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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 operator with 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].

Introduction

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

Among these progresses, the integrated density of states $\mathfrak{N}(E)$ 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 canonically associated von Neumann algebra [2]. If the energy belongs to the resolvent set, where $\mathfrak{N}(E)$ 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 from the quasi periodic hamiltonian.

In the case of a one-dimensional Schrödinger operator with an almost periodic potential V, this group coïncides with the frequency module of V [6, 3]. In this short note, we exhibit an example of a 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 $\mathfrak{N}(E)$ at the steps are really not in the frequency module.

To be precise we deal with a 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 $V\in\mathscr{C}(\mathbb{T})$ and θ is an irrational number. The spectral density in this case is defined by

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

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It has been proven that $\mathfrak{N}(E)$ 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 rational, H would be periodic, and $k = \mathfrak{N}(E)$ could be interpreted as the Bloch wave vector, whereas $E = \mathfrak{N}^{-1}(k)$ 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 occur eventually if k belongs to the reciprocal lattice, which would be here $\mathbb{Z} + \theta\mathbb{Z}$.

If now θ is irrational, the same kind of results occurs: the eventual gaps appear only if $\mathfrak{N}(E) \in \mathbb{Z} + \theta\mathbb{Z} \cap [0, 1]$. 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 these 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 $\mathfrak{A}_\theta$ first described in [8], and for which it has been proven that [4, 7]

$$K_0(\mathfrak{A}_\theta) = \mathbb{Z} + \theta\mathbb{Z}. \tag{I.3}$$

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 not belong to $\mathfrak{A}_\theta$. In this paper we illustrate this fact by the case

$$V(x) = \lambda \chi_{]-\theta', 0]}(x), \qquad \lambda > 0, \qquad x \in \mathbb{T}, \tag{I.4}$$

where χ_I denotes the characteristic function of I, and θ' satisfies the condition of rational independence (R.I.):

1, θ, θ', are rationally independent numbers, satisfying

$$0 < \theta - \varepsilon < \theta' < \theta < 1 \tag{R.I.}$$

for a small enough ε (Sect. II).

Theorem I. *Let θ, θ' satisfy* R.I., *there exists a constant $\lambda_0 > 0$, depending on θ, such that if $\lambda > \lambda_0$, then the density of states $\mathfrak{N}(E)$ of the almost periodic operator on $\ell^2(\mathbb{Z})$*

$$H_x \psi(n) = \psi(n+1) + \psi(n-1) + \lambda \chi_{]-\theta', 0]}(x - n\theta)\psi(n) \tag{I.5}$$

admits steps for which it takes values of the form $m + n\theta + p\theta'$ with $p \neq 0$.

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

II. Coding $\mathbb{T}$ by an Irrational Rotation

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

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

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

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 $a_2, \theta_2, \ldots$.

Now we make the assumption R.I. precise

1, θ, θ' are rationally independent and

$$\theta - \theta\theta_1\theta_2 < \theta' < \theta. \qquad \text{(R.I.)} \tag{II.3}$$

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 $[0, \theta'[$. The 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 $1 \leqq \ell \leqq a_1$; for $0 < \ell\theta \leqq a_1\theta < 1$ and

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

due to

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

Since (everything is given modulo 1)

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

which proves

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

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

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

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

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

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

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

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

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

thus

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

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

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

whereas

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

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)

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

We get the following result:

Lemma II.3 (H. Weyl) [11]. *Let I be an interval of $\mathbb{T}$ and θ be irrational in $]0,1[$. If*

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

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

$$d(N(I)) = |I|, \tag{II.17}$$

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

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 $L_i(x) = \{\ell \in \mathbb{Z}; \exists m \in N_i(x), m < \ell < \hat{m}\}$, 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

$$d(L_i(x)) = (\ell_i - 1)\, d(N_i(x)) = (\ell_i - 1)|I_i|; \tag{II.18}$$

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 Corollary II.4, ii).

III. Computing the Density of States

We come back now to the random operator $H(\lambda) = (H_x(\lambda))_{x \in \mathbb{T}}$ defined by Eq. (I.5). We see easily that $H_x(\lambda) \geqq -2\mathbb{1}$. 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 $\mathscr{H}$ and P be a projection. Then*

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

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

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

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

$$\|R(\lambda)-R(\lambda')\|\leqq\int_{\lambda}^{\lambda'}d\sigma\|R(\sigma)PR(\sigma)\|\leqq\int_{0}^{1/\lambda}dx\left\|\frac{P}{x}R\left(\frac{1}{x}\right)\right\|^2. \tag{III.1}$$

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

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

This gives i) and ii).

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

$$PR(\infty)=R(\infty)P=0\ \Rightarrow\ R(\infty)=(\mathbb{1}-P)R(\infty)(\mathbb{1}-P). \tag{III.3}$$

Now let φ belong to $\mathscr{H}$; then for any $\lambda\geqq 0$:

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

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.

Now if H is replaced by $\Delta=H_0+2$, with

$$H_0\psi(n)=\psi(n+1)+\psi(n-1), \tag{III.6}$$

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

Corollary III.2. *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*

$$N(x)=\{m\in\mathbb{Z};m\theta-x\in[0,\theta'[\}. \tag{III.7}$$

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

Lemma III.3. 1) *The restriction of H_x^D to $\ell^2(\mathbb{Z}-N(x))$ splits into*

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

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*

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

Proof. 1) follows from the fact that $\mathbb{Z}-N(x)$ is partitioned 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 $H^D_{]a,b[}$:

$$\sigma(H^D_{]a,b[})=\{2\cos(k\pi(b-a)^{-1});\, k=1,2,\ldots,b-a-1\}. \tag{III.10}$$

We define now

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

The reduced density of states for H^D_x will be

$$\mathfrak{N}_\infty(E)=\lim_{N\to\infty}(2N+1)^{-1}\operatorname{card}\{\text{eigenvalues } H^D_x\restriction_{\ell^2[\mathbb{Z}-N(x)\cap(-N+N))}<E\}. \tag{III.12}$$

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

Proposition III.4. *The reduced density of states is given by*

$$\mathfrak{N}_\infty(E)=n_1(E)(1+\theta'-(a_1+1)\theta)+n_2(E)(\theta-\theta')+n_3(E)(\theta'-1+a_1\theta),$$

and

$$0\leqq\mathfrak{N}_\infty(E)\leqq 1-\theta'. \tag{III.13}$$

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 $H^D\restriction_{\ell^2(\mathbb{Z}-N(x)\cap[m,m'])}$ smaller than E, is equal to the number of such eigenvalues for $\bigoplus_{\substack{m\leqq m''<m\\ m''\in N(x)}} H^D_{]m'',\hat{m}''[}$, 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 times 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 $R(\infty)=\lim_{\lambda\uparrow\infty}(H_x(\lambda)+3)^{-1}$. By Lemma III.3, we get

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

because $\{0\}$ is an eigenvalue of $R(\infty)$. By III.9 it is not difficult to find that

$$r>2/25\sin^2\left(\frac{\pi}{2}/(a_1+1)(2a_1+1)\right)=r_m. \tag{III.16b}$$

We recall that

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

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

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

If λ_0 is given by $36\lambda_0^{-1}=r_m/4$, which means $\lambda_0=1800\{\sin\pi[2(a_1+1)\cdot(2a_1+1)]^{-1}\}^{-2}$ the spectrum of $R(\lambda)$ for $\lambda\geqq\lambda_0$ is certainly contained into the disconnected intervals $[z_i-r/4, z_i+r/4]$ where z_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

$$\ell_1-1+\ell_2-1+\ell_3-1+1=4a_1 \tag{III.19}$$

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

This implies the existence of $4a_1$ disconnected intervals containing the spectrum of $H_x(\lambda)$. 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 $H_x(\lambda)$ is dominated by $\lambda+2$, it is certainly contained in $[\lambda/36-3,\lambda+2]$. Thus, there is a sequence $(E_{4a_1}^{(1)}=\lambda/36-3)$

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

such that

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

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

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

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

$$E_{4a_1-1}^2<E<\lambda/36-3, \tag{III.23}$$

then

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

due to the Proposition III.4.

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

2) From heuristic considerations about the maximal length of an interval in which the perturbation theory applies, Aubry finds that the eigenfunctions of $H_x(\lambda)$ should decrease exponentially with a Liapounov exponent of the order $\exp-4\pi/\lambda$ as far as $\lambda>0$ [10]. If the argument holds, the spectrum is expected to be pure point at any λ, at least for most values of θ and θ'.

3) The family $H(\lambda)=(H_x(\lambda))_{x\in\mathbb{T}}$ belongs to the C^*-algebra $\mathfrak{A}_{\theta,\theta'}$ of operators generated by U, the translation by 1, and the multiplication by $\chi_{I'}(x-n\theta)$ on $\ell^2\mathbb{Z}$. All these operators have the form $A=(A_x)_{x\in\mathbb{T}}$ with $x\mapsto A_x$ norm-measurable and

$$UA_xU^{-1}=A_{x+\theta}.$$

Thus $\frac{1}{2N+1}\sum_{n=-N}^{N}\langle n|A_x|n\rangle$ converges, as $N\to\infty$ to

$$T(A)=\int_{\mathbb{T}} dx\langle 0|A_x|0\rangle\,.$$

This is a trace on $\mathfrak{A}_{\theta\theta'}$.

Let $\mathfrak{M}_{\theta\theta'}$ be the von Neumann algebra of the GNS representation of $\mathfrak{A}_{\theta\theta'}$ given by this trace, and let $P_\lambda(E)$ be the eigenprojection (in $\mathfrak{M}_{\theta\theta'}$) of $H(\lambda)$ on the energies less than E. Then in [3] we prove that

$$\mathfrak{N}_\lambda(E)=T(P_\lambda(E))\,.$$

If $E\notin \mathrm{Sp}\,H(\lambda)$, $P_\lambda(E)$ belongs in fact to $\mathfrak{A}_{\theta\theta'}$ and since $H(\lambda)$ is norm continuous with respect to λ, $P_\lambda(E)$ is norm continuous in λ, and therefore its trace is constant [12] as long as E does not meet the spectrum of $H(\lambda)$.

4) If χ_I is approximated by a sequence V_n of continuous functions, Theorem 1 is no longer true. At first sight this seems surprising. Actually, the density of states $\mathfrak{N}^{(n)}$ is a continuous increasing function of E, and as $n\to\infty$ it approaches uniformly the limit even though no steps at the values $m+n\theta+p\theta'$ $(p\neq 0)$ occur. There is no contradiction.

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