

The Symmetry of Ground States Under Perturbation

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We consider a two-body potential which has only periodic ground states and prove that it can be perturbed, by an arbitrarily small perturbation, so as to have only aperiodic ground states.

KEY WORDS: Crystal; ground state; symmetry.

1. INTRODUCTION AND STATEMENT OF RESULTS

It is one of the more significant open problems in the theory of matter to derive the observed crystalline structure of low-temperature matter from the interactions of the constituent atoms or molecules.⁽¹⁾ Using classical mechanics and a phenomenological two-body interaction potential $W(\mathbf{r})$, one would like to show that the ground state of a system of N particles [i.e., the configuration of positions $\mathbf{r}_j(N)$ that minimizes the energy $E = \sum_{i < j} W(\mathbf{r}_i - \mathbf{r}_j)$] has (approximately) a periodic structure. To be precise, one wants to prove that for each fixed j , $\mathbf{r}_j(N)$ has a limit $\tilde{\mathbf{r}}_j$ as $N \rightarrow \infty$ and that the $\tilde{\mathbf{r}}_j$ lie at the vertices of some lattice (not necessarily Bravais).

To the best of our knowledge, the only published proof of this sort is in Ref. 2, which treats the one-dimensional problem, with Lennard-Jones potential $W(x) = |x|^{-12} - |x|^{-6}$ (see Ref. 3 for related work).

The purpose of this paper is to demonstrate the extreme sensitivity, of the qualitative property of periodicity, to perturbation of the potential (even) in one dimension.

We consider first a one-dimensional interaction potential V (trivial in the sense that only nearest neighbors play any effective role—there are no “cooperative effects”) which gives rise to periodic ground states, and show that with an *arbitrarily small* perturbation V_ϵ , the potential $\tilde{V}_\epsilon \equiv V + V_\epsilon$ has only *aperiodic* ground states. [We say the perturbation is “arbitrarily

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small" because V_ϵ and dV_ϵ/dx are continuous, go to zero at infinity, and both $\sup_x |V_\epsilon(x)|$ and $\sup_x |dV_\epsilon(x)/dx|$ go to zero as $\epsilon \downarrow 0$.]

As the details of the construction can be somewhat burdensome, we suggest the reader note the following brief outline. The perturbation V_ϵ consists of gentle depressions located at points chosen in an irregular pattern so as to favor aperiodic ground states. More specifically (note the role of the sequence $\{r_j\}$), the depressions are centered at points $\pm(2^{\lfloor m/2 \rfloor} + r_m)$, m in $\mathbb{N}$. It is proven that any ground state $\{\tilde{x}_j\}$ of $\tilde{V}_\epsilon$ must satisfy $|x_j - x_{j+2^k}| = 2^k + r_{2^k}$ or $2^k + r_{2^k+1}$, and by the choice of $\{r_k\}$ this implies the aperiodicity result. As part of the proof it is shown that there are ground states of $\tilde{V}_\epsilon$ embedded in a certain sequence $\{x_j^0\}$.

2. NOTATION

Throughout this paper, variables denoted j , k , m , or n take values in the set, $\mathbb{Z}$ of integers (or some subset if indicated), and K and N take values in the set $\mathbb{N}$ of natural numbers.

The number ϵ is fixed throughout the paper, and subject only to $0 < \epsilon < \frac{1}{8}$.

Let s_n , $n \geq 0$, be the coefficients in the 2-adic expansion of the irrational number $\alpha = \sum_{n=1}^{\infty} 2^{-v(n)}$, where $v(n) = \sum_{j=2}^{n+1} j$; i.e., $s_n = 0$ or 1 and $\sum_{n=0}^{\infty} s_n 2^{-n} = \alpha$.

Let r_n , $n \geq 0$, be defined by

$$r_{2m} = -2^m \epsilon / 2 + \epsilon \sum_{j=0}^m s_j 2^{m-j}, \quad m \geq 0$$

$$r_{2m+1} = r_{2m} + \epsilon, \quad m \geq 0$$

Let a_n , $n \neq 0$, be defined, with values $1 \pm \epsilon/2$ only, as follows. For $n \geq 1$ we define a_n recursively by setting $a_1 = 1 - \epsilon/2$ and, assuming a_n determined for $1 \leq n \leq 2^m$, $m \geq 0$, setting

$$a_n = a_{n-2^m}, \quad 2^m < n < 2^{m+1}$$

$$a_{2^{m+1}} \begin{cases} = a_{2^m} & \text{if } s_{m+1} + s_{m+2} = 0 \\ \neq a_{2^m} & \text{if } s_{m+1} + s_{m+2} = 1 \end{cases}$$

For $n \leq -1$ and $m \geq 0$ we define

$$a_n = a_{n+1+2^{m+1}}, \quad -2^{m+1} < n < -2^m$$

$$a_{-2^m} = 1 - \epsilon/2$$

Let x_n^0 be defined by

$$x_n^0 = \begin{cases} 0, & n = 0 \\ \frac{n}{|n|} \sum_{j=1}^n a_{jn/|n|}, & n \neq 0 \end{cases}$$

We define the function f_ϵ on $\mathbb{R}$ by

$$f_\epsilon(x) = \begin{cases} -20\epsilon^2[\cos(2\pi x/\epsilon) + 1], & |x| \leq \epsilon/2 \\ 0, & \epsilon/2 < |x| \end{cases}$$

3. THE EXAMPLE

Consider the pair of two-body potentials V and V_ϵ defined by

$$V(x) = \begin{cases} +\infty, & |x| < 3/4 \\ -1 - \cos[4\pi(|x| - 1)], & 3/4 \leq x \leq 5/4 \\ 0, & 5/4 < |x| \end{cases}$$

$$V_\epsilon(x) = \sum_{m=0}^{\infty} 2^{-[m/2]^2 - [m/2]} f_\epsilon(|x| - 2^{[m/2]} - r_m)$$

where $[t]$ denotes the integral part of $t \geq 0$. Note that $V, \tilde{V}_\epsilon \equiv V + V_\epsilon$, and their first derivatives are continuous (except at the hard core) and go to zero at infinity. Also note that $\sup_x |V_\epsilon(x)| = -V_\epsilon(1 \pm \epsilon/2) = 40\epsilon^2$ and $\sup_x |dV_\epsilon(x)/dx| = 40\pi\epsilon$, both of which go to zero as $\epsilon \downarrow 0$.

With the potentials V and $\tilde{V}_\epsilon$ in mind, we make the following definitions.

By a *state* we mean a finite ordered set $\rho = \{x_m, x_{m+1}, x_{m+2}, \dots, x_{n-1}, x_n\}$, where $x_j \in \mathbb{R}$ and $3/4 \leq x_k - x_j$ if $k > j$.

A *bond of type k* , $k \geq 0$ (in a state $\rho = \{x_j\}$) is an ordered pair of numbers $\{x_m, x_n\} (\subseteq \rho)$ such that

$$2^k + r_{2k} - \epsilon/2 \leq x_n - x_m \leq 2^k + r_{2k+1} + \epsilon/2$$

A bond of type k , $\{x_m, x_n\}$, is *simple* if $n \geq m + 2^k$.

Finally, the *strength* of a bond $\{x_m, x_n\}$ is $\tilde{V}_\epsilon(x_n - x_m)$.

In a (finite) system of particles interacting through V , each particle can interact (directly) only with its nearest neighbors, because of the hard core. It is therefore evident that the ground state of such a system is unique (up to translation) and consists of the positions of particles evenly spaced at distance 1 from each other.

For the remainder of the paper we will only consider states of particles interacting through $\tilde{V}_\epsilon$. Note that now the ground state of cardinality N (i.e., with N particles) is *not* unique (if $N \geq 2$). We will show, however, that a ground state can be obtained as the ordered set of *any* N consecutive terms in the (two-sided) sequence $\{x_n^0\}$ defined above. Now let $\bar{\rho}_N = \{\bar{x}_{j_N}, \dots, \bar{x}_{j_N + N - 1}\}$

be any sequence (labeled by N) of ground states such that $\bar{x}_k$ has a limit $\tilde{x}_k$ for each fixed k in $\mathbb{Z}$ as $N \rightarrow \infty$. (For example, $\tilde{x}_j = \bar{x}_j = x_j^0$.) We prove that no such sequence $\{\bar{x}_k\}$ (labeled by k) is periodic, even though $\tilde{V}_\epsilon$ is an arbitrarily small perturbation of V .

4. PROOF OF RESULTS

We begin with a result concerning the sequence $\{x_j^0\}$.

Lemma 1. For each $k \geq 0$ and n ,

$$|x_{n+2^k}^0 - x_n^0| = 2^k + r_{2k} \quad \text{or} \quad 2^k + r_{2k+1}$$

Proof. An equivalent form of the lemma is the assertion (A):

(A) In every block D of 2^k consecutive terms in the sequence

$$\{a_n\}, n(D) = A_k \quad \text{or} \quad A_k + 1$$

Here $n(D)$ is the number of terms in D of value $1 + \epsilon/2$ and $A_k \equiv \sum_{j=0}^k s_j 2^{k-j}$. We consider three kinds of block: (1) where $n > 0$ for all a_n in the block; (2) where $n < 0$ for all a_n in the block; (3) where a_{-1} and a_1 are in the block. We will first prove (A) for case (1) by induction on $k \geq 0$, where the size of the block is 2^k . Assertion (A) holds by inspection for $k = 0$. Now note that the sequence $\{a_n | n > 0\}$ is built up by recursion: once a "basic block" $B_k \equiv \{a_1, a_2, \dots, a_{2^k}\}$ is constructed, B_{k+1} is obtained by joining to B_k either a duplicate of B_k or (if $s_{k+1} + s_{k+2} = 1$) a duplicate except for the last term. Assume all blocks of size 2^m , $0 \leq m \leq k$, in B_k satisfy (A). If $s_{k+1} + s_{k+2} = 0$, then all blocks of size 2^m , $0 \leq m \leq k$, in B_{k+1} satisfy (A), since they are either subsets of one of the two B_k 's which make up B_{k+1} or else they overlap the junction and are thus "translates" of blocks in the B_k 's. The block of size 2^{k+1} is just B_{k+1} , and satisfies (A) by construction; in fact, as is easily established using $A_{j+1} = 2A_j + s_{j+1}$, we have, for all j , the special case of (A):

$$(B) \quad n(B_j) = A_j + s_{j+1}.$$

Next we establish the remaining subcase, $s_{k+1} + s_{k+2} = 1$, as follows. First note that the only size 2^m block not covered by the previous argument is

$$B_{k+1,m} \equiv \{a_{2^{k+1}-2^m+1}, \dots, a_{2^{k+1}}\}$$

But from (B) we have $n(B_j) = A_{j+1} - A_j$, and so

$$\sum_{j=m}^k n(B_j) = A_{k+1} - A_m$$

which implies

$$n(B_{k+1,m}) = n(B_{k+1}) - \sum_{j=m}^k n(B_j) = A_m + s_{k+2}$$

which completes case 1. Next we reduce cases 2 and 3 to case 1. Case 2 follows from case 1 since each block $C_m \equiv \{a_{-2^m}, a_{-2^m+1}, \dots, a_{-1}\}$ appears as the first half of B_{m+1} if $s_{m+1} = 0$, and the second half if $s_{m+1} = 1$. Finally, case 3 follows since any block of type 3, of size 2^k , can be considered to lie in every block

$$D_m \equiv \{a_{-2^{m-1}}, a_{-2^{m-1}+1}, \dots, a_{2^{m-1}}\}$$

for $m \geq k + 1$. But we can always find an $m \geq k + 1$ such that $s_m + s_{m+1} = 0$, in which case D_m is a "translate" of B_m . This completes the proof of the lemma.

Lemma 2. For any $k \geq 0$, $\sum_{j=k+1}^{\infty} 2^j b_j < b_k$, where $b_j = \epsilon^2 2^{-j^2-j-1}$ is the maximum value of $|V_\epsilon(x_n - x_m)|$ if $\{x_m, x_n\}$ is a bond of type j .

Proof. Elementary.

Lemma 3. If ρ is a ground state of cardinality N , it contains exactly $N - 2^k$ bonds of type k for each $k \geq 0$, and they are all simple.

Proof. We will prove the lemma by induction on the bond type k . Assume the lemma holds for all $0 \leq k \leq K$. Comparing ρ to any of the states $\rho^0 = \{x_j^0\}$ of cardinality N , which latter have $N - 2^k$ bonds of type k each of maximum possible strength, we see that ρ must have at least $N - 2^{K+1}$ bonds of type $K + 1$ since in any case it must have less than N , and by Lemma 2 the sum total of the contributions to the energy of ρ of all bonds of type k for $k \geq K + 2$ cannot make up for the lack of a bond of type $K + 1$. (This argument also proves that $k = 0$ satisfies the lemma, simplicity being trivial.) It remains to show simplicity for $k = K + 1$. Let $\{x_m, x_n\}$ be a bond of type $K + 1$ in ρ . Since $N - 2^k$ is the maximum possible number of simple, type k bonds, and since by assumption there are this number for $k = K$, there must be terms x_s and x_t in ρ (possibly $s = t$) such that $\{x_m, x_s\}$ and $\{x_t, x_n\}$ are bonds of type K . But then by geometry, $|x_t - x_s| < 4\epsilon$, which implies that $s = t$. This then implies $\{x_m, x_n\}$ is simple, which completes the proof.

Proposition 1. Any collection ρ^0 of N consecutive terms in $\{x_j^0\}$ constitutes a ground state (with respect to $\tilde{V}_\epsilon$).

Proof. From Lemma 3 and the fact that there are at most $N - 2^k$ simple, type k bonds in any state of cardinality N , and noting again that for any bond $\{x_m, x_n\}$ of type k , $V(x_n - x_m)$ is the maximum possible if $\{x_m, x_n\} \subseteq \rho^0$, the proposition follows.

It follows from our proofs, in particular from (A), that if a sequence of ground states of increasing cardinality is selected from $\{x_j^0\}$, then it will not

be periodic in the limit. We will next show this for *any* convergent sequence of ground states.

Proposition 2. Let $\bar{\rho}_N = \{\bar{x}_{k_j} | j = 1, 2, \dots, N\}$ be any sequence (labeled by N) of ground states of cardinality N such that $\bar{x}_k$ has a limit $\tilde{x}_k$ as $N \rightarrow \infty$ for each k in $\mathbb{Z}$. Then $\{\tilde{x}_k\}$ is not periodic.

Proof. From the above proofs it follows that

$$|\tilde{x}_j - \tilde{x}_{j+2^k}| = 2^k + r_{2k} \quad \text{or} \quad 2^k + r_{2k+1}$$

for all $k \geq 0$. But then in the block $\{\tilde{x}_0, \tilde{x}_1, \dots, \tilde{x}_{2^k}\}$ the proportion of “nearest neighbor distances” (i.e., numbers $|\tilde{x}_{j+1} - \tilde{x}_j|$, $0 \leq j \leq 2^k - 1$) that have value $1 + \epsilon/2$ is either $\sum_{j=0}^k s_j 2^{-j}$ or $2^{-k} + \sum_{j=0}^k s_j 2^{-j}$, and so approaches the irrational number α as $k \rightarrow \infty$. This completes the proof.

5. CONCLUSION

We have shown that the qualitative property of having periodic ground states can be destroyed by an arbitrarily small perturbation of the interaction potential. This result is of particular significance since, when examining such problems using classical mechanics (the use of which is necessary at present considering that even the *existence* of ground states is still unproven in many-body quantum theory) one must use phenomenological potentials which even in principle cannot be justified in detail.

Finally we wish to comment on two features of our method. Because only nearest neighbors interact directly through V , we used perturbations V_ϵ , which perturbed the minimum of V and in fact split the minimum into a double minimum. However, if V were longer range (such as the Lennard-Jones potential) the particles in a ground state would have nearest neighbors closer than the distance to the minimum of the potential, and this is the point we would perturb (if we could do the calculation!); the perturbed potential would then still have a unique minimum. We should also note that although our perturbations V_ϵ are physically of order ϵ , since the energy $V_\epsilon(x)$ and the force $dV_\epsilon(x)/dx$ are both uniformly of order ϵ , it is a fact that (at least as a general method of perturbation) we could not hope to have $d^2V_\epsilon(x)/dx^2$ also uniformly of order ϵ . For example, it follows from the proof in Ref. 2 that such a perturbation would not alter the qualitative features of the ground states of the Lennard-Jones potential.

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