The Ground State for Sticky Disks

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It is proven that the ground state of the two-dimensional sticky potential is the triangular lattice.

1. INTRODUCTION AND STATEMENT OF RESULTS

It is one of the classical unsolved problems in statistical and solid state physics to show why real matter is in crystalline form at low temperature.[1] The full quantum problem is well beyond known techniques, so, as in most discussions of such matters, we consider the problem in the framework of classical mechanics with phenomenological potentials of the Lennard-Jones type. For such a potential V we want to show that the configuration of particle positions $\{\mathbf{r}_j\}$ that minimizes the energy

$$E = \tfrac{1}{2} \sum_{\substack{i,j \\ i \neq j}} V(|\mathbf{r}_i - \mathbf{r}_j|)$$

(i.e., the "zero-temperature state" or "ground state") is roughly periodic, and becomes a perfect lattice as the number of particles grows beyond bound. We call this the "ground state problem" (for the potential V), and note that in some sense it is the attempt to determine (one of) the origins of spatial symmetry in matter.

In one space dimension the ground state problem is trivial for potentials of sufficiently short range. To be specific: *if*, because of a hard core or a priori estimates, one can show that in any ground state for a potential each particle can only interact directly with its nearest neighbors, then, under very mild further conditions on the potential, the ground state is unique (up to translation) and consists of evenly spaced particles. The ground state problem for

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such a potential is trivial (in one dimension) because one can minimize E *locally*, i.e., for each pair of particles separately, and join the results together. The ground state problem is much harder for longer range potentials and/or in higher dimensions.

For longer range potentials the ground state problem is clearly global (or "many-body") in an essential way. The known results in one dimension are the following. For the Lennard-Jones potential $V(r) = r^{-12} - r^{-6}$ it has been shown [2] that each finite system of particles has a unique ground state (up to translation) which becomes evenly spaced as the number of particles grows beyond bound. It is further shown in Ref. 3, again in one dimension, that the qualitative property of having periodic ground states can be destroyed by arbitrarily small perturbations of a potential. There are also interesting related results in Refs. 4 and 5 for one-dimensional systems of *infinitely* many particles.

In two or three dimensions the ground state problem is essentially global or many-body even for very short-range potentials. Consider, for example, the "sticky potential":

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

If we want to minimize E for this potential we can imagine an impenetrable sphere centered at each particle, and the problem consists in showing that those configurations of n spheres in which the maximum possible number are touching (n fixed) are periodic.

In two dimensions each sphere (or, more properly, disk) can touch at most six others, and in three dimensions at most twelve others. [6] It is easy to construct periodic finite arrays where all "interior" spheres touch the maximum possible number of others, but of course each boundary sphere touches fewer than the maximum. It is not hard to check that if one starts by constructing a minimum size boundary (by having the boundary spheres approximate a spherical shell) and then works inward, the spheres will not mesh correctly in the middle—but of course this could still conceivably give a lower value of E than obtained by insisting that *all* the interior spheres touch maximally many neighbors. (Note that in one dimension this conflict disappears since one can easily arrange for a minimal size boundary, namely two, without implication for the interior.)

It is thus by no means clear whether or not the ground states for the sticky potential are periodic (i.e., "crystalline") and the above considerations illustrate the essentially global nature of the ground state problem in two and three dimensions.

In this paper we will give the first derivation of the existence of a crystal in two dimensions—for the sticky potential defined in (1).

2. NOTATION

In accordance with the previous section, we are concerned with configurations C of unit-diameter impenetrable disks in $\mathbb{R}^2$. Each pair of disks that is touching determines a "bond," which we represent by the closed, unit-length line segment between the centers of the pair. By $\hat{C}_g$ we denote the set whose elements are the bonds of C, while C_g, the "graph" of C, denotes the set of all points contained in any of the bonds. The cardinality of $\hat{C}_g$ is denoted C_b. The set of "vertices" of C, i.e., the centers of the disks, is denoted C_v.

For each integer $n \geqslant 1$, $B(n)$ denotes the supremum of C_b over all C containing n disks. It has been shown by Harborth[7] that

$$B(n) = [3n - (12n - 3)^{1/2}]$$

where $[x]$ denotes the greatest integer less than or equal to the real number x. (Note: a variable represented by a lower case letter is assumed to vary through $\mathbb{Z}$ unless otherwise indicated.) A configuration C of n disks will be called "maximal" if $C_b = B(n)$. We will reproduce Harborth's proof (which yields the ground state energy) in order to extend it to obtain properties of the maximal configurations (i.e., ground states). Specifically, we will show that the particles in a ground state lie on the vertices of a "triangular lattice," i.e., the points in the complex plane of the form $m + n \exp(i\pi/3)$, m and n in $\mathbb{Z}$.

3. A CONSTRUCTION

We begin with the computation of C_b for a special class of configurations which will prove to be maximal.

Assume $s \geqslant 1$, $0 \leqslant k \leqslant 5$, and $0 \leqslant j \leqslant s$ are fixed. Let $n = 3s^2 + 3s + 1 + (s + 1)k + j$, so that n can be thought of as the number of disks in the configuration C obtained by nestling more disks around the boundary of a "close-packed hexagon of disks with $s + 1$ disks on each side" [i.e., the hexagon has centers at the points

$$H_s = \{e^{ip\pi/3}(m + ne^{i\pi/3}) | m \geqslant 0, n \geqslant 0, m + n \leqslant s, 0 \leqslant p \leqslant 5\}$$

in the complex plane]. Specifically,

$$C_v = H_s \cup \{e^{ir\pi/3}(m + ne^{i\pi/3}) | m \geqslant 0, n \geqslant 1, m + n = s + 1, 0 \leqslant r \leqslant k - 1\}$$
$$\cup \{e^{ik\pi/3}(m + ne^{i\pi/3}) | m \geqslant 0, 1 \leqslant n \leqslant j, m + n = s + 1\}$$

It is easy to check that $C_b = H(n)$, where

$$H(n) = \begin{cases} 9s^2 + 3s & \text{if } j = k = 0 \\ 9s^2 + 3s + (3s + 2)k - 1 + 3j & \text{if } j + k \neq 0 \end{cases}$$

and that

$$H(n) = [3n - (12n - 3)^{1/2}] \tag{2}$$

4. PROPERTIES OF THE GROUND STATES OF THE STICKY POTENTIAL

Theorem. (1) $B(n) = H(n) = [3n - (12n - 3)^{1/2}]$ (Harborth[7]).

(2) For any maximal configuration C of n disks, $n \geqslant 3$: (a) C_g has a simple closed polygonal boundary with vertices on a triangular lattice and C_v consists of all the lattice points inside and on this polygon. (b) C_g contains exactly $-[3 - (12n - 3)^{1/2}]$ boundary vertices.

Proof. The cases $n = 1$ and 2 for part (1) are trivial so we assume $n \geqslant 3$. Let C be a maximal configuration of n disks. Clearly each disk in C touches at least two others, so C_g decomposes $\mathbb{R}^2$ into elementary polygons with *unit sides*, where "elementary" means that no element of C_v is contained in the polygon's interior. From the maximal property of C it follows that C_g is a connected set and furthermore that this property would persist in the configuration obtained by removing any one disk from C. Therefore C_g has a simple closed polygonal boundary, $\partial C_g \subseteq C_g$, and we denote by a the number of boundary vertices, i.e., the cardinality of $C_v \cap \partial C_g$.

If f_j is the number of elementary j-gons in C_g and $f = \sum_j f_j$, then by Euler's formula

$$n + f = C_b + 1 \tag{3}$$

If the number of all (unit-length) sides of all f elementary j-gons are added, the boundary sides would be counted once and the interior sides twice, so

$$a + 2(C_b - a) = 3f_3 + 4f_4 + \cdots \geqslant 3f$$

Multiplying (3) by 3, this inequality yields

$$n - a \geqslant C_b + 3 - 2n \tag{4}$$

or equivalently

$$C_b \leqslant 3n - a - 3 \tag{$\tilde{4}$}$$

Note that (4) and ($\tilde{4}$) are equalities if and only if there are only triangles in C_g.

By a "vertex of type j" we mean a point in C_v contained in exactly j bonds, and we let k_j be the number of vertices of type j in ∂C_g. Then

$$a = k_2 + k_3 + k_4 + k_5 \tag{5}$$

Since every angle between intersecting bonds is at least $\pi/3$, the interior angle of ∂C_g at a vertex of type j is at least $(j - 1)\pi/3$, so that (from a standard formula) $3/\pi$ times the sum of all interior angles of ∂C_g is

$$3a - 6 \geqslant k_2 + 2k_3 + 3k_4 + 4k_5 \tag{6}$$

Note that (6) is an equality if and only if every interior angle of ∂C_g is $(j - 1)\pi/3$.

If the boundary disks are removed from C, leaving C' with $C_b' \geqslant 0$ bonds, we have

$$C_b' \geq C_b - a - (k_3 + 2k_4 + 3k_5)$$

and from (5) and (6) we get

$$C_b \leq C_b' + k_2 + 2k_3 + 3k_4 + 4k_5$$

and

$$C_b \leqslant C_b' + 3a - 6 \tag{7}$$

Assume for induction that $B(t) \leqslant 3t - (12t - 3)^{1/2}$ for $0 < t < n$. If $a = n$, it follows from (4) that $C_b \leqslant 3n - (12n - 3)^{1/2}$, so until we prove (9) we will assume $a \neq n$. Then since $C_b = B(n)$ by assumption, (7) gives

$$B(n) \leqslant C_b' + 3a - 6 \leqslant B(n - a) + 3a - 6$$

From the induction, then,

$$B(n) \leqslant 3n - 6 - \{12(n - a) - 3\}^{1/2}$$

Note for future reference that we get a strict inequality here if $C_b' < B(n - a)$ or if some interior angle of ∂C_g is $> (j - 1)\pi/3$. Now, using (4),

$$B(n) \leqslant 3n - 6 - (12\{B(n) + 3 - 2n\} - 3)^{1/2}$$

or

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

Therefore

$$\{B(n) - 3n + 6\}^2 \geqslant 12B(n) + 33 - 24n$$

or

$$B^2(n) - 6nB(n) + 9n^2 - 12n + 3 \geqslant 0$$

Let $P(b) = b^2 - 6nb + 9n^2 - 12n + 3$. Then $P(b)$ has roots at $b = 3n \pm (12n - 3)^{1/2}$, and is positive for $b \leqslant 3n - (12n - 3)^{1/2}$ and $b \geqslant 3n +$

$(12n - 3)^{1/2}$. Since clearly $B(n) < 3n$, $[B(n) = 3n$ would require *all* disks to touch six others, including those on the boundary], we have

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

so with (2) we have

$$B(n) = H(n) = [3n - (12n - 3)^{1/2}] \tag{9}$$

which is part (1) of the Theorem.

The essence of our method for proving part (2) is that inequalities (4) and (6) cannot both be strict; if they were, one could obtain (8), and then (9), with $B(n)$ replaced by $\{B(n) + 1\}$, which of course would be false.

Assume n is the smallest nonnegative integer for which there exists a maximal configuration C such that $f_j \neq 0$ for some $j \geqslant 4$ (this will lead to a contradiction). From the assumption that $f_j \neq 0$ for some $j \geqslant 4$, we have, as in the proof of $(\tilde{4})$,

$$(C_b + 1) \leqslant 3n - a - 3 \tag{$\tilde{4}'$}$$

or equivalently

$$n - a \geqslant (C_b + 1) - 2n + 3 \tag{4'}$$

Since by assumption there is a nontriangle in C_g, either it touches ∂C_g or it lies in C_g'. In the former case we get a strict inequality from (6), which leads to

$$(C_b + 1) \leqslant C_b' + 3a - 6 \tag{7'}$$

and then, using $C_b' \leqslant B(n - a)$, to

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

If the latter were the case, then by the minimality of n we have $C_b' \leqslant B(n - a) - 1$, and again we have (8'). So in any case we have (8'). But then just as (8) implies (9), so (8') implies

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

which is in contradiction with the maximality of C and which thus proves part (2a) of the Theorem. And since now (4) is seen to be an equality, part (2b) of the Theorem is also proven, and our proof is complete.

Remark. Part (2) of the Theorem implies that as n is made larger, the ground state fills out *all* of the triangular lattice.

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