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THE STATISTICAL MECHANICS OF ANHARMONIC LATTICES

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I. INTRODUCTION

The equilibrium and non-equilibrium properties of regular harmonic crystals are well understood (Montroll, 1956, Lanford and Lebowitz, 1974). For them it is possible to define an infinite volume equilibrium state for dimensionality three and higher. This state is a Gaussian measure. For one (resp. two) dimensions it is not possible to define such a state because the mean square displacement of any particle diverges as $|\Lambda|$ (resp. $ln|\Lambda|$) as $|\Lambda|\to\infty$, where $|\Lambda|$ is the volume of the system. In all dimensions, however, it is possible to define a state on the algebra generated by the difference variables (Lanford and Lebowitz, 1974).

It is natural to ask, as we do here, whether this dependence on dimensionality, and essential independence of the detailed properties of the harmonic force matrix, remains true for anharmonic forces. In one dimension, the only case for which the answer can be computed explicitly, anharmonic and harmonic yield the same result: there is no long-range order — by which we mean that the expected value of the square displacement of a particle at the center diverges as $|\Lambda|\to\infty$. It seems likely that this analogy also holds in two and three dimensions, and in this paper we present some evidence that it does.

To simplify the situation as much as possible we restrict ourselves to nearest neighbor interactions on a simple cubic lattice and we assume the displacement of each particle to be one-dimensional; really it should be a vector. Most of our results can be readily generalized to more complicated situations.

The setting is the lattice Z^ν, $\nu=1$, 2 or 3. Associated with each point $n\in Z^\nu$ is a variable $x_n\in R$ which we call the particle coordinate at n. Let Λ be the cube in Z^ν, centered at the origin 0, of side $2L+1$ and volume $|\Lambda|=(2L+1)^\nu$. Finally, let $v:R\to R$ be a function such that

$$I(\alpha)=\int e^{-\alpha v}<\infty, \forall\alpha>0,$$

and $v(x)=v(-x)$. We set $X=\{x_i\}_{i\in\Lambda}$.

The potential energy of the particles in Λ is

$$H(X) = \sum_{<i,j>} v(x_i - x_j) \tag{1}$$

with the summation being over all distinct pairs of points $<i,j>$, $i \in \Lambda$, $j \in Z^\nu$, i and j nearest neighbors in Z^ν, i.e. $|i-j| = 1$. If $j \notin \Lambda$ we set $x_j = 0$ in (1). Thus, the particles at the boundary of Λ are "tied down".

With $dX = \prod_{i \in \Lambda} dx_i$, let

$$Z_\Lambda = \int dX \exp[-H(X)] \tag{2}$$

be the partition function. We are interested in knowing whether the marginal distribution of x_0 has a limit as $\Lambda \to \infty$. E.g. does

$$<x_0^2>_\Lambda = \int dX x_0^2 \exp\ [-H(X)]/Z_\Lambda \tag{3}$$

have a finite limit? When $\nu = 1$ the situation is clear because the increments are essentially independent. Asymptotically, $<x_0^2>_\Lambda \sim |\Lambda|$.

Consider the **harmonic** crystal wherein $v(x) = ax^2$, $\alpha > 0$. In this case all the integrals are Gaussians and can be calculated exactly in terms of normal modes (Montroll, 1956). As $\Lambda \to \infty$

$$\frac{1}{|\Lambda|} \ln Z_\Lambda \to -\frac{1}{2}(2\pi)^{-\nu} \int d^\nu k \ln\left[\nu - \sum_{j=1}^{\nu} \cos k_j\right] - \frac{1}{2} \ln(2a/\pi) \tag{4}$$

where the integration is over the cube $[-\pi, \pi]^\nu$. Similarly,

$$<x_0^2>_\Lambda \to (4\alpha)^{-1}(2\pi)^{-\nu} \int d^\nu k \left[\nu - \sum_{j=1}^{\nu} \cos k_j\right]^{-1} \tag{5}$$

which diverges for $\nu = 1$ and 2 but converges for $\nu = 3$. A more careful estimate shows that the divergence is proportional to $|\Lambda|$ (resp. $\ln|\Lambda|$) for $\nu = 1$ (resp. 2).

In Section V we shall show that for $\nu = 2$, $<x_0^2>_\Lambda$ goes to infinity at least as fast as $\ln|\Lambda|$ for potentials that satisfy the hypothesis of Theorem 4. This is a large class, including non-convex potentials, but it does not include potentials with hard walls, i.e. $v(x) = \infty$, $|x| > M$. For $\nu = 3$ our results, in Section VI, are more meager and are confined to convex potentials which increase at least as fast as x^2 as $|x| \to \infty$. However, if the potential is too flat near $x = 0$, it must increase precisely as x^2 for large x. For a decorated lattice, and convex $v(x)$, we can prove that $<x_0^2>_\Lambda$ is bounded in three dimensions.

Our theorems do not prove the **conjecture** that $<x_0^2>_\Lambda$ **always** diverges when $\nu = 2$ and **always** stays bounded when $\nu = 3$, but they make it plausible. We have been unable to find a counterexample.

A noteworthy point is that the integral in (5) occurs in the theory of the random walk and is related to the reciprocal of the probability of not returning to the origin. This leads us to suspect that for general $v(x)$ there is also some connection between the random walk problem and $<x_0^2>_\Lambda$, but we do not know what it is. We shall, however, have a little to say about this in Section VII.

II. THE THERMODYNAMIC LIMIT OF THE FREE ENERGY

One question that is easy to dispose of is that if $g_\Lambda \equiv |\Lambda|^{-1} \ln Z_\Lambda$ then

$$\lim_{\Lambda \to \infty} g_\Lambda = g \tag{6}$$

exists. We shall discuss the two-dimensional case, but the argument is general. An upper bound to Z_Λ is obtained by writing $\exp(-H) = \exp(-H_1)$ $\exp(-H_2)$ where H_1 (resp. H_2) contains all the "horizontal" (resp. "vertical") terms in (1). By Schwarz's inequality $Z_\Lambda^2 \leqslant \int \exp(-2H_1) \int \exp(-2H_2)$. Using the same inequality, $\int \exp(-2H_1) = \int \exp(-2H_2) \leqslant I(2)^{2L(2L+1)} I(4)^{2L+1}$. Thus $g_\Lambda <$ const. $< \infty$.

Now consider a sequence of domains Λ_j with $L_j = 2^j, j = 1, 2, \ldots$, and define $g_j = |\Lambda_j| g_{\Lambda j} 2^{-2j-2}$. In the integral for Z_j, do the integral over all x_n except when $n = (0, m)$. With $Y = \{x_{o,m} - 2^j \leqslant m \leqslant 2^j\}$, Z_j has the form $Z_j = \int W(Y)^2 \exp[-H(Y)]\, dY$ and H is the energy of the middle column. Clearly, $\int W(Y) \exp[-H(Y)] \times \exp[-K(Y)] = \hat{Z}_j$, where $\hat{Z}_j$ is the partition function of a $(2^{j+1}+1) \times (2^j+1)$ rectangle and $K(Y) = \sum_m \Lambda(x_{0,m})$. Using Schwarz's inequality, $\hat{Z}_j^2 \leqslant Z_j \int \exp[-2K(Y) - H(Y)]\, dY \leqslant Z_j I(2)^{2j} I(4)^{2j+1}$. Now splitting $\hat{Z}_j$ again into two pieces, we finally get

$$g_j \geqslant g_{j-1} - R_j \tag{7}$$

where $|R_j| <$ (const.) 2^{-j}. Since g_j is bounded above, (7) implies that g_j has a limit. Since $|\Lambda_j| 2^{-2j-2} \to 1$, $g_{\Lambda j}$ has the same limit.

III. A COMPARISON THEOREM

We return to the problem of evaluating $<x_0^2>_\Lambda$, and ask if there is any way to relate it to the calculation (5) for the pure harmonic case. A useful theorem is the following (Brascamp and Lieb, 1974, 1975).

T h e o r e m 1: *Let* $G = \exp[-(x, Bx)]$, $B > 0$, *be a Gaussian on* R^n *with covariance matrix* $1/2\ B^{-1}$. *If* $V(x)$ *is convex (resp. concave) and if* M *is the covariance matrix of* $G \exp(-V)$, *then* $M \leqslant 1/2 B^{-1}$ (*resp.* $M \geqslant 1/2 B^{-1}$).

This theorem can settle the question for $\nu = 3$ when $v''(x) \geqslant 2\alpha > 0, \forall x$. In this case $<x_0^2>_\Lambda \leqslant$ eqn. (5). See Section VI.

The following two theorems will also be useful in dealing with convex potentials. A function $F(x)$ is said to be log concave if $F(x) = \exp[-f(x)]$, with $f(x)$ convex.

Theorem 2: (*Prékopa, 1971, 1973, Leindler, 1972, Rinott, 1973, Brascamp and Lieb, 1974, 1975*): *Let $F(x, y)$ be log concave in $(x, y) \in R^m \times R^n$. Then*

$$G(x) \equiv \int F(x, y)dy$$

is log concave in $x \in R^m$.

Theorem 2 is the basic for proving Theorem 1 (Brascamp and Lieb, 1974).

An important consequence of Theorem 2 is that when $v(x)$ is convex, the distribution of x_0 is log concave and, of course, even and monotone non-increasing on $(0, \infty)$. In this case, it is easy to see that if $<x_0^2>_\Lambda$ stays bounded, then all moments, $<x_0^n>_\Lambda$, stay bounded.

A sharpened version of Theorem 2 is the following (Brascamp and Lieb, 1975).

Theorem 3: *Let $f(x, y)$ be convex in $(x, y) \in R \times R$, and let $f \in C^2(R^2)$. Define $F(x, y) = exp[-f(x, y)]$,* and

$$exp[-g(x)] = \int F(x, y)dy.$$

The last integral and the integrals

$$\int f_{xx} F\, dy, \quad \int (f_x)^2 F\, dy$$

are assumed to converge uniformly in a neighborhood of a given point x_0. Then $g(x)$ is twice continuously differentiable near x_0. Its second derivative at x_0 satisfies

$$g''(x_0) \geqslant <f_{xx} - (f_{xy})^2/f_{yy}> \geqslant 0; \tag{8}$$

the average is taken with the normalized weight proportional to $F(x_0, y)$.

Remarks: 1. Theorem 3 generalizes to $(x, y) \in R^m \times R^n$; for the purpose of this paper, however, we can restrict ourselves to the given case.

2. Since f is convex,

$$f_{yy} \geqslant 0 \text{ and } (f_{xy})^2 \leqslant f_{xx} f_{yy}.$$

Thus, if we set

$$[f_{xx} - (f_{xy})^2/f_{yy}](x_0, y) = 0$$

when $f_{yy}(x_0, y) = 0$, the inequality (8) is true.

IV. STIFFENING THE SPRINGS DOES NOT NECESSARILY DECREASE $<x_0^2>$

It would be very helpful, if true, to know that increasing some of the terms in (1) decreases $<x_0^2>$. Consider the harmonic case and allow each term in (1) to be different, i.e.

$$H = \sum_{<i,j>} \alpha_{ij}(x_i - x_j)^2, \quad \alpha_{ij} \geqslant 0.$$

It is elementary to see that increasing any α_{ij} does not increase $<x_0^2>$, because the total covariance matrix is decreased in the sense of forms. (As the following example shows, however, it is possible that $<x_0^2>$ is independent of some α_{ij}.)

Now let us do the same thing for a general $v(x)$, i.e.

$$H \to \sum_{<i,j>} \alpha_{ij} v(x_i - x_j)$$

and we can even assume that v is convex. We shall give a simple counter-example to the proposal that increasing any α_{ij} does not increase $<x_0^2>$.

Consider the following case with three particles, i.e. $H = v(x) + v(x-y) + v(y-z) + v(z) + \alpha v(x-z)$ and $x_0 = y$. Let $v(x) = x^2 + \varepsilon x^4$, $\varepsilon > 0$. We want to show that increasing α from 0 can decrease $<x_0^2>$. Let g_∞ (resp. g_0) be $<x_0^2>$ for $\alpha = \infty$ (resp. $\alpha = 0$). Then $g_\infty = 2 \int y^2 G(y)/\int G(y)$ and $g_0 = \int y^2 F(y)/\int F(y)$, with $G(y) = \exp(-2v(y))$ and $F(y) = R(y)^2$ where $R = \exp(-v) * \exp(-v)$. A simple calculation shows that for the pure harmonic case $(\varepsilon = 0)$, $g_0 = g_\infty = 1/2$. When $\varepsilon > 0$ it is impossible to calculate the integrals, but it is possible to calculate $g_i = dg_i/d\varepsilon|_{\varepsilon=0}$. One finds that $g_\infty = -3/4$ and $g_0 = -9/8$. Thus, for small, positive ε, $g_\infty > g_0$, which is the contradiction we wished to demonstrate.

V. TWO DIMENSIONS

We shall show that, for a large class of potentials v, $<x_0^2>_\Lambda$ increases at least as fast as $ln|\Lambda|$ as $|\Lambda| \to \infty$. The method given here follows the argument by Hohenberg (1967), Mermin and Wagner (1966), Mermin (1967, 1968). We thank Dr. B. Halperin for showing us how the ideas in these references apply to the present problem.

Let φ_1, φ_2 be vectors in R^n with $\|\varphi_1\| = 1$, and define

$$y_i = (\varphi_i, X); \quad \partial H/\partial y_i = (\varphi_i, \nabla H). \tag{9}$$

Let T be a linear orthogonal transformation, T: $x_i \to \tilde{x}_i$, such that $\tilde{x}_1 = y_1$. Then, an integration by parts given that

$$\int dX y_2(\partial H/\partial y_1)\exp(-H(X)) = \int dX \exp[-H(X)]\partial y_2/\partial y_1. \tag{10}$$

In this section we shall assume $v \in C^2$ and, to justify eliminating the boundary terms when integrating by parts, we assume that

$$[|x| + |v'(x)|]\exp[-v(x)] \to 0 \text{ as } |x| \to \infty. \tag{11}$$

Now $\partial y_2/\partial y_1 = (\varphi_1, \varphi_2)$. Application of Schwarz's inequality to the left side of (10) gives

$$<y_2^2> \geqslant (\varphi_1, \varphi_2)^2/<(\partial H/\partial y_1)>^2. \tag{12}$$

Consider the matrix

$$(M)_{ij} = <(\partial H/\partial x_i)(\partial H/\partial x_j)> = <\partial^2 H/\partial x_i \partial x_j>, \tag{13}$$

where the last equality follows from an integration by parts and (11). Obviously, M is a real, positive definite matrix. In terms of M, (12) reads

$$<y_2^2> \geqslant (\varphi_1, \varphi_2)^2/(\varphi_1, M\varphi_1) \tag{12a}$$

If we let $\varphi = \varphi_2$, $y = (\varphi, X)$ and $\varphi_1 = M^{-1}\varphi/\|M^{-1}\varphi\|$, then we obtain

$$<y^2>_\Lambda \geqslant (\varphi, M^{-1}\varphi). \tag{14}$$

Let us investigate the matrix M. By (13),

$$M_{ii} = \sum_{j:\,<i,j>} <v''(x_i-x_j)>,\ \text{if } i\in\Lambda \tag{15}$$

$$\begin{aligned} M_{ij} &= -<v''(x_i-x_j)>, \text{ if } i,j \text{ are nearest neighbors and } i,j\in\Lambda,\\ M_{ij} &= 0, \quad \text{otherwise.}\end{aligned}$$

The sum in (15) is over the 4 nearest neighbors of i; if $i\in\partial\Lambda$, it should be understood that $x_j = 0$ if $j\notin\Lambda$. Note that

$$(\varphi, M\varphi) = \sum_{<i,j>} (\varphi_i-\varphi_j)^2 <v''(x_i-x_j)>_\Lambda.$$

Let us assume, for the moment, that there is a positive constant A, independent of i, j and Λ, such that

$$<v''(x_i-x_j)>_\Lambda \leqslant A < \infty \tag{16}$$

Then we have the matrix inequality

$$M \leqslant -A\Delta \tag{17}$$

where $\Delta \leqslant 0$ is defined by

$$\begin{aligned}\Delta_{ii} &= -4, i\in\Lambda,\\ \Delta_{ij} &= 1, \text{ if } i,j \text{ are nearest neighbors and } i \text{ and } j\in\Lambda,\\ \Delta_{ij} &= 0, \text{ otherwise.}\end{aligned}$$

The matrix Δ arises precisely in the case of pure harmonic forces,

$$H(X) = \sum_{<i,j>} (x_i-x_j)^2 = -(X,\Delta X),$$

so that for harmonic forces

$$<y^2>_\Lambda = -(\varphi,\Delta^{-1}\varphi)/2. \tag{18}$$

By (14, 17, 18), and with $y = x_0$, $<x_0^2>_\Lambda(v) \geqslant (2/A) <x_0^2>_\Lambda(v=x^2)$. Since the latter behaves as $ln|\Lambda|$ as $\Lambda\to\infty$, our statement is proved under the assumptions (11, 16). Let us give some simple conditions on v that are sufficient for (16).

Obviously, it suffices that

$$v''(x) \leqslant A,\ \forall\, x. \tag{19}$$

On the other hand, since

$$<v''(x_i-x_j)> = <v'(x_i-x_j)\,(\partial H/\partial x_i)>,$$

(16) is certainly satisfied if, for all i, j,

$$<[v'(x_i-x_j)]^2> \leqslant A/4. \tag{20}$$

Thus another sufficient condition is that

$$|v'(x)| \leqslant B < \infty,\ \forall\, x. \tag{21}$$

We finally consider convex potentials $v(x)$. Write

$$\int dX \exp[-H(X)]\,\delta(x_i-x_j-x) = \exp[-v(x)]\,W(x),$$

which defines $W(x)$. By Theorem 2, $W(x)$ is log concave if v is assume[d] to be convex. We always assume $v(x)$ to be even, which implies tha[t] $W(x)$ is even. Hence, $W(x)$ is decreasing for $x>0$. Note further tha[t] $v'(x)$ is positive and increasing for $x>0$, since $v(x)$ is even and convex Altogether,

$$\begin{aligned}<[v'(x_i-x_j)]^2> &= \int_0^\infty dx\,[v'(x)]^2\, W(x)\exp[-v(x)]\Big/\int_0^\infty dx\, W(x)\exp[-v(x)]\\ &\leqslant \int_0^\infty dx\,[v'(x)]\exp[-v(x)]\Big/\int_0^\infty dx\exp[-v(x)].\end{aligned} \tag{22}$$

The last inequality follows from the fact that $[v'(x)]^2$ is increasing an[d] $W(x)$ is decreasing. Thus, in the case of convex potentials, it suffices tha[t] the last member of (22) is finite.

We summarize the results of this section:

Theorem 4: *In two dimensions, $<x_0^2>_\Lambda$ increases at least as $ln|\Lambda|$ as $\Lambda\to\infty$ if $v(x)$ satisfies*

(i) $[|x|+|v'(x)|]\,exp[-v(x)]\to 0$ *as* $|x|\to\infty$

(ii) One of the following three conditions:

$$\begin{aligned}&(a)\, v''(x) \leqslant A < \infty,\ \forall\, x\\ &(b)\, |v'(x)| \leqslant B < \infty,\ \forall\, x\\ &(c)\, v(x) \text{ is convex and}\\ &\int dx\,[v'(x)]^2\,exp[-v(x)] < \infty.\end{aligned}$$

By taking suitable limits this class includes such diverse potentials a[s] $|x|^\gamma$, $1 \leqslant \gamma < \infty$, $x^2-|x|$ (which has a double minimum) and max $(|x|^\gamma, 1)$ $\forall\,\gamma > 0$ (which has a flat bottom). It does not include $|x|^\gamma$, $0<\gamma<$ [1] or $|x|^\gamma$, $\gamma = \infty$. By the last expression we mean the hammoc[k] potential, i.e.

$$\begin{aligned} v(x) &= 0,\ |x| \leqslant 1\\ &\ \ \infty,\ |x| > 1\end{aligned}$$

A final remark is that when $v(x)$ satisfies the hypothesis of Theorem [4] then, by the methods of Section VI, $<x_0^2>_\Lambda$ does not diverge fast[er] than $ln|\Lambda|$.

VI. THREE DIMENSIONS

As already remarked after Theorem 1, $<x_0>_A$ is bounded in three dimensions if $v(x)$ is convex in the following strict sense:

$$v''(x) > 2a \geqslant 0, \forall x.$$

We exploit this idea a bit further for functions $v \in C^2$.

Let us split the lattice points $n = (n_1, n_2, n_3) \in Z^3$ according to whether $|n| \equiv n_1 + n_2 + n_3$ is even or odd. To emphasize the distinction, let us write $x_n = y_n$, if $|n|$ is even; $x_n = z_n$, if $|n|$ is odd. Then we can write

$$H(X) = \sum_{|m| \text{odd}} \sum_{n:<m,n>} v(y_n - z_m),$$

so that

$$\int \exp[-H(X)]\,dZ = \prod_{|m| \text{odd}} w(Y_m), \tag{23}$$

where Y_m stands for the 6 nearest neighbors of m, and

$$w(Y_m) = \int dz_m \exp[-\sum_{n:<n,m>} v(y_n - z_m)]. \tag{24}$$

Notice that the y' s occupy a face-centered cubic lattice, consisting of the points n with n_1, n_2, n_3 even, together with the centres of the faces of the resulting $2\times2\times2$ cubes.

We shall show (Theorem 5) that, under certain conditions on $v(x)$,

$$w(Y_m) = \exp[-\frac{1}{2}a \sum_{n:<n,m>} \sum_{k:<m,k>} (y_n - y_k)^2 - f(Y_m)], \tag{25}$$

where f is a convex function (of its 6 variables jointly) and a is a suitable positive constant.

Let us further split the variables $\{Y_m\}$ into $\{u_i\}$ and $\{v_j\}$, with the u_i corresponding to the corners of the $2\times2\times2$ cubes and the v_i to the centres of the faces. Then it follows from (23, 24, 25) and Theorem 2 that

$$\int \exp[-H(X)]\,dZ\,dV = \exp[-a \sum_{<i,j>} (u_i - u_j)^2 - g(U)]. \tag{26}$$

where g is a convex function of the U-variables and where the summation is over all pairs of nearest neighbors on the lattice, $(2Z)^3$, of $2\times2\times2$ cubes.

Since the required $<x_0^2>$ is obviously equal to $<u_0^2>$ with the weight (26), Theorem 1 implies that $<x_0^2>$ is bounded above by (5) and is thus bounded.

Let us now give a sufficient condition on $v(x)$ so that (25) is satisfied.

T h e o r e m 5: *Let $v(x)$ be convex, and let*

(i) $0 < A \leqslant v''(x) \leqslant B < \infty$, if $|x| \geqslant M$

(ii) $|v(x) - Cx^2| \leqslant D < \infty$, $\forall x$

with strictly positive constants A,B,C and M. Define

$$\exp[-g(y_1, \dots, y_k)] = \int dz \exp[-\sum_{j=1}^{k} v(y_j - z)].$$

Then

$$g(y_1, \dots, y_k) = \frac{1}{2}a \sum_{i,j=1}^{k} (y_i - y_j)^2 + h(y_1, \dots, y_k),$$

with a constant $a>0$ and with the function h convex.

P r o o f: Apply Theorem 3 to the second derivative of g in a direction $(\lambda_1, \dots, \lambda_k)$ at a given point. Thus

$$\sum_{i,j} \lambda_i \lambda_j \partial^2 g/\partial y_i \partial y_j \geqslant \Big< \sum_i \lambda_i^2 v''(y_i - z) - \frac{\sum_{i,j} \lambda_i \lambda_j v''(y_i - z) v''(y_j - z)}{\sum_l v''(y_l - z)} \Big> =$$

$$= \Big< \frac{\sum_{i,j} (\lambda_i - \lambda_j)^2 v''(y_i - z) v''(y_j - z)}{2 \sum_l v''(y_l - z)} \Big>.$$

By condition (i), this exceeds

$$\frac{A^2}{2kB} \sum_{i,j} (\lambda_i - \lambda_j)^2 \int_{|z - y_i| > M} dz \exp[-\sum_l v(y_l - z)] / \int dz \exp[-\sum_l v(y_l - z)].$$

Condition (ii) in turn implies that this is not smaller than

$$\frac{A^2}{2kB} \exp(-2kD) \sum_{i,j} (\lambda_i - \lambda_j)^2 \int_{|z| > kM} dz \exp(-kCz^2) / \int dz \exp(-kCz^2) \equiv \frac{1}{2} a \sum_{i,j} (\lambda_i - \lambda_j)^2.$$

This proves Theorem 5. Q.E.D.

R e m a r k s: 1. Theorem 5 obviously fails if $v(x)$ increases slower than quadratically as $|x| \to \infty$, because then also $g'' \to 0$ as $|y_i - y_j| \to \infty$.

2. It is less obvious, but true, that Theorem 5 also fails if $v(x)$ increases faster than quadratically, and if $v'' = 0$ somewhere.

Take, for example, $v(x) = x^4$, and let

$$\exp[-g(x, y)] = \int dz \exp[-z^4 - (x - z)^4 - (y - z)^4].$$

By Theorem 2, $g_{xx} \geqslant 0$. Also, simple differentiation gives that

$$g_{xx} \leqslant 12 <(x - z)^2>.$$

In particular, for $y = 2x$

$g_{xx}(x, 2x) < 12 \int dz\, z^2 \exp[-3z^4 - 12z^2x^2] / \int dz \exp[-3z^4 - 12z^2x^2]$.

Hence, $g_{xx}(x, 2x) \to 0$ as $|x| \to \infty$. Note however, that $g_{xx}(x, y) \to \infty$ as $(x, y) \to \infty$ in any other direction than $y = 2x$. The situation is a bit worse when there are 6 neighbors, but in any case Theorem 5 only just barely fails for $v(x) = x^4$. This supports the conjecture that $<x_0^2>$ is bounded for the x^4 interaction. More evidence in this direction is supplied by the fact that $<x_0^2>$ can be proved to be bounded if some interactions are removed.

Namely, remove all the lattice points that do not lie on a corner or on an edge of some $2\times2\times2$ cube. Then we have what is called a *decorated lattice* and the points in the middle of an edge have only two nearest neighbors. One can use the fact that

$$\int dz \exp[-v(x-z)-v(y-z)] = \exp[-a(x-y)^2 - f(x-y)] \qquad (27)$$

with f convex, for a much wider class of potentials than ones in Theorem 5. For example, (27) holds true $v(x) = |x|^\gamma, \gamma > 2$, including the hammock potential ($\gamma = \infty$).

Theorem 6: *In three dimensions,* $<x_0^2>_\Lambda$ *is bounded in* Λ *if* $v(x)$ *satisfies one of the following conditions*

(a) $v(x) = ax^2 + f(x)$, f *convex*, $a > 0$

(b) *conditions* (i) *and* (ii) *of Theorem* 5.

As we said above, x^4 just fails. However, $v(x) = x^4, |x| \leqslant 1$; $2x^2 - 1, |x| \geqslant 1$ does satisfy the hypothèses of Theorem 6 and therefore, if x^4 fails in reality, it cannot be due to small amplitude fluctuations alone.

VII. A TENUOUS CONNECTION WITH THE RANDOM WALK PROBLEM

As we said in the introduction, the various tricks we have employed to show that $<x_0^2>_\Lambda$ goes to infinity in one and two dimensions and stays bounded in three dimensions do not really go to the heart of the problem. Somehow there must be a more immediate connection with some property of the lattice more directly related to its geometry.

To this end, let Δ be the second difference operator on Z^ν with zero boundary conditions on Λ. I.e., for $n \in \Lambda$,

$$(\Delta f)(n) = -2\nu f(n) + \sum_j f(j)\chi(n,j) \qquad (28)$$

where $f(j) \equiv 0$ if $j \notin \Lambda_n$ and $\chi(n,j) = 1$ if n and j are nearest neighbors and zero otherwise. Consider the Green function for n, $m \in \Lambda$

$$-\Delta_n G(n,m) = \delta_{n,m}$$

with δ being the Kronecker delta. If a random walker starting at n is observed for a very long time, then $G(n,m)$ is proportional to the number of times, on the average, that the walker visits the site m. Clearly $G(n,m) = G(m,n)$ and as $\Lambda \to \infty$, $G(n,n)$ remains finite for $\nu = 3$ and goes to infinity for $\nu = 1, 2$.

To use G, we write

$$x_0 = \int_{j\in\Lambda} x_j \delta_{j,0} = -\sum_{j\in\Lambda} x_j (\Delta G(\cdot,0))(j) \qquad (29)$$

$$= (1/2)\sum_j \sum_n (\nabla x)(j,n)\,(\nabla G(\cdot,0))(j,n) \qquad (30)$$

$$= -\sum_{j\in\Lambda} (\Delta x)(j) G(j,0) \qquad (31)$$

where $(\nabla f)(j,n) \equiv [f(j) - f(n)]\chi(j,n)$, and $f(k) \equiv 0$ if $k \notin \Lambda$.

In one dimension, with $\Lambda = [-L, L]$, $G(n,0) = L + 1 - |n|$, and (30) reads

$$x_0 = 1/2\{(x_0 - x_1) + (x_1 - x_2) + \ldots + (x_L)\} + 1/2\{(x_0 - x_{-1}) + (x_{-1} - x_{-2}) + \\ + \ldots + (x_{-L})\}.$$

We now square the right side of (30) and insert it into (3), the expression for $<x_0^2>_\Lambda$. Suppose we consider only the "diagonal terms", i.e. when $j' = j$ and $n' = n$. Assuming that $<(x_j - x_n)^2>\chi(j,n) \leqslant A < \infty$, these terms would contribute

$$(A/4)\sum_j \sum_n \chi(j,n)\,(\nabla G(\cdot,0))(j,n)^2,$$

and this is finite in three dimensions because $G(j,0) \sim |j|^{-1}$ as $j \to \infty$ and $G(j,0)$ is bounded. For the same reason, using Cauchy's inequality, we could handle any finite number of off-diagonal terms, i.e. those for which $|j - j'| < B$ and B is fixed. We cannot handle all the terms this way because we would end up with $\left(\sum_{n:|n|\geqslant 1} |n|^{-2}\right)^2$ and this diverges at infinity. However, the method would work (by Young's inequality) if we knew that the correlations

$$<(x_j - x_n)(x_k - x_l)>\chi(j,n)\chi(k,l)$$

vanished faster than $|j-k|^{-2-\varepsilon}(\varepsilon > 0)$ as $|j-k| \to \infty$.

We almost have here a proof by contradiction for $\nu = 3$. Loosely speaking, if the correlations do not decay, then we have long-range order. But then one would expect that $<x_0^2>_\Lambda$ remains bounded, because $<x_0^2>_\Lambda \to \infty$ means there is no long-range order, i.e. the center of the crystal does not feel the effect of the tied down boundaries.

When $\nu = 2$, the use of (30) almost shows that $<x_0^2>_\Lambda$ diverges, because $G(j,0) \sim -\ln|j|$ for *small* j and large Λ. This argument is insufficient, however, because there might be a cancellation of alternating terms.

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SUMMARY

It is well known that for a lattice of oscillators coupled harmonically there is no long-range order in one and two dimensions, but there is in three dimensions. Long-range order means that the mean square displacement of an oscillator remains finite as the size of the lattice increases. This fact is related to the probability of return to the origin of a random walk. The question to be discussed here is whether the above facts are a consequence of geometry or whether they depend on the harmonic (i.e. x^2) nature of the potential. In the anharmonic case no explicit solution exists. We show that for a large class of potentials the existence or non-existence of order depends only on dimensionality.

RÉSUMÉ

On sait depuis longtemps que, pour un système d'oscillateurs en interaction harmonique sur un réseau, il existe un ordre macroscopique dans le cas de trois dimensions, mais non dans le cas d'une ou de deux dimensions.

L'existence d'un ordre macroscopique signifie que la moyenne quadratique de l'élongation d'un oscillateur reste finie quand la taille du réseau augmente indéfiniment. Cela est lié à la probabilité pour une marche au hasard de retourner à son point de départ.

La question que nous discutons ici est la suivante: les résultats précédents sont-ils une conséquence de la géométrie, ou dépendent-ils de la nature harmonique (i.e. $\sim x^2$) du potentiel?

Dans le cas d'un potentiel anharmonique, il n'existe pas de solution explicite. Nous montrons que, pour une vaste classe de potentiels, l'existence ou la non-existence d'un ordre macroscopique ne dépend que du nombre de dimensions.