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On Hearing the Shape of a Drum

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ABSTRACT

The problem of determining the shape of a vibrating membrane given all its characteristic frequencies is discussed using a regular array of interacting atoms as a discrete model of a membrane in contrast to the continuum model analyzed recently by Kac. Using elementary methods it is shown how the size, boundary length, and connectivity may be found from the frequencies. The problem is related to the enumeration of closed random walks on a lattice, in analogy with Kac's treatment, and thence to the adjacency matrices of abstract linear graphs.

1. INTRODUCTION

In a delightful lecture entitled "Can You Hear the Shape of a Drum?"[1] Professor Mark Kac recently discussed the problem of determining the shape of a vibrating membrane or "drum skin" from the spectrum of its characteristic frequencies, that is, from a knowledge of the pitch of its fundamental note and all the overtones. To treat this problem mathematically one must formulate the equations governing the motion of the membrane. Kac supposes the membrane is clamped along its

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[1] This lecture was filmed under the auspices of the Committee on Educational Media of the Mathematical Association of America, and an expanded version of the script has been published in *The American Mathematical Monthly*.

boundary I' in the (x, y) plane and that the vertical displacement $\varphi(\mathbf{r}, t)$ of a point $\mathbf{r} \equiv (x, y)$ at time t satisfies the standard wave equation

$$\frac{\partial^2 \varphi}{\partial t^2} = c^2 \nabla^2 \varphi = c^2 \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \right), \tag{1.1}$$

where c^2 depends on the tension and density of the membrane. To each characteristic frequency corresponds a "normal mode" of the system in which every part moves with the same purely harmonic motion so that

$$\varphi(\mathbf{r}, t) = u(\mathbf{r}) \exp(i\omega t). \tag{1.2}$$

By substitution in (1.1) we see that the frequencies are given by

$$\omega_n^2 = 2\, c^2 \lambda_n \tag{1.3}$$

where the λ_n must be determined from the eigenvalue equation

$$\tfrac{1}{2} \nabla^2 u + \lambda u = 0 \qquad \text{for} \qquad \mathbf{r} \text{ in } \Omega \tag{1.4a}$$

which is subject to the boundary condition

$$u(\mathbf{r}) = 0 \qquad \text{for} \qquad \mathbf{r} \text{ on } I'. \tag{1.4b}$$

As is well known, non-trivial solutions of (1.4) are possible only for an infinite sequence of discrete eigenvalues

$$\lambda = \lambda_1 \leq \lambda_2 \leq \lambda_3 \cdots \tag{1.5}$$

Given the spectrum of frequencies λ_n we may calculate the auxiliary generating function

$$G(\tau) = \sum_{n=1}^{\infty} \exp(-\lambda_n \tau), \tag{1.6}$$

the sum being convergent for positive values of the "dummy variable" τ. Now it turns out that the behavior of this function for small τ determines both $|\Omega|$, the area of the membrane, and L, the length of its boundary! This is a consequence of the asymptotic formula

$$G(\tau) \approx \frac{|\Omega|}{2\pi\tau} - \frac{L}{4} \frac{1}{(2\pi\tau)^{1/2}} \qquad (\tau \to 0) \tag{1.7a}$$

which Kac proves in an elegant but sophisticated fashion with the aid

of ideas stemming from the theory of Brownian motion. One can thus certainly tell if the drum skin is circular since the boundary length then (and only then) attains its minimum value $2(\pi|\Omega|)^{1/2}$!

It is possible, however, to go further and to see that the next term appearing in (1.7a) for a drum skin with a *smooth* boundary is the additive constant[2]

$$+\tfrac{1}{6}(C-H), \tag{1.7b}$$

where C is the number of separate *components* of the membrane (our "drum" might really be a family of drums!) and where H is the number of holes in the membrane (the drum is *not* necessarily very musical!). Hence if the drum is known to be all in one piece ($C = 1$) one can also "hear" its connectivity.

At present it is not known how much additional information may be extracted from the spectrum of frequencies nor, indeed, if the frequencies uniquely determine the shape of Ω. Professor Kac believes that one cannot hear the shape in full detail but be is not prepared to bet large sums either way!

A physicist in thinking about this problem will naturally inquire how far the fact that the wave equation (1.1) represents only an idealization of physical reality might affect the answer to the problem or its mode of solution. It must be admitted that the wave equation is a fairly good approximation when the amplitude of vibration is kept low (so that anharmonic effects are unimportant) and when precautions are taken to reduce the damping (for example by vibrating the membrane in vacuo). Evidently, however, it completely neglects the discrete, atomic nature of real materials by assuming implicitly that the membrane is a perfectly uniform two-dimensional continuum. Suppose, on the other hand, we regard a membrane as an array of point masses or "atoms" held in equilibrium by their mutual pairwise interactions. The continuum wave equation (1.1) must then be replaced by the set of equations of motion of the atoms. For small displacements from equilibrium, however, such a system should still display normal modes with characteristic frequencies and we may again ask: "What can be learnt from the spec-

[2] Kac actually discusses only the case of a single component membrane ($C = 1$) with a convex polygonal perimeter and one or more convex polygonal holes. As he observes the result (1.7 b) follows formally by letting the polygons approach smooth curves while the extension to $C > 1$ is obvious from his analysis.

trum about the size and shape of the array?" It is to this question that we shall devote attention.

For simplicity we will consider, in the main, just a single layer of atoms which in equilibrium lie on a regular plane lattice (although even a very thin membrane will, in reality, consist of many interacting and partially irregular layers). Equally it is natural to assume in first approximation that each atom interacts only with its spatially nearest neighbors and that the restoring forces are linearly related to the relative out-of-plane displacements. Although this discrete model of a membrane is still rather far from reality in its details, it should serve to reveal the main effects of the "lumpy nature" of physical matter.

It transpires, as we shall demonstrate, that it is still possible to find the size and boundary length of the membrane (or rather their discrete analogs) and also the connectivity. Furthermore the theory of the discrete model is much simpler than that needed in the continuum case, relying on no more than the elementary properties of finite matrices. Once again the ideas of Brownian motion provide a key to the solution but this time in the conceptually simpler guise of random walks on a lattice. The analysis thus throws light on the more elaborate arguments used with the continuum wave equation and on the possibilities of extending them to three or more dimensions, to calculate higher order terms, and to answer the general uniqueness question.

2. Formulation of the Discrete Problem

To derive the equations of motion of our discrete model of a membrane, we will specify it in more detail as follows. At equilibrium the atoms forming the membrane lie on the sites of a regular two-dimensional lattice of coordination number q, nearest neighbor lattice spacing h and cell area a. We will have in mind mainly the plane square and triangular lattices for which $q = 4$ and 6, respectively, but we may with equal ease consider a general d-dimensional lattice. The N lattice sites occupied by atoms free to move will be called *interior sites* and will be labeled $j = 1, 2 \ldots N$. The *area* of the membrane may now be taken as

$$|\Omega| = Na. \tag{2.1}$$

Nearest neighbor atoms will be regarded as interacting through the

bonds of the lattice. The *boundary* of the membrane will consist of B *perimeter bonds* which connect a free atom to one of its neighboring *boundary atoms* which are clamped to the *boundary sites* labeled $j = N + 1,\ N + 2, \ldots$. The length of the boundary may be written

$$L = Bb, \tag{2.2}$$

where b is the length corresponding to a single perimeter bond. (On the square lattice $b = h$ while on the triangular lattice $b = h/\sqrt{3}$.)

If $\varphi_j(t)$ is the (transverse) displacement at time t of the atom associated with the j-th site, i.e., the j-th atom, the force tending to reduce the relative displacement between this atom and a neighbor $k(j)$ is

$$F_{jk} = -K[\varphi_j(t) - \varphi_k(t)], \tag{2.3}$$

where K is the effective "spring constant." When k denotes a boundary site, we have $\varphi_k(t) = 0$ always. If the mass of an atom is m, the equations of motion are therefore

$$m\frac{d^2\varphi_j}{dt^2} = -K\sum_{k(j)}^{q}(\varphi_j - \varphi_{k(j)}), \tag{2.4}$$

where $j = 1, 2, \ldots, N$ and the sum runs over the nearest neighbors of the lattice site j. We have assumed the atoms obey classical mechanics but quantum mechanics would not change the present problem in a fundamental way. As in the continuum case, the characteristic frequencies of the system are found by trying a pure harmonic solution of the form

$$\varphi_j(t) = u_j \exp(i\omega t) \qquad (j = 1, 2, \ldots, N). \tag{2.5}$$

The frequencies are then

$$\omega_n^2 = (qh^2K/md)\,\lambda_n, \tag{2.6}$$

where d takes the value 2 for a plane lattice but more generally is the dimensionality, and where the λ_n are the eigenvalues of the set of homogeneous equations

$$\tfrac{1}{2}(2d/qh^2)\sum_{k(j)}^{q}(u_{k(j)} - u_j) + \lambda u_j = 0, \tag{2.7a}$$

which are subject to the conditions

$$u_k = 0 \qquad \text{if } k \text{ is a boundary site.} \tag{2.7b}$$

We have written the equations in this form in order to point the analogy with the continuum eigenvalue equation (1.4). By considering the well-known finite difference approximation

$$(\partial^2/\partial x^2)\, u(x, y) \simeq h^{-2}[u(x + h, y) + u(x - h, y) - 2u(x, y)] \tag{2.8}$$

one sees that the first term in (2.7) represents merely the discrete analog of the Laplacian operator $\frac{1}{2}\nabla^2$ acting on the function $u_i \simeq u(\mathbf{r})$

On introducing the column vector

$$\mathbf{u} = [u_i], \qquad i = 1, 2, \ldots, N, \tag{2.9}$$

Eqs. (1.7) may be written compactly as

$$\tfrac{1}{2}\mathbf{L}\mathbf{u} + \mathbf{u} = 0, \tag{2.10}$$

where the $N \times N$ "Laplacian matrix" $\mathbf{L}$ has the elements

$$\begin{aligned} L_{jj} &= -(2d/h^2), \\ L_{jk} &= (2d/qh^2), \text{ if } j \text{ and } k \text{ are nearest neighbors,} \\ &= 0 \text{ otherwise} \quad (j \neq k). \end{aligned} \tag{2.11}$$

Notice that with this definition the boundary conditions (2.7b) are automatically taken into account in (2.10).

The theory may be simplified further by defining the square matrix $\mathbf{T}$ by

$$\begin{aligned} T_{jk} &= 1, \quad \text{if } j \text{ and } k \text{ are nearest neighbors,} \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{2.12}$$

The eigenvalues μ_n and eigenvectors $\mathbf{w}_n$ of this matrix are defined in the standard way as the non-trivial solutions of the equation

$$\mathbf{T}\mathbf{w} = \mu\mathbf{w}. \tag{2.13}$$

By comparison with (2.11) we have

$$\mathbf{L} = (2d/qh^2)\,(\mathbf{T} - q\mathbf{I}), \tag{2.14}$$

where $\mathbf{I}$ is the $N \times N$ unit matrix, so that the eigenvalues and characteristic frequencies are related by

$$\mu_n = q[1 - (h^2/d)\,\lambda_n] \tag{2.15}$$

$$= q - (m/K)\,\omega_n^2. \tag{2.16}$$

Knowledge of the characteristic frequencies thus tells us the eigenvalues of the basic matrix $\mathbf{T}$, which in turn embodies all the available information on the shape of the membrane.

3. Relation to Random Walks

As in the continuum case we may define an auxiliary function in terms of the eigenvalues μ_n. A simple choice, related to (1.6), is

$$M(z) = \sum_n \exp(\mu_n z). \tag{3.1}$$

For small z this has the expansion

$$M(z) = M_0 + M_1(z/1!) + M_2(z^2/2!) + \cdots \tag{3.2}$$

where in general the coefficient of $z^s/s!$ is evidently given by

$$M_s = \sum_n \mu_n{}^s. \tag{3.3}$$

The behavior of $M(z)$ for small z is thus determined by the s-th moments of the set of eigenvalues. (These moments could, of course, be computed directly from the ω_n.)

Now recall (*a*) that the eigenvalues of the s-th power of a matrix are just the s-th powers of the eigenvalues of the matrix itself[3] and (*b*) that the sum of the eigenvalues of a matrix is equal to the trace of the matrix, that is, the sum of its diagonal elements.[4] Combining these two results shows that

$$M_s = \mathrm{Tr}\,\{\mathbf{T}^s\} = \sum_{j=1}^{N} (\mathbf{T}^s)_{jj}\,. \tag{3.5}$$

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[3] This follows by iterating the defining equation $\mathbf{T}\mathbf{w}_n = \mu_n \mathbf{w}_n$.

[4] It is easily shown that the trace $\mathrm{Tr}\{A\} = \sum_{j=1}^{N} A_{jj}$ of a matrix $\mathbf{A}$ is invariant under the similarity transform $\mathbf{A}' = \mathbf{S}\mathbf{A}\mathbf{S}^{-1}$. On choosing $\mathbf{S}$ to diagonalize $\mathbf{A}'$ the A'_{jj} becomes the eigenvalues, thereby proving the result.

Our task is hence reduced to studying the traces of the powers of the "shape matrix" **T**. To do this in an elementary way we introduce another, and at first sight, unrelated problem.

Consider a walker (traditionally a drunken man!) who walks at random on sites $j = 1, 2, ..., N$ of the lattice, always taking a step from a site to one of its nearest neighbors. If the walker starts off from an interior site j, how many different paths may he follow which will bring him to site k on his m-th step? In counting the number of such paths, say $p_m(j \to k)$, we will suppose that, when the walker steps along a perimeter bond from an interior site to a boundary site, he "falls off" the lattice and does not return! Such paths must therefore be excluded.

To obtain a formula for the number of possible paths note first that before he takes any steps the walker is sure to be at site j. This may be expressed by

$$\begin{aligned} p_0(j \to k) = \delta_{jk} &= 1 \text{ if } j = k = 1, 2, ..., N, \\ &= 0 \text{ if } j \neq k. \end{aligned} \tag{3.6}$$

Next suppose we know the complete distribution of paths of m steps but wish to determine the number of paths leading to site l in $m + 1$ steps. To reach this site on his $(m + 1)$-th step the walker must have been at one of the neighboring sites $k(l)$ on his previous steps. The number of paths thus satisfies the recurrence relation

$$p_{m+1}(j \to l) = \sum_{k(l)}^{q} p_m(j \to k(l)), \tag{3.7}$$

where the sum runs over the q neighbors of site l unless, of course, one of these is a boundary site from which the walker cannot return.

To solve this recurrence relation a matrix notation is perspicuous. On defining an $N \times N$ matrix $\mathbf{P}_m$ with elements

$$(\mathbf{P}_m)_{kj} = p_m(j \to k) \tag{3.8}$$

we may rewrite (3.6) and (3.7) as

$$\mathbf{P}_0 = \mathbf{I} \tag{3.9}$$

and

$$\mathbf{P}_{m+1} = \mathbf{T}\mathbf{P}_m, \tag{3.10}$$

where the "transition matrix" **T** is just the same as the "shape matrix"

defined previously in (2.12)! Iterating (3.10) and using (3.9) yields the complete solution to our random walk problem, namely,

$$\mathbf{P}_m = \mathbf{T}^m\mathbf{I} = \mathbf{T}^m. \tag{3.11}$$

Conversely we may use the definition of $\mathbf{P}_m$ to rewrite this result as

$$(\mathbf{T}^m)_{jj} = p_m\,(j \to j) \tag{3.12}$$

so that, in words, the j-th diagonal element of $\mathbf{T}^m$ is just the number of possible paths that leave the interior site j but return to it on the m-th step without being lost over the boundary. By (3.5) the moments may hence be expressed as

M_s = total number of paths of s steps which end on their starting points and never leave the interior sites. (3.13)

As we will now show, this result enables us to relate the moments in a simple way to the area, boundary length, and various topological and shape-dependent features of the array of sites which represents the membrane.

4. Evaluation of the Moments

We will utilize the relation (3.13) by enumerating directly the number of closed paths. Consider the zeroth moment M_0. This is equal to the number of paths with no steps; but by the convention (3.6) there is just one such "path" for every interior site and so

$$M_0 = N. \tag{4.1}$$

Consequently the *area of the membrane* is determined immediately by

$$|\,\Omega\,| = M_0 a. \tag{4.2}$$

The value of M_0 may also be found directly from the definition (3.3), since $\mu_h{}^0 \equiv 1$ so that M_0 is also the *number* of eigenvalues or characteristic frequencies. This in turn is equal to the number of degrees of freedom of the membrane which must clearly be N.

There can be no closed walks consisting of just one step, since a single step carries the walker away from his starting point, and so

$$M_1 = 0. \tag{4.3}$$

With two steps the only paths which return are those consisting of a step followed by its *immediate reversal.* From each interior site of the lattice there are $r_2 = q$ such paths making a total of qN, but precisely one of these walks sets out along each perimeter bond and is thus lost! Consequently we have

$$M_2 = qN - B, \tag{4.4}$$

which determines the *length of the boundary* as

$$L = (qM_0 - M_2)b. \tag{4.5}$$

Thus the two leading moments formed from the characteristic frequencies determine the area and the boundary length. In analogy with the continuum formula (1.7a) we might write, from (3.1), (3.2), and (2.16),

$$\begin{aligned} M(z) &= \sum_n \exp\{[q - (m/K)\,\omega_n^2]z\} \\ &= |\Omega|/a + \tfrac{1}{2}[(q|\Omega|/a) - (L/b)]\,z^2 + O(z^3). \end{aligned} \tag{4.6}$$

Whereas in the continuum case we can tell from a knowledge of $|\Omega|$ and L whether the membrane is circular or not, the analogous statement here depends on the lattice structure. Thus, if on the square lattice it is found that $N = n^2$ while $B = 4n$ for some integral n, the membrane must be a perfect square. Similarly, on the triangular lattice it will be a perfect hexagon if and only if $N = 3n(n-1) + 1$ and $B = 6(2n-1)$. At other extreme of shape we can conclude that the atoms are connected in the form of a "Cayley tree" (with no closed circuits of bonds) if $B = (q-2)N + 2$ and we know there is only one connected component: such a "membrane" would, of course, hardly resemble a drum skin!

To derive the higher moments it is convenient to let r_s denote the number of s-step returns when all sites are interior sites. Then we can write

$$M_s = Nr_s - L_{s1} - L_{s2} - \cdots - L_{ss} \tag{4.7}$$

where L_{st} is the total number of the possible s-step closed walks which are lost by passing across a perimeter bond on the t-th step. We see at once that a walk cannot be lost on its last step since it would have to depart from a boundary site which could have been reached only by

crossing a perimeter bond at an earlier stage. Consequently we have

$$L_{ss} = 0. \tag{4.8}$$

On the other hand, as we have seen, a walk can be lost on its first step if its origin is adjacent to a boundary site. The fraction of the r_s possible returns which leave a site along any particular bond is $1/q$ and so for all s

$$L_{s1} = B(r_s/q). \tag{4.9}$$

To complete the derivation of the third moment we only need L_{32}, the number of walks lost on the second step that would have returned on the third step. Such a walk must form a triangle with one vertex on a boundary site and two vertices on adjacent interior sites. Each such "A-triangle" contains two perimeter bonds and hence corresponds to two lost walks (tracing the triangle in opposite senses). If A is the total number of A-triangles we therefore have $L_{3,2} = 2A$ and

$$M_3 = r_3 N - (r_3/q)B - 2A. \tag{4.10}$$

This result may be simplified further by considering specific lattices. On the plane square lattice there are no triangles and hence A, r_3, and M_3 all vanish (as do the higher order odd moments). More interesting is the plane triangular lattice for which

$$q = 6, \quad r_3 = 12 \qquad \text{(triangular lattice)}. \tag{4.11}$$

In this case, as may be seen by inspecting the simple example in Figure 1,

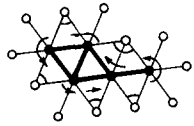

FIG. 1. A configuration of atoms on the triangular lattice with $N = 5$, $B = 18$, and $A = 6$. Interior atoms and bonds are shown by solid circles and heavy lines, boundary atoms and perimeter bonds by open circles and light lines. An angle of each A-triangle has been marked.

each A-triangle defines an *edge bond* connecting its two interior sites. If the edge bonds are traced in sequence, say in an anti-clockwize sense, the number of edge sites passed is equal to A. (Note that a particular

lattice site may be encountered two or even three times as the *edge* is traversed, but each passing is counted separately. An example of such a doubled edge site occurs at the base of the "spike" in Figure 1.) Suppose the edge sites are labeled $\alpha = 1, 2, 3, \ldots, A$ and b_α is the number of perimeter bonds meeting the corresponding site. Evidently we have[5]

$$\sum_{\alpha=1}^{A} b_\alpha = B. \tag{4.12}$$

Notice now that as the edge passes the site α its direction is turned toward the interior through an angle

$$\delta\theta_\alpha = (b_\alpha - 2)(\pi/3). \tag{4.13}$$

This relation between b_α and $\delta\theta_\alpha$ may be checked in Figure 1, where all the possibilities for b_α occur.[5] Summing (4.13) over α yields

$$B - 2A = (3/\pi)\,\Delta\theta, \tag{4.14}$$

where $\Delta\theta$ is the total rotation of the edge or, equally, of the boundary itself. But on tracing the boundary of any simply connected finite region of the plane the total rotation is simply 2π. Thus each separate connected component of the membrane contributes 2π to $\Delta\theta$. Conversely the boundary of any hole contributes a rotation of 2π in the *opposite* sense. Thus, if C is the number of components and H the total number of holes, we have

$$\Delta\theta = 2\pi(C - H) \tag{4.15}$$

so that

$$B - 2A = 6(C - H). \tag{4.16}$$

(This may be checked in Figure 1.)

Combining these results with (4.10) yields

$$M_3^{\text{triangular}} = 12N - 3B + 6(C - H), \tag{4.17}$$

which gives the next term in (4.6). Finally the net connectivity is determined from the first three moments by

[5] Notice that in the case of doubled or trebled edge sites b_α includes only those bonds crossed as the boundary passes the site.

$$C - H = \tfrac{1}{6} M_3 - \tfrac{1}{2} M_2 + M_0 \quad \text{(triangular lattice).} \quad (4.18)$$

Thus we have demonstrated that the information about the shape which can be extracted from the three leading terms of the generating function (1.6) for a continuum membrane model can also be found and, indeed, in a simpler way from the corresponding terms for the discrete model.

5. Further Questions

It is natural to ask whether in the case of a *three*-dimensional lattice containing triangles, such as the face-centered cubic lattice, it is also possible to distinguish the topological features with a knowledge of the third moment. Formula (4.10) remains valid but it does not seem possible to express the number A simply in terms of, for example, the solid angle swept out by a normal to the "surface" of what is now a "crystal" rather than a "membrane." The difficulty may be seen, in the case of the f.c.c. lattice, by contrasting "flat" surfaces parallel to the hexagonal and to the square lattice planes, respectively.

The result (4.17) applies only to the triangular lattice. Can the net connectivity $(C - H)$ be determined from the fourth moment of the square lattice? Similarly, what extra information, if any, can be found from the fourth moment of the triangular lattice? To answer these questions we need general expressions for $L_{4,2}$ and $L_{4,3}$, the number of four-step closed walks lost on their second and third steps. By the same kind of elementary reasoning used before we find

$$L_{4,2} = \sum_{\beta=1}^{B} (c_\beta + d_\beta),$$

$$L_{4,3} = 2S + \sum_{\beta=1}^{B} c_\beta, \quad (5.1)$$

where β labels the perimeter bonds, c_β is the number of interior bonds meeting the bond β, d_β is the number of squares passing through the bond β with at least two vertices on interior sites, and S is the total number of squares with one vertex on a boundary site and three on interior sites. (Compare with the definition of an A-triangle.)

To obtain reasonably simple results it now becomes necessary to impose certain *smoothness conditions* on the boundary of the mem-

brane. (Similar sorts of conditions are in fact needed for the continuum model.) In the case of the square net we suppose there are no isolated sites and no spikes or chains of single bonds. If such "fur" is clipped off we find, by examining the various possible different configurations of an edge site,[6] that

$$M_{\frac{1}{4}}^{\text{square}} = 36N - 14B - 16(C - H) - 2S \tag{5.2}$$

Consequently it is *not* possible to determine the net connectivity unless S is known. Inspection of examples shows that S is essentially a total "surface roughness" or "concavity" parameter which remains zero if the boundary runs parallel to the lattice axes but reaches large values when the boundary runs in staircase fashion at appreciable angles to the axes. If the boundaries of all holes and connected components are rectangular, however, $S = 4H$ and the combination $(2C - H)$ may be found.

For the triangular lattice the situation is not dissimilar in that only certain combinations of surface curvature parameters can be determined. Once again we suppose there are no isolated sites, chains, or pendant bonds. There are then six possible configurations for an interior site and its first neighbor shell which are illustrated in Figure 2.

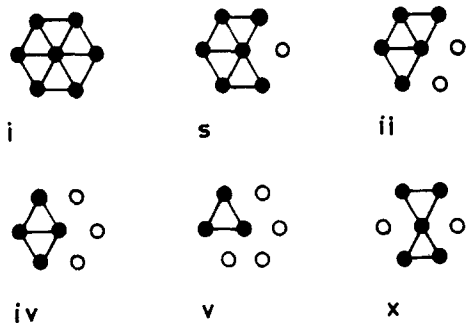

FIG. 2. Possible configurations of an interior atom and its six neighboring sites on the triangular lattice when isolated sites, pendant bonds, and chains are excluded,

Notice that the configuration (x) corresponds to the "crossing" of two boundaries, while (v) represents a sharp point of the boundary and

[6] There are essentially only three configurations.

(s) is associated with a S-square containing three *edge* sites. If the overall numbers of these configurations are X, V, and S respectively, we find

$$M_4^{\text{triangular}} = 90N - 27B + 60(C - H) + 4(X + V + S). \quad (5.3)$$

The information gained from the fourth moment is thus somewhat involved unless the boundaries are not allowed to turn sharply so that configurations (x) and (v) are forbidden. In that case one may determine the parameter S, which has much the same significance as on the square net (where, however, it could not be resolved from $(C - H)$ if only the fourth moment was known).

Since the analysis of the discrete model is so straightforward and elementary one might wonder whether the basic asymptotic formula (1.7) for the continuum case could not be derived, at least formally, merely by letting the lattice spacing h approach zero. The finite differecne approximation (2.8) then becomes exact. In fact it is quite easy to check for special shapes that the n-th characteristic frequency $\omega_n(h)$ of the discrete system approaches the n-th frequency ω_n of the continuous system in the limit $h \to 0$ while $N \to \infty$ so that $|\Omega|$, being proportional to Nh^2, remains constant. Physically this is not surprising and should hold for fairly arbitrary shapes. By comparing (1.6), (2.15), and (3.1) we thus see that one might hope to prove

$$\lim_{h \to 0} e^{-(d/h^2)\tau} M\left[\tau\left(\frac{d}{h^2 q}\right)\right] = G(\tau) \quad (5.4)$$

$$\approx \frac{|\Omega|}{2\pi\tau} - \frac{L}{4(2\pi\tau)^{1/2}} + \frac{1}{6}(C - H).$$

The difficulty in carrying this program through stems, however, from the fact that as $h \to 0$ the number of atoms N and of perimeter bonds B must become infinite. Consequently the moments M_s themselves diverge and the simple expansion (3.2) for $M(z)$ loses its meaning! An indication of this is the appearance in (5.4) of negative and fractional powers of τ, whereas (3.1) contains only positive integral powers of z. To take the limit $h \to 0$ it is, in fact, necessary to know the contributions made by N and B to the moments of *all* orders and hence to study returning paths of indefinitely many steps. This may be seen clearly if we rewrite the result for the triangular lattice in the form required in (5.4) as

$$e^{-qz}M(z) = Ne^{-qz}\left[1 - r_2\frac{z^2}{2!} + r_3\frac{z^3}{3!} - r_4\frac{z^4}{4!} + \cdots\right]$$
$$- B^{-qz}\left[\frac{z^2}{2!} + 3\frac{z^3}{3!} - 27\frac{z^4}{4!} - \cdots\right]$$
$$+ (C - H)\,e^{-qz}\left[6\frac{z^3}{3!} + 60\frac{z^4}{4!} + \cdots\right]$$
$$+ (X - V + S)\,e^{-qz}\left[4\frac{z^4}{4!} + \cdots\right]$$
$$+ \cdots \qquad (5.5)$$

With a little labor one may prove that the first line in (5.5) does yield the term proportional to $|\Omega|$ in (5.4) in the limit $h \to 0$. The divergence as τ approaches zero is found to be determined only by the behavior of r_s for *large* s.[7] The analysis of the term proportional to B is, however, much more involved and one soon concludes that Kac's method, which uses the continuum model at the outset (and considers a continuous diffusion process or Brownian motion in place of discrete random walks), is much to be preferred!

6. Relation to Graph Theory

Finally we may ask: Does the discrete model throw any light on the uniqueness of the frequency spectrum for a given shape, that is, for a given configuration of atoms on the lattice? This problem falls into two parts since on the one hand it is clear that the spectrum of N eigenvalues cannot possibly do more than determine the positions of the "ones" and "zeros" in the shape matrix **T**, while on the other hand this is not necessarily sufficient to determine the lattice configuration.

Fundamentally the matrix **T** is best regarded as the *adjacency matrix* of the *abstract linear graph* underlying the configuration of interior atoms

[7] It may be shown generally for two-dimensional walks that $r_s \approx Dq^s/(s-1)$ as $s \to \infty$ where D is a constant. Consequently the first term in (5.5) is approximately $DNe^{-qz}\,\Sigma_s(qz)^s/(s+1)!$ which for large z approximates.

$$DNe^{-qz}(e^{-qz} - 1)/qz \simeq DNh^2/d\tau = D'|\Omega|/\tau$$

as required by (5.4).

and bonds. Thus with each of the N interior atoms or lattice sites we associate an abstract *point* (or vertex) while each bond joining adjacent atoms or sites is associated with a *line* (or edge) of the graph incident with the corresponding points. Two graphs are considered to be the same (isomorphic) if they differ only by a permutation of the labels of the points. The elements T_{jk} of the adjacency matrix of a graph are unity if there is a (single) edge (j, k) between the point j and k but zero if there is no edge. Now the set of eigenvalues of a matrix is unchanged by permutations of the row and column labels. Consequently the eigenvalues of the adjacency matrix are an intrinsic property of the graph.

Even after allowing for permutations of the labels of the atoms, however, it is obvious that the underlying graph need *not* specify the lattice configuration fully. We may say that there are various different *embeddings* of the graph in the lattice.[8] Thus it is clear that $\mathbf{T}$ yields no information on the relative separations and orientations of different components of a disconnected configuration. Equally the reflection or rotation of parts of a connected component about an *articulation* (or cutting) point of the graph, as illustrated in Figure 3, cannot be dis-

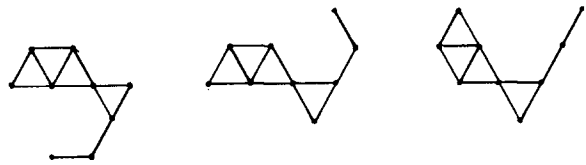

FIG. 3. Various configurations on the triangular lattice corresponding to the same underlying linear graph.

tinguished. Less obviously certain *articulation pairs* of points may form a "pivot" allowing a partial inversion of the configuration but leaving $\mathbf{T}$ invariant, as shown in Figure 4. Such relatively trivial ambiguities might well be ignored. Alternatively they may be excluded by disallowing pendant bonds and (x)-type configurations (see Figure 2), which correspond to the crossing of boundary curves. With

[8] It is necessary here to consider *strong* embeddings in which points placed on adjacent lattice sites must always be incident on an edge corresponding to the lattice bond.

these latter restrictions it seems quite probable that the matrix of a configuration specifies it essentially uniquely.

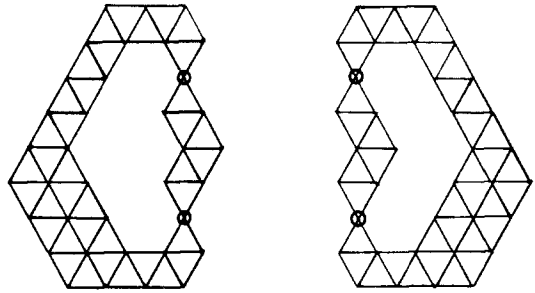

FIG. 4. Two distinct configurations with the same underlying graph illustrating a "pivot" formed by an articulation pair.

The more difficult part of our problem may be rephrased by asking if there exist two $N \times N$ symmetric matrices of zeros and ones which have the same eigenvalues but correspond to different graphs. We also wish to impose the further conditions (*a*) that there be no points of degree one (and hence no pendant bonds), and, for two-dimensional membranes, (*b*) that the graphs be planar, and (*c*) that they can be embedded in the triangular (or other) lattice[8] using only the "contiguous" configurations (i), (s), (ii), (iv), and (v) of Figure 2 (i.e., excluding the crossing configuration).

By our relation (3.13) the identity of the first three eigenvalue moments M_s of two graphs implies immediately that they must contain the same number of points, lines, and triangles (that is subgraphs isomorphic to a triangle). With the aid of a systematic list of graphs[9] one may examine the possible returns in three and more steps and check that *all* connected graphs of six or fewer points satisfying condition (*a*), are in fact uniquely determined by their eigenvalue spectra. It is tempting to conjecture that this will hold for all N. Such a conjecture, however, is false! Thus in Figure 5 two graphs are exhibited[10] for

[9] See, for example, the article by G. E. Uhlenbeck and G. W. Ford in *Studies in Statistical Mechanics* I, North-Holland, Amsterdam, 1962, edited by J. De Boer and G. E. Uhlenbeck. Note the first graph of six points and seven lines in this list is drawn incorrectly with one line too many.

[10] It might be mentioned that the clue leading to the discovery of these two graphs was the interesting (and related) fact that the number of n-step returns to the origin

which the eigenvalues of the adjacency matrices are in both cases given by the $5n$ roots of the equation

$$(\lambda^2 - \Theta\lambda - 1)(\lambda^3 - 2\Theta\lambda^2 - 5\lambda + \Theta\lambda + \Theta) = 0$$

with

$$\Theta = 2\cos(2\pi r/n), \qquad r = 1, 2, \ldots, n, \tag{6.1}$$

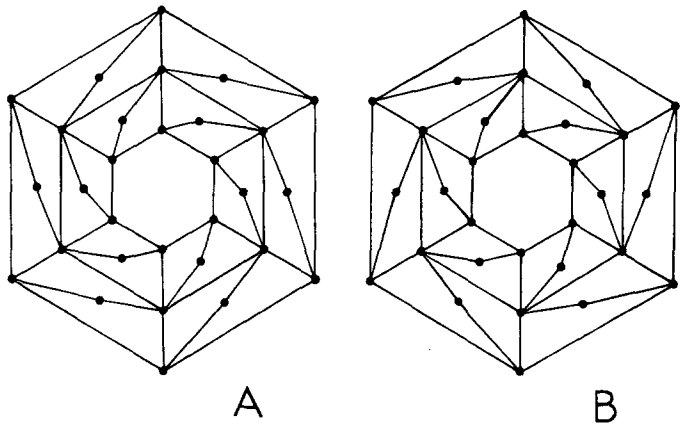

FIG. 5. Two distinct graphs whose adjacency matrices have the same set of eigenvalues.

where, for the case illustrated, $n = 6$. The smallest graphs of this general form have threefold ($n = 3$) rather than sixfold symmetry and hence have only fifteen points.[11] They are equally good counterexamples to

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of the face-centered cubic lattice is the same for all n as on the close-packed hexagonal lattice. This has been proved by M. F. Sykes and M. E. Fisher; see C. Domb, *Advances in Phys.* **9**, No. 34 (1960), 315–317.

[11] Other counterexamples have been given in the literature. Professor Frank Harary has kindly told me of the work of L. Collatz and U. Sinogowitz, *Abh. Math. Sem. Univ. Hamburg* **21** (1957) 63, who list two nonisomorphic trees, not therefore satisfiying condition (*a*), which have the same spectrum. (These trees have eight points and may be specified by the lines (1, 2) (2, 3) (3, 4) (4, 5) (4, 6) (4, 7) (4, 8) and (1,4) (2, 4) (3, 4), (4, 5) (5,6) (5, 7) (5, 8) and their characteristic equation is $\lambda^4(\lambda^4 - 7\lambda^2 + 9) = 0$.) In his paper, *SIAM Rev.* **4** (1962), 202, Harary mentions other known pairs of graphs each with 16 points. He asks what is the smallest number of points that such pairs must have and suggests the answer might be 16. Our examples, however, show this cannot be so. Indeed, if the graphs are allowed to have double lines (i.e., two bonds between the same pair of points) we may construct an example with only 9 points.

the conjecture but their representations in the plane are less easy to disentangle at first glance.

The two graphs (*A*) and (*B*) do appear rather similar and indeed they become identical, although differently drawn, if the twelve points of coordination number two are removed from the (diagonal) lines upon which they sit. It is thus perhaps not so surprising that they "sound identical." To prove that the graphs really are distinct, note that graph (*A*) has subgraphs of the type shown in Figure 6 while graph (B) has none.

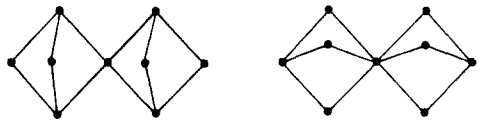

FIG. 6. Two graphs which are subgraphs of (A) in Figure 5 but not of (B).

These counterexamples also satisfy conditions (*a*) and (*b*) in that they are evidently planar and without pendant bonds. They are not embeddable in the triangular lattice (as may be proved by considering the points of sixfold coordination[8]) but they could clearly be embedded in a sufficiently complex regular plane lattice. It is not implausible, however, that examples could be devised along these lines which were embeddable in the triangular lattice. On the other hand, the final condition of (*c*) forbidding (x) or boundary-crossing configurations, looks as if it might then be a more severe obstacle to the construction of counterexamples. One may hope, however, that such graphs, if they exist, will come to light in the not-so-distant future since the increasing interest in the applications of linear graphs is leading to the extensive tabulation and

It is obtained from the analogs of Figure 5 with $n = 3$ by replacing each site of coordination number two and its two incident lines by a double line between the same terminal points. *Note added in proof*: More recently Dr. G. A. Baker kindly pointed out two connected graphs of 6 points and 7 lines with identical spectra [although not both satisfying condition (*a*)] whose identity was missed in the original check of the author. Baker (to be published) has also found simpler examples of graphs with the same spectra that satisfy both conditions (*a*) and (*b*). Professor P. W. Kasteleyn has observed that, if multiple lines of higher order, or loops and/or disconnected graphs are allowed, then counterexamples with very few points exist.

classification of their properties.[9,12] If a counterexample can be found satisfying all the conditions it would be strong presumptive evidence that one cannot always hear the shape of drum!

ACKNOWLEDGMENT

It is a pleasure to acknowledge the stimulation received in conversation and correspondence with Professor Mark Kac. I am most grateful to Professor Frank Harary, Dr. G. A. Baker, Jr., and Professor P. W. Kasteleyn for correspondence and comments on the spectra of graphs.

[12] See, for examples of applications in statistical mechanics, W. G. Hoover and A. G. De Rocco, *J. Chem. Phys.* **36** (1962), 3141, and M. F. Sykes, J. W. Essam, B. R. Heap, and B. J. Hiley, Lattice Constant Systems in Crystal Statistics, *J. Math. Phys.* **7** (1966), in press, and, more generally, C. Berge, *The Theory of Graphs and Its Applications*, Methuen, London, 1962.