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1985 J. Phys. A: Math. Gen. 18 L403

(http://iopscience.iop.org/0305-4470/18/7/014)

J. Phys. A: Math. Gen. 18 (1985) L403-L408. Printed in Great Britain

LETTER TO THE EDITOR

Metal-insulator transition and self-similarity in the Aubry model

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Received 17 December 1984

Abstract. The Aubry model near the critical region is analysed with the numerical renormalisation group method. The transition is shown to be energy dependent and the self-similarity is demonstrated.

Among recent work on almost periodic systems, the Aubry (1978) model has been studied the most. The model Hamiltonian is simply a one-dimensional tight-binding one with a sinusoidal modulation potential incommensurate with the lattice

$$H = \sum_{n=-\infty}^{\infty} \{E_n a_n a_n + t(a_{n+1}^{\dagger} a_n + a_{n-1}^{\dagger} a_n)\}, \tag{1}$$

$$E_n = V \cos(Qn), \tag{2}$$

where Q is incommensurate to π. Based on the localisation criterion of Thouless (1972), Aubry and André (1980) have shown that all states are localised if $2t < V$, while all states are extended if $2t > V$. Therefore, at any eigen energy there is a metal-insulator transition at the critical value $2t = V$. On the other hand, Azbel (1979) has obtained the energy spectrum of the devil's staircase type, with both localised and extended states separated by mobility edges. More controversy was added by Suslov (1982, 1983), who showed the absence of such a mobility edge in his renormalisation group study. In the last five years many authors have contributed to the dispute over whether there are mobility edges in the regime $2t > V$ (Sokoloff 1980, 1981a, Dy and Ma 1982, Soukoulis and Economou 1982).

Another important feature of the Aubry model is the self-similarity of the energy spectrum. Besides the devil's staircase structure mentioned above, Sokoloff (1981b) has shown that near the metal-insulator transition the band contains a hierarchy of gaps of every decreasing magnitude. In terms of the mathematical language, Bellissard and Simon (1982) have proved that the Aubry Hamiltonian (1) has a nowhere dense spectrum. In this letter we will present a renormalisation group calculation to clarify some microscopic properties of the Aubry model near the critical region $2t \simeq V$, especially regarding the metal-insulator transition and the self-similarity.

We consider the equation of motion of the Green function $G(z)_{mn}$ with $z = \varepsilon + i\eta$

$$(z - E_{n+\mu}^0) G(z)_{n+\mu,n} = \delta_{\mu,0} + t_{n+\mu,n+\mu-1}^0 G(z)_{n+\mu-1,n} + t_{n+\mu,n+\mu+1}^0 G(z)_{n+\mu+1,n} \tag{3}$$

0305-4470/85/070403+06$02.25

where $E_n^0 = E_n$, $t_{n,n\pm1}^0 = t$, and $\mu = 0, \pm1, \pm2, \ldots$. From (3) it is easy to see that for fixed n, all the Green functions $G(z)_{mn}$ with even m can be expressed in terms of the Green functions $G(z)_{mn}$ with odd m, and *vice versa*. Hence, we can eliminate half of the Green functions to obtain the equations of motion for the rest half of the Green functions

$$(z - E_{n+\nu_1\mu}^1)G(z)_{n+\nu_1\mu,n} = \delta_{\nu_1\mu,0} + t_{n+\nu_1\mu,n+\nu_1(\mu-1)}^1 G(z)_{n+\nu_1(\mu-1),n} + t_{n+\nu_1\mu,n+\nu_1(\mu+1)}^1 G(z)_{n+\nu_1(\mu+1),n}, \tag{4}$$

where $\nu_1 = 2^1 = 2$, and

$$E_{n+\nu_1\mu}^1 = E_{n+\nu_1\mu}^0 + t_{n+\nu_1\mu,n+\nu_1\mu-1}^0 (z - E_{n+\nu_1\mu-1}^0)^{-1} t_{n+\nu_1\mu-1,n+\nu_1\mu}^0 + t_{n+\nu_1\mu,n+\nu_1\mu+1}^0 (z - E_{n+\nu_1\mu+1}^0)^{-1} t_{n+\nu_1\mu+1,n+\nu_1\mu}^0, \tag{5}$$

$$t_{n+\nu_1\mu,n+\nu_1(\mu\pm1)}^1 = t_{n+\nu_1\mu,n+\nu_1\mu\pm1}^0 (z - E_{n+\nu_1\mu\pm1}^0)^{-1} t_{n+\nu_1\mu\pm1,n+\nu_1(\mu\pm1)}^0. \tag{6}$$

By properly renormalising the site indices $n + \nu_1\mu \to n + \mu$, the equation of motion (4) is mapped onto the original equation of motion (3) with renormalised site energies and hopping integrals. Equation (4) simply describes the behaviour of Green functions in a one-dimensional lattice with double lattice constant. Therefore, the hopping integral (6) between two lattice sites in the renormalised system is less than $t_{n,n\pm1}^0 = t$ of the original system.

We can repeat this process and the equation of motion at the α-step is

$$(z - E_{n+\nu_\alpha\mu}^\alpha)G(z)_{n+\nu_\alpha\mu,n} = \delta_{\nu_\alpha\mu,0} + t_{n+\nu_\alpha\mu,n+\nu_\alpha(\mu-1)}^\alpha G(z)_{n+\nu_\alpha(\mu-1),n} + t_{n+\nu_\alpha\mu,n+\nu_\alpha(\mu+1)}^\alpha G(z)_{n+\nu_\alpha(\mu+1),n}, \tag{7}$$

where $\nu_\alpha = 2^\nu$. The new site energy $E_{n+\nu_\alpha\mu}^\alpha$ and hopping integral $t_{n+\nu_\alpha\mu,n+\nu(\mu\pm1)}^\alpha$ are related to their old counterparts via two equations of the same form as (5) and (6). Since each renormalisation operation doubles the lattice constant, the fixed point is determined by $t_{n+\nu_\alpha\mu,n+\nu_\alpha(\mu\pm1)}^\alpha \to 0$ as $\alpha \to \infty$. The Green functions at the fixed point are then diagonal

$$\lim_{\alpha\to\infty} [G(z)_{n+\nu_\alpha\mu,n}] = \left[\lim_{\alpha\to\infty} (z - E_n^\alpha)^{-1}\right]\delta_{\mu,0}. \tag{8}$$

In the actual calculation the fixed point is reached when the computer sets the small hopping integral ($<10^{-39}$) equal to zero. Near the critical region $2t \geqslant V$, α can be as large as 19-20 in order to reach such a small hopping integral. That is, we need almost $\mathcal{N} = 10^6$ sites to get convergent results.

In this letter we only need the diagonal Green functions $G(z)_{n,n}$, from which one obtains the density of states

$$\rho(\varepsilon) = \lim_{\mathcal{N}\to\infty}\left[\frac{1}{\mathcal{N}}\sum_{n=1}^{\mathcal{N}}\left(-\frac{1}{\pi}\right)\lim_{\eta\to0}\operatorname{Im} G(\varepsilon + i\eta)_{n,n}\right]. \tag{9}$$

The numerical computation scheme is very tedious and has been given elsewhere (Chao *et al* 1984). Earlier, Soukoulis and Economou (1982) have set $V = 1.9$, $t = 1$ and $Q = 0.7$ in their calculation and found nine well defined energy bands. We will use this result as the starting point of our investigation. We first study the critical case $V = 1.9$ and $t = 0.95$ for $Q = 0.7$. Since $9Q = 6.3 \simeq 2\pi$, if we plot the density of states $\rho(\varepsilon)$ with an

energy increment $\Delta\varepsilon$ not sufficiently small, we obtain nine bands distributed symmetrically with respect to $\varepsilon = 0$. With increasing ε these bands are labelled as band 1 to band 9. The bandwidth decreases rapidly with increasing $|\varepsilon|$.

Now we consider the number $\xi = NQ - 2\pi M$ for positive integers N and M. The combination $(N; M; \xi) = (9; 1; 0.002\,676)$ corresponds to the gross nine-band structure mentioned above. If we keep $\xi < 0.0025$, then we found the following interesting combinations:

$$(N: M: \xi) = (368; 41; 0.001\,687),\quad (377; 42; 0.000\,989),\quad (745; 83; 0.000\,697),$$
$$(754; 84; 0.001\,979),\quad (1113; 124; 0.002\,384),\quad (1122; 125; 0.000\,292),$$
$$(1490; 166; 0.001\,394),\quad (1499; 167; 0.001\,282), \ldots .$$

This finding suggests that if we continuously decrease the energy increment $\Delta\varepsilon$, the density of states should be resolved into 9 bands, 368 bands, 377 bands, 745 bands, 754 bands, 1113 bands, ... This is indeed what we have obtained as shown in figure 1 where the density of states (in logarithmic scale) of the bands 6, 7, 8 and 9 (because of symmetry the same structure for bands 4, 3, 2 and 1) are plotted. Each band splits into exactly 41 subbands with the positions of the outermost subbands marked by numbers. In order to resolve these structures, we have to use very small $\Delta\varepsilon = 0.0005$

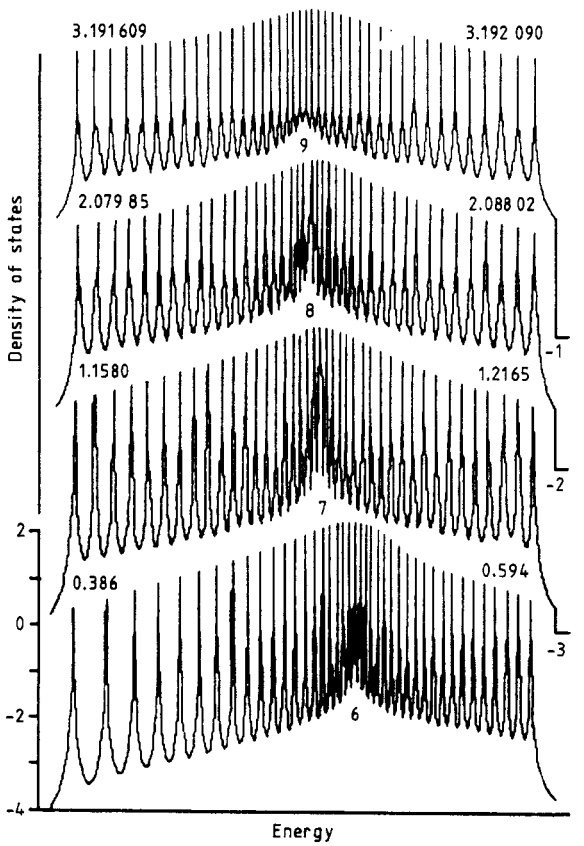

Figure 1. The density of states (logarithmic scale) for bands 6, 7, 8 and 9. Numbers mark the outermost peak positions.

for band 6 and $\Delta\varepsilon = 0.000\,002$ for band 9. The middle plot (indicated by 0.95) in figure 2(a) demonstrates the subband structure of band 5 for $\varepsilon > 0$. There are 20 subbands in this energy region, and so altogether 40 subbands in band 5. The missing subband at $\varepsilon = 0$, as we conjecture, is related to the unusual behaviour discussed by Avron and Simon (1982). We thus obtain the total number of subbands $40 + (8 \times 41) = 368$ as predicted. Although in principle we can decrease $\Delta\varepsilon$ (to much less than 0.000 002) to resolve even finer structure, it is not practical to do so concerning the computer time. Nevertheless, it is reasonable to regard our result as a direct evidence of the devil's staircase character of the Aubry model. Similar evidence was obtained by Azbel and Rubinstein (1983) for the Kronig-Penny model with an incommensurate potential.

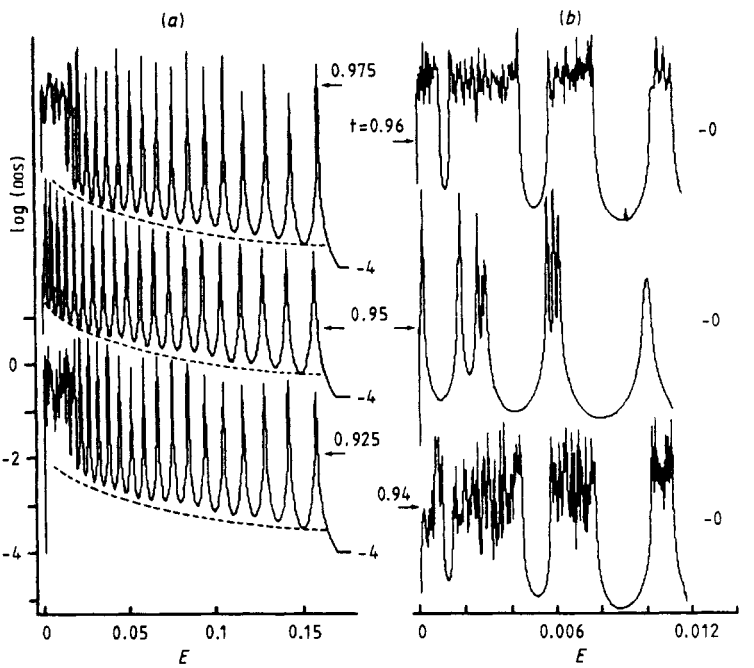

Figure 2. The density of states with resolution $\Delta\varepsilon = 0.0005$ (a) and $\Delta\varepsilon = 0.000\,05$ (b) for various values of t. Reference values -4 (a) and 0 (b) are indicated for different DOS curves.

The density of states in the vicinity of the critical region $2t \simeq V$ are shown in figure 2 for $\Delta\varepsilon = 0.0005$ ((a) with reference value -4 marked for each plot) and for $\Delta\varepsilon = 0.000\,05$ ((b) with reference value 0 marked for each plot). The values of t for various curves are also indicated. At the level of resolution $\Delta\varepsilon = 0.0005$, we see in figure 2($a$) that a deviation from the critical $2t = V$ (here we have $2t/V = 1.95/1.9 = 1.0263$ and $1.85/1.9 = 0.9736$) causes the merge of subbands around the centre of the band 5. This phenomenon also appears in other bands. Therefore, across the critical value $2t = V$ the transition can hardly be energy independent as claimed by Aubry and André (1980). We will return to this point later. At higher resolution $\Delta\varepsilon = 0.000\,05$ we have investigated the region around $\varepsilon = 0$ of band 5, and have found the beautiful fine structure. The results are demonstrated in figure 2(b) for $t = 0.94$, 0.95 and 0.96.

In order to illustrate the energy dependence of the transition across the critical value $2t = V$, we have calculated not only the local density of states $\rho_{E_n}(\varepsilon) =$

$-(1/\pi)\lim_{\eta\to 0}\mathrm{Im}\,G(\varepsilon+\mathrm{i}\eta)_{n,n}$ from the imaginary part of the Green function, but also its real part Re $G_{E_n}(\varepsilon)$. For given value of ε, the relation $\rho_E(\varepsilon)$ against Re $G_E(\varepsilon)$ is shown in figure 3 for $\varepsilon = 0.002\,805$ (plot a), 0.002 971 (plot b), 0.004 396 (plot c), 0.160 192 (plot d), 0.159 253 (plot e) and 0.158 5167 (plot f). The value of t is 0.96 for a and d, 0.95 for b and e, and 0.94 for c and f. For each value of E_n the result is represented by a dot. The energies for cases d, e and f are the positions of the outermost peak in band 5 for $t = 0.96$, 0.95 and 0.94, respectively. The energies for cases a, b and c lie deep in the middle of band 5. While cases d, e and f are almost exactly the same, cases a, b and c are drastically different (notice the logarithmic scales). Hence across the critical value $2t = V$ ($t = 0.95$), the change of physical properties is energy dependent. In other words, the transition is energy dependent.

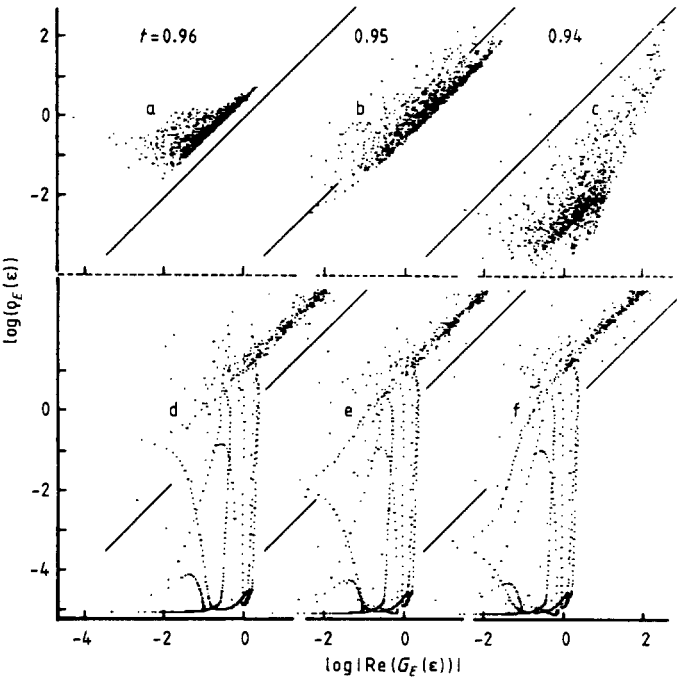

Figure 3. Characteristic properties of Green functions for various eigen energies (details see text). The full lines are for $\log\{\rho_E(\varepsilon)\} = \log|\mathrm{Re}\,G_E(\varepsilon)|$.

Finally, we provide another important piece of information regarding the characteristic feature of the transition. The step of renormalisation to reach the fixed point is 7–9 for all the cases d, e and f, is 11–12 for case c, is 15–16 for case b, and is 19–20 for case a. Evidently, across the critical value $2t = V$, there is practically no change of localisation in the energy region near the band edges of each band. On the other hand, in the vicinity of the band centre, a drastic delocalisation of the electronic wavefunction occurs when $2t/V$ increases from $1.88/1.9 = 0.989\,47$ to $1.92/1.9 = 1.010\,52$ across the critical value $2t/V = 1$. The transition is certainly energy dependent.

This work is financially supported by the Swedish Natural Science Research Council under grant No NFR FFU 3996-121.

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