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Perturbation theory for the random dimer model

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Abstract. We study a one-dimensional tight binding model with a random potential taking two values $\pm v$, with the restriction that on pairs of two neighbouring sites the potentials take the same value. This random dimer model, proposed by Dunlap, Phillips and Wu, has a vanishing Lyapunov exponent for the energy $E = \pm v$. We compute the Lyapunov exponent and the density of states perturbatively in the vicinity of this energy using the invariant measure formalism.

1. Introduction

In a series of recent articles Dunlap *et al* [1, 2] have considered a number of onedimensional disordered tight-binding models which exhibit some exceptional and maybe surprising features; in particular, they may have extended states at particular energies. These models may serve to explain the properties of certain one-dimensional conductors such as polyaniline. Apart from these direct physical applications, the analysis of these models shows that even in the context of one-dimensional discrete random Schrödinger operators, there are still a lot of interesting phenomena to discover, which are not immediately covered by the general results. In this note we consider the simplest of the models proposed by Dunlap *et al* the random dimer model [1] using methods of the invariant measure and perturbation theory from [3] and [4]. This will allow us to calculate more precisely the Lyapunov exponent and the density of states near the exceptional energies. It is our purpose to illustrate that these methods, although developed for the standard Anderson model [5], are really powerful tools to investigate these more exotic situations.

Let us first define the random dimer model and give a qualitative review of its main features. The Hamiltonian of this model is given as

$$H = -\Delta + V \tag{1.1}$$

on $l^2(\mathbb{Z})$, where Δ is the (off-diagonal) discrete Laplacian, i.e.

$$(-\Delta u)(n) = u(n+1) + u(n-1)$$

and V is a diagonal matrix whose entries v_n are given by

$$v_{2k} = v\varepsilon_k \qquad v_{2k+1} = v\varepsilon_k \tag{1.2}$$

where the ε_k are independent, identically, distributed random variables, taking the values +1 and -1 with, say, equal probability $\frac{1}{2}$. The binary nature of the random

[†] More generally, we might consider the case where ε_k takes the values 1 and p/(p-1) with probability p and (1-p), respectively.

variable ε_k is crucial and we will exhibit the effect of smoothening of the distribution later in some detail.

As usual, the associated Schrödinger equation can be written in first-order vector form as

$$\begin{pmatrix} \psi(n+1)\\ \psi(n) \end{pmatrix} = P(E, v_n) \begin{pmatrix} \psi(n)\\ \psi(n-1) \end{pmatrix}$$
(1.3)

with

$$P(E, v) = \begin{pmatrix} E - v & -1 \\ 1 & 0 \end{pmatrix}.$$
 (1.4)

The solution of the Schrödinger equation with initial data $(\psi(0), \psi(-1))$ is then written as

$$\begin{pmatrix} \psi(n+1)\\ \psi(n) \end{pmatrix} = \prod_{k=0}^{n} P(E, v_k) \begin{pmatrix} \psi(0)\\ \psi(-1) \end{pmatrix}.$$
(1.5)

Due to our choice of v_n , the product appearing in (1.5) can be expressed for *n* even or *n* odd as,

$$\prod_{k=0}^{2l+1} P(E, v_k) = \prod_{k=0}^{l} P(E, v\varepsilon_k)^2$$

$$\prod_{k=0}^{2l} P(E, v_k) = P(E, v\varepsilon_l) \prod_{k=0}^{l-1} P(E, v\varepsilon_k)^2.$$
(1.6)

Dunlap et al noted that for E = v (and similarly for E = -v), the two matrices appearing in the product are

$$P(v, -v)^2 = P(2v, 0)^2$$
 and $P(v, v)^2 = P(0, 0)^2 = -1.$ (1.7)

Therefore, for this energy, the product of matrices trivializes to

$$\prod_{k=0}^{l} P(v, v\varepsilon_k)^2 = -1^{l+1+S_l} P(2v, 0)^{2(l+1-S_l)}$$
(1.8)

where $S_l \equiv \sum_{i=0}^{l} \varepsilon_i$. For $|2v| \le 2$, P(2v, 0) has two eigenvalues of modulus one, implying that there exists a bounded solution of the Schrödinger equation for this energy. For |2v| > 2, the two eigenvalues are real, one of them being larger, the other smaller than one, and no bounded solution exists.

While one extended state will not have a significant influence on the transport properties of this model, it is argued in [2] that in a finite sample of length N, a number of states proportional to \sqrt{N} will have a localization length superior to the sample size and thus contribute to transport. To make these claims more precise, we must therefore observe the behaviour of the Lyapunov exponent (inverse localization length) and the density of states in the vicinity of $E = \pm v$. We propose to do this here using perturbation theory for the invariant measure developed in [3, 4]. This will allow us to calculate systematically an expansion in powers of (E-2v) for the density of states and Lyaponov exponent. We shall show that for 2v < 2, the Lyaponov exponent behaves like $(E-v)^2$, while for v=1 it shows a behaviour with leading term (E-1) [1]. As the density of states will be seen to behave like c+c'(E-2v) and $c+c'|E-1|^{1/2}$, respectively, the predictions of [1] will be confirmed in both cases.

2. The invariant measure

Let $\psi_E(n)$ denote the solution of the Schrödinger equation with energy E. We put $r_k = \psi_E(k)/\psi_E(k-1)$. The projective variables r_k satisfy the recursive equation

$$r_{k+1} = E - v_k - \frac{1}{r_k} \equiv \tau_{E, v_k}(r_k).$$
(2.1)

The complex Lyapunov exponent $\tilde{\gamma}(E, v)$ is then defined as

$$\tilde{\gamma}(E,v) = \lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \ln(r_k)$$
(2.2)

where the complex logarithm is chosen such that $\ln(-x) = i\pi + \ln x$, if x is real and positive. $\tilde{\gamma}(E, v)$ is then related to the density of states N(E, v) and the Lyapunov exponent $\gamma(E, v)$ by (see e.g. [6])

$$\tilde{\gamma}(E, v) = \gamma(E, v) + i\pi N(E, v).$$
(2.3)

Contrary to the situation in the standard Anderson model, the r_k here do not form a Markov chain; however, if we put $x_k \equiv r_{2k}$, then these satisfy

$$\boldsymbol{x}_{k+1} = \boldsymbol{\tau}_{E, \upsilon e_k}^2(\boldsymbol{x}_k) \tag{2.4}$$

and since ε_k are i.i.d. random variables form a Markov chain. We denote by $\nu_{E,v}$ an invariant measure with respect to this process, i.e. a measure such that for all measurable functions f

$$\int f(x)\nu_{E,\nu}(\mathrm{d}x) = IE_{\varepsilon} \int f(\tau_{E,\nu}^2(x))\nu_{E,\nu}(\mathrm{d}x).$$
(2.5)

As a consequence of Fürstenberg's theorem [7], this measure will be unique, except when $E = 2 \cos \pi \alpha$ with α rational and v = 0 or $v = \pm E$. To express the complex Lyapunov exponent in terms of this invariant measure, we rewrite it as

$$\tilde{\gamma}(E, v) = \lim_{n \to \infty} \frac{1}{2n} \sum_{k=1}^{n} \left[\ln(r_{2k}) + \ln(r_{2k-1}) \right]$$
$$= \lim_{n \to \infty} \frac{1}{2n} \sum_{k=1}^{n} \ln x_k + \lim_{n \to \infty} \frac{1}{2n} \sum_{k=1}^{n} \ln(\tau_{E, v \in k-1}(x_{k-1})).$$
(2.6)

Therefore

$$\hat{\gamma}(E, v) = \frac{1}{2} \int \ln x \nu_{E,v}(\mathrm{d}x) + \frac{1}{2} I E_{\varepsilon} \int \ln(\tau_{E,v\varepsilon}(x)) \nu_{E,v}(\mathrm{d}x).$$
(2.7)

This formula allows us to calculate the density of states and Lyapunov exponent in our model from the invariant measure $\nu_{E,v}$.

To compute this invariant measure, let us assume that it has a density, $\phi_{E,v}$. Equation (2.5) yields the following equation for ϕ :

$$\frac{1}{2}[T_{E+v}^2 + T_{E-v}^2]\phi_{E,v}(x) = \phi_{E,v}(x)$$
(2.8)

where

$$T_E f(x) = \frac{1}{(x-E)^2} f\left(\frac{1}{E-x}\right).$$
 (2.9)

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Note that $T_0^2 = 1$ and that therefore, for $E = \pm v$, (2.8) takes the simple form

$$\Gamma_{\pm 2v}^{2}\phi_{\pm v,v}(x) = \phi_{\pm v,v}(x). \tag{2.10}$$

Thus, the invariant measure at these energies is exactly that of the free Laplacian at the energy $\tilde{E} = \pm 2v$. If \tilde{E} is of the form $\tilde{E} = 2 \cos \alpha \pi$, α irrational, then $T_{\tilde{E}}\phi = \phi$ has the unique solution

$$\phi_E = \frac{1}{\pi} \frac{\sqrt{1 - \tilde{E}^2/4}}{x^2 - \tilde{E}x + 1}.$$
(2.11)

Thus for $E = \pm v$, $v = \cos \alpha \pi$ (note this implies |v| < 1!) with irrational α , then

$$\phi_{\pm v,v}(x) = \frac{1}{2x} \frac{\sqrt{1-v^2}}{x^2 - 2vx + 1}.$$
(2.12)

In the case $v = \cos \alpha \pi$ with $\alpha = p/q$, equation (2.10) does not have a unique solution, however, one can show easily that the one given by (2.12) is still appropriate.

If $|v| \ge 1$, the situation changes in that now the invariant measure does no longer have a density. Instead, we get

$$\nu_{v,v} = \delta_{x_+(v)} \tag{2.13}$$

where

$$x_+(v)=v+\sqrt{v^2-1}.$$

We may now compute, for E = v, the Lyapunov exponent using (2.7). We get, for |v| < 1,

$$\tilde{\gamma}(v,v) = \frac{i\pi}{4} + \frac{1}{2\pi} \int \ln x \frac{\sqrt{1-v^2}}{x^2 - 2vx + 1} dx$$
(2.14)

and thus

$$\gamma(v, v) = \int \ln |x| \frac{\sqrt{1 - v^2}}{x^2 - 2vx + 1} \, \mathrm{d}x = 0 \tag{2.15}$$

and

$$N(v, v) = \frac{1}{4} + \frac{1}{2\pi} \int_0^\infty \frac{\sqrt{1 - v^2}}{x^2 - 2vx + 1} \, \mathrm{d}x = \frac{3}{4} - \frac{\alpha}{2}.$$
 (2.16)

For $|v| \ge 1$ we have simply

$$\tilde{\gamma}(v,v) = \frac{3i\pi}{4} + \ln|x_{+}(v)|.$$
(2.17)

We recover thus the vanishing of the Lyapunov exponent if $|v| \le 1$, whereas for |v| > 1 it is always positive. In the next section we will derive the perturbation expansion around this exceptional energy.

3. Perturbation theory for |v| < 1

In this section we derive the perturbation expansion for the invariant measure, and consequently the Lyapunov exponent and the density of states, about the energy E = v.

The ideas follow closely those developed in [3] and [4] for the perturbation expansion in the standard Anderson model (the perturbation there being the small random potential), and the reader may find it useful to consult these references for supplementary details.

We put $E = v + \varepsilon$, with $|\varepsilon| \ll 1$. We may then write (2.8) as

$$(T_{2\nu+\varepsilon}^2 - 1)\phi_{\nu+\varepsilon,\nu}(x) = (1 - T_{\varepsilon}^2)\phi_{\nu+\varepsilon,\nu}(x)$$
(3.1)

the idea being that $(1 - T_{\varepsilon}^2)$ is 'small'. It is convenient to set $2v + \varepsilon = \tilde{E}$ fixed, and to expand only in the ε on the right-hand side of (3.1). Then, if $\phi_{v+\varepsilon,v}$ has an asymptotic expansion of the form

$$\phi_{\nu+\varepsilon,\nu}(x) = \sum_{n=0}^{\infty} \frac{\varepsilon^n}{n!} \phi_{\bar{E}}^{(n)}(x)$$
(3.2)

the coefficients $\phi_E^{(n)}$ satisfy the equations

$$(T_{\tilde{E}}^{t}-1)\phi_{E}^{(n)}(x) = \sum_{k=1}^{n} {\binom{n}{k}} \frac{\partial^{k}}{\partial \varepsilon^{k}} T_{\varepsilon}^{2} \phi_{E}^{(n-k)}(x)$$
$$= -\sum_{k=1}^{n} (-1)^{k} {\binom{n}{k}} \sum_{l=0}^{k} {\binom{k}{l}} \frac{d^{l}}{dx^{l}} \left(\frac{d}{dx} x^{2}\right)^{k-l} \phi_{E}^{(n-k)}(x)$$

where we have used that $T_{\varepsilon} = e^{-r d/dx} T_0$. The system of equations (3.4) can now be solved recursively, provided we can invert $(T_{\tilde{E}}^2 - 1)$. Assuming \tilde{E} irrational[†] this can conveniently be done by expanding $\phi_{\tilde{E}}^{(n)}$ in a basis of eigenfunctions of $T_{\tilde{E}}$. It is somewhat advantageous to do this by changing variables from $x \in IR$ to $\theta \in S_1$, via

$$x = \frac{\sin(\theta + \pi\alpha)}{\sin \theta} \qquad \text{where } 2\cos \pi\alpha = \tilde{E}. \tag{3.5}$$

Note that this entails

$$\frac{\mathrm{d}}{\mathrm{d}x} \rightarrow -\frac{\mathrm{d}}{\mathrm{d}\theta} \frac{\sin^2\theta}{\sin\pi\alpha}$$

and

$$T_{\tilde{E}} \rightarrow \tau_{\alpha}$$
: $\tau_{\alpha} h(\theta) = h(\theta - \pi \alpha).$

Note that also

$$\phi_{\tilde{E}}^{(0)}(x)\,\mathrm{d}x \to \frac{1}{\pi}\,\mathrm{d}\theta.$$

We set $h(\theta) d\theta = \phi_E(x) dx$. Equation (3.4) then becomes

$$(1-\tau_{\alpha}^{2})h^{(n)}(\theta) = \sum_{k=1}^{n} \binom{n}{k} \sum_{l=0}^{k} \binom{k}{l} \left(\frac{\mathrm{d}}{\mathrm{d}\theta} \frac{\sin^{2}\theta}{\sin\pi\alpha}\right)^{l} \left(\frac{\mathrm{d}}{\mathrm{d}\theta} \frac{\sin^{2}(\theta+\pi\alpha)}{\sin\pi\alpha}\right)^{k-l} h^{(n-k)}(\theta).$$
(3.6)

If we now expand h in its Fourier series via

$$h^{(n)}(\theta) = \frac{1}{\pi} \sum_{m=-\infty}^{\infty} e^{2im\theta} \hat{h}(n)(m)$$
(3.7)

† If \tilde{E} is rational we can easily modify the expansion to accommodate this energy too.

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we obtain

$$(1 - e^{-4i\pi\alpha m})\hat{h}^{(n)}(m) = \sum_{k=1}^{n} {n \choose k} \sum_{l=0}^{k} {k \choose l} \frac{1}{(\sin \pi \alpha)^{k}} (D^{l}M^{k-l}\hat{h}^{(n-k)})(m)$$
(3.8)

where D and M are matrices with entries

$$D_{ml} = \frac{im}{2} \left[\delta_{m,l+1} + \delta_{m,l-1} - 2\delta_{m,l} \right]$$
(3.9)

and

$$M_{ml} = \frac{im}{2} \left[\delta_{m,l+1} \, \mathrm{e}^{2\mathrm{i}\,\pi\alpha} + \delta_{m,l-1} \, \mathrm{e}^{-2\mathrm{i}\,\pi\alpha} - 2\delta_{m,l} \right]. \tag{3.10}$$

Note that as in previous examples [4] the structure of these equations is such that

$$\hat{h}^{(n)}(m) = 0 \qquad \text{for } |m| > n.$$

Equations (3.8) are now trivial to resolve. We will only use the first two orders here which are given explicitly by

$$\hat{h}^{(0)}(m) = \delta_{m,0}$$

$$\hat{h}^{(1)}(0) = 0$$

$$\hat{h}^{(1)}(\pm 1) = \frac{1}{\sin \pi \alpha} \frac{\pm i}{2} \frac{(1 + e^{\pm 2i\pi \alpha})}{1 - e^{\pm 4i\pi \alpha}}$$
(3.11)

or

$$h^{(1)}(\theta) = \frac{\cos(2\theta + 3\pi\alpha)}{2\pi\sin^2 \pi\alpha}.$$

We now use these results to compute the Lyapunov exponent and the density of states to second order in ε . Consider first the Lyapunov exponent. From (2.7) we obtain

$$\gamma(v+\epsilon, v) = \frac{1}{2} \int \ln|x| \nu_{v+\epsilon,v}(dx) + \frac{1}{2} \int \frac{1}{2} (\ln|\tau_{\epsilon}(x)| + \ln|\tau_{\bar{E}}(x)|) \nu_{v+\epsilon,v}(dx)$$
$$= \frac{1}{4} \int \ln|x| (1+T_{\epsilon}) \phi_{v+\epsilon,v}(x) dx$$
$$+ \frac{1}{4} \int \ln|x| (1+T_{\bar{E}}) \phi_{v+\epsilon,v}(x) dx \equiv I + II.$$
(3.12)

Note that by putting $y = \sqrt{x^2 - \tilde{E}x + 1}$, we get $|x| = y(x)/y(\tilde{E} - 1/x)$, so that the second term in (3.12) may be written as

$$H = \frac{1}{4} \int (\ln y(x) - \ln y(\tau_{\tilde{E}}(x)))(1 + T_{\tilde{E}})\phi_{v+e,v}(x) dx$$

$$= \frac{1}{4} \int \ln y(x)(1 - T_{\tilde{E}}^{2})\phi_{v+e,v}(x) dx$$

$$= \frac{1}{4} \int \ln y(x)(T_{e}^{2} - 1)\phi_{v+e,v}(x) dx. \qquad (3.13)$$

The first term becomes

$$I = \frac{1}{4} \int \ln|x| (1 + T_0 + (T_e - T_0)) \phi_{v + \varepsilon, v}(x) dx$$

= $\frac{1}{4} \int \ln|x| (T_e - T_0) \phi_{v + \varepsilon, v}(x) dx.$ (3.14)

We expand now everything in ε and keep only terms up to order ε^2 . This gives

$$I = \varepsilon \frac{1}{4} \int \ln|x| \frac{d}{dx} x^2 \phi_{\tilde{E}}^{(0)}(x) dx - \varepsilon^2 \frac{1}{4} \int \ln|x| \left(\frac{1}{2} \left(\frac{d}{dx} x^2\right)^2 \phi_{\tilde{E}}^{(0)}(x) - \frac{d}{dx} x^2 \phi_{\tilde{E}}^{(1)}(x)\right) dx$$
(3.15)

and

$$II = -\varepsilon \frac{1}{4} \int \ln y(x) \frac{d}{dx} (1+x^2) \phi_{\tilde{E}}^{(0)}(x) dx + \varepsilon^2 \frac{1}{4} \int \ln y(x) \left(-\frac{d}{dx} (1+x^2) \phi_{\tilde{E}}^{(1)}(x) + \left[\frac{d^2}{dx^2} x^2 + \frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \left(\frac{d}{dx} x^2 \right)^2 \right] \phi_{\tilde{E}}^{(0)}(x) \right) dx.$$
(3.16)

 $\phi_{\tilde{E}}^{(0)}$ and $\phi_{\tilde{E}}^{(1)}$ are known, so that the terms in (3.15), (3.16) can be computed explicitly. As could be expected, the terms proportional to ε sum to zero, and some lengthy but straightforward calculations show that

$$\gamma(v+\varepsilon,v) = \varepsilon^2 \left(\frac{20\cos 2\pi\alpha - 9}{32\sin^2 \pi\alpha} - \frac{\sin 3\pi\alpha (4\sin^2 \pi\alpha + 1)}{32\sin^3 \pi\alpha} \right) + O(\varepsilon^3).$$
(3.17)

This computation confirms the claim by Phillips et al [1] that the Lyapunov exponent vanishes quadratically.

For the density of states we obtain similarly that

$$N(v+\varepsilon, v) = \frac{1}{4} \int_{0}^{\infty} dx ((1+T_{\varepsilon})+(1+T_{\tilde{E}}))\phi_{v+\varepsilon,v}(x)$$

$$= \frac{1}{4} \int_{0}^{\infty} dx ((1+T_{0})+(1+T_{\tilde{E}}))\phi_{v+\varepsilon,v}(x) + \frac{1}{4} \int_{0}^{\infty} dx (T_{\varepsilon}-T_{0})\phi_{v+\varepsilon,v}(x)$$

$$= N(v+\varepsilon, v+\varepsilon) + \frac{1}{4} \int_{0}^{\infty} dx (1+T_{\tilde{E}})(\phi_{v+\varepsilon,v}-\phi_{\tilde{E}}^{(0)})$$

$$+ \frac{1}{4} \int_{0}^{\infty} dx (T_{\varepsilon}+T_{0})\phi_{v+\varepsilon,v}.$$
 (3.18)

We compute only the terms up to order ε explicitly. Using (3.11), one finds that

$$\int_0^\infty (1+T_{\tilde{E}})\phi_{\tilde{E}}^{(1)}(x)\,\mathrm{d}x = 0$$

and thus

$$N(v+\varepsilon, v) = N(v+\varepsilon, v+\varepsilon) - \varepsilon \frac{1}{2\pi} \sqrt{1-v^2} + O(\varepsilon^2)$$
$$= \frac{3}{4} - \frac{1}{2\pi} \cos^{-1} v + \frac{\varepsilon}{4\pi} \frac{(2-v^2)}{\sqrt{1-v^2}} + O(\varepsilon^2).$$
(3.19)

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Thus, we see that in spite of the vanishing of the Lyapunov exponent, the density of states behaves at this energy in a completely regular way. This is in strong contrast to, for example, the model with off-diagonal disorder [8], where the vanishing of the Lyaponov exponent at the band centre is accompanied by a divergence of the differentiated density of state.

Of course, as one would expect, this behaviour is somewhat altered as v approaches ± 1 ; in fact, a divergence appears in (3.17) and (3.19). But taking into account that for $\tilde{E} = 2 - \varepsilon$, $\alpha = \cos^{-1}(v - \varepsilon/2) \approx \sqrt{\varepsilon}$, one finds that in fact

$$N(1-\varepsilon,1) = \frac{3}{4} + \frac{\sqrt{\varepsilon}}{2\pi} + O(\varepsilon)$$
(3.20)

and

$$\gamma(1-\varepsilon,1) = \frac{\varepsilon}{4\pi} + O(\varepsilon^2). \tag{3.21}$$

Notice that in all cases the above formulas show that the number of states in an energy interval around E = v for which $\gamma \leq \delta$ is proportional to $\sqrt{\delta}$. Thus, for a finite system the number of states for which the localization length exceeds the size, L, of the system is proportional to $L^{1/2}$, as argued in [1].

4. Conclusions

The random dimer model provides a simple example for a disordered one-dimensional tight binding model where at an exceptional energy the localization length diverges. We have shown here the perturbation theory involving the invariant measure provides a useful tool to compute precisely the behaviour of the Lyapunov exponent and the density of states near this exceptional point. The results obtained support the argument of Dunlap *et al* [2] for an anomalous finite-size conductance at these energies since \sqrt{N} states are extended over the entire sample of size N. Still, a more refined analysis of the transport properties remains desirable.

We would like to stress that the particular properties of this model depend crucially on the fact that the potential can take on only two values. Any modification of the potential distribution enlarging its support will render the Lyapunov exponent strictly positive. For distributions that are small perturbations of the binary distribution treated here (e.g. two narrow Gaussians concentrated near $\pm v$), the general perturbative framework laid out above may of course be used to compute this effect.

The model considered here may be generalized in many directions. The general strategy would be to consider several allowed patterns ('words') of potentials over blocks of size, say n, and to distribute these words at random over the lattice. For appropriate choices of those words, one may achieve that the corresponding transfer matrices all commute at certain energies (the larger the blocks, the richer this set of energies can be made) what may allow for a vanishing of the Lyapunov exponent at these points. A particularly interesting scenario may arise if those blocks are taken as finite pieces of quasiperiodic structures; the resulting models then interpolate between random and quasiperiodic models. An analysis of this situation is in progress.

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