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Exact evaluation of the causal spectrum and localization properties of electronic states on a scale-free network

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HIGHLIGHTS

- Exact and numerical spectral analysis of a scale invariant tree's adjacency matrix.
- Exact expression for localization property of tight-binding eigenfunctions.
- Localization properties impact design of experimental devices like photonic crystals.

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ABSTRACT

A deterministic network with tree structure is considered, for which the spectrum of its adjacency matrix can be exactly evaluated by a recursive renormalization approach. It amounts to successively increasing number of contributions at any finite step of construction of the tree, resulting in a causal chain. The resulting eigenvalues can be related the full energy spectrum of a nearest-neighbor tight-binding model defined on this structure. Given this association, it turns out that further properties of the eigenvectors can be evaluated, like the degree of quantum localization of the tight-binding eigenstates, expressed by the inverse participation ratio (IPR). It happens that, for the current model, the IPR's are also suitable to be analytically expressed in terms in corresponding eigenvalue chain. The resulting IPR scaling behavior is expressed by the tails of eigenvalue chains as well.

1. Introduction

Most physical systems living on heterogeneous structure behaves quite different from those living on homogeneous backgrounds with translational invariance and other symmetries, as exemplified by the analysis of several quantum models in the past few decades [1–6]. The anomalies include, for instance, the multifractal properties of the energy spectrum, the low-dimensional Bose–Einstein condensation, and the log-periodic oscillation of thermodynamic properties [7–9]. These unique properties are usually related to exact or statistical scale invariance.

The scale-free distribution of node-degree in a large class of complex networks stands among the most interesting properties entailed by heterogeneity and, correspondingly, has received a huge attention of the community working in many different branches of science [10–13]. Many real-world networks with the scale-free properties usually show self-similarity

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under a scale transformation, which leads to interesting critical behaviors for some statistical models [14–17,6,18]. On the other hand, it is possible to construct scale-free networks following an iterative self-repeating pattern [19,20] according to some simple rules. The resulting deterministic network topology has a clear hierarchical structure [21], making it possible to evaluate the properties of physical systems with a chosen complexity using both theoretical and numerical approaches. For a long time lapse, experimental setups based on optical lattices could not adequately reproduce a complex network with no translational symmetry. Thus, it was rather difficult to test a non-homogeneous theory defined on a deterministic scale-free network. However, recent advances in experimental implementation [22] of large-scale photonic chips cast new light on the testing of non-homogeneous quantum walks and similar theories. By tracking the dynamics of photons trapped by deterministic waveguide networks, one should directly observe the distribution of walking bosons and their localization properties. Also, because the fabrication of photonic circuits introduces a controllable disorder in the correlation of sites, photonic chips can simulate a scale-free "crystal structures" with disorder.

This study is focused on the localization properties of non-interacting particles trapped on a hierarchical tree. This choice is justified by the fact that, compared to other complex hierarchical structures studied before [23–25], a loopless tree is much easier to be implemented inside a photonic chip. Therefore, this allows our results to be tested by more sophisticated, large-scale photonic chips in the future. We use a tight-binding approach, where the Hamiltonian takes into account nearest neighbor interactions. The energy spectrum of such Hamiltonian models has been exactly solved for a number of self-similar scale-free networks by using renormalization techniques [26,27]. In most cases, the spectrum has a hierarchical structure that increases in complexity along with the iteratively constructed underlying network. The hierarchical relation among eigenvalues can be usually expressed by means of simple formulae, from which one can derive the spectrum as a one-dimension Julia set [28,29] invariant under iteration. For other non-scale-free networks such as the Sierpinski gasket and Koch curve, similar hierarchical spectra also exist [30–32]. Along the same lines, the degree of localization of a corresponding eigenstates should depend on the hierarchical structure as well.

Despite several numerical investigations based on the use of the inverse participation ratio (IPR) to characterize the degree of quantum localization [33–37], we were unable to identify any contribution providing an explicit dependence between the hierarchical spectrum and corresponding eigenvector's IPR for scale-free networks. Here we consider a tight-binding model defined on an specific tree structure, for which it is possible to establish a analytical relation between the IPR and the corresponding energy eigenvalue. Due to the hierarchical structure, both the eigenvalues and corresponding IPR are expressed in successive generations by means of "causal" chains, resulting in what we call the causal spectrum of a network.

This paper is organized as follows. First we iteratively construct the scale-free tree structure and explore its several basic properties. Then we define a heterogeneous tight-binding model on the structure we construct in Section 2. Without perturbing disorder, we solve the spectrum and find its causal structure. The IPR is determined analytically given any eigenvalue chain in the spectrum.

2. Network construction

The hierarchical tree we consider here is constructed iteratively in a self-similar pattern.

Actually, this structure corresponds to the particular case $G(m = 1, \theta = 0)$ of a general tree defined in [38]. Following the introduced definition and notation, $\mathcal{G}_0$ is a line with two nodes. For $t > 0$, $\mathcal{G}_t$ is obtained by attaching a new vertex to the end of each edge in $\mathcal{G}_{t-1}$, as shown in Fig. 1. The final infinite tree is defined as $\mathcal{G} = \lim_{t\to\infty}\mathcal{G}_t$. The total number of the vertices for any finite iteration $\mathcal{G}_t$ is

$$N_t = 3^t + 1. \tag{1}$$

A vertex introduced at the tth iteration is called a hierarchy-t vertex, and their total number is precisely $2 \times 3^{t-1}$. Now we label all vertices in $\mathcal{G}_t$ by $v_1^{(t)}, v_2^{(t)}, \ldots, v_{N_t}^{(t)}$, and define the adjacency matrix $A^{(t)}$ with elements $a_{ij}^{(t)} = 1$ for adjacent $v_i^{(t)}$ and $v_j^{(t)}$, and $a_{ij}^{(t)} = 0$ otherwise. The degree of any vertex $v_i^{(t)}$ in $\mathcal{G}_t$ is $d_i^{(t)} = \sum_j a_{ij}^{(t)}$. The degree of any hierarchy-n vertex in $\mathcal{G}_t$ is $d^{(t,n)} = 2^{t-n}$. Thus G is scale-free with the degree distribution $P(k) \sim k^{-\gamma}$ that $\gamma = 1 + \frac{\ln 3}{\ln 2}$. Let us also define the diagonal degree matrix $D^{(t)}$ with elements $\delta_{ij}d_i^{(t)}$.

The normalized stochastic matrix [39] for Markov chains on $\mathcal{G}_t$ is $P^{(t)} = (D^{(t)})^{-\frac{1}{2}}A^{(t)}(D^{(t)})^{-\frac{1}{2}}$. Obviously, the i,jth entry of $P^{(t)}$ is $p_{ij}^{(t)} = \frac{a_{ij}^{(t)}}{\sqrt{d_i^{(t)}d_j^{(t)}}}$. Again, we define $P = \lim_{t\to\infty}P^{(t)}$.

3. Tight binding models on $\mathcal{G}$

A typical heterogeneous tight-binding model on $\mathcal{G}_t$ for a single electron is written as

$$\tilde{H}_t = \sum_i d_i^{(t)}c_i^\dagger c_i + \sum_{i\sim j} a_{ij}^{(t)}c_i^\dagger c_j, \tag{2}$$

where the first sum is taken over all vertices and the second sum is taken over all nearest neighbors of the network. $c_i^\dagger$ and c_i are the electron creation and annihilation operators on site i. Note that the eigen-energy of any vertex is not constant,