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LETTER TO THE EDITOR

A new type of transition between critical and extended states in one dimension

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Abstract. We study a tight-binding model, $\Psi_{n+1}+\Psi_{n-1}+\lambda_n V_n \Psi_n = E\Psi_n$, where V_n is a Fibonacci array of two potentials and $\lambda_n = F^{-1/2}n^{-\alpha}$. For $\alpha = 1/2$, this model is asymptotically equivalent at large n to a continuous Schrödinger equation with an electric field F and a quasiperiodic potential. We find that for this value of α, almost all states are changed from critical to extended states as the field strength is increased. However, some states still remain critical and coexist with most extended states. We also discuss the results for other values of α.

Recently much attention has been paid to the electronic structure of one-dimensional quasiperiodic systems [1,2]. For example, it is generally believed that the energy spectrum of a Fibonacci chain is singular continuous and that all eigenstates are critical [1,2]. Critical states show self-similar or chaotic behaviour [2] and are neither localized nor extended. However, the effect of the electric fields on the eigenstates of the quasiperiodic system has not been studied before. In this letter we consider a quasiperiodic Kronig–Penney model with a constant electric field. The Schrödinger equation is given as follows:

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\Psi(x)+\sum_{n=1}^{N} V_n\delta(x-n)\Psi(x)-Fx\Psi(x)=E\Psi(x) \tag{1}$$

where $\hbar^2 = 2m$, $e = 1$, F is the strength of the electric field, and V_n is a Fibonacci array of two potentials V_L and V_S. Potential $V_n = V_s + (V_L - V_S)([(n+1)/\tau] - [n/\tau])$, with $\tau = (\sqrt{5}-1)/2$. Transport properties can be used to determine the nature of the eigenstates of this system. But, except for small fields, the Landauer formula [3] may not be adequate to calculate the resistance R_N of this system. As an alternative to this difficulty, Delyon *et al* [4] showed that this Schrödinger equation is asymptotically equivalent for large n to the following tight-binding model:

$$\Psi_{n+1}+\Psi_{n-1}+\lambda_n V_n\Psi_n = E\Psi_n \tag{2}$$

where Ψ_n is the amplitude of the wavefunction at $x = n$, and $\lambda_n = F^{-1/2}n^{-\alpha}$ with $\alpha = 1/2$. The benefit of this tight-binding model is that Landauer formula can be

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used to find the resistance for all values of F. Since the effect of the electric field is included only in the site energies, the original site energies V_n are modulated by the factor $\lambda_n = F^{-1/2}n^{-1/2}$. We can also derive this tight-binding model using the Poincaré map [5] which is obtained by equation (1) with the step function approximation of electric potential Fx [6]. To test the validity of equation (2), we first studied the periodic system with $V_n = V_0$ for all n. One finds that equation (2) shows Wannier–Stark ladder resonances [7,8] for small fields, consistent with the known results.

We study equation (2) with quasiperiodic potentials by the second-order perturbation theory and numerical calculations. It is found that when $\alpha = 1/2$, almost all states are changed from critical to extended states as the field strength is increased. However, there are some states which seem to be critical at the largest length scales we have examined, and it appears that they are critical in the infinite limit. For $\alpha > 1/2$, all states are extended for large fields.

As Kim *et al* [9] have found in a certain quasiperiodic system, critical states can change to localized states and coexist with them in one dimension. In this paper we show for the first time the transition between critical and extended states. The study of this transition seems to be very important both for understanding the electronic properties of quasicrystals and for understanding the geometric and external field effects on the electronic states of solid states.

For large field limit, λ_n and the site energies are small and we can apply the perturbation theory of Thouless [10] to this system. Up to the second order of $F^{-1/2}$, the inverse localization length ξ^{-1} of the unperturbed energy $E_0 = 2\cos\theta$, is given by

$$\xi^{-1} = \frac{F^{-1}}{8N\sin^2\theta}\left|\sum_{k=1}^{N}\frac{\mathrm{e}^{\mathrm{i}2k\theta}}{k^\alpha} + \frac{1}{\tau}\sum_{k=1}^{N}\frac{[(k+1)/\tau]-[k/\tau]}{k^\alpha}\mathrm{e}^{\mathrm{i}2k\theta}\right|^2 \qquad (3)$$

where $V_n = 1 + 1/\tau([(n+1)/\tau] - [n/\tau])$, with $\tau = (\sqrt{5}-1)/2$. This perturbation theory is valid except for the regions near edges ($\theta = 0, \pi$). When the sample length N is sufficiently large, the first term inside the absolute value is $\mathrm{O}(\theta^{\alpha-1})$ [11]. The second term can be transformed to the following form

$$\frac{1}{\tau^2}\sum_{k=1}^{N}\frac{\mathrm{e}^{\mathrm{i}2k\theta}}{k^\alpha} + \sum_{k=1}^{N}\frac{\mathrm{e}^{\mathrm{i}2k(\theta-m\pi/\tau)}}{k^\alpha}\sum_{m=-\infty}^{\infty}{}' \mathrm{e}^{-\mathrm{i}m\pi/\tau}\frac{\sin(m\pi/\tau)}{m\pi/\tau}.$$

$\sum'$ means the omission of $m = 0$. By the properties of trigonometric series [12] we can get the following expression

$$\xi^{-1} \simeq \frac{F^{-1}}{8N\sin^2\theta}\left|\zeta'_N(\alpha)\delta_{\theta,\theta_{pq}} + \mathrm{O}(\theta^{\alpha-1})\right|^2. \qquad (4)$$

$\zeta'_N(\alpha) = \sum_{k=1}^{N} 1/k^\alpha, (\alpha \geqslant 0)$, and $\theta_{pq} = p\pi \pm q\pi/\tau$ with p and q being an integer and a positive integer, respectively. This expression shows that the inverse localization length of most states is zero. Especially for $\theta = \theta_{pq}$, the inverse localization length ξ^{-1} has a finite value. When $\alpha = 0$, this system is essentially a quasiperiodic system without an electric field. As expected, perturbation theory shows that for most values of θ, ξ^{-1} is zero, so the states are critical [13]. For a specific values of θ, ξ^{-1}

diverges, which means $\theta = \theta_{pq}$ corresponds to a gap. For $\alpha = 1/2$, $\zeta'_N(1/2)$ is $O(\sqrt{N})$. And ξ^{-1} has still a finite value for $\theta = \theta_{pq}$. We obtain two results for $\alpha \leqslant 1/2$. One is that ξ^{-1} is zero for most values of θ, and the other is that there are gap structures in the energy spectrum. Because of the existence of the gap, we conjecture that for $\alpha \leqslant 1/2$ there are some critical states. For $\alpha > 1/2$, ξ^{-1} is zero for all θ. Therefore all gaps die out, implying that all states are extended. Note that for smooth potentials in an electric field, the spectrum is absolutely continuous from $-\infty$ to ∞ and that there are no gaps [14].

To study equation (2) beyond the perturbation theory, we first calculate the scaling behaviours of total bandwidth B_l numerically, when the system is successively approximated by a periodic system with a period F_l. F_l denotes the lth Fibonacci number. We approximate τ in V_n by $\tau_l = F_{l-1}/F_l$. V_L and V_S are -1, and 1, respectively. Figure 1 shows the scaling behaviours of B_l for $F = 1$. For $\alpha \leqslant 0.3$ B_l scales to zero as l is increased. This means the spectrum is singular continuous and all states are critical for one equal to infinity. For $\alpha \geqslant 0.4$, B_l decreases for small length scales, but it increases again after some critical length. Therefore we can expect the spectrum for $\alpha \geqslant 0.4$ may be absolutely continuous in the infinite limit. However, by the perturbation theory, for $\alpha \leqslant 0.5$ there are some gap structures, which shows that there may also be some critical states. As figures 2(b) and 3 show, there are critical states among most extended states. For smaller fields there are more critical states. In the mean time, the corresponding spectra also show the Wannier–Stark ladder resonances for small fields [15]. This behaviour is similar to that of the disordered system with an electric field [16]. In that case, resonances are believed to be related to power-law localized states.

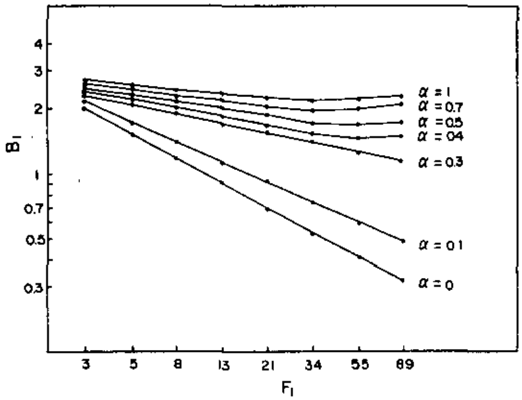

Figure 1. Scaling behaviours of total band width B_l for various values of α as this system is successively approximated by a periodic system of period F_l. Note that x- and y-axis are logarithmic scales.

To investigate the nature of the eigenstates, we calculate the resistance of an electron impinging this sample with an energy E. Figure 2 shows the N dependence of the average resistance $\overline{R} = (1/N)\sum_{i=1}^{N} R_i$ with respect to the sample length for $F = 10.0, \alpha = 0.5$, and $N = 80\,000$. Figures 2 (a) and (b) represent $E = -1.8485$, and $E = 1.920\,005\,56$ respectively. The behaviour of the average resistance has been demonstrated to be a good criterion to distinguish the three types

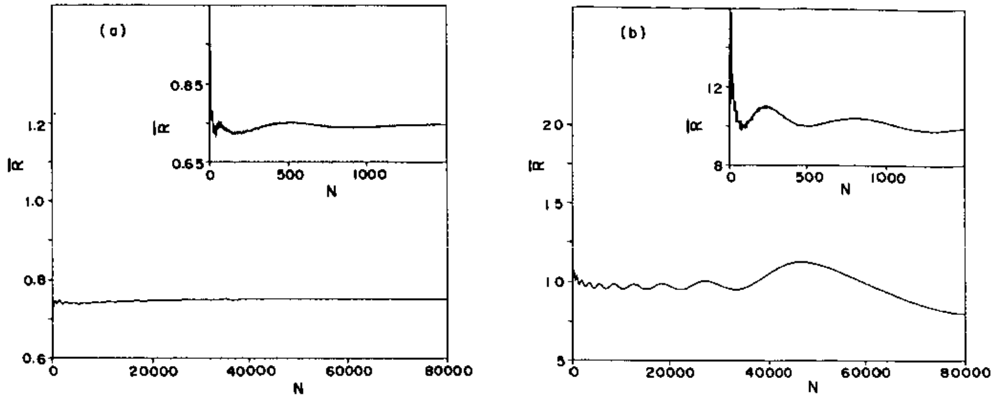

Figure 2. N dependence of the average resistance $\overline{R}$ for (*a*) $E = -1.8485$ and (*b*) $E = 1.920\,005\,56$ when $\alpha = 0.5$ and $F = 10$. The detailed behaviour is shown in the inset.

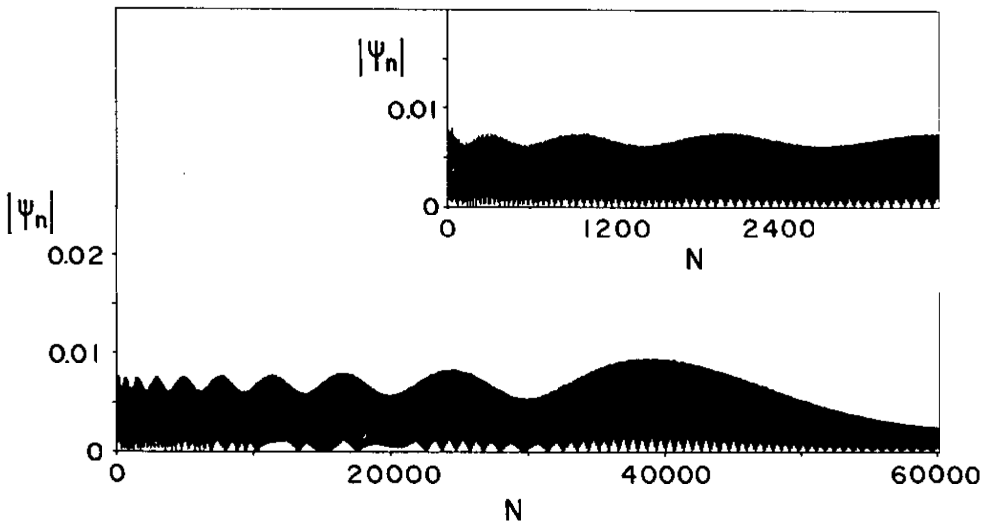

Figure 3. The behaviour of the wavefunction at $E = 1.920\,005\,56, \alpha = 0.5$, and $F = 10$.

of states [9, 17]. For short length scales, as can be seen in the inset of figure 2(*a*), it shows a highly fluctuating behaviour. However, when the sample length is increased, fluctuations die out showing an extended behaviour. For $F = 10$, the average resistance of most states shows the extended behaviour. We can understand this easily, because for large sample length the energy from the electric field is large enough to overcome potential energies.

We expected from the previous perturbative approach some critical states for $\alpha = 1/2$. From figure 2(*b*), we find the average resistance behaves as in figure 2(*a*) in a small length scale. But it displays large fluctuations even for large length scales, which means the state is critical for the sample length going to infinity. These fluctuations come from the clustering of the energy levels and are the evidence of the singular continuous spectrum. There are indeed some critical states coexisting with most other extended states. As we increase F, these critical states change to extended states.

Figure 3 displays the wavefunction of the critical state for the same parameters as figure 2(*b*). For the large sample lengths it shows self-similarity and fluctuations on larger scales. In contrast to that of the usual Fibonacci chain, [2] small fluctuations are weakened as the sample length is increased. These behaviours of the average resistance and the wavefunction are consistent with our previous results [9, 17] on critical states and confirm that the state is indeed critical.

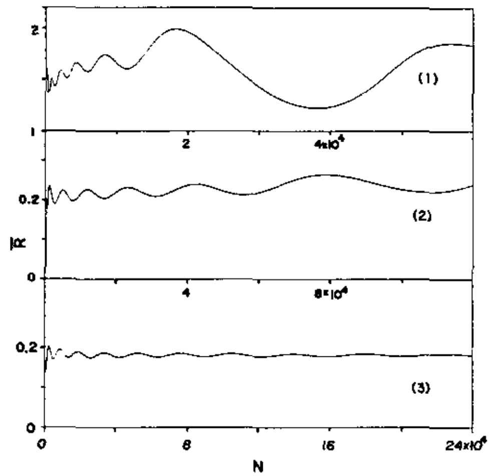

Figure 4. N dependence of $\overline{R}$ for (1) $E = 0.0399465, F = 1$; (2) $E = 0.04108, F = 5$; and (3) $E = 0.04130, F = 10$.

Next we study the transition between critical and extended states as a function of the electric field F. Figure 4 shows the changing behaviours of the average resistance $\overline{R}$ for $\alpha = 1/2, E = 0.0399465$ and $N = 60000$, as F is increased. The electric field for the curves (1), (2), and (3) is 1, 5, and 30, respectively. When $F = 1$, we can see many coupled oscillations. As F is increased, the oscillations with longer periods die out. The curve for $F = 30$ clearly shows that the state is extended. There seems to be a critical field after which the state is extended. In this figure we disregarded the energy shift due to the change of the eletric field strength F. Since the energy spectrum is nearly symmetric with respect to $E = 0$, this result seems to be qualitatively correct. Experimentally this transition might be found in the Fibonacci superlattice [18] with an electric field. For small fields most states are critical. And for large fields most states are extended. Therefore the transition between critical and extended states can be found by changing the electric field in photoluminesence experiment [19].

In conclusion, we have studied the asymptotically equivalent tight-binding model of a one-dimensional quasiperiodic system with an electric field. We find the coexistence [20, 21] of the critical and extended states and, more interestingly, the transition between the two states as a function of the electric field. This transition might be checked in a Fibonacci superlattice. The energy spectrum shows the Wannier–Stark ladder structure for small fields.

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