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The Ground State for Soft Disks[1]

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We consider some two-dimensional models of point particles interacting through short-range two-body potentials and prove that their zero temperature, zero pressure states are crystalline.

KEY WORDS: Ground state; crystal; symmetry.

1. INTRODUCTION

It is often said that the study of the solid–fluid phase transition is hampered by the impossibility(1) of relevant models in one and two dimensions. We refer here to classical mechanical models of point particles in $\mathbb{R}^n$, interacting through "reasonable" two-body potentials, i.e., with strong repulsion at short separation, a unique minimum, and weak attraction at large separation. (Such models are meant to simulate molecular bonded matter; there are other types of classical mechanical models relevant to metallic bonding—see, e.g., Ref. 2. The preference of classical over quantum mechanical models is dictated by the relative lack of computational power in the latter.)

Although Mermin's theorem(1) seems to rule out the possibility of true crystal ordering in two dimensions (at nonzero temperature), there has been growing interest(2) in recent years in the possibility of a weaker form of ordering termed "orientational;" the former refers to long-range positional correlation, as evidenced in material crystals by X-ray scattering, while the latter refers to the long-range correlation of bond angles, as is evidenced in material crystals by the angles between faces.

Although much theoretical work has been done predicting the behavior of the two-dimensional systems, there is in fact the noticeable lack of a

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demonstration that any "reasonable" model actually exhibits orientational ordering. (There is an "unreasonable" model with the property in Ref. 1.)

This paper is meant to contribute in this direction. Herein we consider some models and show that at least they behave well at zero temperature and pressure—they are shown to be perfectly crystalline under these circumstances. We have previously shown this for a "sticky disk" model[3] (see also Refs. 4–6) but since this model has a delta function interaction it is not well suited to nonzero temperatures. The present models are so suited and it is hoped that the techniques developed here will be of help for computations at nonzero temperatures.

Finally we note that although from the group invariance point of view one might expect there to be advantages in working directly with infinite systems of particles, there does not seem to be a formalism well enough developed; see Ref. 7. However, see Refs. 8–10 for related work on the type of crystal to be expected for given potentials.

2. NOTATION AND STATEMENT OF RESULTS

We consider configurations of $n \geqslant 1$ points in the plane: p_j, $j = 1, \ldots, n$. They interact through a potential, V, dependent only on the distance of separation $r_{jk} = |p_j - p_k|$. V will have a hard core (radius 1) and will be of strictly finite range $R > 1$. Although our proofs will clearly hold for a class of potentials, the class does not seem of particular interest. Thus the results will refer only to the following specific example:

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

Each pair of points whose separation r satisfies $1 \leqslant r < R$ $(= 25/24)$ will define a "bond" which is represented by the shortest line segment containing the two points. A configuration of n points will be called "minimal" or a "ground state" if, for that configuration, the total potential energy

$$E = \frac{1}{2} \sum_{j \neq k} V(r_{jk})$$

is minimal as compared with all configurations with n points (n fixed).

If we restrict consideration to configurations with all bonds of unit length, then it has been shown[3,11] that the minimal energy is $-[3n - (12n - 3)^{1/2}]$ (where $[x]$ is the greatest integer less than or equal to the real number x), and also[3] that for any minimal configuration there is some orientation of the triangular lattice containing all the points. In this paper we extend these results as follows.

Theorem. In a ground state for V all bonds are necessarily of unit length.

Corollary. The ground states for V are subsets of the triangular lattice, thus crystalline.

Our arguments are basically geometrical and concern the planar "bond graphs" of configurations, i.e., the graphs composed of the bonds of configurations. It will therefore be useful to call the points of a configuration "vertices" of the corresponding graph.

Finally we note that it is easy to check that every minimal configuration has the following properties: (a) each vertex is contained in at least two bonds; (b) the bond graph decomposes the plane into "elementary" polygons with each side being a bond (a polygon is elementary if it contains no vertex in its interior); (c) the bond graph has a simple closed polygonal boundary.

3. THE GROUND STATE ENERGY

It will be convenient to "associate" a certain energy with each boundary vertex of a minimal configuration, namely, the sum of half the energy of each of the two boundary bonds containing it together with the energy of all other bonds containing it.

Lemma 1. If E_k is the energy associated with the kth boundary vertex of a minimal configuration and if A_k is the internal angle of the boundary at that vertex, then

$$|E_k| \leqslant A_k/(\pi/3) \tag{1}$$

Proof. If the vertex is contained in exactly j bonds, consider E_k as the sum, over each of the $(j-1)$ subangles A of A_k, of half the energy of each of the two bonds defining A. If every A is at least $\pi/3$ (1) is obvious, so assume that at least one of them has the value $A = (1-z)\pi/3$, $0 < z < 1/22$. (This range for z is easily seen to suffice for all possibilities.) Of the two bonds defining A, one sees that at least one has length L satisfying

$$L \geqslant 1/2\sin((1-z)\pi/6)$$

But then

$$\begin{aligned} L &\geqslant 1/(2\sin(\pi/6)\cos(z\pi/6) - 2\cos(\pi/6)\sin(z\pi/6)) \\ &> 1/(1 - 3^{1/2}z/2) \end{aligned}$$

where we used the fact that $0 < z\pi/6 < \pi/6$ so that $\sin(z\pi/6) > z/2$. Since the absolute value of the energy associated with A is less than or equal to $\frac{1}{2} + |V(L)|/2$, if we show that $|V(L)|/2 < \frac{1}{2} - z$ for $0 < z < 1/22$ the proof is complete. But this inequality follows if

$$|V(1/(1 - 3^{1/2}z/2))| \leqslant 1 - 2z = 1 - (4/3^{1/2})(3^{1/2}z/2)$$

or

$$|V(1/(1 - y))| \leqslant 1 - (4/3^{1/2})y$$

or

$$|V(r)| \leqslant 1 - (4/3^{1/2})(1 - 1/r) = 1 - 4/3^{1/2} + 4/(3^{1/2}r)$$

It is easily seen that the given potential V satisfies this last inequality over the necessary range, $1 < r < 50/(50 - 3^{1/2})$, which completes the proof. ■

We note the following corollary of the proof.

Corollary. The inequality (1) is strict unless all subangles of A_k are exactly $\pi/3$.

The next three lemmas are extensions of the methods of Refs. 3 and 11.

Lemma 2. The energy of any configuration of n points is bounded below by $-(3n - (12n - 3)^{1/2})$.

Proof. Let E be the energy of a minimal configuration C of n points, exactly d of which are boundary vertices of the associated bond graph. Let E' be the energy of the configuration C' obtained from C by removing the boundary points. We have

$$E = E' + \sum_{k=1}^{d} E_k$$

where E_k is the energy associated with the kth boundary vertex. From Lemma 1 and the elementary formula for the sum of the internal angles of a polygon we get our first basic inequality:

$$|E| \leqslant |E'| + 3d - 6 \tag{2}$$

Next apply Euler's formula to the bond graph of C: if F_j is the number of elementary polygons in the graph with j sides, if $F = \sum_j F_j$, and B is the number of bonds in C,

$$n + F = B + 1 \tag{3}$$

If the number of sides of all elementary polygons are added, boundary sides are counted once and interior sides twice, yielding

$$d + 2(B - d) = \sum_{j\geqslant 3} jF_j \geqslant 3F \tag{4}$$

Eliminating F between (3) and (4) implies the other basic inequality:

$$B \leqslant 3n - d - 3 \tag{5}$$

or

$$n - d \geqslant B - 2n + 3 \tag{5'}$$

from which we obtain

$$|E| \leqslant 3n - d - 3 \tag{6}$$

or

$$n - d \geqslant |E| - 2n + 3 \tag{6'}$$

We are attempting to prove

$$|E| \leqslant 3n - (12n - 3)^{1/2} \tag{7}$$

which we will do by induction on n. (7) clearly holds for $n = 1$. Assume it holds for all m, $1 \leqslant m < n$. It follows that

$$|E'| \leqslant 3(n - d) - (12(n - d) - 3)^{1/2}$$

From (2)

$$\begin{aligned} |E| &\leqslant 3(n - d) - (12(n - d) - 3)^{1/2} + 3d - 6 \\ &\leqslant 3n - 6 - (12(n - d) - 3)^{1/2} \end{aligned}$$

Then using (6′) this becomes

$$|E| \leqslant 3n - 6 - (12|E| - 24n + 33)^{1/2} \tag{8}$$

It is easy to check by eliminating the square root that the only solution of the equation $x = f(x)$, where $f(x) = 3n - 6 - (12x - 24n + 33)^{1/2}$, is $x = 3n - (12n - 3)^{1/2}$. Since f is a decreasing function of x, (8) implies (7), which completes the induction and proves the lemma. ■

Note: the basic argument, whereby (2) and (6′) imply an upper bound for $|E|$, will be used four more times below with variations.

Lemma 3. For $1 \leqslant n \leqslant 12$, the number of bonds in any configuration of n points and finite energy is bounded above by $[3n - (12n - 3)^{1/2}]$.

Proof. Defining a maximal configuration to be one with the maximal possible number of bonds in the class of all configurations of finite energy and the same number of points, it is easily seen that a maximal configuration has a bond graph with the same properties (a), (b), and (c) we noted for minimal configurations at the beginning of this section. Let K be a maximal configuration of n points, d boundary points, and B bonds. Our justification of

$$B \leqslant 3n - d - 3 \tag{5}$$

carries over to maximal configurations such as K. But we will need a replacement of (2).

A vertex will be said to be "of type j" if it is contained in exactly j bonds, and k_j will be the number of type-j vertices in the boundary of K. Let K' be the configuration obtained from K by removing the boundary points, and assume K' has B' bonds. Then

$$B \leqslant B' + \sum_{j=2}^{6} (j-1)k_j \tag{9}$$

From Ref. 3 or 11 we know how to construct configurations $\tilde{K}$ with n points, $\tilde{d}$ boundary points, and $\tilde{B}$ bonds such that

$$\tilde{B} = 3n - \tilde{d} - 3 \tag{$\tilde{5}$}$$

and we note that $\tilde{d} \leqslant 9$ for $n \leqslant 12$. Clearly then, $d \leqslant 9$ since we are assuming $n \leqslant 12$. Consider the interior angle at a boundary vertex of type j for K. Using the range of V such an angle is seen to be larger than $(j-1)(\pi/3)(21/22)$. The sum of all interior angles of the boundary of K is then

$$\pi d - 2\pi > \sum_{j=2}^{6} (j-1)(\pi/3)(21/22)k_j$$

and so

$$\sum_{j=2}^{6} (j-1)k_j < (3d-6)(22/21)$$

Since $d \leqslant 9$, we have the integer inequality $\sum_{j=2}^{6}(j-1)k_j \leqslant 3d-6$ which together with (9) yields

$$B \leqslant B' + 3d - 6 \tag{$\tilde{2}$}$$

Now just as (2) and (5) lead to (7), ($\tilde{2}$) and ($\tilde{5}$) lead to $B \leqslant 3n - (12n - 3)^{1/2}$, which concludes the proof on noting that B is integral. ■

Lemma 4. The energy of any minimal configuration of n points is $-[3n - (12n-3)^{1/2}]$.

Proof. Let C be a minimal configuration with n points, d boundary points, and energy E. As noted above, configurations with $[3n - (12n - 3)^{1/2}]$ unit length bonds are constructable for any n, so we need only prove

$$|E| \leqslant \left[3n - (12n-3)^{1/2}\right] \tag{$\tilde{7}$}$$

From Lemma 3 we know this holds for $1 \leqslant n \leqslant 12$. To prove ($\tilde{7}$) for $n \geqslant 13$ we use induction. Assume ($\tilde{7}$) holds for $1 \leqslant m < n$, in particular for $|E'|$.

Then from (2)

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

Then using (6′) this becomes

$$|E| \leqslant \left[3n-6-(12|E|-24n+33)^{1/2}\right]$$

Consider again the equation $x=f(x)$, where $f(x)=3n-6-(12x-24n+33)^{1/2}$. In the proof of Lemma 2 we noted that $x=3n-(12n-3)^{1/2}$ is a solution of the equation $x=f(x)$. We now show that $x=[3n-(12n-3)^{1/2}]$ is a solution of the equation $x=[f(x)]$ if $n \geqslant 13$. Since $[f(x)]$ is decreasing in x, this will complete the induction and the proof.

Since the inequality

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

follows from the solution of $x=f(x)$, we need only show

$$\left[3n-(12n-3)^{1/2}\right] \geqslant \left[3n-6-\left(12\left[3n-(12n-3)^{1/2}\right]-24n+33\right)^{1/2}\right]$$

Let $s=3n-(12n-3)^{1/2}-[3n-(12n-3)^{1/2}]$. Then

$$\begin{aligned}
&\left[3n-6-\left(12\left[3n-(12n-3)^{1/2}\right]-24n+33\right)^{1/2}\right]\\
&\quad=\left[3n-6-\left(12\left(3n-(12n-3)^{1/2}\right)-12s-24n+33\right)^{1/2}\right]\\
&\quad=\left[3n-6-\left(\left((12n-3)^{1/2}-6\right)^2-12s\right)^{1/2}\right]\\
&\quad=\left[3n-6-\left((12n-3)^{1/2}-6\right)\left(1-12s/\left((12n-3)^{1/2}-6\right)^2\right)^{1/2}\right]
\end{aligned}$$

Since $12s/((12n-3)^{1/2}-6)^2<1$ for $n \geqslant 13$,

$$\begin{aligned}
&\left[3n-6-\left((12n-3)^{1/2}-6\right)\left(1-12s/\left((12n-3)^{1/2}-6\right)^2\right)^{1/2}\right]\\
&\qquad\leqslant\left[3n-6-\left((12n-3)^{1/2}-6\right)\left(1-6s/\left((12n-3)^{1/2}-6\right)^2\right)\right]\\
&\qquad\leqslant\left[3n-6-\left(\left((12n-3)^{1/2}-6\right)-6s/\left((12n-3)^{1/2}-6\right)\right)\right]\\
&\qquad\leqslant\left[3n-6-\left((12n-3)^{1/2}-6\right)\right]
\end{aligned}$$

since $6s/((12n-3)^{1/2}-6)<s$ and so cannot affect the integer part of $((12n-3)^{1/2}-6)$. This concludes the proof. ■

4. THE SPATIAL FORM OF THE GROUND STATES

Let C be a minimal configuration of n points. We want to prove that all bonds in C must be of unit length. For $n \leqslant 12$ this follows from Lemmas 3 and 4. So we assume $n \geqslant 13$ and use induction on n. Assume the result for all m, $1 \leqslant m < n$. Now assume further that there is an elementary polygon in the bond graph of C with at least four sides. (This will lead to a contradiction.) From (4) we get

$$2B - d \geqslant 3F + 1$$

which together with (3) implies

$$(n-d) \geqslant (|E|+1) - 2n + 3 \tag{$\tilde{6}'$}$$

Consider

$$|E| \leqslant |E'| + \sum_{k=1}^{d} |E_k| \tag{10}$$

If the nontriangle is in C', then from Ref. 3 we know that

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

If on the other hand the nontriangle meets the boundary of C, we know from the corollary of Lemma 1 that

$$\sum_{k=1}^{d} |E_k| < 3d - 6$$

In either case then, (10) implies

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

which, with ($\tilde{6}'$) yields

$$|E| < \left[3n - 6 - (12(|E|+1) - 24n + 33)^{1/2}\right]$$

But then there exists $c > 0$ such that

$$|E| + c \leqslant \left[3n - 6 - (12(|E|+c) - 24n + 33)^{1/2}\right]$$

As in the proof of Lemma 4, this implies

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

which is in contradiction with C being minimal, showing that all elementary polygons in C must be triangles. Thus any nonboundary vertex of the bond graph of C is contained in six bonds. Also it now follows from (4) that the number of bonds in C satisfies

$$B = 3n - d - 3 \tag{$\tilde{\tilde{5}}$}$$

Adding over the vertices the number of bonds containing each vertex, we get

$$2B \geqslant 6(n-d) + 2d + (B - B' - d)$$

or

$$B \geqslant 6n - 5d - B' \tag{11}$$

Eliminating n from (11) and $(\tilde{\tilde{5}})$ we again get

$$B \leqslant B' + 3d - 6 \tag{$\tilde{2}$}$$

Now just as (2) and (5) lead to (7), $(\tilde{2})$ and $(\tilde{\tilde{5}})$ lead to

$$B \leqslant 3n - (12n-3)^{1/2}$$

or

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

since B is integral. But then, as with $n \leqslant 12$, we can use Lemma 4 to complete the induction and conclude as follows.

Theorem. In any ground state of V all bonds are of unit length.

As stated in Section 2, this together with Ref. 3 implies the following.

Corollary. The ground states for V are subsets of the triangular lattice, thus crystalline.

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