

Solvable Isotherms for a Two-Component System of Charged Rods on a Line

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The Coulomb system consisting of an equal number of positive and negative charged rods confined to a one-dimensional lattice is studied. The grand partition function can be calculated exactly at two values of the coupling constant $\Gamma \equiv q^2/k_B T$ (q denoting the magnitude of the charges). The exact results lead to the conjecture that in the complex scaled fugacity plane ξ , all the zeros of the grand partition function lie on the negative real axis for $\Gamma < 2$, on the point $\xi = -1$ for $\Gamma = 2$, and on the unit circle for $\Gamma > 2$. In addition, for $\Gamma > 4$, we conjecture in general and prove at $\Gamma = 4$ that the zeros pinch the real axis in the thermodynamic limit, with an essential singularity in the pressure at the reduced density $1/2$.

KEY WORDS: Random matrices; quantum Brownian motion; partition function zeros; phase transition.

1. INTRODUCTION AND SUMMARY

In 1962 Dyson⁽¹⁻³⁾ defined three types of ensembles of random matrices: orthogonal, unitary, and symplectic. These matrix ensembles were used to formulate a statistical theory of energy levels in complex nuclei and, subsequently, small metal particles.⁽⁴⁾ The physical observables of the theory can be expressed in terms of the probability density function of the eigenvalues, which, since the matrices are unitary, lie on the unit circle in the complex plane.

The probability of finding the eigenvalues $e^{i\phi_j}$ within the intervals $\phi_j \in [\theta_j, \theta_j + d\theta_j]$, $j = 1, \dots, N$, is given by

$$P_N^{(1)}(\theta_1, \dots, \theta_N) d\theta_1 \cdots d\theta_N \quad (1.1)$$

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where

$$P_{NF}^{(1)} = C_{NF}^{(1)} \prod_{1 \leq j < k \leq N} |e^{i\theta_j} - e^{i\theta_k}|^\Gamma \quad (1.2)$$

Here $\Gamma=1$ for the orthogonal, $\Gamma=2$ for the unitary, and $\Gamma=4$ for the symplectic ensemble. $C_{NF}^{(1)}$ is a constant fixed by normalization.

It was immediately observed by Dyson that P_{NF} is identical (up to a normalization constant) to the Boltzmann factor for the one-component log-gas on a circle. This is a classical Coulomb system of N mobile particles of charge $q_k = q$ confined to a circle of radius R . With $\theta_1, \theta_2, \dots, \theta_N$ specifying the positions of the particles, the interaction potential is the two-dimensional Coulomb potential corresponding to charged rods

$$V(\theta_j, \theta_k) = -q_j q_k \log[(R/L) |e^{i\theta_j} - e^{i\theta_k}|] \quad (1.3)$$

Here L is an arbitrary length scale, which we take to equal unity. Also present is a neutralizing background charge density, which is necessary to obtain thermodynamic stability. Since the background only contributes a constant to the Hamiltonian, we see immediately from (1.3) that (1.2) corresponds to the Boltzmann factor for this system if we take

$$\Gamma = q^2/k_B T \quad (1.4)$$

A third physical interpretation of the probability density (1.2) is as the ground-state wave function of an N -body Schrödinger equation. Let us write

$$P_{NF}^{(1)} = (\psi_0)^2 \quad (1.5)$$

It was observed by Sutherland⁽⁵⁾ that ψ_0 is the ground-state wave function of the Schrödinger equation with Hamiltonian

$$H = - \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + \frac{g\pi^2}{L^2} \sum_{1 \leq j < k \leq N} \frac{1}{\sin^2 \pi(x_k - x_j)/L} \quad (1.6)$$

with $x_k = L\theta_k/2\pi$. [Note that in the limit $L \rightarrow \infty$ the potential becomes $V(r) = g/r^2$.] The wave function is subject to periodic boundary conditions, and is defined to be positive in the region $0 \leq x_1 \leq x_2 \leq \dots \leq x_N \leq L$, the choice of ψ_0 in other regions depending on the particle type—boson or fermion. The coupling constants Γ and g are related by the equation

$$\Gamma = 1 + (1 + 2g)^{1/2}, \quad g \geq -1/2 \quad (1.7)$$

The probability density (1.2) at $\Gamma = 1, 2,$ and 4 has a remarkable solvability property: the n -particle distributions, which are defined in terms of the integrals

$$\prod_{l=p}^N \int_0^{2\pi} d\theta_l P_{N\Gamma}, \quad 1 \leq p \leq N \tag{1.8}$$

can all be calculated in closed form.⁽⁶⁾ In principle, these distributions can be observed directly from the energy level data.⁽⁷⁾ It is our purpose to study three further probability densities which share solvability properties comparable with (1.2).

These probability densities have $2N$ variables and are defined by

$$P_{N\Gamma}^{(2)} = C_{N\Gamma}^{(2)} |A_N(e^{i\theta_1}, \dots, e^{i\theta_N}, e^{i\phi_1}, \dots, e^{i\phi_N})|^\Gamma \tag{1.9}$$

where

$$A_N(x_1, \dots, x_N; y_1, \dots, y_N) = \prod_{1 \leq j < k \leq N} (x_k - x_j)(y_k - y_j) \Big/ \prod_{j=1}^N \prod_{k=1}^N (x_j - y_k) \tag{1.10}$$

and again the solvability properties are special to the couplings $\Gamma = 1, 2,$ and 4 . This expression diverges if $\theta_j = \phi_\alpha$ for any $j, \alpha = 1, 2, \dots, N$, so we must impose a short-distance cutoff to prevent this from happening. To accomplish this and obtain the solvability properties, it is necessary to define the θ_j and ϕ_α on interpenetrating sublattices.

The most obvious interpretation of (1.9) is as the Boltzmann factor of a Coulomb gas of positive and negative charged rods confined to a circle. This is a two-parameter system, characterized by the coupling Γ [given by (1.4)] and the quantity $\rho\tau$, which is the ratio of the short-range cutoff τ to the average interparticle spacing $1/\rho$. In the thermodynamic limit the solvability properties at $\Gamma = 2$ for all values of $\rho\tau$ have been obtained by Gaudin.^(8,9)

If the charges are arranged so that they alternate in sign around the circle, that is,

$$\theta \leq \theta_1 < \phi_1 < \dots < \theta_N < \phi_N \leq 2\pi \tag{1.11}$$

the probability density (1.9) offers further physical interpretations. Such a system first arose in studies of the Kondo problem.^(10,11) In a mapping valid in the low-density, $\rho\tau \rightarrow 0$ limit, the pressure and dipole moment of the Coulomb gas were related to the ground-state energy and susceptibility, respectively, of the Kondo problem. Furthermore, the length of the circle

containing the charges is inversely related to the temperature in the Kondo problem, so the thermodynamic limit of the Coulomb gas reproduces the zero-temperature properties of the Kondo problem. More recently,⁽¹²⁾ the probability density (1.9) with the ordering (1.10) has arisen in work on two-state quantum systems.

In a previous study⁽¹³⁾ we showed that for the probability density (1.9) at $\Gamma=1$, for all $\rho\tau$, the integrals of the form (1.8) representing the grand partition function and two- and three-particle correlations can be calculated exactly, provided we adopt the ordering (1.11). Here we will exhibit the same solvability properties of the probability density (1.9) at $\Gamma=2$ and 4 without any ordering restriction on the charges. Like the system with the charges constrained to alternate in sign, the unrestricted system also has a quantum mechanical analogue.⁽¹⁴⁾ Consider the motion of a quantum mechanical particle in the presence of a periodic potential with frictional forces proportional to the particle's velocity, which couple to the environment. Using the Feynman path integral in "imaginary" time, we can integrate out the coordinates of the environment and we are left with the effective action $S_{\text{eff}} = S_0 + S_{\text{int}}$, where

$$S_0 = \int d\tau \frac{1}{2} m(\dot{q}_\tau)^2 + \frac{\eta}{4\pi} \int d\tau d\tau' \left(\frac{q_\tau - q_{\tau'}}{\tau - \tau'} \right)^2 \quad (1.12)$$

$$S_{\text{int}} = \int d\tau V(q_\tau)$$

Here q_τ denotes the particle's coordinate. With the potential chosen as

$$V(q_\tau) = -g \cos q_\tau \quad (1.13)$$

the generating functional Z for the system can be written as

$$Z = C \sum_{N=0}^{\infty} \left(\frac{g}{2} \right)^{2N} \prod_{l=1}^{2N} \int d\tau_l \exp \left[- \sum_{1 \leq i < j \leq 2N} q_i q_j U(|\tau_i - \tau_j|) \right] \quad (1.14)$$

where

$$q_j = \begin{cases} 1 & \text{for } 1 \leq j \leq N \\ -1 & \text{for } N+1 \leq j \leq 2N \end{cases} \quad (1.15)$$

$$U(r) = \begin{cases} -[1/(2\eta)]r, & r \ll 1 \\ -(1/\pi\eta) \log r, & r \gg 1 \end{cases}$$

and C is a constant.

For small g , when the short-range behavior of the potential U is unimportant, (1.14) is the grand partition function of the two-component system of charged rods on a line.

At high temperature a system of oppositely charged rods exists in a conducting phase, which means that the charges are free to respond to and screen an external charge density in the long-wavelength limit. At low temperatures the oppositely charged rods form dipoles, so the system is polar and thus in an insulating state. On the basis of some approximate analysis,^(15,16) it has been conjectured that the transition temperature, for small values of $\rho\tau$ at least, occurs at $\Gamma=2$ with an insulating phase for $\Gamma>2$ and a conducting phase for $\Gamma<2$. In the quantum analogue noted above, insulating and conducting phases correspond to a localized and mobile phase, respectively. The conjectured phase diagram⁽¹⁷⁻¹⁹⁾ has the properties noted above of the charged-rod phase diagram.

Our exact results are consistent with these predictions for the phase diagram, and furthermore strongly suggest a remarkable mathematical mechanism for the transition.

Consider the finite system defined on two interpenetrating sublattices of M sites with periodic boundary conditions. We conjecture that the zeros of the grand partition function all lie on the negative real axis for $\Gamma<2$, on the point $\xi = -1$ [ξ denotes the scaled fugacity; see (4.1)] for $\Gamma=2$ (the perfect-gas result for a lattice with M sites), which we prove, and on the unit circle in the complex ξ plane for $\Gamma>2$, which we prove at $\Gamma=4$. Furthermore, for $\Gamma>2$, we conjecture that the zeros pinch the real axis in the thermodynamic limit, with an essential singularity in the pressure at the reduced density $\rho\tau = 1/2$.

Let us proceed to detail the exact calculations at $\Gamma=2$ and 4. We begin with $\Gamma=2$, for which the calculation is quite straightforward.

2. THE GRAND PARTITION FUNCTION AT $\Gamma=2$

As remarked in the Introduction, for the purposes of a short-range cutoff and the solvability property, it is necessary to define the system on a lattice.

Divide a line of length L into M intervals so that there are sites at the points nL/M , $n=1, 2, \dots, M$. Introduce an interlacing lattice at the points $(n-\frac{1}{2})L/M$, $n=1, 2, \dots, M$. Denote these lattices \mathcal{L}_1 and \mathcal{L}_2 , respectively. Allow N ($\leq M$) positive charges to occupy \mathcal{L}_1 , and N negative charges to occupy \mathcal{L}_2 . Impose periodic boundary conditions, so that the pair potential is

$$V(\theta_1, \theta_2) = -q_1 q_2 \log[|e^{2\pi i\theta_1/L} - e^{2\pi i\theta_2/L}| (L/2\pi)] \quad (2.1)$$

(this is equivalent to defining the system on a circle of circumference L).

Denote the coordinates of the positive charges by $m_k L/M$ and the coordinates of the negative charges by $(l_k - \frac{1}{2})L/M$, where $m_k, l_k = 1, 2, \dots, M$. Further, denote

$$w_k = e^{2\pi i m_k/M}, \quad z_k = e^{2\pi i (l_k - 1/2)/M} \tag{2.2}$$

With this notation, the Boltzmann factor of the system for general Γ [recall (1.4)] is

$$W_{N\Gamma} = (2\pi/L)^{N\Gamma} |A_N(w_1, \dots, w_N; z_1, \dots, z_N)|^\Gamma \tag{2.3}$$

where A_N is given by (1.10).

This is the probability density (1.9) after suitable choice of normalization and θ and ϕ .

The partition function $Z_{N\Gamma}$ is given by

$$Z_{N\Gamma} = \sum_{m_1, \dots, m_N=1}^M \sum_{l_1, \dots, l_N=1}^M W_{N\Gamma}/(N!)^2 \tag{2.4}$$

and the grand partition function is given by

$$\Xi_\Gamma = \sum_{N=0}^M \zeta^{2N} Z_{N\Gamma} \tag{2.5}$$

where ζ denotes the activity. We will now transform (2.3)–(2.5) into manageable forms for $\Gamma = 2$.

Using the Cauchy double alternant determinant formula⁽²⁰⁾

$$\det \left[\frac{1}{w_j - z_k} \right]_{j,k=1, \dots, N} = (-1)^{N(N-1)/2} A_N(w_1, \dots, w_N; z_1, \dots, z_N) \tag{2.6}$$

with A_N given by (1.10), we have

$$W_{N2} = (2\pi/L)^{2N} |\det[(w_j - z_k)^{-1}]|^2 \tag{2.7}$$

If we introduce a parameter $\mu, |\mu| \leq 1$, as a factor of z_k in each term of the determinant, they can each be Taylor-expanded, and after familiar manipulation^(21,22) we obtain

$$\begin{aligned} W_{N2} &= (2\pi/L)^{2N} \sum_{P=1}^{N!} \sum_{Q=1}^{N!} \varepsilon(P) \varepsilon(Q) \\ &\times \lim_{\mu \rightarrow 1^-} \sum_{0 \leq \alpha_1, \dots, \alpha_N}^{\infty} \sum_{0 \leq \beta_1, \dots, \beta_N}^{\infty} \left(\prod_{j=1}^N \mu^{\alpha_j + \beta_j} \right) \\ &\times \exp[-2\pi i(l_k - \frac{1}{2})(\alpha_{P(k)} - \beta_{Q(k)})/M] \exp[2\pi i m_k(\alpha_k - \beta_k)/M] \end{aligned} \tag{2.8}$$

Writing

$$\begin{aligned} \alpha_j &= \gamma_j + k_j M, & 0 \leq \gamma_j \leq M-1, & \quad k_j = 0, 1, 2, \dots \\ \beta_j &= \nu_j + l_j M, & 0 \leq \nu_j \leq M-1, & \quad l_j = 0, 1, 2, \dots \end{aligned} \tag{2.9}$$

it is straightforward to take the limit $\mu \rightarrow 1^-$ and we obtain

$$\begin{aligned} W_{N2} &= (\pi/L)^{2N} \sum_{P=1}^{N!} \sum_{Q=1}^{N!} \varepsilon(P) \varepsilon(Q) \sum_{0 \leq \gamma_1, \dots, \gamma_N}^{M-1} \sum_{0 \leq \nu_1, \dots, \nu_N}^{M-1} \\ &\times \prod_{k=1}^N \exp[-2\pi i(l_k - \frac{1}{2})(\gamma_{P(k)} - \nu_{Q(k)})/M] \exp[2\pi i m_k(\gamma_k - \nu_k)/M] \end{aligned} \tag{2.10}$$

Substituting (2.10) in (2.4), we see that we have an expression of the form

$$\sum_{P=1}^{N!} \sum_{Q=1}^{N!} \varepsilon(P) \varepsilon(Q) \prod_{l=1}^N a_{P(l), Q(l)} \tag{2.11}$$

which we recognize as⁽²⁰⁾

$$N! \text{Det}[a_{j,k}]_{j,k=1, \dots, N} \tag{2.12}$$

Thus

$$\begin{aligned} Z_{N2} &= \frac{1}{N!} \left(\frac{\pi}{L}\right)^{2N} \sum_{0 \leq \gamma_1, \dots, \gamma_N}^{M-1} \sum_{0 \leq \nu_1, \dots, \nu_N}^{M-1} \left(\prod_{k=1}^N \sum_{m=1}^M \exp \frac{2\pi i m(\gamma_k - \nu_k)}{M} \right) \\ &\times \text{Det} \left[\sum_{l=1}^M \exp \frac{-2\pi i(l - \frac{1}{2})(\gamma_j - \nu_k)}{M} \right]_{j,k=1, \dots, N} \end{aligned} \tag{2.13}$$

Consider the expression (2.13). The sum over m gives

$$M \delta_{\gamma_k, \nu_k} \tag{2.14}$$

so we can replace ν_k by γ_k in the sum over l and ignore the sums over the ν_k . Observe that if $\gamma_k = \gamma_{k'}$ for $k \neq k'$, then two rows of the determinant are identical, so we can restrict $\gamma_k \neq \gamma_{k'}$. Furthermore, the summand is symmetric in the γ_k , so we can adopt the ordering

$$0 \leq \gamma_1 < \gamma_2 < \dots < \gamma_N \leq M-1 \tag{2.15}$$

provided we multiply by $N!$. Since $|\gamma_k - \gamma_{k'}| < M$, the only non-zero term in the determinant is the diagonal. We thus obtain

$$\begin{aligned} Z_{N2} &= (M\pi/L)^{2N} \sum_{0 \leq \gamma_1 < \gamma_2 < \dots < \gamma_N \leq M-1} 1 \\ &= \text{coefficient of } \zeta^{2N} \text{ in the expansion of } [1 - (\pi M \zeta/L)^2]^M \end{aligned} \tag{2.16}$$

From (2.5), the product in (2.16) is the grand canonical partition function. Defining the scaled fugacity at $\Gamma = 2$ by

$$\xi = (\pi M \zeta / L)^2 \tag{2.17}$$

we thus, remarkably, have the perfect-gas result for M particles on a lattice of M sites,

$$\mathcal{E}_2 = (1 + \xi)^M \tag{2.18}$$

3. THE GRAND PARTITION FUNCTION AT $\Gamma = 4$

The calculation in this case requires techniques beyond those necessary at $\Gamma = 2$. Here we draw on past experience^(23,13) and familiarity with the calculation of $C_{N4}^{(1)}$ in (1.2) as given by Dyson and Mehta.^(24,25)

3.1. A Confluent Cauchy Double Alternant

Our first objective is to express the Boltzmann factor (2.3) at $\Gamma = 4$ as a special type of determinant. To do this, consider the Cauchy double alternant formula (2.6) with determinant size $2N$,

$$(-1)^N A_{2N}(x_1, \dots, x_{2N}; y_1, \dots, y_{2N}) = \det \left[\frac{1}{x_k - y_j} \right]_{k, j=1, 2, \dots, 2N} \tag{3.1}$$

We will have us for a confluent form of (3.1).

Suppose we take the limits

$$x_{j+N} \rightarrow x_j, \quad y_{j+N} \rightarrow y_j, \quad j = 1, 2, \dots, N \tag{3.2}$$

It is easy to see that the leading order behavior of the left-hand side of (3.1) is

$$\left[\prod_{j=1}^N (x_{j+N} - x_j)(y_{j+N} - y_j) \right] [A_N(x_1, \dots, x_N; y_1, \dots, y_N)]^4 \tag{3.3}$$

On the right-hand side of (3.1), interchange the rows of the determinant so that the $(2j - 1)$ th row contains the x_j and the $2j$ th row contains the x_{N+j} . Then interchange the columns so that the $(2j - 1)$ th column contains the y_j and the $2j$ th column contains the y_{N+j} . Since the number of such interchanges is even, the value of the determinant is unchanged.

The $(2j - 1)$ th and $(2j)$ th rows are then

$$\frac{1}{x_j - y_1} \quad \frac{1}{x_j - y_{N+1}} \quad \dots \quad \frac{1}{x_j - y_N} \quad \frac{1}{x_j - y_{2N}} \tag{3.4}$$

and

$$\frac{1}{x_{N+j}-y_1} \frac{1}{x_{N+j}-y_{N+1}} \dots \frac{1}{x_{N+j}-y_N} \frac{1}{x_{N+j}-y_{2N}} \tag{3.5}$$

respectively. If we subtract (3.4) from (3.5) for each j and take the first of the limits in (3.2), to leading order the right-hand side of (3.1) has a factor of

$$\prod_{l=1}^N (x_l - x_{N+l}) \tag{3.6}$$

and the $(2j)$ th row becomes

$$\frac{1}{(x_j - y_1)^2} \frac{1}{(x_j - y_{N+1})^2} \dots \frac{1}{(x_j - y_N)^2} \frac{1}{(x_j - y_{2N})^2} \tag{3.7}$$

The $(2j-1)$ th and $(2j)$ th columns are now

$$\frac{1}{x_1 - y_j}, \frac{1}{(x_1 - y_j)^2}, \dots, \frac{1}{x_N - y_j}, \frac{1}{(x_N - y_j)^2} \tag{3.8}$$

and

$$\frac{1}{x_1 - y_{N+j}}, \frac{1}{(x_1 - y_{N+j})^2}, \dots, \frac{1}{x_N - y_{N+j}}, \frac{1}{(x_N - y_{N+j})^2} \tag{3.9}$$

respectively. If we subtract (3.8) from (3.9) for each j and take the second of the limits in (3.2), to leading order the right-hand side of (3.1) has, as well as (3.6), a factor of

$$\prod_{l=1}^N (y_{N+l} - y_l) \tag{3.10}$$

and the $(2j)$ th column becomes

$$\frac{1}{(x_1 - y_j)^2}, \frac{2}{(x_1 - y_j)^3}, \dots, \frac{1}{(x_N - y_j)^2}, \frac{2}{(x_N - y_j)^3} \tag{3.11}$$

Canceling the factors (3.6) and (3.10) with the corresponding terms in (3.3) and reading off from (3.8) and (3.11) the columns of the determinant, we have thus derived, by taking the limits (3.2) in (3.1), the identity

$$D^4 \equiv [A_N(x_1, \dots, x_N; y_1, \dots, y_N)]^4$$

$$\times \begin{vmatrix} \frac{1}{x_1 - y_1} & \frac{1}{(x_1 - y_1)^2} & \frac{1}{x_1 - y_2} & \frac{1}{(x_1 - y_2)^2} & \dots \\ \frac{1}{(x_1 - y_1)^2} & \frac{2}{(x_1 - y_1)^3} & \frac{1}{(x_1 - y_2)^2} & \frac{2}{(x_1 - y_2)^3} & \dots \\ \frac{1}{x_2 - x_1} & \frac{1}{(x_2 - y_1)^2} & \frac{1}{x_2 - y_2} & \frac{1}{(x_2 - y_2)^2} & \dots \\ \frac{1}{(x_2 - y_1)^2} & \frac{2}{(x_2 - y_1)^3} & \frac{1}{(x_2 - y_2)^2} & \frac{2}{(x_2 - y_2)^3} & \dots \\ \vdots & \vdots & \vdots & \vdots & \dots \end{vmatrix} \quad (3.12)$$

2N × 2N

Suppose all the x_k and y_k have modulus one. Then, analogous to the work that led to (2.8), we can Taylor-expand each term in the determinant, provided we introduce a parameter μ , $|\mu| < 1$, by replacing each y_k by μy_k . Using the elementary formulas

$$\begin{aligned} (1 - t)^{-1} &= \sum_{k=0}^{\infty} t^k \\ (1 - t)^{-2} &= \sum_{k=0}^{\infty} (k + 1) t^k \\ 2(1 - t)^{-3} &= \sum_{k=0}^{\infty} (k + 2)(k + 1) t^k \end{aligned} \quad (3.13)$$

we can expand each term in (3.12) column by column to obtain

$$D^4 = \left(\prod_{l=1}^N x_l^{-3} \right) \lim_{\mu \rightarrow 1^-} \sum_{\alpha_1, \dots, \alpha_{2N}=0}^{\infty} \prod_{l=1}^N (\mu y_l)^{\alpha_{2l} + \alpha_{2l-1}}$$

$$\times \begin{vmatrix} x_1^{-\alpha_1} & (\alpha_2 + 1) x_1^{-1 - \alpha_2} & x_1^{-\alpha_3} & \dots \\ (\alpha_1 + 1) x_1^{-\alpha_1} & (\alpha_2 + 2)(\alpha_2 + 1) x_1^{-1 - \alpha_2} & (\alpha_3 + 1) x_1^{-\alpha_3} & \dots \\ x_2^{-\alpha_1} & (\alpha_2 + 1) x_2^{-1 - \alpha_2} & x_2^{-\alpha_3} & \dots \\ \vdots & \vdots & \vdots & \dots \end{vmatrix} \quad (3.14)$$

2N × 2N

From the $(2j)$ th column of the determinant in (3.14) a common factor of $(\alpha_{2j} + 1)$ can be extracted for each $j = 1, 2, \dots, N$. Now replace α_{2j} by

$\alpha_{2j} - 1$. Then the summation over α_{2j} must begin from $\alpha_{2j} = 1$. But since there is a factor of α_{2j} in the summand, the $\alpha_{2j} = 0$ term can be included in the sum. Doing this for each $j = 1, 2, \dots, N$, we thus have from (3.14)

$$D^4 = \left(\prod_{l=1}^N x_l^{-3} \right) \lim_{\mu \rightarrow 1^-} \sum_{\alpha_1, \dots, \alpha_{2N} = 0}^{\infty} \prod_{l=1}^N (\mu y_l)^{\alpha_{2l} + \alpha_{2l-1}} \alpha_{2l} \times \begin{vmatrix} x_1^{-\alpha_1} & x_1^{-\alpha_2} & x_1^{-\alpha_3} & \dots \\ (\alpha_1 + 1) x_1^{-\alpha_1} & (\alpha_2 + 1) x_1^{-\alpha_2} & (\alpha_3 + 1) x_1^{-\alpha_3} & \dots \\ x_2^{-\alpha_1} & x_2^{-\alpha_2} & x_2^{-\alpha_3} & \dots \\ \vdots & \vdots & \vdots & \vdots \end{vmatrix} \quad (3.15)$$

$2N \times 2N$

Let us relate this to the Boltzmann factor (2.3) at $\Gamma = 4$. With

$$x_k = w_k, \quad y_k = z_k \quad (3.16)$$

where w_k and z_k are defined by (2.2), we can easily show that

$$W_{N4} = (2\pi/L)^{4N} \left[\prod_{j=1}^N (w_j z_j)^2 \right] [A_N(w_1, \dots, w_N; z_1, \dots, z_N)]^4 \quad (3.17)$$

Hence, by the definition in (3.12) and the identity (3.15), the Boltzmann factor can be written in terms of the right-hand side of (3.15) with the replacements (3.16).

Now, as in (2.9), write the summation in (3.15) as

$$\alpha_j = \gamma_j + k_j M, \quad 0 \leq \gamma_j \leq M - 1, \quad k_j = 0, 1, 2, \dots \quad (3.18)$$

The summation over the k_j can be performed column by column (the j th column depends on k_j only). Since

$$\lim_{\mu \rightarrow 1^-} \sum_{k=0}^{\infty} (-\mu)^k (\gamma + 1 + kM) = \frac{1}{2} a_1(\gamma) \quad (3.19)$$

$$\lim_{\mu \rightarrow 1^-} \sum_{k=0}^{\infty} (-\mu)^k (\gamma + kM)(\gamma + kM + 1) = \frac{1}{2} a_2(\gamma) \quad (3.20)$$

where

$$a_1(\gamma) = \gamma + 1 - M/2, \quad a_2(\gamma) = \gamma^2 + (1 - M)\gamma - M/2 \quad (3.21)$$

we have from (3.15) and (3.17)–(3.21) the identity

$$\begin{aligned}
 W_{N4} &= 2^{-2N} (2\pi/L)^{4N} \sum_{\gamma_1, \gamma_2, \dots, \gamma_{2N} = 0}^{M-1} \prod_{k=1}^N z_k^{\gamma_{2k} + \gamma_{2k-1} + 1} w_k^{-1} \\
 &\times \begin{vmatrix} w_1^{-\gamma_1} & [a_1(\gamma_1) - 1] w_1^{-\gamma_2} & w_1^{-\gamma_3} & \dots \\ a_1(\gamma_1) w_1^{-\gamma_1} & a_2(\gamma_2) w_1^{-\gamma_2} & a_1(\gamma_3) w_1^{-\gamma_3} & \dots \\ w_2^{-\gamma_1} & [a_1(\gamma_2) - 1] w_2^{-\gamma_2} & w_2^{-\gamma_3} & \dots \\ \vdots & \vdots & \vdots & \dots \end{vmatrix}_{2N \times 2N} \tag{3.22}
 \end{aligned}$$

Note that if $\gamma_{2j} = \gamma_{2j'}$ or $\gamma_{2j-1} = \gamma_{2j'-1}$ for any $j \neq j'$, the determinant vanishes, so we can take

$$\gamma_{2j} \neq \gamma_{2j'} \quad \text{and} \quad \gamma_{2j-1} \neq \gamma_{2j'-1} \quad \text{for all } j \neq j' \tag{3.23}$$

Now define

$$\chi(k) = \begin{cases} 1, & k \text{ odd} \\ 2, & k \text{ even} \end{cases} \tag{3.24}$$

Then, we can use the definition of a determinant as a sum over permutations to write (3.22) in the form

$$\begin{aligned}
 W_{N4} &= 2^{-2N} (2\pi/L)^{4N} \sum_{\gamma} \prod_{k=1}^N z_k^{\gamma_{2k-1} + \gamma_{2k} + 1} w_k^{-1} \\
 &\times \sum_{P=1}^{(2N)!} \varepsilon(P) \prod_{k=1}^N w_k^{-\gamma_{P(2k-1)} - \gamma_{P(2k)}} a_{\chi(P(2k))}(\gamma_{P(2k)}) \\
 &\times [a_1(\gamma_{P(2k-1)}) - 1]^{\chi_{P(2k-1)} - 1} \tag{3.25}
 \end{aligned}$$

where γ denotes the range

$$0 \leq \gamma_1, \gamma_2, \dots, \gamma_{2N} \leq M-1, \quad \gamma_{2j} \neq \gamma_{2j'}, \quad \gamma_{2j-1} \neq \gamma_{2j'-1} \tag{3.26}$$

We obtain our final working identity by restricting the permutations to the class X , where

$$X = \{P: P(2l) > P(2l-1) \text{ each } l = 1, 2, \dots, N\} \tag{3.27}$$

Then, from (3.25),

$$\begin{aligned}
 W_{N4} &= 2^{-2N} (2\pi/L)^{4N} \sum_{\gamma} \prod_{k=1}^N z_k^{\gamma_{2k} + \gamma_{2k-1} + 1} \\
 &\times \sum_X \varepsilon(P) \prod_{k=1}^N w_k^{-\gamma_{P(2k-1)} - \gamma_{P(2k)} - 1} \{ a_{\chi(P(2k))}(\gamma_{P(2k)}) \\
 &\times [a_1(\gamma_{P(2k-1)}) - 1]^{\chi_{P(2k-1)} - 1} \\
 &- a_{\chi(P(2k-1))}(\gamma_{P(2k-1)}) [a_1(\gamma_{P(2k)}) - 1]^{\chi_{P(2k)} - 1} \} \tag{3.28}
 \end{aligned}$$

where W_{N4} is given by (2.3); w_k and z_k by (2.2); a_1 and a_2 by (3.21); χ by (3.24); γ by (3.26); and X by (3.27).

3.2. The Partition Function

To evaluate Z_{N4} as defined by (2.4), we first substitute (3.28). The sum over the l_k in (2.4) can now be done immediately. From the definition (2.2) of z_k , and since, from (3.26), $0 \leq \gamma_k \leq M - 1$, we have

$$\sum_{l_1, \dots, l_N=1}^M \prod_{k=1}^N z_k^{\gamma_{2k} + \gamma_{2k-1} + 1} = (-M)^N \prod_{k=1}^N \delta_{\gamma_{2k} + \gamma_{2k-1}, M-1} \tag{3.29}$$

where $\delta_{a,b}$ denotes the Kronecker delta.

Now consider the sum over the m_k in (2.4). By considering the conditions (3.26) and the delta functions in (3.29), we see that there are two classes of nonzero contributions:

$$\begin{aligned} \text{Type 1} \quad P(2l) &= 2r \\ P(2l-1) &= 2r-1 \end{aligned} \tag{3.30}$$

$$\begin{aligned} \text{Type 2} \quad P(2l) &= 2r, \quad P(2l') = 2r-1 \\ P(2l-1) &= 2r', \quad P(2l'-1) = 2r'-1 \end{aligned} \tag{3.31}$$

To compute the sum over the m_k we first consider the contribution from N type 1 permutations, and then introduce in order 1, 2, ..., $[N/2]$ (in this context $[\cdot]$ denotes integer part) type 2 permutations. Let us call the contribution to (2.5) from k type 2 permutations S_k , so that

$$Z_{N,4} = \frac{(-M)^N}{(N!)^2} \left(\frac{2\pi}{L}\right)^{4N} \sum_{k=0}^{[N/2]} S_k \tag{3.32}$$

For S_0 we can have

$$\begin{aligned} P(2l) &= 2Q(l) \\ P(2l-1) &= 2Q(l) - 1, \quad Q(l) \in \{1, 2, \dots, N\} \end{aligned} \tag{3.33}$$

which has $\varepsilon(P) = 1$. Thus, from (2.4), (3.28), (3.29), and (3.32)

$$S_0 = M^N \sum_{\gamma_2, \gamma_4, \dots, \gamma_{2N}=0}^{M-1} \sum_{Q=1}^{N!} \prod_{l=1}^{N!} A_1(\gamma_{2Q(l)}) \tag{3.34}$$

where

$$\begin{aligned} A_1(\gamma) &= a_2(\gamma) - a_1(M-1-\gamma)[a_1(\gamma)-1] \\ &= 2\gamma^2 + 2\left(\frac{1}{2} - M\right)\gamma + M^2/4 - M/2 \end{aligned} \tag{3.35}$$

The summand in (3.34) is independent of the particular permutation, so we can choose $Q(l) = l$ and multiply by $N!$. The summand is also symmetric in the γ 's, so we can choose a particular ordering provided we multiply by $N!$. Thus,

$$S_0 = M^N (N!)^2 \sum_{0 \leq \gamma_2 < \gamma_4 < \dots < \gamma_{2N} \leq M-1} \prod_{l=1}^N A_1(\gamma_{2l}) \tag{3.36}$$

For general S_k , from (3.30)–(3.32), we have

$$\begin{aligned} P(2l) &= 2Q(l); & Q(l) &\in \{1, 2, \dots, N\} - \{r_1, r_2, \dots, r_{2k}\} \\ P(2l-1) &= 2Q(l) - 1 & \text{for } l &\neq m_1, \dots, m_{2k} \end{aligned} \tag{3.37}$$

and

$$\begin{aligned} P(2m_t) &= 2r_{R(2t-1)}, & P(2m_{t+k}) &= 2r_{R(2t-1)} - 1 \\ P(2m_t - 1) &= 2r_{R(2t)}, & P(2m_{t+k} - 1) &= 2r_{R(2t)} - 1 \end{aligned} \tag{3.38}$$

where

$$\begin{aligned} R(t) &\in \{1, 2, \dots, 2k\}, & t &= 1, 2, \dots, k, & 1 \leq m_t \leq N \\ m_t &\neq m_{t'}, & r_{R(2t-1)} &> r_{R(2t)}, & r_t \neq r_{t'} \end{aligned} \tag{3.39}$$

By considering the number of interchanges, we have that

$$\varepsilon(P) = (-1)^k \tag{3.40}$$

All choices of m_1, \dots, m_{2k} give the same contribution to S_k , so we can choose $m_j = j$ provided we multiply by the number of such choices, which is $N!/(N-2k)!$. Thus, from (2.4), (3.28), (3.32), and (3.37)–(3.40)

$$\begin{aligned} S_k &= (-1)^k \frac{N! M^N}{(N-2k)!} \sum_{Q=1}^{(N-2k)!} \sum_{\substack{R=1 \\ t=1, 2, \dots, k}}^{(2k)!} \sum_{r_{R(2t-1)} > r_{R(2t)} \gamma_2, \gamma_4, \dots, \gamma_{2N} = 0} \sum_{\substack{M-1 \\ \gamma_{2j} \neq \gamma_{2j'}}} \\ &\times \prod_{l=1}^N A_1(\gamma_{2Q(l)}) \left\{ \prod_{m=1}^k A_2(\gamma_{2r_{2m}}) \delta_{\gamma_{2r_{2m}} + \gamma_{2r_{2m-1}}, M-1} \right\} \end{aligned} \tag{3.41}$$

where $A_1(\gamma)$ is given by (3.35) and

$$\begin{aligned} A_2(\gamma) &= \{a_2(\gamma)[a_1(M-1-\gamma) - 1] - a_2(M-1-\gamma) \\ &\quad \times [a_1(\gamma) - 1]\} \{[a_1(M-1-\gamma) - a_1(\gamma)]\} \\ &= (M-1-2\gamma)^2 [\gamma^2 + (1-M)\gamma - M/2] \end{aligned} \tag{3.42}$$

In (2.59) we can choose

$$N \geq r_1 > r_2 > \dots > r_{2k} \geq 1 \tag{3.43}$$

provided we multiply by the factor

$$(2k - 1)(2k - 3) \dots 1 = \frac{(2k)!}{2^k k!} \tag{3.44}$$

which is the number of ordered pairs $(r_{R(1)}, r_{R(2)})$, $(r_{R(3)}, r_{R(4)})$, ..., $(r_{R(2k-1)}, r_{R(2k)})$ with the constraint (3.43) such that $r_{R(2t-1)} > r_{R(2t)}$ for each $t = 1, 2, \dots, k$ and $R(t) \in \{1, 2, \dots, 2k\}$. But the summand in (3.41) is independent of the particular choice of r 's in (3.43), so we can choose $r_t = t$ provided we multiply by

$$\sum_{N \geq r_1 > \dots > r_{2k} \geq 1} 1 = \binom{N}{2k} \tag{3.45}$$

Also, the summand in (3.41) is independent of the particular choice of Q , so we can choose $Q(l) = l$ provided we multiply by $(N - 2k)!$. Hence

$$S_k = (-1)^k \frac{N! M^N}{(N - 2k)!} \frac{(2k)!}{2^k k!} \binom{N}{2k} (N - 2k)! \\ \times \sum_{\gamma^*} \prod_{l=1}^k A_2(\gamma_{4l}) \sum_{\gamma^{**}} \prod_{l=2k+1}^{M-1} A_1(\gamma_{2l}) \tag{3.46}$$

where γ^* denotes the range

$$0 \leq \gamma_4, \gamma_8, \dots, \gamma_{4k} \leq M - 1$$

provided

$$\gamma_{4j} \neq \gamma_{4j'}, \quad M - 1 - \gamma_{4j} \tag{3.47}$$

for any $j \neq j'$ ($j, j' = 1, 2, \dots, k$) and γ^{**} denotes the range

$$0 \leq \gamma_{4k+2}, \gamma_{4k+4}, \dots, \gamma_{2N} \leq M - 1$$

provided

$$\gamma_{4k+2j} \neq \gamma_{4k+2j'}, \quad \gamma_{4j'}, \quad M - 1 - \gamma_{4j} \tag{3.48}$$

for any $j \neq j'$ ($j, j' = 1, 2, \dots, N$).

Using the symmetry

$$A_2(\gamma) = A_2(M - 1 - \gamma) \tag{3.49}$$

the condition (3.47), and the fact, which follows from (3.47) and (3.48), that for M odd, $\gamma_{4j} \neq (M - 1)/2$ (M odd), we have

$$\begin{aligned} \sum_{\gamma^*} \prod_{l=1}^k A_2(\gamma_{4l}) &= 2^k \sum_{\substack{\gamma_4, \gamma_8, \dots, \gamma_{4k} = 0 \\ \gamma_{4j} \neq \gamma_{4j'} \ (j, j' = 1, \dots, k)}}^{[M/2] - 1} \prod_{l=1}^k A_2(\gamma_{4l}) \\ &= 2^k k! X_k \end{aligned} \tag{3.50}$$

where

$$X_k = \sum_{0 \leq \gamma_4 < \gamma_8 < \dots < \gamma_{4k} \leq [M/2] - 1} \prod_{l=1}^k A_2(\gamma_{4l}) \tag{3.51}$$

Equation (3.51) follows by using the symmetry of the summand in (3.50) with respect to the γ 's $(\gamma_4, \gamma_8, \dots, \gamma_{4k})$.

The summand in (3.46) is also symmetric with respect to $\gamma_{4k+2}, \gamma_{4k+4}, \dots, \gamma_{2N}$, so if we define

$$\begin{aligned} Y_{k,N} &= \sum_{0 \leq \gamma_{4k+2} < \dots < \gamma_{2N} \leq M - 1} \prod_{l=2k+1}^N A_1(\gamma_{2l}) \\ \gamma_{4k+2j} &\neq \gamma_{4j'}, \quad M - 1 - \gamma_{4j'}, \quad j = 1, 2, \dots, N - 2k; \quad j' = 1, 2, \dots, k \end{aligned} \tag{3.52}$$

and agree on the conventions

$$X_0 = 1, \quad Y_{k,N} = 0 \text{ for } k > [N/2], \quad Y_{N/2,N} = 0 \text{ for } N \text{ even} \tag{3.53}$$

we have from (3.32), (3.46), and (3.50)–(3.53) the result

$$Z_{N,4} = (-1)^N \left(\frac{M}{2}\right)^{2N} \left(\frac{2\pi}{L}\right)^{4N} \sum_{k=0}^{[M/2] - 1} (-1)^k X_k Y_{k,N} \tag{3.54}$$

3.3. The Grand Partition Function

From the definition (2.5), the evaluation (3.54), and the properties (3.53) we have

$$\Xi_4 = \sum_{k=0}^{[M/2]} (-1)^k X_k \sum_{N=2k}^M (-1)^N \zeta^{2N} \left(\frac{M}{2}\right)^{2N} \left(\frac{2\pi}{L}\right)^{4N} Y_{k,N} \tag{3.55}$$

From (3.52), the sum over N in (3.55) is simply

$$\begin{aligned} & \left(\frac{M\zeta}{2}\right)^{4k} \left(\frac{2\pi}{L}\right)^{8k} \left\{ \prod_{l=0}^{M-1} \left[1 - \left(\frac{M\zeta}{2}\right)^2 \left(\frac{2\pi}{L}\right)^4 A_1(l) \right] \right\} \\ & \times \left\{ \prod_{l=1}^k \left[1 - \left(\frac{M\zeta}{2}\right)^2 \left(\frac{2\pi}{L}\right)^4 A_1(\gamma_{4l}) \right] \right\} \\ & \times \left[1 - \left(\frac{M\zeta}{2}\right)^2 \left(\frac{2\pi}{L}\right)^4 A_1(M-1-\gamma_{4l}) \right] \Big\}^{-1} \end{aligned} \tag{3.56}$$

Substituting this result in (3.55) and using (3.51) gives us the evaluation

$$\begin{aligned} \mathcal{E}_4 &= \prod_{l=0}^{M-1} \left[1 - \left(\frac{M\zeta}{2}\right)^2 \left(\frac{2\pi}{L}\right)^4 A_1(l) \right] \\ & \times \prod_{k=0}^{[M/2]} \left[1 - \frac{(M\zeta/2)^4 (2\pi/L)^8 A_2(k)}{\left([1 - (M\zeta/2)^2 (2\pi/L)^4 A_1(k)] \right. \right.} \right. \\ & \quad \left. \left. \times [1 - (M\zeta/2)^2 (2\pi/L)^4 A_1(M-1-k)] \right) \right] \end{aligned} \tag{3.57}$$

The terms in (3.57) can be combined into the single product

$$\begin{aligned} \mathcal{E}_4 &= \prod_{k=0}^{[M/2]-1} \{ [1 - (M\zeta/2)^2 (2\pi/L)^4 A_1(k)] \\ & \times [1 - (M\zeta/2)^2 (2\pi/L)^4 A_1(M-1-k)] - (M\zeta/2)^4 (2\pi/L)^8 A_2(k) \} \\ & \times \begin{cases} 1, & M \text{ even} \\ \{1 - (M\zeta/2)^2 (2\pi/L)^4 A_1[(M-1)/2]\}, & M \text{ odd} \end{cases} \end{aligned} \tag{3.58}$$

Recalling the definitions of A_1 and A_2 as given by (3.35) and (3.42), we have thus derived the result

$$\begin{aligned} \mathcal{E}_4 &= \prod_{l=0}^{[M/2]-1} \left\{ 1 - \xi \frac{4}{M^2} \left[4l^2 - 4l(M-1) + \frac{M^2}{2} - 2M + 1 \right] + \xi^2 \right\} \\ & \times \begin{cases} 1, & M \text{ even} \\ 1 + \xi, & M \text{ odd} \end{cases} \end{aligned} \tag{3.59}$$

where, in analogy to (2.17), we have defined the scaled fugacity at $\Gamma = 4$ by

$$\xi = (\pi M/L)^4 \zeta^2 \tag{3.60}$$

4. PROPERTIES OF THE EXACT SOLUTIONS

4.1. Significance of the Scaled Fugacity ξ

In (2.17) and (3.60) we defined a scaled fugacity ξ , which can be summarized in the one equation

$$\xi = (\pi M/L)^F \zeta^2 \quad (4.1)$$

To understand the significance of this choice, first consider a general one-component lattice gas with an arbitrary two-body potential V in periodic boundary conditions. Let W_n denote the Boltzmann factor of a configuration of n particles at positions x_1, x_2, \dots, x_n . Let W_{M-n} denote the Boltzmann factor of the same configuration, but with the holes and particles interchanged (M denotes the number of lattice sites), and denote the positions of the particles by $x'_1, x'_2, \dots, x'_{M-n}$. Then

$$e^{n\beta E_0} W_n = e^{(M-n)\beta E_0} W_{M-n} \quad (4.2)$$

where

$$E_0 = \sum_{k \neq k'} V(|x_k - x_{k'}|) \quad (4.3)$$

The sum is over all lattice sites $k \neq k'$. Note that, by the assumption of V being periodic, E_0 is independent of k' . To see this, simply multiply both sides of (4.2) by

$$\prod_{k=1}^n \prod_{j=1}^{M-n} \exp[-\beta V(|x_k - x'_j|)] \quad (4.4)$$

Then, from the definition (4.3), (4.2) is evident. By the same argument, the relationship (4.2) holds for two-component charged systems, provided each species of charge is restricted to a particular sublattice.

From (4.2) we have the relationship between partition functions

$$e^{n\beta E_0} Z_n = e^{(M-n)\beta E_0} Z_{M-n} \quad (4.5)$$

Hence, the grand partition function can be written

$$\Xi = \sum_{n=0}^M \xi^n Z_n^* \quad (4.6)$$

where

$$\xi = e^{-\beta E_0} \zeta \quad (4.7)$$

($\xi = e^{-\beta E_0 \zeta^2}$ for two-component charged systems) and

$$Z_n^* = e^{\beta E_0} Z_n \tag{4.8}$$

Since $Z_n^* = Z_{M-n}^*$, the grand partition function is reciprocal in the variable ξ , so that if ξ_0 is a zero of Ξ , so is $1/\xi_0$.

For the two-component charged-rod system under consideration here, with the potential (2.1), the formula (4.3) gives

$$E_0/q^2 = \log(L/2\pi) - \log \prod_{n=1}^{M-1} |1 - e^{2\pi i n/M}| + \log \prod_{n=1}^M |1 - e^{2\pi i(n-1/2)/M}| \tag{4.9}$$

From the identity

$$\prod_{m=1}^M (x - e^{2\pi i m/M} a) = x^M - a^M \tag{4.10}$$

with the $m = M$ term taken to the left-hand side, by taking $a = 1$ and the limit $x \rightarrow 1$, we obtain

$$\prod_{m=1}^{M-1} |1 - e^{2\pi i m/M}| = M \tag{4.11}$$

while $a = e^{-\pi i/M}$ and $x = 1$ in (4.10) gives

$$\prod_{m=1}^M |1 - e^{2\pi i(n-1/2)/M}| = 2 \tag{4.12}$$

Hence

$$E_0/q^2 = \log(L/M\pi) \tag{4.13}$$

and so from (4.7) the scaled fugacity is given by (4.1).

4.2. The Zeros of the Grand Partition Function

We are interested in the location of the zeros of the grand partition function for a particular value of M (the number of lattice sites on each sublattice) as a function of the scaled fugacity (4.1).

At $I = 2$, from (2.18) we see that the M zeros all occur at the point

$$\xi = -1 \tag{4.14}$$

At $\Gamma = 4$, from (3.59), the zeros lie at the zeros of the quadratic

$$1 - \xi \frac{4}{M^2} \left[4l^2 - 4l(M - 1) + \frac{M^2}{2} - 2M + 1 \right] + \xi^2 \tag{4.15}$$

for $l = 0, 1, 2, \dots, [M/2] - 1$, as well as at $\xi = -1$ if M is odd. These zeros all lie on the unit circle in the complex ξ plane. To see this, we note that it is equivalent to saying

$$\left| \frac{4}{M^2} \left\{ 4l^2 - 4l(M - 1) + \frac{M^2}{2} - 2M + 1 \right\} \right| \leq 2 \tag{4.16}$$

for each $l = 0, 1, 2, \dots, [M/2] - 1$. Since the left-hand side of (4.16) is quadratic in l , it is simple to check this explicitly.

For general Γ , it is straightforward to compute Ξ_Γ for small values of M from (2.3)–(2.5). We have

$$M = 2: \quad \Xi_\Gamma = 1 + 2^{2-\Gamma/2} \xi + \xi^2 \tag{4.17a}$$

$$M = 3: \quad \Xi_\Gamma = (1 + \xi) \{ 1 + [3^{1-\Gamma}(2^{\Gamma+1} + 1) - 1] \xi + \xi^2 \} \tag{4.17b}$$

$$M = 4: \quad \Xi_\Gamma = 1 + a\xi + b\xi^2 + a\xi^3 + \xi^4 \tag{4.17c}$$

where

$$\begin{aligned} a &= 8(2^{-3\Gamma/2})[(2 + \sqrt{2})^{\Gamma/2} + (2 - \sqrt{2})^{\Gamma/2}] \\ b &= 2^{-2\Gamma} \{ 16(2^{\Gamma/2}) + 4(2^\Gamma) + 8(2^{-\Gamma/2})[(2 - \sqrt{2})^\Gamma + (2 + \sqrt{2})^\Gamma] \} \end{aligned} \tag{4.18}$$

From (4.17a) and (4.17b) we can calculate immediately that the zeros of Ξ_Γ all lie on the unit circle in the complex ξ plane for $\Gamma > 2$ and on the negative real axis for $\Gamma < 2$. To show that this is true in (4.17c), we note that we can write in this case

$$\Xi_\Gamma = (1 + t_+ \xi + \xi^2)(1 + t_- \xi + \xi^2) \tag{4.19}$$

where

$$t_\pm = \frac{1}{2} \{ a \pm [a^2 - 4(b - 2)]^{1/2} \} \tag{4.20}$$

It is a simple exercise in quadratic equations to show that if t_\pm are real, then the zeros of (4.19) all lie on the circle $|\xi| = 1$ if and only if

$$2a \leq b + 2 \tag{4.21}$$

and

$$a^2/2 \leq b + 2 \tag{4.22}$$

We can check from (4.18) that (4.21) and (4.22) hold for all $\Gamma \geq 2$, while (4.22) breaks down for $\Gamma < 2$. Under the latter circumstance, with (4.21) remaining valid, the zeros all lie on the negative real axis.

The above results are all consistent with the conjecture announced in the Introduction: the M zeros of the polynomial Ξ_Γ as a function of the scaled fugacity ξ all lie on the negative real axis for $\Gamma < 2$, and on the unit circle in the complex $-\xi$ plane for $\Gamma > 2$. At $\Gamma = 2$ the M zeros occur at the point $\xi = -1$.

4.3. The Thermodynamic Limit

In general, for a one-dimensional system of length L , the pressure is given in terms of the grand partition function by

$$\beta P = \lim_{L \rightarrow \infty} \frac{1}{L} \log \Xi \quad (4.23)$$

and the density is given by

$$\rho = \zeta \partial \beta P / \partial \zeta \quad (4.24)$$

Hence, from (2.18), at $\Gamma = 2$

$$\beta P = \frac{1}{\tau} \log(1 + \xi) \quad (4.25)$$

$$\rho_+ = \rho_- = \frac{\xi}{\tau(1 + \xi)} \quad (4.26)$$

where

$$\tau = L/M \quad (4.27)$$

is the lattice spacing on each sublattice and ρ_+ (ρ_-) refers to the particle density on the sublattice for the positive (negative) charges. From (4.25) and (4.26) the equation of state for a noninteracting lattice gas is

$$\beta P = \frac{1}{\tau} \log \left(1 + \frac{\rho_+ \tau}{1 - \rho_+ \tau} \right) \quad (4.28)$$

in agreement with Gaudin's result.⁽⁸⁾

From (3.59), and noting that the sum implied by the formula (4.23) is just an example of a Riemann integral, we have at $\Gamma = 4$

$$\beta P = \frac{1}{\tau} \int_0^{1/2} dt \log [1 - 4\xi(4t^2 - 4t + \frac{1}{2}) + \xi^2] \quad (4.29)$$

Changing variables

$$t = \sin^2(\theta/4) \quad (4.30)$$

we find that (4.29) becomes

$$\beta P = \frac{1}{4\tau} \int_0^\pi d\theta \left(\sin \frac{\theta}{2} \right) \log(1 - 2\xi \cos \theta + \xi^2) \quad (4.31)$$

and from (4.24)

$$\rho_+ = \rho_- = \frac{\xi}{2\tau} \int_0^\pi d\theta \left(\sin \frac{\theta}{2} \right) \frac{\xi - \cos \theta}{1 - 2\xi \cos \theta + \xi^2} \quad (4.32)$$

From (4.31) we read off that the density of zeros of the grand partition function on the unit circle at $\Gamma = 4$ is given by

$$\frac{1}{4} \sin(\theta/2) d\theta \quad (4.33)$$

Thus, the zeros cross the real axis at $\Gamma = 4$ in the thermodynamic limit (although with zero density), and thus, according to the Yang–Lee theory,⁽²⁶⁾ the system exhibits a phase transition as a function of density.

The singularities at $\Gamma = 4$ and $\xi = 1$ are calculated by expanding the integrands in (4.31) and (4.32) near $\theta = 0$. We thus find for $\xi \sim 1$

$$\beta P \sim \frac{1}{\tau} \left[2 \log 2 - 1 - \frac{(1 - \xi)^2}{8} \log |1 - \xi| \right] \quad (4.34)$$

and

$$\rho_+ \sim \frac{1}{2\tau} + \frac{1}{4\tau} (1 - \xi) \log |1 - \xi| \quad (4.35)$$

Hence, defining

$$\beta P_c = \frac{1}{\tau} (2 \log 2 - 1), \quad \rho_c = \frac{1}{2\tau} \quad (4.36)$$

we have

$$\begin{aligned} \beta(P - P_c) &\sim -\frac{1 - \xi}{2} (\rho_+ - \rho_c) \\ &= -\frac{1}{2} f(4\tau(\rho_+ - \rho_c)) (\rho_+ - \rho_c) \end{aligned} \quad (4.37)$$

where $f(x)$ is the inverse function of $x \log x$ for small, positive x . Thus, as a function of density, the pressure exhibits an essential singularity at the critical point $\rho_+ = 1/(2\tau)$. It would seem likely that this feature persists for all $\Gamma > 2$.

4.5. The Phase Diagram

A proper discussion of the phase diagram, in the form of identifying the conducting and insulating regimes, requires the study of correlation functions. We defer this to a subsequent paper, in which we will calculate the two-particle correlations at $\Gamma = 2$ and 4 for all values of $\rho\tau$.

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