

## Circle Theorem for Hard-Core Binary Lattice Gases

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We study the distribution of zeros in a symmetric, two-component Widom–Rowlinson lattice system (any number of dimensions). We show that for sufficiently large mean activity the system partition function cannot vanish if the magnitude of the ratio of the two (complex) activities is different from one.

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**KEY WORDS:** Widom–Rowlinson; lattice gas; phase transition; partition function; Asano contraction.

### 1. INTRODUCTION

Two-component lattice gases of the general type introduced by Widom and Rowlinson<sup>(1)</sup> and their continuum analog have been of considerable interest in the study of phase transitions and cooperative phenomena.<sup>(2–7)</sup> For the simplest case of two symmetric components  $A$  and  $B$  with repulsive hard cores between unlike particles and a smaller (point) hard core between like particles, a demixing phase transition was proven using the Peierls method on the lattice<sup>(2)</sup> and a very clever generalization of it for the continuum case.<sup>(3)</sup> These were proven for the case where the fugacities of the two components are the same,  $z_A = z_B$ , and large. While it has been presumed that no phase transition is possible for such a system away from the symmetry line of equal fugacities for the two components, it has only recently been proven for high values of the fugacities.<sup>(8)</sup>

There are conceptual similarities between these two-component lattice gases and ferromagnetic Ising systems.<sup>(2,6)</sup> For the latter we have the well-known Lee–Yang “circle theorem”<sup>(9)</sup> that says that nonanalytic thermodynamics is possible only if  $e^H$  (where  $H = \beta \times$  magnetic field) is of magnitude one. Hence for the logarithm of the partition function of the ferromagnetic Ising system to be nonanalytic, it is necessary that  $H$  be pure imaginary; if it is

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also (on physical grounds) required to be real, it must be zero. In zero magnetic field the Ising spin system has an up-down symmetry, just as the Widom-Rowlinson system is symmetric under the interchange of the two components if their fugacities are equal.

It is natural to wonder if the analogy can be pushed further by proving analyticity of the pressure and correlation functions unless  $z_A/z_B$  is of magnitude one. It also seems natural to approach the question in the Lee-Yang manner of locating the complex zeros of the system partition function. It is the purpose of this paper to prove such a theorem, at least for the case when the mean fugacity  $(z_A z_B)^{1/2}$  is sufficiently large.

Dunlop's result<sup>(8)</sup> is closely related to ours, although obtained quite differently. If a field  $H$  is defined by  $z_A/z_B = e^{2H}$ , Dunlop shows the partition function to be nonzero in the portion of the complex  $H$  plane defined by  $\text{Re } H \geq |\text{Im } H|$ , provided also that the mean fugacity is large. Dunlop's lower bound for the mean fugacity is smaller by a factor of two than ours, but the region of the complex  $H$  plane proved analytic is also smaller.

## 2. MODELS AND TRANSFORMATIONS

Let  $\Lambda$  denote some finite lattice, with sites  $x, y, \dots$ , in any number of dimensions. Our Widom-Rowlinson type lattice model is characterized by two (hard-core) conditions: each site can be vacant or occupied by at most one particle of either  $A$  type or  $B$  type, and unlike particles are excluded from certain nearby sites around each occupied site. There is no interaction between two like particles at different sites and there are no three-body or higher interactions.

Various geometries have been considered for the exclusion "sphere" for unlike particles. The geometry appears to be a more important factor in penetrating questions dealing with the nature of the equilibrium states<sup>(7)</sup> than in questions dealing only with the existence of a phase equilibrium.<sup>(2,3,8)</sup> Consistent with this observation, our present analysis—bearing essentially only on phase transitions—is insensitive to detailed geometry and requires only that we specify the number  $b$  of different sites excluded to  $B$  ( $A$ ) particles by a particle of type  $A$  ( $B$ ) at some site. Notationally, it is also helpful to refer to the collection  $\mathcal{B} \subset \Lambda \times \Lambda$  of "bonds"; that is, the pair of sites  $(x, y) \in \mathcal{B}$  if an  $A$  particle at  $x$  excludes a  $B$  particle at  $y$  (and vice versa).

It is furthermore helpful to introduce at the very beginning a double-site representation of  $\Lambda$  such that for each  $x \in \Lambda$  we imagine *two* sites which we shall consistently denote  $x'$  and  $x''$ . If  $\Lambda$  itself is two-dimensional, it is convenient to think of two horizontal layers of sites with  $x''$  lying over  $x'$ . For three (or more) dimensions we may think of one copy being slightly displaced from the other. We will say that the corresponding sites  $x'$  and  $x''$  are *partners*.

We now imagine that each of the  $2|\Lambda|$  sites bears an Ising spin  $\frac{1}{2}$ , taking values of  $\pm 1$  and denoted by  $\sigma_{x'}$  or  $\sigma_{x''}$ . We shall define the interactions between these Ising spins in such a way that the partition function for the  $2|\Lambda|$  Ising spins will be proportional to the partition function of our Widom–Rowlinson (WR) model on the original lattice  $\Lambda$ . An analysis of the spin system for possible singularities (phase transitions) can then be translated into a corresponding analysis for the WR model. In particular, zero magnetic field for the spin system will translate to equal chemical potentials for the two types of particles,  $A$  and  $B$ .

Guided by spin-1 descriptions of WR models,<sup>(2,7)</sup> the correspondence is fairly obvious:  $\sigma_{x'} = \sigma_{x''}$  corresponds to the presence of a particle at  $x$ , while  $\sigma_{x'} \neq \sigma_{x''}$  means  $x$  is vacant:  $\sigma_{x'} = \sigma_{x''} = +1$  corresponds to an  $A$  particle, while  $\sigma_{x'} = \sigma_{x''} = -1$  means a  $B$  particle. The hard-core interaction between  $A$  and  $B$  particles corresponds to an exclusion of any configuration for which  $\sigma_{x'}\sigma_{x''} = +1 = \sigma_{y'}\sigma_{y''}$  and  $\sigma_{x'}\sigma_{y'} = -1$  if  $(x, y) \in \mathcal{B}$ . Rather than introduce infinitely repulsive four-body interactions to effect this exclusion, we shall simply agree that no such configurations will be included in any sum over spin configurations.

We introduce a ferromagnetic interaction  $-J\sigma_{x'}\sigma_{x''}$  with  $J > 0$  between partner spins: large  $J$  favors spin configurations  $(+, +)$  and  $(-, -)$ , which correspond to particles of the two types. In order to distinguish between the two types of particles, we need magnetic fields acting on the spins through terms  $-h_{x'}\sigma_{x'}$  and  $-h_{x''}\sigma_{x''}$ . By permitting all  $2|\Lambda|$  magnetic fields to be independent variables we are able to use the Asano contraction technique described below to study the zeros of the partition function.

The partition function of the spin system is thus

$$\Xi_s = \sum'_{\sigma} \prod_{x \in \Lambda} \exp(h_{x'}\sigma_{x'} + h_{x''}\sigma_{x''} + J\sigma_{x'}\sigma_{x''}) \quad (1)$$

Here  $\sigma$  stands for the  $2|\Lambda|$  spin variables  $\{\sigma_{x'}\}_{x \in \Lambda}$  and  $\{\sigma_{x''}\}_{x \in \Lambda}$  and the prime on the summation sign is to remind us of the exclusion of spin configurations for which any bonded pair of sites has configuration  $(+, +)$  at one site and  $(-, -)$  at the other.

Before relating  $\Xi_s$  to the WR partition function we first make a more usual connection with a lattice gas (LG) on the *double* lattice. Here the correspondence is  $\sigma = +$  means a particle,  $\sigma = -$  means a vacancy. To that end we write Eq. (1) as

$$\Xi_s = \{\exp[(J - 2\bar{h})|\Lambda|]\} \sum'_{\sigma} \prod_x \tau_{x'}^{(\sigma_{x'} + 1)/2} \tau_{x''}^{(\sigma_{x''} + 1)/2} Z^{(\sigma_{x'}\sigma_{x''} - 1)/2} \quad (2)$$

where

$$\tau_{x'} = \exp(2h_{x'}), \quad \tau_{x''} = \exp(2h_{x''}), \quad Z = \exp(2J)$$

and

$$\bar{h} = (2|\Lambda|)^{-1} \sum_{x \in \Lambda} (h_{x'} + h_{x''})$$

We can thus write

$$\Xi_s = \{\exp[(J - 2\bar{h})|\Lambda|]\} \Xi_{LG}(\tau', \tau''; Z) \quad (3a)$$

where

$$\Xi_{LG}(\tau', \tau''; Z) = \sum_{\sigma'} \prod_x \zeta_x(\sigma_{x'}, \sigma_{x''}; Z) \quad (3b)$$

and where  $\zeta_x$  is  $\tau_{x'}\tau_{x''}$ ,  $\tau_{x'}/Z$ ,  $\tau_{x''}/Z$ , or 1 according to whether  $(\sigma_{x'}, \sigma_{x''})$  is  $(+, +)$ ,  $(+, -)$ ,  $(-, +)$ , or  $(-, -)$ . It is with  $\Xi_{LG}$  that the Asano analysis of zeros will be carried out.

To obtain the WR partition function we first rewrite Eq. (1) as

$$\begin{aligned} \Xi_s = & [\exp(-J|\Lambda|)] \sum_{\sigma'} \prod_x \exp[(h_{x'} + h_{x''})(\sigma_{x'} + \sigma_{x''})/2] \\ & \times \exp[(h_{x'} - h_{x''})(\sigma_{x'} - \sigma_{x''})/2] \exp[J(\sigma_{x'}\sigma_{x''} + 1)] \end{aligned} \quad (4)$$

so that

$$\Xi_s = (2e^{-J})^{|\Lambda|} \Xi_{WR}(\mathbf{z}_A, \mathbf{z}_B; \Delta h) \quad (5a)$$

where

$$\Xi_{WR}(\mathbf{z}_A, \mathbf{z}_B; \Delta h) = \sum_{\sigma'} \prod_x \eta_x(\sigma_{x'}, \sigma_{x''}) \quad (5b)$$

Here  $\eta_x$  is  $z_{A,x}$ ,  $e^{\Delta h_x}/2$ ,  $e^{-\Delta h_x}/2$ , or  $z_{B,x}$  according to whether  $(\sigma_{x'}, \sigma_{x''})$  is  $(+, +)$ ,  $(+, -)$ ,  $(-, +)$ , or  $(-, -)$ . Also

$$\begin{aligned} z_{A,x} &= [\exp(h_{x'} + h_{x''}) \exp(2J)]/2 \\ z_{B,x} &= \{\exp[-(h_{x'} + h_{x''})] \exp(2J)\}/2 \\ \Delta h_x &= h_{x'} - h_{x''} \end{aligned} \quad (5c)$$

From Eqs. (3) and (5) we have the relationship between  $\Xi_{LG}$  and  $\Xi_{WR}$ :

$$\Xi_{WR} = [\exp(2J - 2\bar{h})/2]^{|\Lambda|} \Xi_{LG}$$

In the next section we look for possible zeros of  $\Xi_{LG}$ , which will then be interpreted in terms of zeros of  $\Xi_{WR}$ . The real WR partition function is  $\Xi(\mathbf{z}_A, \mathbf{z}_B) = \Xi_{WR}(\mathbf{z}_A, \mathbf{z}_B; 0)$ , i.e.,  $h_{x'} = h_{x''}$  for all  $x$ .

### 3. ZEROS OF $\Xi_{LG}$

The trick in determining (bounds for) the zeros of a partition function begins with describing it as the “Asano contraction”<sup>(10)</sup> of partition functions describing small, finite portions of the lattice. These small systems must jointly cover the entire original lattice in the sense that every interaction (including the one-body chemical potential terms) must be included in at least one of the small systems.

Here partition function always means one for which each site is represented by a different independent fugacity variable as in Eqs. (3b) and (5b). While it contains many more variables than the ordinary partition function, such a multivariable partition function has one great simplification: it is linear in each of the different activity variables. (Of course, the ordinary partition function may always be obtained from the multivariable one by setting all activities equal to the same common value.)

Asano contractions deal precisely with such linear functions. Very simply, if

$$f(x, y) = axy + bx + cy + d \tag{6a}$$

where  $x$  and  $y$  are complex variables, and  $a, b, c, d$  are complex constants, then the Asano contraction of  $f$  is

$$f^{AC}(z) = az + d \tag{6b}$$

(Heuristically, it may help to think of  $x$  and  $y$  as duplicates of the “true” variable  $z$ ; only those terms for which both duplicates are present, or neither is present, could be “valid” descriptions of the “true” variable.)

The application to statistical mechanics of lattice systems is usually one of “gluing together” a lattice dismembered at some site  $x$ . If  $Az_x + B$  and  $Cz_{x'} + D$  are the partition functions of the two pieces, the partition function of the composite system (with the pieces still treated as independent) is  $ACz_x z_{x'} + AD_{x'} + BCz_{x'} + BD$ , but the “true” partition function of the rejoined pieces is the Asano contraction  $ADz_x + BD$ .

The motivation behind this method is the theorem of Asano and Ruelle<sup>(11)</sup> relating the zeros of  $f(x, y)$  and those of  $f^{AC}(z)$ . It may be stated: Let  $D_x$  and  $D_y$  be closed regions of the complex plane, not containing 0, with the property that  $f(x, y) \neq 0$  as long as  $x \notin D_x$  and  $y \notin D_y$ . Then  $f^{AC}(z) \neq 0$  as long as  $z \notin D_z$ , where

$$D_z = -(D_x \times D_y) = \{z | z = -\xi\eta, \quad \xi \in D_x, \eta \in D_y\} \tag{7}$$

The most significant feature of this technique is that for finite-range interactions, a finite number of contractions at each site—and consequently a finite number of applications of the theorem—suffices to produce a result for

an infinite lattice. Notice that if  $D_x$  and  $D_y$  are each the interior or exterior of the unit circle,  $D_z$  is the same.

In the above simple illustration the factors  $A$  and  $C$  include Boltzmann-type terms for the various interactions involving a particle at site  $x$ . That they should be multiplied together in the partition function of the composite system follows from the independence of the interactions represented by those terms.

Now, regarding Eq. (3b), we use four-site governing sets—one for each bond in  $\mathcal{B}$ —as the small systems that generate the total partition function  $\Xi_{\text{LG}}$  through the Asano contraction procedure. For a bond  $(x, y) \in \mathcal{B}$ , the small system consists of the four sites  $x', x'', y',$  and  $y''$  and has a partition function

$$\sum_{\substack{\sigma_{x'}, \sigma_{x''} \\ \sigma_{y'}, \sigma_{y''}}} \xi_x \xi_y = [\tau_{x'} \tau_{x''} + Z^{-1}(\tau_{x'} + \tau_{x''}) + 1][\tau_{y'} \tau_{y''} + Z^{-1}(\tau_{y'} + \tau_{y''}) + 1] \\ - \tau_{x'} \tau_{x''} - \tau_{y'} \tau_{y''} \quad (8)$$

An apparent difficulty lies in the fact that the only interaction terms present (the  $Z^{-1}$  factors) appear like an interaction between a vacant site and an occupied site. These factors would erroneously become  $Z^{-2}$  after multiplication of the small partition functions and one contraction.

There is, fortunately, a simple way out of this difficulty. Suppose the lattice  $\Lambda$  were one-dimensional. There would then be just one contraction needed at each site  $x'$  or  $x''$  and if in the functions in Eq. (8),  $Z$  were replaced by  $Z^{1/2}$ , the resulting contracted partition function would be correct.

There are, it is true, some incorrect terms present at intermediate stages, when the contractions have been performed at only one of the partner sites  $x'$  and  $x''$ . An example of such an erroneous term is

$$(\cdots + \tau_{x_1}/Z^{1/2} + \cdots)(\tau_{x_2} \tau_{x_2''} + \cdots) = \cdots + \tau_{x_1} \tau_{x_2} \tau_{x_2''}/Z^{1/2} + \cdots$$

which then becomes  $\tau_{x'} \tau_{x_2''}/Z^{1/2}$  after the contraction at  $x'$ . This term is eliminated, however, by the contraction at  $x''$ —since it contains  $\tau_{x_2''}$  but not  $\tau_{x_1''}$ .

The generalization to higher dimensions is (for this technique!) trivial—we must simply replace  $Z^{1/2}$  by  $Z^{1/b}$ , where  $b$  is number of sites excluded to a  $B$  ( $A$ ) particle by an  $A$  ( $B$ ) particle, in addition to the site on which the reference particle sits. Thus  $b$  is one greater than the number of contractions needed at each site to reconnect the (double-site) lattice after initially splitting it into four-site covering sets. For the square lattice with nearest neighbor exclusions between unlike particles,  $b = 4$ . In three dimensions suppose an  $A$  particle excludes a  $B$  particle from all 27 sites of the  $3 + 3$  cube with  $A$  at its central site. Then  $b = 26$ . This is the model known to have non-translation-invariant equilibrium states associated with a “sharp interface” between the phases.<sup>(7)</sup>

We now must analyze the zeros of the “small” partition function of Eq. (8), with  $Z$  replaced by  $Z^{1/b}$ . Changing notation slightly, we actually study

$$F_w(x, \xi, y, \eta) = [Wx\xi + \frac{1}{2}(x + \xi) + W][Wy\eta + \frac{1}{2}(y + \eta) + W] - W^2x\xi - W^2y\eta \quad (9)$$

where  $2W = Z^{1/b}$  and  $\tau_x$  has been replaced by  $x$ , etc. For this analysis we need the *theorem of Grace*<sup>(12)</sup>:

Let  $f(x, y) = f(y, x) = axy + bx + by + c$ , where  $a, b$ , and  $c$  are complex constants, and let  $g(x) = f(x, x)$ . If the zeros of  $g$  are contained in a closed circular region  $C$  of the complex plane, then  $f(x, y) \neq 0$  if  $x \notin C$  and  $y \notin C$ . We remark that it is crucial that  $f$  be first order in both  $x$  and  $y$  and that  $f$  be symmetric in  $x$  and  $y$ . The theorem can be generalized to an arbitrary (finite) number of variables, for first-order functions *totally* symmetric in all variables.

While  $F_w(x, \xi, y, \eta)$  is not invariant to *all* permutations of its arguments, it is covered by the following corollary of Grace’s theorem.

**Corollary.** Let  $F(x, \xi, y, \eta)$  be first order in each of the four complex variables and satisfy  $F(x, \xi, y, \eta) = F(x, \xi, \eta, y) = F(\xi, x, y, \eta)$ . Let

$$G(x, y) = F(x, x, y, y)$$

and suppose that  $G(x, y) \neq 0$  if  $x \notin C_x$  and  $y \notin C_y$ , where  $C_x$  and  $C_y$  are closed circular regions of the plane; then  $F(x, \xi, y, \eta) \neq 0$  if  $x \notin C_x$ ,  $\xi \notin C_x$ ,  $y \notin C_y$ , and  $\eta \notin C_y$ .

*Proof.* Two applications of Grace’s theorem are required.  $F(x, \xi, y, y) \neq 0$  if  $x \notin C_x$ ,  $\xi \notin C_x$  (for fixed  $y \notin C_y$ ) since  $F(x, \xi, y, y)$  is symmetric in  $x$  and  $\xi$ . But  $F(x, \xi, y, y) \neq 0$  if  $y \notin C_y$ —and fixed  $x \notin C_x$ ,  $\xi \notin C_x$ —implies  $F(x, \xi, y, \eta) \neq 0$  if  $y \notin C_y$ ,  $\eta \notin C_y$  (along with  $x \notin C_x$ ,  $\xi \notin C_x$ ) since  $F$  is symmetric in  $y$  and  $\eta$ . This concludes the proof.

To apply this corollary to  $F_w$  defined in Eq. (9), we must produce circular regions  $C_x$  and  $C_y$ . Actually, we are able to do this only if  $W$  is sufficiently large ( $W > 1 + 2^{-1/2}$ ) and then we may take the unit circle for both  $C_x$  and  $C_y$ . The crucial step is the following.

**Proposition.** If  $G_w(x, y) = F_w(x, x, y, y)$  and  $W \geq 1 + 2^{-1/2}$ , then  $G_w(x, y) = 0$  and  $|y| = 1$  imply that  $|x| = 1$ .

*Proof.* We simply solve  $G_w(x, y) = 0$  for  $x$  in terms of  $y$  using the quadratic formula, to obtain

$$x = \frac{-(Wy^2 + y + W) \pm i[4W^2(Wy^2 + y)(y + W) - (Wy^2 + y + W)^2]^{1/2}}{2(Wy^2 + y)W} \quad (10)$$

We then calculate  $x/y$  making use several times of the fact that  $y^{-1} = y^*$  (= complete conjugate) since  $|y| = 1$ . We obtain

$$\frac{x}{y} = \frac{-(Wy + 1 + Wy^*) \pm i(4W^2|W + y|^2 - |Wy + 1 + Wy^*|^2)^{1/2}}{2W(Wy^2 + y)}$$

In the numerator  $Wy + 1 + Wy^*$  is real, as is the square root, *provided*

$$4W^2|W + y|^2 \geq |Wy + 1 + Wy^*|^2$$

for all  $|y| = 1$ . It may be verified that this is true if  $W \geq 1 + 2^{-1/2}$ . Finally,

$$\left| \frac{x}{y} \right|^2 = \frac{4W^2|W + y|^2}{4W^2|Wy^2 + y|^2} = \frac{|W + y|^2}{|W + y^*|^2} = 1$$

which completes the proof of the proposition since  $W$  is real. Clearly  $G_w = 0$  and  $|x| = 1$  also imply  $|y| = 1$  for  $W \geq 1 + 2^{-1/2}$ .

We can now demonstrate a lemma about the zeros of  $F_w$ .

**Lemma.** Let  $F_w(x, \xi, y, \eta)$  be as defined in Eq. (9) and let  $W \geq 1 + 2^{-1/2}$ ; also let  $C_e$  ( $C_i$ ) be the closed exterior (interior) of the unit circle. If  $q \notin C_e$  is true for  $q$  equaling *each* of the four variables  $x, \xi, y,$  and  $\eta$ , then  $F_w(x, \xi, y, \eta) \neq 0$ . Also, if  $q \notin C_i$  for all four variables,  $F_w \neq 0$ .

*Proof.* Again let  $G_w(x, y) = F_w(x, x, y, y)$  and notice that  $G_w(x, y) = 0$  and  $y = 0$  imply that  $|x| > 1$  for  $W \geq 1 + 2^{-1/2}$  for either branch of Eq. (10). Actually, one branch approaches infinity as  $y \rightarrow 0$  and the other approaches  $-W$ . Either branch is a continuous function of  $y$  that has modulus one when  $|y| = 1$  (by the above proposition) and *only* when  $|y| = 1$  (by the symmetry of  $G_w$  with respect to interchanging  $x$  and  $y$ ). We thus conclude that the mapping (10) carries  $C_i$  into  $C_e$  (inside of unit circle to outside). To obtain the corresponding result for  $C_e$ , we notice that

$$x^2 y^2 G_w(1/x, 1/y) = G_w(x, y)$$

which transforms the small- $y$  results into large- $y$  results; Eq. (10) therefore maps the exterior of the unit circle  $C_e$  into  $C_i$ . We can thus conclude that if  $x$  and  $y$  are both strictly inside or strictly outside the unit circle,  $G_w$  cannot vanish. The corollary to Grace's theorem applies to  $F_w$  of Eq. (9), which concludes the proof of the lemma.

The principal result of this paper is the following theorem.

**Theorem.** The lattice gas partition function  $\Xi_{\text{LG}}(\tau', \tau''; Z)$ , for  $Z \geq (2 + 2^{1/2})^b$ , does not vanish if  $\tau_{x'} < 1$  and  $\tau_{x''} < 1$  for all  $x \in \Lambda$ . It also does not vanish if  $\tau_{x'} > 1$  and  $\tau_{x''} > 1$  for all  $x \in \Lambda$  with  $Z$  in the same range.

*Proof.*  $\Xi_{\text{LG}}$  is the Asano contraction of  $b\Lambda/2$  small partition functions of the form (8) with  $Z$  replaced by  $Z^{1/b} \equiv 2W$ . There are  $b - 1$  contractions at



each site of the (double-site) lattice, so Eq. (7) must be invoked  $b - 1$  times. But each of the closed regions is always the same—the closed exterior (or interior) of the unit circle—so the regions neither grow nor shrink at each contraction. As long as the lemma holds, i.e., if  $W \geq 1 + 2^{-1/2}$ , then the conclusion will be that all fugacities  $\tau_{x'}$  and  $\tau_{x''}$  strictly greater than 1 (or alternatively all strictly less than 1) in magnitude will ensure that  $\Xi_{LG} \neq 0$ .

Consequently, if the fugacities are all the same, say  $\tau$ , and the partition function vanishes, it must be true that  $|\tau| = 1$ . If it is further specified that  $\tau$  is real, then the only possibility, for  $\Xi_{LG}$  to vanish, is that  $\tau = 1$ .

#### 4. CONCLUSIONS AND DISCUSSION

For all lattice gas fugacities  $\tau_{x'}$  and  $\tau_{x''}$  to be of unit modulus, all fields  $h_{x'}$  and  $h_{x''}$  must be pure imaginary [see Eq. (2)]. But this means, for the isomorphic WR system [see Eq. (5c)], that  $z_A$  and  $z_B$  must be equal in magnitude. Alternatively, the ratio

$$z_{A,x}/z_{B,x} = \exp(2h_{x'} + 2h_{x''}) = \tau_{x'}\tau_{x''}$$

obeys a “circle theorem” in the sense that this ratio must be of unit magnitude; and, of course, if the fields are real, they must vanish so that the two fugacities are strictly equal. The preceding statements have been here proven under the condition that the parameter  $Z = e^{2J}$  be real and equal to or greater than  $(2 + 2^{1/2})^b$ . In the WR representation  $Z$  is related to the mean fugacity by

$$Z = 2(z_{A,x}z_{B,x})^{1/2}$$

from Eq. (5c).

The significance, as usual, of statements regarding the zeros of the partition function is the assurance of analytic thermodynamic properties—derivable from the logarithm of the partition function—inside open regions free of zeros. If the fugacities of the two types of WR particles are each real, then they must be equal for a phase separation to be possible. We have proved this only in the high-mean-fugacity region,  $Z \geq (2 + 2^{1/2})^b$ , although we believe it to be true for all real activities.

While there are no calculations or good estimates of the transition fugacities  $z_t = z_A = z_B$  for real lattices in two or more dimensions, they surely lie below the value  $(2 + 2^{1/2})^b/2$  calculated here for the validity of the “circle theorem.” It is to be presumed that some other locus of zeros besides the unit circle (in the  $\tau$  plane) is correct for lower mean fugacities, but that locus most likely still intersects the positive real axis only at  $\tau = 1$ . Dunlop’s work<sup>(8)</sup> verifies this statement down to mean fugacity  $(2 + 2^{1/2})^b/4$ .

Some evidence bearing on these questions is supplied by the one-dimensional lattice with nearest neighbor exclusions between unlike particles.<sup>(13)</sup> This model, of course, has no phase transition (no zeros on the positive real axis). The partition function does have complex zeros, however, which may be studied analytically. Under the simplifying assumptions of (1) periodic boundary conditions and (2)  $z_A z_B = Z^2/4$  is real, the partition function and its zeros were studied as functions of the complex variable  $z_A/z_B = \tau^2$ . There are, for low values of  $z_A z_B$ , zeros of the partition function for values of  $|z_A/z_B|$  different from one. However, for  $(z_A z_B)^{1/2} \geq 3^{3/2} = 5.196\dots$ , the only partition function zeros correspond to  $|z_A| = |z_B|$ . This is consistent with the conclusion of this paper, that  $|z_A|$  must equal  $|z_B|$  for the partition function to vanish if  $(z_A z_B)^{1/2} \geq (2 + 2^{1/2})^2/2 = 5.828\dots$ . In the one-dimensional case ( $b = 2$ ), at least, the bound obtained by the present method appears to be a quite good one.

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