrac{E}{2\lambda}(-1)^{n'} e^{-n'Y_0} & \text{for} \quad \lambda<0\end{cases} \tag{91}$$

We see that $\langle q(n)\rangle = 0$ in the bulk of the lattice in the thermodynamic limit. At the surfaces these are screened surface charge distributions proportional to the electric field, with (in the case $\lambda > 0$) a positive charge near $n = N+1$, where the external potential is negative, and a negative charge near $n = 1$, where the external potential is positive. Notice that if the potential due to this external field were finite as $N \to \infty$ so that $E = O(N^{-1})$, we would be able to compare the results directly with those below on Λ_2. In that case the surface charges would be small, $O(N^{-1})$, a reflection of the effect of the Neumann boundary condition.

On Λ_2, the one-charge distribution function is given by Eqs. (36) and (23) and these results may be reduced to

$$\langle q(n)\rangle = -\frac{V}{8(N+1)\lambda} \sum_{k=-N}^{N+1} \frac{1+(-1)^k}{\nu - \cos[\pi k/(N+1)]} \times \left\{ \exp\left[\frac{\pi i k(n-1)}{N+1}\right] - \exp\left[\frac{\pi i k}{N+1}(n+1)\right] \right\} \tag{92}$$

Writing this as a contour integral around C_1 using $p_-(\zeta, N+1)$, distorting the contour to C_2, and evaluating the integral gives

$$\langle q(n)\rangle = \begin{cases} -\dfrac{V}{2\lambda} \dfrac{\sinh\{[(N+1)/2 - n]\, y_0\}}{\sinh[\frac{1}{2}(N+1)\, y_0]} & \text{for} \quad \lambda > 0 \\ -\dfrac{V}{2\lambda}(-1)^n\, t_N(N, n, Y_0) & \text{for} \quad \lambda < 0 \end{cases} \tag{93}$$

with

$$t_N(N, n, Y_0) = \begin{cases} \cosh\left[\left(\dfrac{N+1}{2} - n\right) Y_0\right] \Big/ \cosh\left(\dfrac{N+1}{2}\, Y_0\right) & \text{for } N \text{ even} \\ \sinh\left[\left(\dfrac{N+1}{2} - n\right) Y_0\right] \Big/ \sinh\left(\dfrac{N+1}{2}\, Y_0\right) & \text{for } N \text{ odd} \end{cases} \tag{94}$$

In the limit $N \to \infty$ with n finite or $n' = N+1-n$ finite these results reduce to, for n finite.

$$\langle q(n)\rangle = \begin{cases} -(V/2\lambda)\, e^{-n y_0}, & \lambda > 0 \\ -(V/2\lambda)(-1)^n\, e^{-n Y_0}, & \lambda < 0 \end{cases} \tag{95}$$

and for n' finite

$$\langle q(n)\rangle = \begin{cases} (V/2\lambda)\, e^{-n' y_0} & \lambda > 0 \\ (V/2\lambda)(-1)^{n'}\, e^{-n' Y_0}, & \lambda > 0 \end{cases} \tag{96}$$

These results show that in the bulk of the system $\langle q(n)\rangle = 0$ in the thermodynamic limit, because the charge distributions at either end screen the system. The magnitude of $\langle q(1)\rangle$ and $\langle q(N)\rangle$ is $(V/2\lambda)\, e^{-y_0}$ (or e^{-Y_0}) and this is $O(1)$ in an applied field $E = V/(N+1)$. If the field E were $O(1)$, then these would be charge densities $O(N+1)$ to screen it. This is quite different from the case on Λ_1. Here, on Λ_2 the Dirichlet boundary conditions have a much stronger effect on the surface charge densities than do the Neumann conditions on Λ_1.

5.2. Two-Charge Distribution Functions

Here we use Eqs. (41) and (42). These may be written as

$$P_{(2)}(m, n) = -\frac{1}{4\Gamma} D_{\mathbf{n}}^2 \sum_{\mathbf{k} \in R_1} \frac{F(\mathbf{k}, \mathbf{m})\, F(\mathbf{k}, \mathbf{n})}{\omega_d/4 + \lambda\xi(\mathbf{k})} \tag{97}$$

on Λ_1. The usual constraint $\mathbf{k} \neq \mathbf{0}$ has been omitted because $D_{\mathbf{n}}^2 F(\mathbf{0}, \mathbf{n}) = 0$.

On Λ_2 we have

$$P_{(2)}(m, n) = -\frac{1}{4\Gamma} D_{\mathbf{n}}^2 \sum_{\mathbf{k} \in R_2} \frac{G(\mathbf{k}, \mathbf{m})\, G^*(\mathbf{k}, \mathbf{n})}{\omega_d/4 + \lambda\eta(\mathbf{k})} \tag{98}$$

At $\lambda = 0$, these sums may be evaluated using the orthonormality property of the appropriate eigenfunctions. Thus, at $\Gamma = 2d/\omega_d$

$$P_{(2)}(\mathbf{m}, \mathbf{n}) = \delta_{\mathbf{m},\mathbf{n}} - \frac{1}{2d} \sum_{\alpha=1}^{d} (\delta_{\mathbf{m},\mathbf{n}+\mathbf{e}_\alpha} + \delta_{\mathbf{m},\mathbf{n}-\mathbf{e}_\alpha}) \tag{99}$$

This means that the two-charge distribution function is of range 1 at $\Gamma = \Gamma_0(d) = 2d/\omega_d$.

On both lattices, in the thermodynamic limit with $\mathbf{m}$ and $\mathbf{n}$ in the bulk interior of the lattice, the two-charge distribution function may be written for $\lambda > 0$ as

$$\begin{aligned} P_{(2)}(\mathbf{m}, \mathbf{n}) &= p(\mathbf{m} - \mathbf{n}) \\ &= -\frac{1}{4\Gamma\lambda} D_{\mathbf{n}}^2 (2\pi)^{-d} \int_{[-\pi,\pi]^d} d^d\mathbf{k}\, \frac{\exp[i\mathbf{k}\cdot(\mathbf{m}-\mathbf{n})]}{\mu - \sum_{\alpha=1}^{d} \cos(k_\alpha)} \end{aligned} \tag{100}$$

where $\mu = d + \omega_d/4\lambda$. For $\lambda < 0$ some rearrangement of the integrals gives an alternative form

$$p(\mathbf{m}) = \frac{1}{4\Gamma\lambda} D_{\mathbf{n}}^2 (2\pi)^{-d} \int_{[-\pi,\pi]^3} d^d\mathbf{k}\, \frac{\exp(-i\mathbf{k}\cdot\mathbf{m})}{|\mu| - \sum_{\alpha=1}^{d} \cos(k_\alpha)} \prod_{\alpha=1}^{d} (-1)^{m_\alpha} \tag{101}$$

provided λ is not close to its critical value $\lambda_c(d) = -\omega_d/8d$, if $d \geqslant 3$. We should remember here that $\mu < -d$. Thus, for $\lambda > 0$ and $|\mathbf{m}|$ large

$$p(\mathbf{m}) \sim -\frac{1}{2\Gamma\lambda} D_{\mathbf{n}}^2 \frac{1}{(2\pi)^d} \int d^d\mathbf{k} \frac{\exp(i\mathbf{k}\cdot\mathbf{m})}{\omega_d/2\lambda + \mathbf{k}^2} \tag{102}$$

since the major contribution to the integral comes from near $\mathbf{k} = \mathbf{0}$. Thus,

$$p(\mathbf{m}) \sim \exp(-|\mathbf{m}|/L_{D+}) \tag{103}$$

where $L_{D+} = (2\lambda/\omega_d)^{1/2}$. These correlation functions decay monotonically with a correlation length that decreases with decreasing temperature until $\Gamma = \Gamma_0(d)$. For $\lambda < 0$ the correlation function is modulated by a factor $\prod_{\alpha=1}^d (-1)^{m_\alpha}$ and while $\lambda \neq \lambda_c(d)$ (if $d \geqslant 3$),

$$p(\mathbf{m}) \sim \prod_{\alpha=1}^{d} (-1)^{m_\alpha} \exp(-|\mathbf{m}|/L_{D-}) \tag{104}$$

where

$$L_{D-} = \left(\frac{2|\lambda|}{\omega_d}\right)^{1/2} \left(1 + \frac{8d\lambda}{\omega_d}\right)^{-1/2}$$

so that this correlation length increases as the temperature decreases further, diverging as $\lambda \to \lambda_c(d) = -\omega_d/8d$.

With these thermodynamic limit correlation functions, we may consider the quantity

$$g_{\mathrm{SL}}(\Gamma) = \sum_{\mathbf{n}} \mathbf{n}^2 p(\mathbf{n}) \tag{105}$$

which is expected to be $-2d/\Gamma\omega_d$ from the Stillinger–Lovett sum rule. We may use the identity $x^{-1} = \int_0^\infty dt \exp(-tx)$ to obtain

$$p(\mathbf{n}) = -\frac{1}{4\Gamma\lambda} D_{\mathbf{n}}^2 \int_0^\infty dt\, e^{-\mu t} \prod_{\alpha=1}^{d} I_{n_\alpha}(t) \tag{106}$$

from Eq. (100), which holds for all $\lambda > 0$. The relevant sum of Bessel functions that occur in the sum for $g_{\mathrm{SL}}(\Gamma)$ is[21]

$$\sum_{n=-\infty}^{\infty} I_n(t) = e^t \tag{107}$$

This gives

$$g_{\mathrm{SL}}(\Gamma) = -2d/\omega_d\Gamma \tag{108}$$

The manipulations required for $\lambda < 0$ are a little more complicated, but they still give Eq. (108). Thus, in both boundary conditions the bulk of the system has correlations that obey the standard form of the second Stillinger–Lovett sum rule.[11]

6. THE CHARGE ORDERED PHASE IN THREE DIMENSIONS

In this section we consider $d = 3$ and concentrate to begin with on the model on Λ_2. We are concerned with the bulk properties of the system. From Eq. (29) the critical value of λ is $\lambda_c(3) = -\omega_3/4\eta(\mathbf{k}_0)$, where $\mathbf{k}_0 = (N, M, M)$, and thus in the thermodynamic limit, $\eta(\mathbf{k}_0) = 6$. The parameter λ is then, for $\Gamma \geqslant \Gamma_c(3)$

$$\lambda = \lambda_c(3) + z/\|\Lambda_3\| \tag{109}$$

where $z = 2/[\Gamma - \Gamma_c(3)]$ [Eq. (63b)]. In the sum in Eq. (42) for $P_{(2)}(\mathbf{m}, \mathbf{n})$ with $\Gamma > \Gamma_c(3)$, the contributions of the four-vectors $\mathbf{k}$ with $\eta(\mathbf{k}) = \eta(\mathbf{k}_0)$ must be separated off and treated differently. We define, for vectors $\mathbf{n}_0 = (\gamma N, 0, 0)$ and $\mathbf{m}_0 = \mathbf{n}_0 + \mathbf{m}$,

$$p(\mathbf{m}, \gamma) = \lim_{\|\Lambda_2\| \to \infty} P_{(2)}(\mathbf{m}_0, \mathbf{n}_0) = p^0(\mathbf{m}, \gamma) + p(\mathbf{m}) \tag{110}$$

where $p^0(\mathbf{m}, \gamma)$ is the contribution from the four-vectors $\mathbf{k}$ with $\eta(\mathbf{k}) = \eta(\mathbf{k}_0)$. The limit is taken with $0 < \gamma < 1$ and γN an integer. First we have

$$p^0(\mathbf{m}, \gamma) = (1 - T/T_c)[1 - \cos(2\pi\gamma)] \prod_{\alpha=1}^{3} (-1)^{m_\alpha} \tag{111}$$

The remainder of the two-charge distribution function is, after taking the thermodynamic limit and rearranging the integrand,

$$p(\mathbf{m}) = -\frac{6}{\omega_3 \Gamma} D_{\mathbf{m}}^2 \prod_{\alpha=1}^{3} (-1)^{m_\alpha} \frac{1}{(2\pi)^3} \int_{[-\pi,\pi]^3} d^3\mathbf{k} \, \frac{\exp(-i\mathbf{k} \cdot \mathbf{m})}{3 - \sum_{\alpha=1}^{3} \cos(k_\alpha)} \tag{112}$$

This may be estimated for large $|\mathbf{m}|$ by expanding the integrand about $\mathbf{k} = \mathbf{0}$, since the small-$|\mathbf{k}|$ region dominates the integral at large $|\mathbf{m}|$. This gives

$$p(\mathbf{m}) \sim \frac{9}{\pi^2 \Gamma |\mathbf{m}|} \prod_{\alpha=1}^{3} (-1)^{m_\alpha} \tag{113}$$

Thus, for $\Gamma > \Gamma_c(3)$, the three-dimensional system develops long-range order: charges oscillate in sign across the lattice. The correlation length remains infinite, which is characteristic of spherical models. The critical exponent for the order parameter is $\beta = \frac{1}{2}$, as expected. The value of the order parameter varies on a thermodynamic scale across the lattice, as can be seen from Eq. (111). The factor $[1 - \cos(2\pi\gamma)]$ there reflects the amplitude $|G(\mathbf{k}_0, \mathbf{m})|^2$ of the eigenvectors selected out by the constraint equation when $\Gamma > \Gamma_c(d)$. On Λ_1 a similar behavior is seen with $\mathbf{n}_0 = (\gamma_1, \gamma_2, \gamma_3)\, N$, $\mathbf{m}_0 = \mathbf{n}_0 + \mathbf{m}$, and

$$p(\mathbf{m}, \gamma) = \lim_{\|\Lambda_1\| \to \infty} P_{(2)}(\mathbf{m}_0, \mathbf{n}_0) = p^0(\mathbf{m}, \gamma) + P(\mathbf{m}) \tag{114}$$

The only change is that

$$p(\mathbf{m}, \gamma) = (1 - T/T_c) \prod_{\alpha=1}^{3} [(-1)^{m_\alpha}(1 + \cos 2\pi\gamma_\alpha)] \tag{115}$$

and the condensed phase and order parameter are modulated in all three directions. It is interesting to evaluate

$$g_{\mathrm{SL}}(\gamma) = \sum_{\mathbf{m}} \mathbf{m}^2 p(\mathbf{m}, \gamma) \tag{116}$$

This is not possible: the sums do not converge. However, since these bulk two-charge distribution functions have orientational symmetry, we may consider

$$\bar{g}_{\mathrm{SL}}(\gamma) = \lim_{\mu \to 0} \sum_{\mathbf{m}} \mathbf{m}^2 p(\mathbf{m}, \gamma) \exp(-\mu \mathbf{m}^2) \tag{117}$$

The relevant sums may be evaluated using the ϑ-function formula

$$\sum_{m=-\infty}^{\infty} \exp(imq - \mu m^2) = (\pi/\mu)^{1/2} \sum_{n=-\infty}^{\infty} \exp[-(n + q/2\pi)^2/\mu] \tag{118}$$

The sum of $p^0(m, \gamma)$ then gives zero in the limit $\mu \to 0$, since only the value $q = \pi$ is relevant. The sum over $p(\mathbf{m})$ may be evaluated in the same way, and the integral evaluated asymptotically at small μ. This gives

$$\bar{g}_{\mathrm{SL}}(\gamma) = \lim_{\mu \to 0} -27\pi^4\mu/4\Gamma = 0 \tag{119}$$

Thus, the condensed system has no susceptibility, corresponding to a dielectric constant $\varepsilon = 1$ throughout the bulk of the sample.

7. DISCUSSION

The systems introduced in this paper do behave as Coulombic plasma systems. They screen external electric fields from the center of a thermodynamically large system, and the screening is exponentially fast. The systems obey the first and second Stillinger–Lovett relations in the interior when the thermodynamic limit is taken. The system susceptibility [$g_{(2)}(\Gamma)$ on Λ_1, $G_{(2)}(\Gamma)_{11}$ on Λ_2] obeys the appropriate form of the Stillinger–Lovett relation for the electrostatic boundary conditions applying. At weak coupling the charge–charge distribution functions show exponential decay with distance, with the correlation length decreasing as the coupling Γ increases. These observations establish that we are dealing with Coulombic systems of good standing. The spherical constraint introduces an extra long-range interaction, but this does not interfere with the Coulombic nature of the systems.

The coupling constant Γ separates into three ranges, (i) $0<\Gamma<\Gamma_0(d)$; (ii) $\Gamma_0(d)<\Gamma<\Gamma_c(d)$; (iii) $\Gamma_c(d)<\Gamma$. The third range only occurs in $d\geqslant 3$. For $0<\Gamma<\Gamma_0(d)=2d/\omega_d$, the charge–charge correlation function behaves as in a weakly coupled plasma. At $\Gamma=\Gamma_0(d)$ the two-charge distribution function has a range of one lattice spacing, which corresponds to a correlation length minimum. On $\Gamma_0(d)<\Gamma<\Gamma_c(d)$ [or $\Gamma_0(d)<\Gamma$ for $d=1, 2$], the two-charge distribution function oscillates in sign and decays exponentially with a correlation length that increases as Γ increases. For $d\geqslant 3$ this correlation length diverges as $\Gamma\to\Gamma_c(d)$ from below. This feature of the distribution function suggests that the coupling $\Gamma=\Gamma_0(d)$ corresponds to coupling $\Gamma=2$ in the one-component, two-dimensional plasma. There the correlation function also seems to display a minimum in its correlation length, with monotonic decay of correlations for $\Gamma<2$ and oscillatory decay for $\Gamma>2$. Finding this behavior in both types of model suggests that it may be a general feature of Coulombic systems. It should be noted that in spite of the change in the behavior of the two-charge distribution functions, there is no singularity in the thermodynamic behavior, neither in these spherical models nor in the two-dimensional, one-component plasma.

These charged spherical models are not complete guides to the behavior of Coulombic systems. They do not have a Kosterlitz–Thouless transition in two dimensions, because the charge variables are continuous. In three dimensions they produce a somewhat strange dielectric phase, apparently with dielectric constant $\varepsilon=1$. One way of interpreting this is to say that the system cannot develop any local dipole moment density when in its condensed phase. It is clear at least that it is difficult to define the response of the bulk interior of these systems to an applied external field because any external field is automatically screened by the surface layers. Unfortunately, it is not possible to see slow decay of distribution functions along surfaces in these models. Their boundary conditions correspond to zero and infinite external dielectric constants, and in those cases no slow decay of distribution functions is expected.[22,23]

One feature of spherical models in general is that the spherical constraint spreads inhomogeneities out over thermodynamically large volumes. In the nearest neighbor spherical Ising-spin model, the two-phase interface is delocalized.[24] We see a similar spreading with the dependence of $p^0(\mathbf{m}, \gamma)$ on γ. Nonetheless, we notice that there are localized surface effects in these systems: the surface charge densities are localized exponentially at the system surfaces.

The models introduced in this paper can be expected to give some guide to the behavior of Coulombic systems in general. In particular they allow extensions to the case where the system is confined by walls of some dielectric material with dielectric constant other than $O(A_1)$ or $\infty(A_2)$. Work on these problems is now in progress.

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