

# Appendix A

## Schrödinger Operators with Substitutive Potential

The Schrödinger equation on  $\mathbf{R}^n$  :  $(-\Delta + V(x))\psi(x) = E\psi(x)$ , where  $\Delta$  is the Laplace operator, appears, in many problems related to Quantum Mechanics, as the eigenvalue equation for a one-electron energy operator  $H$ ,  $H\psi = -\Delta\psi + V \cdot \psi$ , when  $V$  describes the potential energy of the electron.

The discovery of Quasicrystals, in 1984, has motivated a great interest in models provided by discrete Schrödinger operators acting on  $\ell^2(\mathbf{Z}^v)$ . The one-dimensional case with potentials taking finitely many values on the infinite chain  $\mathbf{Z}$ , or on the semi-infinite chain  $\mathbf{N}$ , has attracted particular attention and has been considerably studied. It is, of course, impossible to cite all the contributions and progresses. We would just like to explain the role played by substitutions in this area.

### A.1 Classical Facts on 1D Discrete Schrödinger Operators

#### A.1.1 Preliminaries

We consider  $\mathcal{L}$ , the space of bilateral complex sequences, and  $H$ , the *discrete Schrödinger operator* defined on  $\varphi = (\varphi(n))_{n \in \mathbf{Z}} \in \mathcal{L}$  by

$$(H\varphi)(n) = \varphi(n+1) + \varphi(n-1) + v(n)\varphi(n), \quad n \in \mathbf{Z}, \quad (\text{A.1})$$

where the *potential*  $v = (v(n))_{n \in \mathbf{Z}}$  is a bounded and real sequence. It is easily checked that  $H$  restricted to  $\ell^2(\mathbf{Z})$  is a self-adjoint bounded operator.

We are interested in the description of the spectral invariants of  $H \in \mathcal{B}(\ell^2(\mathbf{Z}))$  according to the properties of the sequence  $v$ , more precisely, we wish to have a good knowledge of

1.  $sp(H) = \{\lambda \in \mathbf{R}, H - \lambda I \text{ non-invertible}\};$
2.  $\sigma$ , maximal spectral type of  $H$ .

Recall that the *spectral measure*  $\sigma_{f,g}$  of  $f, g \in \ell^2(\mathbf{Z})$  is defined by

$$\int_{\mathbf{R}} x^k d\sigma_{f,g}(x) = \langle H^k f, g \rangle_{\ell^2(\mathbf{Z})}, \quad k \geq 0$$

( $\sigma_{f,f}$  is denoted by  $\sigma_f$ ) and the maximal spectral type  $\sigma$  is a bounded positive measure on  $\mathbf{R}$ , defined up to equivalence, such that

$$\sigma_{f,g} \ll \sigma \quad \text{for every } f, g \in \ell^2(\mathbf{Z}).$$

As in the unitary case,  $sp(H)$  is the topological support of  $\sigma$  and the possible eigenvalues of  $H$  are the discrete point masses of  $\sigma$ .

### First Observations

1. If  $v \equiv 0$ , then  $H = \Delta$  and  $\sigma$  is equivalent to the Lebesgue measure on  $[-2, 2]$ .

To prove this claim, we observe that  $H$  is conjugate to  $M_\omega$ , the multiplication operator by  $\omega : t \mapsto 2 \cos t$  on  $L^2(\mathbf{T})$ , through the canonical isometric isomorphism  $\varphi \in \ell^2(\mathbf{Z}) \mapsto \Phi \in L^2(\mathbf{T})$  with  $\Phi(t) = \sum_{n \in \mathbf{Z}} \varphi(n) e^{int}$ . It is clear that  $sp(M_\omega) = [-2, 2]$  and so is  $sp(H)$  by conjugation. The maximal spectral type  $\sigma$  of  $H$  is generated by the spectral measures  $\sigma_{e_k}$  with  $e_k(n) = \delta_{nk}$  for  $n, k \in \mathbf{Z}$ ; but, for every  $k \in \mathbf{Z}$ ,  $\sigma_{e_k}$  is the pull-back under  $\omega$  of the Lebesgue measure on  $\mathbf{T}$ . In particular,

$$\begin{aligned} \langle H^n e_0, e_0 \rangle &= \frac{1}{2\pi} \int_0^{2\pi} (2 \cos t)^n dt \\ &= \int_{-2}^2 \frac{x^n}{\pi \sqrt{4-x^2}} dx, \end{aligned}$$

and  $\sigma_{e_0}$  is absolutely continuous with respect to the Lebesgue measure on  $[-2, 2]$  with  $1/\pi \sqrt{4-x^2}$  as its density.

2. On the opposite, the operator  $\varphi \mapsto (v(n)\varphi(n))_{n \in \mathbf{Z}}$  has a pure point spectrum since the  $e_k, k \in \mathbf{Z}$ , form a complete family of eigenvectors.

Thus, in the general case,  $H$  is a perturbation of  $\Delta$  by this operator and all is possible!

3. *General case.* For  $n, m \in \mathbf{Z}$ , we denote by  $\sigma_{n,m}$  the spectral measure  $\sigma_{e_n, e_m}$  and we put  $\sigma_n = \sigma_{n,n}$ .

**Proposition A.1.** *The maximal spectral type (up to equivalence) is*

$$\sigma = \sigma_0 + \sigma_{-1}.$$

This is an easy consequence of the following lemma.

**Lemma A.1.** *For every  $n \in \mathbf{Z}$ ,  $e_n = p_n(H)e_0 + q_n(H)e_{-1}$  where  $p_n$  and  $q_n$  are polynomials in  $\mathbf{R}[X]$ .*

*Proof of the Lemma.* This can be established by induction on  $n$ , starting with

$$\begin{cases} p_{-1}(t) = 0, & q_{-1}(t) = 1 \\ p_0(t) = 1, & q_0(t) = 0 \end{cases}$$

Then,

$$\begin{aligned} H e_n(k) &= e_n(k+1) + e_n(k-1) + v(k)e_n(k) \\ &= e_{n-1}(k) + e_{n+1}(k) + v(k)e_n(k) \end{aligned}$$

so that,  $e_{n+1} = H e_n - v(n)e_n - e_{n-1} = p_{n+1}(H)e_0 + q_{n+1}(H)e_{-1}$  by induction on  $n \geq 0$ , with

$$\begin{cases} p_{n+1}(t) = (t - v(n))p_n(t) - p_{n-1}(t) \\ q_{n+1}(t) = (t - v(n))q_n(t) - q_{n-1}(t) \end{cases} \quad (\text{A.2})$$

Writing  $e_{n-1} = H e_n - v(n)e_n - e_{n+1}$  when  $n \leq 0$  and proceeding in the same way, we see that  $p_n$  and  $q_n$  have degree  $n$  if  $n \geq 0$  and  $-n-1$  if  $n \leq -1$ .  $\square$

*Proof of the Proposition.* If we put  $\mathbf{S} = \begin{pmatrix} \sigma_0 & \sigma_{0,-1} \\ \sigma_{-1,0} & \sigma_{-1} \end{pmatrix}$ , we deduce from the above lemma that

$$\sigma_{n,m} = (p_n, q_n) \mathbf{S} \begin{pmatrix} p_m \\ q_m \end{pmatrix};$$

in particular, we have  $\sigma_{n,m} \ll \sigma_0 + \sigma_{-1}$  for every  $n, m \in \mathbf{Z}$ , which gives the proposition.  $\square$

*Remark A.1.* A system with absolutely continuous spectrum behaves like a conductor while a system with pure point spectrum behaves like an insulator. We shall see that periodic potentials lead to absolutely continuous spectrum; on the opposite, random potentials give rise (almost surely) to pure point spectrum and, for potentials intermediate between those two extreme cases, one may expect the presence of a singular continuous component.

### A.1.2 Schrödinger Equation

We begin by investigating the possible eigenvalues of  $H$ . A good reference for this section is [22].

**Definition A.1.**  $E \in \mathbf{R}$  is an *eigenvalue* of  $H$  if there exists  $\varphi \in \ell^2(\mathbf{Z})$ , called an *eigenvector* of  $H$ , such that  $H\varphi = E\varphi$ ; in other words  $\varphi$  is a solution of the (tight-binding) *Schrödinger equation*

$$\psi(n+1) + \psi(n-1) + v(n)\psi(n) = E\psi(n), \quad n \in \mathbf{Z}. \quad (\text{A.3})$$

Equation (A.3) is nothing but an order-two linear recurrence equation that involves matrices in  $SL(2, \mathbf{R})$  and the solutions form a two-dimensional vector space of  $\mathcal{L}$ . Actually, equation (A.3) for  $\psi$  means,

$$\begin{pmatrix} \psi(n+1) \\ \psi(n) \end{pmatrix} = g_n \begin{pmatrix} \psi(n) \\ \psi(n-1) \end{pmatrix} \quad \text{for every } n \in \mathbf{Z}, \quad (\text{A.4})$$

with  $g_n = \begin{pmatrix} E - v(n) & -1 \\ 1 & 0 \end{pmatrix} \in SL(2, \mathbf{R})$ . By iterating (A.4), we get

$$\begin{pmatrix} \psi(n+1) \\ \psi(n) \end{pmatrix} = S_n \begin{pmatrix} \psi(0) \\ \psi(-1) \end{pmatrix} \text{ if } n \geq 0 \text{ with } S_n = g_n g_{n-1} \cdots g_0$$

and

$$\begin{pmatrix} \psi(n) \\ \psi(n-1) \end{pmatrix} = S_n \begin{pmatrix} \psi(0) \\ \psi(-1) \end{pmatrix} \text{ if } n \leq -1 \text{ with } S_n = g_n^{-1} g_{n-1}^{-1} \cdots g_{-1}^{-1}.$$

Note that, by (A.2),

$$\begin{aligned} S_n := S_n(E) &= \begin{pmatrix} p_{n+1}(E) & q_{n+1}(E) \\ p_n(E) & q_n(E) \end{pmatrix} \quad \text{if } n \geq 0 \\ &= \begin{pmatrix} p_n(E) & q_n(E) \\ p_{n-1}(E) & q_{n-1}(E) \end{pmatrix} \quad \text{if } n \leq -1. \end{aligned}$$

**Definition A.2.** The matrices  $(g_n)$  are called the *transfer matrices*.

**Proposition A.2.** *The eigenvalues of  $H$  are simple : for every  $E \in \mathbf{R}$ , there exists at most one solution  $\varphi \in \ell^2(\mathbf{Z})$  satisfying (A.3) (up to a multiplicative constant).*

*Proof.* Indeed, for every  $E \in \mathbf{C}$ , equation (A.3) admits two solutions in  $\mathcal{L}$ , and if  $\varphi$  and  $\psi$  are two such solutions, the wronskian

$$\begin{aligned} W_n(\varphi, \psi) &= \varphi(n)\psi(n-1) - \varphi(n-1)\psi(n) \quad \text{if } n \geq 0 \\ &= \det \begin{pmatrix} \varphi(n) & \psi(n) \\ \varphi(n-1) & \psi(n-1) \end{pmatrix} = \det S_{n-1} \cdot \det \begin{pmatrix} \varphi(0) & \psi(0) \\ \varphi(-1) & \psi(-1) \end{pmatrix} \\ &= W_0(\varphi, \psi) \end{aligned}$$

and the analogue for  $n \leq -1$ . This proves that the wronskian must be constant and, if  $\varphi$  and  $\psi$  are in  $\ell^2(\mathbf{Z})$ , this constant must be zero. The eigenvectors are proportional.  $\square$

We recall some classical facts on the spectrum of a self-adjoint operator  $H$  on a Hilbert space  $\mathcal{H}$ . If  $E \in sp(H)$  is an isolated point of  $\sigma(H)$  then  $E$  is an eigenvalue. On the other hand, a theorem due to H. Weyl states that a point of  $\sigma(H)$  which is not an eigenvalue is an *approximate eigenvalue* in the following sense :

**Definition A.3.**  $E$  is an *approximate eigenvalue* of  $H$  if there exists a sequence  $(x_k)$  of elements in  $\mathcal{H}$  such that  $\|x_k\| = 1$  and

$$\lim_{k \rightarrow \infty} \|Hx_k - Ex_k\| = 0.$$

Let us get back to the Schrödinger operator.

**Definition A.4.** A solution  $\varphi \in \mathcal{L}$  of (A.3) is said to be *polynomially bounded* if there exists  $k \geq 1$  such that  $\varphi(n) = O(1 + |n|^2)^k$  as  $n \rightarrow \pm\infty$ .

One can prove the following by constructing an approximate sequence with help of a truncation.

**Proposition A.3.** Let  $E \in \mathbf{R}$ . If the equation (A.3) has a polynomially bounded solution  $\varphi$ , then  $E$  belongs to  $sp(H)$ .

If  $\varphi \in \mathcal{L}$  is such a solution,  $E$  is called a *generalized eigenvalue* and  $\varphi$  a *generalized eigenvector* of  $H$ .

This provides a first description of the spectrum of  $H$  that we admit [22].

**Corollary A.1.**  $sp(H)$  is the closure of the set

$$\{E \in \mathbf{R}, \text{ for which (A.3) has a polynomially bounded solution}\}$$

To decide whether  $E$  is an eigenvalue of  $H$  or not, we are thus led to study the behaviour of the sequence  $(S_n(E))$  as  $n \rightarrow \pm\infty$ .

Before continuing, we need some notations and properties of  $SL(2, \mathbf{R})$  or  $SL(2, \mathbf{C})$ , that we summarize below.

1. If  $g \in SL(2, \mathbf{R})$ , we note  $\|g\|$  the operator norm of  $g$ , i.e.  $\|g\| = \sup_{\|x\|_2=1} \|gx\|_2$  where  $\|\cdot\|_2$  is the euclidian norm on  $\mathbf{R}^2$ . If  $r(g)$  denotes the *spectral radius* of  $g$ ,  $r(g) = \lim_{n \rightarrow \infty} \|g^n\|^{1/n}$ .
2. If  $g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL(2, \mathbf{C})$ ,  $\|g\|$  can be computed in terms of the coefficients :

$$\|g\|^2 = \frac{1}{2}(K^2 + \sqrt{K^2 - 4}) \quad \text{where } K^2 = |a|^2 + |b|^2 + |c|^2 + |d|^2,$$

and  $\|g\| = \|g^{-1}\|$ .

3. We shall be needing the Cayley-Hamilton identity

$$g^2 = Tr(g) \cdot g - I \tag{A.5}$$

which infers

$$Tr(g^2) = Tr^2(g) - 2 \tag{A.6}$$

and  $Tr(g) = Tr(g^{-1})$ . By (A.5) indeed,  $g^{-1} = Tr(g) \cdot I - g$  and  $Tr(g^{-1}) = 2Tr(g) - Tr(g) = Tr(g)$ .

4. Another consequence of the Cayley-Hamilton identity is the following inequality : If  $x \in \mathbf{R}^2$ ,

$$\|x\| \leq 2 \sup\{|Tr(g)| \cdot \|gx\|, \|g^2x\|\} \tag{A.7}$$

**5. Fricke Formula :** We shall also need the following generalization of (A.6).

Let  $g, h \in SL(2, \mathbb{C})$ ; then we have (A.8)

$$Tr^2(g) + Tr^2(h) + Tr^2(gh) = Tr(ghg^{-1}h^{-1}) + 2 + Tr(g) + Tr(h) + Tr(gh).$$

**6. Lyapunov exponents.** If  $S_n = T_1 \cdots T_n$  is a product of elements of  $SL(2, \mathbb{C})$ ,  $(\|S_n\|)_{n \geq 1}$  is a sequence of numbers  $\geq 1$  by item 2. and we put

$$\gamma_n = \frac{1}{n} \log \|S_n\|.$$

If the limit  $\gamma$  of  $(\gamma_n)$  exists as  $n \rightarrow \infty$  (for instance, in the ergodic case as we shall see), then  $\gamma$  is called the *Lyapunov exponent* of this product of matrices.

**Theorem A.1 (Oseledec).** *Let  $(g_n)_{n \in \mathbb{N}^*}$  be a sequence of matrices in  $SL(2, \mathbb{C})$  satisfying.*

$$a) \quad \lim_{n \rightarrow +\infty} \frac{1}{n} \log \|g_n g_{n-1} \cdots g_1\| = \gamma$$

$$b) \quad \lim_{n \rightarrow +\infty} \frac{1}{n} \log \|g_n\| = 0.$$

*Then, there exists a nonzero vector  $x$  such that*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \|g_n \cdots g_1 x\| = -\gamma$$

*and, for any  $w$  independent of  $x$ ,*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \|g_n \cdots g_1 w\| = \gamma.$$

Consider now the sequence  $(S_n)_{n \in \mathbb{Z}}$  where  $S_n = S_n(E)$ . If  $\varphi$  and  $\psi$  are two fundamental solutions of (A.3), then, for every  $n \in \mathbb{Z}$ ,

$$\|S_n\|^2 = |\varphi(n)|^2 + |\varphi(n+1)|^2 + |\psi(n)|^2 + |\psi(n+1)|^2,$$

since  $\begin{pmatrix} \varphi(0) & \psi(0) \\ \varphi(-1) & \psi(-1) \end{pmatrix} = I$ , and the asymptotic behaviour of the solutions follows from the asymptotic behaviour of  $\|S_n\|$ . Suppose, for instance, that the positive  $\gamma_n := \gamma_n(E)$  admit a limit  $\gamma := \gamma(E) > 0$  as  $n \rightarrow +\infty$ . By the previous Oseledec theorem, one of the two vectors  $(\varphi(n+1), \varphi(n))$  and  $(\psi(n+1), \psi(n))$  goes to infinity while the other goes to zero, with exponential rate.

### A.1.3 Periodic Potential

The Floquet theory for periodic differential equations can be transposed in this context of difference equation and thus leads to a complete spectral description of  $H$  in this case. Those systems with periodic potential will be useful later, when we aim to study substitutive Schrödinger operators by means of periodic approximations.

Suppose  $v$  to be a periodic sequence with period-length  $p$  :  $v_{n+p} = v_n$  for every  $n \in \mathbf{Z}$ . With our notations,

$$g_{n+p} = g_n \quad \text{for every } n \in \mathbf{Z} \quad \text{where} \quad g_n := g_n(E, v).$$

The block  $S_p = g_p g_{p-1} \dots g_1$  will play a specific role and we put  $\mathbf{t}(E) = \text{Tr}(S_p(E))$ . Note that  $\mathbf{t}$  is a polynomial function of  $E$ , of degree  $p$ , with leading coefficient equal to one. By the Cayley-Hamilton identity,  $S_p$  is a solution of the equation

$$X^2 - \mathbf{t}(E)X + 1 = 0, \quad X \in SL(2, \mathbf{R}).$$

**Proposition A.4.**  $E \in sp(H)$  if and only if  $|\mathbf{t}(E)| \leq 2$ .

*Proof.*  $\triangleleft$  let  $E$  be such that  $|\mathbf{t}(E)| \leq 2$ . Then  $S_p$  has two complex conjugate eigenvalues and it is easily checked that  $|\text{Tr}(S_p^k)| \leq 2$  for all  $k \in \mathbf{Z}$ .

Assume now that  $E$  is not in  $sp(H)$ . For every  $k \in \mathbf{Z}$ , one can find  $\varphi \in \ell^2(\mathbf{Z})$ ,  $\varphi \neq 0$ , such that  $(H - EI)\varphi = e_k$ . In particular, choosing  $k = 0$ , there must exist  $\varphi \in \ell^2(\mathbf{Z})$  such that

$$\varphi(n+1) + \varphi(n-1) + (v(n) - E)\varphi(n) = \begin{cases} 0 & \text{if } n \neq 0 \\ 1 & \text{if } n = 0. \end{cases}$$

This implies that one of the two vectors  $(\varphi(1), \varphi(0))$  or  $(\varphi(0), \varphi(-1))$  is nonzero. Suppose, for instance, that this is the first one, denoted by  $x$ . Since  $S_p^k x = \begin{pmatrix} \varphi(kp+1) \\ \varphi(kp) \end{pmatrix}$  for every  $k \geq 0$ , we get, by applying inequality (A.7) with  $g = S_p^k$ , that

$$\sup \left\{ 2(|\varphi(kp+1)|^2 + |\varphi(kp)|^2), |\varphi(2kp+1)|^2 + |\varphi(2kp)|^2 \right\} \geq \|x\|$$

which is incompatible with  $\varphi \in \ell^2(\mathbf{Z})$ . (If we need to consider the second vector, we would get a contradiction by looking at the negative  $k$ ).

$\triangleleft$  We now assume that  $|\mathbf{t}(E)| > 2$ ; the eigenvalues of  $S_p$  are the real numbers  $\lambda$  and  $1/\lambda$ , where, say,  $|\lambda| > 1$ . There exists  $w \neq 0$  with  $\|S_{np}w\| = \|S_p^n w\| = O\left(\frac{1}{|\lambda|^n}\right)$  and  $\|S_p^n x\| = O(|\lambda|^n)$  for any  $x$  non-proportional to  $w$ . It follows that every solution

of the Schrödinger equation must increase with exponential rate in one direction at least;  $E$  cannot be in  $sp(H)$  in view of corollary A.1.  $\square$

Using the spectral radius formula, one easily sees that the Lyapunov exponent exists and is equal to :

$$\gamma(E) = \frac{1}{p} \log r(S_p(E)).$$

The following alternative to the proposition is clear.

**Proposition A.5.**  $E \in sp(H)$  if and only if  $\gamma(E) = 0$ .

*Remark A.2.* We can precise the previous proposition in the following way :  $E$  is in  $sp(H)$  if and only if there exists  $\varphi \in \ell^\infty(\mathbf{Z})$  and  $\theta$  in  $\mathbf{R}$  such that

$$H\varphi = E\varphi, \quad \text{Tr}(S_p(E)) = 2 \cos \theta \quad \text{and} \quad \tau^p(\varphi) = e^{i\theta} \varphi$$

where  $\tau$  is the backward shift on  $\ell^\infty(\mathbf{Z})$ . This is the discrete version of the *Floquet theorem*.

**Corollary A.2.** *The spectrum of the periodic Schrödinger operator  $H$  is the union of  $p$  closed intervals with disjoint interiors :*

$$sp(H) = \mathbf{t}^{-1}([-2, 2]) =: \bigcup_{m=1}^p J_m.$$

*Proof.*  $H\varphi = E\varphi$  formally means :

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdots & 1 & E - v(-1) & 1 \cdots & & \\ \cdots & \cdot & 1 & E - v(0) & 1 \cdots & \\ \cdots & \cdot & \cdot & 1 & E - v(1) & 1 \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \varphi = 0$$

where the matrix is of the Jacobi type. Now, previous Floquet's theorem says that  $E \in sp(H)$  if and only if  $\det(E - V(\theta)) = 0$  for some real  $\theta$ , where

$$V(\theta) = \begin{pmatrix} v(1) & 1 & \cdot & \cdot & \cdot & e^{-i\theta} \\ 1 & v(2) & 1 & \cdot & \cdot & \cdot \\ 0 & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ e^{i\theta} & \cdot & \cdot & \cdot & 1 & v(p) \end{pmatrix}$$

But  $V(\theta)$  is symmetric, and  $\det(E - V(\theta)) = \mathbf{t}(E) - 2 \cos \theta$ . It follows that, for every  $t \in [-2, 2]$ , the equation  $\mathbf{t}(E) = t$  admits  $p$  real roots, whence the description of  $\mathbf{t}^{-1}([-2, 2])$ .  $\square$



The following theorem gives a final answer to the spectral problem in the periodic case.

**Theorem A.2.** *Let  $H$  be the Schrödinger operator with a periodic potential  $v$ . Then  $H$  has an absolutely continuous spectrum.*

*Proof.* ★ Following the same scheme, we see that  $H$  admits no eigenvalues : a non-trivial solution  $\varphi$  of  $(H - EI)\varphi = 0$  cannot belong to  $\ell^2(\mathbf{Z})$ .

★ In order to describe the maximal spectral type  $\sigma$  of  $H$ , we interpret  $H$  as an operator acting on  $L^2(\mathbf{T}, \mathbf{C}^p)$ . Consider indeed the canonical isomorphism between  $\ell^2(\mathbf{Z})$  and  $L^2(\mathbf{T})$ ,  $\varphi \mapsto \Phi$ , with  $\Phi(t) = \sum_{n \in \mathbf{Z}} \varphi(n) e^{int}$ . By the Fourier inversion formula, the periodic potential  $v$  may be written under the form

$$v(n) = \sum_{j=1}^p a_j e^{2\pi i n j/p} = \hat{v}(n)$$

where  $v$  is the discrete measure  $\sum_{j=1}^p a_j \delta_{\frac{2\pi j}{p}}$ . Therefore,  $H$  is conjugate to the operator  $\hat{H}$  acting on  $L^2(\mathbf{T})$  in this way :

$$\begin{aligned} (\hat{H}\Phi)(t) &= 2 \cos t \Phi(t) + \sum_{n \in \mathbf{Z}} \sum_{j=1}^p a_j e^{2\pi i n j/p} \varphi(n) e^{int} \\ &= 2 \cos t \Phi(t) + \sum_{j=1}^p a_j \Phi\left(t + \frac{2\pi j}{p}\right). \end{aligned}$$

Putting more generally  $F_j(t) = F\left(t + \frac{2\pi j}{p}\right)$  and denoting by  $\mathbf{F}$  the vector-valued function with components  $(F_j)$ ,  $1 \leq j \leq p$ ,  $\hat{H}$  extends to a multiplication operator on  $L^2(\mathbf{T}, \mathbf{C}^p)$  by the following formula :

$$\mathbf{F}(t) \mapsto M(t) \cdot \mathbf{F}(t), \quad \text{where } M(t) = D(t) + G,$$

$D$  being the diagonal matrix  $(d_{jj})_{1 \leq j \leq p}$  with  $d_{jj}(t) = 2 \cos\left(t + \frac{2\pi j}{p}\right)$  and  $G$  the

circulant matrix 
$$\begin{pmatrix} 0 & a_1 & 0 & \cdot & \cdot & 0 \\ 0 & 0 & a_2 & \cdot & \cdot & 0 \\ \cdot & & & & & \cdot \\ \cdot & & & & a_{p-1} & \\ a_p & 0 & 0 & \cdot & \cdot & 0 \end{pmatrix}.$$

In particular,  $\hat{H}$  has an absolutely continuous spectrum and the same holds for  $H$ .  $\square$

*Example A.1.* Consider  $v(n) = (-1)^n$ . Then  $\mathbf{t} = E^2 - 3$  and

$$sp(H) = \{E, -2 \leq E^2 - 3 \leq 2\} = [-\sqrt{5}, -1] \cup [1, \sqrt{5}].$$

In addition, following the proof of the theorem, if we consider

$$\mathbf{F}(t) = (F(t), F(t + \pi)),$$

then  $\widehat{H}\mathbf{F}(t) = M(t) \cdot \mathbf{F}(t)$  with

$$M(t) = \begin{pmatrix} 2\cos t & 1 \\ 1 & -2\cos t \end{pmatrix}$$

The spectrum  $sp(H)$  can be rediscovered as the union of the images of the continuous version of the eigenvalues :

$$sp(H) = \bigcup_{i=1}^2 \lambda_i(\mathbf{T}),$$

$\lambda_1(t), \lambda_2(t)$  being, for each  $t$ , the eigenvalues of  $M(t)$ ; in particular, in our example,

$$\begin{aligned} \lambda_1(t) &= \sqrt{1 + 4\cos^2 t} \\ \lambda_2(t) &= -\sqrt{1 + 4\cos^2 t} \end{aligned}$$

and  $sp(H) = [-\sqrt{5}, -1] \cup [1, \sqrt{5}]$  again.

*Remark A.3.* 1. Note that the action of  $\widehat{H}$  may be expressed by :

$$\widehat{H}(F) = 2\cos t \cdot F + F * v,$$

and clearly,  $\widehat{H}$  extends to an operator on  $M(\mathbf{T})$  by the same formula :  $\widehat{H}(\rho) = 2\cos t \cdot \rho + \rho * v$ , if  $\rho \in M(\mathbf{T})$ , as soon as  $v(n) = \widehat{v}(n)$ , for some  $v \in M(\mathbf{T})$ .

2. In [108], a different point of view is developed, centered on the dynamical system induced by  $\mathbf{t}$ .

## A.2 Ergodic Family of Schrödinger Operators

Henceforth, one will be interested in a potential  $v = (v(n))_{n \in \mathbf{Z}} \in \mathcal{L}$  generating an ergodic subshift  $(\Omega, T, \mu)$ , and in some cases, a strictly ergodic one, that is a compact, uniquely ergodic and minimal dynamical system under the shift's action. To each  $\omega \in \Omega$ , we associate the Schrödinger operator  $H_\omega$  with potential  $\omega = (\omega(n))$  and we put  $H := H_v$ . Before obtaining general results for the specific operators  $H_v$ ,  $\mu$ -almost sure results on the family  $(H_\omega)$ ,  $\omega \in \Omega$ , will be deduced from the ergodic theory. Complements can be found in [22].

### A.2.1 General Properties

We can already make these preliminary simple observations :

1. In all cases, we readily have :

**Proposition A.6.** *If  $(\Omega, T, \mu)$  is a subshift, then*

$$H_{T\omega} = U^* H_\omega U$$

where  $U := U_\tau$  is the unitary operator associated with  $\tau$ , the shift on  $\ell^2(\mathbf{Z})$ .

Thus  $sp(H_\omega) = sp(H_{T\omega})$ . If  $\sigma_\omega$  is the maximal spectral type of  $H_\omega$  and, for  $n \in \mathbf{Z}$ , if  $\sigma_{\omega,n}$  denotes the spectral measure of  $e_n$ , relative to  $H_\omega$ , then  $\sigma_{T\omega,n} = \sigma_{\omega,n+1}$  for every  $n \in \mathbf{Z}$ ,  $\omega \in \Omega$ .

We denote by  $\Sigma$  the spectrum of  $H$  and  $G = \{\omega \in \Omega, sp(H_\omega) = \Sigma\}$ .  $G$  is a non-empty and  $T$ -invariant subset of  $\Omega$  by the previous proposition A.6. If  $(\Omega, T, \mu)$  is ergodic,  $\mu(G) = 0$  or 1 and, finally,

$$sp(H_\omega) = \Sigma \quad \text{for } \mu - a.e. \omega$$

since  $\mu(G) > 0$ .

2. Suppose now the system  $(\Omega, T)$  to be minimal. We have :

**Proposition A.7.** *If  $(\Omega, T, \mu)$  is a minimal subshift, then  $sp(H_\omega) = sp(H_{\omega'})$  for all  $\omega, \omega' \in \Omega$  i.e. the spectrum of  $H_\omega$  does not depend on  $\omega$ .*

This will be a consequence of the following, interesting in itself, lemma.

**Lemma A.2.** *Let  $H_n, H$  be self-adjoint operators on the Hilbert space  $\mathcal{H}$ , such that  $H_n$  tends to  $H$  in the strong operator topology. Then*

$$sp(H) \subset \limsup \text{top}(sp(H_n)) := \bigcap_n \overline{\bigcup_{m \geq n} sp(H_m)}.$$

*Proof of the lemma.* Let  $E \notin \overline{\bigcup_{m \geq n} sp(H_m)}$  for some fixed  $n$ . Then, the distance  $d_n := \text{dist}(E, \bigcup_{m \geq n} sp(H_m))$  must be positive. As  $(H_m - EI)^{-1}$ , in turn, is self-adjoint,

$$\|(H_m - EI)^{-1}\| = \sup_{\mu \in sp(H_m)} \left| \frac{1}{\mu - E} \right| \leq \frac{1}{d_n} \quad (m \geq n).$$

by applying the spectral image theorem. Thus,  $\|H_m f - E f\| \geq d_n \|f\|$  for every  $f \in \mathcal{H}$ . Taking the strong limit on  $m$ , we obtain that

$$\|H f - E f\| \geq d_n \|f\|;$$

$(H - EI)$  being itself self-adjoint, we conclude that  $E \notin sp(H)$ . □

*Proof of the proposition.* As usual,  $\Omega$  is endowed with the metric  $d(\omega, \omega') = \sum_{\mathbf{z}} \frac{1}{2^{|\mathbf{z}|}} |\omega(\mathbf{z}) - \omega'(\mathbf{z})|$ . If  $d(\omega, \omega') \leq \varepsilon$ , there exists  $N$  such that  $\omega_{[-N, N]} = \omega'_{[-N, N]}$ , and for every  $f \in \mathcal{H}$ ,

$$\|H_\omega f - H_{\omega'} f\|^2 \leq C \sum_{|n| > N} |f(n)|^2.$$

This proves that, for any fixed  $f \in \mathcal{H}$ , the map  $\omega \mapsto \|H_\omega f\|$  is continuous on  $\Omega$ . But, by definition of  $\Omega$ ,  $\omega \in \Omega$  if  $\omega = \lim_{i \rightarrow \infty} T^{n_i} v$  for some sequence  $(n_i)$ , so that,  $H_{T^{n_i} v}$  converges strongly to  $H_\omega$ . The lemma, combined with proposition A.6, implies that

$$sp(H_\omega) \subset \limsup_{i \rightarrow \infty} \text{top}(sp(H_{T^{n_i} v})) \subset \Sigma.$$

Since the system is assumed to be minimal,  $\Omega$  is the closed orbit of any of its points, and for every  $\omega \in \Omega$ ,  $v = \lim_{j \rightarrow \infty} T^{m_j} \omega$  for a suitable sequence  $(m_j)$ . Finally,

$$\Sigma \subset sp H_\omega \quad \text{for every } \omega \in \Omega$$

and the proposition is proved.  $\square$

**3.** We do not know whether the spectral measure  $\sigma_\omega$  depends on  $\omega$ , and if it does, how. But one can prove the following.

**Proposition A.8.** *Assume that the system  $(\Omega, T, \mu)$  is ergodic and fix  $E \in \mathbf{R}$ . Then  $\mu\{\omega \in \Omega, \sigma_\omega\{E\} > 0\} = 0$ . As a consequence,  $\kappa = \int_\Omega \sigma_\omega d\mu(\omega)$  is a continuous measure.*

*Proof.* Put  $\Omega_E = \{\omega \in \Omega, \sigma_\omega\{E\} > 0\}$ . The complement set  $\Omega_E^c$  is clearly invariant since  $\sigma_{T\omega}\{E\} = \sigma_{T\omega, 0}\{E\} + \sigma_{T\omega, -1}\{E\} = \sigma_{\omega, 1}\{E\} + \sigma_{\omega, 0}\{E\}$  by proposition A.1; hence  $\sigma_\omega\{E\} = 0$  implies  $\sigma_{T\omega}\{E\} = 0$  in turn. It follows that  $\mu(\Omega_E) = 0$  or 1 by ergodicity of the system. We claim that  $\mu(\Omega_E) = 0$ .

Consider, indeed,  $P_{\omega, E}$  the projection of rank  $\leq 1$  onto the eigenspace corresponding to the eigenvalue  $E$ . We have

$$\begin{aligned} \sum_n \sigma_{n, \omega}\{E\} &= \sum_n \langle P_{\omega, E} e_n, e_n \rangle = \text{Tr}(P_{\omega, E}) = 1 \quad \text{if } \omega \in \Omega_E \\ &= 0 \quad \text{otherwise.} \end{aligned}$$

Thus

$$\mu(\Omega_E) = \int_\Omega \text{Tr}(P_{\omega, E}) d\mu(\omega) = \sum_n \int_\Omega \sigma_{n, \omega}\{E\} d\mu(\omega).$$

But

$$\int_\Omega \sigma_{n, \omega}\{E\} d\mu(\omega) = \int_\Omega \sigma_{n, T\omega}\{E\} d\mu(\omega) = \int_\Omega \sigma_{n+1, \omega}\{E\} d\mu(\omega);$$

hence the sequence  $(\int_{\Omega_E} \sigma_{n,\omega}\{E\} d\mu(\omega))_n$  must be constant, thus identically zero. This implies that  $\Omega_E$  is negligible, and the claim follows.  $\square$

*Remark A.4.* The periodic case may appear as a particular case of the ergodic one. Since the involved measure  $\mu$  has a finite support, the almost-sure results are thus replaced by deterministic ones.

### A.2.2 Lyapunov Exponents

In this section, the system  $(\Omega, T, \mu)$  is supposed to be ergodic. The following sub-additive ergodic theorem will be useful [142, 148].

**Theorem A.3 (Kingman).** *Let  $(X, T, \mu)$  be an ergodic dynamical system and let  $(f_n)$  be a subadditive cocycle in  $L^1(X, \mu)$ , i.e. be such that*

$$f_{n+m}(x) \leq f_n(x) + f_m(T^n x), \quad \mu - a.e., \quad \text{for } n, m \geq 0.$$

*Then,  $f_n(x)/n$  converges, for  $\mu$ -almost all  $x$  and in  $L^1(X, \mu)$ , to the constant  $\inf_n \frac{1}{n} \int_X f_n d\mu$ .*

We introduced the Lyapunov exponent as a measuring instrument, when existing, of the asymptotic behaviour of the solutions to the Schrödinger equation. Since we are now dealing with an ergodic family of Schrödinger equations, the involved product of matrices

$$g_n g_{n-1} \cdots g_0 = S_n := S_n(E, \omega) \quad (n \geq 0)$$

and the analogous for  $n \leq 0$ , also depend on  $\omega$ . We are thus led to distinguish two kinds of exponents.

**Notation :** We consider, for  $n \in \mathbf{Z}$  and  $E \in \mathbf{R}$  (or  $\mathbf{C}$ ), the two quantities :

$$\gamma_n(E, \omega) = \log \|S_n(E, \omega)\|,$$

and

$$\gamma_n(E) = \int_{\Omega} \log \|S_n(E, \omega)\| d\mu(\omega).$$

Observe that  $\gamma_n(E) \geq 0$  since  $\det S_n = 1$  and  $\|S_n\| \geq 1$ . From the multiplicative cocycle equation in  $SL(2, \mathbf{R})$  satisfied by  $(S_n(E, \omega))$  :

$$S_n(E, T^m \omega) \cdot S_m(E, \omega) = S_{n+m}(E, \omega),$$

it follows that  $\|S_{n+m}(E, \omega)\| \leq \|S_n(E, T^m \omega)\| \cdot \|S_m(E, \omega)\|$  for every  $n, m \geq 0$ . Therefore,  $(\gamma_n(E))$  is a subadditive ergodic sequence for  $n \geq 0$ . In addition, note that  $\|S_{-n}(E, T^n \omega)\| = \|S_{n-1}(E, \omega)\|$  if  $n \geq 1$  and

$$\gamma_{-n}(E) = \gamma_{n-1}(E) \quad \text{for } n \geq 1.$$

We easily deduce that

$$\gamma(E) = \lim_{|n| \rightarrow \infty} \frac{1}{|n|} \gamma_n(E) = \inf_{n \geq 1} \frac{1}{n} \gamma_n(E)$$

exists and is nonnegative for every  $E \in \mathbf{R}$  or  $\mathbf{C}$ .

**Definition A.5.** We call *mean Lyapunov exponent* the nonnegative number

$$\gamma(E) = \lim_{|n| \rightarrow \infty} \frac{1}{|n|} \int_{\Omega} \log \|S_n(E, \omega)\| d\mu(\omega)$$

which is defined for every  $E \in \mathbf{R}$  or  $\mathbf{C}$ .

It has been remarked that the function  $E \in \mathbf{C} \mapsto \gamma(E)$  is subharmonic, that is uppersemicontinuous and submean; indeed,  $S_n(E)$  is an holomorphic matrix in  $E$ , therefore  $\log \|S_n(E, \omega)\|$  is subharmonic as well as  $\int_{\Omega} \log \|S_n(E, \omega)\| d\mu(\omega)$ ; finally,  $\gamma(E)$  is subharmonic as the limit of such ones.

Now, since we have, for every  $n, m \geq 0$  and fixed  $E$ ,

$$\log \|S_{n+m}(E, \omega)\| \leq \log \|S_m(E, \omega)\| + \log \|S_n(E, T^m \omega)\|$$

we may apply the subadditive ergodic theorem to  $\omega \mapsto \log \|S_n(E, \omega)\|$  and get the following.

**Proposition A.9.** *Let  $E$  be a fixed real or complex number. Then, for  $\mu$ -almost  $\omega$ , the sequence  $\frac{1}{|n|} \log \|S_n(E, \omega)\|$  converges to  $\gamma(E)$  as  $|n| \rightarrow \infty$ .*

**Definition A.6.** We could speak of the *individual Lyapunov exponent* for

$$\lim_{|n| \rightarrow \infty} \frac{1}{|n|} \text{Log} \|S_n(E, \omega)\| = \gamma(E, \omega)$$

when the limit exists.

*Remark A.5.* 1. This proposition is already contained in the following well-known multiplicative ergodic theorem, due to Furstenberg and Kesten [95], which is a noncommutative generalization of Birkhoff's theorem and can also be obtained as a corollary of the posterior Kingman theorem.

**Theorem A.4 (Furstenberg & Kesten).** *Let  $(X, T, \mu)$  be an ergodic dynamical system and let  $A : X \rightarrow GL_d(\mathbf{R})$  be a measurable function, with both  $\log \|A\|$  and  $\log \|A^{-1}\|$  in  $L^1(X, \mu)$ . Then, the sequence  $\frac{1}{n} \log \|A(T^{n-1}x) \cdots A(x)\|$  converges to a constant  $\Lambda(A)$ , for  $\mu$ -almost all  $x$  and in  $L^1(X, \mu)$ .*

2. When the system is uniquely ergodic, one can ask about the uniform convergence in both Kingman and Furstenberg-Kesten theorems. In this direction we have :

**Theorem A.5 (Furman).** *Let  $(X, T, \mu)$  be a uniquely ergodic system and let  $A : X \rightarrow GL_d(\mathbf{R})$  be a continuous function; then, for every  $x \in X$  and uniformly on  $X$*

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \log \|A(T^{n-1}x) \cdots A(x)\| \leq \Lambda(A)$$

where  $\Lambda(A)$  is the almost-sure constant limit in the previous theorem.

The following will be used [19].

**Theorem A.6 (Avron-Simon).** *When the involved system is uniquely ergodic,*  

$$\int_{\mathbf{R}} |\gamma_n(E, \omega) - \gamma(E)|^2 dE \xrightarrow{|n| \rightarrow \infty} 0 \text{ uniformly in } \omega \in \Omega.$$

### A.2.3 Results from Pastur, Kotani, Last and Simon

The set  $\mathcal{N} = \{E \in \mathbf{R}, \gamma(E) \text{ exists and is zero}\}$  is particularly meaningful. The relation between the positivity of  $\gamma$  and the nature of the spectrum of  $H$  has been first pointed out by Pastur. The following theorem is proved in [22].

**Theorem A.7 (Pastur).** *If  $m(\mathcal{N}) = 0$ , then, for  $\mu$ -almost all  $\omega$ ,  $H_\omega$  has no absolutely continuous part in its spectrum. Also, if there exists a positive measure  $\nu$  on  $\mathbf{R}$  such that  $\nu(\mathcal{N}) = 0$  then  $\sigma_\omega \perp \nu$  for  $\mu$ -almost all  $\omega$ .*

Note the following improvement due to Kotani [149].

**Theorem A.8 (Kotani).** *For  $\mu$ -almost all  $\omega$ , the topological support of  $(\sigma_\omega)_{ac}$  is the essential closure of  $\mathcal{N}$ .*

This theorem admits an important consequence in view to the next section, where substitutive potentials and, more generally, uniformly recurrent ones are involved.

**Theorem A.9 (Kotani).** *Let  $\nu$  be a non-periodic sequence taking finitely many values. If  $(\Omega, T, \mu)$  is an ergodic dynamical system, then, for  $\mu$ -almost all  $\omega$ ,  $H_\omega$  has no absolutely continuous part in its spectrum.*

*Proof.* We just sketch the proof. Suppose on the contrary that  $m(\mathcal{N}) > 0$ ; one can show, using first Kotani's theorem, that every point  $\omega$  in the topological support of  $\mu$  is entirely determined by the knowledge of  $(\omega(n))_{n \leq 0}$  or  $(\omega(n))_{n \geq 0}$  and that the map  $(\omega(n))_{n \geq 0} \mapsto (\omega(n))_{n \leq -1}$  (resp.  $n \leq -1 \mapsto n \geq 0$ ) is continuous on the support of  $\mu$ . In particular, one can find an index  $K$  such that the equalities :  $\omega(n) = \omega'(n)$  for  $n = -1, -2, \dots, -K$  imply  $\omega(0) = \omega'(0)$ , so that, by  $T$ -invariance of the support of  $\mu$ ,  $\omega(n) = \omega'(n)$  for every  $n \geq 0$ . It follows that the support of  $\mu$  is finite, with  $\text{Card Supp}(\mu) \leq K^s$  if  $\nu$  is supposed to take  $s$  distinct values. This exactly means that  $\nu$  is a periodic sequence, whence the theorem.  $\square$

We shall invoke later the following consequence of those two fundamental results A.7 and A.9.

**Corollary A.3.** *Let  $v$  be a sequence taking finitely many values such that  $(\Omega, T, \mu)$  is a strictly ergodic dynamical system. If the individual Lyapunov exponent  $\gamma(E, v)$  exists and is zero for every  $E \in sp(H)$ , then  $m(sp(H)) = 0$ .*

*Proof.* Applying theorem A.6, we know that  $\int_{\mathbf{R}} |\gamma_n(E, v) - \gamma(E)|^2 dE \rightarrow 0$  as  $|n| \rightarrow +\infty$ , thus, for a subsequence  $(n_j)$ ,  $\gamma_{n_j}(E, v)$  tends to  $\gamma(E)$  for almost all  $E$ . Since  $\gamma_{n_j}(E, v)$  tends to zero for every  $E \in sp(H)$ ,  $\gamma(E) = 0$  for  $E \in sp(H) \setminus N$  where  $m(N) = 0$ . Suppose now that  $m(sp(H)) > 0$ ;  $m(sp(H) \setminus N)$  is still positive and  $\gamma(E) = 0$  on a set of positive measure. It follows from Pastur's theorem that, for  $\mu$ -almost all  $\omega$ ,  $\sigma_\omega$  must have an absolutely continuous part. But, the aperiodic sequence  $v$  taking finitely many values, Kotani's theorem applies : for  $\mu$ -almost all  $\omega$ ,  $H_\omega$  has no absolutely continuous part in its spectrum. This contradiction proves that  $m(sp(H)) = 0$ .  $\square$

Thus, if the aperiodic potential takes finitely many values, an absolutely continuous spectrum is excluded for  $\mu$ -almost all  $\omega$  and if, moreover, the system  $(\Omega, T, \mu)$  is minimal, the spectrum  $sp(H_\omega)$  is independent of  $\omega$ .

The problem to know whether the absolutely continuous spectrum itself does not depend on  $\omega$  for strictly ergodic systems has been definitively solved by Last and Simon in [157], after many partial results (see also [115]).

**Theorem A.10 (Last & Simon).** *Let  $v$  be a sequence taking finitely many values such that  $(\Omega, T, \mu)$  is a strictly ergodic dynamical system. Then, the essential support of the absolutely continuous part of the spectrum is independent of  $\omega$ .*

In case of an aperiodic potential  $v$ , it follows from theorems A.9 and A.10 that the absolutely continuous spectrum of  $H_\omega$  is empty for every  $\omega \in \Omega$ .

### A.3 Substitutive Schrödinger Operators

We restrict our attention to potentials  $v$  with  $v(n) = V \cdot u(n)$  where  $u$  is a fixed point of a primitive substitution  $\zeta$  defined on the alphabet  $A$ , and where  $V$  is some real constant. Recall that bilateral substitution subshifts can be constructed so as to obtain a strictly ergodic dynamical system.

**Proposition A.10.** *Let  $\zeta$  be a primitive substitution on  $A$ . If  $\alpha$  and  $\beta$  are letters in  $A$  such that*

$$\beta \text{ is the last letter of } \zeta(\beta) \text{ and } \alpha \text{ is the first letter of } \zeta(\alpha),$$

*then there exists a unique fixed point  $x$  of  $\zeta$  such that  $x_{-1} = \beta$  and  $x_0 = \alpha$ . Moreover, the system  $(X, T)$ , with  $T$  the bilateral shift and  $X$  the closed orbit of  $x$  under  $T$  in  $A^{\mathbf{Z}}$ , is strictly ergodic.*





Among the considerable amount of results, two types of them will be retained, giving sufficient conditions on the potential to ensure the absence of eigenvalues together with a purely singular spectrum. Although they largely exceed the framework of substitutions, they are not exhausting the question for those sequences.

### A.3.1 The Trace Map Method

Historically, it seems that the Fibonacci potential has been first introduced and the interesting trace map first used, to work out the spectral problem. Actually, the three quoted examples (and a class of other ones) can be analyzed exactly in the same way : We begin with a description of  $sp(H)$  with help of the trace map, then we check that eigenvalues cannot exist and finally, we conclude that  $m(sp(H)) = 0$  by estimating the individual Lyapunov exponent. As we said, this scheme of proof can be shortened by using the Last-Simon theorem. But the description of the spectrum by means of the trace map remains interesting as we shall see.

The key point of the proof is an approximation argument by periodic Schrödinger operators whose spectrum is well-known.

**Lemma A.3.** *Let  $v$  be a sequence taking finitely many values and  $H$ , the Schrödinger operator corresponding to  $v$ . For every  $m$  we denote by  $v_m$  the periodic sequence coinciding with  $v$  on the segment  $[a_m, b_m]$  and by  $H_m$  the corresponding operator. If  $b_m \rightarrow +\infty$ ,  $a_m \rightarrow -\infty$ , then  $sp(H) \subset \limsup \text{top}(sp(H_m))$ .*

*Proof.* Since  $\|(H - H_m)\varphi\|^2 \leq C \sum_{|n| \geq \inf(b_m, |a_m|)} |\varphi(n)|^2$ , the lemma is a consequence of lemma A.2.  $\square$

We choose to give the details for the founder Fibonacci case [231].

**Theorem A.11 (A. Sütö).** *Let  $v = V \cdot u$  be a Fibonacci potential, where  $u$  is the bilateral Fibonacci 0 – 1-sequence and  $V \in \mathbf{R}$ . Then the maximal spectral type of  $H := H_v$  is continuous singular.*

Recall the inductive property shared by the elementary words of  $u$  :

$$\zeta^n(0) = \zeta^{n-1}(0) \zeta^{n-1}(1) = \zeta^{n-1}(0) \zeta^{n-2}(0) \quad (\text{A.9})$$

and thus  $|\zeta^n(0)| = F_n$  where  $F_{n+1} = F_n + F_{n-1}$ ,  $F_0 = 1$ ,  $F_1 = 2$ .

This relation directly transposes to the transfer matrices  $g_n$ . Let us put

$$T_n = g_{F_n} g_{F_n-1} \cdots g_1 \quad \text{if } n \geq 1$$

and

$$L_n = (g_1 g_2 \cdots g_{F_n})^{-1} = g_{-F_n-1}^{-1} \cdots g_{-2}^{-1}$$

by the symmetry of  $u$ . Then, if  $\Phi_n = \begin{pmatrix} \varphi(n+1) \\ \varphi(n) \end{pmatrix}$ ,

$$\Phi_{F_n} = T_n \Phi_0 \quad \text{and} \quad \Phi_{-F_n-2} = L_n \Phi_{-2} \quad \text{for } n \geq 1.$$

Finally, put, for  $n \geq 1$ ,

$$x_n = \text{Tr}(T_n), \quad y_n = \text{Tr}(L_n).$$

From a relation between the matrices  $T_n$ ,  $L_n$ , we shall deduce a relation on their traces.

**Lemma A.4 (Trace Map).** *The sequence  $(x_n)$  satisfies the equation :*

$$x_{n+2} = x_n x_{n+1} - x_{n-1} \quad \text{for } n \geq 0, \quad (\text{A.10})$$

if we set  $x_0 = \text{Tr}(g_2)$  and  $x_{-1} = 2$ . Moreover,  $y_n = x_n$  for  $n \geq 1$ .

*Proof.* On the transfer matrices, relation (A.9) can be read as follows.

$$\begin{aligned} T_{n+2} &= T_n T_{n+1} & \text{if } n \geq 1 \\ &= T_n \cdot T_{n-1} T_n & \text{if } n \geq 2 \end{aligned}$$

and

$$\begin{aligned} x_{n+2} &= \text{Tr}(T_{n+2}) = \text{Tr}(T_n^2 T_{n-1}) = \text{Tr}((x_n T_n - I) T_{n-1}) \\ &= x_n \text{Tr}(T_{n-1} T_n) - x_{n-1} \\ &= x_n x_{n+1} - x_{n-1} \quad \text{if } n \geq 2. \end{aligned}$$

For  $n = 0, 1$  this remains true provided that  $x_0 = E - V = \text{Tr}(g_2)$  and  $x_{-1} = 2$ . Analogously,  $L_{n+2} = L_n L_{n+1}$  and  $y_{n+3} = y_{n+2} y_{n+1} - y_n$  if  $n \geq 1$ . By induction on  $n$  it is easily checked that  $y_n = x_n$  for every  $n \geq 1$ .  $\square$

We shall establish the following description of the spectrum.

**Theorem A.12.**  $sp(H) = B_\infty := \{E \in \mathbf{R}, (x_n) \text{ is bounded}\}.$

*Proof of theorem A.12.* First,  $x_n$  being a continuous function of  $E$  for any  $n \in \mathbf{Z}$ , observe that  $B_\infty$  must be closed in  $\mathbf{R}$ .

We successively prove both inclusions.

$\star B_\infty \subset sp(H)$ . We shall need the identities to be proved

$$v(F_n + j) = v(j) \quad \text{if } 1 \leq j \leq F_n \quad \text{and } n \geq 3 \quad (\text{A.11})$$

$$v(-F_{2n} + j) = v(j) \quad \text{if } 1 \leq j \leq F_{2n+1} \quad \text{and } n \geq 1 \quad (\text{A.12})$$

Starting with  $\zeta^{n+2}(0) = \zeta^{n+1}(0) \zeta^n(0) = \zeta^n(0) \zeta^{n-1}(0) \cdot \zeta^n(0)$ , we find for  $n \geq 3$ ,

$$\begin{aligned} \zeta^{n+2}(0) &= \zeta^n(0) \zeta^{n-1}(0) \cdot \zeta^{n-2}(0) \zeta^{n-3}(0) \zeta^{n-2}(0) \\ &= \zeta^n(0) \zeta^n(0) \zeta^{n-3}(0) \zeta^{n-2}(0) \end{aligned}$$

whence (A.11); now (A.12) can be obtained in the same way by using  $\eta = \zeta^2$ . It follows that

$$S_{2F_n} = g_{2F_n} g_{2F_n-1} \cdots g_1 = g_{F_n} \cdots g_1 \cdot g_{F_n} \cdots g_1 = T_n^2$$

and  $S_{2F_n} = x_n T_n - I$ .

Let now  $E \in B_\infty$  and suppose that  $E \notin sp(H)$ . As in the periodic case, we prove that one of the two vectors  $\Phi_0$  or  $\Phi_{-2}$  is non zero, if the sequence  $(\Phi_n)$  derives from a non-trivial solution  $\varphi$  of  $(H - EI)\varphi = e_0$ .

If  $\Phi_0 = w \neq 0$ , then  $\Phi_{2F_n} = T_n^2 w$ , and, according to inequality (A.7),  $0 < \|w\|^2 \leq \sup\{2c\|\Phi_{F_n}\|, \|\Phi_{2F_n}\|\}$  if  $|x_n| \leq c$ , so that  $\varphi \notin \ell^2$ .

If now  $\Phi_{-2} = w \neq 0$ ,  $0 < \|w\|^2 \leq \sup\{2c\|\Phi_{-F_n-2}\|, \|\Phi_{-2F_n-2}\|\}$  and  $\varphi \notin \ell^2$  again.

In both cases, we get a contradiction. Note that the same argument may be used to prove that no point of  $B_\infty$  can be an eigenvalue of  $H$ .

$\star sp(H) \subset B_\infty$ . We approximate  $H$  by the periodic Schrödinger operators  $H_m := H_{v_m}$ , where  $v_m$  is  $F_m$ -periodic with period

$$\overleftarrow{\zeta^m(0)} \quad \overrightarrow{\zeta^m(0)} \quad \text{if } m \text{ is even}$$

and

$$\overleftarrow{\zeta^{m-1}(0)} \quad \overrightarrow{\zeta^{m-2}(0)} \quad \text{if } m \text{ is odd}$$

By lemma A.2,  $sp(H) \subset \limsup_{\text{top}} \Sigma_m$  where  $\Sigma_m = sp(H_m) = \{E, |x_m| \leq 2\}$  according to the characterization established in the periodic case (proposition A.4). The proof of theorem A.12 will be complete if we prove the following :

**Lemma A.5.** *The sequence of subsets  $(\Sigma_m \cup \Sigma_{m+1})_m$  is non-increasing and is contained in  $B_\infty$ .*

Indeed, admitting lemma A.5, we deduce that

$$\Sigma_m \cup \Sigma_{m+1} \supset \bigcup_{k=m}^{\infty} \Sigma_k \quad \text{for every } m$$

and  $B_\infty \supset \overline{\left(\bigcup_{k=m}^{\infty} \Sigma_k\right)}$  since  $B_\infty$  is closed. Hence,  $B_\infty \supset \bigcap_m \overline{\left(\bigcup_{k=m}^{\infty} \Sigma_k\right)} \supset sp(H)$ .

Thus both inclusions are established and theorem A.12 is proved.  $\square$

We turn back to lemma A.5 which happens to be a consequence of the trace map.

**Lemma A.6.** *Consider  $(x_n)_{n \geq 0}$  with  $x_{-1} = 2$ , a solution of (A.10). Then,  $(x_n)$  is unbounded if and only if there exists a unique  $N$  such that*

$$|x_{N-1}| \leq 2, \quad |x_N| > 2 \quad \text{and} \quad |x_{N+1}| > 2 \quad (\text{A.13})$$

In this case,  $|x_n| > 2$  for every  $n \geq N$  and one can find  $C > 1$  such that

$$|x_n| > 2 C^{F_{n-N}} \quad \text{for } n \geq N.$$

Otherwise,

$$|x_n| \leq 2 + |x_{-1} - x_0| = 2 + |V|.$$

*Proof.* ★ Suppose that (A.13) holds; then, from (A.10), we have

$$\begin{aligned} |x_{N+2}| &\geq |x_{N+1}| |x_N| - |x_{N-1}| \\ &\geq \frac{1}{2} |x_{N+1}| |x_N| + \left( \frac{1}{2} |x_{N+1}| |x_N| - |x_{N-1}| \right) \\ &\geq \frac{1}{2} |x_{N+1}| |x_N| > 2. \end{aligned}$$

It follows that  $\log \frac{1}{2} |x_{n+2}| \geq \log \frac{1}{2} |x_{n+1}| + \log \frac{1}{2} |x_n|$  for  $n \geq N$ , and  $\log \frac{1}{2} |x_n|$  grows faster than the Fibonacci sequence initiated at  $N$ .

★ Suppose now that (A.13) is not satisfied : if  $|x_n| > 2$ , then  $|x_{n-1}|$  and  $|x_{n+1}|$  must be  $\leq 2$ . But the nontrivial invariant given by the Fricke formula (A.8) and expressed with  $g = S_n$ ,  $h = S_{n-1}$ , leads to

$$x_{n+1}^2 + x_n^2 + x_{n-1}^2 - x_{n+1} x_n x_{n-1} = V^2 + 4 \quad n \geq 0$$

that we write

$$V^2 + 4 = x_{n+1}^2 + x_{n-1}^2 + \left( x_n - \frac{1}{2} x_{n+1} x_{n-1} \right)^2 - \frac{1}{4} x_{n+1}^2 x_{n-1}^2.$$

Hence,  $\left( x_n - \frac{1}{2} x_{n+1} x_{n-1} \right)^2 = V^2 + \left( 2 - \frac{x_{n+1}^2}{2} \right) \left( 2 - \frac{x_{n-1}^2}{2} \right)$  and

$$|x_n| \leq \frac{1}{2} |x_{n+1} x_{n-1}| + \left( V^2 + \left( 2 - \frac{x_{n+1}^2}{2} \right) \left( 2 - \frac{x_{n-1}^2}{2} \right) \right)^{1/2}.$$

If  $|x_{n-1}|$  and  $|x_{n+1}|$  are  $\leq 2$ , the maximum of  $|x_n|$  is reached as  $|x_{n-1}| = |x_{n+1}| = 2$  so that  $|x_n| \leq 2 + |V| = 2 + |x_0 - x_{-1}|$ .

We end this part by the proof of lemma A.5. From the above estimates, it is clear that

$$B_\infty^c \subset \bigcup_{m \geq 0} (\Sigma_m^c \cap \Sigma_{m+1}^c)$$

and that

$$\Sigma_m^c \cap \Sigma_{m+1}^c \subset \Sigma_{m+1}^c \cap \Sigma_{m+2}^c.$$

Finally, the remaining lemma A.5 is proved.  $\square$

*Proof of theorem A.11.* We already observed that  $H$  has no eigenvalue. Thus, Sütö's theorem will be deduced for  $H$ , from the computation of the individual Lyapunov exponent, by a now standard process, as pointed out in section A.2.3.

**Theorem A.13.** *The individual Lyapunov exponent  $\gamma(E, v)$  exists and is equal to zero for every  $E \in sp(H)$ .*

*Proof.* Since the potential satisfies the symmetry relation  $v_{-n} = v_{n-1}$ , we only consider the behaviour of  $\frac{1}{n} \gamma_n(E, v) := \frac{1}{n} \log \|S_n(E, v)\|$  as  $n \rightarrow +\infty$ . We first study (ommitting the dependence on  $E$  and  $v$ )

$$t_n = \frac{1}{F_n} \log \|T_n\| \quad \text{where} \quad T_n = g_{F_n} g_{F_n-1} \cdots g_1.$$

From the relation

$$\begin{aligned} T_{n+1} &= T_{n-1} T_n = T_{n-2}^{-1} T_n^2 \\ &= x_n T_{n-2}^{-1} T_n - T_{n-2}^{-1} \\ &= x_n T_{n-1} - T_{n-2}^{-1} \end{aligned}$$

we obtain that

$$1 \leq \|T_{n+1}\| \leq |x_n| \|T_{n-1}\| + \|T_{n-2}\|.$$

If  $E \in B_\infty$ , say,  $|x_n| \leq C_0$  for every  $n$ , then  $1 \leq \|T_n\| < C^n$  for some constant  $C$ . We already have the fact that

$$t_n \leq \frac{1}{F_n} n \cdot \log C \xrightarrow{n \rightarrow +\infty} 0 \quad \text{if} \quad E \in sp(H). \quad (\text{A.14})$$

Now, consider more generally  $S_n = g_n g_{n-1} \cdots g_1 g_0$ . In order to exploit the previous step, we decompose  $n$  in the Fibonacci base :

$$n = F_{n_k} + F_{n_{k-1}} + \cdots + F_{n_0} \quad (\text{actually with } n_k - n_{k-1} \geq 2)$$

and, reminding identity (A.11)

$$v(F_n + j) = v(j) \quad \text{if} \quad 1 \leq j \leq F_n \quad (n \geq 3)$$

we get,

$$\begin{aligned} S_n &= S_\ell T_{n_k} \quad \text{where} \quad n - F_{n_k} =: \ell < F_{n_k-1} \\ &= T_{n_0} T_{n_1} \cdots T_{n_k} \quad (\text{where } T_{n_0}, T_{n_1} \text{ may be distinct}) \end{aligned}$$

Finally, by (A.14),

$$0 \leq \log \|S_n\| \leq \sum_{j=0}^k \log \|T_{n_j}\| =: \sum_{j=0}^k F_{n_j} t_{n_j}$$

$$\begin{aligned} &\leq \left( \sum_0^k n_j \right) \log C \quad \text{if } E \in B_\infty \\ &\leq C' (\log n)^2 \end{aligned}$$

and  $\gamma(E, v) = 0$ . □

*Remark A.7.* 1. This method has been worked out by Bovier and Ghez in [39] where they obtain sufficient combinatorial conditions on the involved sequence  $v$  to ensure singular continuous spectrum; this condition, in terms of *powers* of words, is rather technical.

2. Finally, the result holds for a dense  $G_\delta$  set of  $\omega$  : by minimality, the set of  $\omega$  for which  $H_\omega$  has no eigenvalues is dense since it contains the orbit  $O(v)$  and it is a countable intersection of open sets [229]. So, by using the Last-Simon theorem, we get a purely continuous spectrum for a dense  $G_\delta$  set of  $\omega$ 's.

### A.3.2 The Palindromic Density Method

In [116], the authors exhibit a new combinatorial condition on the strictly ergodic orbit  $X := \overline{O(v)}$  to exclude eigenvalues in the spectrum of  $H := H_v$  (and, consequently, in the spectrum of  $H_\omega$  for a dense  $G_\delta$  set of  $\omega$ 's). Recall that a *palindrome* in the infinite word  $v$  on the alphabet  $A$  is a symmetric word. Following the authors, we say that :

**Definition A.8.** The infinite word  $v \in A^{\mathbb{Z}}$  is *palindromic* if  $v$  contains arbitrarily long palindromes.

**Theorem A.14 (Hof, Knill & Simon).** *Let  $v \in A^{\mathbb{Z}}$  be an aperiodic and palindromic sequence generating a strictly ergodic system  $(X, T)$ . Then, the Schrödinger operator  $H_\omega$  has a purely singular continuous spectrum for a dense  $G_\delta$  set of values of  $\omega$ .*

*Proof.* According to a previous remark, it is sufficient to exclude eigenvalues in the spectrum of *one* operator, for instance,  $H := H_v$ . The proof rests on the following combinatorial improvement that we admit.

**Lemma A.7.** *Under the assumptions of the theorem, one can find, for every constant  $C > 1$ , infinitely many palindromes  $w_i$  of length  $L_i$ , centered on  $m_i$ , such that :  $|m_i| \rightarrow \infty$  and  $C^{m_i}/L_i \rightarrow 0$ .*

Let  $E$  be an eigenvalue of  $H$  and  $H\varphi = E\varphi$  where  $\varphi \in \ell^2(\mathbb{Z})$ ,  $\|\varphi\| = 1$ .

★ Suppose first that the palindromes  $w_i := v_{[m_i - \ell_i, m_i + \ell_i]}$  have odd length  $L_i := 2\ell_i + 1$  and are centered on  $m_i$ . To each  $w_i$ , we associate the element  $\varphi_i \in \ell^2(\mathbb{Z})$  defined by  $\varphi_i(n) = \varphi(2m_i - n)$ , the reflecting word at  $m_i$ . Finally, we put  $\Phi(n) = \begin{pmatrix} \varphi(n+1) \\ \varphi(n) \end{pmatrix}$  and  $\Phi_i(n) = \begin{pmatrix} \varphi_i(n+1) \\ \varphi_i(n) \end{pmatrix}$  for  $n \in \mathbb{Z}$ . Without loss of generality, we may assume that the  $m_i$  are nonnegative indices.

The symmetry of the word  $w_i$  results into the following on the transfer matrices  $(g_n)$  :

$$g_{m_i-k} = g_{m_i+k} \quad \text{for } 0 \leq k \leq \ell_i;$$

thus,

$$A_i := g_1^{-1} \cdots g_{m_i}^{-1} = g_{2m_i-1}^{-1} \cdots g_{m_i}^{-1}$$

and since  $\Phi_i(m_i) = \begin{pmatrix} \varphi(m_i-1) \\ \varphi(m_i) \end{pmatrix}$ , we get

$$A_i \Phi(m_i) = \Phi(0) \quad \text{and} \quad A_i \Phi_i(m_i) = \Phi_i(0). \quad (\text{A.15})$$

Moreover, because of the symmetry of  $w_i$  again, we check that

$$\varphi_i(n+1) + \varphi_i(n-1) = (E - v(n))\varphi_i(n)$$

for every  $n \in [m_i - \ell_i, m_i + \ell_i]$ , so that the wronskian  $W := W(\varphi, \varphi_i)$  is constant on the interval  $[m_i - \ell_i, m_i + \ell_i]$ . From that property, we deduce an estimate of  $W(m_i)$  : since  $\|\varphi\| = \|\varphi_i\| = 1$ , we derive

$$|W(m_i)|L_i \leq \sum_{n \in \mathbb{Z}} |W(n)| \leq 2$$

from the Cauchy-Schwarz inequality. But  $W(m_i) = \varphi(m_i)(\varphi(m_i+1) - \varphi(m_i-1))$ , thus  $|\varphi(m_i)|$  and  $|\varphi(m_i+1) - \varphi(m_i-1)|$  cannot be simultaneously greater than  $(2/L_i)^{1/2}$ . Whence the discussion :

If  $|\varphi(m_i+1) - \varphi(m_i-1)| \leq (2/L_i)^{1/2}$ , then

$$\|(\Phi - \Phi_i)(m_i)\| = |\varphi(m_i+1) - \varphi(m_i-1)| \leq (2/L_i)^{1/2};$$

If  $|\varphi(m_i)| \leq (2/L_i)^{1/2}$ , then, in turn,

$$\|(\Phi + \Phi_i)(m_i)\| \leq K(L_i)^{-1/2}$$

since  $(\Phi + \Phi_i)(m_i) = \varphi(m_i) \begin{pmatrix} E - v(m_i) \\ 2 \end{pmatrix}$ . In both cases, we deduce from (A.15) that

$$\begin{aligned} \|\Phi(0)\| - \|\Phi(2m_i)\| &\leq K\|A_i\|(L_i)^{-1/2} \\ &\leq C^{m_i}/L_i^{1/2} \end{aligned}$$

where  $\|g_n\| < C$  for all  $n$  and  $E$ . If  $C, m_i$  and  $L_i$  are such that  $C^{m_i}/L_i^{1/2}$  tends to zero, then

$$\lim_i (\|\Phi(0)\| - \|\Phi(2m_i)\|) = \|\Phi(0)\| = 0$$



since  $\varphi \in \ell^2(\mathbf{Z})$  and  $m_i$  tends to infinity. But  $\varphi$  must then be zero, which leads to a contradiction.

★ Suppose now that the palindromes  $w_i$  have even length  $L_i := 2\ell_i$  and are centered on  $m_i + 1/2$ . Then

$$g_{2m_i-n+1} = g_n \quad \text{for } m_i - \ell_i \leq n \leq m_i + \ell_i + 1,$$

and we consider  $\varphi_i(n) = \varphi(2m_i - n + 1)$ . The previous proof can be arranged in such a way to get the same contradiction.  $\square$

**Examples and Problem :** This last result covers many examples of potentials arising from primitive substitutions such as : Thue-Morse, Fibonacci, Period doubling, binary and ternary non-Pisot as well as sequences defined by circle maps, of the form  $v_n = \mathbf{1}_{[0, \beta[}(n\alpha + \theta)$ , with  $\alpha$  irrational and suitable  $\theta$ .

The Rudin-Shapiro sequence seems to escape those processes : Actually J.P. Allouche proved that neither the Rudin-Shapiro sequence, nor generalized ones in sense of [184], are palindromic [9]; also numerical experiments indicate that there might be eigenvalues in the spectrum of the associated Schrödinger operator [116]. Thus, the nature of the spectrum of  $H$  for the Rudin-Shapiro potential is an open question.

## Appendix B

### Substitutive Continued Fractions

Some algebraic properties of real numbers can be read on a suitable expansion, adic-expansion, continued fraction expansion or other one. In this chapter, we focus on the continued fractions viewed as sequences taking integer values, and, more specifically, on such sequences taking finitely many values, then we ask for algebraic properties of the underlain real numbers. In this framework too, the initial study of substitutive sequences has led to a more general interest in combinatorics of words and the parallel with the previous appendix is powerful. We just aim to gain a glimpse into this subject and we address the reader to [4, 11, 14] for more information, also on the adic-expansions [3, 86].

#### B.1 Overview on Continued Fraction Expansions

Let  $a_1, a_2, \dots$  be a sequence taking values in a finite alphabet  $A = \{1, 2, \dots, s\}$  which may be viewed as the *continued fraction expansion* of some positive real number; which algebraic properties does it enjoy? We already know that the rational numbers are real numbers with finite continued fraction expansion and that the numbers with eventually periodic continued fraction expansion are exactly the quadratic irrational ones by Lagrange's theorem. What else? In particular, what can we say about irrational numbers whose continued fraction expansion is an automatic sequence on a finite alphabet? We begin with usual definitions and general facts on the continued fractions.

It is well-known that every real number  $x$  is the limit of the sequence of rational numbers, called *convergents*,

$$\frac{p_n(x)}{q_n(x)} = a_0(x) + \frac{1}{a_1(x) + \frac{1}{a_2(x) + \dots + \frac{1}{a_n(x)}}} =: [a_0(x); a_1(x), \dots, a_n(x)],$$

where  $a_0(x) = [x]$ ; the integers  $a_n(x)$  are called the *partial quotients* of  $x$ . Rational numbers have a terminating continued fraction and we usually write for an irrational  $x \in [0, 1]$  :

$$x = \frac{1}{a_1(x) + \frac{1}{a_2(x) + \dots}} =: [0; a_1(x), a_2(x), \dots].$$

This expansion involves linear recurrences of order two and by the way, matrices in  $SL(2, \mathbf{Z})$  : if we put

$$A_k(x) = \begin{pmatrix} a_k(x) & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad M_n(x) = A_n(x) \dots A_1(x),$$

then we get, by induction on  $n \geq 1$ ,

$$M_n(x) = \begin{pmatrix} q_n(x) & p_n(x) \\ q_{n-1}(x) & p_{n-1}(x) \end{pmatrix}, \quad \text{with } q_0(x) = 1, \quad p_0(x) = 0 \text{ if } x \in (0, 1]. \quad (\text{B.1})$$

The following identities can easily be obtained from (B.1).

1. By taking the determinant of  $M_n(x)$ ,

$$q_n(x)p_{n-1}(x) - p_n(x)q_{n-1}(x) = (-1)^n.$$

2. By using the symmetry of the  $A_k(x)$ ,

$$\frac{q_{n-1}(x)}{q_n(x)} = [0; a_n(x), \dots, a_1(x)]. \quad (\text{B.2})$$

3. Now, palindromes have a nice expression : if  $[0; a_1, \dots, a_n] = p_n/q_n$ , then

$$[0; a_1, \dots, a_n, a_n, \dots, a_1] = \frac{p_n^2 + p_{n-1}^2}{p_n q_n + p_{n-1} q_{n-1}} \quad (\text{B.3})$$

and

$$[0; a_1, \dots, a_n, c, a_n, \dots, a_1] = \frac{p_n(c p_n + 2 p_{n-1})}{c p_n q_n + p_n q_{n-1} + p_{n-1} q_n}. \quad (\text{B.4})$$

4. From above, one can deduce the striking identity [235]

$$[0; a_1, \dots, a_{n-1}, a_n + 1, a_n - 1, a_{n-1}, \dots, a_1] = \frac{p_n}{q_n} + \frac{(-1)^n}{q_n^2} \quad (\text{B.5})$$

### B.1.1 The Gauss Dynamical System

We consider  $\mathcal{X} = [0, 1] \setminus \mathbf{Q}$  and the *Gauss map*  $T$  defined by

$$Tx = \frac{1}{x} \bmod 1 \quad \text{for } x \in \mathcal{X}.$$

Then,  $a_1(x) = [\frac{1}{x}]$  and  $a_{n+1}(x) = a_1(T^n x)$  for every  $n \geq 1$ , so that  $x$  can be expressed in the form

$$x = \frac{1}{a_1(x) + \frac{1}{a_2(x) + \cdots + \frac{1}{a_n(x) + T^n x}}} =: [0; a_1(x), \dots, a_n(x) + T^n x], \quad (\text{B.6})$$

with

$$T^n x = [0; a_{n+1}(x), a_{n+2}(x), \dots] \quad \text{for every } n \geq 0.$$

We recall that  $T$  on  $\mathcal{X}$  preserves the so-called *Gauss measure*  $\mu$ , which is absolutely continuous with respect to the Lebesgue measure on  $[0, 1]$ , with density  $\frac{1}{\log 2} \frac{1}{1+x}$ . This probability measure is  $T$ -ergodic, even mixing [29] and it is the unique absolutely continuous  $T$ -invariant one; in fact,  $\frac{1}{\log 2} \frac{1}{1+x}$  is the fixed point of the Perron-Frobenius operator on  $L^1([0, 1])$  associated with  $T$  [46].

**Definition B.1.** The ergodic dynamical system  $(\mathcal{X}, \mu, T)$  is the *Gauss dynamical system*. This system is conjugate to the backward shift on  $\mathbf{N}^{\mathbf{N}}$ .

From identity (B.6), we derive that

$$x = \frac{p_n(x) + T^n x p_{n-1}(x)}{q_n(x) + T^n x q_{n-1}(x)}, \quad (\text{B.7})$$

and

$$\begin{aligned} xq_{n-1}(x) - p_{n-1}(x) &= q_{n-1}(x) \frac{p_n(x) + T^n x p_{n-1}(x)}{q_n(x) + T^n x q_{n-1}(x)} - p_{n-1}(x), \\ &= \frac{(-1)^n}{q_n(x) + T^n x q_{n-1}(x)}. \end{aligned}$$

We deduce from above the important following bounds :

$$\frac{1}{2} < q_n(x) |xq_{n-1}(x) - p_{n-1}(x)| < 1. \quad (\text{B.8})$$

On the other hand, from (B.7) again, we see that

$$T^n x = -\frac{xq_n(x) - p_n(x)}{xq_{n-1}(x) - p_{n-1}(x)}.$$

so that, for  $n \geq 1$ ,

$$xTx \cdots T^n x = (-1)^n (xq_n(x) - p_n(x)) = |xq_n(x) - p_n(x)|. \quad (\text{B.9})$$

Combining (B.8) and (B.9), we get that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log q_n(x) + \frac{1}{n} (\log x + \cdots + \log T^{n-1} x) = 0.$$

But now, according to the pointwise ergodic theorem, for almost all  $x \in [0, 1]$ ,

$$\lim_{n \rightarrow \infty} \frac{1}{n} (\log x + \cdots + \log T^{n-1} x) = \int_0^1 \log x \, d\mu(x) = -\frac{\pi^2}{12 \log 2},$$

and we have proved the Paul Lévy's statistical estimate on the denominators  $q_n(x)$  :

**Theorem B.1 (P. Lévy).** : *For almost all  $x \in [0, 1]$ ,*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log q_n(x) = \frac{\pi^2}{12 \log 2}, \quad (\text{B.10})$$

where  $(q_n(x))_n$  is the sequence of denominators of the convergents of  $x$ .

**Definition B.2.** We call a *Lévy number*, any  $x \in [0, 1]$  for which the limit in (B.10) exists and  $\beta(x) := \lim_{n \rightarrow \infty} \log q_n(x)/n$  is then called the *Lévy constant* of  $x$ .

Note that the irrational quadratic numbers are Lévy numbers [82].

The behaviour of the sequence  $(a_n(x))$  itself is less rigid but, as a consequence of Fatou's lemma, the following can be proved.

**Proposition B.1.** *For almost all  $x \in [0, 1]$ ,  $\lim_{n \rightarrow \infty} (a_1(x) + \cdots + a_n(x))/n = +\infty$ .*

### B.1.2 Diophantine Approximation and BAD

From now on, we omit to mention the dependence on  $x$  in the continuous fraction expansion. The behaviour of the denominators  $(q_n)_n$  is relevant for rational approximation and, consequently, for transcendence, as we briefly summarize. Recall the classical result of Dirichlet :

**Theorem B.2 (Dirichlet).** *For any  $x \in [0, 1]$ , there exist infinitely many  $q \in \mathbf{N}$  such that  $||qx|| \leq 1/q$ , where  $|| \cdot ||$  denotes the distance to the nearest integer.*

From (B.8), we see that

$$\frac{1}{a_{n+1} + 2} \leq q_n ||q_n x|| \leq \frac{1}{a_{n+1}} \quad (\text{B.11})$$

and the convergents provide explicit rational approximates satisfying Dirichlet's theorem. Moreover, they are the best ones in sense that  $||qx|| \geq ||q_n x||$  for any  $q < q_{n+1}$ .

The inequality in Dirichlet's result is best possible (up to a multiplicative constant), more precisely, there exist real numbers  $x$  for which the inequality  $||qx|| \leq c/q$  has at most a finite number of solutions for any given  $c < 1/\sqrt{5}$ . If we denote by BAD the set of *badly approximable numbers* that is

$$\text{BAD} := \{x \in [0, 1], ||qx|| > cq^{-1} \text{ for some constant } c := c(x)\},$$

the following can be deduced from (B.11) :

**Proposition B.2.** *The real number  $x \in \text{BAD}$  if and only if the sequence of its partial quotients is bounded.*

All quadratic irrationals are in BAD since they have an ultimately periodic expansion. The problem whether an algebraic non-quadratic number could belong to BAD remains open, but in fact, the converse assertion is conjectured.

Note that BAD is uncountable with zero Lebesgue measure by proposition B.1. Whence, transcendental numbers do exist in BAD. Many explicit examples of such numbers have been constructed (see [6]) and we just mention a historical example [235].

**Theorem B.3.** *Let  $u$  be an integer  $\geq 2$ . The number  $g = \sum_{k=0}^{\infty} \frac{1}{u^{2^k}}$  is transcendental, with partial quotients bounded by  $u + 2$  if  $u \geq 3$ , and by 6 if  $u = 2$ .*

*Proof.* The transcendence of those numbers has been established by Mahler and we refer to [14] for a proof. It remains to show that they belong to BAD.

We fix  $u \geq 2$  and we put  $g_n = \sum_{k=0}^n u^{-2^k}$ . The computation of the first terms gives

$$\begin{aligned} g_0 &= u^{-1}, \\ g_1 &= u^{-1} + u^{-2} = [0; u-1, u+1], \\ g_2 &= [0; u-1, u+2, u, u-1]. \end{aligned}$$

Writing  $g_n = P_n/Q_n = [0; a_1, \dots, a_N]$  with  $P_n/Q_n$  irreducible, then  $Q_n = u^{2^n}$  so that  $g_{n+1} = g_n + u^{-2^{n+1}}$ . Now we remark by induction on  $n \geq 1$  that  $N = 2^n$  and

$$\frac{P_{n+1}}{Q_{n+1}} = \frac{P_n}{Q_n} + \frac{1}{Q_n^2} = [0; \underbrace{a_1, \dots, a_{N-1}}, a_N + 1, a_N - 1, \underbrace{a_{N-1}, \dots, a_1}],$$

using (B.5) for the last equality. Then the bounds on the partial quotients arise by induction on  $n$  again.  $\square$

## B.2 Morphic Numbers

Aperiodic substitutive words constitute a class of sequences very close to periodic ones, and one may think reasonably that the arithmetical study of real numbers with such expansions could be carried out. Of course, according to the conjecture, the expected conclusion is the transcendence of those numbers, but, beyond this conclusion, growth estimates of the denominators  $q_n$  could be useful in view to Koksma's and Mahler's classifications (see [51]).

### B.2.1 Schmidt's Theorem on Non-Quadratic Numbers

We shall consider numbers whose continued fraction expansion is the fixed point of some aperiodic primitive substitution, and call them *morphic numbers*. For such non-quadratic numbers, approximation by quadratic irrational numbers instead of rational ones proves to be more effective. The idea for getting transcendence goes as follows : suppose that the real number of  $[0, 1]$

$$x = [0; a_1, a_2, \dots]$$

has bounded partial quotients. Besides suppose that the sequence  $(a_n)_{n \geq 1}$  presents properties of "repetition". More precisely this sequence begins by arbitrarily long prefixes which are "almost-squares":

$$a_1 a_2 \dots = V_n V'_n \dots$$

where the length  $|V_n|$  goes to infinity, and where  $V'_n$  is a "big" prefix of  $V_n$ . Approach the sequence  $(a_n)_{n \geq 1}$  by the periodic one :  $V_n V_n V_n \dots$ , and let  $\xi_n$  be the real (quadratic) number whose partial quotients are given by the letters of the periodic sequence  $V_n V_n V_n \dots$ . Then, using the same notation for the sequence and the so-associated real number, the coincidence between  $x$  and  $\xi_n$  is apparently reduced to

$$\begin{aligned} x &= \underbrace{V_n} \mid \dots \\ \xi_n &= \underbrace{V_n} \mid \underbrace{V_n} \underbrace{V_n} \dots \end{aligned}$$

though in fact it is better (don't forget that  $V'_n$  is a prefix of  $V_n$ )

$$\begin{aligned} x &= \underbrace{V_n} \underbrace{V'_n} \mid \dots \\ \xi_n &= \underbrace{V_n} \underbrace{V'_n} \mid \dots \end{aligned}$$

The approximation of  $x$  by quadratic numbers is good enough to say something on  $x$  by using a powerful Schmidt's theorem just below.

Recall the following notation.

**Definition B.3.** Let  $\xi$  be a root of the minimal equation  $a\xi^2 + b\xi + c = 0$ , with  $a, b, c \in \mathbf{Z}$ , and  $\gcd(|a|, |b|, |c|) = 1$ . The *height* of  $\xi$ , denoted by  $H(\xi)$ , is defined by  $H(\xi) = \max(|a|, |b|, |c|)$ .

**Theorem B.4 (W.M. Schmidt).** Let  $x$  be a real number in  $[0, 1]$ . We suppose that  $x$  is neither rational, nor quadratic irrational. If there exist a real number  $B > 3$ , and infinitely many quadratic irrational numbers  $\xi_k$  such that

$$|x - \xi_k| < H(\xi_k)^{-B}$$

then  $x$  is transcendental.

We shall need the following classical lemmas on continued fraction expansions.

**Lemma B.1.** Let  $\xi \in [0, 1]$  be a number with purely periodic continued fraction expansion

$$\xi = [0, a_1, a_2, \dots, a_k, a_1, a_2, \dots, a_k, \dots].$$

Then the (quadratic irrational) number  $\xi$  satisfies  $H(\xi) \leq q_k$ .

**Lemma B.2.** If  $x, y \in [0, 1]$  have the same first  $k$  partial quotients  $a_1 a_2 \dots a_k$ , then

$$|x - y| \leq \frac{1}{q_k^2}.$$

*Proof.* : 1. By assumption,  $\xi = [0, a_1, a_2, \dots, a_k, \frac{1}{\xi}]$  that is  $\xi = \frac{p_k + \xi p_{k-1}}{q_k + \xi q_{k-1}}$  and

$$q_{k-1}\xi^2 + \xi(q_k - p_{k-1}) - p_k = 0.$$

It follows that

$$H(\xi) \leq \max(q_{k-1}, |q_k - p_{k-1}|, p_k) \leq q_k,$$

since  $p_n \leq q_n$  for all  $n \geq 1$ .

2. Since  $p_k/q_k = [0, a_1, a_2, \dots, a_k]$ , we have simultaneously  $|x - p_k/q_k| \leq 1/q_k^2$  and  $|y - p_k/q_k| \leq 1/q_k^2$  by (B.11). Moreover,  $x - p_k/q_k$  et  $y - p_k/q_k$  having same sign depending on  $k$  only, we may write :  $|x - y| = \left| |x - p_k/q_k| - |y - p_k/q_k| \right| \leq 1/q_k^2$ .  $\square$

Now, we refer to section 5.3 for definitions and notations related to the substitutions. If  $M := M(\zeta)$  is the matrix of the primitive substitution  $\zeta$  on  $A$ , and if  $\theta$  is the Perron-Frobenius eigenvalue of  $M$ , recall that  $d = (d_\alpha)_{\alpha \in A}$  denotes the positive associated eigenvector corresponding to  $\theta$  and normalized by  $\sum_{\alpha \in A} d_\alpha = 1$ ;  $d$  is thus the vector of frequencies of letters. Also,  $g$  denotes the corresponding left eigenvector uniquely defined by  $\sum_{\alpha \in A} g_\alpha d_\alpha = 1$ .



**Definition B.4.** If  $W = w_1 \dots w_\ell \in \mathcal{L}(\zeta)$ , the *weighted norm* of  $W$  is,

$$||W|| := \sum_{1 \leq i \leq \ell} g_{w_i} = \lim_{n \rightarrow \infty} \frac{|\zeta^n(W)|}{\theta^n}.$$

The equivalence between both writings results from corollary 5.1. Indeed, for every  $\alpha, \beta \in A$ , it is proved that  $d_\alpha \cdot g_\beta = \lim_{n \rightarrow \infty} m_{\alpha\beta}^{(n)} / \theta^n$  where  $m_{\alpha\beta}^{(n)} := (M^n)_{\alpha\beta}$  is nothing but the occurrence number of  $\alpha$  in the word  $\zeta^n(\beta)$ . It follows that

$$g_\beta = \lim_{n \rightarrow \infty} \sum_{\alpha \in A} \frac{m_{\alpha\beta}^{(n)}}{\theta^n} = \lim_{n \rightarrow \infty} \frac{|\zeta^n(\beta)|}{\theta^n}$$

whence the second form of the weighted norm.

The following theorem states one of the first results in this direction. We identify  $x$  with its expansion.

**Theorem B.5.** *Let  $x \in [0, 1]$  be a non-quadratic number whose continued fraction expansion is the fixed point of some primitive substitution  $\zeta$ . If there exists a prefix of  $x$ ,  $U := W_1 W_2 W_1$  where the words  $W_1$  and  $W_2$  satisfy  $||W_1|| > ||W_2||$ , then  $x$  is a transcendental number.*

*Proof.* : From our assumption and because  $x = \zeta^n(x)$  for each  $n \geq 1$ ,  $x$  begins for every  $n$  with the word  $V'_n = \zeta^n(W_1 W_2)$  whose length is denoted by  $\ell_n$ . If  $\xi_n$  is the purely periodic sequence with period  $V'_n$ ,  $\xi_n$  is a *reduced* quadratic irrational and, by lemma B.1, we have  $H(\xi_n) \leq q_{\ell_n}$ .

Now, since  $W_1 W_2 W_1$  is a prefix of  $x$ ,  $x$  begins with  $V_n = \zeta^n(W_1 W_2 W_1)$  for every  $n$ , so that  $x$  and  $\xi_n$  have the same  $L_n = |V_n|$  first partial quotients. It follows from lemma B.2, that

$$|x - \xi_n| \leq \frac{1}{q_{L_n}^2}.$$

If there exists some number  $\theta > 3$  such that  $q_{\ell_n}^\theta < q_{L_n}^2$  for infinitely many  $n$ , then

$$|x - \xi_n| \leq \frac{1}{q_{L_n}^2} < q_{\ell_n}^{-\theta} \leq H(\xi_n)^{-\theta},$$

and the theorem is a direct consequence of W.M. Schmidt's theorem.

We are left with estimates of both  $q_{\ell_n}$  and  $q_{L_n}$ .

First of all, observe that, by primitivity,  $\beta := \lim_{n \rightarrow \infty} \frac{1}{n} \log q_n$  exists. More generally we have the following.

**Lemma B.3.** *Let  $(\Omega, S, \nu)$  be the uniquely ergodic substitution system, associated with  $\zeta$ , and, for every  $\omega \in \Omega$ , denote by  $x_\omega \in [0, 1]$  the number whose continued fraction expansion is  $[0; \omega_1, \omega_2, \dots]$ ; then,*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log q_n(\omega) \quad \text{exists for every } \omega \in \Omega.$$

Moreover, all the numbers of the closed orbit are Lévy numbers with the same Lévy constant.

Put now  $\rho = \lim_{n \rightarrow \infty} |\zeta^n(W_2)|/|\zeta^n(W_1)|$ ; under our assumption on the words  $W_i$ , we have  $\rho < 1$  and

$$\lim_{n \rightarrow \infty} \frac{L_n}{\ell_n} = \lim_{n \rightarrow \infty} \frac{2 + \frac{|\zeta^n(W_2)|}{|\zeta^n(W_1)|}}{1 + \frac{|\zeta^n(W_2)|}{|\zeta^n(W_1)|}} = \frac{2 + \rho}{1 + \rho} > \frac{3}{2}.$$

Combining these remarks, we obtain that

$$\lim_{n \rightarrow \infty} \frac{\log q_{\ell_n}}{\log q_{L_n}} = \lim_{n \rightarrow \infty} \frac{\ell_n}{L_n} < \frac{2}{3}$$

which ends the proof.

*Proof of the lemma.* Actually, we can see more precisely that, for every  $\omega \in \Omega$ ,  $\beta(x_\omega)$  exists and is equal to

$$\beta = - \lim_{n \rightarrow \infty} \sum_{\alpha_1 \dots \alpha_n \in \Omega_n} \log[0; \alpha_1, \dots, \alpha_n] \nu([\alpha_1 \dots \alpha_n]), \quad (\text{B.12})$$

where  $\Omega_n$  is the set of  $n$ -factors of elements in  $\Omega$ . If  $\varphi$  is the natural map  $\omega \in \Omega \mapsto x_\omega = [0; \omega_1, \omega_2, \dots] \in [0, 1]$ ,  $\varphi$  is continuous by lemma B.2 and  $\varphi(\Omega)$  is a compact subset of  $[0, 1]$  avoiding 0. Hence the function  $\log \varphi$  is continuous on  $\Omega$  and obviously,  $\varphi \circ S = T \circ \varphi$ . As a consequence of Oxtoby's ergodic theorem,

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n < N} \log \varphi(S^n \omega) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n < N} \log T^n \varphi(\omega)$$

exists for every  $\omega \in \Omega$  and is equal to  $\int_\Omega \log \varphi(\omega) d\nu(\omega)$ . It follows that every  $x_\omega$  admits a Lévy constant

$$\beta(x_\omega) = \lim_{n \rightarrow \infty} \frac{1}{n} \log q_n(\omega) = - \int_\Omega \log \varphi(\omega) d\nu(\omega).$$

By using the following remark :  $|\log y - \log(p_n(y)/q_n(y))| \leq \frac{1}{2^{n-2}}$  for  $n \geq 1$  and  $y \in \mathcal{X}$  [29], and invoking the uniform convergence, we get

$$\begin{aligned} \int_\Omega \log \varphi(\omega) d\nu(\omega) &= \lim_{n \rightarrow \infty} \int_\Omega \log \frac{p_n(\omega)}{q_n(\omega)} d\nu(\omega) \\ &= \lim_{n \rightarrow \infty} \int_\Omega \log[0; \omega_1, \dots, \omega_n] d\nu(\omega). \end{aligned}$$

The lemma is proved. □

The proof of the theorem is complete. □

The statement can be simplified when the continued fraction expansion of  $x$  is an automatic sequence.

**Corollary B.1.** : *Let  $x \in ]0, 1[$  be a non-quadratic number whose continued fraction expansion is the fixed point of some primitive substitution of constant length. If there exists a prefix of  $x$ ,  $U = W_1 W_2 W_1$  where the words  $W_i$  satisfy  $|W_1| > |W_2|$ , then  $x$  is a transcendental number.*

*Proof.* In case of a constant-length substitution,  $g_\alpha = 1$  for every  $\alpha$ , so that the weight norm of the word  $W = w_1 \dots w_l$  reduces to  $|W|$ .  $\square$

*Example B.1.* Most of the classical examples of substitutive sequences satisfy this criterion and provide transcendental numbers. However, once again, the Rudin-Shapiro automaton seems to escape this procedure and the algebraic nature of the Rudin-Shapiro continued fractions will be deduced from a next result.

*Remark B.1.* The method developed above involves properties of prefixes of the fixed point  $\zeta^\infty(a)$ , and, consequently, cannot be used to establish the transcendence of any limit point in the closed orbit  $x$  in  $[0, 1]$ , although all these numbers are Lévy numbers.

As a generalization of this method, the next theorem establishes the transcendence for a broader class of sequences enjoying suitable combinatorial properties ([11] and see also [14]).

**Theorem B.6.** *Let  $x \in [0, 1]$  be an irrational number with continued fraction expansion :  $x = [0; a_1, a_2, \dots]$  and denominators  $(q_n)_{n \geq 0}$ . We suppose that the sequence  $(a_n)_{n \geq 1}$  contains infinitely many prefixes of the form  $U_k V_k$  such that*

- (i)  $\lim_{k \rightarrow \infty} |U_k| = +\infty$ ,
- (ii)  $V_k$  itself is a prefix of  $U_k$ .

*We put  $\gamma = \liminf_{k \rightarrow \infty} (|U_k| + |V_k|)/|U_k| \geq 1$ ,  $M = \limsup_{k \rightarrow \infty} q_{|U_k|}^{1/|U_k|}$  and  $m = \liminf_{k \rightarrow \infty} q_{|U_k V_k|}^{1/|U_k V_k|}$ . Then, if  $\gamma > 3 \log M / 2 \log m$ , the number  $x$  is transcendental.*

*Example B.2.* One can check that sturmian sequences, in turn, provide transcendental numbers since they meet the conditions of theorem B.6.

## B.2.2 The Thue-Morse Continued Fraction

We consider the specific number whose continued fraction expansion is the Thue-Morse sequence on the alphabet  $\{a, b\}$ , where  $a, b$  are integers  $\geq 2$ . We already observed that this number must be transcendental and a quick proof of this fact will be given in the next section. But, because of the rigidity and of the symmetry of this sequence, we are able to get rather precise growth estimates of the associated denominators [204].

We denote by  $A$  and  $B$  the matrices  $\begin{pmatrix} a & 1 \\ 1 & 0 \end{pmatrix}$  and  $\begin{pmatrix} b & 1 \\ 1 & 0 \end{pmatrix}$  respectively. If  $\|\cdot\|$  is the operator norm on matrices, recall that, for symmetric matrices,  $\|X\| = \rho(X)$ , where  $\rho(X)$  is the spectral radius of  $X$ , that is  $\rho(X) = \sup\{|\lambda|, \lambda \text{ eigenvalue of } X\}$  for the symmetric matrix  $X$ ; in particular  $\rho(A) = \frac{a+\sqrt{a^2+4}}{2}$ .

The first lemma below already appears in [67]. We always identify the number  $x$  and the sequence of its partial quotients.

**Lemma B.4.** *If the letters  $a$  and  $b$  occur in  $x$  with frequency  $\alpha$  and  $\beta$  respectively, then*

$$\limsup q_n^{\frac{1}{n}} \leq \|A\|^\alpha \|B\|^\beta.$$

*Proof.* For  $n \geq 1$ , let  $u_n$  be the vector  $\begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix}$ , with  $u_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ , so that

$$u_n = \begin{pmatrix} a_n & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_{n-1} & 1 \\ 1 & 0 \end{pmatrix} \cdots \begin{pmatrix} a_1 & 1 \\ 1 & 0 \end{pmatrix} u_0 =: W_n u_0,$$

where  $W_n := W_n(A, B)$  is the product of matrices. It follows that

$$\|u_n\| \leq \|W_n\| \leq \|A\|^m \|B\|^{n-m}$$

if  $m$  is the occurrence number of  $A$  in  $W_n$ . Thus  $\|u_n\|^{\frac{1}{n}} \leq \|A\|^{\frac{m}{n}} \|B\|^{1-\frac{m}{n}}$  and

$$\limsup \|u_n\|^{\frac{1}{n}} \leq \|A\|^\alpha \|B\|^\beta.$$

Since  $q_n < \|u_n\| < \sqrt{2} q_n$ , we get

$$\frac{1}{\sqrt{2}} \|u_n\| < q_n < \|u_n\|, \quad (\text{B.13})$$

whence the lemma.  $\square$

We deduce the first estimate for the Thue-Morse number .

**Proposition B.3.** *If  $(q_n)_n$  is the sequence of denominators of the Thue-Morse sequence on  $\{a, b\}$ , then*

$$\limsup_{n \rightarrow \infty} q_n^{1/n} \leq \sqrt{\|AB\|}.$$

*Proof.* Since the Thue-Morse sequence on  $\{a, b\}$  is a fixed point of  $\zeta$  on the alphabet  $\{ab, ba\}$  as well, the proposition follows from the previous lemma applied with  $W_{2n}$  and  $W_{2n+1}$ .  $\square$

For the lower bound, we shall make use of the trace map equation (see appendix A). Let us denote by  $\zeta^n(A) = A_n$  the product of the matrices corresponding to the word  $\zeta^n(a)$  and by  $\zeta^n(B) = B_n$  the analogue for  $\zeta^n(b)$ . Then,

$A_0 = A$ ,  $B_0 = B$ , and we obviously have  $A_{n+1} = B_n A_n$  and  $B_{n+1} = A_n B_n$  for  $n \geq 0$ . It is easily checked by induction on  $n$  that  $A_n$  and  $B_n$  are symmetric if  $n$  is even, and that  $B_n = A_n^*$  otherwise,  $X^*$  denoting the transpose of  $X$ .

**Lemma B.5.** *For every  $n \geq 1$ , we have  $\rho(A_n) \geq (\rho(AB))^{2^{n-1}}$ .*

*Proof.* The lemma follows from some properties of the spectral radius of square matrices. For any such  $X$  and  $Y$ , then  $\rho(XY) = \rho(YX)$  and  $\rho(XX^*) = \|XX^*\| = \|X\|^2 \geq \rho(X)^2$ .

Suppose first that  $n = 2k + 2$ . Thus,

$$\rho(A_{2k+2}) = \rho(B_{2k+1}A_{2k+1}) = \rho(A_{2k+1}^*A_{2k+1}) \geq \rho(A_{2k+1})^2.$$

Suppose now  $n = 2k + 1$ . Then

$$\begin{aligned} \rho(A_{2k+1}) &= \rho(B_{2k}A_{2k}) = \rho(B_{2k-1}A_{2k-1}A_{2k-1}B_{2k-1}) \\ &= \rho(B_{2k-1}^2A_{2k-1}^2) = \rho((A_{2k-1}^*)^2A_{2k-1}^2) \\ &= \rho((A_{2k-1}^2)^*A_{2k-1}^2) \geq \rho(A_{2k-1}^2)^2 = \rho(A_{2k-1})^4. \end{aligned}$$

A combination of those inequalities gives the result since :  $\rho(A_{2k+1}) \geq \rho(A_{2k-1})^4 \geq \rho(A_1)^{2^{2k}} = \rho(A_1)^{2^{n-1}}$  if  $n = 2k + 1$ , and  $\rho(A_{2k+2}) \geq \rho(A_{2k+1})^2 \geq \rho(A_1)^{2^{2k+1}} = \rho(A_1)^{2^{n-1}}$  if  $n = 2k + 2$ .  $\square$

We deduce the following lower estimate.

**Proposition B.4.** *If  $(q_n)_n$  is the sequence of denominators of the Thue-Morse sequence on  $\{a, b\}$ , and  $c_k = 5.2^k$ , then  $\liminf_{k \rightarrow \infty} q_k^{1/c_k} \geq \sqrt{\rho(AB)}$ .*

*Proof.* We start with the obvious inequality :  $q_n > \text{Tr}(W_n)/2$ . Indeed, remember that  $\begin{pmatrix} q_n & p_n \\ q_{n-1} & p_{n-1} \end{pmatrix} = W_n \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$  since  $p_0 = 0$  and  $p_{-1} = 1$ , so that  $2q_n > q_n + q_{n-1} \geq q_n + p_{n-1} = \text{Tr}(W_n)$ , whence the claim.

But the trace of a product of matrices in  $SL(2, \mathbf{Z})$  is computable by iteration of the Cayley-Hamilton identity, as we already did in appendix A. Denote by  $\alpha_k$  and  $\beta_k$  the trace of  $A_k$  and  $B_k$  respectively; then,  $\alpha_0 = a, \beta_0 = b$ , and  $\alpha_k = \beta_k$  for  $k \geq 1$ . If  $X \in SL(2, \mathbf{R}^+)$  is such that  $\rho(X) > 1$ , then  $\text{Tr}(X) \geq \rho(X)$ ; this shows that  $\lim_{k \rightarrow \infty} \alpha_k = +\infty$ . Now, put  $Z_k = B_k A_k B_k A_k$ , associated with the word  $\zeta^k(abab)$  of length  $c_k$ , so that, with our notations,  $Z_k = W_{c_k}$ . Then we readily obtain with help of (A.5)

$$\begin{aligned} \text{Tr}(Z_k) &= \text{Tr}(A_{k+1}B_kA_{k+1}) = \text{Tr}(A_{k+1}^2B_k) \\ &= \alpha_{k+1}\text{Tr}(A_{k+1}B_k) - \text{Tr}(B_k) \\ &= \alpha_{k+1}\text{Tr}(A_kB_k^2) - \text{Tr}(B_k) \\ &= \alpha_{k+1}\alpha_k\text{Tr}(A_kB_k) - \alpha_k - \alpha_{k+1}\alpha_k, \end{aligned}$$

finally

$$\text{Tr}(Z_k) = \alpha_{k+1}^2 \alpha_k - \alpha_{k+1} \alpha_k - \alpha_k. \quad (\text{B.14})$$

Since  $\alpha_k$  tends to infinity with  $k$ , we deduce from (B.14) that  $\text{Tr}(Z_k) \sim \alpha_{k+1}^2 \alpha_k$  as  $k$  goes to  $+\infty$ . Keeping in mind that  $q_{c_k} \geq \frac{1}{2} \text{Tr}(Z_k)$ , we may write

$$\begin{aligned} \liminf q_{c_k}^{\frac{1}{c_k}} &\geq \liminf \text{Tr}(Z_k)^{\frac{1}{c_k}} \geq \liminf (\rho(A_{k+1})^2 \rho(A_k))^{\frac{1}{c_k}} \\ &\geq \liminf \rho(AB)^{\frac{5 \cdot 2^{2k-1}}{c_k}} = \sqrt{\rho(AB)}, \end{aligned}$$

since, by lemma B.5,

$$\rho(A_{k+1})^2 \rho(A_k) \geq \rho(A_1)^{2^{2k+1} + 2^{2k-1}} = \rho(A_1)^{5 \cdot 2^{2k-1}}.$$

□

**Corollary B.2.** *The Lévy constant  $\beta$  of the Thue-Morse number satisfies*

$$\log \sqrt{\rho(AB)} \leq \beta \leq \log \sqrt{\|AB\|}$$

When  $a = 1$ , and  $b = 2$  for example, those estimates lead to  $0.658 \leq \beta \leq 0.676$ . By applying the formula (B.12) with  $n = 5$ , we get the approximation  $\beta \simeq 0.669$ .

### B.3 Schmidt Subspace Theorem

B. Adamczewski and Y. Bugeaud have obtained in [4] significant improvements of theorem B.6 by using a more powerful theorem of W. Schmidt, usually called the Schmidt subspace theorem [222].

**Theorem B.7 (W.M. Schmidt).** *Let  $m \geq 2$  be an integer and  $\varepsilon > 0$ . Let  $L_j, 1 \leq j \leq m$ , be  $m$  linear forms on  $\mathbf{R}^m$ , with algebraic coefficients and linearly independent on  $\overline{\mathbf{Q}}$ . Then, the solutions  $x = (x_1, \dots, x_m)$  in  $\mathbf{Z}^m$  to the inequality*

$$|L_1(x) \cdots L_m(x)| \leq \max\{|x_1|, \dots, |x_m|\}^{-\varepsilon}$$

*lie in finitely many proper subspaces of  $\mathbf{Q}^m$ .*

The benefit of the Schmidt subspace theorem, as explained by the authors of [4], rests in the arbitrary number of concerned linear forms. Actually, taking  $m = 2$  in this statement leads to the famous Roth theorem on algebraic numbers. Indeed, let  $\alpha$  be an irrational algebraic number and suppose that there exist infinitely many distinct solutions  $(p_n/q_n)$  to the inequality  $0 < |\alpha - \frac{p}{q}| < \frac{1}{q^{2+\varepsilon}}$ ; this condition can

be expressed in the form  $q_n|q_n\alpha - p_n| < q_n^{-\varepsilon}$ , and for  $n$  large enough, modifying  $\varepsilon$  if necessary,

$$q_n|q_n\alpha - p_n| < \max\{|p_n|, q_n\}^{-\varepsilon}$$

since  $|p_n| \leq q_n(|\alpha| + 1)$  as soon as  $|\alpha - p_n/q_n| < 1$ . We can write this inequality as

$$|L_1(p_n, q_n)| |L_2(p_n, q_n)| < \max\{|p_n|, q_n\}^{-\varepsilon},$$

where  $L_1(x, y) = x - \alpha y$ ,  $L_2(x, y) = y$  are linear forms on  $\mathbf{R}^m$ , with algebraic coefficients and linearly independent on  $\mathbf{Q}(\alpha)$ . By applying the previous theorem, we deduce that infinitely many  $p_n/q_n$  lie in a same vector line of  $\mathbf{Q}^2$ : one can find two integers  $x, y$ ,  $(x, y) \neq (0, 0)$  such that  $xp_n + yq_n = 0$  for those  $n$ ; but there is only a finite number of such rational numbers whence a contradiction. We have thus got the following famous result:

**Theorem B.8 (Roth).** *If  $\alpha$  is such that, for every  $\varepsilon > 0$ , the inequality*

$$0 < \left| \alpha - \frac{p}{q} \right| < \frac{1}{q^{2+\varepsilon}}$$

*holds for infinitely many rational numbers, then  $\alpha$  is transcendental.*

But Roth's theorem is of no use for the transcendence of irrational numbers in BAD.

We select below a few of the results in [3, 4] related to our purpose.

### B.3.1 Transcendence and Repetitions

If  $V$  is a word on the alphabet  $A$  and  $\alpha \geq 1$ , we denote by  $V^\alpha$  a partial repetition of  $V$ :  $V^\alpha = VV'$  where  $V'$  is a prefix of  $V$  with  $|VV'|/|V| = \alpha$ . A square corresponds to  $\alpha = 2$ . The first improvement is the next theorem that we admit [4].

**Theorem B.9 (Adamczewski & Bugeaud).** *Let  $x$  be the real number identified with its continued fraction expansion  $x = [0; a_1, a_2, \dots]$  and suppose that  $x$  is neither quadratic nor rational. Then  $x$  is transcendental in both cases:*

- (i)  $x$  begins with arbitrary large squares.
- (ii) The sequence  $(q_n^{1/n})_{n \geq 0}$  is bounded and there exists a rational number  $\omega > 1$  such that  $x$  begins with arbitrary large words  $V_n^\omega$ .

**Remark B.2.** 1. The condition on the sequence of denominators in (ii) is satisfied for almost all  $x$  by Lévy's theorem for instance. In addition, it is trivially true for numbers in BAD since the sequence then is lacunary.

- 2. In this version, the repetitions, once more, must appear at the very beginning of the infinite word and this constraint has to be released if one is interested in points of the closed orbit for instance. The authors obtained a second version

where a controlled shift of the repetitions is allowed; in counterpart, the numbers are supposed to be Lévy's numbers and the constraint on the growth of the denominators must be increased.

We deduce from theorem B.9 (ii) the following result which solves the question of morphic numbers in the constant-length case.

**Theorem B.10 (Adamczewski & Bugeaud).** *The continued fraction expansion of an algebraic number of degree at least three cannot be a recurrent fixed point of some constant-length substitution.*

*Proof.* Let  $\zeta$  be a constant-length substitution on the alphabet  $A$  and suppose that  $a = (a_j)_{j \geq 1}$  is a fixed point of  $\zeta$ ; necessarily,  $a_1$  is the first letter of  $\zeta(a_1)$  and by definition of a recurrent sequence,  $a_1$  occurs in  $a$  at least twice; in particular, there exists  $W \in \mathcal{L}_a$  such that the factor  $a_1 W a_1$  appears as a prefix of  $a$ . Clearly, the assumptions of theorem B.9 (ii) are satisfied by taking  $V_n = \zeta^n(a_1 W)$ . Note that this result admits an extension to automatic sequences, i.e. the image letter-by-letter of such fixed points.  $\square$

*Example B.3.* The image of the Rudin-Shapiro sequence by some map  $\{\pm 1\} \mapsto \{a, b\}$ , where  $a, b$  are distinct integers  $\geq 2$ , cannot be the continued fraction expansion of an algebraic number.

### B.3.2 Transcendence and Palindromes

In 1840, Liouville has shown that  $e$  is not a quadratic irrational number by exhibiting “good” simultaneous rational approximations of  $e$  and  $e^{-1}$ . In the prolongation of Liouville's result, one can prove the following by using the Schmidt subspace theorem.

**Theorem B.11 (W.M. Schmidt).** *Let  $\xi$  be an irrational number. Suppose that  $\xi$  and  $\xi^2$  admit good simultaneous rational approximations in sense that there exist infinitely many distinct rational numbers  $(p_n/q_n)$ ,  $(p'_n/q_n)$  such that*

$$|q_n \xi - p_n| < \frac{1}{q_n^\sigma} \quad \text{and} \quad |q_n \xi^2 - p'_n| < \frac{1}{q_n^\tau},$$

where  $\sigma + \tau > 1$ ; then  $\xi$  is either quadratic or transcendental.

*Proof.* Suppose  $\xi$  to be an algebraic number of degree  $\geq 3$ . We manage to make use of the Schmidt subspace theorem, so we consider the three linear forms on  $\mathbf{Q}$

$$\begin{cases} L_1(X_1, X_2, X_3) = X_1, \\ L_2(X_1, X_2, X_3) = \xi X_1 - X_2, \\ L_3(X_1, X_2, X_3) = \xi^2 X_1 - X_3. \end{cases}$$



From our assumption, those forms have algebraic coefficients and are linearly independent on  $\mathbf{Q}$ . If the sequences  $(p_n/q_n)$ ,  $(p'_n/q_n)$  satisfy

$$|q\xi - p| < \frac{1}{q^\sigma}, \quad |q\xi^2 - p'| < \frac{1}{q^\tau}$$

with  $\sigma + \tau > 1$  as assumed in the statement, we get,

$$\prod_{1 \leq j \leq 3} |L_j(q_n, p_n, p'_n)| < \frac{1}{q_n^{\sigma+\tau-1}}.$$

Now, applying Schmidt's theorem, we conclude that infinitely many  $(q_n, p_n, p'_n)$  lie in a same vector plane of  $\mathbf{Q}^3$ : one can thus find an infinite sequence  $(n_k)$  and three integers  $x_1, x_2, x_3$  with  $(x_1, x_2, x_3) \neq (0, 0, 0)$  such that, for every  $n \in (n_k)$ ,  $x_1 q_n + x_2 p_n + x_3 p'_n = 0$ , or, equivalently,

$$x_1 + x_2 \frac{p_n}{q_n} + x_3 \frac{p'_n}{q_n} = 0.$$

Taking the limit as  $k \rightarrow \infty$  we get  $x_1 + x_2 \xi + x_3 \xi^2 = 0$ , whence a contradiction.  $\square$

As a corollary, following [5], we shall establish a property of palindromic continuous fractions.

Recall that a palindrome is a symmetric word :

$$W := a_1 a_2 \dots a_{n-1} a_n = a_n a_{n-1} \dots a_2 a_1 =: \overline{W}.$$

If  $W$  is a palindrome and  $p_n/q_n = [0; a_1 a_2 \dots a_{n-1} a_n]$ , then we have  $p_n/q_n = q_{n-1}/q_n$  from (B.2) so that  $p_n = q_{n-1}$ . If now  $x$  begins with  $W$ , this remark can be used to provide an excellent simultaneous approximation to the number  $x$  and its square. Indeed, since  $|x - p_n/q_n| < 1/q_n^2$ , then

$$\begin{aligned} |x^2 - \frac{p_{n-1}}{q_n}| &= |x^2 - \frac{p_{n-1}}{q_{n-1}} \frac{p_n}{q_n}| \\ &\leq |x - \frac{p_n}{q_n}| |x + \frac{p_{n-1}}{q_{n-1}}| + \frac{1}{q_n q_{n-1}} \leq \frac{a_n + 3}{q_n^2} = \frac{a_1 + 3}{q_n^2}. \end{aligned}$$

It follows that the infinite sequences  $(p_n/q_n)$  and  $(p_{n-1}/q_n)$  satisfy theorem B.11 and  $x$  must be either quadratic or transcendental. This proves the next statement.

**Theorem B.12 (Adamczewski & Bugeaud).** *The continued fraction expansion of an algebraic number of degree at least three never begins with arbitrarily large palindromes.*

*Example B.4.* This theorem provides a very short proof of the transcendence of the Thue-Morse continued fractions.

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# Glossary

$L_C(B)$	occurrence number of $C$ in $B$ , 130
$A^* = \cup_{k \geq 0} A^k$	all words on the alphabet $A$ , 97
$C(\zeta) = (C_{\alpha\beta}^{\gamma\delta})$	coincidence matrix, 244
$H(\mu)$	translation group of $\mu$ , 58
$H(\xi)$	height of the algebraic number $\xi$ , 324
$M(\mathbf{T})$	algebra of the regular Borel complex measures on $\mathbf{T}$ , 1
$M(\zeta)$	composition matrix of $\zeta$ , 131
$M_0(\mathbf{T})$	Rajchman measures, 3
$M_c(\mathbf{T})$	convolution-ideal of continuous measures on $\mathbf{T}$ , 2
$M_d(\mathbf{T})$	sub-algebra of discrete measures in $M(\mathbf{T})$ , 2
$O(u)$	orbit of $u$ , 98
$R_\theta$	irrational rotation, 29
$SL(2, \mathbf{R})$	group of $2 \times 2$ -real matrices with $\pm 1$ determinant, 295
$S_q$	$q$ -shift, 52
$U_T$	operator $f \rightarrow f \circ T$ on $L^2$ , 21
$Z = (\sigma_{\alpha\beta}^{\gamma\delta})$	bi-correlation matrix, 256
$[U, f]$	cyclic subspace spanned by $f \in H$ , 22
$[\alpha_0 \alpha_1 \cdots \alpha_k]$	cylinder set, 85
$[\mu]$	type of the measure $\mu$ , 31
$[\sigma_{\max}]$	maximal spectral type, 34
$\Delta$	Gelfand spectrum of the Banach algebra $M(\mathbf{T})$ , 6
$\Sigma = (\sigma_{\alpha\beta})_{\alpha, \beta \in A}$	correlation matrix, 197
$\chi = (\chi_\mu)_{\mu \in M(\mathbf{T})}$	generalized character, 7
$\delta_t$	Dirac measure at $t$ , 2
$\ell^2(\mathbf{Z})$	space of square summable bi-infinite sequences, 293
$\ell^\infty(\mathbf{Z})$	space of bounded bi-infinite sequences, 300
$\hat{\mu}(n)$	$n^{th}$ Fourier coefficient of the measure $\mu$ , 2

<b>T</b>	$\mathbf{R} \setminus 2\pi\mathbf{Z}$ , 1
$\mu * \nu$	convolution of $\mu$ and $\nu$ , 1
$\mu \ll \nu$	$\mu$ is absolutely continuous with respect to $\nu$ , 2
$\mu \perp \nu$	$\mu$ and $\nu$ are mutually singular, 3
$\mu \sim \nu$	$\mu$ and $\nu$ are equivalent, 2
$\overline{\Gamma}$	closure of $\Gamma$ in $\Delta$ , 9
$\rho(\mu, \nu)$	affinity between $\mu$ and $\nu$ , 3
$\sigma_0$	reduced maximal spectral type, 49
$\sigma_f$	spectral measure of $f \in H$ , 21
$\sigma_{f,g}$	spectral measure of $f, g \in H$ , 22
$h(\zeta)$	height of $\zeta$ , 162
$h_d$	discrete idempotent in $\Delta$ , 15
$m(U)$	spectral multiplicity of $U$ , 37
$sp(A)$	spectrum of the operator $A$ , 21
$u_{[m,n]}$	factor $u_m u_{m+1} \cdots u_n, m \leq n$ , 98
$\mathbf{1}^\perp$	orthogonal of the constants, 49
$\mathcal{L}(X)$	language of $X$ , 98
$\mathcal{L}(u)$	language of $u$ , 98
$\mathcal{L}_\zeta$	language of the substitution $\zeta$ , 125
$\mathcal{S}$	Wiener space, 104
$\mathbf{Z}_2$	2-adic integers, 85
$\mathbf{Z}_q$	$q$ -adic integers, 226
<b>BAD</b>	badly approximable numbers, 323

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