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Crystallinity in Two Dimensions: A Note on a Paper of C. Radin

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To demonstrate the crystallinity of the soft disk ground state, a modified treatment of this model is given, as Radin's proof of a crucial lemma can be shown to be incorrect.

KEY WORDS: Crystal; ground state; soft disks; symmetry.

1. INTRODUCTION AND STATEMENT OF RESULTS

Recently there has been much work which shows that—in the framework of classical mechanics—some classes of two-body potentials give rise to crystalline ground states. As surface tension produces notorious difficulties in dimensions greater than one,(1) to the best of my knowledge there are only two attempts to show crystallinity of ground states in two dimensions(2,3) based on some considerations given by Harborth.(4)

In Ref. 3 Radin constructs a soft disk model, using the two-body potential

$$V(r) = \begin{cases} +\infty, & \text{for } 0 \leqslant r < 1 \\ 24r - 25, & \text{for } 1 \leqslant r < 25/24 \\ 0, & \text{for } 25/24 \leqslant r \end{cases}$$

in two dimensions, and tries to show the following:

Theorem. In any ground state of V all separations of two points are

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of unit length and the ground states for V are subsets of the triangular lattice, thus crystalline.

Radin's proof of his Lemma 4 and his examination of the spatial form of a ground state make use of the inequality

$$x \leqslant \left[3n - 6 - (12x - 24n + 33)^{1/2}\right] =: \left[f(x)\right]$$

where $[t]$ denotes the integral part of t.

For $n \in \mathbb{N}$, $n \geqslant 13$, $x < 3n$ the inequality is asserted to imply $x \leqslant [3n - (12n - 3)^{1/2}]$. This is manifestly incorrect as the reader may verify by inserting $x = 209/8$; $n = 13$ or $x = 73/2$; $n = 17$.

Fortunately the above theorem can be shown to remain valid. In the following we shall see that the appearance of the inequality $x \leqslant [f(x)]$ can be avoided. By consideration of some geometrical properties of n-point configurations it is replaced by the inequality $[y] \leqslant f([y])$, which is much easier to handle. Thus the proof of the theorem turns out to be essentially shorter than Radin's attempt. However, two basic inequalities correctly derived in Ref. 3 are still needed.

2. DEFINITIONS AND PROOFS

We have to examine configurations of n points which minimize the total potential energy. These configurations will be called "minimal."

Each pair of points with separation $1 \leqslant r < 25/24$ will define a "bond," represented by the shortest line segment containing the two points. If such a bond is not of unit length, it will be called "exceptional." In a minimal configuration the bond graph must have a simple closed polygonal boundary, so we can restrict ourselves to this case.

In Ref. 3 the following two inequalities are rigorously proven:

(a) Let E be the energy of an n-point configuration C which has exactly d boundary vertices in the associated bond graph. Let E' be the energy of the configuration C' obtained from C by removing the boundary points. Then we have

$$|E| \leqslant |E'| + 3d - 6 \tag{1}$$

The inequality is strict if there exists an angle $\alpha \neq \pi/3$ between two neighboring bonds containing the same boundary vertex.

(b) Let B be the number of bonds in C. Then we obtain

$$n - d \geqslant B - 2n + 3 \tag{2}$$

The inequality is strict if C contains a j-gon, $j \geqslant 4$, a "nontriangle."

These inequalities now allow us to proceed as follows.

Lemma 1. Suppose the graph of C contains only triangles and at least one bond is exceptional. This implies $|E| < [3n - (12n - 3)^{1/2}]$.

Proof. First of all, we note that $V(r)$ has a unique minimum at $r = 1$ with $V(r) = -1$ and that the range of finite values for $V(r)$ is $-1 \leqslant V(r) \leqslant 0$. So in any configuration of finite energy we have $|E| \leqslant B$. As one bond is exceptional, we have $|E| < B$ and from (2) we get $n - d > |E| - 2n + 3$ or

$$n - d \geqslant \left[|E| + 1 \right] - 2n + 3 \tag{3}$$

Now we can use Harborth's induction technique.[4] If $n < 3$, the lemma is trivial, so we can state $n \geqslant 3$. We assume the lemma holds for all t-point configurations, if $t < n$, and we have to show it holds for any n-point configuration.

Now let C be an n-point configuration. Then the above assumption especially implies that the lemma holds for the configuration C' derived from C as in (a) above, if $n - d > 0$. If C contains only boundary points, then we have $n - d = 0$ and the lemma can be proven directly, as (3) then implies

$$\left[|E| + 1 \right] \leqslant 3n - (n + 3) \leqslant \left[3n - (12n - 3)^{1/2} \right]$$

If $n - d > 0$, there are two possible cases:

(i) C' contains an exceptional bond. With the induction assumption and (1) we get

$$\begin{gathered} |E| \leqslant |E'| + 3d - 6 < \left[3(n-d) - (12(n-d) - 3)^{1/2} \right] + 3d - 6 \\ \left[|E| + 1 \right] \leqslant 3(n-d) - (12(n-d) - 3)^{1/2} + 3d - 6 \end{gathered} \tag{4}$$

Together with (3) this leads to $[|E| + 1] \leqslant 3n - 6 - (12[|E| + 1] - 24n + 33)^{1/2}$. $[|E| + 1]$ is an integer, so from Refs. 2 and 4 we know that this inequality implies

$$\left[|E| + 1 \right] \leqslant \left[3n - (12n - 3)^{1/2} \right] \tag{5}$$

(ii) The exceptional bond touches the boundary and (i) does not hold. In this case C' is a configuration already examined in Refs. 2 and 4 and from there we know that

$$|E'| \leqslant \left[3(n-d) - (12(n-d) - 3)^{1/2} \right] \tag{6}$$

Furthermore at least one of the boundary angles is not $\pi/3$, so we get from (1)

$$|E| < |E'| + 3d - 6 \leqslant \left[3(n-d) - (12(n-d)-3)^{1/2}\right] + 3d - 6$$

This is again (4), which leads together with (3) to (5). So the lemma is proven. ■

Lemma 2. Suppose the graph of C contains at least one nontriangle. This implies $|E| < [3n - (12n-3)^{1/2}]$.

Proof. As there is a nontriangle in C, from (2) we get $n - d \geqslant (B + 1) - 2n + 3$. Of course, $|E| \leqslant B$ again, so the inequality immediately leads to (3). Again induction is used. As (3) is still valid, the lemma holds for all configurations containing only boundary points. As in the proof of Lemma 1 we assume the lemma holds for C' derived from a given configuration C.

(i) The graph of C' contains at least one nontriangle or at least one exceptional bond. Then with the induction assumption or Lemma 1

$$|E| \leqslant |E'| + 3d - 6 < \left[3(n-d) - (12(n-d)-3)^{1/2}\right] + 3d - 6$$

This is (4) for another time.

(ii) The nontriangle touches the boundary and (i) does not hold. Reasoning as in the proof of Lemma 1 we can use (6) in this case and again at least one boundary angle is not $\pi/3$. So we can proceed as in Lemma 1 and the proof is complete. ■

From Refs. 2 and 4 we know that there exist configurations with $|E| = [3n - (12n-3)^{1/2}]$ which are subsets of the triangular lattice. Combining this with the two lemmas, we see that the theorem stated in the introduction is proven.

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