Dynamical upper bounds in quantum mechanics

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Let H be a discrete self-adjoint Schrödinger operator on separable Hilbert space $l^2(\mathbb{Z})$ into himself.

$$[H\psi](n) = \psi(n+1) + \psi(n-1) + V(n)\psi(n)$$

V is a function $\mathbb{Z} \to \mathbb{R}$, the so-called potential.

In this work, we consider only Sturmian potential :

$$V(n) = (\lfloor (n+1)\beta \rfloor - \lfloor n\beta \rfloor) V$$

V is a positive constant called strength of potential or couplage. β is an irrationnal number.

Link to physics : Modeling electron/phonon spectrum in a quasicrystal.

Only 2 values possible for the potential.

Quasiperiodical potential : no period but any sequence repeats infinitly many times

Potential construction :

By graphic means : line with β slope, iterated rotation by angle β.

By word concatenation : The potential coincide with sturmian words,

$$W_{-1} = V$$

$$W_0 = 0$$

$$W_{k+1} = W_k^{a_{k+1}} W_{k-1}, \quad k \geq 0.$$

Unitary dynamical evolution :

$$\psi(t) = e^{-itH}\psi(0).$$

In this case, ψ is known to spread out with time over the canonical basis of $l^2(\mathbb{Z})$.

Dynamical field consist to quantify how fast it spreads.

The probability for the system to be in n over the time T (in average) :

$$a(n, T) = \frac{2}{T}\int_0^{\infty} e^{-2t/T} |\langle e^{-itH}\psi(0), \delta_n\rangle|^2 dt.$$

We denote the time average outside probabilities

$$P(N, T) = \sum_{|n|>N} a(n, T),$$

For $p > 0$, one defines moments of order p

$$\langle |X|^p_{\psi(0)} \rangle = \sum_n |n|^p a(n, T),$$

And their growth exponents :

$$\beta^-_{\psi(0)}(p) = \liminf_{T\to\infty} \frac{\log \langle |X|^p_{\psi(0)} \rangle}{p \log T}$$

$$\beta^+_{\psi(0)}(p) = \limsup_{T\to\infty} \frac{\log \langle |X|^p_{\psi(0)} \rangle}{p \log T}.$$

For all $\alpha \in [0, +\infty]$,

$$S^{-}(\alpha) = -\liminf_{T\to\infty} \frac{\log P(T^{\alpha} - 2, T)}{\log T}$$

and

$$S^{+}(\alpha) = -\limsup_{T\to\infty} \frac{\log P(T^{\alpha} - 2, T)}{\log T}$$

The following critical exponents are particular of interest :

$$\alpha_l^{\pm} = \sup\{\alpha \geq 0 : S^{\pm}(\alpha) = 0\},$$

$$\alpha_u^{\pm} = \sup\{\alpha \geq 0 : S^{\pm}(\alpha) < \infty\}.$$

$\alpha_l^\pm$ is the (lower and upper) rates of propagation of the essential part of the wavepacket and $\alpha_u^\pm$ as the rates of propagation of the fastest part.
In particular, if $\gamma > \alpha_u^+$ then $P(T^\gamma, T)$ goes to 0 faster than any inverse power of T.

They verify $0 \leq \alpha_l^\pm \leq \alpha_u^\pm$.

$$\lim_{p \to 0} \beta_\psi^\pm(p) = \alpha_l^\pm$$

$$\lim_{p \to \infty} \beta_\psi^\pm(p) = \alpha_u^\pm.$$

(B. Simon) For this model,

$$\alpha_u^{\pm} \leq 1.$$

Until 2005, it was an open question, if one can improve this so-called balistic bound.

In this work, we improve upper bounds for the fast part of the wavepacket under assumption on the irrational number.

$$q_{-1} = 0, q_0 = 1,$$

$$q_{k+1} = a_{k+1} q_k + q_{k-1}$$

Let β be an irrational number and H_β with a sturmian potential associated to β. $V > 20$. If $D = \limsup_k \frac{\log q_k}{k}$ is finite then

$$\alpha_u^+ \leq \frac{2D}{\log\left(\frac{V-8}{3}\right)}.$$

$$\psi(n+1)+\psi(n-1)+V(n)\psi(n)=z\psi(n) \tag{1}$$

with $z \in \mathbb{C}$ and ψ a non-zero vector.

One can reformulate this in terms of transfer matrix.

$$\begin{pmatrix}\psi(n+1)\\ \psi(n)\end{pmatrix} = F(n,z)\begin{pmatrix}\psi(1)\\ \psi(0)\end{pmatrix}$$

$$F(n,z)=\begin{cases} T(n,z)\dots T(1,z) & n\geq 1,\\ Id & n=0,\\ [T(n,z)]^{-1}\dots.[T(0,z)]^{-1} & n\leq -1.\end{cases}$$

$$T(m,z)=\begin{pmatrix} z-V(m) & -1\\ 1 & 0\end{pmatrix}$$

The transfer matrix play a key role in all the theory.

Of course, in eigenvalue/vector study, and spectrum study.

But also in dynamical field, with this estimate : (Damanik, Tcheremtchansev)

$$P(N,T) \lesssim \exp(-cN) + T^3 \int_{-K}^{K} \left(\max_{1 \leq k \leq N} \left\| F(k, E + \frac{i}{T}) \right\|^2 \right)^{-1} dE,$$

$$p_{-1} = 1, p_0 = 0,$$

$$q_{-1} = 0, q_0 = 1,$$

$$p_{k+1} = a_{k+1} p_k + p_{k-1}$$

$$q_{k+1} = a_{k+1} q_k + q_{k-1}$$

We denote

$$M_k(z) = F(q_k, z)$$

$$M_{k+1}(z) = M_{k-1}(z) M_k(z)^{a_{k+1}}$$

Let $t_{k,p}$ be the trace of the matrix $M_{k-1}M_k^p$. The evolution along the p index is given by

$$t_{k,p+1} = t_{k+1,0}t_{k,p} - t_{k,p-1},$$

and consequently,

$$t_{k,p+1} = S_p(t_{k+1,0})t_{k,1} - S_{p-1}(t_{k+1,0})t_{k,0}$$

S_p denotes the p^{th} Tchebychev polynomial of the second kind

The evolution along the k index is related to the p-evolution by

$$t_{k+1,0} = t_{k,a_{k+1}},$$

The behavior of the sequence of trace $t_{k,0}$ is interesting in dynamics but also for the spectrum of the operator H.

$$\sigma = \{E \in \mathbb{R}, s.t. \{t_{k,0}(E)\}_k bounded\}$$

We can be more precise and tell with the next criteria when this sequence is bounded or not.

A necessary and sufficient condition that $\{t_{k,0}(E)\}_k$ be unbounded is that

$$|t_{N+1,0}(E)| > 2, |t_{N,0}(E)| > 2, |t_{N-1,0}(E)| \leq 2$$

for some $N \geq 0$. This N is unique. Denote

$$G_k = G_{k-1} + a_k G_{k-2}, G_0 = 1, G_{-1} = 1.$$

We have

$$|t_{k,0}(E)| \geq e^{cG_{k-N}} \quad \forall k > N.$$

Denote $\sigma_{k,p} = \{E \in \mathbb{R}, |t_{k,p}(E)| \leq 2\}$.

(i) the set $\sigma_{k,p}$ is made of $pq_k + q_{k-1}$ distinct intervals,

(ii) the $\sigma_{k,0}$ coincide with the spectrum of periodic operator H_k replacing β with p_k/q_k in definition)

(iii) $\sigma \subset \sigma_{k+1,0} \cup \sigma_{k,0}$

Moreover, σ the spectrum of H verify
$\sigma = \cap_{k=N}^{\infty}(\sigma_{k+1,0} \cup \sigma_{k,0})$

For a given k, we call
type I gap : a band of $\sigma_{k,1}$ included in a band of $\sigma_{k,0}$ and therefore in a gap of $\sigma_{k+1,0}$,
type II band : a band of $\sigma_{k+1,0}$ included in a band of $\sigma_{k,-1}$ and in a gap of $\sigma_{k,0}$,
type III band : a band of $\sigma_{k+1,0}$ included in a band of $\sigma_{k,0}$ and in a gap of $\sigma_{k,1}$.

(Raymond) At a given level k,
(i) a type I gap contains an unique type II band of $\sigma_{k+2,0}$.
(ii) a type II band contains $(a_{k+1} + 1)$ bands of type I of $\sigma_{k+1,1}$. They are alternated with (a_{k+1}) type III bands of $\sigma_{k+2,0}$
(iii) a type III band contains (a_{k+1}) bands of type I of $\sigma_{k+1,1}$. They are alternated with $(a_{k+1} - 1)$ type III bands of $\sigma_{k+2,0}$

(Liu, Wen) Each band length has a lower bound with coefficient of Q_n and an upper bound with coefficient of P_n.

$$P_n = \begin{pmatrix} 0 & c_1^{a_n-1} & 0 \\ c_1/a_n & 0 & c_1/a_n \\ c_1/a_n & 0 & c_1/a_n \end{pmatrix}$$

with $c_1 = \frac{3}{V-8}$

$$Q_n = \begin{pmatrix} 0 & c_2^{a_n-1} & 0 \\ c_2(a_n+2)^{-3} & 0 & c_2(a_n+2)^{-3} \\ c_2(a_n+2)^{-3} & 0 & c_2(a_n+2)^{-3} \end{pmatrix}$$

with $c_2 = \frac{1}{V+5}$.

By now, we define the periodic approximants spectrum not only in $\mathbb{R}$ but in $\mathbb{C}$.

$$\sigma_{k,0} = \{z \in \mathbb{C} : |t_{k,0}(z)| \leq 2\}$$

If $k \geq 3$, and $V > 20$ then there exist constants $c,d > 0$ such that

$$\bigcup_{j=1}^{q_{k-1}} B(x_k^{(j)}, r_k) \subseteq \sigma_{k,0} \subseteq \bigcup_{j=1}^{q_{k-1}} B(x_k^{(j)}, R_k)$$

where $\{x_k^{(j)}\}_{1 \leq j \leq q_{k-1}}$ are the zeros of $t_{k,0}$,
$r_k = c.$ min band length and $R_k = d.$max band length.

As $x_k^{(j)}$ are real, we have

$$\sigma_{k,0} \subseteq \{z \in \mathbb{C} : |Imz| < R_k\} \subseteq \{z \in \mathbb{C} : |Imz| < dq_k^{-\gamma(V)}\}.$$

for a suitable $\gamma(V)$. This implies

$$\sigma \subset \sigma_{k,0} \cup \sigma_{k+1,0} \subseteq \{z \in \mathbb{C} : |Imz| < dq_k^{-\gamma(V)}\}. \qquad (2)$$

We should have $R_k < dq_k^{-\gamma(V)}$ so a suitable γ can be chosen by taking :

$$\gamma(V) \leq \limsup_k -\frac{k \log c_1}{2 \log q_k}.$$

For $T > 1$, denote by $k(T)$ the unique integer with

$$\frac{q_{k(T)-1}^{\gamma(V)}}{d} \leq T \leq \frac{q_{k(T)}^{\gamma(V)}}{d}$$

and let

$$N(T) = q_{k(T)+\lfloor\sqrt{k(T)}\rfloor}.$$

$$N(T) \lesssim C_\nu T^{\frac{1}{\gamma(V)}} T^{\nu}. \quad (3)$$

$$P(N(T), T) \lesssim exp(-cN(T)) + T^3 \int_{-K}^{K} \left(\max_{1 \leq q_n \leq N(T)} \left\| M_n(E \right. \right.$$

$$\lesssim exp(-cN(T)) + T^3 e^{-2cG_{\lfloor \sqrt{k(T)} \rfloor}}$$

From this bound, we see that $P(N(T), T)$ goes to 0 faster than any inverse power of T. As

$$N(T) \lesssim C_\nu T^{\frac{1}{\gamma(V)}} T^{\nu}.$$

we have

$$\alpha_u^+ \leq \frac{1}{\gamma(V)} + \nu$$

Let β be an irrational number and H_β with a sturmian potential associated to β. $V > 20$. If $D = \limsup_k \frac{\log q_k}{k}$ is finite then

$$\alpha_u^+ \leq \frac{2D}{\log\left(\frac{V-8}{3}\right)}.$$

Moreover, for an irrational with continued fraction expansion containing no 1, the dynamical upper bound becomes

$$\alpha_u^+ \leq \frac{D}{\log\left(\frac{V-8}{3}\right)}.$$

It is clear that taking V large enough, one can obtain a non trivial bound that is smaller than 1.
The condition D finite is true for almost all irrational.
Moreover,
(Khintchin) For almost all β with respect to Lebesgue measure,

$$D = \limsup_{k} \frac{\log q_k}{k} = D_K = \frac{\pi^2}{12 \log 2}.$$

There exist an irrational number β with $D = +\infty$ such that for any $V > 20$.

$$\alpha_u^+ = 1.$$

Proof :
Sturmian potentials of operator H_β and H_{β_n} have the same first $p_{n+1} + q_{n+1}$ values.

(Last) Let $H_1 = \Delta + V_1$ and $H_2 = \Delta + V_2$ on $l^2(\mathbb{Z})$, and such that $|V_1(k)|, |V_2(k)| < C$ for all $k \in \mathbb{Z}$ and C a constant. Let $T > 0$ and $\varepsilon > 0$ be fixed so there exist $L(T, \varepsilon), \delta > 0$ such that $|V_1(k) - V_2(k)| < \delta$ for all $|k| < L$, then

$$|\langle |X|^2_{H_1,\psi(0)} \rangle - \langle |X|^2_{H_2,\psi(0)} \rangle| < \varepsilon.$$

As H_{β_n} is a periodic potential operator, one has

$$\langle |X|^2_{\beta_n} \rangle_T > C_n T^2$$

choose T_n big enough such that

$$C_n > \frac{1}{\log T_n}.$$

One can then choose a_{n+1} such that $L(T_n, \varepsilon) \leq p_{n+1} + q_{n+1}$. Inductively, we have a sequence T_n going to infinity and an irrational number β with

$$\langle |X|^2_{\beta} \rangle_{T_n} > \frac{T_n^2}{\log T_n} - \varepsilon > T_n^{2-\delta}, \forall \delta > 0$$

$$\alpha_u^+ \geq \beta^-_{\delta_1}(2) > 1 - \delta, \forall \delta > 0.$$