Transactions of the Materials Research Society of Japan 25 [4] 1061-1064 (2000)

ELECTRONIC STATES IN QUASIPERIODIC LATTICE, WHICH IS CONSIDERED TO CONSIST OF A SET OF A FEW KINDS OF CLUSTERS

Noriyuki Chiba and Toshiyuki Ninomiya

Department of Physics, Faculty of Science and Engineering, Chuo University, Kasuga 1-13-27 Bunkyo-ku, Tokyo 112-8551, JAPAN
Fax: 81-3-3817-1792, e-mail: chiba@phys.chuo-u.ac.jp

The electronic states in the lattice which consists of a few kinds of clusters are studied with regard to how the eigen states in the lattice are obtained from those of individual clusters. We show that the energies at which the Green's function is zero play the same role as the eigen energies. Then, we clarify the process of energy band formation associated with accumulation of atoms one by one. Addition of atoms is accompanied with migration of eigen states from one band to a neighboring band, and the patterns of this migration is discussed in relation with the structure of clusters.
Key words: Quasiperiodic lattice, Fibonacci lattice, Electronic states, Tight-binding model

1 INTRODUCTION

Fibonacci lattice, a typical one-dimensional version of quasicrystal, has been extensively studied since the discovery of quasicrystal as a real material by Shechtman *et al.*[1] Fibonacci sequence is constructed recursively as $S_{i+1} = S_i S_{i-1}$. It is well known that the energy spectrum of the electronic states in the Fibonacci lattice is a Cantor-like set of zero Lebesgue measure and all the the eigen states are neither localized nor extended,but critical. These results have mainly been obtained by trace mapping [2, 3] or renomarization technique [4, 5] based on the self-similarity of its structure. It seems that less attention has been paid to how the eigen states of the cluster S_{i+1} are given from those of S_i and S_{i-1} when connecting these clusters.

In the present work we develop a theory of electronic states in a cluster S_γ obtained by connection of two one-dimensional clusters of any type, S_α and S_β, and it is found that not only the eigen energies of S_α and S_β but also the energies at which their Green's functions are zero play important role in determining the eigen energies of the newly obtained cluster S_γ (Fig.1). The case of connection of mirror symmetric clusters, in which the Fibonacci sequence is included, is also discussed in Sec.3. In numerical calculation, atoms are accumulated one by one on a Fibonacci lattice, and we observe migration of the eigen states from a band to a neighboring band when the structure has a certain kind of patterns (Sec.4), that is, an eigen state is emitted from one band, when the end of the cluster has some special structure by adding an atom, and is absorbed by the neighboring band when one more atom is accumulated.

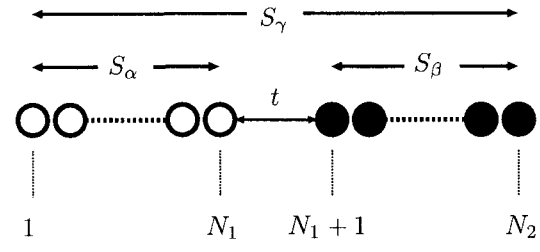


Figure 1: Open circles and solid circles represent S_α, S_β respectively. S_γ is obtained by connecting S_α with S_β by hopping integral t.

2 ELECTRONIC STATES OF A COMBINED CLUSTER

In this section we discuss a case of connection of two clusters of arbitrary array of atom A and B , including periodic lattice, and give the condition which should be satisfied by eigen energies of a newly obtained cluster S_γ from S_α and S_β (Fig.1). For the electronic states we use the on-site tight-binding model defined by

$$\phi_\alpha(n+1) + \phi_\alpha(n-1) + V_n\phi_\alpha(n) = E_\alpha\phi_\alpha(n) \quad \text{for} \quad 1 \le n \le N_1 \quad (2.1)$$

where $\phi_\alpha(N_1+1) = 0$ and

$$\phi_\beta(n+1) + \phi_\beta(n-1) + V_n\phi_\beta(n) = E_\beta\phi_\beta(n) \quad \text{for} \quad N_1+1 \le n \le N_2 \quad (2.2)$$

where $\phi_\beta(N_1) = 0$. $\phi_\alpha(n)$ and $\phi_\beta(n)$ denote wave function of S_α, S_β at the nth site.

Perturbation in the Hamiltonian caused by connection of S_α and S_β by hopping integral t between site N_1 and N_1+1 is given by

$$\Delta(N_1, N+1) = t|N_1\rangle\langle N_1+1| + t|N_1+1\rangle\langle N_1|, \tag{2.3}$$

here, $t=1$ for the Fibonacci sequence.

Now in order to obtain electronic states of S_γ, we expand the defined region of ϕ_α and ϕ_β to $1 \le n \le N_2$, and ϕ_α and ϕ_β are given to satisfy

$$\phi_\alpha(n) = 0 \qquad n \ge N_1+1, \tag{2.4}$$
$$\phi_\beta(n) = 0 \qquad n \le N_1. \tag{2.5}$$

Then, $\phi_\alpha(n)$ and $\phi_\beta(n)$ are orthogonal.

The Green's function $\mathrm{G}(z)$ for S_γ satisfies the Dyson expansion

$$\mathrm{G}(z) = \mathrm{G}_0(z) + \mathrm{G}_0(z)\Delta(N_1, N_1+1)\,\mathrm{G}(z), \tag{2.6}$$

and we obtain

$$\begin{aligned}\mathrm{G}(n,n';z) &= \mathrm{G}_0(n,n';z) \\ &\quad + t\,\mathrm{G}_0(n,N_1;z)\,\mathrm{G}(N_1+1,n';z) \\ &\quad + t\,\mathrm{G}_0(n,N_1+1;z)\,\mathrm{G}(N_1,n';z),\end{aligned} \tag{2.7}$$

where $\mathrm{G}(n,n';z) \equiv \langle n|\,\mathrm{G}(z)|n'\rangle$. $\mathrm{G}_0(n,n';z)$ is the Green's function for S_α in the case of $n,n' \le N_1$ and for S_β in the case of $n,n' \ge N_1+1$ and $\mathrm{G}_0(n,n';z)=0$ for $n \le N_1$ and $n' \ge N_1+1$.

Then the poles of $\mathrm{G}(n,n';z)$ which indicate E_γ are given by

$$\mathrm{G}_\alpha(E_\gamma)\,\mathrm{G}_\beta(E_\gamma) = t^{-2}, \tag{2.8}$$

or

$$\sum_\alpha \frac{|\phi_\alpha(N_1)|^2}{E_\gamma - E_\alpha} \sum_\beta \frac{|\phi_\beta(N_1+1)|^2}{E_\gamma - E_\beta} = t^{-2}, \tag{2.9}$$

where

$$\mathrm{G}_\alpha(z) \equiv \mathrm{G}_0(N_1, N_1; z), \tag{2.10}$$
$$\mathrm{G}_\beta(z) \equiv \mathrm{G}_0(N_1+1, N_1+1; z). \tag{2.11}$$

Because right hand side of (2.8) is positive, both $\mathrm{G}_\alpha(E_\gamma)$ and $\mathrm{G}_\beta(E_\gamma)$ must be positive or negative. Then the region in which the eigen states E_γ exist are given by configuration of E_α, E_β and E_α^*, E_β^* where E_α^*, E_β^* are the energy at which $\mathrm{G}_\alpha(E_\alpha^*)=0$, $\mathrm{G}_\beta(E_\beta^*)=0$ respectively (Fig.2). Every masked region contains one eigen state.

3 ELECTRONIC STATES OF MIRROR SYMMETRIC CLUSTERS

Fibonacci lattice can be divided into the three kinds of clusters of mirror symmetry which are called *singular words* w_n.[6] For example, the clusters are

$$w_1 = AA, w_2 = BAB, w_3 = AABAA \ . \tag{3.1}$$

And w_n satisfies

$$w_n = w_{n-2}w_{n-3}w_{n-2} \qquad n \ge 1. \tag{3.2}$$

If we use the similar way of description for mirror symmetric cluster S_α and S_β, this corresponds to

$$S_\gamma = S_\beta S_\alpha S_\beta \ . \tag{3.3}$$

Using the method discussed in Sec.2, eigen energies of S_γ can be obtained from S_β, S_α. The Green's function for S_γ has the poles at the energy which is given by

$$(\mathrm{G}_\alpha(E_\gamma) \pm \mathrm{G}_0(N_1+1, N_2; E_\gamma))\,\mathrm{G}_\beta(E_\gamma) = t^{-2}. \tag{3.4}$$

Considering the symmetry, $\mathrm{G}_\alpha(z), \mathrm{G}_0(N_1+1, N_2; z)$ can be divided into symmetric and antisymmetric part as follows

$$\mathrm{G}_\alpha(z) = \mathrm{G}_{\alpha_+}(z) + \mathrm{G}_{\alpha_-}(z), \tag{3.5}$$
$$\mathrm{G}_0(N_1+1, N_2; z) = \mathrm{G}_{\alpha_+}(z) - \mathrm{G}_{\alpha_-}(z), \tag{3.6}$$

where $\mathrm{G}_{\alpha_+}(z)$ and $\mathrm{G}_{\alpha_-}(z)$ are symmetric and antisymmetric parts of $\mathrm{G}_\alpha(z)$ respectively. From these we obtain symmetric and antisymmetric eigen states shown as

$$\mathrm{G}_{\alpha_+}(E_\gamma)\,\mathrm{G}_\beta(E_\gamma) = \frac{t^{-2}}{2}, \tag{3.7}$$
$$\mathrm{G}_{\alpha_-}(E_\gamma)\,\mathrm{G}_\beta(E_\gamma) = \frac{t^{-2}}{2}. \tag{3.8}$$

Therefore the regions in which eigen energies exist are given similarly to Fig.2.

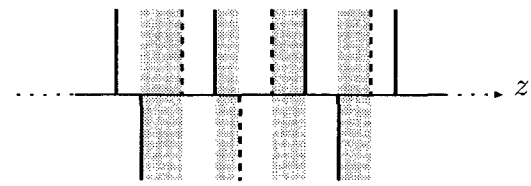
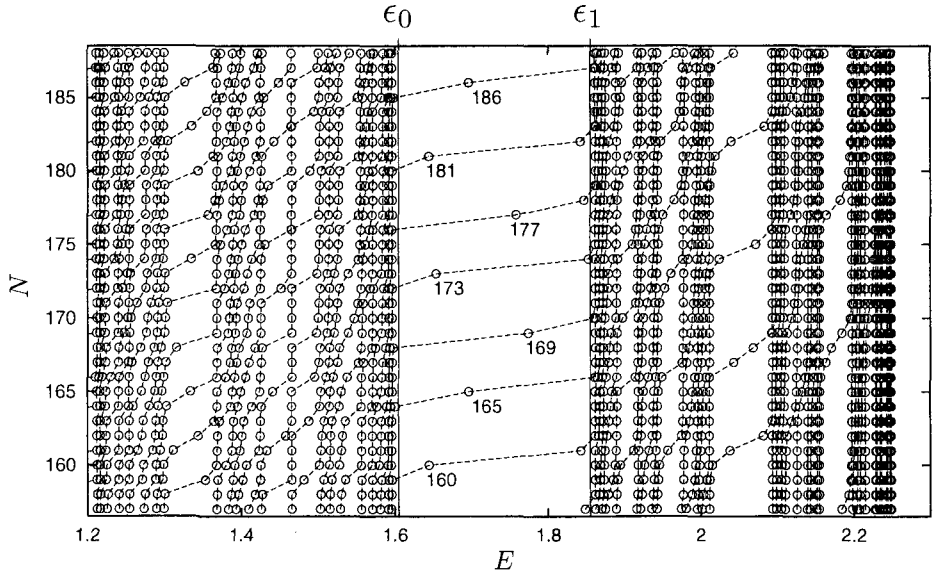


Figure 2: The solid and broken lines give the energy E_α, E_β and E_α^*, E_β^* respectively, where the upper and lower section of the horizontal line are for S_α and S_β. Eigen states exist only in the masked region.

(a).



(b).

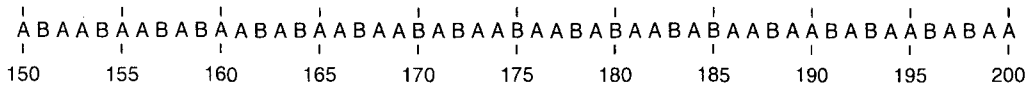


Figure 3: The numerical results on shift of eigen energies when adding atoms one by one. Circles denote eigen energies of system size N. Here we take $V_A = -V_B = 0.6$.

4 THE PROCESS OF ENERGY BAND FORMATION ASSOCIATED WITH ACCUMULATING ATOMS ONE BY ONE

Figure 3 shows results of numerical calculation on shift of eigen energies from a band to a neighboring band via localized states when atom are accumulated one by one to grow a Fibonacci lattice (Fig.3b). If S_β is only one atom, which has the potential $V(= V_A$ or $V_B)$,

$$\mathrm{G}_\beta(z) = \frac{1}{z - V} \qquad (4.1)$$

and from (2.8) the poles of the present system are given by

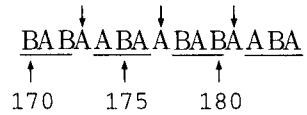
$$\mathrm{G}_\alpha(E) = t^{-2}(E - V). \qquad (4.2)$$

Shift of the energies due to addition of one atom A or B is generally summarized as follows :

a). Eigen energies E_α higher than V shift to higher side but not beyond E^*_α, and E_α lower than V shift to lower side but not beyond E^*_α.

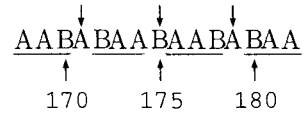
b). An eigen state is generated near V.

Here we discuss the shift observed in the energy gap ranging ($\epsilon_0 \sim \epsilon_1$) in more detail (Fig.3a). As shown in (3.1) the Fibonacci sequence consists of $w_1 = AA$, $w_2 = BAB$, and $w_3 = AABAA$, and AA and $AABAA$ have BAB on their both sides. Since the number of $AABAA$, N_{w_3}, is as large as τN_{w_1} ($\tau = (\sqrt{5}+1)/2$),[6] we may roughly consider that main character is determined by the sequence $\cdots w_2 w_3 w_2 w_3 \cdots$. Then, the sequence is considered to have the structure in which ABA and BAB are separated with single A. For example, atoms at 170th through 184th site is given as



(Case A).

This structure is also regarded as



(Case B),

where AAB's are arranged with alternating direction and are separated with single A or B.

The wave function $\psi(n)$ at the edge of the band ϵ_0 is such that given in Fig.4: that is, the wave function has a small value at the sites where ABA and BAB are separated. This situation takes place because one of the eigen energies of ABA and BAB have the same magnitude $\sqrt{2+V^2}$, which is very near the energy at the band edge. Then, the wave functions must have the opposite phase but the same magnitude at the sites just before and after the site where the wave function disappears. We have a similar result on the wave function at the band edge ϵ_1 (Case B). Here the wave function disappears at the site 171, 175 and 179th.

Figure 3 shows that the emission of an eigen state from the band edge ϵ_0 to the middle of the band gap take place when an atom A is added on BAB or ABA at end of the Fibonacci lattice. Second step, that is, the absorption of the state by the band edge ϵ_1 take place because of further addition of A on $BABA$ or B on $ABAA$ (This implies the formation of BAA or AAB). This also gives that we have the migration from ϵ_0 to ϵ_1 by the accumulation four atoms, which is in agreement with computer simulation. In the case of 165th and 186th atoms the migration occurs by accumulation of five atoms after the emission due to the 160th and 181th atoms. This reflects that the Fibonacci sequence is not purely of $\cdots w_2w_3w_2w_3\cdots$.

5 CONCLUSIONS

We have developed the theory which gives the eigen energies of a combined clusters and found that the energy at which the Green's function is zero is important in determining the eigen energies. We also found that accumulation of atoms one by one on a Fibonacci lattice clarifies the process of energy band formation through the migration of eigen states from one band to a neighboring band.

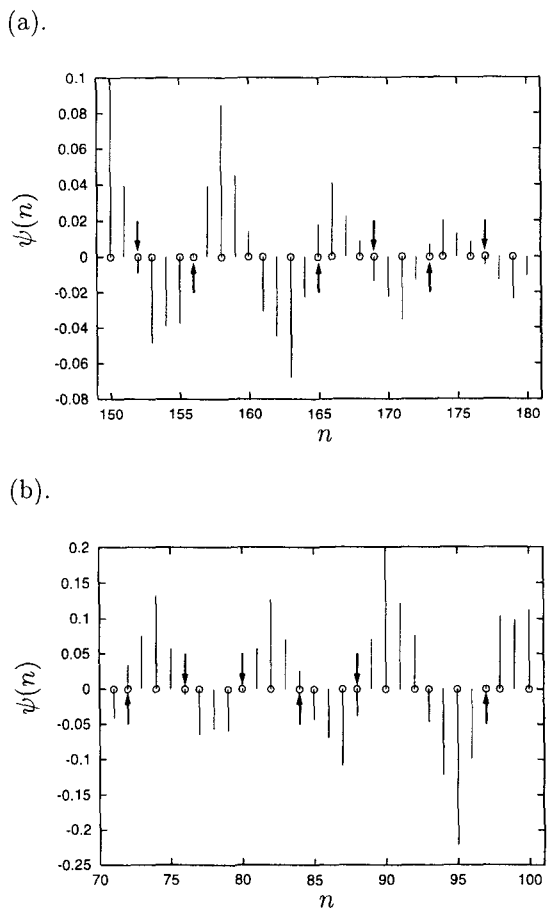


Figure 4: Wave function $\psi(n)$ of system size $N = 180$ at energy $E = 1.597$. Circles indicate A-site. Arrows indicate the sites which separate ABA and BAB. The wave function has a small value at these sites.

References

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

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

[3] M. Kohmoto, B. Sutherland and C. Tang Phys. Rev. B**35**, 1020 (1987).

[4] Q. Niu and F. Nori Phys. Rev. B**42**, 10329 (1990).

[5] Y. Liu and W. Sritrakool Phys. Rev. B**43**, 1110 (1991).

[6] Wen Zhi-Ying,"BEYOND QUASICRYSTALS" Ed. by F.AXIEL, D.GRATIAS, Springer-Verlag, Berlin Heidelberg New York (1995) pp. 433-440.

(Received December 17, 1999; Accepted August 16, 2000)