Scaling properties of coupled optical interface modes in Fibonacci dielectric superlattices

1996 J. Phys.: Condens. Matter 8 10285

(http://iopscience.iop.org/0953-8984/8/49/019)

J. Phys.: Condens. Matter **8** (1996) 10285–10292. Printed in the UK

Scaling properties of coupled optical interface modes in Fibonacci dielectric superlattices

G J Jin†‡, Z D Wang‡, A Hu† and S S Jiang†

† Department of Physics and National Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, People's Republic of China

‡ Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong

Received 24 June 1996, in final form 16 September 1996

Abstract. The scaling properties of coupled optical interface modes in Fibonacci dielectric superlattices are investigated. In the dielectric continuum approximation, the frequency spectra are found to have two sets of dual triadic Cantor structures. This duality is also reflected in the distributions of electric fields. Scaling and multifractal analyses are used to establish that the frequency spectra are all singular continuous and the eigenstates are critical.

Quasiperiodic structures present us with a new type of system which is intermediate between periodic and disordered structures. A lot of interesting physical properties in the quasiperiodic systems have been explored theoretically and experimentally for the last decade [1–8]. Among them, elementary excitations, such as electron, phonon, plasmon, and spin wave, in the Fibonacci chains or superlattices have attracted much attention. The energy spectra and the wave functions are two important aspects to show quasiperiodic behaviours. To characterize them, many new theoretical methods, especially scaling and multifractal analyses, have proven successful [9–15].

Optical phonons in layered structures and periodic superlattices have been addressed for many years [16, 17]. However, only a few studies on the optical phonons in quasiperiodic structures have been reported [18]. In this paper, we first derive the transfer matrix expressions and the trace map formulae for the coupled optical interface modes in Fibonacci dielectric superlattices. Then we present scaling and multifractal analyses for the frequency spectra and the eigenstates by numerical calculations

A Fibonacci superlattice is a one-dimensional quasiperiodic structure with two building blocks which can be denoted by L and S. As a structure considered here, each of them is a bilayer [6, 7] composed of an A layer and a B layer. The B layers in L and S blocks have the same thickness d, but the A layers have thickness d_L in L blocks and d_S in S blocks, respectively. Using these two blocks, a Fibonacci dielectric superlattice is formed in terms of the rule $S_{j+1} = \{S_j, S_{j-1}\}$, $S_1 = \mathrm{L}$, $S_2 = \mathrm{LS}$, where j is the generation number. For example, $S_3 = \mathrm{LSL}$, $S_4 = \mathrm{LSLLS}$, $S_5 = \mathrm{LSLLSLSL}$.... A and B are two kinds of dielectric materials with different dielectric functions ε_A and ε_B. ε_A and ε_B are the same as for the corresponding infinite media and may be frequency dependent. In the electrostatic limit and dielectric continuum approximation, there is an electrostatic potential Φ to satisfy the Laplace equation $\nabla^2\Phi(\boldsymbol{r}, t) = 0$, and the electric field caused by the vibration of the crystal polarization is determined by $E = -\nabla\Phi$.

Take z as the quasiperiodic direction, and assume that the system is homogeneous and isotropic in xy planes. Without loss of generality, we consider that only a plane wave

0953-8984/96/4910285+08$19.50

$\exp(\mathrm{i}kx)$ propagates along the x direction in the superlattice planes with k as the in-plane wave vector. If we write $\Phi(\boldsymbol{r}, t) = \phi(z)\exp\{\mathrm{i}(kx - \omega t)\}$, the Laplace equation becomes

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2} - k^2\right)\phi(z) = 0. \tag{1}$$

The electrostatic continuum conditions at the interface of nth and $(n+1)$th layers take the form

$$\phi_n(z) = \phi_{n+1}(z) \qquad \varepsilon_n \frac{\mathrm{d}\phi_n(z)}{\mathrm{d}z} = \varepsilon_{n+1}\frac{\mathrm{d}\phi_{n+1}(z)}{\mathrm{d}z}. \tag{2}$$

The solutions of equation (1) can be written as $\phi_l(z) = g_l \mathrm{e}^{kz} + h_l \mathrm{e}^{-kz}$ in the A layers, and $\phi_l(z) = p_l \mathrm{e}^{kz} + q_l \mathrm{e}^{-kz}$ in the B layers, where l denotes the block index. If a local coordinate is taken for each layer and its origin is positioned at the centre of this layer, a transfer matrix representation

$$\begin{pmatrix} g_{l+1} \\ h_{l+1} \end{pmatrix} = T_{l+1,l}\begin{pmatrix} g_l \\ h_l \end{pmatrix} \tag{3}$$

for A layers is obtained, where

$$T_{l+1,l} = \begin{pmatrix} \alpha\, \mathrm{e}^{k(d_{l+1}+d_l)/2} & \beta \mathrm{e}^{k(d_{l+1}-d_l)/2} \\ -\beta \mathrm{e}^{-k(d_{l+1}-d_l)/2} & \gamma\, \mathrm{e}^{-k(d_{l+1}+d_l)/2} \end{pmatrix} \tag{4}$$

with $d_l = d_L$ for an L block and d_S for an S block, and

$$\begin{aligned} \alpha &= \cosh kd + \frac{1}{2}\left(\frac{\varepsilon_B}{\varepsilon_A} + \frac{\varepsilon_A}{\varepsilon_B}\right)\sinh kd \\ \beta &= \frac{1}{2}\left(\frac{\varepsilon_B}{\varepsilon_A} - \frac{\varepsilon_A}{\varepsilon_B}\right)\sinh kd \\ \gamma &= \cosh kd - \frac{1}{2}\left(\frac{\varepsilon_B}{\varepsilon_A} + \frac{\varepsilon_A}{\varepsilon_B}\right)\sinh kd. \end{aligned} \tag{5}$$

Note that all the effects of B layers are included in equation (5). We find that for $T_{l,l+1}$ there are only three types of unimodular transfer matrix $T_{L,L}$, $T_{S,L}$ and $T_{L,S}$. As usual, we take $M_1 = T_{L,L}$ and $M_2 = T_{L,S}T_{S,L}$, and according to the recursion relation [4]

$$M_{j+1} = M_{j-1}M_j \tag{6}$$

we can conversely deduce the expression of $M_0 = M_2 M_1^{-1}$, and subsequently, $M_{-1} = M_1 M_0^{-1}$.

By defining $\chi_j = \frac{1}{2}\operatorname{Tr} M_j$, it was shown by Kohmoto *et al* that $I = \chi_{j+1}^2 + \chi_j^2 + \chi_{j-1}^2 - 2\chi_{j+1}\chi_j\chi_{j-1} - 1$ is an invariant which remains constant at every step of the recursive procedure [4]. In the present system, we can find that

$$\begin{aligned} \chi_{-1} &= \cosh k(d_L - d_S) \\ \chi_0 &= \cosh kd \cosh kd_S + \frac{1}{2}\left(\frac{\varepsilon_B}{\varepsilon_A} + \frac{\varepsilon_A}{\varepsilon_B}\right)\sinh kd \sinh kd_S \\ \chi_1 &= \cosh kd \cosh kd_L + \frac{1}{2}\left(\frac{\varepsilon_B}{\varepsilon_A} + \frac{\varepsilon_A}{\varepsilon_B}\right)\sinh kd \sinh kd_L \end{aligned} \tag{7}$$

and thus the invariant for the Fibonacci dielectric superlattice is

$$I = \frac{1}{4}\left(\frac{\varepsilon_B}{\varepsilon_A} - \frac{\varepsilon_A}{\varepsilon_B}\right)^2 \sinh^2 kd \sinh^2 k(d_L - d_S). \tag{8}$$

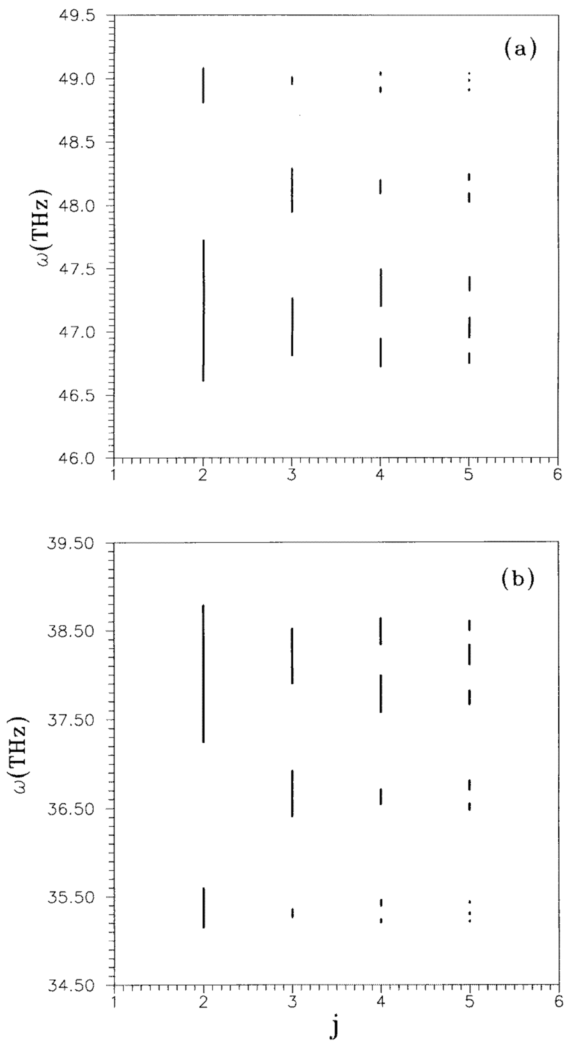

Figure 1. Two sets of dual bands in the Fibonacci dielectric superlattices with generation number $j = 2$–5: (a) ω_+ band; (b) ω_- band.

From equation (6), it is straightforward to demonstrate the well known recursion relation of a nonlinear trace map [4]

$$\chi_{j+1} = 2\chi_j\chi_{j-1} - \chi_{j-2}. \tag{9}$$

For example, it is direct to verify that $\chi_2 = 2\chi_1\chi_0 - \chi_{-1}$. (7) and (9) are quite useful in the following numerical analyses. In the numerical calculation of the coupled optical interface modes of Fibonacci dielectric superlattices, the number of Fibonacci generations can only be taken to be a finite value. So there are two types of boundary condition: one is the periodic boundary condition, and the other is the free boundary condition. The former, which is also referred to as a rational approximation, is employed in the present work.

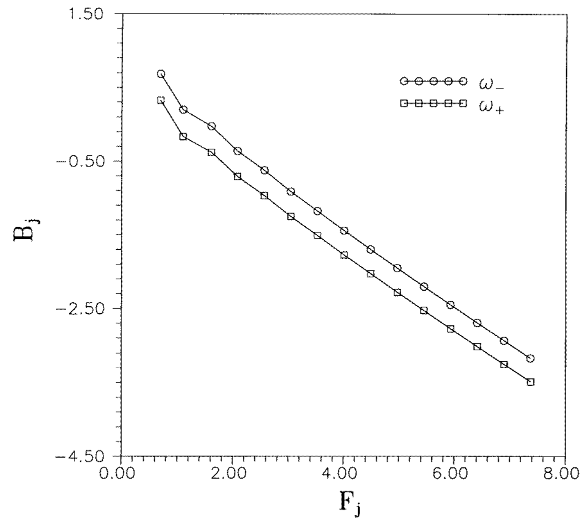

Figure 2. Scaling relations of the total bandwidths B_j against the Fibonacci number F_j ($j = 2$–16) for the ω_+ bands and ω_- bands.

The recursion equation for the quasiperiodic structure can be formally written as

$$\begin{pmatrix} g_{N+1} \\ h_{N+1} \end{pmatrix} = M_j \begin{pmatrix} g_1 \\ h_1 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} g_1 \\ h_1 \end{pmatrix} = \mathrm{e}^{\mathrm{i}QD} \begin{pmatrix} g_1 \\ h_1 \end{pmatrix} \tag{10}$$

where the m_{ij} $(i, j = 1, 2)$ are all complicated functions of wave vector, thicknesses and frequency and Q and D are the wavevector and thickness of the whole superlattice, respectively. Based on (3)–(10), further theoretical analyses of the coupled optical interface modes can be made. To obtain the concrete numerical results, we choose the dielectric function of A to be frequency independent, but the one of B to be frequency dependent: $\varepsilon_B(\omega) = \varepsilon_{B,\infty}(\omega^2 - \omega_{B,LO}^2)/(\omega^2 - \omega_{B,TO}^2)$, as for alkali halide or polar semiconductor materials. The relevant parameters are chosen as the following: $\varepsilon_A = 2.1$, as the value of SiO_2; $\varepsilon_{B,\infty} = 2.34, \varepsilon_{B,0} = 5.9, \omega_{B,TO} = 32.01$THz and $\omega_{B,LO} = 50.74$ THz, which correspond to the values of NaCl; $\varepsilon_C = 1$ as the value of vacuum; $kd_L = 2.0,\ kd_S = 1.0$ and $kd = 0.5$.

If the Fibonacci generation number j is chosen, then under the rational approximation, the eigenfrequency equation reads

$$\chi_j = \cos QD. \tag{11}$$

Some specific cases, like $QD = 0, \pm\pi$, correspond to the band edges. The trace map equation (9) provides us with a powerful tool to calculate the frequency spectra. The numerical results for $j = 2, 3, 4, 5$ are shown in figure 1. The results for $j = 6$–20 are also obtained, but not displayed here. Being different from the electron, phonon, plasmon and spin wave [1–6], in the present system, the allowed frequencies form two dual Cantor structures and the total number of subbands is $2F_j$, where F_j is a Fibonacci number which satisfies the recursion relation $F_j = F_{j-2} + F_{j-1}$, and $F_0 = F_1 = 1$. In addition, these two dual band structures are all nonuniform scaling. For the band ω_+, at lower frequencies, there are larger bands and smaller gaps, while at higher frequencies, the bands are narrower. As for the band ω_-, the case is reversed. The characteristics are closely related to the invariant I which is qualitatively different from the other elementary excitations [2, 3, 6].

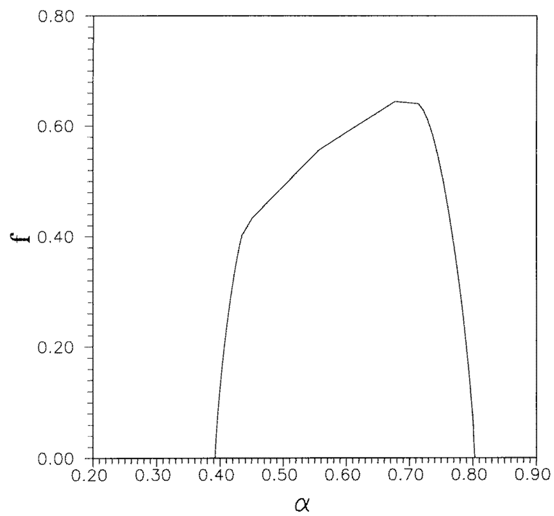

Figure 3. Multifractal spectra $f \sim \alpha$ curve of ω_- bands.

From the relationship between the total bandwidth and the period of the system, extended, localized and critical states can be identified for a quasiperiodic structure [7]. In our Fibonacci dielectric superlattice with F_j blocks representing the period of the system, it is straightforward to evaluate the width of each subband, then sum them over to get the total bandwidth B_j. Figure 2 shows the log–log relation between B_j and F_j for the two dual Cantor structures. Clearly, there exists a scaling relation between the total bandwidths and the Fibonacci number

$$B_j \sim F_j^{-\delta}$$

with $\delta \approx 0.5$. When j becomes larger and larger, B_j, that is to say, the Lebesque measure of the energy band, approaches zero, so all the states are critical. This result stems from the quasiperiodicity and is essentially the same as those in systems of electrons [9], phonons [12] and plasmons [13]. However, the ω_+ and ω_- bands have almost the same exponential δ, which is due to the fact that the duality for two bands is strict.

At this stage, we address the multifractality of the spectra. For this process, we need to calculate the partition function [8]

$$\Gamma(q, \tau, \{s_i\}, l) = \sum_{i=1}^{N} \frac{p_i^q}{l_i^\tau} \tag{12}$$

under the condition

$$\Gamma(q, \tau) = \lim_{l \to 0} \Gamma(q, \tau, \{s_i\}, l) = C \tag{13}$$

where s_i is the subset with measure l_i, $l \leqslant l_i$ and C is a finite constant. Once the mass exponent $\tau(q)$ is determined, the implicit relation $f(\alpha)$ can be obtained from

$$\alpha(q) = \frac{\mathrm{d}\tau(q)}{\mathrm{d}q} \qquad f(q) = q\alpha(q) - \tau(q). \tag{14}$$

We here use l_i to represent the width of the ith subband, and $p_i = 1/F_j$ in equation (12). Figure 3 shows the multifractal spectra of the eigenfrequency distribution. To improve the

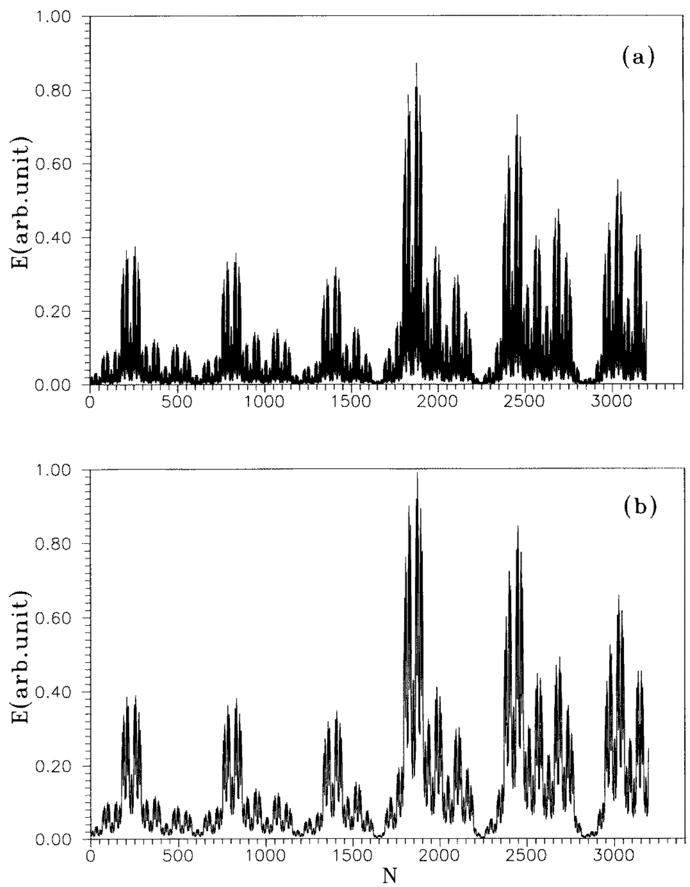

Figure 4. The distribution of electric field in a Fibonacci dielectric superlattice with $j = 16$, $QD = 0.5$: (a) sixth mode counted from the bottom of the ω_+ band; (b) sixth mode counted from the top of the ω_- band.

convergence, we made use of the trick suggested by Halsey *et al* [10] by taking $\Gamma_{13}/\Gamma_{16} = 1$. We can see from figure 3 that the singularity index α is distributed between 0.392 06 and 0.800 89, so the spectrum is singular continuous. The fractal dimension of the support is $f_{max} = f(0.676\,90) = D_0 = 0.644\,28$. For simplicity, only the multifractal spectrum for the ω_- band is presented; the result for the ω_+ band is the same because of the duality.

On the other hand, each of the eigenfrequencies can create a special distribution of potential, or equivalent field, which represents an eigenstate of the system. As the thickness of each layer of the superlattice is small, the layer-averaged potential or field is concerned. In the recursive procedure, the only important issue is to determine what the layer is when l changes, which we solved by using an algebraic method. We focus on the electric field in the following, as it relates directly to the long-wave optical vibrations.

From $E = -\nabla\Phi$, the distribution of the electric field can be expressed as

$$|E_l^A|^2 = 2k^2(|g_l|^2 + |h_l|^2)\sinh kd_l/kd_l$$
$$|E_l^B|^2 = 2k^2(|p_l|^2 + |q_l|^2)\sinh kd/kd \tag{15}$$

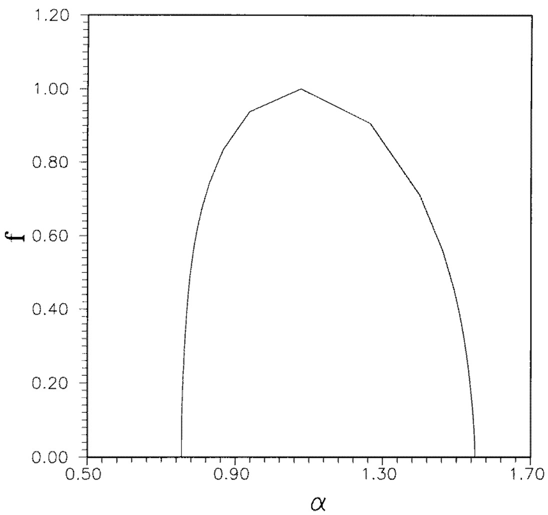

Figure 5. Multifractal spectra $f \sim \alpha$ curve of the distribution of the electric field in figure 4(b).

where

$$\begin{aligned} p_l &= \frac{1}{2}\left(1+\frac{\varepsilon_A}{\varepsilon_B}\right) \mathrm{e}^{k(d+d_l)/2}\, g_l + \frac{1}{2}\left(1-\frac{\varepsilon_A}{\varepsilon_B}\right) \mathrm{e}^{k(d-d_l)/2}\, h_l \\ q_l &= \frac{1}{2}\left(1-\frac{\varepsilon_A}{\varepsilon_B}\right) \mathrm{e}^{-k(d-d_l)/2}\, g_l + \frac{1}{2}\left(1+\frac{\varepsilon_A}{\varepsilon_B}\right) \mathrm{e}^{-k(d+d_l)/2}\, h_l. \end{aligned} \tag{16}$$

Under the periodic boundary condition, equation (10) leads to

$$g_1 = -\frac{m_{22} - \mathrm{e}^{\mathrm{i}QD}}{m_{21}} h_1. \tag{17}$$

Once the m_{ij} $(i,\ j = 1,\ 2)$ are recursively obtained, g_1 is determined by h_1 which is chosen as a unit. Here we can obtain any set of (g_l, h_l) by using the transfer matrix.

In terms of (3)–(5) and (15)–(17), we have examined the distribution of electric field for $j = 16$ and $QD = 0.5$. There are $2F_j = 3194$ states and they are all critical states, some appearing to be quasilocalized. This does not seem strange because the invariant takes a finite value for all eigenfrequencies between 0.4 and 4.5. More interestingly, all the states are one to one correspondent for two dual bands ω_+ and ω_-, as shown in figure 4. Figures 4(a) and (b) are adopted from the ω_+ and ω_- bands, respectively. The former is the sixth mode from the bottom of the ω_+ band, while the latter is the sixth mode from the top of the ω_- band. As far as we know, these dual eigenstates have not been declared in the study on electrons, phonons, plasmons or spin waves in one-dimensional systems.

Similarly, the multifractal spectra of the distribution of electric field can be calculated. We choose $p_i = |E_i|/\sum_i |E_i|$ and $l_i = l = 1/2F_j$. The numerical result of $f(\alpha)$ for the distribution of the electric field in figure 4(b) is shown in figure 5. The range of α is between $\alpha_{min} = 0.754\,29$ and $\alpha_{max} = 1.5498$. Figure 5, together with figure 4, tells us that the eigenstates are neither extended nor localized, but are critical, although its fractal dimension of support is $f_{max} = f(1.0760) = D_0 = 1$. It is clear that the duality ensures that the $f(\alpha)$ spectrum for the distribution of the electric field in figure 4(a) closely resembles figure 5.

In summary, the scaling properties of coupled optical interface modes in Fibonacci dielectric superlattices have been investigated for the first time. Except for the general characteristics of quasiperiodicity, we have found that the frequency spectra as well as the eigenstates all have dualities, in contrast to other elementary excitations in Fibonacci structures so far studied. These dualities have obvious impact on the scaling and multifractal behaviours of the frequency spectra and the eigenstates. The origin of these dualities is believed to be the dielectric properties of the alkali halide or polar semiconductor materials used to compose the Fibonacci superlattices.

Acknowledgments

This work was supported by Hong Kong RGC grant under No. HKU262/95P, the National Natural Science Foundation of China, and the Provincial Natural Science Foundation of Jiangsu.

References

[1] Kohmoto M, Kadanoff L P and Tang C 1983 *Phys. Rev. Lett.* **50** 1870
[2] Kohmoto M and Banavar J R 1986 *Phys. Rev.* B **34** 563
[3] Hawrylak P and Quinn J J 1986 *Phys. Rev. Lett.* **57** 380
[4] Kohmoto M, Sutherland B and Tang C 1987 *Phys. Rev.* B **35** 1020
[5] Johnson B L and Camley R E 1991 *Phys. Rev.* B **44** 1225
[6] Feng J W, Jin G J, Hu A, Kang S S, Jiang S S and Feng D 1995 *Phys. Rev.* B **52** 15312
[7] Merlin R, Bajema K, Clarke R, Juang F-Y and Bhattacharya P K 1985 *Phys. Rev. Lett.* **55** 1768
[8] Hu A, Tien C, Li X, Wang Y and Feng D 1986 *Phys. Lett.* **119A** 313
[9] Kohmoto M 1983 *Phys. Rev. Lett.* **51** 1198
[10] Halsey T C, Jensen M H, Kadanoff L P, Procaccia I and Shraiman B I 1986 *Phys. Rev.* A **33** 1141
[11] Tang C and Kohmoto M 1986 *Phys. Rev.* B **34** 2041
[12] Janssen T and Kohmoto M 1988 *Phys. Rev.* B **38** 5811
[13] Hiramoto H and Kohmoto M 1988 *Phys. Rev. Lett.* **62** 2714
[14] Tong P Q 1995 *Phys. Rev.* B **52** 16301
[15] Peng R W, Wang M, Hu A, Jiang S S, Jin G J and Feng D 1995 *Phys. Rev.* B **52** 13310
[16] Sood A K, Menéndez J, Cardona M and Ploog K 1985 *Phys. Rev. Lett.* **54** 2115
[17] Huang Kun and Zhu Banfen 1988 *Phys. Rev.* B **38** 13377
[18] Jin G J, Kang S S, Wang Z D, Hu A and Jiang S S 1996 *Phys. Rev.* B **54**