Fractal spectra for incommensurate systems

1986 J. Phys. A: Math. Gen. 19 2907

(http://iopscience.iop.org/0305-4470/19/14/026)

J. Phys. A: Math. Gen. 19 (1986) 2907-2912. Printed in Great Britain

COMMENT

Fractal spectra for incommensurate systems

K A Chao

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

Received 18 November 1985, in final form 20 December 1985

Abstract. A scaling rule has been proposed to study the energy spectrum of the Aubry model $H=\Sigma_n[(V\cos Qn)a_n^\dagger a_n + t(a_{n+1}^\dagger a_n + a_{n-1}^\dagger a_n)]$ for a class of irrational numbers $Q=1/(\mu+Q)$, where μ is a positive integer. The scaling rule is universal in the sense that it is independent of the ratio V/t and has been confirmed via a large scale numerical calculation. A fractal dimensionality D_f of the energy spectrum is defined and has been found to be $D_f=1$.

Recently there has been considerable interest in the spectral structure of the one-dimensional Aubry model (Aubry 1978)

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

where $E(Q,n)=V\cos(Q2\pi n)$, and Q is an irrational number. Many authors (Sokoloff 1981a, Sokoloff and José 1982, Dy and Ma 1982, Suslov 1983, Llois *et al* 1984, Dy and Wang 1984, Wiecko and Roman 1984, Weaire and Kermode 1983) have calculated the energy spectrum of $H(Q)$ using various approaches. One novel feature of the spectrum is the existence of a hierarchy of subbands with decreasing bandwidths. This has been demonstrated under the name of either the devil's staircase, Cantor set, or hierarchical recursion by Azbel (1979), Sokoloff (1981b), Bellissard *et al* (1982), Bellissard and Simon (1982), Azbel and Rubinstein (1983), de Lange and Janssen (1983) and Chao *et al* (1985). The application of scaling theory by Suslov (1982), Thouless and Niu (1983), Kohmoto (1983) and Ostlund and Pandit (1984), together with the so-obtained empirical scaling results have revealed some detailed structures of the eigensolutions of the model Hamiltonian.

The irrational number Q can be expressed as a continued fraction

$$Q=[\mu_1,\mu_2,\mu_3,\ldots]=\cfrac{1}{\mu_1+\cfrac{1}{\mu_2+\cfrac{1}{\mu_3+\ldots}}} \tag{2}$$

where μ_i are positive integers. Azbel (1964a, b, 1979) predicted that the spectrum splits into (approximately) μ_1 bands, each of which splits into μ_2 subbands, each of which splits into μ_3 subbands, etc. If one truncates the continued fraction, Q can be approximated by a rational number $Q\simeq\nu/N$, where ν and N are integers. Under this approximation the energy spectrum splits into N bands and each band contains the same number of eigenstates. Such spectra were studied by Hofstadter (1976) and Wilkinson (1984).

0305-4470/86/142907+06$02.50

In this comment we will consider a special class of *quadratic irrational numbers* $\{Q(\mu);\ \mu = 1, 2, \ldots\}$ defined as

$$Q \equiv Q(\mu) = [\mu, \mu, \mu, \ldots] = \frac{1}{\mu + Q(\mu)} \equiv \frac{1}{\mu + Q}. \tag{3}$$

For given μ there are two solutions $Q_+ > 0$ and $Q_- < 0$. Since $Q_+ + Q_- = \mu$ and $E(Q, n) = V\cos(Q2\pi n)$, the spectra of $H(Q_+)$ and $H(Q_- = \mu - Q_+)$ (or $H(1 - Q_+)$) are identical. Hence, the spectra of $H(Q)$ are symmetric with respect to $Q = 0.5$. For this class of Q, we propose a scaling hypothesis to demonstrate the fractal (or self-similar) properties of the energy spectra of $H(Q)$. If the total number of eigenstates is N_t (N_t can be arbitrarily large), and we use $Q^\eta N_t$ (with $\eta = 0, 1, 2, \ldots$) as a scale to measure the number of eigenstates in each subband, we can derive a fractal (or self-similar) pattern of band splitting. The scaling hypothesis is *universal* in the sense that it is valid as long as $2t > V$.

Before we study the case of integer μ, it is helpful to consider $Q = 0$ (or $\mu = \infty$) first, corresponding to a periodic system with period 1. The energy spectrum is just a single tight-binding band. From

$$E(Q, n) = E\left(\frac{1}{\mu + Q}, n\right) = V\cos\left(\frac{2\pi n}{\mu + Q}\right)$$

the case $Q = 0$ can also be interpreted as a splitting of the original single energy band into μ ($\to\infty$) subbands and each subband contains only one eigenenergy. Next, we consider the case that μ is not an integer and $Q \neq 0$, but Q is a rational number ν/N. One simple example is $\mu = 2.1$ and $Q = 0.4 = \frac{2}{5}$. In this case the system is also periodic with a superperiodicity N, and the original single energy band splits into N subbands. The number of eigenstates in each subband is equal to $1/N$ of the total number of eigenstates.

For the case of integer μ to be investigated in this comment, the expression $E(Q, n) = E(2\pi n/(\mu + Q))$ suggests the following ansatz. The original single energy band corresponding to $\mu = \infty$ splits into $\mu + 1$ subbands when μ takes the value of a finite positive integer. Among them, μ subbands are equivalent in the sense that an equal fraction $f_s = 1/(\mu + Q) = Q$ of the total number of eigenstates is contained in each of these μ subbands. The remaining non-equivalent subband contains a fraction $f_m = 1 - \mu f_s = 1 - \mu Q$ of the total number of eigenstates. From (3) we have $1 - \mu Q = Q^2$, and so $f_m/f_s = Q$. Consequently, if we use N_T (total number of eigenstates of the system) as a scale to measure the number of eigenstates in each band, we simply obtain the original single energy band. Then, if we use QN_T as a scale to measure the number of eigenstates in each band, we expect the original single band splitting into $\mu + 1$ subbands. It is important to point out that Azbel (1964a, b, 1979) predicted only μ subbands. If we approximate the irrational Q by the rational number $1/\mu$ (the crudest approximation), we also get μ subbands. We will return to this point later.

Before we generalise the results by applying the ansatz again to each subband, we first have to satisfy the symmetry requirement. The spectrum of eigenenergy ε of the Hamiltonian $H(Q)$ is symmetric with respect to $\varepsilon = 0$. If μ is even, the symmetry is satisfied with the non-equivalent subband located at the centre of the spectrum, and the μ equivalent subbands symmetrically placed at both sides of the non-equivalent subband. Therefore, for even μ we can apply the ansatz again to each subband. Now we will display an equation for the scaling assumption for even integer μ. At the nth stage of band splitting, the number of eigenstates in each subband is either $N_t Q^n$ or

$N_t Q^{n+1}$, where N_t is the total number of eigenstates of the system. Let α_n (or β_n) be the number of subbands containing $N_t Q^n$ (or $N_t Q^{n+1}$) eigenstates at the nth stage. At the next stage of band splitting, there are α_{n+1} (or β_{n+1}) subbands containing $N_t Q^{n+1}$ (or $N_t Q^{n+2}$) eigenstates. The recursion relation between $(\alpha_{n+1}, \beta_{n+1})$ and (α_n, β_n) can be derived. For example, if μ is even, we have

$$\begin{pmatrix} \alpha_{n+1} \\ \beta_{n+1} \end{pmatrix} = \begin{pmatrix} \mu & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} \tag{4}$$

with $\alpha_0 = 1$ and $\beta_0 = 0$. If we denote $x = N_t Q^n$ as the independent variable, then $\alpha(x) = \alpha_n$ and $\beta(x) = \beta_n$ are functions of x. Equation (4) can be rewritten as

$$\alpha(x) = (1/Q - Q)\alpha(x/Q) + \beta(x/Q) \tag{5a}$$

and

$$\beta(x) = \alpha(x/Q) \tag{5b}$$

or simply

$$\alpha(x) = (1/Q - Q)\alpha(x/Q) + \alpha(x/Q^2) \tag{6a}$$

and

$$\beta(x) = (1/Q - Q)\beta(x/Q) + \beta(x/Q^2). \tag{6b}$$

For odd μ, we have to treat $\mu = 1$ and $\mu \geq 3$ separately. If $\mu \geq 3$, we must have both the non-equivalent subband and one of the μ equivalent subbands located around $\varepsilon = 0$ and overlapping each other. The overall middle subband thus contains a fraction $f_s + f_m = Q + Q^2$ of the total number of eigenstates. When this resultant middle subband splits again, the equivalent subband component produces μ equivalent subbands and one non-equivalent subband. Each of these newly appearing μ equivalent subbands contains a fraction $f_s f_s = Q^2$ of the total number of eigenstates, while the newly appearing non-equivalent subband contains only a fraction $f_s f_m = Q^3$ of the total number of eigenstates. At this stage, the resultant middle subband can be well separated into $\mu + 1$ equivalent subbands, each with a fraction factor Q^2, and one non-equivalent subband with the fraction factor Q^3. The non-equivalent subband will stay at the middle and the $\mu + 1$ equivalent subbands stay symmetrically at both sides. Now, we can continue to apply the ansatz to all subbands. The scaling assumption can be expressed in similar equations

$$\alpha(x) = (1/Q - Q - 1)\alpha(x/Q) + (1/Q - Q + 1)\alpha(x/Q^2) + \alpha(x/Q^3) \tag{7a}$$

and

$$\beta(x) = (1/Q - Q - 1)\beta(x/Q) + (1/Q - Q + 1)\beta(x/Q^2) + \beta(x/Q^3). \tag{7b}$$

For $\mu = 1$ one can imagine that the original single energy band actually consists of two overlapping subbands. Both subbands are symmetrically located around $\varepsilon = 0$. The fraction factor of one subband is Q and the fraction factor of the other is Q^2. Therefore, at the first step of subband identification, the original single energy band can be well separated into $\mu + 1 = 2$ equivalent subbands with fraction factor Q^2 each and one non-equivalent subband with fraction factor Q^3. Again, the non-equivalent subband stays at the centre around $\varepsilon = 0$. From now on, each equivalent subband will split into two subbands with relative fraction factors Q and Q^2. On the other hand, the central non-equivalent subband starts to play the role of the original single energy

band and will split into $\mu+1=2$ equivalent subbands plus one central non-equivalent subband. The equation for scaling assumption can be derived without difficulty, though it is a little more complicated than the cases $\mu \neq 1$.

If the above scaling hypothesis is correct, when a parent band splits into subbands with predicted partition of number of eigenstates, these subbands must be well separated by energy gaps. Furthermore, if we analyse only one of the subbands each time and continue the process step by step, not only should the pattern of band splitting be correct, it should also exhibit a hierarchical structure of monotonically decreasing bandgaps. In other words, starting from any subband, the application of the scaling hypothesis should reproduce the entire band structure of the whole system. From the following numerical experiment, we see that the energy spectrum indeed has this fractal (or self-similar) property.

We should point out that the above scaling hypothesis is independent of the ratio $V/2t$. Since Aubry and Andre (1980) have shown that all eigenstates of $H(Q)$ are localised if $2t < V$, we hesitate to apply the concept of *energy band* in this region. Therefore, we will restrict our scaling hypothesis to the region $2t \geqslant V$ only. For given values of $2t/V \geqslant 1$ and integer μ, we have used the so-called negative-eigenvalue-counting method (Martin 1961) to calculate the number of eigenstates in a given energy interval ΔE. ΔE is reduced step by step in order to detect the formation of subbands. The numerical accuracy is 10^{-6}.

We have studied the cases $\mu = 1, 2, 3, 4, 5, 6$, and five randomly chosen values of μ between $\mu = 7$ and $\mu = 20$. For every value of μ, we have considered twenty values of $V/t = 0.1m$ with $m = 1, 2, \ldots, 20$. In every case the band splitting follows our proposed scaling hypothesis. Here we show in figure 1 only the results of the first few splittings for $2t/V = 1$ and $\mu = 1, 2$ and 3. Each subband is represented by a vertical bar with both band edges marked by numbers. Because of the symmetry, only the part of the spectrum with positive eigenenergies is plotted. When a band splits into subbands, the relative fraction factors ($1, Q$ or $1-Q$) of numbers of eigenstates in these subbands are indicated next to the bars. The fractal (or self-similar) structure of the spectrum is clearly seen in figure 1. In particular, we would like to point out that at any stage of band splitting, the original band edges (and the original bandgaps) do not change at all. Therefore, the spectrum has a hierarchical feature of monotonically decreasing bandgaps as predicted by the scaling hypothesis. With decreasing $V/2t$, we found that the fractal structure of the spectrum remains intact, but every bandgap gets narrower. At $V/2t = 0$, all bandgaps disappear.

With the numerical accuracy 10^{-6}, there is at least one eigenstate in an energy interval $\Delta E = 10^{-6}$. Hence, we have to compute the energy spectrum of a chain of about 10^6 atoms. For given values of μ and $V/2t$, it takes about 45 min of CPU time to calculate the spectrum on a VAX 780 computer. We have checked 11 different values of μ and 20 different values of $V/2t$. The whole numerical work took about 160 h CPU time.

Recently, the fractal dimensionality has been extensively studied from the topological point of view (Mandelbrot 1977). In the theory of fractal dimensionality, the two quantities which play the fundamental roles are the scale of measurement and the number of units measured with the scale. To my knowledge the concept of a fractal has not been generalised and applied to energy spectra. In our calculation to detect the band splitting, we reduce the scale of measuring the number of eigenstates by a factor Q, and then count the increase of the number of subbands. Therefore, we can use the scaling hypothesis to define the fractal dimensionality of the energy spectrum

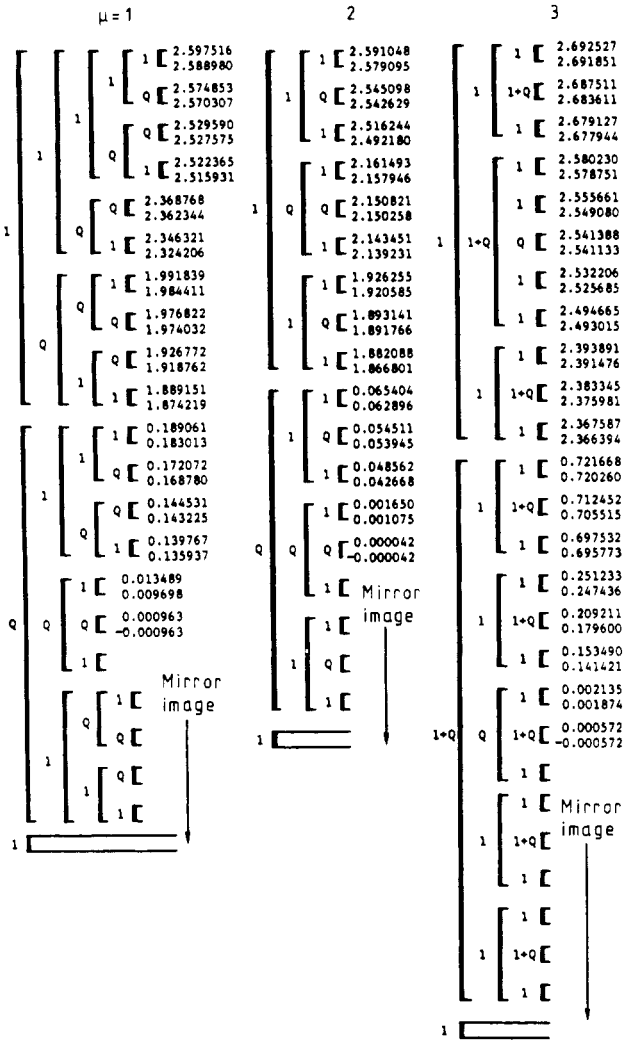

Figure 1. The fractal (or scaling) properties of the energy spectra for various values of μ and $2t/V = 1$.

as

$$D_f = \log[(\alpha(Qx)+\beta(Qx))(\alpha(x)+\beta(x))^{-1}]/\log(1/Q). \tag{8}$$

From equations (6*a*, *b*) and (7*a*, *b*) it is easy to show that $D_f = 1$. It can also be proved without difficulty that $D_f = 1$ for $\mu = 1$.

A generalisation of the scaling is to consider the cases

$$Q = -[-\mu, -\mu, -\mu, \ldots] = 1/(\mu - Q) \tag{9}$$

and

$$Q = [\mu_1, \mu_2, \mu_1, \mu_2, \ldots] = \cfrac{1}{\mu_1 + \cfrac{1}{\mu_2 + Q}}. \tag{10}$$

The results are very complicated due to the overlap of subbands and will not be discussed here.

To close this comment, we would like to remark on the approximation in which the irrational Q is approximated by a rational number ν/N. Within this approximation, the original single energy band always splits into N (and only N)subbands, and each subband contains an equal number of eigenstates. The fractal structure of the spectrum is then quite different from what we have derived for the class of Q defined by (3), although within this approximation the fractal dimensionality of the spectrum is still $D_f = 1$.

This work was supported by the Swedish Natural Science Research Council under Grant No NFR-FFU-3996-121.

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
Azbel M Ya 1964a *Zh. Eksp. Teor. Fiz.* **46** 929 (*Sov. Phys.-JETP* **19** 634–45)
—— 1964b *Dokl. Akad. Nauk* **159** 703 (*Sov. Math.-Dokl.* **5** 1549–52)
—— 1979 *Phys. Rev. Lett.* **43** 1954–7
Azbel M Ya and Rubinstein M 1983 *Phys. Rev.* B **27** 6530–3
Bellissard J, Bessis D and Moussa P 1982 *Phys. Rev. Lett.* **49** 701–4
Bellissard J and Simon S 1982 *J. Funct. Anal.* **48** 408–19
Chao K A, Riklund R and Wahlström G 1985 *J. Phys. A: Math. Gen.* **18** L403–8
de Lange C and Janssen T 1983 *Phys. Rev.* B **28** 195–209
Dy K S and Ma T C 1982 *J. Phys. C: Solid State Phys.* **15** 6971–80
Dy K S and Wang J Y 1984 *J. Phys. C: Solid State Phys.* **17** 421–6
Hofstadter D R 1976 *Phys. Rev.* B **14** 2239–49
Kohmoto M 1983 *Phys. Rev. Lett.* **51** 1198–201
Llois A M, Cohan N V and Weissmann M 1984 *Phys. Rev.* B **29** 3111–6
Mandelbrot B B 1977 *Fractals: Form, Chance and Dimension* (San Francisco: Freeman)
Martin J L 1961 *Proc. R. Soc.* A **260** 139–46
Ostlund S and Pandit R 1984 *Phys. Rev.* B **29** 1394–414
Sokoloff J B 1981a *Phys. Rev.* B **23** 6422–9
—— 1981b *Solid State Commun.* **40** 633–6
Sokoloff J B and José J V 1982 *Phys. Rev. Lett.* **49** 334–7
Suslov I M 1982 *Zh. Eksp. Teor. Fiz.* **83** 1079–88 (*Sov. Phys.-JETP* **56** 621–7)
—— 1983 *Zh. Eksp. Teor. Fiz.* **84** 1792–805 (*Sov. Phys.-JETP* **57** 1044–51)
Thouless D J and Niu Q 1983 *J. Phys. A: Math. Gen.* **16** 1911–9
Weaire D and Kermode J P 1983 *Phys. Stat. Solidi* b **118** K163–6
Wiecko C and Roman E 1984 *Phys. Rev.* B **30** 1603–5
Wilkinson M 1984 *Proc. R. Soc.* A **391** 305–50