

# Dynamical Upper Bounds for the Fibonacci Hamiltonian

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(Dated: February 22, 2005)

We consider transport exponents associated with the dynamics of a wavepacket in a discrete one-dimensional quantum system and develop a general method for proving upper bounds for these exponents in terms of the norms of transfer matrices at complex energies. Using this method, we prove such upper bounds for the Fibonacci Hamiltonian. Together with the known lower bounds, this shows that these exponents are strictly between zero and one for sufficiently large coupling and the large coupling behavior follows a law predicted by Abe and Hiramoto.

PACS numbers: 72.10.-d, 72.15.-v

## I. INTRODUCTION

The spreading of a quantum mechanical wavepacket has been the focus of intense research both in the physics and mathematics communities. The free case and, more generally, the case where the spectral measure of the initial state has an absolutely continuous component are well understood. More recently, the case of point spectrum has received a lot of attention and the question whether spectral localization leads to dynamical localization has been answered quite satisfactorily [1]. As a consequence, dynamical localization was shown in most systems for which spectral localization had been established earlier. The most prominent exception to this rule is given by the random dimer model [2], which displays spectral localization and dynamical delocalization and, in fact, super-diffusive transport.

Between these two extreme cases there are a lot of models for which intermediate spectral and dynamical behavior has been observed; for example, Bloch electrons in a magnetic field [3] and one-dimensional quasicrystals [4, 5]. The spreading of a wavepacket in such systems is much less understood. There are a number of works based on heuristics and numerics for the Harper and Fibonacci models devoted to this issue. As a consequence it is expected that transport in the Harper model is almost diffusive and transport in the Fibonacci model is anomalous in the sense that the transport exponents take values other than zero (which would be the case in a dynamically localized system), one-half (diffusive transport), and one (ballistic transport). In fact, these exponents decrease as the coupling constant is increased and their behavior for large values of the coupling constant  $\lambda$  is expected to be of order  $1/\log \lambda$  [6, 7].

For the Harper model, there are no explicit rigorous bounds for the transport exponents. Bellissard et al.

show a lower bound in terms of the multifractal dimensions of the density of states, [8], but they do not have lower bounds for these dimensions. On the other hand, there are some explicit rigorous results for the Fibonacci model. However, they are limited to bounding the transport exponents from below. The question of whether the expected upper bounds, and hence anomalous transport, hold has been open from a rigorous standpoint. In fact, there was no general method for proving upper bounds on transport exponents, and finding such a method (that is applicable to models of interest) is one of the most important problems in this field.

In any event, quantum dynamics for models with singular continuous spectra supported on Cantor sets with critical eigenfunctions is a rich subject and has been studied by many authors, with most papers focusing on the Harper model and the Fibonacci model or generalizations thereof. A nice discussion of “what determines the spreading of a wavepacket,” particularly in these intermediate cases, may be found in [9].

It is the purpose of this Letter to report on rigorous work concerning these issues. We have developed a general approach for proving upper bounds on transport exponents in terms of the norms of transfer matrices. These matrices are the standard tool, in one dimension, to study spectral (and dynamical) properties of a given model. Essentially, it is always the ultimate goal to reduce a problem at hand (such as studying dynamical quantities) to properties of transfer matrices or, which is essentially equivalent, solutions of the associated difference equation. The first rigorous results on lower bounds for transport exponents could only be established after Jitomirskaya and Last had found such a general correspondence [10]. See [10] for the first explicit lower bounds for transport exponents in the Fibonacci model and [11] for the best bounds known to this date. We will describe our general method for proving upper bounds on transport exponents in Theorem 1 below. Secondly, we have applied this method to the Fibonacci model and proved upper bounds on transport exponents that are indeed of order  $1/\log \lambda$  in the large coupling regime. See The-

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orem 2 for the detailed statement. Together with the known lower bounds, this establishes the first rigorous anomalous transport result.

The organizations is as follows: We recall the definitions of the transport exponents and some of the known rigorous lower bounds for them in Section II, describe our general upper bound for these exponents in terms of transfer matrix norms in Section III, and discuss the application of this general result to the case of the Fibonacci model in Section IV.

## II. TRANSPORT EXPONENTS

Consider a discrete one-dimensional Schrödinger operator,

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

on  $\ell^2(\mathbb{Z})$ . A number of recent papers (e.g., [10–17]) were devoted to proving lower bounds on the spreading of an initially localized wavepacket, say  $\psi = \delta_1$ , under the dynamics governed by  $H$ , typically in situations where the spectral measure of  $\delta_1$  with respect to  $H$  is purely singular and sometimes even pure point.

A standard quantity that is considered to measure the spreading of the wavepacket is the following: For  $p > 0$ , define  $\langle |X|_{\delta_1}^p \rangle(T) = \sum_n |n|^p a(n, T)$ , where  $a(n, T) = \frac{2}{T} \int_0^\infty e^{-2t/T} |\langle e^{-itH} \delta_1, \delta_n \rangle|^2 dt$ . Clearly, the faster  $\langle |X|_{\delta_1}^p \rangle(T)$  grows, the faster  $e^{-itH} \delta_1$  spreads out, at least averaged in time. One typically wants to prove power-law bounds on  $\langle |X|_{\delta_1}^p \rangle(T)$  and hence it is natural to define the following quantity: For  $p > 0$ , define the *lower transport exponent*  $\beta_{\delta_1}^-(p)$  by

$$\beta_{\delta_1}^-(p) = \liminf_{T \rightarrow \infty} \frac{\log \langle |X|_{\delta_1}^p \rangle(T)}{p \log T}$$

and the *upper transport exponent*  $\beta_{\delta_1}^+(p)$  by

$$\beta_{\delta_1}^+(p) = \limsup_{T \rightarrow \infty} \frac{\log \langle |X|_{\delta_1}^p \rangle(T)}{p \log T}.$$

Both functions  $\beta_{\delta_1}^\pm(p)$  are non-decreasing. Numerical studies suggest that for some models, they may exhibit non-trivial growth [9, 18, 19]. Such a multiscaling phenomenon was termed *quantum intermittency* by Guarneri and Mantica [18]. For the two main models of interest, numerics show that there is non-trivial growth for the Harper model, but no growth for the Fibonacci model [9].

Another way to describe the spreading of the wavefunction, which turns out to capture the limiting behavior of  $\beta_{\delta_1}^\pm(p)$  for small and large values of  $p$ , respectively, is in terms of probabilities. We define time-averaged *outside probabilities* by  $P(N, T) = \sum_{|n| > N} a(n, T)$ . Denote  $S^-(\alpha) = -\liminf_{T \rightarrow \infty} \frac{\log P(T^\alpha - 2, T)}{\log T}$  and  $S^+(\alpha) = -\limsup_{T \rightarrow \infty} \frac{\log P(T^\alpha - 2, T)}{\log T}$  for any  $\alpha \in [0, +\infty]$ . They

obey  $0 \leq S^+(\alpha) \leq S^-(\alpha) \leq \infty$ . These numbers control the power decaying tails of the wavepacket. In particular, the following critical exponents are of interest:

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

and

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

We have that  $0 \leq \alpha_l^- \leq \alpha_u^- \leq 1$ ,  $0 \leq \alpha_l^+ \leq \alpha_u^+ \leq 1$ , and also that  $\alpha_l^- \leq \alpha_l^+$ ,  $\alpha_u^- \leq \alpha_u^+$ .

One can interpret  $\alpha_l^\pm$  as 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 (polynomially small) part of the wavepacket. In particular, if  $\alpha > \alpha_u^+$ , then  $P(T^\alpha, T)$  goes to 0 faster than any inverse power of  $T$ . Since a ballistic upper bound holds in our case (for any potential  $V$ ), Theorem 4.1 in [17] yields  $\lim_{p \rightarrow 0} \beta_{\delta_1}^\pm(p) = \alpha_l^\pm$  and  $\lim_{p \rightarrow \infty} \beta_{\delta_1}^\pm(p) = \alpha_u^\pm$ . In particular, since  $\beta_{\delta_1}^\pm(p)$  are nondecreasing, we have that  $\beta_{\delta_1}^\pm(p) \leq \alpha_u^\pm$  for every  $p > 0$ .

When one wants to bound all these dynamical quantities for specific models, it is useful to connect them to the qualitative behavior of the solutions of the difference equation

$$u(n+1) + u(n-1) + V(n)u(n) = zu(n) \quad (2)$$

since there are effective methods for studying these solutions. Presently, the known general results are limited to one-sided estimates of the transport exponents. Namely, a number of approaches to lower bounds on  $\beta_{\delta_1}^\pm(p)$  have been found in recent years. The papers [10, 14, 15] derive such bounds in terms of the behavior of solutions to (2) with real energies  $z$ , with a link furnished by Hausdorff-dimensional properties of spectral measures due to results of Guarneri, Combes, and Last [12]. In fact, what is proven in these papers (although not stated in this form) are lower bounds on  $\alpha_l^-$ . Therefore, the lower bounds for  $\beta_{\delta_1}^-(p)$  obtained in this way are constant in  $p$ . There is also work by Guarneri and Schulz-Baldes [13], who bound  $\alpha_l^+$  from below in terms of the packing dimension of the spectral measure.

Further developments of these ideas by Guarneri and Schulz-Baldes, Barbaroux et al., and Tcheremchantsev [16] allowed these authors to obtain better lower bounds for  $\beta_{\delta_1}^\pm(p)$  which are growing in  $p$ . These results elucidate the phenomenon of quantum intermittency.

On the other hand, [11] develop a direct approach without an intermediate step. These papers use power-law upper bounds on solutions corresponding to energies from a set  $S$  to derive lower bounds for  $\beta_{\delta_1}^-(p)$ . The set  $S$  can even be very small. One already gets non-trivial bounds when  $S$  is not empty. If  $S$  is not negligible with respect to the spectral measure of  $\delta_1$ , the bounds are stronger, but there are situations of interest (e.g., random polymer models [2]), where the spectral measure assigns zero weight to  $S$ .

### III. TRANSFER MATRICES AND UPPER BOUNDS FOR TRANSPORT EXPONENTS

It should be stressed that there were no general rigorous methods for bounding  $\alpha_l^\pm$ ,  $\alpha_u^\pm$ , or  $\beta_{\delta_1}^\pm(p)$  non-trivially from above. In the present paper we propose a first general approach to proving upper bounds on  $\alpha_u^\pm$  (which in turn bound  $\alpha_l^\pm$  and  $\beta_{\delta_1}^\pm(p)$  for all  $p > 0$  from above, as well). This approach relates the dynamical quantities introduced above to the behavior of the solutions to the difference equation (2) for complex energies  $z$ . To state this result, let us recall the reformulation of (2) in terms of transfer matrices. These matrices are uniquely determined by the requirement that

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

for every solution  $u$  of (2). Consequently,

$$\Phi(n, z) = \begin{cases} T(n, z) \cdots T(1, z) & n \geq 1, \\ \text{Id} & n = 0, \\ [T(n+1, z)]^{-1} \cdots [T(0, z)]^{-1} & n \leq -1, \end{cases}$$

where

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

We have the following result:

**Theorem 1** *Suppose  $H$  is given by (1), where  $V$  is a bounded real-valued function, and  $K \geq 4$  is such that  $\sigma(H) \subseteq [-K+1, K-1]$ . Suppose that, for some  $C \in (0, \infty)$  and  $\alpha \in (0, 1)$ , we have*

$$\int_{-K}^K \left( \max_{3 \leq n \leq CT^\alpha} \|\Phi(n, E + \frac{i}{T})\|^2 \right)^{-1} dE = O(T^{-m})$$

and

$$\int_{-K}^K \left( \max_{3 \leq -n \leq CT^\alpha} \|\Phi(n, E + \frac{i}{T})\|^2 \right)^{-1} dE = O(T^{-m})$$

for every  $m \geq 1$ . Then  $\alpha_u^+ \leq \alpha$ . In particular,  $\beta_{\delta_1}^+(p) \leq \alpha$  for every  $p > 0$ .

*Remarks.* (a) If the conditions of the theorem are satisfied for some sequence of times,  $T_k \rightarrow \infty$ , we get an upper bound for  $\alpha_u^-$ .

(b) The proof of Theorem 1 is based on the well-known formula  $a(n, T) = \frac{1}{T\pi} \int |\langle (H - E - \frac{i}{T})^{-1} \delta_1, \delta_n \rangle|^2 dE$  and the fact that resolvent decay is closely related to lower bounds on transfer matrix growth. Details will be given in [20].

### IV. THE FIBONACCI HAMILTONIAN

The Fibonacci Hamiltonian is an operator of the form (1), where the potential is given by  $V(n) = \lambda \chi_{[1-\alpha, 1)}(n\alpha \bmod 1)$  with  $\alpha = (\sqrt{5} - 1)/2$ . This potential belongs to the more general class of Sturmian potentials, given by  $V(n) = \lambda \chi_{[1-\alpha, 1)}(n\alpha + \theta \bmod 1)$  with general irrational  $\alpha \in (0, 1)$  and arbitrary  $\theta \in [0, 1)$ . These sequences provide standard models for one-dimensional quasicrystals. (See [5] for the discovery of quasicrystals.) Early studies of the spectral properties of the Fibonacci model were done by Kohmoto et al. and Ostlund et al. [4]. It was suggested that the spectrum is always purely singular continuous and of zero Lebesgue measure. This was rigorously established by Sütő for the Fibonacci case [21] and by Bellissard et al. [22] and Damanik et al. [14] in the general Sturmian case. Abe and Hiramoto studied the transport exponents for the Fibonacci model numerically [6]; see also Geisel et al. [7]. They found that they are decreasing in  $\lambda$  and their work suggests that

$$\alpha_l^\pm, \alpha_u^\pm \sim \frac{\text{const}}{\log \lambda} \quad (3)$$

as  $\lambda \rightarrow \infty$ .

The general approaches to lower bounds for the transport exponent described above have all been applied to the Fibonacci Hamiltonian (and some Sturmian models). The best lower bound for  $\alpha_l^-$  was obtained by Killip et al. in [15]. It reads  $\alpha_l^- \geq \frac{2\kappa}{\zeta(\lambda) + \kappa + 1/2}$ , where

$$\kappa = \frac{\log \frac{\sqrt{17}}{4}}{5 \log \left( \frac{\sqrt{5}+1}{2} \right)} \approx 0.0126 \text{ and } \zeta(\lambda), \text{ chosen so that one}$$

can prove a result like  $\sum_{n=1}^L \|\Phi(n, E)\|^2 \leq CL^{2\zeta(\lambda)+1}$  for energies in the spectrum of  $H$  (our definition differs from that of [15]), obeys  $\zeta(\lambda) = \frac{3 \log \sqrt{5}}{\log \left( \frac{\sqrt{5}+1}{2} \right)} (\log \lambda + O(1))$ . This

shows in particular that  $\alpha_l^-$  admits a lower bound of the type (3).

The best lower bound for  $\alpha_u^-$  was found in [11], where it was shown that  $\alpha_u^- \geq \frac{1}{\zeta(\lambda)+1}$ . In terms of the exponents  $\beta_{\delta_1}^-(p)$ , the best known lower bounds are (see [11])

$$\beta_{\delta_1}^-(p) \geq \begin{cases} \frac{p+2\kappa}{(p+1)(\zeta(\lambda)+\kappa+1/2)} & p \leq 2\zeta(\lambda) + 1, \\ \frac{1}{\zeta(\lambda)+1} & p > 2\zeta(\lambda) + 1. \end{cases}$$

We also want to mention work on upper bounds for the slow part of the wavepacket by Killip et al. [15]. More precisely, they showed that there exists a  $\delta \in (0, 1)$  such that for  $\lambda$  large enough,  $P(C_2 T^{p(\lambda)}, T) \leq 1 - \delta$ . Here,  $p(\lambda) = \frac{6 \log \frac{\sqrt{5}+1}{2}}{\log \xi(\lambda)}$  and

$$\xi(\lambda) = \frac{\lambda - 4 + \sqrt{(\lambda - 4)^2 - 12}}{2}. \quad (4)$$

See [15, Theorem 1.6.(i)]. However, this result does not say anything about the fast part of the wavepacket, and

in particular, no statement for any of the transport exponents can be derived.

With the help of Theorem 1 we can prove upper bounds for  $\alpha_u^+$  for the Fibonacci model at sufficiently large coupling. These upper bounds show that (3) is indeed true.

The precise result is as follows:

**Theorem 2** *Consider the Fibonacci Hamiltonian and assume that  $\lambda \geq 8$ . Let  $\alpha(\lambda) = \frac{2 \log \frac{\sqrt{5}+1}{2}}{\log \xi(\lambda)}$ , where  $\xi(\lambda)$  is as in (4). Then,  $\alpha_u^+ \leq \alpha(\lambda)$ , and hence  $\beta^+(p) \leq \alpha(\lambda)$  for every  $p > 0$ .*

*Remarks.* (a) One can observe that  $\alpha(\lambda) < p(\lambda)$ .

(b) Note that  $\xi(\lambda) = \lambda + O(1)$  as  $\lambda \rightarrow \infty$ . Moreover,  $\alpha(8) = \frac{2 \log \frac{\sqrt{5}+1}{2}}{\log 3} \approx 0.876$  and  $\alpha(\lambda)$  is a decreasing function of  $\lambda$  for  $\lambda \geq 8$ . Thus, we establish anomalous transport for the Fibonacci Hamiltonian with coupling  $\lambda \geq 8$

and confirm the asymptotic dependence of the transport exponents  $\alpha_u^\pm$  on the coupling constant  $\lambda$  that was predicted by Abe and Hiramoto. We emphasize again that this is the first model for which anomalous transport can be shown rigorously.

(c) Their key idea is to study the well-known trace map as a complex dynamical system and prove upper bounds on the imaginary width of the (complex) canonical approximants of the spectrum. Denote  $x_n(z) = \text{Tr } \Phi(F_n, z)$ , where  $F_n$  is the  $n$ -th Fibonacci number and  $z \in \mathbb{C}$ , and  $\sigma_n = \{z \in \mathbb{C} : |x_n(z)| \leq 2\}$ . Then we prove that  $\sigma_n \subseteq \{z \in \mathbb{C} : |\text{Im } z| < C\xi(\lambda)^{-n/2}\}$ . Outside of the sets  $\sigma_n \cup \sigma_{n+1}$ , the traces grow super-exponentially and this yields the lower bounds on the norms of transfer matrices that we need. The claimed upper bound on  $\alpha_u^+$  then follows from Theorem 1. A detailed proof of Theorem 2 may be found in [20].

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