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THE DENSITY OF STATES FOR ALMOST PERIODIC SCHRÖDINGER OPERATORS AND THE FREQUENCY MODULE : A COUNTER-EXAMPLE

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ABSTRACT : We exhibit an example of a one-dimensional discrete Schrödinger with an almost periodic potential for which the steps of the density of states do not belong to the frequency module. This example is suggested by the K-theory [3].

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INTRODUCTION

The problem of investigating the spectrum of quantum almost periodic hamiltonian operators, increased very recently in importance due to new informations obtained by several authors.

Among these progresses, the integrated density of states $\mathcal{N}(E)$ has been interpreted in the algebraic framework [9,3] : the trace of the spectral measure associated with the random hamiltonian as an element of the canonical associated von Neumann algebra [2]. *If the energy belongs to the resolvent set,* where $\mathcal{N}(E)$ is locally constant, the density of states takes values in the K_0-group (precisely in its image by the trace) of the canonical C*-algebra constructed form the quasi periodic hamiltonian.

In the case of a one-dimensional Schrödinger operator with an almost periodic potential V , this group coincides with the frequency module of V [6,3]. In this short note, we exhibit an example of one-dimensional Schrödinger operator with a "discontinuous quasi-periodic" potential for which the K-group is different from the frequency module, and we show that the values of $\mathcal{N}(E)$ at the steps are really not in the frequency module.

To be precise we deal with an hamiltonian $(H_x)_{x\in\mathbb{T}}$ acting on $\ell^2(\mathbb{Z})$ by

$$H_x\psi(n) = \psi(n+1) + \psi(n-1) + V(x-n\theta)\,\psi(n) \tag{I.1}$$

where $V\in\mathcal{C}(\mathbb{T})$ and θ is an irrational number. The spectral density in this case is defined by

$$\mathcal{N}(E) = \lim_{N\to\infty} (2N+1)^{-1}\ \mathrm{card}\left\{\text{eigenvalues of } H_x \restriction_{\ell^2(-N,N)} < E\right\} \tag{I.2}$$

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It has been proven that $\mathcal{N}(E)$ exists ; it is independent of $x \in \mathbb{T} = \mathbb{R}/\mathbb{Z}$, and it is a continuous increasing function of E [9]. Moreover, it is locally constant on the resolvent set of H_x, which in this case is independent of x .

If θ was rationnal, H would be periodic, and $k = \mathcal{N}(E)$ could be interpreted as the Bloch wave vector, whereas $E = \mathcal{N}^{-1}(k)$ would give the dispersion law for the energy as the function of the frequency. As it is well known a gap in the energy would occurs eventually if k belongs to the reciprocal lattice, which would be here $\mathbb{Z} + \theta\mathbb{Z}$.

If now θ is irrationnal, the same kind of results occurs : the eventual gaps appears only if $\mathcal{N}(E) \in \mathbb{Z} + \theta\mathbb{Z} \cap [0,1]$. This result could be heuristically obtained by a perturbative argument following the line of the periodic situation. In the continuous analog of this model, the set $\mathbb{Z} + \theta\mathbb{Z}$ is the frequency module of V , i.e. the group of frequencies in $\mathbb{R}$ appearing in the Fourier expansion of V . Then, the perturbative arguments can be sharpened to prove this results [6]. In [3] it has been related to the K-theory of the C*-algebra attached to $H = (H_x)_{x \in \mathbb{T}}$. In the example I.1 this C*-algebra is $\mathcal{A}_\theta$ first described in [8], and for which it has been proven that [4,7]

$$K_0(\mathcal{A}_\theta) = \mathbb{Z} + \theta\mathbb{Z} \tag{1.3}$$

If now we replace V by a function on $\mathbb{T}$ which has some points of discontinuity the K-theory is no longer equal to $\mathbb{Z} + \theta\mathbb{Z}$, because the hamiltonian I.1 does belong to $\mathcal{A}_\theta$. In this paper we illustrate this fact by the case

$$V(x) = \lambda \, \chi_{]-\theta',0]}(x) \qquad \lambda > 0, \; x \in \mathbb{T} \tag{1.4}$$

where χ_I denotes the characteristic function of I , and θ'

satifies

R.I.) $1, \theta, \theta'$, are rationnally independent numbers, satisfying

$$0 < \theta - \varepsilon < \theta' < \theta < 1$$

for a small enough ε (section II).

<u>Theorem 1</u>

The density of states for the almost periodic operator on $\ell^2(\mathbb{Z})$

$$H_x \psi(n) = \psi(n+1) + \psi(n-1) + \lambda \chi_{]-\theta',0]}(x - n\theta)\, \psi(n) \qquad (1.5)$$

where θ, θ' satisfy R.I., admits steps at the values $m + n\theta + p\theta'$ $m, n, p \in \mathbb{Z}$, where $p \neq 0$ provided λ is big enough.

The proof of this theorem will be done by hand without reference to the C*-algebraic approach. The Section II is devoted to some facts on number theory ; the Section III concerns the proof of the theorem.

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II. CODING $\mathbb{T}$ BY AN IRRATIONNAL ROTATION

We need first to recall some well known facts about the continued fraction expansion of an irrationnal number [5].

Let θ be an irrationnal number in $]0,1[$. We then define a_1 by

$$a_1 = [1/\theta_1] \tag{II.1}$$

where $[x]$ denotes the biggest integer dominated by x . We put

$$\theta_1 = \theta^{-1} - a_1 \tag{II.2}$$

and we can define recursively $a_2, \theta_2, \dots$

Now we precise the assumption R.I. .

R.I.) $1, \theta, \theta'$ are rationnaly independent and

$$\theta - \theta\theta_1\theta_2 < \theta' < \theta \tag{II.3}$$

In what follows we shall denote $[a,b[$ the set of points of $\mathbb{T} = \mathbb{R}/\mathbb{Z} = S_1$, between a and b when we run along the circle in the anticlockwise direction.

Lemma II.1

Let x be a point in $[0,\theta'[$, then smallest integer $\ell(x) \neq 0$ such that $x + \ell\theta$ belongs to $[0,\theta'[$ is :

1) $\ell(x) = a_1 + 1 = \ell_1$ if $x \in I_1 = [0, \theta\theta_1 - \theta + \theta'[$

2) $\ell(x) = 2a_1 + 1 = \ell_2$ if $x \in I_2 = [\theta\theta_1 - \theta + \theta', \theta\theta_1[$

3) $\ell(x) = a_1 = \ell_3$ if $x \in I_3 = [\theta\theta_1, \theta'[$

Proof : 1) Let us assume $x \in I_1$. Since $\theta > \theta'$ we get $x + \ell\theta \notin [0,\theta'[$ as far as $1 \leq \ell \leq a_1$, for $0 < \ell\theta \leq a_1\theta < 1$ and

$$x + \ell\theta \leq \theta\theta_1 - (\theta - \theta') + a_1\theta \leq 1 - (\theta - \theta') < 1 \tag{II.4}$$

due to

$$a_1\theta + \theta\theta_1 = 1 \tag{II.5}$$

Since (everything is given modulo 1)

$$0 < (a_1+1)\theta \leq x + a_1\theta + \theta < \theta - \theta\theta_1 + \theta\theta_1 - \theta + \theta' = \theta' \tag{II.6}$$

which proves

$$\ell(x) = a_1 + 1 \tag{II.7}$$

2) If $x \in I_2$, we get in much the same way for $1 \leq \ell \leq a_1$ since $x < \theta\theta_1$,

$$0 < x + \ell\theta < \theta\theta_1 + a_1\theta = 1 \tag{II.8}$$

Thus $\ell(x) \geq a_1 + 1$. However since $x \in I_2$

$$\theta' = \theta\theta_1 - \theta + \theta' + (a_1+1)\theta - 1 \leq x + (a_1+1)\theta - 1 < \theta \tag{II.9}$$

Therefore $\ell(x) \neq a_1 + 1$. In order to come back to the interval $[0,\theta'[$ we need to turn again of $a_1\theta$ at least. For if $a_1+1 \leq \ell \leq 2a_1$ we get

$$x + \ell\theta - 1 < (\ell - a_1)\theta \leq a_1\theta < 1 \tag{II.10}$$

On the other hand, for $\ell = 2a_1 + 1$, we obtain

$$0 < \theta' - \theta\theta_1 \leq x + (2a_1+1)\theta - 2 < \theta + a_1\theta - 1 < \theta' \tag{II.11}$$

thus

$$\ell(x) = 2a_1 + 1 \tag{II.12}$$

3) At last if $x \in I_3$ and $0 \leq \ell \leq a_1 - 1$

$$\theta\theta_1 \leq x + \ell\theta < \theta' + (a_1-1)\theta = \theta' - \theta + 1 - \theta\theta_1 < 1 \tag{II.13}$$

whereas

$$0 \leq x + a_1\theta - 1 < \theta' - \theta\theta_1 < \theta' \tag{II.14}$$

Thus

$$\ell(x) = a_1. \tag{II.15}$$

Definition II.2

Let A be a subset of $\mathbb{Z}$. The density of A is the number (if it exists)

$$d(A) = \lim_{N\to\infty} (2N+1)^{-1} \operatorname{card}\left(A \cap [-N,N]\right)$$

We get the following result.

Lemma II.3

Let I be an interval of $\mathbb{T}$ and θ be irrationnal in $]0,1[$.
If

$$N(I) = \left\{ m \in \mathbb{Z} ; \quad m\theta \ (\mathrm{mod}\ 1) \in I \right\} \tag{II.16}$$

the density of $N(I)$ exists and is given by

$$d(N(I)) = |I| \qquad \text{(II.17)}$$

(where $|\cdot|$ denotes the Lebesgue measure).

Proof : We define by ℓ the Lebesgue measure on $\mathbb{T}$, by ℓ_N the probability measure

$$\ell_N(f) = (2N+1)^{-1} \sum_{m=-N}^{N} f(m\theta) \qquad f \in \mathcal{C}(\mathbb{T}) \qquad \text{(II.18)}$$

If $f(x) = \exp(2i\pi mx)$, clearly we find by hand that $\ell_N(f) \to \ell(f)$ for $N \to \infty$. Since ℓ_N and ℓ are probability measures, a $3\cdot\varepsilon$ argument shows that this is true for any f in $\mathcal{C}(\mathbb{T})$.

Now we see easily that

$$d(N(I)) = \lim_{N\to\infty} \ell_N(\chi_I) \qquad \text{(II.19)}$$

Since I is an interval there is an increasing sequence $(f_n)_{n\geq 0}$ and a decreasing sequence $(g_n)_{n\geq 0}$ in $\mathcal{C}(\mathbb{T})$ such that

$$\sup_n f_n(x) = \chi_I(x) = \inf_n g_n(x) \qquad x \notin \partial I \qquad \text{(II.20)}$$

This implies

$$\ell(f_n) \leq \liminf_{N\to\infty} \ell_N(\chi_I) \leq \limsup_{N\to\infty} \ell_N(\chi_I) \leq \ell(g_n) \qquad \text{(II.21)}$$

Taking the supremum of the l.h.s. and the infimum of the r.h.s., the dominated convergence theorem shows that the limit in (II.19) exists and is equal to $\ell(\chi_I) = |I|$.

An immediate consequence is :

Corollary II.4

For $x \in T$ we put $N_i(x) = \{m \in \mathbb{Z} ; m\theta - x \in I_i\}$. Then

i) $d(N_i(x)) = |I_i|$

ii) $\sum_{i=1,2,3} d(N_i(x)) = \theta'$

Corollary II.5

If $L_i(x) = \{ \ell \in \mathbb{Z} ; \exists m \in N_i(x) \quad , m < \ell < \hat{m} \}$, where $\hat{m}$ denotes the smallest integer such that $m < \hat{m}$ and $\hat{m}\theta - x \in [0, \theta'[$, then :

i) $d(L_i(x)) = (\ell_i - 1)\ |I_i|$

ii) $\sum_{i=1,2,3} d(L_i(x)) = 1 - \theta'$

Proof- : By Lemma II.1, if $m \in N_i(x)$ then $\hat{m} - m = \ell_i$. Thus for each $m \in N_i(x)$ there are $\ell_i - 1$ points in $L_i(x)$ which proves that

$$d(L_i(x)) = (\ell_i - 1)\ d(N_i(x)) = (\ell_i - 1)|I_i| \tag{II.21}$$

ii) follows from the fact that $(L_i(x))_{i=1,2,3}$ is a partition of $\mathbb{Z} - \bigcup_{i=1,2,3} N_i(x)$, and of the Corollary II.4, ii).

III. COMPUTING THE DENSITY OF STATES

We come back now to the random operator $H(\lambda) = (H_x(\lambda))_{x\in T}$ defined by eq.(1.5). We see easily that $H_x(\lambda) \geq -2\mathbb{1}$. We claim that $H(\lambda)$ converges in the norm resolvent sense if $\lambda \uparrow \infty$. For :

Lemma III.1

Let H be a positive bounded operator on the Hilbert space $\mathcal{H}$ and P be a projection. Then

i) $\mathcal{R}(\infty) = \lim_{\lambda\uparrow\infty} (H + \mathbb{1} + \lambda P)^{-1}$ exists in the norm sense.

ii) $\| \mathcal{R}(\infty) - (H + \mathbb{1} + \lambda P)^{-1} \| \leq \lambda^{-1} (1 + \|H + \mathbb{1}\|)^2$

iii) $\mathcal{R}(\infty) P = P \mathcal{R}(\infty) = 0$ and the restriction of $\mathcal{R}(\infty)$ to the subspace $(P\mathcal{H})^\perp$ is $((\mathbb{1}-P)H(\mathbb{1}-P) + \mathbb{1})^{-1}$

Proof : We denote by $\mathcal{R}(\lambda)$ the operator $(H + \mathbb{1} + \lambda P)^{-1}$. Then $\mathcal{R}(\lambda)$ is decreasing in λ. If $\lambda' > \lambda$ we have

$$\|\mathcal{R}(\lambda) - \mathcal{R}(\lambda')\| \leq \int_\lambda^{\lambda'} d\sigma \; \|\mathcal{R}(\sigma) P \mathcal{R}(\sigma)\| \leq \int_0^{1/\lambda} dx \; \left\|\frac{P}{x} \mathcal{R}\left(\frac{1}{x}\right)\right\|^2 \qquad \text{(III.1)}$$

But we have, since $\mathcal{R}(\lambda) \leq \mathbb{1}$,

$$\left\|\frac{P}{x} \mathcal{R}(x^{-1})\right\| = \|(Px^{-1} + H + \mathbb{1})\mathcal{R}(x^{-1}) - (H + \mathbb{1})\mathcal{R}(x^{-1})\| \leq 1 + \|H + \mathbb{1}\| \qquad \text{(III.2)}$$

This gives i) and ii).

From (III.2), if $x \to 0$, we get

$$P\mathcal{R}(\infty) = \mathcal{R}(\infty) P = 0 \Rightarrow \mathcal{R}(\infty) = (\mathbb{1} - P)\mathcal{R}(\infty)(\mathbb{1} - P) \qquad \text{(III.3)}$$

Now let φ belongs to $\mathcal{H}_\gamma$; then for any $\lambda \geq 0$:

$$(\mathbb{1}-P)\varphi = R(\lambda)[H+\mathbb{1}+\lambda P](\mathbb{1}-P)\varphi = R(\lambda)(H+\mathbb{1})(\mathbb{1}-P)\varphi \tag{III.4}$$

If $\lambda \to \infty$ we get together with (III.3)

$$(\mathbb{1}-P)\varphi = R(\infty)(\mathbb{1}-P)[H+\mathbb{1}](\mathbb{1}-P)\varphi \tag{III.5}$$

which is the end of the Lemma.

If now H is replaced by $\Delta = H_o + 2$, with

$$H_o \psi(n) = \psi(n+1) + \psi(n-1) \tag{III.6}$$

and P by $\chi_{[0,\theta'[}(n\theta - x)$ we get

<u>Corollary III.2</u>

If $\lambda \uparrow \infty$, $H_x(\lambda)$ converges in the norm resolvent sense to the Laplace operator $\Delta^D - 2 = H_x^D$ with Dirichlet boundary condition on

$$\mathcal{N}(x) = \{ m \in \mathbb{Z} ; m\theta - x \in [0,\theta'[\} .$$

The spectrum of H_x^D is very simple, due to:

<u>Lemma III.3</u>

i) The restriction of H_x^D to $\ell^2(\mathbb{Z} - \mathcal{N}(x))$ splits into

$$H_x^D = \bigoplus_{m \in \mathcal{N}(x)} H^D_{]m,\hat{m}[} \tag{III.8}$$

where $H^D_{]a,b[}$ is the Laplace operator $\Delta - 2$ on the interval $[a,b]$ with zero boundary conditions at $\{a\}$ and $\{b\}$.

2) $H^D_{]m,\hat{m}[}$ is unitarily equivalent to $H^D_{]0,\ell_i[}$ if $m \in N_i(x)$.

3) The spectrum of H_x^D (restricted to $\ell^2(\mathbb{Z}-N(x))$) is

$$S(\infty)=\bigcup_{i=1,2,3}\left\{2\cos(k\pi\,\ell_i^{-1});\ k=1,2,\dots,\ell_i-1\right\} \qquad \text{(III.9)}$$

<u>Proof</u> : 1) follows from the fact that $\mathbb{Z}-N(x)$ is partitionned into $\bigcup_{m\in N(x)}]m,\hat{m}[$, since by Lemma III.1, $R(\infty)$ leaves $\ell^2(\mathbb{Z}-N(x))$ invariant and that the Laplace operator has only nearest neighbours interaction, we get the decomposition (III.8).

2) is elementary.

3) comes from the explicit calculation of the spectrum of $H^D_{]a,b[}$:

$$\sigma(H^D_{]a,b[})=\left\{2\cos\left(k\pi(b-a)^{-1}\right)\ ;\ k=1,2,\dots,b-a-1\right\}. \qquad \text{(III.10)}$$

We define now

$$n_i(E)=\text{card}\left\{k\in[1,\ell_i-1]_{\mathbb{N}}\ ;\ 2\cos(k\pi\,\ell_i^{-1})<E\right\} \qquad \text{(III.11)}$$

The reduced density of states for H_x^D will be

$$n_\infty(E)=\lim_{N\to\infty}(2N+1)^{-1}\ \text{card}\left\{\text{eigenvalue } H_x^D\restriction_{\ell^2([\mathbb{Z}-N(x)]\cap[-N,N])}\leq E\right\} \qquad \text{(III.12)}$$

The reduced density of state consists formally in taking the density of states of H_x^D when we extend it on $\ell^2(N(x))$ by the operator "equal" to $+\infty$.

<u>Proposition III.4</u>

The reduced density of states is given by

$$\left\{\begin{array}{l} \mathcal{N}_\infty(E) = n_1(E)\left(1+\theta' - (a_1+1)\theta\right) + n_2(E)(\theta-\theta') + n_3(E)\left(\theta' - 1 + a_1\theta\right) \\ \text{and} \qquad 0 \leq \mathcal{N}_\infty(E) \leq 1-\theta' \end{array}\right. \tag{III.13}$$

Proof : Instead of picking the interval $[-N,N]$ in (III.12), we can pick any interval of the form $[m,m']$ with $m,m' \in N(x)$ and $m'-m \to +\infty$. Then, the number of eigenvalues of $H^D \upharpoonright \ell^2(\mathbb{Z} - N(x) \cap [m,m'])$ smaller than E, is equal to the number of such eigenvalues for $\bigoplus_{\substack{m \leq m'' < m' \\ m'' \in N(x)}} H^D_{]m'',\hat{m}''[}$, which is equal to

$$\sum_{i=1,2,3} n_i(E)\, d_i \tag{III.14}$$

where $(d_i)_{i=1,2,3}$ counts the number of time an m'' belonging to $N_i(x)$ occurs in $[m,m'] \cap N(x)$. If $m'-m \to \infty$ the ratio $d_i(m'-m)^{-1}$ converges to the density of $N(x)$. By Corollary II.4, and Lemma II.1, one can easily compute this density which gives (III.13) if we take into account the identity

$$\theta\theta_1 = 1 - a_1\theta \tag{III.15}$$

Proof of Theorem I : We denote by r the smallest distance between two eigenvalues of $\mathcal{R}(\infty) = \lim_{\lambda\uparrow\infty} (H_\lambda(\lambda)+3)^{-1}$.

By Lemma III.3, we get

$$r = \operatorname{Inf}\left\{ \left|(E_1+3)^{-1} - (E_2+3)^{-1}\right| ;\ E_1, E_2 \in S(\infty) \cup \{\infty\} \right\} \tag{III.16}$$

because $\{0\}$ is an eigenvalue of $\mathcal{R}(\infty)$. We recall that

$$0 \leq \Delta \leq 4 \tag{III.17}$$

Thus, due to the Lemma III.1, with $H = \Delta$, and $P = \chi_{[0,\theta'[}(n\theta - x)$ we get

$$\| (H_2(\lambda) + 3)^{-1} - R(\infty) \| \leq 36\, \lambda^{-1} \tag{III.18}$$

If we define λ_0 such that $36\lambda_0^{-1} = r/4$, the spectrum of $R(\lambda)$ for $\lambda \geq \lambda_0$ is certainly contained into the disconnected intervals $[\gamma_i - \frac{r}{4}, \gamma_i + \frac{r}{4}]$ where γ_i belongs to the eigenvalues of $R(\infty)$. This choice of λ_0 says that each of these intervals is disconnected from each other. The number of them is equal to

$$l_1 - 1 + l_2 - 1 + l_3 - 1 + 1 = 4a_1 \tag{III.19}$$

due to the eigenvalue $\{0\}$ for $R(\infty)$.

This implies the existence of $4a_1$ disconnected interval containing the spectrum of $H_2(\lambda)$. Among them $4a_1 - 1$ are closed to the points of $S(\infty)$. The last one is at a distance bigger than $\lambda/36 - 3$. Since the norm of $H_2(\lambda)$ is dominated by $\lambda + 2$, it is certainly contained in $[\lambda/36 - 3, \lambda + 2]$. Thus, there is a sequence $(E^{(1)}_{4a_1} = \lambda/36 - 3)$

$$E_i^1(\lambda) < E_i^2(\lambda) < E_{i+1}^1(\lambda) \qquad i = 1, \dots, 4a_1 - 1 \tag{III.20}$$

such that

$$\sigma(H_2(\lambda)) \subset \bigcup_{i=1}^{4a_1-1} [E_i^1(\lambda), E_i^2(\lambda)] \cup [\lambda/36 - 3, \lambda + 2] = S(\lambda) \tag{III.21}$$

Now if $E \notin S(\lambda)$ the density of states $\mathcal{N}_\lambda(E)$ of $H_2(\lambda)$ is locally constant and independent of $\lambda \geq \lambda_0$ (see, [3]) ; therefore it is given by the Proposition III.4, which is precisely of the form

$$\mathcal{N}_\lambda(E) = m + n\theta + p\theta' \qquad m, n, p \in \mathbb{Z} \tag{III.22}$$

In order to prove that the last term is effectively present, we remark that if

$$E^{1}_{4a_1-1} < E < \lambda/36-3 \tag{III.23}$$

then

$$\mathcal{N}_{\lambda}(E) = 1-\theta' \tag{III.24}$$

due to the Proposition III.4 .

REMARKS

1) The other part of the spectrum of $H_{x}(\lambda)$ have not been investigated here. A nowhere dense spectrum is expected. If $\lambda \neq \infty$ it is true that $H_{x}(\lambda)$ have no eigenvalue of infinite multiplicity. Thus $E \mapsto \mathcal{N}_{\lambda}(E)$ is a continuous increasing function.

2) From heuristic arguments this Schrödinger operator is expected to have a pure point spectrum as far as $\lambda > 0$ [10], at least if θ and θ' are chosen in a right way (for instance they have good diophantine properties).

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[10] of us (J.B.) is indebted to S. Aubry for giving him this information.