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LETTER TO THE EDITOR

Anomaly and singular continuous spectrum in a one-dimensional incommensurate system

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Abstract. We study a tight-binding model given by $\Psi_{n+1}+\Psi_{n-1}+V\cos(2\pi Qn+\theta)\Psi_n = E\Psi_n$, where Q is a Liouville number. It is demonstrated that all eigenstates are critical with singular continuous spectra for all values of V. These critical states appear to be composed of 'connected extended states'. We also find a band-centre anomaly: the resistance of the band centre displays coupled oscillations and is much larger than that of other states.

One-dimensional Schrödinger equations with two incommensurate periods have attracted much attention from physicists and mathematicians (Azbel 1964, Aubry and Andre 1980, Simon 1982, Sokoloff 1986). A typical model is given by the almost-Mathieu equation

$$\Psi_{n+1}+\Psi_{n-1}+V\cos(2\pi Qn+\theta)\Psi_n = E\Psi_n \tag{1}$$

where Q is an irrational number. Aubry and Andre (1980) studied this equation and showed that for $0<V<2$, the spectrum is absolutely continuous and all eigenstates are extended while for $V>2$, the spectrum is point-like and all states are localised. At the dual point $V=2$, the spectrum is singular continuous and the states are critical. In the meantime, Avron and Simon (1982, hereafter referred to as AS) proved that when Q is a Liouville number satisfying the condition

$$|Q-p_k/q_k| \leqslant k^{-q_k} \tag{2}$$

with p_k/q_k the kth convergent to Q, the energy spectrum is singular continuous instead of point-like for $V>2$. (See also Thouless and Niu (1983).) This property was then conjectured to be true for all values of V. They also showed that the eigenstates are critical but do not decay to zero at large distances, in contrast to usual critical wavefunctions found in quasiperiodic systems (Kohmoto *et al* 1983).

Singular continuous spectra can also be found in quasiperiodic systems like Fibonacci chains and hierarchical systems (Ceccato *et al* 1989, Schneider *et al* 1989). These systems are known to possess only singular continuous spectra and critical eigenstates, which can be either self-similar and algebraic or chaotic. Meanwhile, the precise nature of the proposed critical states in equation (1) for the Liouville number Q is not known yet. Liouville numbers constitute a set of measure zero, and there exist many irrational numbers arbitrarily close to them. This implies that eigenstates of the system display highly singular behaviour as Q is varied.

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This letter investigates numerically equation (1) for two types of Liouville numbers (Baker 1975): (1) a general Liouville number given by $Q_n = \sum_{\nu=1}^{\infty} n^{-\nu!}$ and (2) $\tilde{Q}$ satisfying equation (2). In the case of $\tilde{Q}$, we confirm that for all V the energy spectrum is singular continuous and all states are critical as conjectured by AS. This critical wavefunction seems to be of a third type in that it is self-similar but not an algebraic function of the distance. It looks rather like extended wavefunctions connected to each other. This type of wavefunction was also reported in a one-dimensional quasiperiodic system (Kim *et al* 1989a). For a general Liouville number Q_n which does not satisfy equation (2), we obtain the same results: the energy spectrum is singular continuous, and all states are critical regardless of V. In addition, we find that the resistance of the band centre displays oscillations coupled with other large oscillations, and is almost 100 times larger than those of other states (including states near the band edge) at large distances. This anomaly can also be seen in the case of $\tilde{Q}$, but it is not on such a large scale. This is in contrast to the band-centre anomaly in disordered systems where both the density of states and the localisation length diverge (Gorkov and Dorokov 1976, Kappus and Wegner 1981).

A Liouville number is a transcendental number which can be well approximated by rationals (Baker 1975). It is in general defined by the inequality $|Q - p_k/q_k| < 1/(q_k)^k$ with p_k and $q_k \to \infty$ as $k \to \infty$. We can easily see that Q_n satisfies this inequality and therefore is a Liouville number. The Liouville numbers considered by AS satisfy the inequality in equation (2) and constitute a subclass of general Liouville numbers. Such numbers $\tilde{Q}$ can be obtained through the use of the continued fraction expansion $\tilde{Q} = [a_0, a_1, a_2, \ldots]$ (Hua 1982). It we choose, for example, $a_{k+1} = k^{q_k}, k^{q_k-1}, k^{q_k-1}+1$, etc, in the expansion of $\tilde{Q}$, where q_k is the denominator of the kth convergent of $\tilde{Q}$, then it is straightforward to show that equation (2) is satisfied. Thus we obtain $\tilde{Q}_1 = [0, 1, 2, 27, 4^{82}, \ldots]$, $\tilde{Q}_2 = [0, 1, 1, 3, 4096, 5^{28673}, \ldots]$, $\tilde{Q}_3 = [1, 2, 3, 730, 4^{720}+1, \ldots]$ which correspond to the choices $a_{k+1} = k^{q_k}$, k^{q_k-1}, and $k^{q_k-1}+1$, respectively. It is thus obvious that these numbers are extremely close to rationals. For example, $\tilde{Q}_3$ and the rational $[1, 2, 3, 730] = 7303/5112$ differ from each other only by 10^{-400}, and are essentially equal within finite precision.

To study nature of the energy spectrum, we use two different methods. One method is to investigate scaling of B_k, the sum of allowed energy spectra. We find that $B_k \sim q_k^{-\delta}$ like a quasiperiodic system (Kohmoto *et al* 1983). Table 1 shows values of δ for some values of V and for both types of Liouville numbers, Q_2 and $\tilde{Q}_1$. The values of δ for $\tilde{Q}_1$ are similar to those in usual incommensurate systems obtained by Kohmoto (1983). But this scaling can be continued only up to two or three stages. The other method uses the resistance incident on the sample with a certain energy. The dimensionless resistance R is given by the Landauer formula (Landauer 1970) $R = |r|^2/|t|^2$, where r and t denote the reflection and transmission amplitudes, respectively. Figure 1(a) shows the logarithm of geometrical average resistances $\overline{\ln R} \equiv (1/N)\sum_{i=1}^{N} \ln R_i$, where R_i is the resistance of the system with i lattices, at two incident energies $E_1 = -1.678\,204\,063\,944\,9003$ and $E_2 = E_1 + 10^{-15}$, when $Q = \tilde{Q}_3$ and $V = 2.01$. It is remarkable that the behaviour of the resistance at the two energies is strikingly different in spite of the very small difference in energy, $\delta E \sim 10^{-15}$. E_1 and E_2 correspond to an eigenstate and a gap, respectively. Note that the escaping point N_{es} is exactly given by 5112. It is similar to the escaping problem of the transfer matrix (Kohmoto *et al* 1983), where the trace grows rapidly for forbidden states but remains bounded at eigenenergies. The eigenenergies of the system with the lattice size N less than 5112 are almost escaping points, and an extremely small portion is not escaping. Even when

Table 1. The indices δ for various values of V when Q is equal to Q_2 or $\tilde{Q}_1$.

	$V=1.95$	$V=2.00$	$V=2.05$
$Q=Q_2$	0.933 65	1.225 90	1.368 00
$Q=\tilde{Q}_1$	0.764 83	0.974 59	1.286 49

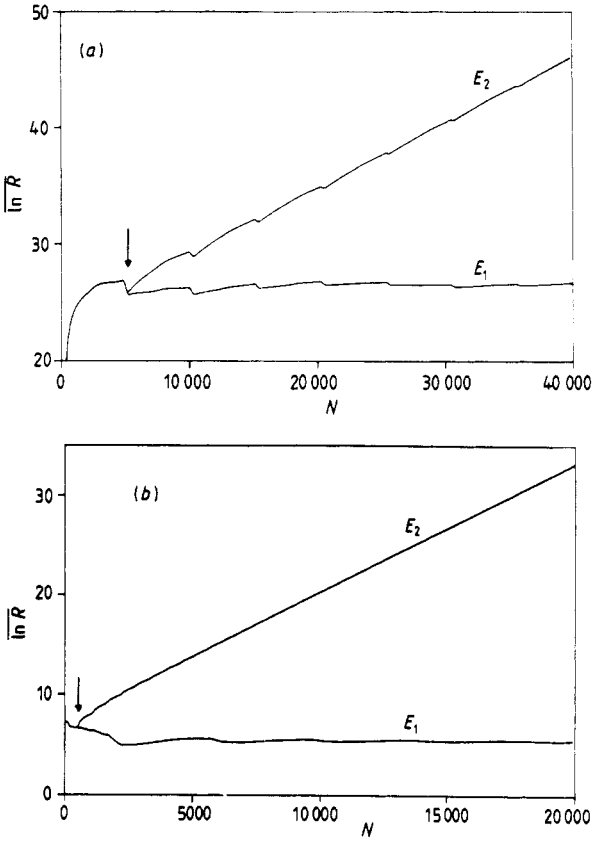

Figure 1. (*a*) N dependence of the logarithm of the geometrical average resistance $\overline{\ln R}$ for $Q=\tilde{Q}_3=7303/5112$ and $V=2.01$, for an eigenenergy $E_1=-1.678\,204\,063\,944\,9003$ and a forbidden energy $E_2=E_1+10^{-15}$. The arrow denotes the escaping point, $N_{es}=5112$. (*b*) $\overline{\ln R}$ for $Q=Q'=7303/5113$ and $V=1.9$, for $E_1=2.519$ and $E_2=E_1+10^{-4}$. The arrow denotes the escaping point $N_{es}=595$.

$v\leqslant 2$, the same behaviour is found with $\delta E=10^{-9}$ and 10^{-6} for $V=2.0$ and 1.90, respectively.

For comparison, we show in figure 1(*b*) the logarithm of average resistances at two energies $E_1=2.5219$ A and $E_2=E_1+10^{-4}$ when $Q=Q'\equiv 7303/5113\simeq\tilde{Q}_3+10^{-4}$. In this case the escaping point is not 5113 but 595, as can be seen from the continued fraction expansions of Q' and $\tilde{Q}_3$; i.e. $7303/5113=[1,2,2,1,80,2,4]$ and $7303/5112=[1,2,3,730]$ respectively. Note that the numbers 2 and 4 appearing after 80 in the expansion of Q' change the spectrum only slightly. Thus almost all eigenenergies of the system with $N=595$ survive even when N becomes 5113. If we combine blocks of 5113 sites (or, almost equivalently, blocks of 595 sites) in this case ($Q=Q'$), we

would obtain finite or absolutely continuous spectra in contrast to the previous case ($Q = \tilde{Q}_3$), where infinitesimal or singular continuous spectra would be obtained. This shows the striking difference between singular continuous and absolute continuous spectra, and suggests that the energy spectra for Q equal to a Liouville number are singular continuous regardless of V.

Figure 2 shows behaviour of the wavefunctions when $Q = \tilde{Q}_3$ and (a) $V = 1.90$, $E = -2.521\,987$; (b) $V = 2.0$, $E = -2.579\,085\,843\,24$; (c) $V = 2.01$, $E = -1.678\,204\,063\,994\,9003$. Periodic boundary conditions have been imposed and wavefunctions have been normalised. It appears in figure 2(a) that the states are composed of many extended states connected to each other. Note that there exists a singularity at every lattice site $5112n$, where n is an integer. The insets show the detailed behaviour up to first 7 and 5112 sites. ($\tilde{Q}_3$ can be successively approximated by 10/7 and 7303/5112.) Self-similarity is obvious. Figures 2(b) and 2(c) also display features in general similar to those of figure 2(a) except for bulging of the central region of blocks. We believe that these are critical wavefunctions of the type suggested by AS. They are self-similar and almost extended-like, not decaying to zero at large distances.

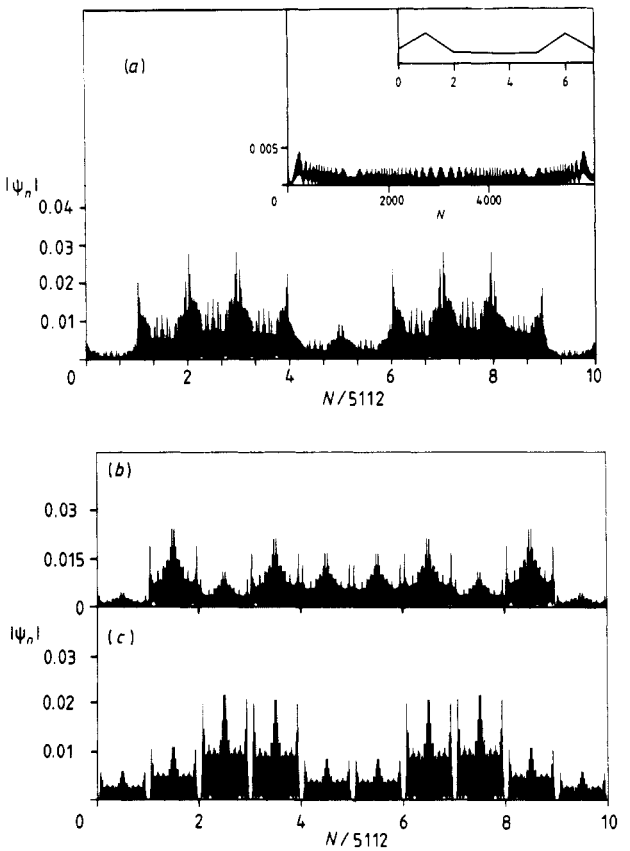

Figure 2. Behaviour of the wavefunction when $Q = \tilde{Q}_3$, and (a) $V = 1.90$, $E = -2.521\,978$; (b) $V = 2.0$, $E = -2.579\,085\,8434$; (c) $V = 2.01$, $E = -1.678\,204\,063\,944\,9003$. The insets in ($a$) exhibit the wavefunctions of one block (of 5112 sites and of 7 sites). Self-similarity can be observed.

Figure 3 shows N-dependence of the average resistance $\bar{R}$ for the states (a) at the band centre and (b, c) near the edge when $Q = Q_2$. In small scales, as can be seen in the inset of figure 3(a), it converges rapidly to a constant value like that of extended states. In large scales, however, it converges to another value, which is almost 100 times larger. We expect that this behaviour appears self-similarly as in the case of critical states in a quasiperiodic system of which the average resistance has been reported to show self-similar oscillations (Schneider *et al* 1987, Sutherland and Kohmoto 1987, Kim *et al* 1989a, b). Note, however, that the second oscillation length is very large compared with that of critical states in a quasiperiodic system. This anomaly exists only in those states very near the band centre, and disappears when $V < 1.26$ or $V > 2.7$. In contrast, the curves in figures 3(b) and 3(c), which correspond to $V = 1.62$ and 1.90, respectively, apparently converge to a single constant value. The convergence is not uniform but composed of coupled oscillations, implying critical states (Kim *et al* 1989a, b). It is remarkable that when the sample length is large, as can be seen from figure 3, the resistance of the band centre is almost 100 times larger than that of the states near the band edge. This is presumably due to the large difference between denominators of successive rational approximants of a Liouville number Q_2.

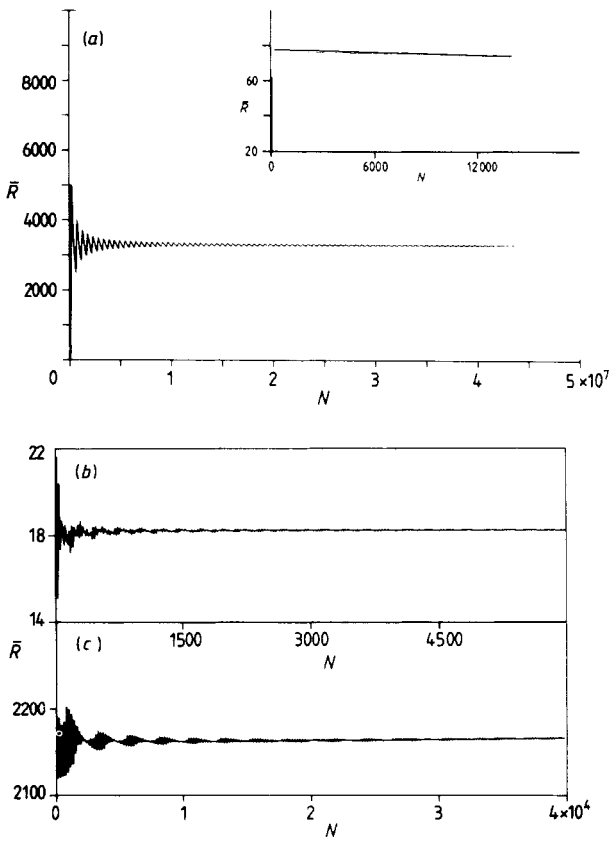

Figure 3. N dependence of the average resistance $\bar{R}$ when $Q = Q_2$: (a) at the band centre for $V = 1.62$, $E = 0$; (b) at the band edge for $V = 1.62$, $E = -1.02$; (c) at the band edge for $V = 1.90$, $E = -2.745$.

To find the origin of this anomaly, we consider the equation describing the inverse localisation length α (Lambert and Thorpe 1982, Stone *et al* 1983)

$$\alpha = \alpha_1 + \alpha_2(\varphi)$$

$$\alpha_1 = \sum_{i=1}^{N} \ln(1+\rho_i) \tag{3a}$$

$$\alpha_2(\varphi) = \frac{1}{N}\sum_{i=1}^{N} \ln(1+t_i+2t_i^{1/2}\cos\varphi_i) \tag{3b}$$

where

$$\rho_i = \varepsilon_i^2/(4-E^2)$$

$$t_i = b_i^2 a_{i-1}^2 \qquad a_i = [R_i/(1+R_i)]^{1/2} \qquad b_i = [\rho_i/(1+\rho_i)]^{1/2}$$

and ε_i denotes the site energy $V\cos(2\pi Qn+\theta)$. The recursion relation of the phase φ is given by

$$a_i \exp[\mathrm{i}(\varphi_{i+1}-\delta_{i+1})] = [b_i + a_{i-1}\exp(\mathrm{i}\varphi_i)]/[1+b_i a_{i-1}\exp(\mathrm{i}\varphi_i)] \tag{4}$$

where

$$\delta_i = \mu_i + \mu_{i-1} - \nu_i + \nu_{i-1}$$

$$\mu_i = \tan^{-1}[\varepsilon_i/(4-E^2)^{1/2}]$$

and $\nu_i = \pi/2 - 2ik + \pi/2(1-\varepsilon_i/|\varepsilon_i|)$ with k given by the relation $E = 2\cos k$. We can see from (3*a*) that α_1 at the band centre is smaller than that near the band edge and they converge rapidly to constant values. Thus the anomaly is due to α_2, where the phase φ plays an important role. Equation (3*b*) shows that the φ in the range $\pi/2 < \varphi < 3\pi/2$ give negative contribution to α_2, while the φ near 0 or 2π give a large positive contribution to α_2. Indeed, in strongly disordered systems (Stone *et al* 1983), all the φ populate near 0, leading to strong localisation. Figure 4 shows $P(\varphi)$, the probability distribution of φ for $N = 10^5$, $V = 1.62$ and $E = 0.0$. Note that there are many φ near 0 and 2π as in the case of strongly disordered systems. Such a distribution of phase correlations leads to the anomaly. Without the peaks near 0 and 2π, the anomaly would not exist.

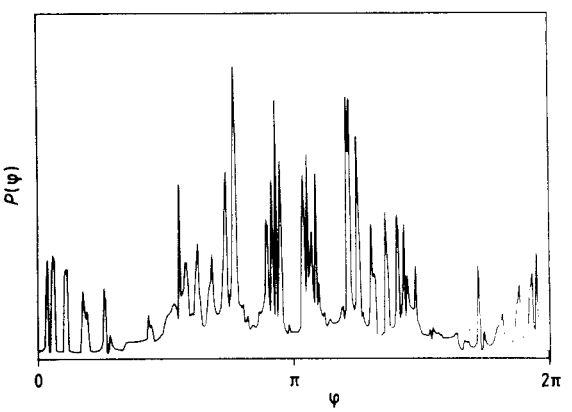

Figure 4. Probability distribution $P(\varphi)$ for $N = 10^5$, $V = 1.62$ and $E = 0.0$. The peaks near $\varphi = 0$ and 2π are peculiar to this system.

In conclusion, we studied the almost-Mathieu equation for two types of the Liouville numbers. It is demonstrated that the energy spectrum is singular continuous and all states are critical regardless of V. We also found an unusual band-centre anomaly, the resistance of the states at the band centre displaying oscillations coupled with other large oscillations.

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