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On the mobility edges in one-dimensional incommensurate systems

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Abstract. The transfer matrix method and successive average resistivity criterion for localisation of electronic states have been used to study the Soukoulis–Economou model of the one-dimensional system with incommensurate potentials. Numerical studies show that, for a case studied extensively, where $E_n = 1.9[\cos(0.7n) + \frac{1}{3}\cos(1.4n)]$, all electronic states of the middle sub-bands are extended and there is no so-called 'local mobility edge'.

1. Introduction

The recently discovered incommensurate phenomena in some physical systems possessing at least two periodicities which are incommensurate with each other have generated considerable theoretical interest. Examples of such physical systems are crystals containing a charge-density wave (Bruesch *et al* 1975) and a spin-density wave (Wilson *et al* 1975), mercury chain compounds (Chiang *et al* 1977) and certain crystals that have distortion waves which are incommensurate with the underlying Bravais lattice (de Wolff *et al* 1981). Incommensurability also plays a role in the electronic properties in high magnetic fields (Hofstadter 1976). In some sense, the incommensurate systems are intermediate between periodic and random systems. Therefore, unlike amorphous materials, there is quasi-periodic long-range order in an incommensurate crystal, which gives the crystal very unusual physical properties. The dependence of the electronic properties on the type of incommensurate potential has been examined by Llois *et al* (1984), and the ground-state properties of a tight-binding Hamiltonian with incommensurate site energy have been extensively investigated—a detailed review article has recently been published on this field (Sokoloff 1985).

The Aubry model, a single-particle tight-binding model with incommensurate potential, has been extensively studied (Aubry and Andre 1979, Sokoloff 1985). The Hamiltonian of the model is simply

$$H = \sum_{n=-\infty}^{\infty} E_n |n\rangle\langle n| + \sum_{n=-\infty}^{\infty} t(|n\rangle\langle n+1| + |n+1\rangle\langle n|) \tag{1}$$

where $|n\rangle$ is the Wannier state, t is the nearest-neighbour hopping integral and the site

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energy $E_n = V\cos(Qn)$. V is the potential strength and the wavevector Q is incommensurate with π. Although the sinusoidal potential of the single-particle Aubry model is not expected to be an exact description of the potential seen by the electrons when the crystal is incommensurate, this is a simple and successful model which contains the main characters of the incommensurate systems. The Aubry model possesses very interesting electronic properties. Azbel (1979) has shown that its energy spectrum has the structure of a devil's staircase, and Bellissard and Simon (1982) have proved that it has an energy spectrum which is nowhere dense. Firstly, the whole energy spectrum consists of sub-bands, the number of which depends on the wavevector Q. If we increase the resolution of the eigen-energy, each sub-band will split into sub-sub-bands. With a further increase in the resolution, each sub-sub-band splits again. In this way a hierarchical structure, or so-called self-similar structure, of the energy spectrum is shown. Therefore, the spectrum is Cantor set like. For the Aubry model, on the contrary, in contrast with a one-dimensional random system in which all the states are localised, Aubry and Andre (1979) have shown by duality theory that a metal–insulator transition occurs for $V = 2t$; this is called the critical point and means that, for $V > 2t$, all states are localised and, for $V < 2t$, all states are extended. Consequently, for a fixed V the electronic spectrum has such a property that all states have the same degrees of localisation and no mobility edge exists. The localisation of the electronic states is independent of the energy. However, it should be pointed out that the duality theory is not a rigorous theory with full generality. A striking result has been given by Avron and Simon (1982) who prove exactly that, if $Q/2\pi$ is a Liouville number, then for any Q in the region $V > 2t$ the spectrum is singular continuous (intermediate state) but not a pure point spectrum (localised state). At the same time, Azbel (1979) and Sokoloff (1981) have claimed that in the region $V < 2t$ the eigenstates are not all extended and there is a mobility edge. However, Suslov (1982) has performed a renormalisation group study to show the absence of such a mobility edge. On the contrary, all the numerical results based on different criteria of localisation for the Aubry model confirm the conclusion of the duality theory that all states are extended in the region $V < 2t$ and there is no mobility edge (Llois *et al* 1984, Liu 1988). The absence of the mobility edge, i.e. the fact that the localisation of states is independent of energy, is quite a surprising result. A plausible explanation is that, on the one hand, the incommensurate systems are the same as random systems in which the states at the tails of the energy band become localised more easily than those at the centre. On the other hand, for the Aubry model $E_n = V\cos(Qn)$, the local site-energy spacings $\Delta E_n = V\{\cos[Q(n+1)] - \cos(Qn)\}$ become smaller near the band edges and this facilitates electronic propagation. It seems that these two opposing tendencies cancel each other so that the localisation of electronic states would be independent of the energy and there is no mobility edge. To check this physical explanation, Soukoulis and Economou (1982) have suggested a modified model which contains two sinusoidal potentials as follows:

$$E_n = V[\cos(Qn) + V_1\cos(2Qn)]. \tag{2}$$

It is easy to see that, for this modified model, the superposition of the two sinusoidal potentials with different wavevectors destroys the symmetry in the Aubry model and makes the local site-energy spacings far smaller at low energies than at high energies. Consequently, the eigenstates with higher energies are easier to localise than those with lower energies and one can expect the mobility edge to appear. If the mobility edge does appear, this would be a very remarkable result because it would be the first time that a mobility edge had been found in one-dimensional systems. To justify their conjecture

numerically, Soukoulis and Economou calculated the following case which contains nine sub-bands:

$$E_n = 1.9[\cos(0.7n) + \tfrac{1}{3}\cos(1.4n)] \qquad t = 1. \tag{3}$$

They found a mobility edge at around $E = 0.7$ between sub-bands 6 and 7 numbered from the low-energy side. All states from the first to sixth sub-bands are extended and all are localised from the seventh to ninth sub-bands. We call this mobility edge which separates the extended states from the localised states in the whole spectrum the 'global mobility edge'. Using the real-space renormalisation group decimation method and the Thouless criterion of localisation, Chao *et al* (1985) have reported that there were two global mobility edges in the same system: one between sub-bands 6 and 7 as detected by Soukoulis and Economou and an additional one between sub-bands 2 and 3. Moreover, they found that in sub-bands 3, 4, 5 and 6 the states in the centre of the sub-band are extended but that states in the edges are localised. This means that each of the sub-bands 3, 4, 5 and 6 has two mobility edges which separates extended states from localised states in the sub-band. Chao *et al* call these mobility edges which appear in the sub-bands 'local mobility edges'. Zheng and Zhu (1986, 1987) by using the criterion of localisation of the self-energy convergent lengths have confirmed the existence of the local mobility edges of sub-bands 3, 4, 5 and 6 and the global mobility edge between sub-bands 6 and 7, but not the global mobility edge between sub-bands 2 and 3. Furthermore, they conjecture that a 'hierarchical structure of the mobility edges' may also exist. This means that the sub-bands in any hierarchy of the energy spectrum which has a hierarchical structure would have their own two local mobility edges. If this conjecture is confirmed, the self-similarity, which is characteristic of the energy spectrum of the incommensurate systems, would be far more pronounced. It should exist not only in the energy spectrum but also in the electronic transport properties. In this paper, we concentrate on a study of the existence of the local mobility edge for the Soukoulis–Economou model.

2. Localisation and mobility edge

For the Aubry model at the critical point $V = 2$ the total bandwidth of the energy spectrum (measure of spectrum) is zero (Bellissard *et al* 1983). This means, rigorously speaking, that the eigenstates no longer condense to form a continuous band. For the studied case $V = 1.9$, although the total bandwidth of the spectrum is not zero, all the sub-bands have split up into satellite-like sub-sub-bands. This is also so for the Soukoulis–Economou model. Therefore, to locate the sub-sub-bands correctly and to determine their widths is extremely important for the study of the electronic localisation of the incommensurate systems.

In the same way as in previous work (Soukoulis and Economou 1982, Chao *et al* 1985, Zheng and Zhu 1986) we study the case in equation (3), which contains nine sub-bands. To search for the local mobility edges, we investigate the three middle sub-bands 4, 5 and 6, for which the bandwidths are wider. Using the method of Dean (1972), we locate the sub-bands and calculate the density of states (DOS). The fine structure of the three sub-bands is shown in figure 1. The DOSs are calculated for the energy interval $\Delta E = 0.001$ and are in agreement with previous work (Zheng and Zhu 1986). In figure

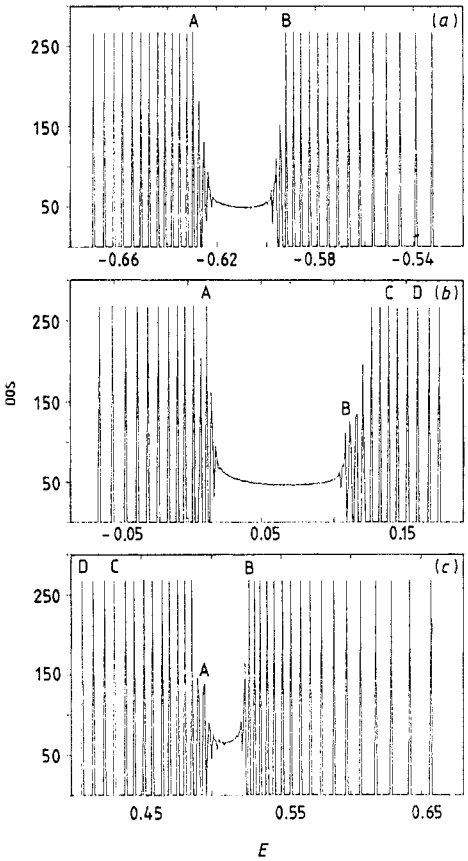

Figure 1. The energy spectrum for (*a*) sub-band 4, (*b*) sub-band 5 and (*c*) sub-band 6. The sub-sub-bands labelled A, B, C and D are the same as those listed in table 1.

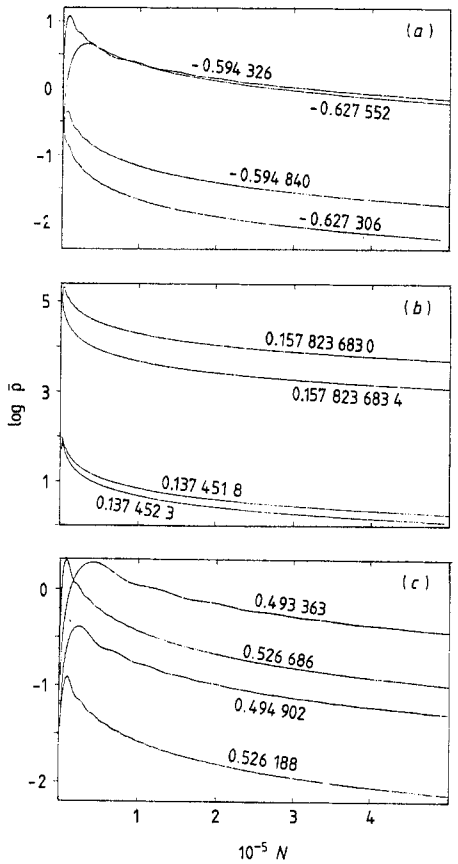

Figure 2. Plots of the logarithmic average resistivity against system length N for (*a*) sub-band 4, (*b*) sub-band 5 and (*c*) sub-band 6. The fact that the average resistivity monotonously decreases with increasing N shows that these states are extended.

1, we can see that each sub-band consists of a group of sub-sub-bands, of which the broadest is in the centre and is surrounded by other narrower satellite sub-sub-bands. The figure seems also to show that the satellite sub-sub-bands have the same DOSs, but we should point out that this is not true. The fact that they have the same DOSs is because by definition the DOS equals $\Delta N/\Delta E$ and so by Dean's method we should firstly choose an energy interval ΔE and then calculate the number of eigenstates ΔN in ΔE. For the present case, every sub-sub-band has almost the same number of eigenstates and the real bandwidth of sub-sub-bands, except the middle ones, are smaller than the chosen energy interval $\Delta E = 0.001$. Therefore the numerical results of the DOSs of most sub-sub-bands would have the same values. In fact, the real widths of the sub-sub-bands are so different that the differences between the DOSs could even reach seven orders of magnitude (table 1). The calculation to determine the widths of the sub-sub-bands requires much computer time. We have chosen some satellite sub-sub-bands from each sub-band for study. Table 1 shows the numerical results, and we can see that, the further the satellite sub-sub-band is from the centre, the narrower is its width. For example,

Table 1. Numerical results.

Sub-band	Energy range	Sub-sub-band	Energy range
4	From −0.670 to −0.532	A	From −0.627552 to −0.627305
		B	From −0.594841 to −0.594325
5	From −0.059 to 0.173	A	From 0.012055 to 0.012493
		B	From 0.109797 to 0.111920
		C	From 0.1374518 to 0.1374523
		D	From 0.15782368300 to 0.15782368334
6	From 0.407 to 0.657	A	From 0.493363 to 0.494902
		B	From 0.526188 to 0.526686
		C	From 0.43090583801 to 0.43090583833
		D	From 0.40791766876460 to 0.40791766876477

sub-sub-band D of sub-band 6 has a bandwidth of only 10^{-13}. This suggests to us that, if we could not exactly determine the location and width of the sub-sub-bands, we could easily choose the incorrect eigen-energies in the gaps, which will lead to inaccurate determination of the localisation.

To study the localisation of the eigenstates for the Soukoulis–Economou model, as a powerful criterion of the localisation, we choose the 'successive average resistivity' which was developed by one of the present authors and co-workers (Liu and Chao 1986, Liu and Riklund 1987). For this purpose, we have to calculate the resistivity which is a reliable physical quantity to estimate the localisation and can be examined by experiment. To calculate the resistivity, the formula of Landauer (1970) combined with the transfer matrix method is a very powerful technique and has been used extensively.

We study a finite incommensurate system containing $N+1$ atoms and of length N (here the lattice spacing is taken as unity) and embed this finite system as an incommensurate segment in an infinite, perfectly conducting ordered chain. For this system the tight-binding Hamiltonian is

$$H = \sum_{n=-\infty}^{\infty} E_n |n\rangle\langle n| + \sum_{n=-\infty}^{\infty} t(|n\rangle\langle n+1| + |n+1\rangle\langle n|) \tag{4}$$

where t is the hopping integral and E_n are the site energies. In the perfectly ordered chain, we take E_n to be zero; in the embedded incommensurate segment, E_n is given by the Soukoulis–Economou model: $E_n = V[\cos(Qn) + V_1 \cos(2Qn)]$.

In the tight-binding base and if we choose $t = 1$, the equation of motion for the amplitudes of the eigenfunction $\Psi = \Sigma_n a_n |n\rangle$ is

$$(\varepsilon - E_n)a_n - a_{n+1} - a_{n-1} = 0. \tag{5}$$

We define the promotion matrix as follows:

$$P^{(n)} \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix} \equiv \begin{pmatrix} \varepsilon - E_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_n \\ a_{n-1} \end{pmatrix} = \begin{pmatrix} a_{n+1} \\ a_n \end{pmatrix}. \tag{6}$$

The relation which connects both ends of the incommensurate segment is

$$\begin{pmatrix} a_{N+2} \\ a_{N+1} \end{pmatrix} = \left(\prod_{i=1}^{N+1} P^{(i)} \right) \begin{pmatrix} a_1 \\ a_0 \end{pmatrix} \equiv \mathbf{P}_N \begin{pmatrix} a_1 \\ a_0 \end{pmatrix}. \tag{7}$$

It can be proved (Liu and Chao 1986, Liu and Riklund 1987) that the Landauer formula

for the energy-dependent dimensionless resistance $R(E, N)$ of a finite one-dimensional system embedded in a perfectly ordered chain is

$$R(E, N) = R_N/T_N = |(T_N)_{12}|^2 \tag{8}$$

where $(T_N)_{ij}$ is an element of the transfer matrix $\mathbf{T}_N$.

$$\mathbf{T}_N = \boldsymbol{\theta}\mathbf{S}^{-1}\mathbf{P}_N\mathbf{S}$$

$$\boldsymbol{\theta} = \begin{pmatrix} \exp[ik(N+1)] & 0 \\ 0 & \exp[-ik(N+1)] \end{pmatrix} \qquad \mathbf{S} = \begin{pmatrix} \exp(-ik) & \exp(ik) \\ 1 & 1 \end{pmatrix}. \tag{9}$$

We define the average resistivity as

$$\bar{\rho}_N = \sum_{i=1}^{N} \frac{\rho_i}{N} = \frac{1}{N}\left(\frac{R(E,1)}{1} + \frac{R(E,2)}{2} + \ldots + \frac{R(E,N)}{N}\right) \tag{10}$$

where N is the length of the embedded incommensurate segment, i.e. the incommensurate system studied, $R(E, j)$ is the dimensionless resistance which is determined by the Landauer formula (8).

For metallic crystalline solids, ρ_i should be independent of the size of the system; so, at zero temperature, $\bar{\rho} = \rho_i = \rho = 0$. For an extended state in an incommensurate system, the reflection coefficient is smaller than unity, and we have

$$\rho_N = (R_N/1 - R_N)(1/N) \xrightarrow{N\to\infty} 0$$

and

$$\bar{\rho}_N \xrightarrow{N\to\infty} 0.$$

Therefore, if we successively calculate the respective average resistivities with increasing N, after reaching some value of N the average resistivity will monotonically decrease if the state is extended. Quite the contrary is true if the state is localised and the wavefunction is exponentially localised. The dimensionless resistance can be written as

$$R(E, N) = R_N/1 - R_N \propto \exp(N/L)$$

where L is the localisation length. Both the resistance and the last term of the average resistivity (10) will diverge if N goes to infinity. In this case, if we successively calculate the respective average resistivities with increasing N, the average resistivities will monotonically and quickly increase. Consequently, the trend of the successive average resistivities sharply distinguishes the extended state from the localised state and the energy gap. We can use this trend of successive average resistivities as the criterion of the extended state. Using the successive average resistivity criterion, we have carefully investigated the electronic states of the sub-sub-bands listed in table 1 from the edges to the centre of bands. It was found that the curves of the successive average resistivities for all studied states monotonically decrease after a small value of the system length N, which means that all states in these sub-sub-bands are extended. In figure 2, we have plotted several typical graphs of logarithmic average resistivity. The behaviour of the curve, which first increases for a small range of system lengths N, results from the existence of the boundary resistance (Azbel 1983). Because there is no localised state to

be found, our conclusion is that all states are extended for the three sub-bands studied and no so-called local mobility edge exists.

3. Summary and discussion

Let us recall all the previous work on the subject under study. Soukoulis and Economou (1982) found that all states of sub-bands 1–6 are extended, and there exists a mobility edge (a global mobility edge) between sub-bands 6 and 7 at around $E = 0.7$. By using the renormalisation group method, Chao *et al* (1985) confirmed the existence of this global mobility edge. Moreover, they reported that in the sub-bands 3, 4, 5 and 6, the localisation of electronic states is not unique, but at the same time there exist extended states (the centre of each of the sub-bands) and localised states (the edges of each of the sub-bands). This means that in each of sub-bands 3, 4, 5 and 6 there are two mobility edges which they called local mobility edges. By using the criterion of localisation of the self-energy convergent length, Zheng and Zhu (1986, 1987) confirmed the existence of the local mobility edge. Considering the self-similarity of the energy spectrum (or the hierarchical structure of an energy spectrum) for incommensurate systems, they furthermore conjectured that a hierarchical structure of the local mobility edge may exist. If we review this problem, we see that the existence of the local mobility edge relies on the coexistence of two kinds of electronic state with different localisations, i.e. extended states and localised states, in each of the studied sub-bands. Therefore the investigation of this coexistence is the key to the problem. Because of the Cantor-set-like property of the spectrum for an incommensurate system, it is therefore extremely important to determine correctly the structure of the sub-bands. For this purpose, we determined the bandwidth of sub-sub-bands up to 10^{-13} and then examined the localisation using the successive average resistivity criterion. The calculation shows that all the states of the studied sub-bands are extended. This result implies that there is no so-called local mobility edge, which is different from the results of Chao *et al* and Zheng and Zhu. The question is how easy is it to see, if we compare the calculations performed by the different groups, whether the different conclusions drawn by different workers mainly arise from the chosen accuracy of calculation. It is most evident that, for example, if we could not exactly locate the satellite sub-sub-bands with an extremely high accuracy, it would be possible to take the 'energy value' in the band gaps as the eigen-energy. Certainly this false 'eigenstate' is 'localised' by any criterion of localisation; then, misleadingly, the 'localised states' and the extended states would 'coexist' in the studied sub-band and a so-called local mobility edge would be found. Of course, this is not true. We believe that, following an improvement in the chosen accuracy of computation, the same conclusion could be drawn even from different calculation methods and criteria of localisation.

Now we give a brief comment on the controversial local mobility edge and the hierarchical structure of the local mobility edge conjectured by Zheng and Zhu (1986, 1987). It is well known that the self-similar or hierarchical structure of the energy spectrum for incommensurate systems comes from the quasi-periodicity of the system. If we rewrite the wavevector $Q = 2\pi\alpha$ and use for α the continued-fraction expansion, then α would be approximated by a series of rational numbers. In this way, the incommensurate systems could be approximated by a series of commensurate systems with definite periodicity. These serial periodicities result in self-similarity (or hierarchical structure) of the energy spectrum (Liu and Chao 1986). On the contrary, the appearance

of localised electronic states is due to multiple scattering of the impurities or aperiodic potentials of the studied system, which should not have self-similarity. In our opinion, the local mobility edge discussed and the conjectured hierarchical structure appearing in the mobility edges lack the necessary physical foundation. Our highly-accurate calculation has proved this point.

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