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Spectra and Transport in Almost Periodic Dimers

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We study spectral properties of discrete Schrödinger operators with potentials obtained via dimerization of a class of aperiodic sequences. It is shown that both the nature of the autocorrelation measure of a regular sequence and the presence of generic (full probability) singular continuous spectrum in the hull of primitive and palindromic (four block substitution) potentials are robust under dimerization. Generic results also hold for circle potentials. We illustrate these results with numerical studies of the quantum mean square displacement as a function of time. The numerical techniques provide a very fast algorithm for the time evolution of wave packets.

KEY WORDS: Dimer operators; almost periodicity; substitution potentials; singular continuous spectra.

1. INTRODUCTION

It is well known that the general rule for bounded random potentials $V = (V_n)_{n\in\mathbb{Z}}$ is the presence of Anderson localization and pure point spectrum for the corresponding Schrödinger operators $H_V: l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$

$$(H_V\psi)_n = \psi_{n+1} + \psi_{n-1} + \lambda V_n \psi_n \tag{1}$$

with potential intensity $\lambda > 0$. This holds, in particular, for potentials assuming only two values $V_n \in \{-1, +1\}$, $\forall n$.[(1)] Such strong lack of correlation along different sites forbids long range tunneling and the *mean square displacement*

$$m_2(t) = \sum_{n\in\mathbb{Z}} n^2 \, |\psi_n(t)|^2 \tag{2}$$

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is usually a bounded function of time, a property which turns out to be one of the most used to probe (de)localization.

On the other hand, aperiodic potentials with long range correlation, e.g., almost periodic potentials, have shown many instances of weak delocalization, marked by the presence of singular continuous spectra of the corresponding Schrödinger operators. This is in particular noted for substitution potentials assuming a finite number of values.[2–7] In such cases the delocalization can be characterized by the exponent

$$m_2(t) \sim t^{2\alpha}, \qquad \text{for large } t \tag{3}$$

with $0 \leqslant \alpha \leqslant 1$. Of course $\alpha = 0$ in case of localization, while for $\alpha = 1$ the so-called ballistic motion occurs, a fact that has been related to absolutely continuous spectrum of H_V.

The discovery that random dimer potentials, which have strict local correlations, are able to show delocalization for some potential intensities with (numerically found) exponent $\alpha \approx 3/4$,[8,9] generated some surprise. Recall that a dimer potential $W = (W_n)_{n \in \mathbb{Z}}$ is built upon V by the rule

$$W_{2n} = W_{2n+1} = V_n, \qquad \forall n \in \mathbb{Z} \tag{4}$$

Although the spectra of the random dimer operators H_W (assuming only the values $W_n = \pm 1$) are still pure point,[10] for some potential intensities, in particular for $\lambda \leqslant 1$, the local correlations introduced by dimerization cause the appearance of the so-called *critical energies*, i.e., energies with null Lyapunov exponent, opening the door for the numerical found delocalization.

In this work we address the influence of the dimerization on spectral properties of a class of almost periodic potentials which are sequences with long range order. For concreteness the potentials considered are generated by some substitution sequences,[2,6] a convenient choice since there are plenty of examples of such sequences assuming only two values. These are models of one-dimensional quasicrystals. Recall that the purely singular continuous spectrum is the general rule for Schrödinger operators with substitution potentials (see refs. 2–5, 7 and references therein).

The main questions discussed here are:

1. How does the dimerization affect the asymptotic conductance on the lattice as specified by $m_2(t)$? More precisely, does the dimerization change (and how) the exponent α in Eq. (3)?

2. What are the influences of dimerization on the spectral type of the original Schrödinger operator? Is the singular continuous spectrum robust under dimerization?

3. To what extent the dimerization modify the correlation measure of the sequence itself?

We discuss these questions in the reverse order they were presented. On the last question above, we shall conclude that dimerization has a small effect on the randomness (or lack thereof) of a given sequence. The appropriate quantity to measure randomness of the sequence $u = (u_n)$ is an *autocorrelation measure*, defined in Section 2, and denoted by σ_u. We refer the reader to Section 2 for the relevant definitions, and the proof of the next theorem.

Theorem 1. Let $u = (u_n)$ be a bounded sequence of complex numbers such that the autocorrelation measure is unique. Then, the corresponding dimerized sequence $w = (w_n)$ has a unique autocorrelation measure. Moreover, if σ_u has a single component (pure point, absolutely continuous or singular continuous), then σ_w has the same component, and conversely.

Now we look upon the second question. In ref. 10 it is proven that for a large class of random Schrödinger operators the dimerization does not change the pure point character of its spectrum. It is also clear that periodic potentials keep periodic after dimerization, so that we have instances of Schrödinger operators with absolutely continuous spectrum before and after dimerization. Here we present examples of Schrödinger operators with singular continuous spectrum which are (in some sense) robust under dimerization; we consider palindromic[5] and also "four block"[11] substitution potentials. It is also important to recall that the autocorrelation functions do exist for primitive substitution sequences, so that Theorem 1 applies. In Section 3 we provide the pertinent definitions and prove

Theorem 2. Let $u = (u_n)_{n \in \mathbb{Z}}$ be an aperiodic substitution sequence with hull $\Omega(u)$ palindromic and strictly ergodic, and $w = (w_n)_{n \in \mathbb{Z}}$ its dimerization. Then there exist generic sets G_u in $\Omega(u)$, and G_w in $\Omega(w)$, for which (for any $\lambda \neq 0$) H_v has purely singular continuous for each $v \in G_u$ and also for each $v \in G_w$.

We remark that the conclusion in Theorem 2 about $v \in G_u$ is a result of ref. 5, and in Section 3 it is shown that that proof can be adapted for $v \in G_w$. It is in this sense we have found the singular continuous spectrum is robust under dimerization (see also Theorem 3).

We note in particular that Fibonacci ($\xi(a) = ab$, $\xi(b) = a$; see Section 3 for the definition of substitution sequences), Thue–Morse ($\xi(a) = ab$, $\xi(b) = ba$)[5] and the nonprimitive[4] $\zeta(a) = aabaa$, $\zeta(b) = b$, substitution sequences

are in the class for which Theorem 2 applies. We notice that in the recent article[12] there are uniform spectral results for the case of dimerization of Sturmian potentials.

The following theorem is an immediate application of the results of ref. 11:

Theorem 3. Let $u = (u_n)_{n \in \mathbb{Z}}$ be an aperiodic primitive substitution sequence such that there exists a finite word q with $qqqq$ occurring in u. If $w = (w_n)_{n \in \mathbb{Z}}$ denotes its dimerization, then for almost every v in $\Omega(w)$ (with respect to the unique invariant probability measure), H_v has purely singular continuous spectrum (for any $\lambda \neq 0$).

This theorem applies, in particular, to the binary non-Pisot substitution ($\xi(a) = ab$, $\xi(b) = aaa$) and simple adaptations (e.g., $a \to ab$, $b \to a^n$ with $n \geqslant 4$, and the "generalized Fibonacci" $a \to a^n b$, $b \to a$ with $n \geqslant 3$). We also remark that the hypotheses of Theorem 3 also imply the generic presence of pure singular continuous spectrum for potentials in the respective hull.

The first question above is addressed from the numerical point of view in Section 4. There it is also proposed an efficient algorithm for the time evolution of wave packets according to Hamiltonian (1); it allowed us to consider lattices of size $2^{15} \approx 32000$ on a Macintosh G4 microcomputer. It consists of the fusion of a numerical technique originally proposed for the kicked rotator[13] with sympletic integrators.[14] The numerical results are summarized in Figs. 1 and 2. In Section 5 we draw our concluding remarks and state the spectral results for circle potentials.

2. AUTOCORRELATION OF DIMERIZED SEQUENCES

In this section we show that the spectral type of a sequence does not modify after dimerization. A bounded sequence of complex numbers $v = (v_k)_{k \in \mathbb{N}}$ (with suitable adaptations if k runs over $\mathbb{Z}$) is called regular if its *autocorrelation function*,[6, 15, 16] defined by the sequence

$$C_v(k) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} v_{n+k} \overline{v_n}, \qquad k \geqslant 0$$

exists; extend it for negative integers by the expression $C_v(-k) = \overline{C_v(k)}$. If v is regular then, by Bochner–Herglotz Theorem, there exists only one Borel positive measure σ_v on the interval $[0, 1]$, called its *autocorrelation measure*, such that the Fourier transform

$$\hat{\sigma}_v(k) \equiv \int_0^1 e^{i2\pi kt} \, d\sigma_v(t) = C_v(k), \qquad \forall k \in \mathbb{Z}$$

The autocorrelation measures can be used to characterize regular sequences qualitatively from "ordered to random:" σ_v is pure point for periodic sequences, while for independent random sequences it is purely absolutely continuous, and in between one would put sequences with singular continuous autocorrelation measure. Notice that there are autocorrelation measures of each spectral type within the almost periodic substitution sequences; for example, Fibonacci's is pure point, Thue–Morse's is singular continuous and Rudin–Shapiro's is Lebesgue measure.[2, 6, 15]

With these preliminaries, we are in position to prove Theorem 1. Denote by $w = (w_n)$ the dimerization, as indicated in (4) (but here restricted to $n \in \mathbb{N}$), of a fixed regular sequence $u = (u_n)$. Direct calculation results in $C_w(0) = C_u(0)$; now

$$\begin{aligned} C_w(1) &= \lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} w_{n+1}\overline{w_n} \\ &= \lim_{N\to\infty} \frac{1}{N} \left[\sum_{k=0}^{[N/2]} w_{2k+1}\overline{w_{2k}} + \sum_{k=0}^{[N/2]} w_{2k+2}\overline{w_{2k+1}} \right] \end{aligned}$$

and since $w_{2k+1} = w_{2k} = u_k$, it follows that the limit defining $C_w(1)$ exists and

$$C_w(1) = \tfrac{1}{2}\,(C_u(0) + C_u(1))$$

In a similar way, one obtains that $C_w(2)$ exists and

$$C_w(2) = C_u(1)$$

The same kind of argument applies for all values of k, and one gets that the autocorrelation function of w exists and satisfy

$$\begin{aligned} C_w(2k) &= C_u(k) \\ C_w(2k+1) &= \tfrac{1}{2}\,(C_u(k) + C_u(k+1)) \end{aligned}$$

Therefore w is also regular. We shall denote by σ and $\boldsymbol{\sigma}$ the autocorrelation measures of the sequences u and w, respectively. It remains to show that if σ has a single component, then $\boldsymbol{\sigma}$ also has only that kind of component, and conversely.

The above relations can be rewritten in terms of the Fourier transform components $\hat{\sigma}$ and $\hat{\boldsymbol{\sigma}}$,

$$\hat{\boldsymbol{\sigma}}(2k) = \hat{\sigma}(k) \tag{5}$$

$$\hat{\boldsymbol{\sigma}}(2k+1) = \tfrac{1}{2}\,(\hat{\sigma}(k) + \hat{\sigma}(k+1)) \tag{6}$$

which resembles a relation in Allouche and Mendès–France's approach to the autocorrelation of the Thue–Morse sequence.[15]

Set $f(t) = 2t$ and $g(t) = 2t-1$, and for a measure μ denote its image under f by $f_*\mu = \mu \circ f^{-1}$ (analogously for $g_*\mu$). By using relation (5)

$$\begin{aligned}\hat{\sigma}(2k) &= \int_0^1 e^{2\pi i 2kx}\, d\sigma(x)\\ &= \int_0^{1/2} e^{2\pi ik(2x)}\, d\sigma(x) + \int_{1/2}^1 e^{2\pi ik(2x)}\, d\sigma(x)\\ &= \int_0^1 e^{2\pi ikt} d[f_*\sigma(t) + g_*\sigma(t)] = \hat{\sigma}(k)\\ &= \int_0^1 e^{2\pi ikt}\, d\sigma(t)\end{aligned}$$

Therefore

$$\sigma = f_*\sigma + g_*\sigma$$

Now Theorem 1 follows from the uniqueness of Lebesgue decomposition of positive measures.

3. SPECTRUM OF SOME DIMER SCHRÖDINGER OPERATORS

In this section we prove Theorem 2; at the end we comment upon Theorem 3. Let us recall some facts about substitution potentials, referring the reader to the papers[2, 3, 5, 6] for further details. Since we consider only potentials taking two values we mostly restrict ourselves to substitutions $\xi: \mathscr{A} \mapsto \mathscr{A}^*$ on an alphabet $\mathscr{A} = \{a, b\}$; $\mathscr{A}^*$ is the set of all words of finite length on $\mathscr{A}$. Given $x \in \mathscr{A}^*$, its length is denoted by $|x|$. ξ is *primitive* if there exists k such that both $\xi^k(a)$ and $\xi^k(b)$ contain all letters of $\mathscr{A}$. Denote by $\mathscr{A}^{\mathbb{N}}$ ($\mathscr{A}^{\mathbb{Z}}$) the set of all (two-sided) sequences of letters in $\mathscr{A}$; the substitution ξ have natural extensions, by concatenation, to $\mathscr{A}^*$, $\mathscr{A}^{\mathbb{N}}$ and $\mathscr{A}^{\mathbb{Z}}$; for example, $\xi(ab) = \xi(a)\,\xi(b)$. A *substitution sequence* is a fixed point v of ξ in $\mathscr{A}^{\mathbb{N}}$ or $\mathscr{A}^{\mathbb{Z}}$, i.e., $\xi(v) = v$. Consider on $\mathscr{A}^{\mathbb{N}}$ ($\mathscr{A}^{\mathbb{Z}}$) the point convergence topology generated by the metric

$$d(u, v) = \sum_n \frac{|u_n - v_n|}{2^{|n|}}, \qquad u = (u_n), \quad v = (v_n)$$

with $n \in \mathbb{N}$ ($n \in \mathbb{Z}$). The existence of a fixed point follows from the assumption, which we now make, that $\xi(a)$ begins with a and that $|\xi^k(a)|$ goes to infinity as $k \to \infty$ (ξ^k denotes the kth iterate of ξ; see, for instance, Proposition V.1 in ref. 6).

Given a substitution sequence $\bar{v}$ in $\mathscr{A}^{\mathbb{N}}$, pick any $v \in \mathscr{A}^{\mathbb{Z}}$ such that $v_n = \bar{v}_n$ for $n \geqslant 0$. If T: $\mathscr{A}^{\mathbb{Z}} \mapsto \mathscr{A}^{\mathbb{Z}}$ denotes the left shift $(Tu)_n = u_{n+1}$, the *hull* Ω of such sequence is defined as ref. 17 (see refs. 4, 16, and 18 for different ways of dealing with this definition)

$$\Omega = \{u \in \mathscr{A}^{\mathbb{Z}} : \text{there exists } n_j \to \infty, \lim_{j \to \infty} T^{n_j} v = u\}$$

i.e., it is the set of limit points of $\{T^n v\}$ as $n \to \infty$; the hull does not depend on the particular extension v of $\bar{v}$ considered, and is a compact subset of $\mathscr{A}^{\mathbb{Z}}$. Recall that in important situations, for example for primitive substitutions (Chap. V in ref. 6; see also ref. 4 for nonprimitive cases), $T\Omega = \Omega$ and the dynamical system (Ω, T) is *strictly ergodic*, i.e., it is minimal (every orbit is dense) and has just one probability invariant measure.

If $p(a) = +1$ and $p(b) = -1$, we associate a *substitution potential* to each $u = (u_n)_{n \in \mathbb{Z}} \in \Omega$ by $(p(u_n))_{n \in \mathbb{Z}}$, which we again denote by u. For a subset of almost periodic substitution sequences, we investigate the spectral properties of the Schrödinger operator H_u, given by (1), after dimerization.

We introduce the *dimerization operator* D: $\mathscr{A} \to \mathscr{A}_2 = \{aa, bb\}$, $D(a) = aa$, $D(b) = bb$, and its natural extensions, by concatenation, to $\mathscr{A}^*$, $\mathscr{A}^{\mathbb{N}}$ and $\mathscr{A}^{\mathbb{Z}}$. The image of D on $\mathscr{A}^{\mathbb{N}}$ is the set of *dimerized sequences* $\mathscr{A}_2^{\mathbb{N}}$, that is, sequences for which the occurrence of a given letter appears always in even lengths (with clear interpretations of $\mathscr{A}_2^*$ and $\mathscr{A}_2^{\mathbb{Z}}$). Notice that D, restricted to each of such sets, is injective, so we can define

$$\begin{aligned} \tilde{\xi}&: \mathscr{A}_2^{\mathbb{N}} \to \mathscr{A}_2^{\mathbb{N}} \\ v &\mapsto D \circ \xi \circ D^{-1}(v) \end{aligned} \tag{7}$$

and we have $\tilde{\xi}^n = D \circ \xi^n \circ D^{-1}$. If $w = (w_n)$ is the dimerization, $w_{2n} = w_{2n+1} = u_n$, of a sequence $u = (u_n) \in \mathscr{A}^{\mathbb{N}}$, then $w = \lim_{n \to \infty} \tilde{\xi}^n(aa) = D(u)$, since D is continuous (one can see that D is actually a contraction in balls of radius less than $1/2$). It is clear that we can carry this construction to $\mathscr{A}^{\mathbb{Z}}$, and we shall not continue to mention this explicitly.

Given finite words $A = a_0 \cdots a_n$ and $B = b_k \cdots b_m$, we denote by $\#_A B$ the number of occurrences of A in B; if A occurs (somewhere) in B, it will be indicated by the notation $A \subset B$. Given W a finite word, we remark that the *cylinder sets*

$$[W] = \{y \in \mathscr{A}^{\mathbb{Z}} : y_0 \cdots y_n = W\}$$

are open and closed. In particular, they form a basis for the point convergence topology.

Recall also that an element $x \in \mathscr{A}^{\mathbb{Z}}$ is *almost periodic* if for each $\epsilon > 0$ the set of $r \in \mathbb{Z}$ for which

$$d(T^r(x), x) < \epsilon$$

is relatively dense, meaning that there is a $K = K(\epsilon)$ such that every interval of length K contains at least one such r. Such K's are called *ϵ-periods* of x.

From now on we set u a fixed point of the substitution $\xi: \mathscr{A} \to \mathscr{A}^*$ and $w = D(u)$. The following lemma is important for a reduction in the proof of unique ergodicity (see below).

Lemma 1. (i) The cylinders $T^j[\xi^n(a)]$ (resp. $T^j[\tilde{\xi}^n(aa)]$), $\forall j, n$, generate the measurable sets of $\Omega(u) \subset \mathscr{A}^{\mathbb{Z}}$ (resp. $\Omega(w) \subset \mathscr{A}_2^{\mathbb{Z}}$).

(ii) A sequence $v \in \mathscr{A}^{\mathbb{Z}}$ is almost periodic if, and only if, the dynamical system $(\Omega(v), T)$ is minimal.

Proof. Recall that the cylinders are a basis for the topology of $\Omega(v)$ (or $\Omega(w)$). For an alphabet of N letters, $\mathscr{A} = \{l_1, \ldots, l_n\}$, an arbitrary cylinder is the intersection of a finite number of suitable translates $T^j[l_i]$, for $i = 1, \ldots, n$. A further reduction is possible since $[l_n]$ is the complement of $\bigcup_{i=1}^{n-1} [l_i]$. Therefore, for a two letter alphabet, it is enough to produce the cylinder $[a]$, which for the dimer is given by the union $[aa] \cup T[aa]$.

Proofs of (ii), i.e., Gottschalk's theorem, can be found in refs. 6 and 19. ▮

Remark 1. This lemma can be adapted to "any-mers," i.e., for any $n \in \mathbb{N}$, $D(a) = a \cdots a$, with n factors, for all $a \in \mathscr{A}$.

Proposition 1. If $(\Omega(u), T)$ is strictly ergodic, then so is $(\Omega(w), T)$.

Proof. By Lemma 1, u is almost periodic; given $\epsilon > 0$, twice the ϵ-period of u will work for w, so w is also almost periodic; again by Lemma 1, $(\Omega(w), T)$ is minimal.

To prove unique ergodicity of $(\Omega(w), T)$, we use Lemma 5.4 in Chap. 4 of ref. 20, or Corollary IV.14 of ref. 6, so that it is enough to prove that the frequency of $\tilde{\xi}^m(aa)$ in any finite word B of w approaches a uniform positive limit when $|B| \to \infty$. Take $B_n \subset w$ with $k_n = |B_n|$ and k_n a

monotone increasing sequence; it is then enough to prove that for each m there is $\mu_m > 0$ such that

$$\lim_{n\to\infty} \frac{\#_{\tilde{\xi}^m(aa)} B_n}{k_n} = \mu_m \tag{8}$$

For any such word B_n, there are dimerized words $A_n, C_n \subset w$ such that $A_n \subset B_n \subset C_n$ with $|A_n| \geqslant |B_n| - 2$ and $|C_n| \leqslant |B_n| + 2$; hence

$$\#_{\tilde{\xi}^m(aa)} A_n \leqslant \#_{\tilde{\xi}^m(aa)} B_n \leqslant \#_{\tilde{\xi}^m(aa)} C_n \tag{9}$$

Since for any dimerized word Z

$$\#_{\tilde{\xi}^m(aa)} Z = \#_{\xi^m(a)} D^{-1}(Z)$$

we have that $D^{-1}(C_n)$ is a word of length $(|C_n|/2)$, and $D^{-1}(A_n)$ has length, at least, $(|C_n|/2 - 1)$, both occurring in u. From such relations we get

$$\lim_{n\to\infty} \frac{\#_{\tilde{\xi}^m(aa)} A_n}{k_n} = \lim_{n\to\infty} \frac{\#_{\tilde{\xi}^m(aa)} C_n}{k_n} = \lim_{n\to\infty} \frac{1}{2} \frac{\#_{\xi^m(a)} D^{-1}(C_n)}{|C_n|/2} = \frac{\nu_m}{2}$$

with the relative frequency of $\xi^m(a)$ in u indicated by $\nu_m > 0$ (since $(\Omega(u), T)$ is strictly ergodic). Now relation (9) shows that the limit (8) exists and with $\mu_m = \nu_m/2 > 0$. ▌

Remark 2. The same reasoning applies for alphabets with more than 2 letters; one just has to evaluate the relative frequency of the smallest set of words a, for which the cylinders $T^j[a]$ generate the σ-algebra of measurable sets.

Applying Proposition 1 and the results of Kotani–Last–Simon[21, 22] on ergodic and minimal Schrödinger operators to our aperiodic potentials assuming finitely many values (see also ref. 5), we conclude that for any potential intensity $\lambda \neq 0$:

Corollary 1. If u is an aperiodic substitution sequence such that $(\Omega(u), T)$ is strictly ergodic, then the Schrödinger operator H_v has no absolutely continuous spectrum for any dimerized potential $v \in \Omega(w)$.

Our goal now is to exclude point spectrum of H_v for some $v \in \Omega(w)$. Following ref. 5 we shall consider strongly palindromic potentials. A finite word is a *palindrome* if it is the same whichever direction it is read: from left to right or from right to left. An element $v \in \mathscr{A}^{\mathbb{Z}}$ is called *palindromic*

if v contains arbitrarily long palindromes, and the corresponding hull $\Omega(v)$ is called palindromic. Finally, $v \in \mathcal{A}^{\mathbb{Z}}$ is *strongly palindromic* if it contains a sequence of palindromes of length l_i centered at $m_i \to \infty$ such that $e^{Bm_i}/l_i \to 0$, for a certain constant $B \geqslant 1$, which in our case is determined by the parameter λ (see the proof of Theorem 8.1 in ref. 5).

Proposition 2. If $\Omega(u)$ is minimal and palindromic, then there exists a generic set $G \subset \Omega(w)$ such that H_v has no eigenvalues for any $v \in G$.

Proof. Since the proof is a simple adaptation of results contained in ref. 5 we just outline it. Being $\Omega(u)$ palindromic, there is a palindromic sequence $p \in \Omega(u)$, and so $D(p)$ is a palindromic sequence in $\Omega(w)$. By Proposition 2.1 of ref. 5, there exists a strongly palindromic sequence $s \in \Omega(w)$ for which H_s has no eigenvalues (Theorem 8.1 of ref. 5).

Since $H_{T^j s}$ has the same spectrum as H_s for any j and, by minimality, it is a dense set in $\Omega(w)$, it follows by the "Wonderland results"[23] the existence of the generic set $G \subset \Omega(w)$ for which H_v has no eigenvalues for any $v \in G$. ▌

The proof of Theorem 2 follows readily from the combination of Corollary 1 and Proposition 2.

Proof of Theorem 3. It is clear that the presence of a Gordon-type block, as in ref. 24, also occurs after dimerization, and an infinite number of them (with increasing length) for a given potential exclude eigenvalues; following ref. 11, a four block *qqqq* in the primitive substitution guarantees the applicability of such Gordon-type argument in a set of positive invariant measure; since the set of potentials for which the associated operators have no eigenvalues is invariant, by ergodicity it has full invariant measure. The aperiodicity of the sequence implies the absence of absolutely continuous spectrum for such operators. From the proof of Proposition 1 it follows that the dimerization of a full (invariant) measure set also has full measure, concluding the proof of Theorem 3. ▌

4. NUMERICAL RESULTS

In this section we display the numerical results for the mean square displacement, showing super-diffusive behavior for the almost periodic and dimerized almost periodic potentials.

In order to consider larger finite basis approximations for the problem in $l^2(\mathbb{Z})$, we propose a combination of techniques that resulted in a very fast algorithm for quantum time evolution, with no matrix diagonalization; two time steps will be involved, the first one being the decomposition of the

final time evolution t is an integer multiple of Δt. We begin by recalling the Trotter product formula for the propagator of a quantum Hamiltonian. We decompose our Hamiltonian in its free $(K\psi)_n = \psi_{n-1} + \psi_{n+1}$ and "contact" $V = \lambda u$ parts, so that $H_V = K + V$,

$$e^{-i\,\Delta t\,H_V} = \mathrm{s}-\lim_{N\to\infty} (e^{-i\,\Delta t\,K/N} e^{-i\,\Delta t\,V/N})^N$$

which was estimated (see below) for each fixed *large* time step Δt.

From the proof of this formula,[25] one sees that in general we can consider subsequences on its right hand side that have a different factorization for the *small* time step $s = \Delta t/N$; for instance, with (see ref. 25)

$$e^{-i\,\Delta t\,V/2N} e^{-i\,\Delta t\,K/N} e^{-i\,\Delta t\,V/2N}$$

one gets the so-called *sympletic propagator* of second order.[14] Factorizing in more terms and using the Baker–Campbell–Hausdorff formula, one is able to construct sympletic integrators of higher orders. We write each factor in the Trotter formula as

$$e^{-is(K+V)} = \prod_{j=1}^{8} e^{-isd[j]K} e^{-isc[j]V} + O(s^7) \tag{10}$$

where $c[j]$, $d[j]$ are positive real numbers with $\sum c[j] = \sum d[j] = 1$. We have used this sixth order setting with an optimal number of factors (see details in ref. 14). In terms of the disorder λ, the bound $N = 14$, $\lambda\,\Delta t \leqslant 7$, has proved enough for convergence of the Trotter formula; we have used $\Delta t = 5$ for $\lambda \leqslant 1$ and $\Delta t = 3$ for $1.1 \leqslant \lambda \leqslant 2$.

The factor $e^{-isd[j]K}$ is diagonal in "momentum" representation, while $e^{-isc[j]V}$ is diagonal in "position" representation. Fixing the size of the lattice as a power of 2, we can use fast Fourier transforms to jump the propagator from position to momentum representation, and vice versa. With such procedure it was possible to use bases of size $L = 2^{15}$, on a Macintosh G4 microcomputer, with a reasonable running time.

In our numerical calculations we have considered Fibonacci and Thue–Morse potentials (assuming the values $\pm\lambda$). The initial condition was concentrated on the zeroth position of each finite basis approximation $[-L/2, L/2-1] \cap \mathbb{Z}$, and its time evolution computed as indicated above. The maximum time span for the evolution was either 10^5 or less in case the packet hits the border with probability 10^{-8}.

The values of α in (3) were obtained from line fittings on the plots of $\ln m_2(t) \times \ln t$. For large values of the potential λ (the effective disorder intensity is then 2λ) such plots can present large oscillations and it was

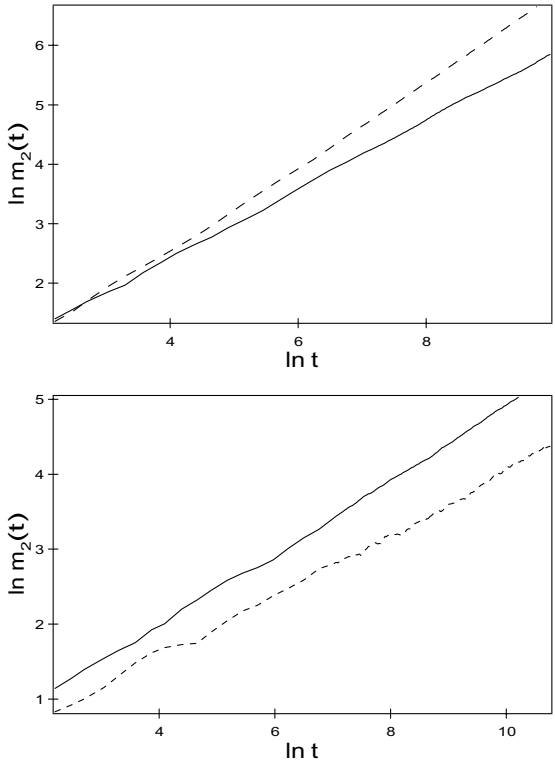

Fig. 1. The mean square displacement for the Fibonacci potential, for $\lambda = 1.2$ averaged over 5 realizations (top), and $\lambda = 1.7$ averaged over 10 realizations. The dimerized cases are plotted with a dashed line. Note the ln–ln scale.

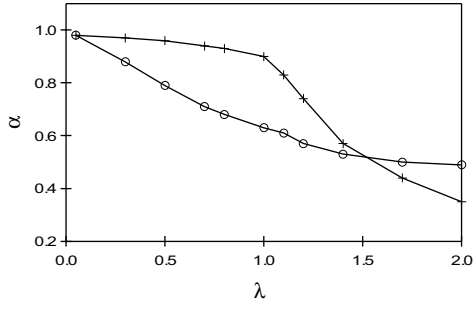

Fig. 2. The exponent α for the Fibonacci sequence as function of the potential intensity λ: (○) no dimerization; (+) after dimerization.

necessary to employ averages over different initial conditions on the lattice (we took up to ten realizations for each average), in order to get effective straight line curves; notice that due to the almost periodicity of the potentials, such averages correspond to ensemble averages over the hull. It is remarkable that the plots in the Thue–Morse case present larger oscillations than the corresponding Fibonacci cases, so that we have restricted $\lambda \leqslant 1.3$ for Thue–Morse potentials, while $\lambda \leqslant 2.0$ for Fibonacci ones. In all cases we have got $\alpha < 1$, as expected from the absence of absolutely continuous spectrum for those Hamiltonians.

In Fig. 1 $m_2(t)$ is shown for the Fibonacci Hamiltonian with $\lambda = 1.2$ and 1.7. Denote by α_d the values of the exponent α for the dimerized potentials. In the Fibonacci case, for small intensities $\alpha_d > \alpha$, as an expected contribution from the introduced local correlations, but for $\lambda \approx 1.4$ we have $\alpha_d/\alpha \approx 1$, so there is a crossing of such values, and $\alpha_d < \alpha$ for larger intensities. This is shown in Fig. 2, where the values of α and α_d are presented as function of the intensity λ. Notice that the transition is also apparent from the slopes in Fig. 1.

We cannot give a precise justification for this transition, but it appears that the dimerization, in producing a local correlation in the sequence, scrambles the long range order, which is so finely tuned by a substitution rule. In the case of the Thue–Morse potential, however, we obtained numerically that $\alpha_d/\alpha \approx 1$ for $0 \leqslant \lambda \leqslant 1.3$. The Thue–Morse sequence has some symmetries which are close to the dimerization. Note that it is invariant under the substitution $1 \to 1001$ and $0 \to 0110$, so that the basic dimer strings are all present in it. A look at the sequence reveals that even three consecutive dimer strings occur in it. This does not happen in a general substitution sequence, in particular the Fibonacci sequence does not have one of the basic dimer strings.

It is tempting to point out the similarity of the transition in the Fibonacci potential with the random dimer: they both show a change of behavior at potential intensity $\lambda = 1$ (recall that in the random dimer $\alpha = \alpha_d = 0$ for $\lambda > 1$ and if $\lambda < 1$, $\alpha = 0$ and $\alpha_d = 3/4$[8]). To this picture, we may add the (trivial) periodic case which shows no transition, with $\alpha = \alpha_d = 1$ for all λ. But it is still a subtle problem the extent to which local and long range order in the potential affects the propagation in the lattice.

5. FINAL REMARKS

We found that the autocorrelation measures of a given regular sequence u and its dimerization $w = D(u)$ share the same components: notice that this more general version of Theorem 1 was actually proven.

It is also applicable to any-mers, the proof needing just a slight adaptation in the change of variables step.

It was numerically found that the exponent α ruling the algebraic growth of the second moment $m_2(t)$ can present different behaviors after dimerization, depending on the substitution and also on the disorder intensity. So this paper adds some evidence that only the type of the potential autocorrelation measure is not sufficient for a classification of the behavior of physical quantities obtained from the corresponding Schrödinger operator (see also ref. 26).

We note that the dimerization of a (finite valued) strongly palindromic sequence, with parameter $B > 2$, is also strongly palindromic with the new parameter $B/2$, so that the absence of eigenvalues can occur for Schrödinger operators with both sequences as potentials. However, if the original sequence generates a strictly ergodic hull, it is not at all obvious that so does its dimerized version; that was the content of the proof of Theorem 2, which can be adapted to any-mers. It is also worth pointing out that for such results it is enough that the palindromic substitution sequence generates strictly ergodic potentials, so that Theorem 2 holds for the nonprimitive examples discussed in ref. 4.

A closer look at the proof of Theorem 2 reveals that only the properties of almost periodicity, unique ergodicity, aperiodicity and that it takes only finitely many values (two, in fact) were employed, so that, by using results of refs. 5 and 17, we can say something about the spectrum of Schrödinger operators (1) with dimerized potentials generated by circle sequences, i.e., $u_{a,b,\theta} = (u_n)$, with

$$u_n = \chi_{[a,b)}(n\beta + \theta (\mathrm{mod}\ 1))$$

here $\chi_{[a,b)}$ is the characteristic function of the interval $[a, b)$ with $0 \leqslant a < b < 1$, β an irrational number, and $0 \leqslant \theta < 1$. In this case the hull of $u_{a,b,\theta}$ is independent of θ, strictly ergodic and palindromic.[5, 17] Therefore,

Theorem 4. If β is an irrational number and $w_{a,b,\theta}$ is the dimerization of $u_{a,b,\theta}$, then $\Omega(w_{a,b,\theta})$ is aperiodic, strictly ergodic and palindromic. Furthermore, for any $\lambda \neq 0$ the operator H_v, as defined in (1), has pure singular continuous spectrum for v in a generic subset of $\Omega(w_{a,b,\theta})$.

Some interesting questions left for future investigations include the relations of dimerization with Hausdorff dimensional properties of the spectrum, whether uniform spectral results always persist after dimerization (as is the case of Sturmian potentials[12]), and a possible explanation of the results shown in Fig. 5, maybe in terms of the density of states.

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