Energy spectra for one-dimensional quasiperiodic potentials: bandwidth, scaling, mapping and relation with local isomorphism

1989 J. Phys. A: Math. Gen. 22 3267

(http://iopscience.iop.org/0305-4470/22/16/017)

J. Phys. A: Math. Gen. 22 (1989) 3267-3282. Printed in the UK

Energy spectra for one-dimensional quasiperiodic potentials: bandwidth, scaling, mapping and relation with local isomorphism

Frank Wijnands

Institute for Theoretical Physics, University of Nijmegen, 6525 ED Nijmegen, The Netherlands

Received 6 March 1989

Abstract. Energy spectra for one-dimensional tight-binding models, with two types of quasiperiodic potentials, are studied, for which the incommensurability is characterised by quadratic irrationals. One is the step potential model, for which the structure is a generalised Fibonacci chain. For special structures, scaling properties of the spectrum are found numerically; a critical index δ for the total bandwidth is determined. After deriving recursion relations for the trace of transfer matrices, it is shown that generalised Fibonacci chains have the same energy spectrum if and only if they are locally isomorphic. The other potential is sinusoidal, for which the critical index δ is determined at the critical point.

1. Introduction

There has been much interest (Hofstadter 1976, Andre and Aubry 1980, Kohmoto *et al* 1983 and references therein, Thouless 1983, Ostlund *et al* 1983, Ostlund and Pandit 1984, Wilkinson 1987) in a tight-binding model with the Schrödinger equation:

$$\begin{aligned} &\Psi_{m+1}+\Psi_{m-1}+V(m\omega)\Psi_m=E\Psi_m \\ &V(t+1)=V(t). \end{aligned} \tag{1}$$

This is the Schrödinger equation for an electron on a one-dimensional lattice with a periodic site potential. Here m labels the lattice site and E is the energy. The relation between the nature of the wavefunctions and the character of the energy spectrum has been studied for a number of models. If ω is rational, say $\omega=p/q$, p and q being relatively prime integers, the eigenspectrum consists of q bands and all eigenfunctions are extended. If ω is irrational, the question arises: what is the nature of the spectrum? The potential $V(m\omega)=\lambda\tan(2\pi[m\omega-\nu])$ gives localised states for 'typical' irrational ω, and the bands for $\omega=p/q$ have widths proportional to $e^{-\gamma q}$, as $q\to\infty$ (Grempel *et al* 1982). An analytic weak potential $V(m\omega)$ gives extended states for almost every irrational ω (Bellissard *et al* 1983). Rational $\omega=p/q$ give bandwidths proportional to q^{-1}, as $q\to\infty$ (Kohmoto *et al* 1983).

Kohmoto *et al* (1983) studied the case of a step potential:

$$V(t)=\begin{cases} V_0 & \text{for } -\omega<t\leqslant-\omega^3 \\ V_1 & \text{for } -\omega^3<t\leqslant\omega^2 \end{cases}$$

where $\omega=(\sqrt{5}-1)/2$ is the inverse of the golden mean.

Because the bandwidths were proportional to $q^{-(1+\delta)}$, $\delta > 0$, the states were believed to be neither localised nor extended. This has been proven for certain values of $|V_0 - V_1|$ (Casdagli 1986, Delyon and Petritis 1986, Suto 1987). Kohmoto *et al* (1983) analysed the problem also by means of a mapping problem, making use of a recursion relation for the traces of transfer matrices.

The case $V(t) = \lambda \cos(2\pi t)$ has been studied extensively as well. With this choice of the potential, the model is self-dual, since the Fourier coefficients of the wavefunctions Ψ_m obey the same equation, with different coefficients, as the Ψ_m. For $\omega = (\sqrt{5}-1)/2$, Kohmoto (1983) compared $\lambda = 1.98$, 2.00 and 2.02. From the spectrum, the states turned out to be extended for $\lambda = 1.98$, critical for $\lambda = 2.00$ and localised for $\lambda = 2.02$, in agreement with Andre and Aubry (1980) and Avron and Simon (1983).

Now $\omega = (\sqrt{5}-1)/2$ belongs to the family of positive solutions of the following quadratic equation:

$$\phi^2 + n\phi = 1 \tag{2}$$

with n a positive integer. Positive solutions are: $\phi = (\sqrt{(n^2+4)} - n)/2$. These ϕ can be rewritten as a continued-fraction expansion:

$$\phi = 1/(n + 1/(n + \ldots) \ldots)). \tag{3}$$

For $n = 1$, ϕ is the inverse of the golden mean.

The purpose of this paper is twofold. The first aim is to treat the localisation problem for general *n*. For the step potential and for the potential $V(t) = \lambda \cos(2\pi t)$, the values $n = 1$, 2, 3, 4 are studied. For each *n*, energy spectra for systematic commensurate approximants are calculated. The description of the models is given in § 2. Numerical results for the total bandwidth and for scaling properties are presented in § 3. The second aim is to relate energy spectra of generalised Fibonacci chains (in particular, the step potential case) and the concept of local isomorphism (note that generalised Fibonacci chains can be considered as one-dimensional quasicrystals). Levine and Steinhardt (1986) argue that quasicrystals have the same diffraction pattern and the same free energy if and only if they belong to the same local isomorphism class. It will be studied whether generalised Fibonacci chains (not) belonging to the same local isomorphism class, have the same (a different) energy spectrum. Section 4 contains (the derivation of) recursion relations for the traces of transfer matrices, which will be useful in the following section. In § 5, for a given arbitrary generalised Fibonacci chain, we will study which set of chains belongs to the same local isomorphism class and which set of chains has the same energy spectrum as the given one. Comparison of the two sets yields the answer on the relation between energy spectra and local isomorphism.

2. Transfer matrix formulation of the model

First, write the Schrödinger equation (1) in terms of transfer matrices as

$$M(m\phi)\theta_m = \theta_{m+1} \qquad M(t) = \begin{bmatrix} E - V(t) & -1 \\ 1 & 0 \end{bmatrix} \qquad \theta_m = \begin{bmatrix} \Psi_m \\ \Psi_{m-1} \end{bmatrix}. \tag{4}$$

Notice that the matrices $M(t)$ are periodic in t with period 1 and that $\det M(t) = 1$. Lattice sites m and $m+k$ can be related by repeating the procedure given in (4):

$$M^{(k)}(m\phi)\theta_m = \theta_{m+k} \tag{5}$$

where $M^{(k)}(t)$ is defined recursively by

$$M^{(k_1+k_2)}(t) = M^{(k_1)}(t+k_2\phi)M^{(k_2)}(t) \tag{6}$$

and $M^{(1)}(t) \equiv M(t)$. Rational approximants can be achieved by cutting off the continued-fraction expansion (3) after l steps:

$$\phi_l = 1/(n_1+1/(n_2+\ldots+1/n_l)\ldots)) \qquad n_1 = \ldots = n_l = n. \tag{7}$$

Equation (7) can be rewritten in the form: $\phi_l = q_{l-1}/q_l$, where q_l are generalised Fibonacci numbers; q_l obey the recursion relations

$$q_{l+1} = nq_l + q_{l-1} \qquad q_0 = 1 \qquad q_1 = n. \tag{8}$$

For these rational values $\phi_l = q_{l-1}/q_l$, energies are allowed (forbidden) if $|\mathrm{Tr}[M^{(q_l)}(t)]|$ is less than (greater than) two.

In working out the models for the two types of potentials, the further approach is different, so they will be treated separately.

2.1. *The step potential*

The model can be described as follows. The site potential $V(m\phi)$ can take two values: V_0 and V_1. Consider a structure consisting of atoms of type A (then $V(m\phi) = V_1$) and of type B (then $V(m\phi) = V_0$) on sites m $(m = 0, 1, 2, \ldots)$. For a generalised Fibonacci chain, the potential $V(m\phi)$ can be constructed as follows. We consider sequences of symbols A, B. Starting with sequence $S_0 = B$ at site $m = 0$ corresponding to V_0, $S_1 = AB^{n-1}$ at sites $m = 0, \ldots, (n-1)$ corresponding to $V_1, V_0, \ldots, V_0$, the juxtaposition rule is

$$S_{k+1} = S_k^n S_{k-1} \qquad k \geqslant 1. \tag{9}$$

Note that the number of atoms after each step S_k is q_k, and the atoms are put on sites $m = 0, \ldots, (q_k - 1)$. A commensurate approximant is achieved by cutting off the construction after l steps and constructing a periodic structure with unit cell S_l at sites $m = 0, 1, 2, \ldots$; ϕ is replaced by ϕ_l. Energies are allowed if $|\mathrm{Tr}[M^{(q_l)}(0)]| \leqslant 2$ (for convenience, t is put equal to zero). $\mathrm{Tr}[M^{(q_l)}(0)]$ can be calculated by using a recursion relation for $M_k \equiv M^{(q_k)}(0)$ $(k \geqslant 0)$, after defining

$$M_B = \begin{bmatrix} E - V_0 & -1 \\ 1 & 0 \end{bmatrix} \qquad M_A = \begin{bmatrix} E - V_1 & -1 \\ 1 & 0 \end{bmatrix}$$
$$M_{k+1} = M_{k-1}M_k^n \qquad M_0 = M_B \qquad M_1 = M_B^{n-1}M_A \qquad k \geqslant 1. \tag{10}$$

Proof. M_0 corresponds to $S_0 = B \rightarrow M_0 = M_B$. M_1 corresponds to $S_1 = AB^{n-1} \rightarrow M_1 = M^{(q_1)}(0) = M^{(n)}(0) = M((n-1)\phi_l)\ldots M(0) = M_B^{n-1}M_A$. M_2 corresponds to $S_2 = S_1^n S_0 \rightarrow M_2 = M^{(q_2)}(0) = M^{(q_0+nq_1)}(0) = M^{(q_0)}(nq_1\phi_l)M^{(nq_1)}(0) = M_B(M_B^{n-1}M_A)^n = M_0M_1^n$. Equation (9) leads directly to (10) because M_k corresponds to the reverse of S_k for each k.

Note that (10) also holds for the incommensurate limit (then the proof goes with ϕ instead of ϕ_l). Equation (10) holds for general S_0, S_1, with M_0, M_1 corresponding to the reverse of S_0, S_1 respectively. Energies are allowed (forbidden) if $|\mathrm{Tr}\, M_l|$ is less than (greater than) two.

2.2. The sinusoidal potential

We now consider the potential $V(t) = \lambda \cos(2\pi t)$. For rational approximants $\phi_l = q_{l-1}/q_l$, $\mathrm{Tr}(M^{(q_l)}(t))$ has to be calculated. Taking t equal to zero, $M^{(q_l)}(0)$ has the form

$$M^{(q_l)}(0) = \prod_{m=1}^{q_l} \begin{bmatrix} E - \lambda \cos(2\pi[q_l - m]\phi_l) & -1 \\ 1 & 0 \end{bmatrix}. \tag{11}$$

3. Spectra and scaling

For the step potential and for a fixed value of n, the energy spectra can be calculated for various commensurate approximants $\phi_l = q_{l-1}/q_l$ with help of (10). In all calculations, $V_0 = -V_1 = 0.6$ in (10).

Figure 1(a) shows the energy bands for $n = 2$, $l = 1, 2, 3$; and in figure 1(b) the middle bands for $l = 3, 4, 5$ are plotted.

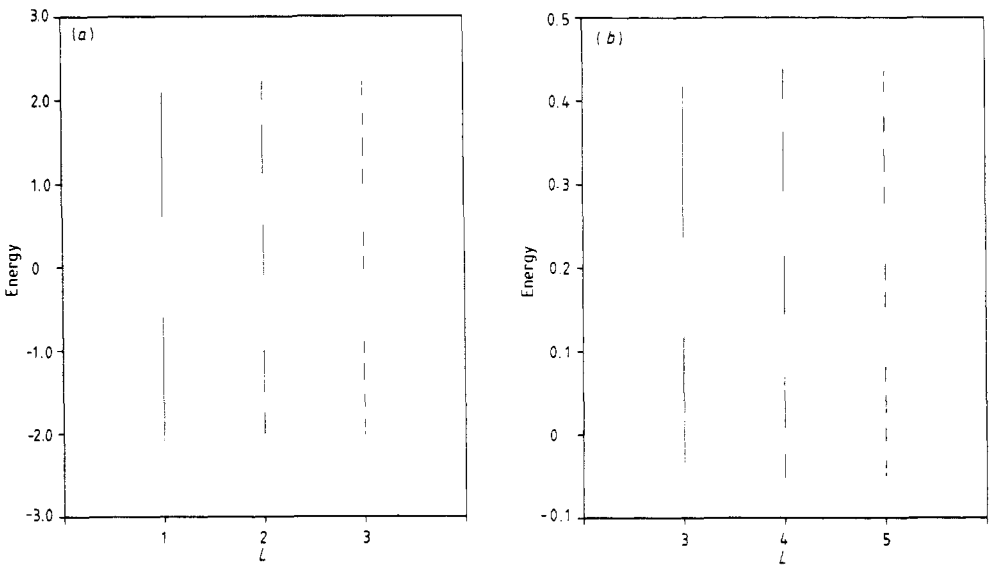

Figure 1. Allowed energies for the step potential, $n = 2$, $V_0 = -V_1 = 0.6$; (a) gives the bands for $l = 1, 2, 3$; (b) gives the middle bands for $l = 3, 4, 5$.

Comparing 1(a) and 1(b), one sees that the spectrum for ϕ_l appears in the spectrum for ϕ_{l+2} in a rescaled version, given by the scaling parameter α. The greater the values of l, the more the scaling parameter α converges (for the middle bands and the middle gaps).

For $n = 1$ and $n = 3$, scaling is found by comparing ϕ_l and ϕ_{l+3} and for $n = 2$ and $n = 4$, ϕ_l and ϕ_{l+2} are compared. This is related to the fact that, for n odd, every third generalised Fibonacci number is even and, for n even, every second generalised Fibonacci number is even.

Table 1 shows the values of the scaling parameter α for $n = 1, 2, 3, 4$; α has been calculated by comparing values of l up to $l = 21, 17, 13, 11$ for $n = 1, 2, 3, 4$ respectively.

Table 1. Scaling parameter α and critical index δ of the step potential and sinusoidal potential for $n = 1, 2, 3, 4$.

	Step potential		Sinusoidal potential	
n	α	δ	α	δ
1	5.618 ± 0.008	0.354 ± 0.005	14.0 ± 0.1	1.00 ± 0.01
2	8.77 ± 0.05	0.349 ± 0.002	39.7 ± 0.2	1.00 ± 0.01
3	80.3 ± 0.5	0.340 ± 0.003	1280 ± 30	1.00 ± 0.01
4	47.3 ± 0.3	0.328 ± 0.002	950 ± 10	1.00 ± 0.01

For the sinusoidal potential, scaling is found at $\lambda = 2.00$ but scaling does not appear at $\lambda = 1.98$ and $\lambda = 2.02$. Figure 2 shows the spectrum for $l = 1, 2, 3$ (figure 2(*a*)) and the middle bands for $l = 3, 4, 5$ (figure 2(*b*)) for $n = 2$ and $\lambda = 2.00$, the self-dual point. In table 1 the values of the scaling parameter α of the middle bands and middle gaps for $n = 1, 2, 3, 4$ are given. For $n = 1, 2, 3, 4$ values of l up to $l = 21, 10, 7, 6$ were compared respectively.

Another quantity is the total bandwidth B_l as a function of different approximants $\phi_l = q_{l-1}/q_l$ and fixed n. For the step potential, B_l is found numerically to go down as: $B_l = c[q_l]^{-\delta}$, as $q_l \to \infty$, in all cases $n = 1, 2, 3, 4$, each with its own value of c and δ. In the incommensurate limit, the wavefunctions seem to be critical: they are neither localised nor extended, according to Grempel *et al* (1982) and Kohmoto *et al* (1983). In table 1, the values of δ, called the critical index of total bandwidth, are given for $n = 1, 2, 3, 4$.

For the sinusoidal potential, at $\lambda = 2.00$, B_l once again decreases as $B_l = c[q_l]^{-\delta}$, as $q_l \to \infty$, in all cases $n = 1, 2, 3, 4$. The values of δ are given in table 1 for $n = 1, 2, 3, 4$. Surprisingly, δ is the same for each $n = 1, 2, 3, 4$. All cases $n = 1, 2, 3, 4$ give

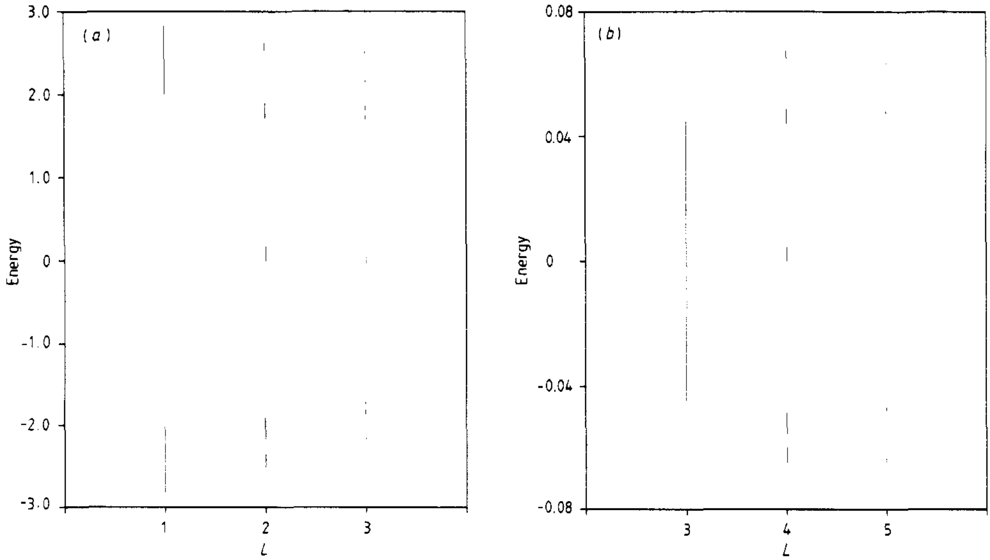

Figure 2. Allowed energies for the sinusoidal potential, $n = 2$, $\lambda = 2.00$; (*a*) shows the spectrum for $l = 1, 2, 3$; (*b*) shows the middle bands for $l = 3, 4, 5$. Notice that the middle band for $l = 3$ consists of two bands that touch each other.

the same picture for $\lambda = 1.98$ and $\lambda = 2.02$: log B_l goes down faster than linearly to zero as a function of l for $\lambda = 2.02$, log B_l goes down slower than linearly to its asymptotic value as a function of l for $\lambda = 1.98$, as $q_l \to \infty$.

4. Recursion relations

In order to treat the spectral problem for $n = 1$, Kohmoto *et al* (1983) converted (10) into a recursion relation for $x_k = \mathrm{Tr}(M_k)$: $x_{k+1} = x_{k-1}x_k - x_{k-2}$, and constructed a three-dimensional mapping operator T. If $\boldsymbol{r}_k = (x_k, x_{k-1}, x_{k-2})$, then $\boldsymbol{r}_{k+1} = T\boldsymbol{r}_k = (x_{k-1}x_k - x_{k-2}, x_k, x_{k-1})$. Starting with $|x_0| \leq 2$ and $|x_1| \leq 2$, an energy has escaped, once $|x_k|$ and $|x_{k+1}|$ are greater than two. Gumbs and Ali (1988) derived similar recursion relations for $n = 2, 3$ and Holzer (1988a, b) derived recursion relations for general n. The author derived similar recursion relations for general n independently. Since they will be of use in § 5, a short proof will follow below.

Taking (10) as the starting point, it holds that

$$M_{k+1} + [M_{k-2}]^{-1} = M_{k-1}[M_k]^n + [M_{k-1}]^n[M_k]^{-1}. \tag{12}$$

Using the relations:

$$\begin{aligned}&\mathrm{Tr}(AB) + \mathrm{Tr}(AB^{-1}) = \mathrm{Tr}(A)\mathrm{Tr}(B) \qquad \mathrm{Tr}(A) = \mathrm{Tr}(A^{-1}) \qquad \text{if } \det A = \det B = 1\\ &Tr(AB) = \mathrm{Tr}(BA) \qquad \text{for every matrix } A,\ B\end{aligned} \tag{13}$$

directly yields

$$\mathrm{Tr}(M_{k-1}[M_k]^m) = \mathrm{Tr}(M_{k-1}[M_k]^{m-1})\mathrm{Tr}\ M_k - \mathrm{Tr}(M_{k-1}[M_k]^{m-2}) \tag{14a}$$

$$\mathrm{Tr}([M_{k-1}]^m[M_k]^{-1}) = \mathrm{Tr}([M_{k-1}]^{m-1}[M_k]^{-1})\ \mathrm{Tr}\ M_{k-1} - \mathrm{Tr}([M_{k-1}]^{m-2}[M_k]^{-1} \tag{14b}$$

Defining

$$x(k) = \mathrm{Tr}(M_k) \qquad y(k, m) = \mathrm{Tr}(M_{k-1}[M_k]^m) \qquad z(k, m) = \mathrm{Tr}([M_{k-1}]^m[M_k]^{-1})$$

equations (12) and (14a, b) can be rewritten as

$$x(k+1) = y(k, n-1)x(k) - y(k, n-2) + z(k, n-1)x(k-1) - z(k, n-2) - x(k-2)$$

$$y(k, m) = y(k, m-1)x(k) - y(k, m-2)$$

$$z(k, m) = z(k, m-1)x(k-1) - z(k, m-2).$$

Substituting $m = n$ in the last relation and using $z(k, n) = x(k-2)$ yields: $x(k-2) = z(k, n-1)x(k-1) - z(k, n-2)$, so that the resulting recursion relations become

$$x(k+1) = y(k, n-1)x(k) - y(k, n-2) \tag{15a}$$

$$y(k, m) = y(k, m-1)x(k) - y(k, m-2) \tag{15b}$$

with initial conditions: $x(1) = \mathrm{Tr}(M_1)$, $x(0) = \mathrm{Tr}(M_0)$, $y(0, n-1) = \mathrm{Tr}(M_1[M_0]^{-1})$. With help of the relations $y(k, 0) = x(k-1)$, $y(k, -1) = y(k-1, n-1)$, all $x(k)$ can be calculated.

Essentially, the recursion relations (15) are relations between variables of the form $x(k_1)$ and $y(k_2, n-1)$, as becomes clear by calculating the recursion relations for $n=1$, 2, 3:

$$n=1: \qquad x(k+1)=x(k-1)x(k)-x(k-2) \tag{16}$$

$$\begin{aligned} n=2: \qquad & x(k+1)=y(k,1)x(k)-x(k-1) \\ & y(k,1)=x(k-1)x(k)-y(k-1,1) \end{aligned} \tag{17}$$

$$\begin{aligned} n=3: \qquad & x(k+1)=y(k,2)x(k)-x(k-1)x(k)+y(k-1,2) \\ & y(k,2)=x(k-1)[x(k)]^2-y(k-1,2)x(k)-x(k-1). \end{aligned} \tag{18}$$

We define $y(k)\equiv y(k, n-1)$ and $\boldsymbol{r}_k \equiv (x(k), x(k-1), y(k-1))$. Analogously to the $n=1$ case, a three-dimensional mapping operator T can be defined with $\boldsymbol{r}_{k+1}=T\boldsymbol{r}_k=(x(k+1), x(k), y(k))$. The $x(k+1)$, $y(k)$ are calculated according to (15). There exists an invariant:

$$-4+x(k)^2+x(k-1)^2+y(k-1)^2-x(k)x(k-1)y(k-1)=(V_1-V_0)^2 \tag{19}$$

for each $k\geq 1$. The proof goes by induction to k. Therefore, for general n, the mapping is on a two-dimensional manifold.

5. Spectra and local isomorphism

Up to now, energy spectra were discussed in relation to the nature of the electronic states. Another question is whether there is a relation between energy spectra of generalised Fibonacci chains, and the concept of local isomorphism.

Definition. Two n-dimensional structures are locally isomorphic if and only if every sphere in one structure can be mapped on a sphere with the same radius and the same contents in the other structure by a translation and/or an orthogonal transformation.

For two generalised Fibonacci chains this means that two chains are locally isomorphic if and only if every sequence in one chain can be mapped on the same sequence in the other chain by a translation and/or an inversion.

Consider an arbitrary generalised Fibonacci chain, as in § 2:

$$\begin{aligned} & S_0=A^{a_1}B^{b_1}\ldots\ldots A^{a_m}B^{b_m} && (a_1,\ldots,b_m=0,1,\ldots) \\ & S_1=A^{c_1}B^{d_1}\ldots A^{c_p}B^{d_p} && (c_1,\ldots,d_p=0,1,\ldots) \\ & S_{k+1}=S_k^nS_{k-1} \qquad (k\geq 1). \end{aligned} \tag{20}$$

The infinite chain is referred to as $S_\infty=\lim_{k\to\infty} S_k$. According to § 2, the energy spectrum for a commensurate approximant S_l consists of energies for which $|\mathrm{Tr}\ M_l|\leq 2$, where M_l is determined by the procedure:

$$\begin{aligned} & M_0=M_B^{b_m}M_A^{a_m}\ldots M_B^{b_1}M_A^{a_1} \qquad M_1=M_B^{d_p}M_A^{c_p}\ldots M_B^{d_1}M_A^{c_1} \\ & M_{k+1}=M_{k-1}M_k^n. \end{aligned} \tag{21}$$

In the following, for a given chain S_∞, the set of chains will be determined, which is locally isomorphic to S_∞, and the set which has the same energy spectrum as S_∞. Comparison of the two sets will provide the relation between energy spectrum and local isomorphism.

5.1. Locally isomorphic structures

In order to determine all T_∞ which are locally isomorphic to a given S_∞, two lemmas will be useful. First, some notation is introduced. With T_∞, a structure is meant which is constructed in the same way as S_∞ (see equation (20)), but with $(T_0, T_1) \neq (S_0, S_1)$. For given S_k, S_k^{r} means the reverse of S_k (for example: if $S_k = A^a B^b$, then $S_k^{\mathrm{r}} = B^b A^a$). For given S_k, let E be a product of A atoms and B atoms. Then ES_kE^{-1} is said to be a positive product if ES_kE^{-1} does not contain A^i or B^i with $i<0$ (E^{-1}: if, for example, $E = A^aB^b$, then $E^{-1} = B^{-b}A^{-a}$). Note that E is not necessarily a positive product.

Lemma 5.1. For given S_∞, let T_∞ be such that $T_0 = ES_0E^{-1}$, $T_1 = ES_1E^{-1}$ with the restriction on E, that T_0, T_1 be positive products.

Then S_∞ and T_∞ are locally isomorphic and

$$T_k = ES_kE^{-1} \qquad k \geqslant 0 \tag{22}$$

Proof. (i) Equation (22) is evident for $k = 0, 1$.

(ii) Suppose (22) holds for $k-1$, k. Then $T_{k+1} = T_k^n T_{k-1} = (ES_kE^{-1})^n ES_{k-1}E^{-1} = ES_k^n S_{k-1}E^{-1} = ES_{k+1}E^{-1}$. Since S_k and T_k differ by the same set of finite sequences at the edges for each k, the two infinite sequences are locally isomorphic.

Lemma 5.2. For given S_∞, let T_∞ be such that $T_0 = S_0^{\mathrm{r}}$, $T_1 = S_1^{\mathrm{r}}$. Then S_∞ and T_∞ are locally isomorphic and:

$$\begin{aligned} (S_0S_1)^{-1}T_k^{\mathrm{r}}(S_1S_0) &= S_k \qquad k \text{ even} \\ (S_1S_0)^{-1}T_k^{\mathrm{r}}(S_0S_1) &= S_k \qquad k \text{ odd.} \end{aligned} \tag{23}$$

The rather lengthy proof is given in appendix 1. Now all T_∞ can be determined, which are locally isomorphic to a given S_∞.

Theorem 5.3. For given S_∞, the structures T_∞ which are locally isomorphic to S_∞ are of one of the following forms:

$$(a) \qquad T_0 = ES_mE^{-1},\ T_1 = ES_{m+1}E^{-1} \qquad m \geqslant 0 \tag{24a}$$

$$(b) \qquad T_0 = ES_m^{\mathrm{r}}E^{-1},\ T_1 = ES_{m+1}^{\mathrm{r}}E^{-1} \qquad m \geqslant 0 \tag{24b}$$

$$(c) \qquad S_0 = ET_mE^{-1},\ S_1 = ET_{m+1}E^{-1} \qquad m > 0 \tag{24c}$$

$$(d) \qquad S_0 = ET_m^{\mathrm{r}}E^{-1},\ S_1 = ET_{m+1}^{\mathrm{r}}E^{-1} \qquad m > 0 \tag{24d}$$

with E an arbitrary product of A atoms and B atoms, such that T_0, T_1 are positive products.

For the proof, see appendix 2.

5.2. Structures with the same energy spectrum

The next question is: for given S_∞, which T_∞ have the same energy spectrum as S_∞? The spectrum for S_∞ consists of energies, for which $|\lim_{k\to\infty} x(k)| \leqslant 2$ (see § 2); $x(k) = \mathrm{Tr}(M_k)$ where M_k and S_k are related according to (20) and (21). The spectrum for T_∞ consists of energies for which $|\lim_{k\to\infty} x'(k)| \leqslant 2$; $x'(k) = \mathrm{Tr}(M'_k)$, where M'_k and T_k are related according to (20) and (21). First, for given S_∞, the structures T_∞ of form (a)-(d) in theorem 5.3 will be proven to have the same spectrum as S_∞. The following lemma will be useful.

Lemma 5.4. If $x'(0)=x(0)$, $x'(1)=x(1)$, $y'(0, n-1)=y(0, n-1)$, then S_∞ and T_∞ have the same energy spectrum.

Proof. According to the recursion relations (15), the starting conditions for $x(k)$ are $x(0)$, $x(1)$, $y(0, n-1)$; for $x'(k)$ they are $x'(0)$, $x'(1)$, $y'(0, n-1)$. If the starting conditions are the same, then $x'(k)=x(k)$ for each k and $\lim_{k\to\infty} x'(k)=\lim_{k\to\infty} x(k)$. Thus S_∞ and T_∞ have the same spectrum.

Theorem 5.5. For given S_∞: S_∞ and the locally isomorphic structures T_∞ in (24) of theorem 5.3, have the same energy spectrum.

For the proof, see appendix 3.

The final step is to prove that the T_∞ in (24) of theorem 5.3 are the only structures having the same energy spectrum as S_∞. Two lemmas will be useful.

Lemma 5.6. For arbitrary S_l and T_k (with corresponding $x(l)=\mathrm{Tr}(M_l)$, $x'(k)=\mathrm{Tr}(M'_k)$ respectively) the energy spectrum is the same if and only if $x(l)=x'(k)$.

Proof. The 'if' part is trivial.

For the 'only if' part: in order to get the same spectrum, S_l and T_k must contain the same number of atoms (since the number of bands equals the number of atoms), say s_l. Then $x(l)$ and $x'(k)$ are both polynomials in E of order s_l. In order to have the same spectrum, $2s_l$ points $(E, x(l)(E))$, $(E, x'(k)(E))$ must be the same. Since a polynomial of order s_l is completely determined by s_l+1 points and since $s_l \geqslant 1$, the polynomials $x(l)$ and $x'(k)$ must be the same.

In order to formulate the following lemma, we introduce some notation. Let s_k be the number of atoms contained in S_k; so s_0, s_1 is the number of atoms in S_0, S_1 respectively and $s_{k+1}=ns_k+s_{k-1}$; note that $s_k=q_k$, defined in (8), if $s_0=1$, $s_1=n$. Similarly, s'_k is the number of atoms contained in T_k. Let $aP(p)$ denote a polynomial of order p with highest-order coefficient a: $aP(p)=aE^p+0(<p)$.

Lemma 5.7. For S_∞ and T_∞ (with corresponding $x(k)=\mathrm{Tr}(M_k)$, $x'(k)=\mathrm{Tr}(M'_k)$ respectively) with $s_k=s'_k$ for each k, then it holds for each $k>1$:

(a) if $x'(0)=x(0)$, $x'(1)=x(1)$, $y'(0, n-1)=y(0, n-1)-a_{-1}P(p_{-1})$, then:

$$\begin{aligned} &x'(k)-x(k)=a_{-1}q_{k-2}P(p_{-1}-s_0-s_1+s_k) \\ &y'(k-1, n-1)-y(k-1, n-1)=a_{-1}(q_{k-2}-q_{k-3})P(p_{-1}-s_0-s_1+s_k-s_{k-1}) \end{aligned} \tag{25a}$$

(b) if $y'(0, n-1)=y(0, n-1)$, $x'(1)=x(1)$, $x'(0)=x(0)-a_0P(p_0)$, then:

$$\begin{aligned} &x'(k)-x(k)=-a_0q_{k-2}P(p_0-s_0+s_k) \\ &y'(k-1, n-1)-y(k-1, n-1)=-a_0(q_{k-2}-q_{k-3})P(p_0-s_0+s_k-s_{k-1}) \end{aligned} \tag{25b}$$

(c) if $y'(0, n-1)=y(0, n-1)$, $x'(0)=x(0)$, $x'(1)=x(1)-a_1P(p_1)$, then:

$$\begin{aligned} &x'(k)-x(k)=-a_1q_{k-1}P(p_1-s_1+s_k) \\ &y'(k-1, n-1)-y(k-1, n-1)=-a_1(q_{k-1}-q_{k-2})P(p_1-s_1+s_k-s_{k-1}). \end{aligned} \tag{25c}$$

For the proof, see appendix 4.

Now, for a given S_∞, the structures T_∞ can be determined, which have the same spectrum as S_∞. In order to have the same energy spectrum for S_∞ and T_∞, it must hold that $\lim_{k\to\infty} x(k) = \lim_{k\to\infty} x'(k)$ with $x(k)$, $x'(k)$ being polynomials of order s_k, s'_k respectively in E. Then there must be a $t \in \mathbb{Z}$, such that $\lim_{k\to\infty}[x'(k) - x(k+t)] = 0$. This means that $s'_k = s_{k+t}$ for $\min(k, k+t) \geq 0$. Since $\lim_{k\to\infty} S_k = \lim_{k\to\infty} S_{k+t}$, we can start with S_0, S_1, T_0, T_1 such that $s_0 = s'_0$, $s_1 = s'_1$. We now assume (assumption 1) that, if an $M \in \mathbb{N}$ can be found such that $x'(k) - x(k) = f(k)P(s_k - M)$ for each k, with $\lim_{k\to\infty} f(k) \neq 0$, then $\lim_{k\to\infty} x(k) \neq \lim_{k\to\infty} x'(k)$.

Consider, for given S_∞, a chain T_∞, with $s_k = s'_k$ for each k. Let $y'(0, n-1) = y(0, n-1) - a_{-1}P(p_{-1})$, $x'(0) = x(0) - a_0 P(p_0)$, $x'(1) = x(1) - a_1 P(p_1)$. Then, according to lemma 5.7

$$x'(k) - x(k) = q_{k-2}[a_{-1}P(p_{-1} - s_0 - s_1 + s_k) - a_0 P(p_0 - s_0 + s_k)] - q_{k-1}a_1 P(p_1 - s_1 + s_k)$$

where only the highest-order terms count. Then $x'(k) - x(k) = f(k)P(\max[p_{-1} - s_0 - s_1, p_0 - s_0, p_1 - s_1] + s_k)$. Now the question is, whether $\lim_{k\to\infty} f(k) \neq 0$. First note that, if we are in case (a), (b) or (c) of lemma 5.7, then $\lim_{k\to\infty} f(k) = \infty$. For combinations of these cases, choose S_0, S_1, T_0, T_1 such that S_{-2}, T_{-2}, S_{-1}, T_{-1} are positive products. Then the a_{-1} term does not provide the highest-order term: $p_{-1} - s_0 - s_1 < \min(p_0 - s_0, p_1 - s_1)$. Then $\lim_{k\to\infty} f(k) = 0$ only if $p_0 - s_0 = p_1 - s_1$ and if $\lim_{k\to\infty}[q_{k-2}a_0 + q_{k-1}a_1] = 0 \to a_1 = -\phi a_0$. If V_0, V_1 are rational, then a_0, a_1 are rational, and $\lim_{k\to\infty} f(k) = \infty$. For given C, D being products of M_A matrices and M_B matrices: if $\mathrm{Tr}\, C = \mathrm{Tr}\, D$, then $D = ECE^{-1}$ or $D = EC^{\mathrm{r}}E^{-1}$ with E being a product of M_A matrices and M_B matrices. Argument: write $D = PCQ$ (such P, Q can always be found). We now assume the following expression to hold (assumption 2): $\mathrm{Tr}\, D = \mathrm{Tr}(PCQ) = \mathrm{Tr}(CQP) \neq \mathrm{Tr}\, C$ if $P \neq Q^{-1}$ since $\mathrm{Tr}\, C$ will then be a different polynomial in E than $\mathrm{Tr}\, D$. Analogously, after noting that $\mathrm{Tr}\, C = \mathrm{Tr}(C^{\mathrm{r}})$ due to theorem 5.5, $\mathrm{Tr}(PC^{\mathrm{r}}Q) \neq \mathrm{Tr} C$ if $P \neq Q^{-1}$ (this is made plausible below theorem 5.8).

Theorem 5.8. For rational V_0, V_1, for given S_∞: the T_∞ which have the same energy spectrum as S_∞ are exactly the T_∞ in (24) of theorem 5.3.

Proof. Suppose T_∞ has the same energy spectrum as S_∞. Then T_∞ must be of one of the following forms, due to assumption 1 and 2:

(a) $\quad T_0 = ES_m E^{-1}$, $T_1 = FS_{m+1}F^{-1}$ $\quad m \geq 0$

(b) $\quad T_0 = ES^{\mathrm{r}}_m E^{-1}$, $T_1 = FS^{\mathrm{r}}_{m+1}F^{-1}$ $\quad m \geq 0$

(c) $\quad S_0 = ET_m E^{-1}$, $S_1 = FT_{m+1}F^{-1}$ $\quad m > 0$

(d) $\quad S_0 = ET^{\mathrm{r}}_m E^{-1}$, $S_1 = FT^{\mathrm{r}}_{m+1}F^{-1}$ $\quad m > 0.$

The final step is to prove that $E = F$. The proof will be given for case (a); the proof for the other cases goes analogously. Define U_∞ by: $U_0 = S_m$, $U_1 = S_{m+1}$, $U_{k+1} = U^n_k U_{k-1}$. Then $U_\infty = S_\infty$. Thus T_∞ and U_∞ must be proven to have the same spectrum, where $T_0 = EU_0E^{-1}$, $T_1 = FU_1F^{-1}$. Let $x(k) = \mathrm{Tr}(M_k)$ and $x'(k) = \mathrm{Tr}(M'_k)$ correspond to U_k and T_k respectively. Then $M'_0 = M_E^{-1}M_0M_E$, $M'_1 = M_F^{-1}M_1M_F$. Since then $x'(0) = x(0)$, $x'(1) = x(1)$, it must hold that $y'(0, n-1) = y(0, n-1)$, due to lemma 5.7. Thus $\mathrm{Tr}(M'_1(M'_0)^{-1}) = \mathrm{Tr}(M_1M_0^{-1}) \to \mathrm{Tr}(M_F^{-1}M_1M_FM_E^{-1}M_0^{-1}M_E) = \mathrm{Tr}(M_1M_0^{-1})$. The same argument as in assumption 2 yields: $M_E = M_F \to E = F$.

The statement that the T_∞ of form (a) have the same spectrum as S_∞ according to theorem 5.5 completes the proof.

It can be proven that theorem 5.8 also holds ($\lim_{k\to\infty} f(k) \neq 0$) for V_0, V_1 not both rational, except for the following case (if it exists!).

(1) Let $s'_k = s_{k+t}$ for each k, for certain t (otherwise S_∞ and T_∞ will not have the same spectrum due to assumption 1);

(2) choose S_0, S_1, T_0, T_1 such that $t = 0$ and $S_{-2}, T_{-2}, S_{-1}, T_{-1}$ are positive products;

(3) $a_1 = -\phi a_0$ and $p_0 - s_0 = p_1 - s_1$;

(4) for each k, S_k and T_k contain the same number of atoms of type A (thus also of type B, since $s_k = s'_k$): suppose $s_k = s'_k$; S_k, T_k contain A_k, A'_k atoms of type A respectively, $A_k \neq A'_k$. Then $x'(k) - x(k) = (A'_k - A_k)(V_0 - V_1)P(s_k - 1)$;

(5) for each k, S_k and T_k are of the form: $S_k = EA^{a_1}B^{b_1} \ldots A^{a_j}B^{b_j}E^{-1}$, $T_k = FA^{c_1}B^{d_1} \ldots A^{c_{j'}}B^{d_{j'}}F^{-1}$ with $j = j'$, where E, F are products of A atoms and B atoms: suppose $A_k = A'_k$, $j \neq j'$. Then $x'(k) - x(k) = (j' - j)(V_0 - V_1)^2 P(s_k - 4)$.

Comparing theorems 5.3 and 5.8 leads to the conclusion that two generalised Fibonacci chains constructed by juxtaposition have the same energy spectrum if and only if they are locally isomorphic (except for the case mentioned below theorem 5.8, for which it is not known). The proof of theorem 5.3 shows that, if S_∞ and T_∞ are locally isomorphic, then there is a $m \in \mathbb{Z}$ such that the commensurate approximants T_k and S_{k+m} differ by a constant finite sequence at the edges for each k, or such that T_k and the reverse of S_{k+m} differ by a finite sequence for each k (constant for each even k, and constant for each odd k), for k large enough.

6. Conclusions

For the step potential, for which the system is critical in the incommensurate limit, and for the $\lambda = 2$ case of the sinusoidal potential, a scaling parameter α and a critical index for the total bandwidth δ is determined for $n = 1, 2, 3, 4$ and the total bandwidth goes down as $c[q_l]^{-\delta}$, where q_l is the number of bands. For the step potential, recursion relations for general n have been derived to treat the spectral problem by means of a mapping problem. Generalised Fibonacci chains are found to have the same energy spectrum if and only if they are locally isomorphic (except for one case, for which it is not known). It has been shown how two locally isomorphic chains are related.

Acknowledgment

I would like to thank Dr T Janssen for very useful and inspiring discussions.

Appendix 1. Proof of lemma 5.2

Proof by induction. Define U_∞ by: $U_0 = S_0 = T_0^r$, $U_1 = S_1 = T_1^r$, $U_{k+1} = U_{k-1}U_k^n$ (the juxtaposition rule for U_k is different from the rule for S_k, T_k).
Then

(i) $(S_0S_1)^{-1}U_2(S_1S_0) = S_2$

(ii) $(S_1S_0)^{-1}U_3(S_0S_1) = S_3$

(iii) $(S_1S_0)^{-1}U_3U_2 = (S_0S_1)^{-1}U_2U_3$.

Proof by substituting $U_2 = S_0 S_1^{n}$, $U_3 = S_1[S_0 S_1^{n}]^{n}$. Induction step; for k even: suppose $(S_0S_1)^{-1}U_{k-2}(S_1S_0) = S_{k-2}$, $(S_1S_0)^{-1}U_{k-1}(S_0S_1) = S_{k-1}$, $(S_1S_0)^{-1}U_{k-1}U_{k-2} = (S_0S_1)^{-1}U_{k-2}U_{k-1}$. Then

(iv) $(S_0S_1)^{-1}U_k(S_1S_0) = S_k$

(v) $(S_0S_1)^{-1}U_kU_{k-1} = (S_1S_0)^{-1}U_{k-1}U_k$.

Proof by substituting $U_k = U_{k-2}U_{k-1}^{n}$ and using the induction assumptions.

Analogously one can prove, using the induction assumptions for odd k:

(vi) $(S_1S_0)^{-1}U_k(S_0S_1) = S_k$

(vii) $(S_1S_0)^{-1}U_kU_{k-1} = (S_0S_1)^{-1}U_{k-1}U_k$.

Relations (i)-(vii) lead to

$$(S_0S_1)^{-1}U_k(S_1S_0) = S_k \qquad \text{for } k \text{ even}$$
$$(S_1S_0)^{-1}U_k(S_0S_1) = S_k \qquad \text{for } k \text{ odd.}$$

The final step in the proof is made by noting that $U_k = T_k^{r}$, $k \geqslant 0$. This leads directly to

$$(S_0S_1)^{-1}T_k^{r}(S_1S_0) = S_k \qquad \text{for } k \text{ even}$$
$$(S_1S_0)^{-1}T_k^{r}(S_0S_1) = S_k \qquad \text{for } k \text{ odd.}$$

Appendix 2. Proof of theorem 5.3

For given S_∞, define U_∞ by: $U_0 = S_m$, $U_1 = S_{m+1}$, $m \geqslant 0$, $U_{k+1} = U_k^{n}U_{k-1}$. Then $U_k = S_{k+m}$ for each k and $U_\infty = S_\infty$.

(*a*) Then T_∞, given by $T_0 = EU_0E^{-1} = ES_mE^{-1}$, $T_1 = EU_1E^{-1} = ES_{m+1}E^{-1}$, is locally isomorphic to S_∞ according to lemma 5.1 and

$$T_k = ES_{k+m}E^{-1} \qquad k \geqslant 0. \tag{A2.1}$$

The only restriction on E is that T_0, T_1 be positive products.

(*b*) Then T_∞, given by $T_0 = EU_0^{r}E^{-1} = ES_m^{r}E^{-1}$, $T_1 = EU_1^{r}E^{-1} = ES_{m+1}^{r}E^{-1}$, is locally isomorphic to S_∞ according to lemmas 5.1, 5.2 and

$$\begin{aligned} &(S_mS_{m+1})^{-1}E^{r}T_k^{r}(E^{-1})^{r}(S_{m+1}S_m) = S_{k+m} \qquad k \text{ even} \\ &(S_{m+1}S_m)^{-1}E^{r}T_k^{r}(E^{-1})^{r}(S_mS_{m+1}) = S_{k+m} \qquad k \text{ odd.} \end{aligned} \tag{A2.2}$$

The restriction on E is that T_0, T_1 be positive products.

(*c*) For given S_∞: if positive products T_0, T_1 can be found such that $S_0 = ET_mE^{-1}$, $S_1 = ET_{m+1}E^{-1}$ for certain E and $m > 0$, then S_∞ and T_∞ are locally isomorphic and

$$S_k = ET_{k+m}E^{-1} \qquad k \geqslant 0, m > 0. \tag{A2.3}$$

(*d*) Analogously, for given S_∞: if positive products T_0, T_1 can be found, such that $S_0 = ET_m^{r}E^{-1}$, $S_1 = ET_{m+1}^{r}E^{-1}$ for certain E and $m > 0$, then S_∞ and T_∞ are locally isomorphic and

$$\begin{aligned} &(T_mT_{m+1})^{-1}E^{r}S_k^{r}(E^{-1})^{r}(T_{m+1}T_m) = T_{k+m} \qquad k \text{ even} \\ &(T_{m+1}T_m)^{-1}E^{r}S_k^{r}(E^{-1})^{r}(T_mT_{m+1}) = T_{k+m} \qquad k \text{ odd.} \end{aligned} \tag{A2.4}$$

The next step is to prove that there are no other structures T_∞, which are locally isomorphic to a given S_∞.

(a) Without inversion. With help of the relation $S_{k-1} = S_k^{-n} S_{k+1}$, S_l can also be defined for $l<0$, if S_l is a positive product. Let $p \in \mathbb{Z}$ be such that S_l is a positive product for $l \geqslant p$, and S_{p-1} is not. Take an arbitrary T_∞ and write: $T_1 = DS_{t+1}C$, where $t+1$ is the largest integer for which S_{t+1} is included in T_1 (so C, D are positive products). If S_{p+1} is not included in T_1, then write $t=p$ (then C, D are not both positive products).

At first, sequences T_k and ET_kE^{-1} $(k \geqslant 0)$ will not be distinguished. Later on, this possibility of getting locally isomorphic chains (according to lemma 5.1) will be taken into account. Since we do not distinguish between T_k and CT_kC^{-1} $(k \geqslant 0)$ at this stage, write: $T_1 = CDS_{t+1}$. Then CD must be a product of sequences S_t and S_{t+1}: $T_1^2 = CDS_{t+1}CDS_{t+1}$ occurs in T_∞. Now S_∞ can be considered as built up out of S_t, S_{t+1}, occurring as powers $(S_{t+1})^n$, $(S_{t+1})^{n+1}$, S_t. Then $T_1 = (S_{t+1})^\gamma$ or $T_1 = (S_{t+1})^{i_1} S_t (S_{t+1})^{i_2} \dots (S_{t+1})^{i_{k-1}} S_t (S_{t+1})^{i_k}$. Since $t+1$ is the largest integer for which S_{t+1} is included in T_1, it holds that

$$T_1 = (S_{t+1})^\gamma \qquad 1 \leqslant \gamma \leqslant n \tag{A2.5}$$

or

$$T_1 = (S_{t+1})^{i_1} S_t (S_{t+1})^{i_2} \qquad i_1 \leqslant n-1,\ 1 \leqslant i_2 \leqslant n.$$

$n=1$. $T_1 = S_{t+1}$ or $T_1 = S_tS_{t+1}$. Suppose $T_1 = S_tS_{t+1}$. Since we do not distinguish between T_k and $S_t^{-1}T_kS_t$ $(k \geqslant 0)$ at this stage, we may write: $T_1 = S_t^{-1}S_tS_{t+1}S_t = S_{t+1}S_t = S_{t+2}$. Due to the fact that $t+1$ is the largest integer for which S_{t+1} is included in T_1, it holds that $T_1 = S_{t+1}$. The next step is to prove that $T_0 = S_t$. $T_1^2T_0T_1^2 = (S_{t+1})^2 T_0 (S_{t+1})^2$ occurs in T_∞. In order to be locally isomorphic to S_∞, it must hold that

$$T_0 = S_t \text{ or } T_0 = S_t(S_{t+1})^{i_1} \dots (S_{t+1})^{i_k} S_t \qquad i_1, \dots, i_k = 1, 2.$$

In the latter case, $i_1 = i_k = 2$, because $T_0T_1T_0$ occurs in T_∞. Also $T_0T_1^2T_0$ occurs in T_∞, which means that $(S_{t+1})^2S_t(S_{t+1})^2S_t(S_{t+1})^2$ occurs; this sequence does not occur in S_∞. So $T_1 = S_{t+1}$, $T_0 = S_t$.

$n>1$. Suppose $T_1 = (S_{t+1})^{i_1}S_t(S_{t+1})^{i_2}$ (see (A2.5)). Now T_1^{n+1} occurs in T_∞. Since $n>1$, $S_t(S_{t+1})^{(i_1+i_2)}S_t(S_{t+1})^{(i_1+i_2)}S_t$ occurs. This sequence only occurs in S_∞ when $i_1+i_2=n$. Write $T_1 = (S_{t+1})^{(n-i)}S_t(S_{t+1})^i$ $(i \geqslant 1)$. Since we do not distinguish between T_k and $(S_{t+1})^iT_k(S_{t+1})^{-i}$ $(k \geqslant 0)$ at this stage, write $T_1 = (S_{t+1})^nS_t = S_{t+2}$. Since $t+1$ was the largest integer for which S_{t+1} is included in T_1, T_1 must be $(S_{t+1})^\gamma$, $1 \leqslant \gamma \leqslant n$. Now T_1^n occurs in T_∞. Since S_{t+1} occurs only as power $(S_{t+1})^n$ or $(S_{t+1})^{n+1}$ in S_∞, it must hold that $\gamma = 1$: $T_1 = S_{t+1}$. The next step is to prove that $T_0 = S_t$. Now $T_1^{n+1}T_0T_1^n = (S_{t+1})^{n+1}T_0(S_{t+1})^n$ and $T_1^nT_0T_1^{n+1} = (S_{t+1})^nT_0(S_{t+1})^{n+1}$ occurs in T_∞, which yields: $T_0 = S_t$ or $T_0 = S_t(S_{t+1})^{i_1} \dots (S_{t+1})^{i_k}S_t$; $i_1 = i_k = n$; $i_2, \dots, i_{k-1} = n$, $n+1$. In the latter case, make use of the fact that $(T_1^nT_0)^n$ occurs in T_∞ and that, if $[(S_{t+1})^{n+1}S_t][(S_{t+1})^nS_t]^i[(S_{t+1})^{n+1}S_t]$ occurs in S_∞, then $i=n$ or $n-1$. This means that T_0 must be of this kind

$$T_0 = S_t[(S_{t+1})^nS_t]^{(n-i-j_0)}[(S_{t+1})^{n+1}S_t][(S_{t+1})^nS_t]^{j_1} \dots [(S_{t+1})^nS_t]^{j_s} \times [(S_{t+1})^{n+1}S_t][(S_{t+1})^nS_t]^i$$

with $i \geqslant 1, j_1, \dots, j_s = n$, $n-1$ and $j_0 = 1, 2$. Now $T_1^{n+1}T_0$ occurs in T_∞. In order to be locally isomorphic to S_∞, it must hold that $n-i-j_0 = n$ or $n-1 \to i \leqslant 0$. Since $i \geqslant 1$, T_∞ and S_∞ cannot be locally isomorphic. So $T_1 = S_{t+1}$, $T_0 = S_t$.

Combining these results with lemma 5.1 gives, as a conclusion, that the T_∞ which are locally isomorphic to S_∞, without taking inversion into account, are of the form (A2.1) $(t \geqslant 0)$ or (A2.3) $(t<0)$.

(b) With inversion. Lemma 5.2 tells us that, with $U_0 = S_0^r$, $U_1 = S_1^r$, $U_{k+1} = U_k^n U_{k-1}$, every finite sequence in S_∞ occurs in the reverse of U_∞ and vice versa. So the task is to search for T_∞ such that every sequence in T_∞ occurs in U_∞ and vice versa. Part (a) of the proof showed that, in order to get locally isomorphic chains T_∞ and U_∞ without taking inversion into account, it must hold that $T_0 = FU_tF^{-1}$, $T_1 = FU_{t+1}F^{-1}$, which means that the T_∞, which are locally isomorphic to S_∞, taking inversion into account, are of the form (A2.2) or (A2.4).

Appendix 3. Proof of theorem 5.5

Suppose $T_0 = ES_tE^{-1}$, $T_1 = ES_{t+1}E^{-1}$; then we are in cases (a) $(t \geq 0)$ and (c) $(t < 0)$ of theorem 5.3. Say $U_0 = ES_0E^{-1}$, $U_1 = ES_1E^{-1}$, $U_{k+1} = U_k^n U_{k-1}$. Then $U_\infty = T_\infty$, since $\lim_{k\to\infty} ES_kE^{-1} = \lim_{k\to\infty} ES_{k+t}E^{-1}$. So we have to prove that U_∞ and S_∞ have the same spectrum.

Let E, S_k, U_k correspond to M_E, M_k, M'_k respectively according to (20) and (21). Then $M'_0 = M_E^{-1}M_0M_E$, $M'_1 = M_E^{-1}M_1M_E$. With use of the relation $\mathrm{Tr}(CD) = \mathrm{Tr}(DC)$ for arbitrary C, D, this directly yields: $x'(0) = x(0)$, $x'(1) = x(1)$, $y'(0, n-1) = y(0, n-1)$. Using lemma 5.4, U_∞ and S_∞ have the same spectrum, thus T_∞ and S_∞ have the same spectrum. Suppose $T_0 = ES_t^rE^{-1}$, $T_1 = ES_{t+1}^rE^{-1}$. Then we are in cases (b) $(t \geq 0)$ and (d) $(t < 0)$ of theorem 5.3. Say $V_0 = E^{-1}T_0E = S_t^r$, $V_1 = E^{-1}T_1E = S_{t+1}^r$, $V_{k+1} = V_k^n V_{k-1}$. Then V_∞ and T_∞ have the same spectrum according to the proof above. So the next step is to prove that V_∞ and S_∞ have the same spectrum. Say $U_0 = S_t$, $U_1 = S_{t+1}$, $U_{k+1} = U_k^n U_{k-1}$. Then $U_\infty = S_\infty$. We have to prove that U_∞ and V_∞ have the same spectrum (note that $V_0 = U_0^r$, $V_1 = U_1^r$).

Let M_k, M'_k correspond to U_k, V_k respectively. It must hold that: (1) $\mathrm{Tr}(M_0^r) = \mathrm{Tr}(M_0)$, (2) $\mathrm{Tr}(M_1^r) = \mathrm{Tr}(M_1)$, (3) $\mathrm{Tr}[M_1^r(M_0^r)^{-1}] = \mathrm{Tr}[M_1M_0^{-1}]$. The relations (1), (2), (3) hold if $\mathrm{Tr}(C) = \mathrm{Tr}(C^r)$ for arbitrary $C = M_A^{a_1} \ldots M_B^{b_m}$ $(a_1, \ldots, b_m \in \mathbb{Z})$. The proof goes by induction. First, $\mathrm{Tr}(C) = \mathrm{Tr}(C^r)$ for $C = M_A^{a_1}M_B^{b_1}$, $C = M_A^{a_1}M_B^{b_1}M_A^{a_2}$, $C = M_B^{b_1}M_A^{a_1}M_B^{b_2}$ for all a_1, a_2, b_1, $b_2 \in \mathbb{Z}$, by using (13). The induction step: suppose $\mathrm{Tr}(M_A^{a_1} \ldots M_A^{a_m}) = \mathrm{Tr}(M_A^{a_m} \ldots M_A^{a_1})$. Then

$$
\begin{aligned}
\mathrm{Tr}(M_A^{a_1} \ldots M_A^{a_m} M_B^{b_m}) \\
&= \mathrm{Tr}(M_A^{a_1} \ldots M_B^{b_{m-1}})\mathrm{Tr}(M_A^{a_m}M_B^{b_m}) - \mathrm{Tr}(M_A^{a_1} \ldots M_B^{(b_{m-1}-b_m)}M_A^{-a_m}) \\
&= \mathrm{Tr}(M_B^{b_{m-1}} \ldots M_A^{a_1})\mathrm{Tr}(M_B^{b_m}M_A^{a_m}) - \mathrm{Tr}(M_A^{-a_m}M_B^{(b_{m-1}-b_m)} \ldots M_A^{a_1}) \\
&= \mathrm{Tr}(M_B^{b_m}M_A^{a_m} \ldots M_A^{a_1})
\end{aligned}
$$

because of the induction assumption and with use of (13).

Appendix 4. Proof of lemma 5.7

First, note that $x'(k)$ and $x(k)$ are polynomials with highest-order term E^{s_k}. The proof will be given for (25a). The other two cases go analogously. The cases $n = 1$ and $n > 1$ are treated separately. Suppose $x'(0) = x(0)$, $x'(1) = x(1)$, $y'(0, n-1) = y(0, n-1) - a_{-1}P(p_{-1})$. The task will be to find the highest-order term of the difference polynomial $y'(k-1, n-1) - y(k-1, n-1)$ and $x'(k) - x(k)$. By 'lower-order terms' will be meant terms which do not contribute to the highest-order term.

n = 1. For $n=1$, $y(0, n-1) = x(-1)$, $y'(0, n-1) = x'(-1)$.

$$x'(2) = x'(0)x'(1) - x'(-1)$$

$$= x(0)x(1) - [x(-1) - a_{-1}P(p_{-1})] = x(2) + a_{-1}P(p_{-1})$$

$$x'(3) = x'(1)x'(2) - x'(0) = x(1)[x(2) + a_{-1}P(p_{-1})] - x(0)$$

$$= x(3) + a_{-1}P(p_{-1} + s_1) = x(3) + a_{-1}P(p_{-1} - s_0 - s_1 + s_3)$$

$$x'(4) = x'(2)x'(3) - x'(1) = \ldots = x(4) + a_{-1}P(p_{-1} - s_0 - s_1 + s_4).$$

The induction step: suppose (25a) holds for $k-1$, $k-2$, $k-3$. Then (25a) also holds for k. Proof by using $x'(k) = x'(k-2)x'(k-1) - x'(k-3)$ and substituting the terms on the right-hand side with help of the induction assumptions.

n > 1.

$$y'(1, n-1) = y'(1, n-2)x'(1) - y'(1, n-3)$$

$$= [y'(1, 0)x'(1) - y'(1, -1)][x'(1)]^{n-2} + \text{lower-order terms}$$

$$= [x'(0)x'(1) - y'(0, n-1)][x'(1)]^{n-2} + \text{lower-order terms}$$

$$= y(1, n-1) + a_{-1}P(p_{-1} + (n-2)s_1)$$

$$x'(2) = y'(1, n-1)x'(1) - y'(1, n-2)$$

$$= x(2) + a_{-1}P(p_{-1} + (n-1)s_1)$$

$$= x(2) + q_0 a_{-1}P(p_{-1} - s_0 - s_1 + s_2);$$

$$y'(2, n-1) = y'(2, n-2)x'(2) - y'(2, n-3)$$

$$= [x'(1)x'(2) - y'(1, n-1)][x'(2)]^{n-2} + \text{lower-order terms}$$

$$= y(2, n-1) + a_{-1}P(p_{-1} + ns_1 + (n-2)s_2)$$

$$+ (n-2)a_{-1}P(p_{-1} + ns_1 + (n-2)s_2)$$

$$= y(2, n-1) + (q_1 - q_0)a_{-1}P(p_{-1} - s_0 - s_1 + s_3 - s_2);$$

$$x'(3) = y'(2, n-1)x'(2) - y'(2, n-2)$$

$$= x(3) + q_1 a_{-1}P(p_{-1} - s_0 - s_1 + s_3).$$

The induction step: suppose (25a) holds for $y(k-2, n-1)$, $x(k-2)$, $x(k-1)$. Then (25a) also holds for $y(k-1, n-1)$, $x(k)$ by using the relations

$$y'(k-1, n-1) = y'(k-1, n-2)x'(k-1) - y'(k-1, n-3)$$

$$= [x'(k-2)x'(k-1) - y'(k-2, n-1)][x'(k-1)]^{n-2} + \text{lower-order terms};$$

$$x'(k) = y'(k-1, n-1)x'(k-1) - y'(k-1, n-2)$$

and using the induction assumptions.

References

Andre G and Aubry S 1980 *Ann. Israel Phys. Soc.* **3** 133
Avron J and Simon B 1983 *Duke Math. J.* **50** 369
Bellissard J, Lima R and Testard D 1983 *Commun. Math. Phys.* **88** 207
Casdagli M 1986 *Commun. Math. Phys.* **107** 295
Delyon F and Petritis D 1986 *Commun. Math. Phys.* **103** 441
Grempel D, Fishman S and Prange R 1982 *Phys. Rev. Lett.* **49** 833
Gumbs G and Ali M 1988 *Phys. Rev. Lett.* **60** 1081
Hofstadter D 1976 *Phys. Rev.* B **14** 2239
Holzer M 1988a *Phys. Rev.* B **38** 1709
—— 1988b *Phys. Rev.* B **38** 5756
Kohmoto M 1983 *Phys. Rev. Lett.* **51** 1198
Kohmoto M, Kadanoff L and Tang C 1983 *Phys. Rev. Lett.* **50** 1870
Levine D and Steinhardt P 1986 *Phys. Rev.* B **34** 596
Ostlund S and Pandit R 1984 *Phys. Rev.* B **29** 1394
Ostlund S, Pandit R, Rand D, Schellnhuber H and Siggia E 1983 *Phys. Rev. Lett.* **50** 1873
Suto A 1987 *Commun. Math. Phys.* **111** 409
Thouless D 1983 *Phys. Rev.* B **28** 4272
Wilkinson M 1987 *J. Phys. A: Math. Gen.* **20** 4337