

# Equilibrium States of a Dimer Model with Angular Forces

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**Abstract.** Several complementary techniques are applied to the study of the orientational transition in a restricted lattice model of rigid linear dimers with finite interactions between contiguous molecules, on the square lattice. The restriction has the effect of forcing the ordered phase to resemble either a smectic or a nematic liquid crystal. It is shown that the symmetry of the equilibrium state is broken for some interactions and that the equilibrium state is unique for others. Thermodynamic analyticity is established for high temperatures.

## 1. Introduction

Considerable effort has been expended in the study of dense fluids and their phase transitions. There has also been considerable interest in various models of liquid crystalline systems. One of these models is the continuum rigid rod model which has the virtue of relative mathematical simplicity. The combination of these two classes of models yields a model of rigid straight polymeric molecules that are constrained to fit on some lattice; dimers on a square lattice represent the simplest example. This system is known to have no phase transition (Heilmann and Lieb [1], Gruber and Kunz [2], Runnels and Hubbard [3]) when all allowed configurations of a specified number of molecules have the same energy. If this restraint is removed and intermolecular interactions permitted, the possibility of an orientational phase transition must be reexamined. It will be shown that for a restricted version of the model, and some interactions, a phase transition does occur. When we refer to the existence of a phase transition, we are actually referring to a breakdown of symmetry in the equilibrium states as discussed by Dobrushin [4] and Lanford and Ruelle [5]. We do not attempt to infer from this symmetry breakdown anything about nonanalyticity of the free energy.

## 2. The Restricted Dimer Model

The underlying lattice for this problem is the two-dimensional square lattice. On that lattice we shall place straight rigid dimers whose width is the edge of the unit cell of the square lattice. The dimer may be of

horizontal or vertical orientation, but no two molecules may overlap. We make a further restriction in the lattice model in the interest of greater mathematical tractability: the left end of a horizontal dimer and the bottom of a vertical dimer must reside at a lattice site whose coordinates  $(x, y)$  satisfy the condition  $x = y \pmod{2}$ . Such a lattice site is denoted a reference site. This restricted lattice system also has no phase transition in the absence of other interactions. (This follows most simply by noticing



Fig. 1. The pair potential  $\phi$  has value  $a$  for the left relative orientation,  $b$  for the middle, and  $c$  for the right. We set  $c = 0$

that under these conditions the molecules interact one-dimensionally – along diagonal lines.)

We now imagine the molecules to interact by way of a short-ranged pair potential  $\phi$ . Specifically, for two adjacent parallel dimers, the pair potential has value  $a$ ; for two adjacent perpendicular dimers, the pair potential is  $b$  (see Fig. 1). We assume that not both  $a$  and  $b$  are zero. A more general model would include an interaction  $c$  for end-to-end molecules; it turns out, however, that any nonvanishing value for  $c$  invalidates a transformation to be introduced below. Consequently we set  $c = 0$ . We also set equal to zero any pair potential for nonadjacent molecules and all higher order many-body potentials.

There are two basic types of close-packed ordered arrangements that this lattice affords. One is reminiscent of a nematic and the other reminiscent of a smectic liquid crystal (see Fig. 2), and we will use these names to identify the two structures. The interaction energy per molecule of the close-packed nematic structure is clearly  $2a$  and that of the smectic close-packed structure if  $a + 2b$ . Obviously the nematic (smectic) structure is favored if  $a < 2b$  (if  $a > 2b$ ).

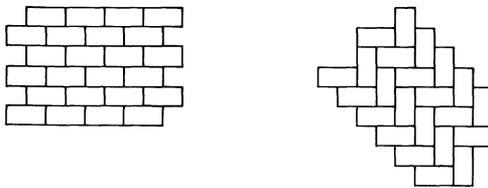


Fig. 2. Two close packed ordered structures. We refer to the one on the left as “nematic” and the one on the right as “smectic”. Each structure has a reflected version that interchanges the roles of horizontal and vertical dimers

### 3. Equilibrium States

We denote by  $V$  a finite portion of the (restricted) square lattice and by  $\alpha$  any allowed configuration of horizontal and vertical molecules. The sum of all pairwise interactions discussed above will be denoted by  $\Phi(\alpha)$ , and the energy of configuration  $\alpha$  by  $U(\alpha)$ :

$$U(\alpha) = -\beta\mu N(\alpha) + \beta\Phi(\alpha), \quad (1)$$

where  $N(\alpha)$  is the number of molecules in configuration  $\alpha$ ,  $\mu$  is the chemical potential and  $\beta = 1/kT$ . We will also refer to  $U$  as the interaction; the interaction so defined includes the chemical potential and the temperature. The grand partition function for the finite system is then

$$Z = \sum_{\alpha} e^{-U(\alpha)},$$

and the pressure (times  $\beta$ ) in the thermodynamic limit is

$$P = \lim_{|V| \rightarrow \infty} |V|^{-1} \log Z.$$

The existence of  $P$  was established by Gruber and Kunz [2]; the important question remaining is the analyticity of its dependence on the interaction  $U$ .

Equivalently, we wish to know the portions of the  $\beta - \mu$  half-plane (positive  $\beta$ ) for which  $P$  is an analytic function of  $\beta$  and  $\mu$ , and which therefore correspond to a single thermodynamic phase. This can be accomplished for a portion of the half-plane by an application of the Yang-Lee-Ruelle theorem (Ruelle [6]) on the zeros of  $Z$ .

Additional information can be obtained through study of the dependence of the equilibrium states of the system on the boundary conditions. Two sorts of result here are possible: for some interactions we can prove that the equilibrium state is unique, independent of boundary conditions and translationally invariant; for others we can prove the existence of two different equilibrium states, depending on the boundary conditions. These situations pertain to two disjoint regions of the  $\beta - \mu$  half-plane, and it is natural (but unproven) to presume that a two-phase coexistence curve passes between the regions.

#### *Region of Analyticity*

The Yang-Lee techniques, generalized by Ruelle [6], is a general and powerful method of determining regions of the complex activity ( $z$ ) plane which are free of zeros of the grand partition function  $Z$  for a lattice system. As is well known, any part of the positive real  $z$  axis which is in a zero free-region is a domain of analyticity of  $Z$  and therefore devoid of thermodynamic anomalies.

Use of the Yang-Lee-Ruelle theorem requires the generation of two collections. The first is a collection of “covering sets”  $A_\alpha$ , each composed of sites and “bonds” – the latter representing interactions between occupied sites. The union of all covering sets must include at least once each site and interaction of the lattice system. The second collection consists of regions  $M_{\alpha,i}$  of the complex plane – one for each site  $i$  included in each covering set  $A_\alpha$ . The regions  $M_{\alpha,i}$  must be closed and must not contain the origin. Finally the covering sets and regions must be chosen so that  $Z_\alpha \neq 0$  if  $z_i \in (\sim M_{\alpha,i})$  for each site  $i$  in  $A_\alpha$ . Here  $\sim$  denotes the complement and  $Z_\alpha$  the multivariant grand partition function for the set  $A_\alpha$ . In the multivariant partition function there is associated a site activity variable  $z_i$  with each site. Thus  $Z_\alpha$  is a linear function of any one site activity.

The Yang-Lee-Ruelle theorem states that the multivariant partition function  $Z_V$  for the entire lattice does not vanish if each activity obeys the requirement

$$z_i \in (\sim R_i)$$

where  $R_i$  is the “set product” region

$$R_i = - \prod_{\alpha} (-M_{\alpha,i}),$$

the product being over all  $\alpha$  for which  $A_\alpha$  contains site  $i$ . By the product  $AB$  of two sets we mean all complex numbers  $z$  which can be represented as  $z = z_1 \cdot z_2$  with  $z_1 \in A$ ,  $z_2 \in B$ .

We may transcribe the geometry of the restricted dimer problem into an equivalent lattice gas problem involving “spherical” molecules. If we locate a dimer by its midpoint, then the location of the midpoint establishes unambiguously the orientation of the dimer. The resulting pattern of midpoint sites without the restriction would define the line graph of the square lattice. With the restriction we have the “lattice” shown in Fig. 3, where hard core interactions are indicated by heavy lines, the parallel interaction (a) by light lines, and the perpendicular interaction (b) by dotted lines. On this lattice we need specify only the occupied sites – the orientations are determined.

It may be seen that each site interacts with ten other sites – two with a hard core interaction, and four each with an  $a$  and a  $b$  interaction. We shall thus employ ten two-point covering sets  $M_{\alpha,i}$  for an arbitrary site  $i$ , where  $1 \leq \alpha \leq 10$  and the index  $\alpha$  is keyed to the labeled sites in Fig. 3. For the hard core interactions we may take (Runnels and Hubbard [3]):

$$M_{9,i} = M_{10,i} = \{z: \operatorname{Re}(z) \leq -1/2\}.$$

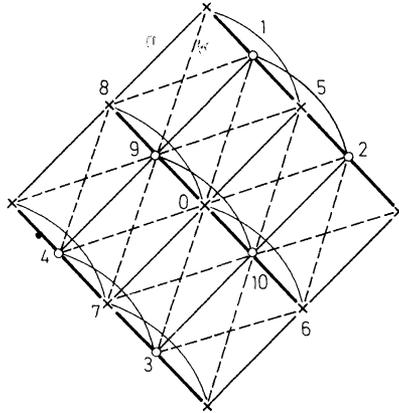


Fig. 3. Line graph of the restricted square lattice. Heavy lines represent hard core overlap, light lines represent the parallel interactions (a), and dotted lines represent the perpendicular interaction (b)

If  $a$  is negative, we may take (Ruelle [6]) for  $1 \leq \alpha \leq 4$

$$M_{\alpha,i} = \{z: |z + 1| \leq (1 - e^{\beta\alpha})^{1/2}\},$$

while if  $a$  is positive, we use

$$M_{\alpha,i} = \{z: |ze^{-\beta\alpha} + 1| \leq (1 - e^{-\beta\alpha})^{1/2}\}.$$

Corresponding choices for  $M_{\alpha,i}$ , with  $5 \leq \alpha \leq 8$ , are obtained by obvious transcription.

We wish to show that for sufficiently small  $\beta$  an arbitrary portion of the positive real  $z$  axis is free of zeros. We may write  $R_i = R$  (all  $i$ ) as

$$R = -M_9^2 M_1^4 M_5^4,$$

where the subscript  $i$  has been suppressed, and the powers represent set products. Now  $-M_9^2$  is the region exterior to the parabola (Runnels and Hubbard [3])

$$z = (-1/4 + t^2) - it, \quad -\infty < t < +\infty,$$

and contains none of the positive real axis. Clearly for sufficiently small  $\beta$  both  $M_1^4$  and  $M_5^4$  are contained within a circle about  $z = 1$  - and so is their product. Furthermore the radius decreases with decreasing  $\beta$  and vanishes at  $\beta = 0$ . It follows that the smallest real  $z_0$  in  $R$  increases to  $+\infty$  as  $\beta \rightarrow 0$ . Translating these statements from activity to chemical potential yields the region of analyticity shown in Fig. 4. Algebraic details about the set products have been worked out by Freasier [7].

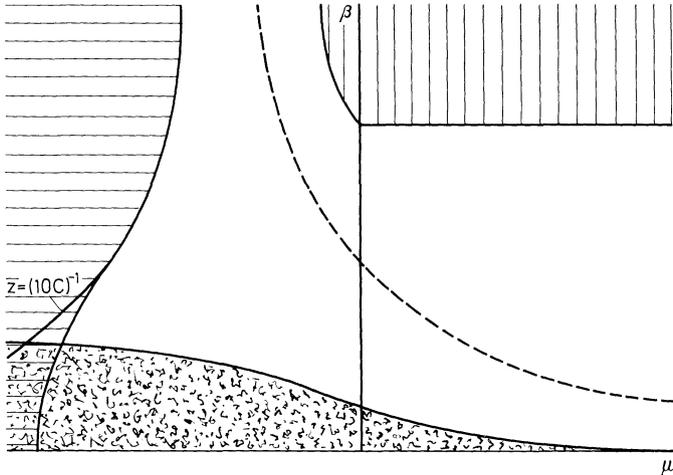


Fig. 4. Equilibrium states. The dotted region at the bottom is the Yang-Lee-Ruelle region of analyticity. In the region with horizontal shading, the equilibrium state is unique. There are at least two equilibrium states in the region with vertical shading, where long range order prevails. The presumed two-phase coexistence curve is also shown, although nothing is known with rigor about it

*Uniqueness of the Equilibrium State.* Dobrushin [4] has obtained a criterion which is sufficient to insure the uniqueness of the equilibrium Gibbsian state. It is admittedly a rather weak theorem but does provide nontrivial results. We wish to follow Dobrushin’s notation as closely as possible and employ the transcribed lattice notation of the preceding section.

A configuration on this lattice is a function  $x$  from the lattice to the discrete space  $\{0, 1\}$ . That is  $x(t) = 1$  if the site  $t$  is occupied and  $x(t) = 0$  if the site is empty. A different configuration is specified by another function  $x(t)$ . The single variable  $x$  with no argument is identical to  $x(0)$  – the characteristic function for the site designated as the origin,  $t = 0$ .

The notation  $q(x|x(t))$  stands for the (grand canonical) conditional probability that the origin has occupancy specified by  $x$ . That is,

$$q(x|x(t)) = \frac{\exp[-U(x; x(t))]}{\sum_{x=0,1} \exp[-U(x; x(t))]},$$

where  $U(x; x(t))$  is given by Eq. (1) with an expanded designation of the configuration. We can now state the uniqueness criterion of Dobrushin as

$$(1/2) \sum_{s \neq 0} (\sup)_s \sum_{x=0,1} |q(x|x(t)) - q(x|\tilde{x}(t))| < 1, \tag{2}$$

where  $(\sup)_s$  means the supremum taken over all pairs of characteristic functions  $x(t)$  and  $\tilde{x}(t)$  which agree everywhere except at  $t = s$ :

$$x(t) = \tilde{x}(t), \quad t \neq s.$$

The qualitative physical significance of Eq. (2) is that the interaction must be weak enough so that there is little correlation between the origin and any other site  $s$ . Translational invariance also follows if Eq. (2) is satisfied.

The summation over  $s$  in Eq. (2) may be limited to those ten sites within the interaction range of the origin, which divide into three equivalence classes (see Fig. 3). Dobrushin [4] has shown that Eq. (2) may be written as

$$\sum_{s \neq 0} (\sup)_s \Delta_s < 1,$$

where

$$\Delta_s = \frac{C_s z |E_s - 1|}{(1 + C_s z)(1 + C_s z E_s)}.$$

Here we have defined

$$z = \exp(\beta\mu) > 0,$$

$$E_s = \exp[-\beta\varphi(s)] \geq 0,$$

$$C_s = C_{s,x(t)} = \exp \sum_{t \neq 0, s} [-\beta\varphi(t)x(t)] \geq 0,$$

with  $\varphi(t)$  having value  $a$ ,  $b$  or  $+\infty$ . [If  $\varphi(s) = +\infty$ , then  $E_s = 0$ .]

We now introduce the function

$$\varphi^*(t) = \begin{cases} \varphi(t) & \text{if } \varphi(t) < 0 \\ 0 & \text{if } \varphi(t) \geq 0, \text{ including } \varphi(t) = +\infty \end{cases}$$

and the number

$$C = \exp \sum_{t \neq 0} -\beta\varphi^*(t).$$

Now for all  $s$  and all functions  $x(t)$  it is clear that

$$\begin{aligned} \Delta_s &\leq C_s z |E_s - 1| \\ &\leq \begin{cases} C_s z & \text{if } \varphi(s) \geq 0 \\ C_s z E_s & \text{if } \varphi(s) < 0. \end{cases} \end{aligned}$$

If  $\varphi(s) \geq 0$ ,  $C_s$  is bounded by  $C$ :

$$\begin{aligned} C_s &\leq \exp \sum_{t \neq 0, s} [-\beta \varphi^*(t)] \\ &= \exp \sum_{t=0} [-\beta \varphi^*(t)] = C. \end{aligned}$$

On the other hand, if  $\varphi(s) < 0$  we have

$$\begin{aligned} E_s C_s &= \exp[-\beta \varphi(s)] \exp \sum_{t \neq 0, s} [-\beta \varphi(t) x(t)] \\ &\leq \exp \sum_{t \neq 0} [-\beta \varphi^*(t)] = C. \end{aligned}$$

We thus conclude that

$$\Delta_s \leq Cz$$

uniformly with respect to  $s$  and  $x(t)$ . If we therefore restrict  $z$  to values less than  $(10C)^{-1}$  we are assured that the inequality (2) is satisfied. The portion of the  $\beta - \mu$  half plane for which uniqueness is thus established is shown in Fig. 4. By more careful arguments (Freasier [7]) the uniqueness region may be enlarged. The asymptote for large  $\beta$  is still  $4[\varphi^*(1) + \varphi^*(5)]$ , but uniqueness holds for all  $\beta$  for

$$\mu < 8[\varphi^*(1) + \varphi^*(5)] - 2[\varphi(1) + \varphi(5)]. \quad (3)$$

*Symmetry Breakdown and Nonuniqueness.* To establish the existence of multiple equilibrium states we employ the method of contours that originated with Peierls [8]. The technique has been successfully employed with various models of magnets and "gases" (Dobrushin [4], Griffiths and Lebowitz [9], Lebowitz and Gallavotti [10], Ruelle [11]). If  $a - 2b$  is negative (positive) we anticipate that the low temperature, high density system will assume the nematic (smectic) structure with high probability. In either case there are two equivalent alignments of the molecules, related to each other by reflection. The technique is to show that boundary conformation of one alignment renders arbitrarily small the probability of the contrary internal alignment at sufficiently low temperature and high chemical potential.

For this demonstration we return to the original square lattice and adopt the pictorial representation shown in Figs. 5 and 6. We represent a vertical dimer's reference site by + and a horizontal dimer's reference site by 0. Unoccupied reference sites are represented by dots, and the other lattice sites are deleted to avoid clutter. Nematic and smectic boundary conditions (of one of two possible alignments) are illustrated

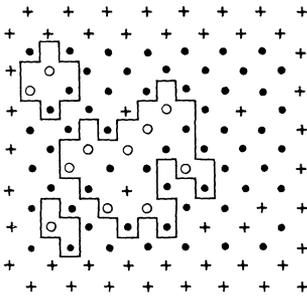


Fig. 5

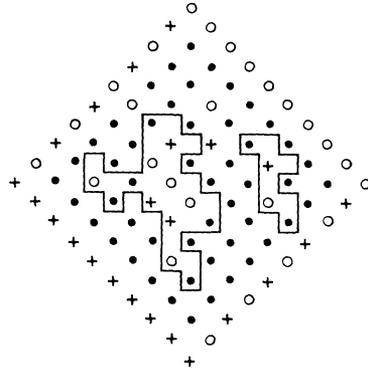


Fig. 6

Fig. 5. A configuration with nematic boundary conditions and three contours

Fig. 6. A configuration with smectic boundary conditions and two contours

in Figs. 5 and 6. “Contours” are defined for a particular configuration in the finite region  $V$  by adding molecules from the “outside in” from the (distant) boundary. The added molecules must conform to the close-packed structure associated with the boundary, and each added molecule must be adjacent to at least one other of a chain of these ordered molecules extending to the boundary of  $V$ . The molecules are added until no more molecules can be added without interfering with a molecule in  $V$ . The limits of these added molecules define the contours of the configuration; the added molecules are removed after the contours have been drawn. Contours so defined are shown in Figs. 5 and 6. It should be noticed that every “misaligned” molecule becomes enclosed inside some boundary. Every contour defined in this way is an “outer contour”; inner contours are not defined or needed for this problem. Two outer contours may never intersect: in fact, there must be room to place “properly aligned” molecules between any two outer contours.

Suppose  $G$  is some contour belonging to the configuration  $\alpha$ ; we denote by  $|G|$  the length of the contour in lattice parameter units. The configuration energy  $U(\alpha)$  may be represented as

$$U(\alpha) = U_{\text{I}} + U_{\text{II}} + U_{\text{III}},$$

where  $U_{\text{I}}$  = self energy of molecules inside  $G$  and interactions with each other,

$U_{\text{II}}$  = self energy of molecules outside  $G$  and interactions with each other,

$U_{\text{III}}$  = interaction of molecules inside  $G$  with those outside  $G$ .

By self energy we mean the negative of the chemical potential  $\mu$ , and it should be recalled that the temperature is included in  $U$ . In order to show that the occurrence of a misaligned molecule is rare, we obtain an estimate of the (grand canonical) probability  $P(G)$  of the contour  $G$ . This probability is given by

$$P(G) = \frac{\sum_{\alpha \subset G} e^{-U(\alpha)}}{\sum_{\alpha} e^{-U(\alpha)}}, \quad (4)$$

where  $\alpha \subset G$  means configurations  $\alpha$  containing the contour  $G$ . Our estimate will be an upper bound, depending only on  $|G|$ , obtained by including only part of the terms of the denominator of Eq. (4).

The terms to be retained in the denominator are those generated from  $\alpha \subset G$  by a transformation  $T: \alpha \rightarrow T_{\alpha}$  defined as follows:

- (a) The orientations of all molecules exterior to  $G$  are unchanged.
- (b) A horizontal molecule at  $(x, y)$  inside  $G$  becomes a vertical molecule at  $(x, y)$ .
- (c) A vertical molecule at  $(x, y)$  inside  $G$  becomes a horizontal molecule at  $(x-1, y+1)$ .
- (d) Around  $G$ , both inside and outside, all possible molecules are added which meet the two requirements: (1) some part of the molecule touches  $G$ , and (2) the molecule is aligned properly with respect to the boundary conditions.

It may readily be determined that  $T$  carries allowed configurations into allowed configurations. In fact, steps (a) through (c) preserve  $U_I$  and  $U_{II}$ , while changing  $U_{III}$ . Step (d), however, renders  $T$  a many to-one transformation and alters all parts of  $U$ . We may easily bound the multiplicity of the transformation by  $4^{|G|}$ , arising from a possible degeneracy of 2 both inside and outside each segment of  $G$ . The effects of transformation  $T$  on the example configurations are shown in Figs. 7 and 8.

We now estimate  $\Delta U = U(T_{\alpha}) - U(\alpha)$ , the goal being a negative change increasing in magnitude linearly with  $|G|$ . Some further notation is convenient: We let  $|G| = G_a + G_b + G_c$  where the subscript denotes the type of interaction across a segment of  $G$  after the transformation. With nematic boundary conditions  $G_a$  is the number of vertical segments, while  $G_c$  is the number of horizontal segment;  $G_b$  vanishes in this case. For smectic boundary conditions  $G_c$  vanishes. In addition, the following inequalities hold for geometrical reasons:

$$\begin{aligned} G_c &\leq |G|/2 \quad (\text{nematic boundary}) \\ G_a &\leq |G|/2 \quad (\text{smectic boundary}). \end{aligned} \quad (5)$$

From this point on we shall assume both  $a$  and  $b$  to be negative, so that all intermolecular interactions will tend to stabilize dense configura-

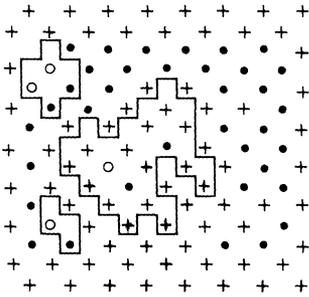


Fig. 7

Fig. 7. The configuration generated from that of Fig. 5 by the transformation  $T$

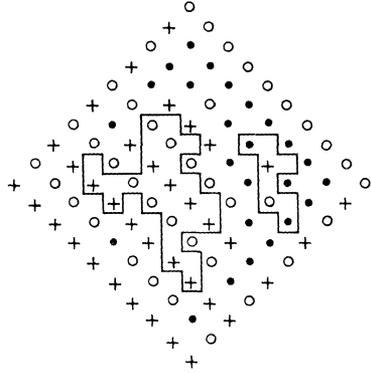


Fig. 8

Fig. 8. The configuration generated from that of Fig. 6 by the transformation  $T$

tions. As previously discussed we decide on nematic or smectic boundary conditions on the basis of the sign of  $a - 2b$  (nematic if negative). It is actually unduly restrictive to assume both to be negative. One can be positive if it is sufficiently small compared to the magnitude of the other (see Freasier [7]).

The simplification resulting from the assumption of negative values of  $a$  and  $b$  is in the interaction part of  $U_I$  and  $U_{II}$ . Step (d) in the definition of the transformation  $T$  alters the interaction part of  $U_I$  and  $U_{II}$  in an essentially unknown manner, but the change must be negative. Step (d) also alters the self energy part ( $-\beta\mu$ ) of  $U_I$  and  $U_{II}$  in a negative way if  $\mu$  is positive and in a way bounded by  $-\mu|G|$  if negative. If we introduce  $\mu^*$  by

$$\mu^* = \begin{cases} \mu & \text{if } \mu < 0 \\ 0 & \text{if } \mu \geq 0 \end{cases},$$

we can summarize the above comments by

$$\begin{aligned} U_I(T_\alpha) &\leq U_I(\alpha) - \beta\mu^*|G| \\ U_{II}(T_\alpha) &\leq U_{II}(\alpha) - \beta\mu^*|G|. \end{aligned} \tag{6}$$

The “surface” term  $U_{III}$  plays the crucial role. From the definition of the contours and the transformation  $T$ , the energy  $U_{III}(T_\alpha)$  is as low as possible:

$$\begin{aligned} U_{III}(T_\alpha) &= \beta a G_a \quad (\text{nematic}) \\ U_{III}(T_\alpha) &= \beta(a G_a + b G_b) \quad (\text{smectic}). \end{aligned} \tag{7}$$

The configuration  $\alpha$  prior to the transformation could have none of these “matched” interactions across the contour (or else the contour would not be there). There can, however, be some “mismatched” interactions across contour lines –  $b$  interactions in the nematic case and  $a$  interactions in the smectic case. An obvious lower bound in the nematic case in

$$U_{\text{III}}(\alpha) \geq \beta b |G| \quad (\text{nematic}). \quad (8)$$

The corresponding bound in the smectic case is not so obvious. Clearly the misfit  $a$  interactions can only arise from contour segments contributing to  $G_b$ ; study of all possibilities reveals that whenever such an interaction is realized, there must be immediately adjacent another  $G_b$  segment which is geometrically inaccessible. Consequently we obtain

$$U_{\text{III}}(\alpha) \geq \beta a (G_b/2) \quad (\text{smectic}). \quad (9)$$

Combining the three contributions to  $U$  we have for the nematic case

$$\Delta U \leq \beta(a - 2b - 4\mu^*) (|G|/2) \quad (10)$$

where we have used  $G_a \geq |G|/2$  from Eq. (5). For the smectic case we find

$$\Delta U \leq \beta(2b - a - 8\mu^*) (|G|/4), \quad (11)$$

using the facts that  $a$  and  $(2b - a)$  are negative and that  $G_b \geq |G|/2$ .

We now return to the estimation of the probability of the contour  $G$ . From Eq. (4) we have

$$\begin{aligned} P(G) &\leq \sum_{\alpha \subset G} e^{-U(\alpha)} / \sum_{\alpha \subset G} 4^{-|G|} e^{-U(T_\alpha)} \\ &= 4^{|G|} e^{\Delta U} \\ &\leq \exp\{(\ln 4 + \beta W) |G|\} \\ &= \hat{P}(|G|), \end{aligned} \quad (12)$$

where  $W$  is given by

$$W = \begin{cases} (a - 2b - 4\mu^*)/2 & (\text{nematic}) \\ (2b - a - 8\mu^*)/4 & (\text{smectic}). \end{cases} \quad (13)$$

The factor  $4^{-|G|}$  in the denominator corrects for the multiplicity of the transformation  $T$ . It is clear that  $P(G)$  is a decreasing function of  $\beta$  if  $W$  is negative, which implies the limits on  $\mu$ :

$$\begin{aligned} \mu &> (a - 2b)/4 & (\text{nematic}) \\ \mu &> (2b - a)/8 & (\text{smectic}). \end{aligned} \quad (14)$$

We are now in a position to obtain an upper bound on the probability  $\varrho^\dagger$  of “misaligned” molecules – that is, of molecules which do not conform to the orientations dictated by the boundary conditions. In the standard way, this bound is obtained by the observation that any misaligned molecule must be inside *some* contour, so that

$$\varrho^\dagger \leq \sum_{|G|} \hat{P}(|G|) K(|G|),$$

where  $K(|G|)$  bounds the number of contours of length  $|G|$  around a specified site, on the square lattice. The function

$$K(|G|) = (|G|/4) 3^{|G|-2},$$

is due essentially to Peierls (see Griffiths and Lebowitz [9]) and leads to

$$\varrho^\dagger \leq (1/36) \sum_{|G|=0}^{\infty} |G| \exp \{ |G| (\ln 12 + \beta W) \}. \quad (15)$$

The series (15) converges, provided

$$\beta > (\ln 12)/(-W), \quad (16)$$

and hence defines in this range a decreasing function of  $\beta$ . It follows that at sufficiently high  $\beta$  the probability of  $\varrho^\dagger$  of a misaligned molecule at any interior site may be arbitrarily small. In particular, at low temperatures  $\varrho^\dagger$  is less than  $\varrho/2$  – which establishes the existence of long ranged order. Identical reasoning with reflected boundary conditions proves that for the portion of the  $\beta - \mu$  plane defined by Eqs. (14) and (16) there are (at least) two equilibrium states.

#### 4. Conclusions

Our state of knowledge about the equilibrium states of the restricted dimer model is summarized in Fig. 4. There is a unique Gibbsian state in the region with horizontal shading; thermodynamic analyticity is guaranteed in the dotted region. Presumably both these regions correspond to the one-phase regime of the “gaseous” state. There are at least two equilibrium states in the region with vertical shading. These two states are not translationally invariant and are obtained from each other by reflection.

It is natural to assume that a two-phase coexistence curve separates the regions as indicated by the dotted line in Fig. 4. Presumably the high  $\beta$  asymptote is at  $\mu = 2a$  in the nematic case and at  $\mu = a + 2b$  in the smectic case, these representing the energy of the ordered solid phase. It is not known whether there is a critical temperature or whether instead the coexistence curve is asymptotic to the positive  $\mu$  axis.

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