Computer experimental evidence for an energy-dependent metal-insulator transition in a one-dimensional incommensurate system

1987 J. Phys. A: Math. Gen. 20 L71

(http://iopscience.iop.org/0305-4470/20/2/006)

J. Phys. A: Math. Gen. **20** (1987) L71-L75. Printed in the UK

LETTER TO THE EDITOR

Computer experimental evidence for an energy-dependent metal–insulator transition in a one-dimensional incommensurate system

K A Chao and G Wahlström

Department of Physics and Measurement Technology, University of Linköping, S-58183 Linköping, Sweden

Received 17 October 1986

Abstract. Based on the Landauer formula for DC conductivity, a computer experiment is performed on a chain of 10^7 atoms to show the energy-dependent metal-insulator transition in the Aubry model. The self-similarity of conducting channels in the conducting phase is also demonstrated.

One of the most discussed issues of the one-dimensional Aubry (1978) model

$$H(Q)=\sum_{n=-\infty}^{\infty}[V\cos(Qn)a_n^{\dagger}a_n+t(a_{n+1}^{\dagger}a_n+a_{n-1}^{\dagger}a_n)] \tag{1}$$

where Q is incommensurate to π, is the characteristic features of the eigenfunctions in the vicinity of $V/t=2$. Aubry and André (1980) showed that the Hamiltonian (1) is self-dual with respect to the Fourier transform. By assuming exponential localisation of all possibly existing localised states, Aubry and André combined the self-duality property and a formula developed by Thouless (1972) to conclude that in the regime $V/t>2$ all eigenstates are exponentially localised, whilst in the regime $V/t<2$ all eigenstates are Bloch-like extended. Although many succeeding works in the field found no disagreement with this conclusion, there are controversial arguments regarding the delocalisation of eigenstates in the region $V/t<2$.

Avron and Simon (1982) and Simon (1982) have shown that if Q/π is extremely well approximated by a rational number (namely, Q/π is a Liouville number), there exists an unusual type of eigenfunction of (1) which we call a *resonance state*. A resonance state has large amplitudes at positions separated by long distances. Even for irrational Q/π resonance, states also appear if $V/t=2$ (Avron and Simon 1982). Furthermore, resonance states were discovered later in other models similar to (1) but with the potential $\cos(Qn)$ replaced by $\tan(Qn)$ (Grempel *et al* 1982, 1984), or by $\cos(Qn)+\frac{1}{3}\cos(2Qn)$ (Chao *et al* 1985).

Resonance states are neither exponentially localised nor Bloch-like extended. Since Thouless' formula (1972) applies only to exponential localisation, the energy-independent metal-insulator transition (MIT) at $V/t=2$ derived by Aubry and André (1980) may be modified. It has been shown that the MIT is energy dependent and so mobility edges exist in some non-self-dual models, for example, the $\cos(Qn)+\frac{1}{3}\cos(2Qn)$ potential model (Soukoulis and Economou 1982, Chao *et al* 1985). In this non-self-dual model, for fixed value of V/t, as the MIT is approached from the metallic side, the DC

0305-4470/87/020071+05$02.50

conductivity $\sigma(E)$ shows a superperiodic structure with superperiod $\mathscr{L}(E)$ (Liu and Chao 1986). If we approximate $Q/2\pi$ sequentially by Liouville numbers l_1/L_1, $l_2/L_2, \ldots$, with $L_i < L_{i+1}$, then when E approaches a mobility edge E_c, $\mathscr{L}(E)$ increases and at well defined energies E_i, has values $\mathscr{L}(E_i) = L_i$. Consequently, via the Liouville number approximation of $Q/2\pi$, the energy-dependent MIT of the $\cos(Qn)+\frac{1}{3}(2Qn)$ potential model is closely related to the existence of resonance states near mobility edges.

If we incorporate these results to the above-mentioned existences of resonance states in the Aubry model, it is worthwhile to perform a careful computer experiment to determine whether the MIT in the vicinity of $V/t = 2$ is energy dependent. This is the purpose of the present letter.

Giving the values of V/t and Q, we use the transfer-matrix method to calculate the energy-dependent total transmission coefficient $T(E)$ of a chain of 10^7 atoms and then use the Landauer formula (1970) to obtain the dimensionless resistance $R(E) = [1 - T(E)]/T(E)$. The computation procedure has already been given earlier (Liu and Chao 1986). If $T(E)$ is less than 10^{-8}, the corresponding eigenstate is classified as non-conducting. It is important to mention that we did not find any value of $T(E)$ between 10^{-8} and 5.3×10^{-5}. Hence, all conducting states have $T(E)$ greater than 10^{-5}. Furthermore, for almost all non-conducting states, $T(E)$ decreases to 10^{-8} within a distance much shorter than the whole chain length.

We set $t = 1$ as our energy units. It is well known that the transfer-matrix method works only for eigenenergies $|E| < 2t = 2$. For a given value of $V^* = (V_c - V)/V_c = (2 - V)/2$, the calculated results will be presented in the Q-E plane. Because of symmetry, we only need to study the region $0 < E < 2$ and $0 < Q < \pi$. Let us first calculate the eigenenergy spectra of (1) with Q/π approximated by rational numbers. In figure 1 the allowed eigenenergies are indicated by black segments for V^* between 0 and 10^{-2}, since spectra for different V^* are indistinguishable within the accuracy of plotting. The same energy-band structures were first obtained by Hofstadter (1976).

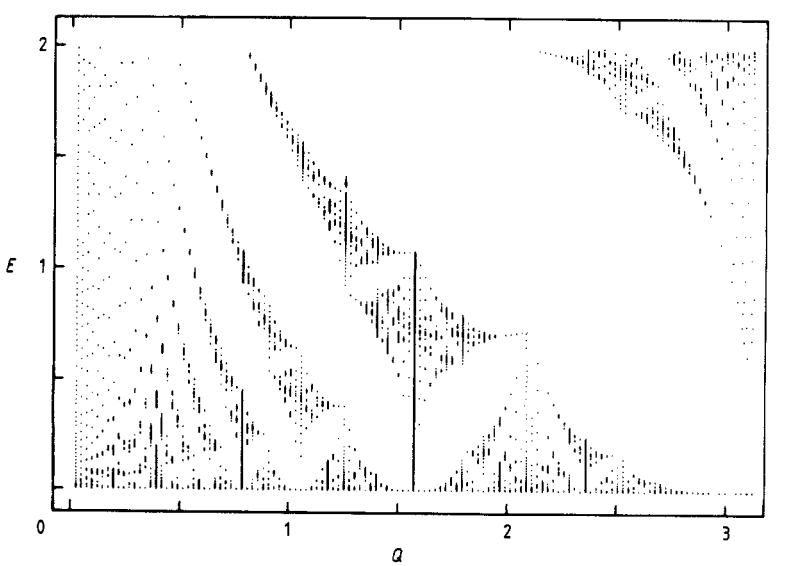

Figure 1. Bands of allowed eigenenergies for $0 < V^* < 10^{-2}$, where $V^* = (V_c - V)/V_c = (2 - V)/2$.

For $V^* = 10^{-2}$ we have calculated the resistance at every point ($Q = n\delta Q$, $E = m\delta E$) in the Q-E plane with $\delta Q = 0.0125$ and $\delta E = 0.000\,25$. The eigenenergies of conducting states are marked by black dots in figure 2. If we compare figures 1 and 2, obviously not all eigenstates are conducting. Similar results on conducting eigenstates are shown in figure 3 for $V^* = 10^{-3}$, but with smaller $\delta Q = 0.0025$ and $\delta E = 0.000\,05$. The inset in figure 3 is for $V^* = 10^{-4}$ with even smaller $\delta Q = 0.0005$ and $\delta E = 0.000\,01$. We see

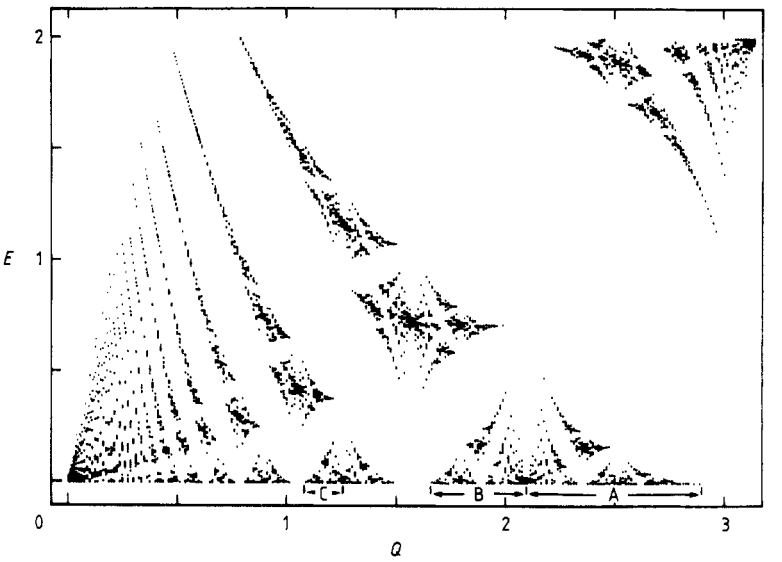

Figure 2. Conducting eigenstates are marked by dots in the Q-E plane with $\delta Q = 0.0125$ and $\delta E = 0.000\,25$, and $V = 10^{-2}$.

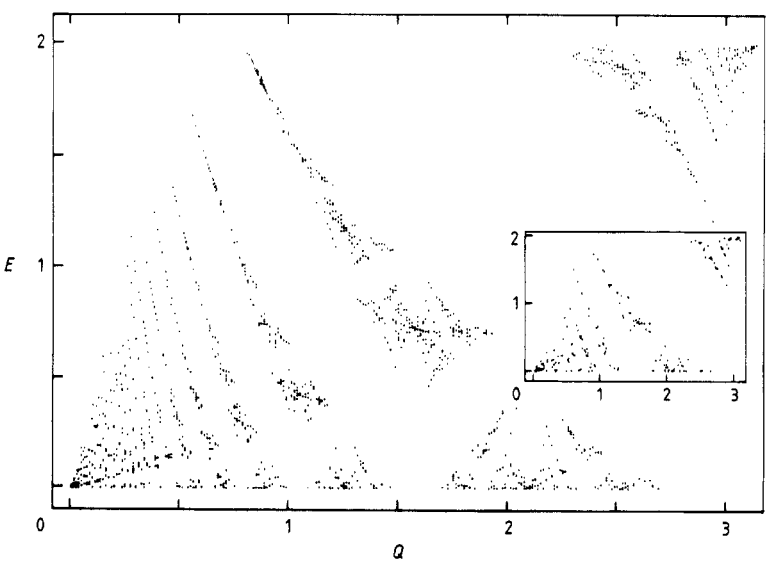

Figure 3. Similar to figure 2 for $V^* = 10^{-3}$ but with $\delta Q = 0.0025$ and $\delta E = 0.000\,05$. Inset is for $V^* = 10^{-4}$ with $\delta Q = 0.0005$ and $\delta E = 0.000\,01$.

a continuous elimination of conducting states as $V^* \to 0$. At $V^* = 0$ we found no conducting states.

Let us investigate more thoroughly the case $Q = 1.2517$ which is very close to the Q value marked by an arrow in figure 1. With $\delta E = 10^{-3}$, the conducting states between $E = 1.342\,342$ and $E = 0.926\,158$ for $V^* = 10^{-2}$ are shown in figure 4 by row A. Now we study the region R in row A for $V^* = 0.02/2^n$ with $n = 1, 2, \ldots, 8$. For $1 \leqslant n \leqslant 5$ we set $\delta E = 10^{-5}$, and for $6 \leqslant n \leqslant 8$ we set $\delta E = 10^{-6}$. The conducting states are shown in figure 4 by the 8 rows of group R. Similarly, we study the region S in row A with $\delta E = 10^{-6}$ for $1 \leqslant n \leqslant 4$. For convenience of presentation, we have shifted the origin of E for each n, and the results are plotted in figure 4 as group S_1. If we further decrease the energy interval to $\delta E = 10^{-7}$, the conducting states for $5 \leqslant n \leqslant 8$ are shown in figure 4 as group S_2, but with the horizontal energy scale expanded by a factor 2.3.

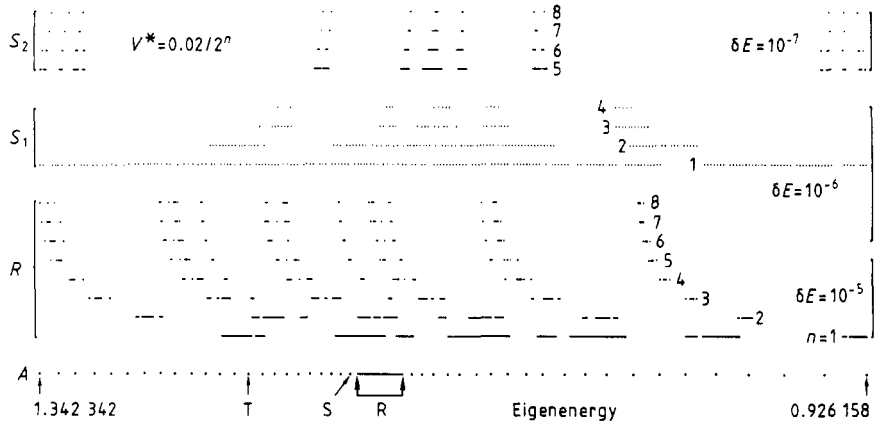

Figure 4. Conducting states for $Q = 1.2517$. See text for details.

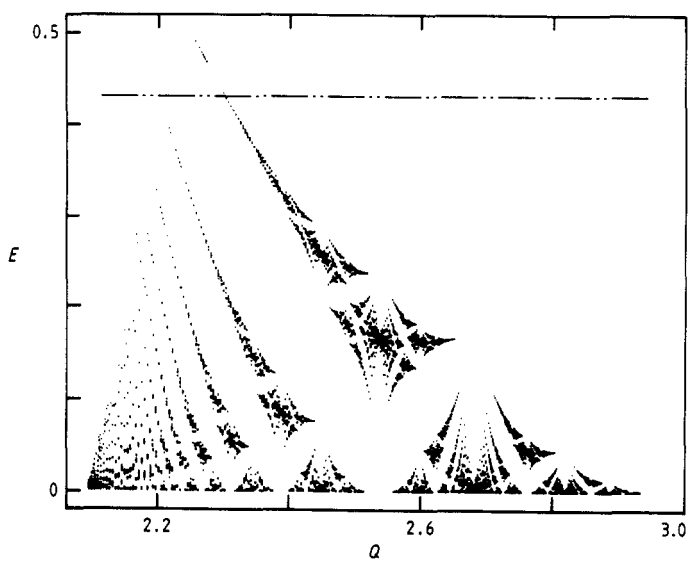

Figure 5. The triangular region A in figure 2 is recalculated with $\delta Q = 0.002$ and $\delta E = 0.0001$. The chain line corresponds to $E = 2$ in figure 2.

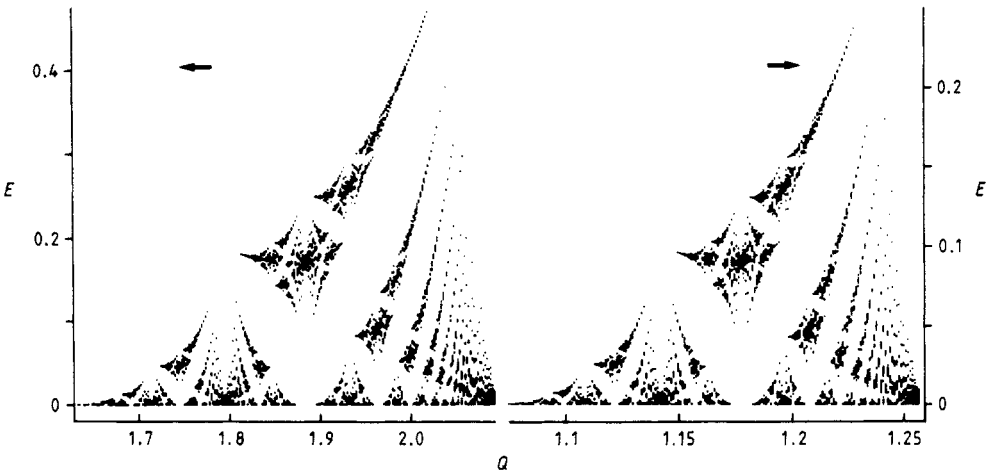

Figure 6. The triangular regions B and C in figure 2 are recalculated with $\delta Q = 0.002$ and $\delta E = 0.0001$ to demonstrate the self-similarity.

Finally, we examine the region T in row A with $\delta E = 10^{-8}$. For $n > 3$, we found no conducting states at all.

The size of a chain of 10^7 atoms is comparable to that of a realistic macroscopic sample. Consequently, our computer experiment provides the evidence of an energy-dependent metal-insulator transition in the vicinity of $V/t = 2$.

We have also set $\delta Q = 0.002$ and $\delta E = 0.0001$ to perform a better calculation over the three triangular regions A, B and C in figure 2. The results for triangle A, shown in figure 5, resemble the original figure 2. The results for triangles B and C, shown in figure 6, are almost identical to each other. Such comparisons demonstrate the self-similarity of the conducting channels of the Aubry model.

This work was financially supported by the Swedish Natural Science Research Council under Grant No NFR-FFU-3996-136.

References

Aubry S 1978 *Solid State Sciences: Solitons and Condensed Matter Physics* vol 8, ed A P Bishop and T Schneider (Berlin: Springer) pp 264-77
Aubry S and André G 1980 *Ann. Israel Phys. Soc.* **3** 133-64
Avron J and Simon B 1982 *Bull. Am. Math. Soc.* **6** 81
Chao K A, Riklund R and Liu You-Yan 1985 *Phys. Rev.* B **32** 5979-86
Grempel D R, Fishman S and Prange R E 1982 *Phys. Rev. Lett.* **49** 833-6
Grempel D R, Prange R E and Fishman S 1984 *Phys. Rev.* A **29** 1639-47
Hofstadter D R 1976 *Phys. Rev.* B **14** 2239-49
Landauer R 1970 *Phil. Mag.* **21** 863-7
Liu You-Yan and Chao K A 1986 *Phys. Rev.* B in press
Simon B 1982 *Adv. Appl. Math.* **3** 463-90
Soukoulis C M and Economou E N 1982 *Phys. Rev. Lett.* **48** 1043-6
Thouless D J 1972 *J. Phys. C: Solid State Phys.* **5** 77-81