Quasiperiodic lattice: Electronic properties, phonon properties, and diffusion

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Results of a renormalization-group analysis augmented by numerical calculations are presented for the electronic and phonon properties of a one-dimensional quasiperiodic lattice. Qualitative differences in the electronic and phonon band structure are predicted analytically and confirmed numerically. An exactly evaluated wave function shows a power-law behavior. Results of a calculation of the diffusion coefficient are also presented.

Following the recent experimental discovery of the quasicrystal phase in metallic alloys,[1] there has been a regeneration of interest in the studies of the physical properties of quasiperiodic systems in one dimension.[2] Even more recently, Merlin *et al.*[3] have succeeded in growing a realization of a quasiperiodic superlattice and have carried out x-ray and raman scattering measurements on it.

In this paper we study the electronic and the phonon problem on a one-dimensional lattice which consists of two types of bonds, A and B. More specifically, the distribution of A and B follows the Fibonacci sequence S_∞ which is constructed recursively as $S_{l+1}=\{S_l,S_{l-1}\}$ with $S_1=\{A\}$ and $S_2=\{A,B\}$. A key result of our analysis is that while we can map one problem onto the other in a straightforward way, the scaling index (to be defined later) for the phonon spectrum depends on the frequency ω, whereas it is independent of the energy E in the electronic problem. This leads to qualitative differences in the two band structures—a result we have confirmed by numerical analysis (Fig. 1). The wave function (normal mode) for a special energy $E(\omega)$ is obtained exactly, and it is shown to be self-similar and therefore intermediate between a localized and extended state (Fig. 2). We calculate the scaling behavior of the density of states for phonons in the $\omega\to 0$ limit and show that the Fibonacci lattice may be characterized by a spectral dimension (d_s) of 1 and a random-walk dimension (d_w) of 2. Results of a calculation of the diffusion coefficient are also presented (Fig. 3).

I. ELECTRONIC AND PHONON SPECTRA

Consider the tight-binding model for the electronic problem

$$t_{n+1}\psi_{n+1}+t_n\psi_{n-1}=E\psi_n \ , \tag{1}$$

where ψ_n denotes the wave function at the nth site and $\{t_i\}$ is the Fibonacci sequence with two kinds of hopping matrix elements t_A and t_B. The phonon problem, on the other hand, is described by an equation of motion

$$-\omega^2\psi_n=K_{n+1}\psi_{n+1}+K_n\psi_{n-1}-(K_{n+1}+K_n)\psi_n \ , \tag{2}$$

where ψ_n now denotes the displacement from its equilibrium position of the nth atom and the K's form a Fibonacci sequence with two kinds of spring constants K_A and K_B. Kohmoto, Kadanoff, and Tang[4] (and also, independently, Ostlund *et al.*[5]) have studied a similar electronic problem: $\psi_{n+1}+\psi_{n-1}+V_n\psi_n=E\psi_n$, where the V_n's follow a Fibonacci sequence. The method of Kohmoto *et al.* is used to study the present problems with some modification.

The tight-binding model (1) may be written in the form $\boldsymbol{\psi}_{n+1}=\underline{M}(t_{n+1},t_n)\boldsymbol{\psi}_n$, where $\boldsymbol{\psi}_n$ is a column vector

$$\begin{bmatrix}\psi_n\\ \psi_{n-1}\end{bmatrix}$$

and $\underline{M}(t_i,t_j)$ is a transfer matrix given by

$$\underline{M}(t_i,t_j)=\begin{bmatrix}E/t_i & -t_j/t_i\\ 1 & 0\end{bmatrix} .$$

For the phonon problem, one simply makes the replacements $t_i\to K_i$ and $E\to -\omega^2+K_i+K_j$, i.e.,

$$\underline{M}(K_i,K_j)=-\begin{bmatrix}(-\omega^2+K_i+K_j)/K_i & -K_j/K_i\\ 1 & 0\end{bmatrix} .$$

The solution to (1) [or (2)] may be written, using products of the matrices, as $\boldsymbol{\psi}_{n+1}=\underline{M}(n)\boldsymbol{\psi}_1$ where

$$\underline{M}(n)=\underline{M}(t_{n+1},t_n)\underline{M}(t_n,t_{n-1})\cdots\underline{M}(t_2,t_1) \ .$$

The key problem is therefore to calculate this transfer matrix $\underline{M}(n)$. The Fibonacci lattice permits an extremely effective method for doing this. The Fibonacci numbers are given by $F_{l+1}=F_{l-1}+F_l$ with $F_0=F_1=1$. When n is a Fibonacci number, $\underline{M}(n)$ can be obtained recursively. Define $\underline{M}_l\equiv\underline{M}(F_l)$, then

$$\underline{M}_{l+1}=\underline{M}_{l-1}\underline{M}_l \ , \tag{3}$$

with $\underline{M}_1=\underline{M}(t_A,t_A)$ and $\underline{M}_2=\underline{M}(t_A,t_B)\underline{M}(t_B,t_A)$. The transfer matrix for a general value of n is given by

$$\underline{M}(n)=\underline{M}_{l_i}\cdots\underline{M}_{l_2}\underline{M}_{l_1} \ , \tag{4}$$

where $n=F_{l_1}+F_{l_2}+\cdots+F_{l_i}$ and $l_1>l_2>\cdots>l_i$.

The recursion relation (3) gives a powerful calculational scheme. However, the essential importance rather lies in the fact that it defines a nonlinear dynamical map and we can therefore use theories and concepts of dynamical systems.[6]

Defining $x_l = \frac{1}{2}\,\mathrm{tr}\underline{M}_l$, one can show that

$$x_{l+1} = 2x_l x_{l-1} - x_{l-2}\ , \tag{5}$$

which leads to the result that on successive iterations the quantity

$$I = x_{l+1}^2 + x_l^2 + x_{l-1}^2 - 2x_{l+1}x_l x_{l-1} - 1$$

is a constant of the motion (i.e., independent of l). It has been shown by Kohmoto and Oono[6] that the map given by (5) yields to a fixed-point analysis. A scaling index α for three iterations was found to be given by

$$\alpha = [1 + 4(1+I)^2]^{1/2} + 2(1+I)\ . \tag{6}$$

Physically, α denotes the scaling index for the self-similar band structure.[7] Also, the quantity I determines the size of the band gaps—a large I implies large gaps and $I \to 0$ implies a vanishing gap.

The key difference between the electronic and phonon problems arises in the expressions for I:

$$I_{\mathrm{el}} = \frac{1}{4}\left[\frac{t_B}{t_A} - \frac{t_A}{t_B}\right]^2\ , \tag{7}$$

and

$$I_{\mathrm{ph}} = \frac{\omega^4}{4}\left[\frac{1}{K_B} - \frac{1}{K_A}\right]^2\ . \tag{8}$$

The important point is that α depends on ω for the phonon case, while it is independent of E for the electronic case. This leads to qualitative differences in the band structure which are best seen in the numerical results shown in Fig. 1. In the electronic case, there is uniform scaling, whereas in the phonon case, at low values of ω, there are large bands and small gaps while for higher values of ω the bands are very narrow.

The phonon problem with the spring constants uniform and the masses in a Fibonacci sequence is dual to the phonon problem discussed above, and has a very similar band structure.

It can be shown for both electronic and phonon problems that the gaps are distributed densely and there are no isolated states such as states in a gap.[8] Sets of this kind are called Cantor sets.

II. SELF-SIMILAR WAVE FUNCTION

We consider the electronic problem at the center of the spectrum, $E=0$. This value of E actually is in the spectrum, and we can exactly evaluate the wave function for this special value of the energy. The mapping (3) for $E=0$ gives the six cycle:

$$\underline{M}_1 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},\quad \underline{M}_2 = \begin{bmatrix} -R & 0 \\ 0 & -1/R \end{bmatrix},$$

$$\underline{M}_3 = \begin{bmatrix} 0 & 1/R \\ -R & 0 \end{bmatrix},\quad \underline{M}_4 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

$$\underline{M}_5 = \begin{bmatrix} 1/R & 0 \\ 0 & R \end{bmatrix},\quad \underline{M}_6 = \begin{bmatrix} 0 & -R \\ 1/R & 0 \end{bmatrix}$$

and $\underline{M}_{l+6} = \underline{M}_l$, where $R = t_B/t_A$. Figure 2 shows a plot of the modulus of ψ_n versus the site label n along the chain for $R=2$. There are a series of peaks which have values of a power of R. These peaks correspond to the transfer matrix (4) which have eigenvalues R^p. First note that

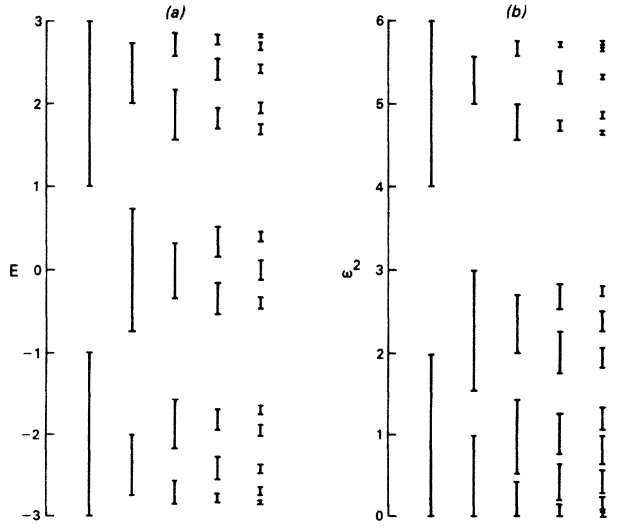

FIG. 1. (a) The allowed energies for the electronic problem for $t_A = 1.0$ and $t_B = 2.0$. (b) The allowed ω^2 for the vibrational problem for $K_A = 1.0$ and $K_B = 2.0$. The band structures for $l = 2$, 3, 4, 5, and 6 are shown.

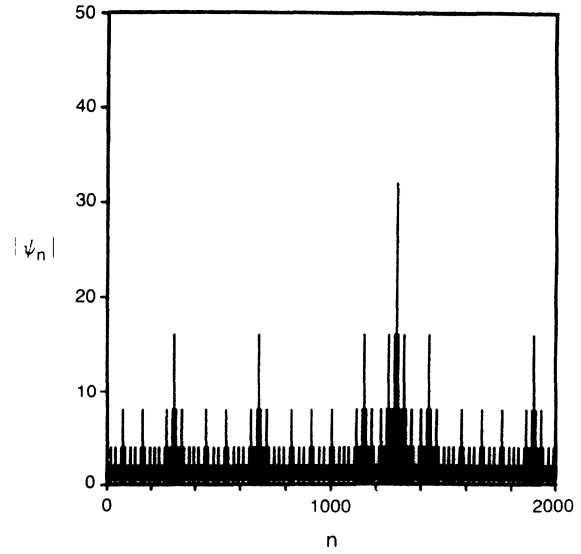

FIG. 2. The self-similar electronic wave function at $E=0$ for $R = t_B/t_A = 2.0$. The figure is a plot of $|\psi|$ versus the site number along the quasiperiodic lattice.

$$\underline{M}_3\underline{M}_6=\begin{bmatrix}1/R^2 & 0\\ 0 & R^2\end{bmatrix}$$

and $\underline{M}_{l+6}=\underline{M}_l$. From this, the transfer matrix

$$\underline{M}(n)=\underline{M}_3\underline{M}_6\cdots\underline{M}_{3\times 2p}$$

with an eigenvalue R^{2p} is constructed where p is an integer. Therefore, there are a series of peaks

$$\psi_n=R^{2p}\psi_0\ , \tag{9}$$

with

$$n=F_3+F_6+F_9+F_{12}+\cdots+F_{3\times 2p}\ .$$

There is another series of the transfer matrices:

$$\underline{M}(n)=\underline{M}_2\underline{M}_6\underline{M}_9\underline{M}_{12}\underline{M}_{15}\cdots\underline{M}_{3\times(2p+1)}\ ,$$

which gives the peaks

$$\psi_n=-R^{2p+1}\psi_1\ , \tag{10}$$

with

$$n=1+F_2+F_6+\cdots+F_{3\times(2p+1)}\ ,$$

and

$$p=1,2,3,\ldots\ .$$

The two series of peaks (9) and (10) give the fundamental structure of the wave function. They are the peaks of order of magnitude R^p which are encountered sequentially as n is increased. The self-similarity of this wave function can be described precisely as follows: take $|\psi_0|=|\psi_1|=1$, for example. Then the modulus of the wave function is invariant under the scale transformation of $n\rightarrow n/\sigma_G^3$ and $|\psi|\rightarrow|\psi|/R$ (if $|\psi|>1$) or $|\psi|\rightarrow R|\psi|$ (if $|\psi|<1$), where σ_G is the golden mean $(\sqrt{5}+1)/2$.

These rescaling parameters σ_G^3 and R are related to the power-law behavior of the peaks (9) and (10):

$$\psi_n\sim n^{\beta}\ ,\qquad \beta=\ln R/\ln\sigma_G^3\ . \tag{11}$$

Although we have the exact wave function only at the special energy $E=0$, there are many other energies at which the wave functions behave similarly. Those energies are at the centers of the clusters. The corresponding orbits for the mapping (3) are attracted to the six cycle. Therefore, the wave functions are similar to the one at $E=0$ on a large length scale.

For these special values of energy, the wave functions are neither extended nor localized in a standard way and are probably characteristic of a wave function at the mobility edge. Some special wave functions have been obtained in other incommensurate models.[9]

There are infinitely many eigenvalues in the energy spectrum of the type described above. However, they are still very rare in a sense that if one picks an element of the spectral set, then, with probability 1, the corresponding orbit is chaotic rather than a limit cycle. An important unresolved issue is to understand the wave functions which correspond to chaotic orbits.[10]

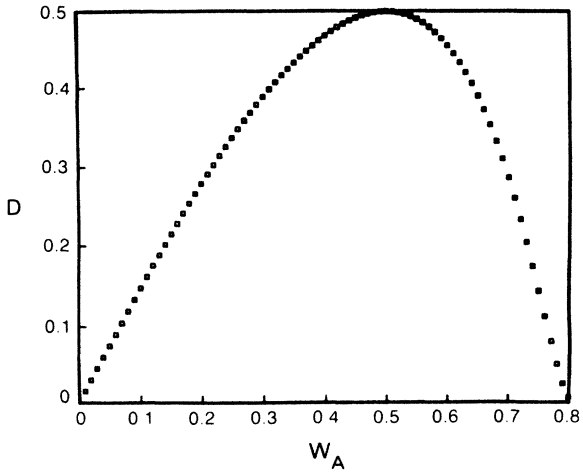

FIG. 3. A plot of the diffusion coefficient versus W_A.

For the phonon problem, ψ_n is regarded as describing the displacement and this behaves similarly to the wave function at the corresponding energy. There is a one-to-one correspondence between the phonon and the electronic spectra.

III. SPECTRAL DIMENSION, FRACTAL DIMENSION, AND DIFFUSION

We now switch to the phonon problem in the low-frequency limit. This part of the spectrum is an edge of the total spectrum and it can be shown that a two cycle of the map (5) governs the edges of the spectrum. Note that as $\omega\rightarrow 0$, $I=0$ and this two cycle becomes the fixed point $x_1=I$. A fixed-point analysis gives the Van Hove—type behavior of the integrated density of states, namely it is proportional to the square root of ω^2. Hence, the low-frequency integrated density of states of the phonons is *linear* in ω. We have verified this analytic result numerically. This implies a linear low-temperature specific heat and a value of the spectral dimension d_s equal to one. It is easy to show using the mass-volume relationship that the Fibonacci lattice has a fractal dimension $d_f=1$. Therefore, one expects that the random-walk dimension $d_w=2(d_f/d_s)$ (defined by $\langle r^2\rangle\sim r^{2/d_w}$) is equal to 2 and that there is no anomalous diffusive behavior.[11]

Using the results for the diffusion coefficient for a periodic one-dimensional hopping model of arbitrary period N derived by Derrida,[12] we have numerically evaluated the velocity and diffusion coefficient on a Fibonacci lattice.

We find, indeed, that the velocity is zero and that the diffusion coefficient is well defined. Figure 3 shows a plot of the diffusion coefficient D versus W_A, where W_A denotes the probability of jumping across an A band per unit time. For convenience, W_A and W_B were normalized as

$$W_A\sigma_G + W_B(1-\sigma_G)=0.5\ ,$$

so that the average of W's on the lattice is constant. The diffusion coefficient has a maximum for $W_A = W_B = 0.5$, a situation corresponding to the usual random walk and is asymmetric about the peak.

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[1]D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).

[2]B. Simon, Adv. Appl. Math. **3**, 463 (1982); B. Simon and B. Soulliard, J. Stat. Phys. **36**, 273 (1984), and references therein.

[3]R. Merlin, K. Bajema, R. Clarke, F-T. Juang, and P. K. Bhattacharya, Phys. Rev. Lett. **55**, 1768 (1985).

[4]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).

[5]S. Ostlund, R. Pandit, D. Rand, H. J. Schellnhuber, and E. Siggia, Phys. Rev. Lett. **50**, 1873 (1983).

[6]M. Kohmoto and Y. Oono, Phys. Lett. **102A**, 145 (1984).

[7]M. Kohmoto, Phys. Rev. Lett. **51**, 1198 (1983).

[8]F. Nori and J. P. Rodriguez (unpublished) have studied both models (1) and (2) numerically. Our results are consistent with their findings except that they find states in gaps. Since they imposed boundary conditions at an arbitrary lattice length, these gap states may probably be attributed to boundary effects; J. M. Luck and D. Petritis [J. Stat. Phys. **42**, 289 (1986)] have also studied the same models and our results agree with their findings; F. Delyon and D. Petritis, Commun. Math. Phys. **103**, 441 (1986) have rigorously proven the absence of localized states (and hence the states in the gap) for related models.

[9]R. E. Prange, D. R. Grempel, and S. Fishman, Phys. Rev. B **29**, 6500 (1984); S. Ostlund and R. Pandit, *ibid.* **29**, 1394 (1984).

[10]J. Bellissard, D. Bessis, and P. Moussa, Phys. Rev. Lett. **49**, 701 (1982); chaotic orbits are obtained also in their model. However, this does not directly imply chaotic wave functions because the orbits represent only selected points on the lattice.

[11]S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43**, L625 (1982).

[12]B. Derrida, J. Stat. Phys. **31**, 433 (1983).