Journal of Statistical Physics, Vol. 60, Nos. 1/2, 1990

Yang–Lee Theory and the Conductor–Insulator Transition in Asymmetric Log-Potential Lattice Gases

P. J. Forrester[1]

Received January 3, 1990

A feature of a conducting phase at low density is that there is a singularity in the fugacity expansion of the pressure, whereas the same expansion in the insulating phase gives an analytic series. The Yang–Lee characterization of a phase transition thus implies that in the conducting phase the zeros of the grand partition function must pinch the real axis in the complex scaled fugacity (ξ) plane at $\xi = 0$, whereas in the insulating phase a neighborhood of $\xi = 0$ must be zero free. Exact and numerical calculations are presented which suggest that for two-component log-potential lattice gases in one dimension with dimensionless coupling Γ, the zeros pinch the point $\xi = 0$ for $\Gamma < 2$, while for $\Gamma \geqslant 2$ a neighborhood of $\xi = 0$ is zero free. The conductor–insulator transition therefore takes place at $\Gamma = 2$ independent of the density and other parameters in the model.

KEY WORDS: Conductor–insulator transition; Yang–Lee theory; exact solvability.

1. INTRODUCTION

The log-potential, two-component Coulomb gas on a one-dimensional lattice is perhaps the simplest system to exhibit a conductor–insulator transition. In addition to the theoretical interest of this feature, it has been shown[(1)] that this system is essentially equivalent to the quantum Brownian motion problem in a periodic potential. The conducting and insulating phases correspond to mobile and trapped states, respectively, of the particle in the quantum problem.

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

0022-4715/90/0700-0203$06.00/0

The two components of the model are the positive and negative two-dimensional Coulomb charges, both of magnitude q, and the dimensionless coupling constant is

$$\Gamma := q^2/k_B T \tag{1.1}$$

Recent studies[2-5] have focused on solvability properties of this system. In ref. 2 the grand partition function Ξ, which is a polynomial in the scaled fugacity ξ, was factorized exactly at $\Gamma = 2$ and 4. These and subsequent exact results suggest further areas of study, two of which will be addressed in this paper.

The first is again exact solvability. The motivation given in ref. 2 for the exact results at $\Gamma = 2$ and 4 was a correspondence with the solvability of the one-component system at $\Gamma = 1$, 2, and 4. For the one-component model, the Boltzmann factors at these three couplings are related to the three classical groups: orthogonal, unitary, and symplectic.[6] Clearly the correspondence is not complete, as at $\Gamma = 1$ in the two-component model no exact solution was given. Here an asymmetric two-component log-potential lattice gas is solved exactly, and it will be shown that in a certain limit the $\Gamma = 1$ symmetric model is recovered.

The second topic suggested to be considered here is an analysis of the phase transition via the location of the zeros of the grand partition function. In ref. 2 it was conjectured that the zeros of the polynomial $\Xi(\xi)$ for the symmetric lattice gas were all on the negative real axis in the conducting phase, and on the unit circle in the insulating phase. In Section 4 of this paper the question of determining the phase from the location of the grand partition function zeros is addressed.

Numerical finite lattice calculations for the asymmetric model show that again in the conducting phase all the zeros lie on the negative real axis in the scaled fugacity plane. Further, for $\Gamma < 2$, evidence is presented which suggests the zero closest to the origin, ξ_1 say, has the expansion

$$\xi_1 = -\frac{1}{M^\gamma}\left[a_0(\Gamma) + \frac{a_1(\Gamma)}{M} + \frac{a_2(\Gamma)}{M^2} + \cdots\right] \tag{1.2}$$

where $a_0(\Gamma)$, $\gamma > 0$ and M is the order of the polynomial $\Xi(\xi)$.

For the symmetric model we conjecture

$$\gamma = 2 - \Gamma \tag{1.3}$$

The key feature to note is that as $M \to \infty$, the zero pinches the real axis at the origin. Assuming a finite density of zeros have the behavior (1.2), this says the pressure is nonanalytic at $\xi = 0$, which is a feature of a conducting phase.

At $\Gamma = 2$ the expansion (1.2) holds with $\gamma = 0$. A gap of magnitude $a_0(2)$ is thus present between the zeros and the positive real fugacity axis. Here the pressure is now an analytic function of ξ in the neighborhood of $\xi = 0$, the Taylor series having radius of convergence $a_0(2)$. This is a feature of an insulating phase, so a conductor–insulator phase transition has taken place.

2. AN ASYMMETRIC LOG-POTENTIAL LATTICE GAS

In addition to the solvable one-component systems of Dyson,[6] a solvable two-component log-potential plasma has been found.[7] Both components have charges of like sign with charge ratio 1:2. In correspondence with this solvable model we propose the following two-component lattice gas.

2.1. Definition of the Model

Consider a line of length L, which is divided into M intervals so that there are lattice sites at the points nL/M, $n = 1, 2,..., M$. Introduce two interlacing lattices, the first at the points $(\phi_0 + l)\, L/M$, the second at the points $(\phi_1 + l)\, L/M$, $l = 0, 1, 2,..., M-1$. Denote these lattices L_1, L_2, and L_3, respectively (see Fig. 1). Allow N $(\leqslant M)$ positive charges of magnitude $2q$ to occupy L_1 and $2N$ negative charges of magnitude q to occupy either L_2 or L_3.

The charges are two-dimensional, so that they interact via the logarithmic potential. In periodic boundary conditions, the potential is

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

Denote the coordinates of the kth positive charge by $m_k L/M$, and the coordinates of the kth negative charge by $(l_k + \phi_0)\, L/M$ if the charge is on L_2 or $(l_k + \phi_1)\, L/M$ if the charge is on L_3. The allowed values of m_k are $m_k = 1, 2,..., M$, while the allowed values of l_k are $l_k = 0, 1,..., M-1$.

Further denote

$$x_k = e^{2\pi i m_k/M} \qquad \text{and} \qquad y_k = e^{2\pi i(l_k + \phi_p)/M} \tag{2.2}$$

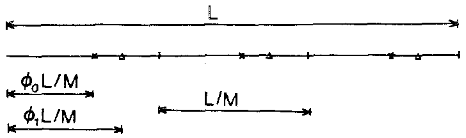

Fig. 1. The lattice geometry and spacings. The sublattices L_1, L_2, and L_3 are denoted by dashes, crosses, and triangles, respectively.

where $p=0, 1$ according to whether the negative charge is on sublattice L_2 or L_3, respectively.

With this notation, the Boltzmann factor $W_{N\Gamma}$ for N particles of charge $+2q$ and $2N$ particles of charge $-q$ is

$$W_{N\Gamma}=(2\pi/L)^{3N\Gamma}\,|F(x_1,..., x_N; y_1,..., y_{2N})|^{\Gamma} \tag{2.3}$$

where

$$F:=F(x_1,..., x_N; y_1,..., y_{2N})$$
$$:=\frac{\prod_{1\leqslant j<k\leqslant N}(x_k-x_j)^4\prod_{1\leqslant j<k\leqslant N}(y_k-y_j)}{\prod_{j=1}^{N}\prod_{k=1}^{2N}(x_j-y_k)^2} \tag{2.4}$$

The partition function $Z_{N\Gamma}$ and grand partition function Ξ_Γ are given by

$$Z_{N\Gamma}=\frac{1}{N!(2N)!}\sum_{m_1,..., m_N=1}^{M}\;\sum_{l_1,..., l_{2N}=0}^{M-1} W_{N\Gamma} \tag{2.5}$$

and

$$\Xi_\Gamma=\sum_{N=0}^{M}\zeta^{2N}Z_{N\Gamma} \tag{2.6}$$

respectively, where ζ denotes the activity.

2.2. Boltzmann Factor As a Determinant

The solvable case to be presented here is $\Gamma=1$, and this feature relies on the following determinant identity.

Theorem 2.1. With the notation (2.4),

$$F=\det\begin{bmatrix}(x_j-y_k)^{-1}\\(x_j-y_k)^{-2}\end{bmatrix}_{\substack{j=1,..., N\\k=1,..., 2N}} \tag{2.7}$$

where the determinant consists of 2×1 blocks, with elements as given.

Proof. Our method of proof is very similar to that used in ref. 2, pp. 464–465, to derive a similar identity. Briefly, we begin with the Cauchy double alternant formula with determinant size $2N$:

$$(-1)^N\frac{\prod_{1\leqslant j<k\leqslant 2N}(x_k-x_j)(y_k-y_j)}{\prod_{j=1}^{2N}\prod_{k=1}^{2N}(y_k-x_j)}=\det[(x_k-y_j)^{-1}]_{k,j=1,..., 2N} \tag{2.8}$$

The identity (2.7) follows by taking the limit $x_j \to x_{j+N}$ for each $j = 1, 2,..., N$. This is straightforward on the left-hand side. On the right-hand side it is necessary to first subtract the jth row from the $(j+N)$th row. Rearranging the order of the rows and canceling the leading-order common factor on both sides then gives (2.7).

Remark. The identity (2.7) occurs in Muir[8] and is due to F. Brioschi in a paper published in 1882.

Suppose all the x_j and y_k in (2.7) have unit modulus. Each term in the determinant can then be Taylor expanded, provided a parameter μ, $|\mu| < 1$, is introduced by replacing each y_k by μy_k. This procedure gives

$$F = \left(\prod_{l=1}^{N} x_l^{-3}\right) \lim_{\mu \to 1^-} \sum_{\alpha_1,...,\alpha_{2N}=0}^{\infty} \prod_{l=1}^{N} \alpha_{2l-1}(\mu^{-1} x_l)^{-\alpha_{2l-1}-\alpha_{2l}} \times \det[y_k^{\alpha_j}]_{k,j=1,...,2N} \tag{2.9}$$

Further, with the assumption of all the x_j and y_k having unit modulus,

$$|F| = (-i)^N \prod_{j=1}^{N} (x_j)^2 \left(\prod_{k=1}^{2N} y_k^{1/2}\right) F \tag{2.10}$$

and so substituting (2.10) and (2.9) in (2.3) gives a determinant identity for W_{N1}.

The limit $\mu \to 1^-$ can be taken by following the procedure of ref. 2, p. 467. Thus, write the summation in (2.9) as

$$\alpha_j = \gamma_j + k_j M, \qquad 0 \leqslant \gamma_j \leqslant M-1, \qquad k_j = 0, 1, 2,... \tag{2.11}$$

With the choices (2.2) of x_k and y_k, this gives

$$x_k^{\alpha_j} = x_k^{\gamma_j} \qquad \text{and} \qquad y_k^{\alpha_j} = e^{2\pi i \phi_p k_j} y_k^{\gamma_j} \tag{2.12}$$

The formulas

$$\lim_{\mu \to 1^-} \sum_{k=0}^{\infty} (\mu e^{2\pi i \phi_p})^k = \frac{1}{1 - e^{2\pi i \phi_p}} \tag{2.13}$$

and

$$\lim_{\mu \to 1^-} \sum_{k=0}^{\infty} k(\mu e^{2\pi i \phi_p})^k = \frac{e^{2\pi i \phi_p}}{(1 - e^{2\pi i \phi_p})^2} \tag{2.14}$$

then show

$$W_{N1} = (-i)^N (2\pi/L)^{3N\Gamma} \prod_{k=1}^{2N} y_k^{1/2} \sum_{\gamma_1,...,\gamma_{2N}=0}^{M-1} \prod_{l=1}^{2N} x_l^{-\gamma_{2l}-\gamma_{2l-1}-1} \times \det[f_p^{(0)} y_k^{\gamma_{2j-1}}, f_p^{(1)}(\gamma_{2j})\, y_k^{\gamma_{2j}}]_{j,k=1,...,2N} \tag{2.15}$$

where

$$f_p^{(0)} = \frac{1}{1 - e^{2\pi i \phi_p}} \tag{2.16}$$

and

$$f_p^{(1)}(\gamma) = \frac{1}{1 - e^{2\pi i \phi_p}} \left(\gamma + 1 + \frac{M e^{2\pi i \phi_p}}{1 - e^{2\pi i \phi_p}} \right) \tag{2.17}$$

3. FACTORIZATION OF THE GRAND PARTITION FUNCTION

3.1. The Partition Function

The factorization of the grand partition function at $\Gamma = 1$ from the identity (2.15) closely parallels that used in ref. 2 to factorize the grand partition function for the symmetric two-component log-potential lattice gas at $\Gamma = 4$. The latter calculation is fairly complicated. However, it has been shown by Rosinberg[4] (see also ref. 5) that a more revealing and simpler calculation is possible. Unfortunately, no progress has been made in modifying Rosinberg's approach to the present situation, so we must resort to the original method. In this section we will derive a tractable expression for Z_{N1}.

Substituting (2.15) in (2.5) shows that the sum over the m_k can be done immediately. Since $0 \leqslant \gamma_k \leqslant M$, we have

$$\sum_{m_1,\dots,m_N = 1}^{M} \prod_{k=1}^{N} x_k^{-(\gamma_{2k-1} + \gamma_{2k} + 1)} = M^N \prod_{k=1}^{N} \delta_{\gamma_{2k-1} + \gamma_{2k}, M-1} \tag{3.1}$$

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

Now consider the sum over the l_k in (2.5). Since the summand is symmetric, we can make the orderings

$$1 \leqslant l_1 \leqslant l_2 \leqslant \cdots \leqslant l_{2N} \leqslant M \tag{3.2}$$

provided we multiply by $(2N)!$. Now do the sum over $l_1, l_3, \dots, l_{2N-1}$ (method of summation over alternate variables[8]). These coordinates occur in the first, third,... rows of the determinant, respectively. For the sum over l_1 there are two possibilities:

(i) l_2 is on the sublattice L_2. In this case we sum l_1 from 0 to $l_2 - 1$ inclusive.

(ii) l_2 is on the sublattice L_3. Here we sum l_1 from 0 up to and including l_2.

Both these seemingly different procedures are the same, since the $l_1 = l_2$ term in (2.5) is zero. Performing the sum according to these rules gives for the jth element of the first row

$$f_0^{(x)} \sum_{l=0}^{l_{2k}-1+p} e^{2\pi i(l+\phi_0)(\gamma_j+1/2)/M} + f_1^{(x)}(\gamma_j) \sum_{l=0}^{l_{2k}-1+p} e^{2\pi i(l+\phi_1)(\gamma_j+1/2)/M} \tag{3.3}$$

where $k = 1$; $x = 0$ or 1 according to whether the column index is even or odd, respectively; and $p = 0$ or 1 according to whether l_2 is on the L_3 or L_2 sublattice, respectively.

The sum over l_3 is from l_2 to l_4. However, by adding the first row (3.3), which leaves the value of the determinant unchanged, the sum can be taken from 0 to l_4. The third row of the determinant is thus (3.3) with $k = 2$. Proceeding similarly, we see that the $(2k-1)$th row is given by (3.3) for each $k = 1, 2, \dots, N$.

Since

$$\sum_{l=0}^{l_{2k}-1+p} e^{2\pi i(l+\phi)(\gamma_j+1/2)/M} = \frac{e^{2\pi i(1/2+\phi)(\gamma_j+1/2)/M}\left(1 - e^{2\pi i(\gamma_j+1/2)(l_{2k}+p)/M}\right)}{-2i \sin \pi(\gamma_j + \frac{1}{2})/M} \tag{3.4}$$

we see that the jth element of the $(2k-1)$th row is

$$G_p^{(x)}(l_{2k}, \gamma_j) := [f_0^{(x)}(\gamma_j)\, e^{2\pi i(1/2+\phi_0)(\gamma_j+1/2)/M} + f_1^{(x)}(\gamma_j)\, e^{2\pi i(1/2+\phi_1)(\gamma_j+1/2)/M}] \times (1 - e^{2\pi i(\gamma_j+1/2)(l_{2k}+p)/M})/[-2i \sin \pi(\gamma_j + \tfrac{1}{2})/M] \tag{3.5}$$

Hence

$$Z_{N1} = (2\pi/L)^{3N} (-iM)^N (N!)^{-1} \sum_{\gamma_2, \gamma_4, \dots, \gamma_{2N}=0}^{M-1} \prod_{k=1}^{N} \delta_{\gamma_{2k-1}+\gamma_{2k}, M-1} \times \sum_{0 \leqslant l_2 \leqslant l_4 \leqslant \cdots \leqslant l_{2N} \leqslant M-1} \det \begin{bmatrix} G_p^{(0)}(l_{2k}, \gamma_{2j-1}) & G_p^{(1)}(l_{2k}, \gamma_{2j}) \\ f_p^{(0)} y_{2k}^{\gamma_{2j-1}} & f_p^{(1)}(\gamma_{2j})\, y_{2k}^{\gamma_{2j}} \end{bmatrix}_{j,k=1,\dots,N} \tag{3.6}$$

The determinant in (3.6) has a 2×2 block structure. If we define

$$\chi(k) = \begin{cases} 0 & k \text{ even} \\ 1 & k \text{ odd} \end{cases} \tag{3.7}$$

then the determinant has the expansion

$$\sum_{P=1}^{(2N)!} \varepsilon(P) \prod_{k=1}^{N} G_p^{\chi(P(2k-1))}(l_{2k}, \gamma_{P(2k-1)}) f_p^{\chi(P(2k))}(\gamma_{P(2k)})\, y_k^{\gamma_{P(2k)}} \tag{3.8}$$

The determinant is symmetric in the l_{2k}, so the sum over each l_{2k} can be taken from 0 to $M-1$ provided we divide by $N!$. Performing the sum gives a contribution with the structure

$$\prod_{k=1}^{N} a_{P(2k-1),P(2k)} \tag{3.9}$$

Further, the sum over the permutations in (3.8) can be restricted to the set

$$X = \{P: P(2l) > P(2l-1) \text{ each } l = 1, 2, \ldots, N\} \tag{3.10}$$

if we replace (3.9) by

$$\prod_{k=1}^{N} (a_{P(2k-1),P(2k)} - a_{P(2k),P(2k-1)}) \tag{3.11}$$

After calculating the explicit form of $a_{P(2k-1),P(2k)}$ we thus have

$$Z_{1N} = (2\pi/L)^{3N} M^{2N}(N!)^{-2} \sum_{\gamma_2,\gamma_4,\ldots,\gamma_{2N}=0}^{M-1} \prod_{k=1}^{N} \delta_{\gamma_{2k-1}+\gamma_{2k},M-1}$$
$$\times \sum_X \varepsilon(P) \prod_{k=1}^{N} [\delta_{\gamma_{P(2k-1)}+\gamma_{P(2k)},M-1} A_1(\gamma_{P(2k)}; \chi(P(2k-1)), \chi(P(2k)))] \tag{3.12}$$

where

$$\begin{aligned}
&A_1(\gamma_{P(2k)}; \chi(P(2k-1)), \chi(P(2k)))\\
&\quad= \frac{1}{\sin \pi(\gamma_{P(2k)} + 1/2)/M} \{ f_0^{\chi(P(2k))}(\gamma_{P(2k)}) f_0^{\chi(P(2k-1))}(M-1-\gamma_{P(2k)})\\
&\qquad \times e^{2\pi i\phi_0} \cos \pi(\gamma_{P(2k)} + \tfrac{1}{2})/M\\
&\qquad + f_0^{\chi(P(2k))}(\gamma_{P(2k)}) f_1^{\chi(P(2k-1))}(M-1-\gamma_{P(2k)})\\
&\qquad \times e^{2\pi i\phi_1} e^{2\pi i(\phi_0-\phi_1)(\gamma_{P(2k)}+1/2)/M} e^{\pi i(\gamma_{P(2k)}+1/2)/M}\\
&\qquad + f_0^{\chi(P(2k-1))}(\gamma_{P(2k)}) f_1^{\chi(P(2k))}(M-1-\gamma_{P(2k)})\\
&\qquad \times e^{2\pi i\phi_0} e^{2\pi i(\phi_1-\phi_0)(\gamma_{P(2k)}+1/2)/M} e^{-\pi i(\gamma_{P(2k)}+1/2)/M}\\
&\qquad + f_1^{\chi(P(2k-1))}(\gamma_{P(2k)}) f_1^{\chi(P(2k))}(M-1-\gamma_{P(2k)})\\
&\qquad \times e^{2\pi i\phi_1} \cos \pi(\gamma_{P(2k)} + \tfrac{1}{2})/M \}
\end{aligned} \tag{3.13}$$

The formula (3.12) has precisely the same structure as the partition function for the symmetric, two-component, log-potential lattice gas at $\Gamma = 4$ (ref. 2, pp. 468–469).

3.2. The Grand Partition Function

The working contained in ref. 2, pp. 469–473, demonstrates the following result for the grand partition function when the partition function has the structure (3.12).

Theorem 3.1. Let Z_{1N} be defined by (3.12) for any function A_1 with the property

$$A_1(\gamma_{P(2k)}; \chi(P(2k-1)), \chi(P(2k))) = A_1(M-1-\gamma_{P(2k)}; \chi(P(2k-1)), \chi(P(2k))) \tag{3.14}$$

Then

$$\begin{aligned} \Xi_1 &:= \sum_{N=0}^{M} \zeta^{3N} Z_{1N} \\ &= \prod_{k=0}^{[M/2]-1} \{[1 + (2\pi\zeta/L)^3\, M^2 A_1(k; 0, 0)] \\ &\quad \times [1 + (2\pi\zeta/L)^3\, M^2 A_1(M-1-k; 0, 0)] \\ &\quad - (2\pi\zeta/L)^6\, A_2(k)\} \\ &\quad \times \begin{cases} 1, & M \text{ even} \\ [1 + (2\pi\zeta/L)^3\, M^2 A_1((M-1)/2; 0, 0)], & M \text{ odd} \end{cases} \end{aligned} \tag{3.15}$$

where

$$A_2(k) = A_1(k; 1, 1)\, A_1(M-k-1; 0, 0) \tag{3.16}$$

Since from (3.13) the property (3.14) holds, the factorization is thus complete once the functional forms of A_1 and A_2 are inserted and some simplification performed. However, before doing this it is desirable to introduce a scaled fugacity ξ, defined so that the grand partition function becomes a polynomial of order M (the number of lattice sites in each sublattice) and the coefficient of the highest power is unity.

As noted in ref. 2, pp. 474–475, these requirements are fulfilled by the choice

$$\xi = (2\pi\zeta/L)^3\, e^{\Gamma(E_1 + E_2 + E_3)} \tag{3.17}$$

where E_j is the energy of a particle on sublattice L_j. (The energy between two particles on different sublattices only counts half, so as to avoid double counting.) A straightforward calculation along the lines of that given in ref. 2, p. 475, shows that

$$e^{\Gamma(E_1+E_2+E_3)} = \left(\frac{M}{2}\right)^{3\Gamma} \left(\frac{\sin \pi(\phi_1-\phi_0)}{\sin^2 \pi\phi_1 \sin^2 \pi\phi_0}\right)^{\Gamma} \tag{3.18}$$

and thus the scaled fugacity is explicitly specified.

Now reconsider the expression (3.15). After some simple calculations, use of (3.13), (3.7), (2.17), (2.16), (3.17), and (3.18) shows that

$$(2\pi\zeta/L)^6 M^4[A_1(k;0,0)\,A_1(M-1-k;0,0)-A_2(k)] = \xi^2 \tag{3.19}$$

$$(2\pi\zeta/L)^3 A_1((M-1)/2);0,0) = \xi \tag{3.20}$$

and

$$(2\pi\zeta/L)^3 M^2[A_1(k;0,0)+A_1(M-1-k;0,0)] = \xi f(k;\phi_0,\phi_1) \tag{3.21}$$

where

$$\begin{aligned} f(k;\phi_0,\phi_1) = &-\frac{8}{M}\frac{\sin^2\pi\phi_1 \sin^2\pi\phi_0}{\sin\pi(\phi_1-\phi_0)}\frac{1}{\sin\pi(k+1/2)/M} \\ &\times\left\{\frac{(2k-M+1)\cos\pi(k+1/2)/M}{4\sin^2\pi\phi_0}\right. \\ &+\frac{(2k-M+1)\cos\pi(k+1/2)/M}{4\sin^2\pi\phi_1} \\ &+\frac{2k+1-M}{2\sin\pi\phi_0\sin\pi\phi_1} \\ &\times\cos\left[\frac{2\pi(\phi_0-\phi_1)[k-(M-1)/2]}{M}+\frac{\pi(k+1/2)}{M}\right] \\ &+\frac{M\sin\pi(\phi_0-\phi_1)}{4\sin^2\pi\phi_0\sin^2\pi\phi_1} \\ &\left.\times\sin\left[\frac{2\pi(\phi_0-\phi_1)[k-(M-1)/2]}{M}+\frac{\pi(k+1/2)}{M}\right]\right\} \end{aligned} \tag{3.22}$$

Hence the grand partition function at $\Gamma = 1$ factorizes as

$$\Xi_1 = \prod_{k=0}^{[M/2]-1} (1+\xi f(k;\phi_0,\phi_1)+\xi^2) \times \begin{cases} 1, & M \text{ even} \\ (1+\xi), & M \text{ odd} \end{cases} \tag{3.23}$$

where f is given by (3.22) and the notation $[\cdot]$ in the product terminal denotes the integer part.

A feature of the polynomial $\Xi_1 = \Xi_1(\xi)$ immediately apparent from (3.23) is that

$$\Xi_1(1/\xi) = (1/\xi)^M \, \Xi_1(\xi) \tag{3.24}$$

which says that Ξ_1 is a reciprocal polynomial. For the symmetric two-component log-potential lattice gas it was shown in ref. 2, p. 474, that in terms of the appropriate scaled fugacity, the grand partition function is a reciprocal polynomial for all Γ. However, this feature does not persist for general asymmetric lattice gases, due to the lack of symmetry between the sublattices available to the same signed charge. (Conversely, if the sublattices L_2 and L_3 are indistinguishable in periodic boundary conditions, as happens with the choices $\phi_0 = 1/3$, $\phi_1 = 2/3$ and $\phi_0 = 1/4$, $\phi_1 = 3/4$, the grand partition function is reciprocal in ξ for all Γ.) Numerical calculations shows that for the present system, the grand partition function is only reciprocal at $\Gamma = 1$ and 2.

3.3. Grand Partition Function of Symmetric Model

Consider a system of N particles of charge $+2q$ and $2N$ particles of charge $-q$ on the lattice described in Section 2.1. In the limit $\phi_1 \to 0$, the leading-order contribution comes from those configurations in which all sites on L_3 next to occupied sites on L_1 are occupied. Thus, each $+2q$ charge is paired with a $-q$ charge. The effective potential at a distance r from such a pair is just the potential of a single positive charge of magnitude $+q$.

By introducing the scaled fugacity (3.17), the grand partition function of this limiting system is precisely the grand partition function of a system of equal numbers of positive charges $+q$ and negative charges $-q$. The fugacity ζ is given in terms of the scaled fugacity ξ by

$$2\pi\zeta/L = \xi(2/(M \sin \pi\phi_0))^\Gamma \tag{3.25}$$

Although the number and magnitude of the charges is symmetric, the domain is still asymmetric: the positive charges can occupy sites on the sublattice L_1 only, but the negative charges can occupy either the sublattice L_1 or L_2 (the latter provided there is no positive charge at the site; see Fig. 2).

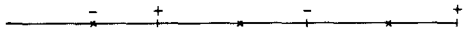

Fig. 2. An allowed configuration for the symmetric lattice gas. Sublattice L_1 is denoted by dashes and L_2 by crosses. The positive charges can occupy sublattice L_2 only, while the negative charges can occupy either sublattice L_1 or L_2.

By taking the limit $\phi_1 \to 0$ in (3.23), we see that at $\Gamma = 1$ of the symmetric model, the grand partition function has the exact factorization

$$
{}_{\text{sym}}\Xi_1 = \prod_{k=0}^{[M/2]-1} (1 + \xi h(k; \phi_0) + \xi^2) \times \begin{cases} 1, & M \text{ even} \\ 1 + \xi, & M \text{ odd} \end{cases} \tag{3.26}
$$

where

$$
\begin{aligned}
h(k; \phi_0) = {} & \frac{2}{M \sin \pi(k + 1/2)/M} \\
& \times \left\{ (M - 1 - 2k) \sin \pi\phi_0 \cos \pi \left(k + \frac{1}{2}\right) \Big/ M \right. \\
& \left. + M \sin \left[\frac{2\pi\phi_0}{M} \left(\frac{M-1}{2} - k \right) + \frac{\pi}{M} \left(k + \frac{1}{2} \right) \right] \right\}
\end{aligned} \tag{3.27}
$$

3.4. Zeros of the Grand Partition Function

From (3.23), the zeros of Ξ_1 occur at the zeros of the quadratic

$$
1 + \xi f(k; \phi_0, \phi_1) + \xi^2 \tag{3.28}
$$

Since f is real, we can immediately conclude that the zeros are either on the negative real axis or unit circle of the complex ξ plane. Numerical calculations indicate that $f(k; \phi_0, \phi_1) \geqslant 2$ for all $0 \leqslant k \leqslant M - 1$. If true, this implies that all the zeros are on the negative real axis.

3.5. Thermodynamic Limit

It is a simple task to obtain the pressure from (3.23) and (3.26), as the operation

$$
\frac{1}{M} \log \Xi_1 \tag{3.29}
$$

gives a Riemann sum approximation to an integral. Thus, for the symmetric model, the dimensionless pressure $\tau\beta P$ ($\tau = L/M$ is the lattice spacing) at $\Gamma = 1$ is given by

$$\tau\beta P = \int_0^{1/2} \log[1 + \xi H(t; \phi_0) + \xi^2]\, dt \tag{3.30}$$

where

$$H(t; \phi_0) = \frac{1}{\sin \pi t}\left\{2(1-2t)\cos \pi t \sin \pi\phi_0 - 2\sin\left[2\pi\phi_0\left(t - \frac{1}{2}\right) - \pi t\right]\right\} \tag{3.31}$$

A similar (but more lengthy) expression for the pressure in the asymmetric case can be written down immediately from (3.23).

Changing variables

$$H(t; \phi_0) = s + 1/s, \qquad 0 < s \leqslant 1 \tag{3.32}$$

in (3.30) gives

$$\tau\beta P = \int_0^1 g(s) \log\left(1 + \frac{\xi}{s}\right)(1 + s\xi)\, ds \tag{3.33}$$

The function $g(s)$ gives the density of zeros at $\xi = -s$. It has the normalization property

$$\int_0^1 g(s)\, ds = \frac{1}{2} \tag{3.34}$$

and can be calculated explicitly from the formula

$$1/g(s) = ds/dt \tag{3.35a}$$

$$= H'(t; \phi_0)/(1 - s^{-2}) \tag{3.35b}$$

where (3.35b) follows from (3.32), provided (3.35b) is regarded as a function of s.

The zeros do not intersect the positive ξ axis, so there is no transition as ξ is varied. However, from (3.35b) we can deduce that at $\xi = 0$ the density of zeros is

$$g(0) = \frac{4 \sin \pi\phi_0}{\pi} \tag{3.36}$$

This means that the pressure is not an analytic function of the scaled fugacity at $\xi = 0$. From (3.33), using integration by parts, the leading-order singular behavior is

$$\tau\beta P \sim -g(0)\xi \log \xi \tag{3.37}$$

4. THE PHASE DIAGRAM AND FINITE-SIZE LATTICE CALCULATIONS

Two-component log-potential lattice gases have two phases—a high-temperature conducting phase and a low-temperature dipole (insulating) phase. The conducting phase is characterized by an analogue of the Stillinger–Lovett sum rule (see, e.g., ref. 9), which is a condition on the asymptotic behavior of the charge–charge correlation. In the dipole phase the Stillinger–Lovett sum rule breaks down and a different decay is expected.[3]

In the low-density limit the conducting and insulating phases can be further distinguished. If the pressure is expanded about zero fugacity in the conducting phase, there is a singularity [as in (3.37)], whereas the same expansion in the insulating phase gives an analytic series. In the analogous continuous, two-dimensional, charge-symmetric Coulomb gas it has been shown in ref. 10 (see also ref. 11) that for $\Gamma \geqslant 2$ all the coefficients of the Mayer series diverge. Between $\Gamma = 2$ and $\Gamma = 4$ the coefficient of ξ^N is finite if and only if $\Gamma > 4 - 2/N$, while the series is analytic above $\Gamma = 4$. In accordance with the Yang–Lee characterization of a phase transition,[12] these features of the phases have immediate consequences for the location of the zeros of the grand partition function: in the conducting phase the zeros must pinch the real axis in the complex ξ plane at $\xi = 0$, whereas in the insulating phase a neighborhood of $\xi = 0$ must be zero free.

Can this characterization be used to locate the transition temperature in two-component log-potential lattice gases? To explore this question, first the symmetric log-potential lattice gas was considered and numerical calculation of the zeros of the grand partition function was performed for various values of Γ and M. The lattice of Fig. 2 with $\phi_0 = 0.5$ was chosen, but the two species were restricted to the distinct sublattices.

Insight into the possible functional form can be obtained by using (3.23) to derive the exact expansion at $\Gamma = 1$. (Although the allowed configurations of the exact solution differ from those of the numerical calculation, we do not expect the functional form to depend on this detail.) For example, with $\phi_0 = 1/2$, factorizing the $k = 0$ quadratic in (3.27) gives

$$\xi_1(M) \sim -\frac{\pi}{8M} - \frac{\pi}{16M^2} + O\left(\frac{1}{M^3}\right) \tag{4.1}$$

Table IA. The Value of the Zero Closest to the Origin, $\xi_1(M)$, in the Symmetric Model for Values of M and Γ As Indicated

M	$\xi_1(M)$, $\Gamma=0.6$	$\xi_1(M)$, $\Gamma=1.1$
10	−0.03889993	−0.09387103
11	−0.03415190	−0.08601634
12	−0.03031837	−0.07943074
13	−0.02716810	−0.07382574
14	−0.02454035	−0.06899467

The exact expansion at $\Gamma=1$ suggests the general form

$$\xi_1(M) \sim \frac{1}{M^\gamma}\left(a_0 + \frac{a_1}{M} + \frac{a_2}{M^2} + \cdots\right) \tag{4.2}$$

where the exponent γ will depend on the coupling Γ. By truncating the expansion to include only three terms, we can determine the constants a_0, a_1, and a_2 uniquely from three values of $\xi_1(M)$. By selecting different sets of data (i.e., different values of M), the accuracy of the choice of γ can be estimated from the stability of the coefficients a_0, a_1, and a_2.

In Table IA, the zeros of the grand partition function for M from 10 to 14 with $\Gamma=1.1$ and 0.6 are given. In Table IB, the corresponding values

Table IB. The Values of a_0, a_1, and a_2 for given γ Values in the Truncated Expansion (4.2)[a]

	{10, 11, 13}	{10, 12, 14}	{12, 13, 14}
$\gamma=0.85$			
a_0	−0.60059	−0.59886	−0.59636
a_1	−0.83245	−0.87140	−0.93650
a_2	1.9287	2.1452	2.5659
$\gamma=0.9$			
a_0	−0.73235	−0.73229	−0.73220
a_1	−0.13433	−0.13575	−0.13794
a_2	0.01448	0.02240	0.03654
$\gamma=0.95$			
a_0	−0.89021	−0.89263	−0.89617
a_1	0.80497	0.85948	0.95137
a_2	−2.6907	−2.9937	−3.5875

[a] Various data sets $\{M_1, M_2, M_3\}$ from Table IA have been used with $\Gamma=1.1$.

Table IIA. The Value of the Zero Closest to the Origin, $\xi_1(M)$, in the Asymmetric Model with $\phi_0=1/4$ and $\phi_1=3/4$ for Values of M and Γ As Indicated

M	$\xi_1(M)$, $\Gamma=0.5$	$\xi_1(M)$, $\Gamma=2$
5	−0.02694465	−0.34015386
6	−0.01916992	−0.32654753
7	−0.01443133	−0.31724446
8	−0.01131261	−0.31048527
9	−0.00914165	−0.30535346

of a_0, a_1, and a_2 are given at $\Gamma=1.1$. We see that the most stable γ value is 0.9.

Using Table IA to perform similar calculations of a_0, a_1, and a_2 at $\Gamma=0.6$ gives that in this case $\gamma=1.4$ is the most stable value. At $\Gamma=1$, (4.1) gives the exact result $\gamma=1$, and since at $\Gamma=2$ all the zeros are at $\xi=-1$,[2] we have the further exact result $\gamma=0$ when $\Gamma=2$. These results provide strong evidence that for $\Gamma\leqslant 2$ in the symmetric model

$$\gamma=2-\Gamma \tag{4.3}$$

Next, numerical calculations of the zeros of the grand partition function of the asymmetric model for certain values of ϕ_0 and ϕ_1 were performed. Here, due to the extra number of configurations contributing

Table IIB. As in Table IB, with Data Sets from Table IIB, and $\Gamma=0.5$

	{5, 6, 8}	{5, 7, 9}	{7, 8, 9}
$\gamma=1.5$			
a_0	−0.16951	−0.16642	−0.16214
a_1	−0.7466	−0.7854	−0.8538
a_2	0.4399	0.5565	0.8259
$\gamma=1.6$			
a_0	−0.24385	−0.24159	−0.23850
a_1	−0.6041	−0.6324	−0.6819
a_2	0.2708	0.3557	0.5505
$\gamma=1.4$			
a_0	−0.11559	−0.11245	−0.10812
a_1	−0.7956	−0.8349	−0.9041
a_2	0.4562	0.5744	0.8471

to each term, the maximum size polynomial obtained was only of order nine. With only small-order polynomials as data, it is more difficult to deduce the value of γ [although from (3.23) we have the exact result that at $\Gamma = 1$, $\gamma = 1$]. We find that values of γ close to the conjectured value (4.3) have similar stability properties (see Table II). Nevertheless, none of the results obtained were inconsistent with (4.3). In particular, at $\Gamma = 2$, with $\phi_0 = 1/4$ and $\phi_1 = 3/4$ the choice $\gamma = 0$ and the data of Table II A give $a_0 = -0.268$, thus indicating a gap between the zeros of the grand partition function and the positive ξ axis. The conductor–insulator transition again takes place at $\Gamma = 2$.

The conjecture (4.3) implies that $\xi_1(M)$ pinches the real ξ axis at $\xi = 0$ in the limit $M \to \infty$. Assuming that a finite density of zeros have similar behavior [as in the exact factorization (3.23)], the density of zeros function $g(s)$ for zeros at $s = -\xi$ thus has the behavior

$$g(s) \sim c_1(\Gamma)\, s^{-1+1/(2-\Gamma)} \qquad \text{as} \quad s \to 0 \tag{4.4}$$

where $c_1(\Gamma)$ is a positive function independent of s. The leading-order singular behavior of the dimensionless pressure $\tau\beta P_{\text{sing}}$ as a function of ξ is therefore

$$\tau\beta P_{\text{sing}} \sim c_2(\Gamma) \begin{cases} \xi^{1/(2-\Gamma)}, & 1/(2-\Gamma) \notin \mathbf{Z}^+ \\ \xi^{1/(2-\Gamma)} \log \xi, & 1/(2-\Gamma) \in \mathbf{Z}^+ \end{cases} \tag{4.5}$$

as $\xi \to 0$, where $c_2(\Gamma)$ is independent of ξ.

For the continuous version of the symmetric model, the expansion (4.5) (without the logarithmic correction) appears in ref. 13, p. 3279.

Note that (4.5) implies that the series expansion of the pressure in terms of ξ has the nonsingular term as its leading behavior for $\Gamma \leqslant 2$, while for $2 - 1/(N+1) > \Gamma > 2 - 1/N$ the pressure to leading order behaves as a series in the first N powers in ξ. This is analogous to the results of ref. 11 for the continuous two-dimensional symmetric Coulomb gas.

ACKNOWLEDGMENTS

Financial support for this project was obtained from the Australian Research Council. Thanks are due to K. Keay for writing most of the software for the numerical computations.

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