Nonmonotonic crossover and scaling behaviors in a disordered 1D quasicrystal

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We consider a noninteracting disordered 1D quasicrystal in the weak disorder regime. We show that the critical states of the pure model approach strong localization in strikingly different ways, depending on their renormalization properties. A finite size scaling analysis of the inverse participation ratios of states (IPR) of the quasicrystal shows that they are described by several kinds of scaling functions. While most states show a progressively increasing IPR as a function of the scaling variable, other states exhibit a nonmonotonic “re-entrant” behavior wherein the IPR first decreases, and passes through a minimum, before increasing. This surprising behavior is explained in the framework of perturbation renormalization group treatment, where wavefunctions can be computed analytically as a function of the hopping amplitude ratio and the disorder. Our results should help to clarify results of recent studies of localization due to random and quasiperiodic potentials.

It is established that, in many quasiperiodic models, electronic states are multifractal or “critical” in the absence of disorder [1–6]. The consequences of adding disorder to a quasiperiodic Hamiltonian have been studied as well, and rigorous arguments [7, 8] predict that the addition of (uncorrelated short-range) disorder, however weak, will result in all states becoming localized. While this statement holds for infinite systems, in this paper we consider finite samples (i.e., smaller than the localization length) to understand how critical states of the pure system change under addition of weak disorder. We will show that the answer to this question is dependent on the renormalization properties of the quasiperiodic chain and that different kinds of scaling functions can be defined for this problem. One motivation for our study comes from work on many-body localization in interacting quasiperiodic systems where the question of differences in the nature of the transition for quasiperiodic (also called pseudorandom) versus random potentials has been raised [9–11]. This question can also be directly addressed experimentally using cold atoms [12–14]. In this paper, we consider the noninteracting model to show that interesting new phenomena can occur when random disorder is added to deterministic but nonperiodic order.

Considering a tight-binding model on Fibonacci approximant chains in the weak disorder regime where the chain length is much smaller than the putative localization length, we show that a large (but sub-extensive) set of states exhibit a nonmonotonic approach to strong localization. This implies that some states are initially delocalized, in the sense that their inverse participation ratio (IPR) starts to decrease with disorder. These states subsequently begin “relocalizing” when the disorder exceeds a certain value, as one expects, and as verified in other studies [15]. We speculate that this type of nonmonotonic behavior could occur in a generic way when the pure quasicrystal is perturbed.

The model considered here is a tight-binding problem of the following form

$$H = \sum_i t_i (|i\rangle \langle i+1| + |i+1\rangle \langle i|) ,$$  \hspace{1cm} (1)

In this Hamiltonian, the hopping amplitudes $t_i = t_i^{(0)} + \epsilon_i$ are perturbed from the values $t_i^{(0)}$, the initial “pure” system hopping amplitudes which can take two values, $t_A$ or $t_B$ according to the deterministic Fibonacci sequence described below. The site energies are all assumed to be equal and can be set to zero by defining the origin suitably. The properties of the pure Hamiltonian depend on a single parameter, namely the hopping ratio $\rho = t_A/t_B$ henceforward supposed to be in the range $0 \leq \rho \leq 1$ (in the following we will set $t_B = 1$ without loss of generality). As customary in the Anderson localization literature, the random bond perturbations, $\epsilon_i$, are chosen as i.i.d. random variables taken from a uniform distribution in the interval $[-W/2, W/2]$, such that $\langle \epsilon \rangle = 0$ and $\langle \epsilon^2 \rangle = W^2/12$. The value of $W$ thus denotes the disorder strength. The sequence of hopping amplitudes $t_A$ and $t_B$ in the pure system corresponds to letters A and B of a specific series of chains leading in the infinite size limit to the Fibonacci quasicrystal. These chains $C_n$, termed approximants, can be built iteratively by concatenation, namely $C_{n+1} = C_n C_{n-1}$. With initial conditions $C_0 = B$ and $C_1 = A$, the next few chains are AB, ABA, ABAAB, and so on. The lengths of these chains then obey the Fibonacci recursion relation $L_{n+1} = L_n + L_{n-1}$ with initial conditions $L_0 = L_1 = 1$, and the ratio of lengths of successive chains $L_n/L_{n+1}$ tends to the (inverse) golden ratio.
mean \( \omega = (\sqrt{5} - 1)/2 \), in the limit \( n \to \infty \).

The properties of the pure model with no disorder (\( \epsilon_j = 0 \ \forall j \)) have been discussed in many classic papers, using a variety of methods, notably the powerful trace map method [3, 4], providing several exact results. It is known that all states are delocalized in the sense of a vanishing Lyapunov exponent [2], but critical. Detailed information on spectrum and states have been obtained using the perturbative renormalization group (RG) introduced by Niu and Nori and Kalugin et al. [16–18]. This approach gives quantitatively good predictions for the spectrum, eigenstates, and the quantum diffusion properties of wave packets for \( \rho \ll 1 \) [19–22]. This approach will be used below to interpret numerical results discussed next.

The averaged IPR corresponding to a given (normalized) eigenstate \( \alpha (\alpha = 1, \ldots, L) \) as a function of the disorder strength \( W \) is defined by

\[
\mathcal{I}_\alpha(W, L) = \left\langle \sum_{i=1}^{L} |\psi_\alpha(i)|^4 \right\rangle,
\]

(2)

where the brackets stand for the average over disorder. \( \mathcal{I} \) is just one of the set of \( q \)-moments of the probability of presence on each site. We consider the IPR (\( q = 2 \)) in this paper, as an indicator of localization adequate for our noninteracting model (for interacting case see [23] for a discussion of the diagnostic tool involving the Kohn localization tensor). Recall that for large system size \( L \), \( \mathcal{I} \to L^{-D_2} \) with \( D_2 \) having the value 1 for an extended state, 0 for a localized state and a value in-between for a critical state. In the Fibonacci chain approximants, the pure system IPR values \( \mathcal{I}_\alpha(0, L_n) \) fluctuate irregularly in a self-similar fractal way with the index \( \alpha \) due to very different properties of states under real space renormalization, as discussed below. In the presence of disorder, the IPR evolve as illustrated in Fig. 1 which shows \( \mathcal{I} \) as a function of \( W \) computed for \( \rho = 0.5 \), and \( n = 10 \) (89 sites). Four different levels are shown to illustrate the different behaviors which are seen. While the level at the lower band edge (\( \alpha = 1 \)) shows a steep increase with \( W \), others (such as \( \alpha = 3 \) and \( \alpha = 7 \)) show nonmonotonic behavior. The character strings in the figure are RG paths of each level, detailed in the next section.

As in the periodic model the critical point corresponds to \( \mathcal{W}_c = 0 \) (any disorder however weak localizes the critical states on the Fibonacci chain) with the localization length given by \( \xi \sim W^{-\nu} \), where the \( \nu \) is the correlation length exponent. In the weak disorder regime, the IPR is expected to have the scaling form

\[
\frac{\mathcal{I}_\alpha(W, L)}{\mathcal{I}_\alpha(0, L)} = f_\alpha(L/\xi)
\]

(3)

(see [24] for a more general discussion of finite size effects for the \( q \)-th moments of wavefunctions near the critical point of the Anderson model). Scaling plots for chains of generations \( n = 10 \) to \( n = 16 \) are presented in Fig. 2 for \( \rho = 1/2 \) (top panel) and \( \rho = 1/3 \) (bottom panel), showing good collapse for all the states when \( \mathcal{I} \) is plotted as a function of the scaling variable \( WL^{1/\nu} \), for the values \( \nu = 1.7 \pm 0.04 \) and \( \nu = 1.9 \pm 0.06 \) respectively [25]. Several different scaling functions \( f_\alpha \) are found, describing the variety of behaviors already seen in Fig. 1. Notice that our IPRs are defined with respect to a given state \( \alpha \) followed from one generation to the next, implying that the energies of the states move towards the band edge as the system size is increased. One can check numerically that the minima of the IPR of the states displaying the nonmonotonic behavior (as well as the wiggles and secondary minima of the other states) occur essentially when their energies start to cross with those of the neighboring levels (i.e., when the gaps become of the order of the fluctuations of energies), thereby suggesting that the changes of the behavior of the IPR are due to level repulsion.

Fig. 3 shows the dependence of the nonuniversal exponent \( \nu \) (blue filled circles) on the ratio of hopping amplitudes, \( \rho \). The values of \( \nu \) descend towards zero as \( \rho \) decreases, possibly logarithmically, to zero. However, this limit is difficult to study as some of the gaps between neighboring levels becomes extremely small leading to computational errors. In the periodic limit where \( \rho = 1 \), we find \( \nu = 2/3 \), in agreement with the result obtained for the disorder driven superfluid-insulator phase transition of noninteracting bosons [26]. This value corresponds, in that model as well, to scaling at the band edge. As noted by them, \( \nu = 2/3 \) violates the bound \( \nu \geq 2/d \) established by Chayes et al. [27] for random (interacting) systems, as well as the generalized Harris-Luck criterion \( \nu \geq 1/d \) [28] for aperiodic systems. This is not surprising since, unlike
the present case, these inequalities apply to transitions at finite disorder. In fact, in contrast with the band edge states, the state in the center of the spectrum at $\langle E \rangle = 0$ ($\alpha = 1 + [L_n/2]$ for $L_n$ odd) scales with the standard universal exponent $\nu = 2$ for all hopping ratios $\rho$ (see SI [29] for more details).

For large enough systems it is usual to define quantities *averaged over states* in the vicinity of fixed energy or chemical potential. An analysis of finite size scaling of the IPR at fixed energy $\langle E \rangle$ shows that it is described by a different exponent $\nu$ for all values of $E$ at fixed $\rho$ (see SI [29] for more details). The dependence of $\nu$ on the ratio of hopping amplitudes is also shown in Fig. 3 (red empty circles), showing that for $\rho \to 1$ we recover the standard value $\nu = 2$. This underscores the importance of distinguishing between the different situations when analyzing a given experimental system.

![Figure 2. Averaged IPR (normalized to $I(0, L)$) of several states ($\alpha = 1, 3, 6, 7, 28$) and system sizes ($n = 10, 12, 14, 16$) and for $t_A/t_B = 1/2$ (top panel) and $t_A/t_B = 1/3$ (bottom panel) showing data collapse as a function of the scaling variable $WL^{1/\nu}$ with $\nu = 1.7$ and $\nu = 1.9$ respectively. A similar behavior is found for all individual levels followed from one generation to the next. The nonmonotonicity of the IPR is more pronounced for smaller $\rho$ and disappears continuously in the periodic limit ($\rho \to 1$).](image)

We now briefly recall (for details see [22, 30]) the steps of the real space RG for the pure system before discussing the addition of randomness. Sites on a given chain are termed either "molecule" sites—pairs of sites coupled via $t_B$—or "atomic" sites—those with $t_A$ on both sides. One defines two different real space decimation procedures: i) decimating all atoms leaving only sites corresponding to molecules (mRG) or ii) decimating all molecules leaving only the atom sites (aRG). The following results are then obtained to lowest nontrivial order in $\rho$. Under mRG, an initial chain $C_n$ transforms to the chain $C_{n-2}$ after decimation, with new effective hopping amplitudes given by $|t'_A| = z t_A$ and $|t'_B| = z t_B$ where $z = \rho/2$. An energy shift of $+t_B$ (resp. $-t_B$) occurs with each molecular RG transformation of bonding (resp. antibonding) levels. Under aRG, an initial chain $C_n$ transforms to the chain $C_{n-3}$ after decimation, with new effective hopping amplitudes given by $|t'_A| = \pi t_A$ and $|t'_B| = \pi t_B$ where $\pi = \rho^2$. The ratio of the hopping amplitudes, $t_A/t_B$, is left invariant in both types of RG. Thanks to these transformations, the spectrum of the $n$-th chain can be built up from the spectra of the $n-2$ and $n-3$ generation chains. In the absence of disorder, the spectrum of an approximant chain has a self-similar structure with three main clusters, which are in turn split into three subclusters and so on.

For each energy level $E_n$ ($\alpha = 1, \ldots, L_n$), one can define the "renormalization path" or set of characters $a, m, \pi, \ldots$. Each element of this RG path is determined by whether the corresponding RG step was atomic or molecular. The bandwidth of this level (the width when periodic boundary conditions are assumed) then scales as $z^n m^{n-a}$, where $n_m$ denotes the total number of molecular RG steps, and $n_a$ the overall number of atomic RG steps in its RG path.

To each level described by some RG path, corresponds a wavefunction with support on sites having the same transformation properties under the RG. A wavefunction for energy $E$ for a given chain can be related to the wavefunction of a state of energy $E'$ on a smaller chain. The scale factors corresponding to mRG and aRG are denoted by $\lambda$ and $\pi$, respectively, with $|\psi^{(n)}(i, E)|^2 = \lambda^2 |\psi^{(n-2)}(i', E'/z)|^2 = \lambda (i', E'/z)^2$ and $|\psi^{(n,a)}(i, E)|^2 = \pi (i, E/\pi)^2$, where $i$ and $i'$ correspond to the site indices in the initial and final chains. The scale factors are $\lambda(\rho) = 1/(1 + 2\rho^2)$ and $\pi(\rho) = 1/(1 + 2\rho^2)$, to order $\rho^2$ [22]. It is the existence of these two distinct scale fac-
tors which leads to multifractality of the wavefunctions.

For a chain of generation $n$, the IPR of a state $\alpha$ corresponding to a given RG path can therefore be written as $I_n \sim (\lambda)^{2n}(\tilde{\lambda})^{2n}$ which is a function only of the number of mRG steps (since $n_a$ is determined by the constraint $2n_m + 3n_a \sim n$). The RG approach also gives the dependence of the IPR with system size: $I(E, L_n) \sim L_n^{-D_2(E)}$ where the exponent $D_2(E)$ measures the “mass scaling” of the atoms associated with the state of energy $E$. An explicit calculation of $D_2(E)$ [21, 22] shows that, in the limit $n \to \infty$, states at the edge of the spectrum (for which $n_m = n/2$) are “more extended”, i.e. have a larger value of $D_2$, than the state in the center (for which $n_m = 0$).

This RG scheme can be extended to the disordered model, for weak disorder on finite chains. We require that $W$ be smaller than the smallest gaps of the spectrum ($W < \pi^{n/3}$). This ensures that the branching hierarchical structure of the spectrum is conserved and the RG path structure of the pure system is not changed (no level crossing due to the random perturbation occurs). A straightforward extension of the degenerate (Brillouin-Wigner) perturbation theory (discussed in the SI [29]) gives the effective hopping amplitudes under mRG and aRG. For small $W$, after the first RG step the onsite energy and the hopping amplitudes are given up to second order in the perturbations as follows:

|        | $m\text{RG}$ | $a\text{RG}$ |
|--------|--------------|--------------|
| $\xi_i$ | $\epsilon$   | 0            |
| $t_B'$  | $\frac{1}{2} \frac{(t_A + \epsilon_i)}{t_B}$ | $- \frac{(t_A + \epsilon_i)(t_A + \epsilon'_{j})}{t_B}$ |
| $t_A'$  | $\frac{1}{2} \frac{(t_A + \epsilon_i)(t_A + \epsilon'_{j})}{t_B}$ | $- \frac{(t_A + \epsilon_i)(t_A + \epsilon'_{j})}{t_B}$ |

where as already stated, the $\epsilon$ are i.i.d. random variables. Disordering the Fibonacci chain therefore leads to small onsite energy corrections $\xi_i$ (zero for aRG at this order) and modified renormalized hopping amplitudes. From Eq. (4) one sees that the average renormalized hopping amplitudes are unchanged from their pure values, but their variance is proportional to $W^2$. The spectrum is broadened—i.e. while the average value or center of mass of minibands of the chain are not shifted at lowest order, their widths increase with the disorder strength. For $W$ small enough that levels do not overlap, the RG can therefore proceed as in the pure case. Wavefunctions are determined by the coupling ratio, whose average value is renormalized to $\rho' = \rho + W^2$ and therefore increases under RG. Since small $\rho$ corresponds to stronger quasiperiodic modulation, one observes that the disorder diminishes the quasiperiodic modulation—as the number of RG steps increases one gets a homogeneously disordered chain in the large distance limit.

For strong values of disorder gaps are filled in progressively, with the two largest gaps of width $\sim t_B - t_A$ being the last to disappear (when $W$ becomes of the order of $t_B$). At large disorder, a disordered band is formed which corresponds to a final molecular state $\alpha$.

The different types of IPR scaling functions seen in Figs. 1 and 2 can be now be explained in terms of the nature of the level after the last RG step, which can be either atomic or molecular. We can distinguish between four cases in fact, since the last RG step can correspond to mRG or aRG. These four classes of levels have wavefunctions with support on sites which have the same RG characteristics—these are shown in the inset of Fig. 4 along with the final form (molecule or atom). The strong bonds (represented by double lines) of each cluster are taken to be $t_B + \epsilon_j$ and the weak bonds (single lines) are $t_A + \epsilon_j$. The variation of the IPR $\Delta I$ can be found by diagonalizing the pure Hamiltonian as a function of $\rho$, and computing wavefunction corrections in standard second order perturbation theory in $\epsilon_j$ (see SI [29] for more details). It is then averaged over all random variables of the cluster. We give below the results for the $m$ level (cluster a and b) and $a$ level (cluster c and d). As the full functions of $\rho$ are cumbersome, we give the results after expansion around a point $\rho_0$:

\begin{align*}
  a) & \quad \frac{\Delta I}{I(0)} \approx [11.32 - \frac{43.83}{\bar{\rho} + 147.12(\bar{\rho})^2}] \bar{W}^2, \\
  b) & \quad \frac{\Delta I}{I(0)} \approx [0.15 + \frac{10.98}{\bar{\rho} - 4.11(\bar{\rho})^2}] \bar{W}^2, \\
  c) & \quad \frac{\Delta I}{I(0)} \approx [-0.77 + \frac{5.25}{\bar{\rho} + 10.19(\bar{\rho})^2}] \bar{W}^2, \\
  d) & \quad \frac{\Delta I}{I(0)} \approx [-0.14 + \frac{13.6}{\bar{\rho} + 3.22(\bar{\rho})^2}] \bar{W}^2,
\end{align*}

with $\bar{\rho} = \rho - \rho_0$, for $\rho_0 = 0.45$. In these expressions,
\(\tilde{W}\) denotes the width of effective renormalized distribution, which increases with the number of RG steps. Fig 4 shows plots of the four functions in Eq. (5) for \(\phi = 0.01\). These curves should be considered, for this value of the hopping ratio only as qualitative indications of the behavior of these states, as the theory is quantitatively accurate only for values \(\rho < 1\). Exact diagonalization results confirm, in fact, that the IPR of all levels depends quadratically on the disorder for \(W \to 0\) (see SI [29] for more details). Comparing with the \(W \to 0\) regime of Fig. 1, these results for the curvature correspond to the initial behavior of the curves: levels of type a) and b) corresponding to molecular final states have positive curvatures, while c) and d) corresponding to atomic final states have negative curvatures. Case (a) describes band edge states, which localize the most rapidly as disorder is increased compared to the other curves. More differences between levels will appear when longer range structural information is included. The results given in Eq. (5) are not qualitatively changed upon adding onsite randomness. To repeat, the behavior shown in Fig. 4 is expected only for very small disorder. For large \(W\), differences between “strong” and “weak” bonds cease to exist and the standard Anderson model is recovered, in which the IPR increases with \(W\) (as discussed above, this occurs when the disorder strength becomes of the order of the gaps with the neighboring states and level repulsion sets in). The negative-curvature \(\Delta(I)/I\) curves will therefore eventually “bottom out” and start increasing with \(W\), as we saw in Fig. 2. [Notice that the IPR of all the states tend to 1/2 in the \(W \to \infty\) limit for the model described by the Hamiltonian (1).]

To sum up, we have shown, by considering finite approximants of the Fibonacci chain, that the addition of disorder in a model with critical states can lead to an effect of delocalization followed by localization of a subset of levels. We have presented an argument to explain the disorder-dependence of IPR for levels as a function of their RG path. The states which exhibit nonmonotonic behavior are those which under RG ultimately are reduced to a single “atom” level \((\alpha = 3, 7, 11, 15, 20, 24, 28, 32, 36, \ldots)\), while the other levels show the expected monotonic increase of the IPR with \(W\). The number of the nonmonotonic “atom” states diverges with the system size as \(L^\beta\), with \(\beta = \ln 2/(2\ln(1/\omega)) \approx 0.72\). Hence they represent a sub-extensive set of all the eigenstates. For stronger values of disorder, an upturn of the curves will eventually occur, as localization lengths become smaller than the chain length, and the usual Anderson localization physics is recovered. The exponent \(\nu\) describing the approach to strong localization depends on the parameter \(\rho\), tending to very small values for \(\rho \to 0\), beyond the region of reliability of the numerical computations. The scaling functions for the IPR are different according to the nature of the level, and are nonmonotonic. These characteristics show that this localization transition is in a different universality class from the standard Anderson model, which is recovered in the limit \(\rho = 1\), with the value \(\nu = 2/3\) as found previously in a different context by Cestari et al. [26]. A similar result has been recently found in [32] where it was shown that Anderson localization in a 2D generalization of the Aubry-André model appears to be in a quite different universality class from the same model with random potentials.

Some works [33, 34] incorporate geometrical forms of disorder where segments of the chains are flipped. From analyzing Lyapunov exponents using RG [34] and by direct transfer matrix methods, it was concluded that localization does not occur in this case. More detailed finite size scaling analyses of the phason-disordered 1D Fibonacci chains are probably necessary before this issue can be definitely settled. In this context, we note that a similar type of geometrical disorder is considered in a 2D model, and shown to lead to localization of all states [35].

The reentrant delocalization-localization of certain states could also be observable in experiments on multilayer systems, by means of precise measurements of the transport in mesoscopic samples. In this context it can be noted that, for three dimensional quasicrystals such as AlCuFe, it was long ago pointed out that structural disorder tends to improve conductivity [36].

Our results can be expected to have relevance for the debate on many-body localization due to disorder versus localization due to pseudo-disorder [9–11]. Questions concerning the critical properties for each case are not just theoretical problems, but are now amenable to experimental verification using cold atoms [12–14]. Our results suggest that the transition might have an intermediate regime, where finite size effects can be anomalous. Generally speaking, adding perturbations to the pure noninteracting Hamiltonian could produce non-monotonic or re-entrant behavior.

In this respect, some important theoretical questions still remain open. A first natural question concerns the robustness of our findings with respect to the nature of the random perturbation. While it is reasonable to expect that the addition i.i.d. onsite disorder and/or the choice of Gaussian vs box distributions should not significantly alter the scenario discussed here, heavy-tailed and/or correlated randomness might drastically change the results. Another intriguing direction would be to study the effect of other kinds of random perturbations, e.g., adding to the pure Hamiltonian (1) weak long-range matrix elements with a small probability, thereby transforming the 1D chain into a sparse random matrix ensemble with a Fibonacci backbone. Preliminary results on this model seem to indicate that the same kind of nonmonotonic behavior of the IPR as a function of the strength of the long-range hopping is observed for the same states (the atomic final states) as for the disordered case, suggesting that the way in which individual levels respond to perturbations might be a specific (and robust)
feature of their individual critical properties. Finally, it would also be interesting to investigate the region of the phase diagram $t_A > t_B$ ($\rho > 1$) for which much less is known even in the pure limit.

Acknowledgments

We are grateful to J.-N. Fuchs, J.-M. Luck, N. Macé, F. Piechon, and J. Vidal for many illuminating discussions. P.J. would like to thank the Idex PALM of University Paris-Saclay for financial support during this project. M.T. is a member of the Institut Universitaire de France.

[1] S. Ostlund et al. Phys. Rev. Lett., 50:1873, 1983.
[2] François Delyon and D. Petritis. Comm. Math. Phys., 103:441, 1986.
[3] Mahito Kohmoto, Leo P. Kadanoff, and Chao Tang. Localization problem in one dimension: Mapping and escape. Phys. Rev. Lett., 50:1870–1872, Jun 1983. doi: 10.1103/PhysRevLett.50.1870. URL https://link.aps.org/doi/10.1103/PhysRevLett.50.1870.
[4] Mahito Kohmoto, Bill Sutherland, and Chao Tang. Critical wave functions and a cantor-set spectrum of a one-dimensional quasicrystal model. Phys. Rev. B, 35:1020–1033, Jan 1987. doi: 10.1103/PhysRevB.35.1020. URL https://link.aps.org/doi/10.1103/PhysRevB.35.1020.
[5] C. Tang and M. Kohmoto. Phys. Rev. B, 34:2041, 1986.
[6] H. H. Hiramoto and M. Kohmoto. Phys. Rev. B, 40:8225, 1989.
[7] François Delyon, Yves-Emmanuel Lévy, and Bernard Souillard. Approach à la borland to multidimensional localization. Phys. Rev. Lett., 55:618–621, Aug 1985. doi: 10.1103/PhysRevLett.55.618. URL https://link.aps.org/doi/10.1103/PhysRevLett.55.618.
[8] S. Kotani and B. Simon. Comm. Math. Phys., 112:103–119, 1987.
[9] Shankar Iyer, Vadim Oganesyan, Gil Refael, and David A. Huse. Many-body localization in a quasiperiodic system. Phys. Rev. B, 87:134202, Apr 2013. doi: 10.1103/PhysRevB.87.134202. URL https://link.aps.org/doi/10.1103/PhysRevB.87.134202.
[10] Mac Lee, Thomas R. Look, S. P. Lim, and D. N. Sheng. Many-body localization in spin chain systems with quasiperiodic fields. Phys. Rev. B, 96:075146, Aug 2017. doi: 10.1103/PhysRevB.96.075146. URL https://link.aps.org/doi/10.1103/PhysRevB.96.075146.
[11] Vedika Khemani, D. N. Sheng, and David A. Huse. Two universality classes for the many-body localization transition. Phys. Rev. Lett., 119:075702, Aug 2017. doi: 10.1103/PhysRevLett.119.075702. URL https://link.aps.org/doi/10.1103/PhysRevLett.119.075702.
[12] Pranjal Bordia, Henrik P. Lüschen, Sean S. Hodgman, Michael Schreiber, Immanuel Bloch, and Ulrich Schneider. Coupling identical one-dimensional many-body localized systems. Phys. Rev. Lett., 116:140401, Apr 2016. doi: 10.1103/PhysRevLett.116.140401. URL https://link.aps.org/doi/10.1103/PhysRevLett.116.140401.
[13] B. Deissler et al. Nature Physics, 6:354, 2010.
[14] Junpeng Hu, Haiping Hu, Kuei Sun, and Chuanwei Zhang. Phys. Rev. Lett., 120:060407, 2018.
[15] Youyan Liu and Rolf Riklund. Electronic properties of perfect and nonperfect one-dimensional quasicrystals. Phys. Rev. B, 35:6034–6042, Apr 1987. doi: 10.1103/PhysRevB.35.6034. URL https://link.aps.org/doi/10.1103/PhysRevB.35.6034.
[16] Q. Niu and F. Nori. Phys. Rev. Lett., 57:2057, 1986.
[17] Q. Niu and F. Nori. Phys. Rev. B, 42:10329, 1990.
[18] P. Kalugin, A. Kitaev, and L. Levitov. Electron spectrum of a one-dimensional quasicrystal. Sov. Phys. JETP, 64(2), 1986. URL http://www.jetp.ac.ru/cgi-bin/e/index/e/64/2/p410a?list.
[19] Frédéric Pichon, Mourad Benakli, and Anuradha Jagannathan. Analytical results for scaling properties of the spectrum of the fibonacci chain. Phys. Rev. Lett., 74:5248–5251, Jun 1995. doi: 10.1103/PhysRevLett.74.5248. URL https://link.aps.org/doi/10.1103/PhysRevLett.74.5248.
[20] Frédéric Pichon. Anomalous diffusion properties of wave packets on quasiperiodic chains. Phys. Rev. Lett., 76:4372–4375, Jun 1996. doi: 10.1103/PhysRevLett.76.4372. URL https://link.aps.org/doi/10.1103/PhysRevLett.76.4372.
[21] Stefanie Thiem and Michael Schreiber. J. Phys. Cond. Mat., 25:075503, 2013.
[22] Nicolas Macé, Anuradha Jagannathan, and Frédéric Pichon. Fractal dimensions of wave functions and local spectral measures on the fibonacci chain. Phys. Rev. B, 93:205153, May 2016. doi: 10.1103/PhysRevB.93.205153. URL https://link.aps.org/doi/10.1103/PhysRevB.93.205153.
[23] V. K. Varma, S. Pilati, and V. E. Kravtsov. Conduction in quasiperiodic and quasirandom lattices: Fibonacci, riemann, and anderson models. Phys. Rev. B, 94:214204, Dec 2016. doi: 10.1103/PhysRevB.94.214204. URL https://link.aps.org/doi/10.1103/PhysRevB.94.214204.
[24] Alberto Rodriguez, Louella J. Vasquez, Keith Slevin, and Rudolf A. Römer. Multifractal finite-size scaling and universality at the anderson transition. Phys. Rev. B, 84:134209, Oct 2011. doi: 10.1103/PhysRevB.84.134209. URL https://link.aps.org/doi/10.1103/PhysRevB.84.134209.
[25] Data are averaged over 262144, 65536, 12288, and 2048 realizations for $n = 10, 12, 14,$ and 16 respectively.
[26] J. C. C. Cestari, A. Foerster, M. A. Gusmão, and M. Continentino. Critical exponents of the disorder-driven superfluid-insulator transition in one-dimensional bose-einstein condensates. Phys. Rev. A, 84:055601, Nov 2011. doi: 10.1103/PhysRevA.84.055601. URL https://link.aps.org/doi/10.1103/PhysRevA.84.055601.
[27] J. T. Chayes, L. Chayes, Daniel S. Fisher, and T. Spencer. Finite-size scaling and correlation lengths for disordered systems. Phys. Rev. Lett., 57:2999–3002, Dec 1986. doi: 10.1103/PhysRevLett.57.2999. URL https://link.aps.org/doi/10.1103/PhysRevLett.57.2999.
[28] J. M. Luck. Europhysics Lett., 24:359, 1993.
[29] Supplementary material.
[30] Stefanie Thiem and Michael Schreiber. Renormalization group approach for the wave packet dynamics in golden-mean and silver-mean labyrinth tilings. Phys. Rev. B, 85:224205, Jun 2012. doi:
[31] Bernhard Kramer and Angus MacKinnon. Rep.Prog. Phys., 56:1469–1564, 1993.

[32] T. Devakul and D.A. Huse. Anderson localization transitions with and without random potentials Phys. Rev. B 96:214201, 2017.

[33] Danhong and Danrung Huang. Phys. Rev. B, 70:205124, 2004.

[34] M. T. Velhinho and I. R. Pimentel. Lyapunov exponent for pure and random fibonacci chains. Phys. Rev. B, 61:1043–1050, Jan 2000. doi:10.1103/PhysRevB.61.1043. URL https://link.aps.org/doi/10.1103/PhysRevB.61.1043.

[35] Jean-Noël Fuchs and Julien Vidal. Hofstadter butterfly of a quasicrystal Phys. Rev. B 94:205437, 2016.

[36] D. Mayou, C. Berger, F. Cyrot-Lackmann, T. Klein, and P. Lanco. Evidence for unconventional electronic transport in quasicrystals. Phys. Rev. Lett., 70:3915–3918, Jun 1993. doi:10.1103/PhysRevLett.70.3915. URL https://link.aps.org/doi/10.1103/PhysRevLett.70.3915.
Nonmonotonic crossover and scaling behaviors in a disordered 1D quasicrystal: 
Supplementary material

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(Dated: September 20, 2018)

In this supplementary material we provide more details and results related to several points discussed in the main text.

FINITE SIZE SCALING

The top panel of Fig. 1 shows the scaling plots of the IPR as a function of the disorder $W$ of the state at the center of the spectrum ($\alpha = 1 + [L_n/2]$ for $L_n$ odd). As for Fig. 2 of the main text, data are averaged over 262144, 65536, 12288, and 2048 realizations for $n = 10, 12, 14,$ and 16 respectively. A good collapse of the data for several system sizes is found in terms of the scaling variable $WL^{0.5}$ (corresponding to the standard exponent $\nu = 2$) for all values of the hopping ratio $\rho$. Note that a nonuniversality of the IPR of the center state starts to appear for $\rho \lesssim 1/2$ and becomes more pronounced as $\rho$ is further decreased.

The bottom panel of Fig. 1 shows instead the scaling behavior of the IPR averaged over a small but finite fraction of the states around a fixed energy. In practice here we considered 1/16 of states around $\langle E \rangle = 0$. In this case the data for several different systems sizes show good collapse when plotted in terms of the scaling variable $WL^{1/\nu}$. We find a nonuniversal $\rho$-dependent exponent $\nu$ which decreases (possibly logarithmically) to zero as $\rho \to 0$ and approaches the standard value $\nu = 2$ in the pure case, $\rho \to 1$ (see Fig. 3 of the main text). A similar behavior is found for other values of the energy $\langle E \rangle$ in the bulk of the spectrum (away from big gaps). Note that no signs of the nonmonotonic behavior is seen in this case.

In Fig. 2 we show the results of exact diagonalizations for $|I_\alpha(W, L) - I_\alpha(0, 0)|$ as a function of $W$ in the small $W$ region for $n = 12$ ($L = 233$) and for several states (the same as Fig. 2 of the main text) and three different values of $\rho$. This plot confirms that the IPR of all states behaves quadratically for $W \to 0$ as

$$I_\alpha(W, L_n) \simeq I_\alpha(0, L_n) + c_\alpha^{(n)} W^2,$$

with positive or negative coefficients $c_\alpha^{(n)}$ depending on the level index (e.g., $c_\alpha^{(n)} < 0$ for $\alpha = 3, 7, 11, 15, 20, 24, 28, 32, 36, \ldots$). This is precisely the behavior predicted by the real space RG approach [see Eq. (5) of the main text].

DEGENERATE PERTURBATION THEORY FOR DISORDERED MODEL

We wish to compute the renormalized hopping amplitudes, $t'_A$ and $t'_B$ obtained for a disordered Fibonacci chain in which the bonds have values of either $t_A + \epsilon_j$ (weak bond) or $t_A + \epsilon_j$ (strong bond) [see Eq. (4) of the main text]. Although the onsite energies in the model are taken to be 0, diagonal terms will be generated under RG, and are denoted $\xi_j$, and we will also calculate their renormalized values. The zero-order Hamiltonian $H_0$ is off-diagonal, and consists only the pure strong couplings $t_B$, while the perturbation $H_1$ contains the weak bonds and diagonal onsite energy terms, $\xi_j$. In Brillouin-Wigner perturbation theory for degenerate states, the effective Hamiltonian is given by [1]

$$H_{\text{eff}} = QH_0 Q + QH_1 Q + QH_1 P \frac{1}{E - H_0} PH_1 Q + \ldots$$

(Supplementary Figure 1. Top panel: Averaged IPR (normalized to $I(0, L)$) of the center state ($\alpha = 1 + [L_n/2]$) for $n = 10$ (circles), $n = 12$ (squares), and $n = 16$ (diamonds)) and for $t_A/t_B = 4/5$ (blue), $t_A/t_B = 1/2$ (red), and $t_A/t_B = 1/3$ (green) showing data collapse as a function of the scaling variable $WL^{0.5}$. Bottom panel: IPR (normalized to $I(0, L)$) averaged over 1/16 of the states around $E = 0$ for $n = 10$ (circles), $n = 12$ (squares), $n = 14$ (diamonds), and $n = 16$ (up triangles) and for $t_A/t_B = 4/5$ (blue), $t_A/t_B = 1/2$ (red), and $t_A/t_B = 1/3$ (green) showing data collapse as a function of the scaling variable $WL^{1/\nu}$.)

in the subspace of energy $E$, where the operator $Q = \sum_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ is the projection operator for states in this subspace, and $P = 1 - Q$.

Figure 3. a) Cluster for strong bond calculation (mRG); b) Cluster for weak bond calculation (mRG).

We now illustrate the calculation of parameters of the effective Hamiltonian after a molecular RG (mRG), namely the onsite energies $\xi'_j$, and the renormalized strong and weak couplings $t'_B, t'_A$. Fig. 3a) shows the cluster of sites which renormalize to give a strong bond after mRG. The three bonds are $t_B + \epsilon_1$, $t_A + \epsilon_2$ and $t_B + \epsilon_3$. The onsite energies are zero in the first RG step, but subsequently acquire nonzero values which are denoted by $\xi_j$ ($j = 1$ to 3). The eigenstates of $H_0$ are $|\psi_1\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$, $|\psi_2\rangle = (|3\rangle + |4\rangle)/\sqrt{2}$, corresponding to $E = t_B$, and $|\psi_3\rangle = (|1\rangle - |2\rangle)/\sqrt{2}$, and $|\psi_4\rangle = (|3\rangle - |4\rangle)/\sqrt{2}$, corresponding to $E = -t_B$.

Using Eq. (1) the onsite energy for the leftmost molecular bonding state, is, to lowest nonvanishing order

$$\xi'_1 = \langle\psi_1|H_{\text{eff}}|\psi_1\rangle = \frac{1}{2}(\xi_1 + \xi_2) + \epsilon_1,$$

with a similar result for the onsite energy for the right molecular state. The effective (strong) hopping amplitude between the two bonding molecular states is

$$t'_B \equiv \langle\psi_1|H_{\text{eff}}|\psi_2\rangle = \frac{1}{2}(t_A + \epsilon_2).$$

The renormalized weak coupling is found by considering the cluster in Fig. 3b) consisting of five sites. The eigenstates of $H_0$ are now $|\psi_1\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$, $|\psi_2\rangle = (|4\rangle + |5\rangle)/\sqrt{2}$, corresponding to $E = t_B$, $|\psi_3\rangle = |3\rangle$, $|\psi_4\rangle = (|1\rangle - |2\rangle)/\sqrt{2}$, and $|\psi_5\rangle = (|4\rangle - |5\rangle)/\sqrt{2}$, corresponding to $E = -t_B$. The effective (weak) hopping amplitude is of second order:

$$t'_A \equiv \langle\psi_1|H_{\text{eff}}|\psi_2\rangle = \frac{1}{2t_B}(t_A + \epsilon_2)(t_A + \epsilon_3).$$

Figure 4. a) Cluster for strong bond calculation (aRG); b) Cluster for weak bond calculation (aRG).

For atomic RG, the clusters to consider for the new strong and weak amplitudes are shown in Fig. 4. The onsite energy and strong and weak hopping amplitudes after aRG are found to be

$$\xi'_1 = \xi_1,$$

$$t'_B = -(t_A + \epsilon_1)(t_A + \epsilon_3)/t_B,$$

$$t'_A = (t_A + \epsilon_1)(t_A + \epsilon_3)(t_A + \epsilon_3)/t_B^2.$$

**IPR CORRECTIONS DUE TO DISORDER**

In this section we provide some details of the calculations the changes of IPR due to disorder for states which renormalize after the ultimate RG step to either a “molecule” or to an “atom”. We consider the hopping model of Eq. (1), where each of the hopping terms is either a perturbed strong ($t_B + \epsilon_j$) or perturbed weak ($t_A + \epsilon_j$) bond, where $\epsilon_j$ are i.i.d. variables uniformly distributed in $[-W/2, W/2]$. In the pure system, the wavefunctions corresponding to the levels of interest have their support primarily (for small $\rho$) on specific groups of sites arranged as in the four clusters shown in the inset of Fig. 4. Weak disorder leads to a small redistribution of amplitudes, that we want to compute, perturbatively. We will be interested in the IPR change of specific states: the band edge molecular level $\alpha = 1$ for clusters (a) and (b), and in the atom level close to/at the center for the clusters (c) and (d). The full Hamiltonian is off-diagonal, with $L$ sites and $L - 1$ bonds. The latter can be strong or weak bonds, with weak disorder in each of the hopping amplitudes, as given in Eq. (1). The aim of the calculations is to compute the changes of IPR due to the disorder for specific states on each of the clusters, using second order perturbation theory.

As contrasted with the Brillouin-Wigner perturbation expansion for degenerate states, in this section, we will
proceed by splitting the Hamiltonian differently as follows: \( H = H_F + H_d \), where the Fibonacci Hamiltonian \( H_F \) includes the pure strong and weak bonds \((t_B \text{ and } t_A)\), and \( H_d \) contains the disordered part, \( \epsilon_j \). For a given cluster of \( L \) sites, the normalized eigenstates of \( H_F \), denoted by \( \{ |\psi_\alpha \rangle \} \) (with \( \alpha = 1, \ldots, L \)) are nondegenerate and can be computed exactly as a function of \( \rho = t_A/t_B \). For each of the clusters the IPR of the state \( \alpha \) at zero order of the perturbation is then given by \( I(0) = \sum_i |\psi_\alpha(i)|^4 \).

Using standard perturbation theory, the first and second order corrections to the wavefunction are

\[
|\psi_\alpha(1)\rangle = \sum_{\beta \neq \alpha} \frac{\langle \psi_\beta | H_d | \psi_\alpha \rangle}{E_\alpha - E_\beta} |\psi_\beta\rangle,
\]

\[
|\psi_\alpha(2)\rangle = \sum_{\beta \neq \alpha} \left[ -\frac{\langle \psi_\alpha | H_d | \psi_\alpha \rangle \langle \psi_\beta | H_d | \psi_\alpha \rangle}{(E_\alpha - E_\beta)^2} + \frac{\langle \psi_\beta | H_d | \psi_\gamma \rangle \langle \psi_\gamma | H_d | \psi_\alpha \rangle}{(E_\alpha - E_\beta)(E_\alpha - E_\gamma)} \right] |\psi_\beta\rangle,
\]

which are combined with the zero order term to give \( |\psi'_\alpha\rangle \). The new IPR is then given by \( I' = \sum_i |\psi'_\alpha(i)|^4 / (\sum_i |\psi_\alpha(i)|^2)^2 \). As there is no convenient closed form expression as a function of \( \rho \) for the fractional change defined by \( \Delta I/I(0) = (I' - I(0))/I(0) \), Eq. (5) of the main text presents the results for each of the four states in terms of an expansion around a point \( \rho = \rho_0 \).

[1] Q. Niu and F. Nori. Phys. Rev. B, 42:10329, 1990.