Electronic states in topologically disordered systems

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Abstract. Networks generated from Voronoi tessellations of space are prototypes for topologically disordered systems. In order to assess the effects of random coordination on the statistical properties of energy spectra, we analyze tight-binding models for planar topologically disordered systems. To this end, the networks are generated by a simple topological model covering a wide range of naturally observed random structures. We find that the energy-level-spacing distributions exhibit level repulsion, similar to the spacings in the energetically disordered Anderson model of localization in the metallic regime.

Keywords: Tessellations; Disorder; Random matrix theory; Spectral statistics

1 Introduction

In most natural structures disorder and random coordination are the rule rather than an exception. Therefore the investigation of random tessellations has become a subject of growing interest [1]. In addition to the structures found in nature, the Voronoi construction, a generalization of the Wigner-Seitz construction, allows to generate tessellations from sets of arbitrarily distributed points [2]. The random Voronoi tessellation has served as the prototype of topologically disordered structures in physics [3]. The aim of this work is a first study of the influence of random coordination on the properties of the electronic spectra in topologically disordered structures. Similar structures are expected in liquid metals or alloys. Here we analyze a tight-binding (TB) model with neighbor hopping on certain two-dimensional (2D) random graphs.

2 Tight-binding model on a random graph

A simple topological model introduced by Le Caër [4] allows to generate efficiently random mosaics that are very similar to Voronoi tessellations generated from disordered arrangements of repulsive particles [5]. Starting point of this model is the triangular structure represented in Fig. 1a (dashed lines). Disorder is achieved by random flips of the diagonal bonds which are performed with probability p, yielding the most disordered structures for $p = 0.5$. As an example, the central bond has

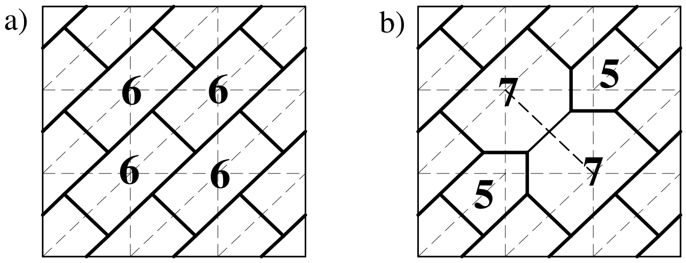

Fig. 1 a): Ordered $p = 0$ triangulation (dashed thin lines) and mosaic (solid bold lines). The numbers indicate the number of edges of a closed loop (mosaic), or, equivalently, the number of neighbors of each vertex (triangulation). b): The same structure after a single flip.

been flipped in Fig. 1b. The dual graphs, the mosaics, obtained by connection of neighboring triangles, are represented as solid lines in Fig. 1.
The TB Hamiltonian is given as

$$H = \sum_{i,j=1}^{N} t_{i,j}\, c_i^\dagger c_j \ , \tag{1}$$

where i, j label the sites of the 2D random graph. The total number of sites is N, and $c_i^\dagger$ (c_i) denotes a fermionic creation (annihilation) operator on site i and we always use periodic boundary conditions. The hopping matrix element between neighboring sites i and j is $t_{i,j} = 1$ and zero otherwise. The eigenvalues and eigenstates of the TB Hamiltonian are calculated employing standard diagonalization methods and Lanczos' algorithm.

3 Density of states

For the regular structures with $p = 0$, the density of states (DOS) can be obtained analytically. The dispersion relation of the triangular structure reads

$$\epsilon_\mathrm{T}(\boldsymbol{k}) = 2\left[\cos(k_x) + \cos(k_y) + \cos(k_x + k_y)\right], \tag{2}$$

where $\boldsymbol{k} = (k_x, k_y)$. In the infinite lattice, the DOS is then given as

$$\rho_\mathrm{T}(E) = \left(4\pi^2\right)^{-1} \int d\boldsymbol{k}\ \delta(E - \epsilon_\mathrm{T}(\boldsymbol{k})) \tag{3}$$

where the integration is performed over the first Brillouin zone, i.e., $k_x, k_y \in [-\pi, \pi)$. This integral can be expressed in terms of complete elliptic integrals of the first kind. The resulting DOS is shown in Fig. 2. Note the logarithmic singularity at $E = -2$. For the mosaic structure at $p = 0$, the dispersion relation is found to be

$$\epsilon_\mathrm{M}(\boldsymbol{k}) = \pm\sqrt{3 + \epsilon_\mathrm{T}(\boldsymbol{k})}. \tag{4}$$

The corresponding DOS

$$\rho_\mathrm{M}(E) = |E|\, \rho_\mathrm{T}(E^2 - 3) \tag{5}$$

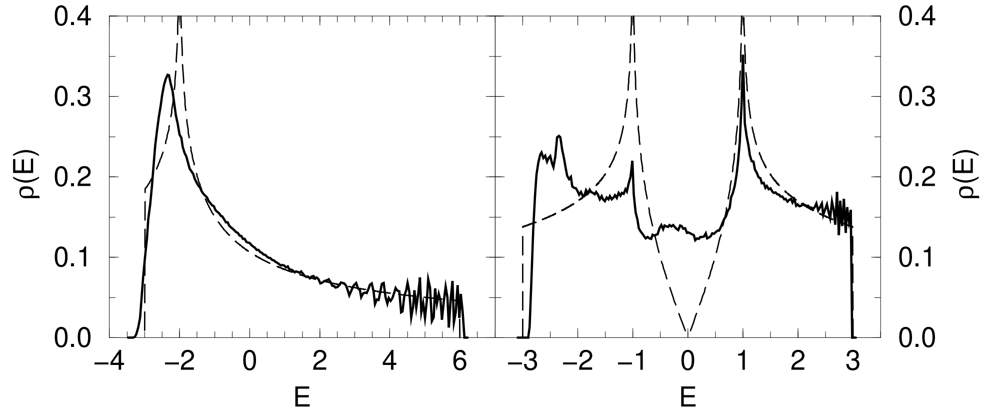

Fig. 2 Left: DOS for the ordered triangulation at $p = 0$ (dashed line) and the disordered triangulation at $p = 0.5$ (solid line). Right: Same as in the left panel but for the mosaic.

with logarithmic singularities at $E = \pm 1$ is also shown in Fig. 2. It is symmetric about $E = 0$ because the ordered mosaic is bipartite.

Fig. 2 also shows the DOS of the most disordered structures with $p = 0.5$, obtained by averaging over 50 realizations on a system of $N = 60 \times 60$ sites. These DOS are rather smooth, apart from oscillations at large energies which also show up in finite-size data for the ordered structures. The logarithmic singularities are washed out by the disorder, and the negative-energy peak for the mosaic structure almost disappears. However, the positive-energy peak for the mosaic structure survives for $p = 0.5$.

4 Energy level distributions

We now turn our attention to the statistical properties of the eigenvalue spectrum of the Hamiltonian (1). Here, we focus on the level-spacing distribution (LSD) $P(s)$ of the normalized energy spacings s. In energetically disordered systems the metal-insulator transition (MIT) in the 3D Anderson model of localization is accompanied by a transition of the LSD. In the metallic regime, one finds level repulsion with $P(s) = P_{\rm GOE}(s)$ of the Gaussian orthogonal random matrix ensemble (GOE) [6], whereas in the insulating regime, there is level clustering described by Poisson's law $P_{\rm P}(s) = \exp(-s)$. Level clustering is also expected for ordered structures. For states at the MIT, an intermediate LSD has been observed [7].

We have computed the LSD of the complete spectrum by properly unfolding the spectrum [8] and averaging over 50 realizations on a system of 60×60 sites. In Fig. 3, we show the results for random graphs with $p = 0.01$ and $p = 0.5$ in comparison to $P_{\rm GOE}(s)$ and $P_{\rm P}(s)$. Both the mosaic and the triangulation data show an enhanced level repulsion with increasing p. The topological structures for $p = 0.01$ are still rather close to the ordered system. Thus it is no surprise that the LSD in Fig. 3 still shows reminiscences of level clustering. However, from an investigation of the system size dependence we expect that even the $p = 0.01$ data tend towards the $P_{\rm GOE}(s)$ result for increasing N. We have also studied the behavior of other spectral

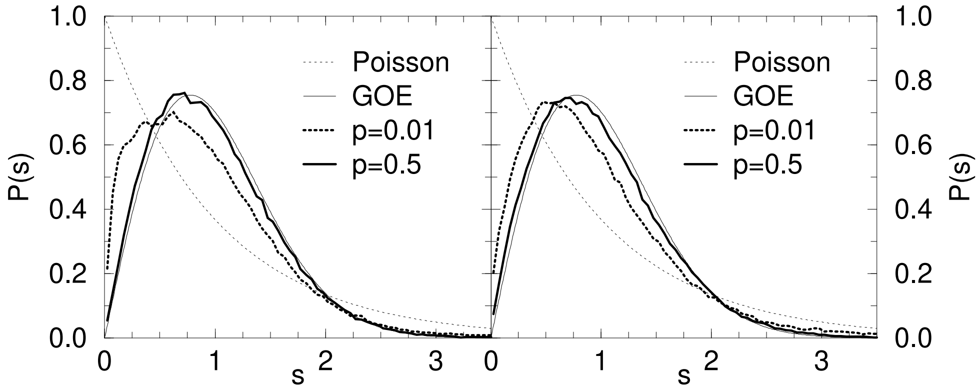

Fig. 3 Left: $P(s)$ for the disordered triangulation at $p = 0.01$ and $p = 0.5$. Thin lines indicate $P_{\mathrm{GOE}}(s)$ and $P_{\mathrm{P}}(s)$. Right: Same for the mosaic.

correlations such as the spectral rigidity Δ_3 [9]. Our results indicate that there are still characteristic deviations from the GOE behavior at the presently considered system sizes, although the system size dependence again shows a tendency towards GOE. This is further corroborated by an analysis of the statistical properties of the eigenfunctions. Results will be published elsewhere.

5 Looking at the eigenstates

In Fig. 4 we show the probability density of a typical eigenfunction $\psi(\boldsymbol{r})$ for the triangular structure at energy $E \approx 1.5$ close to the center of the band. In agreement with the results presented above, we find that the eigenfunction extends over the whole system. This state is of course not a Bloch state, but nevertheless may be viewed as a superposition of eigenstates of the ordered system at energies $E' = E \pm \Delta E$, where ΔE represents an energy level broadening due to the disorder. An eigenstate of the weakly disordered system in Fourier space should therefore exhibit a broadened Fermi surface when interpreting E as the Fermi energy [10]. We also plot the probability density of the Fourier-transformed eigenstate $\tilde{\psi}(\boldsymbol{k})$ in Fig. 4 and compare it to the sharp Fermi surface of the ordered structure. The latter can easily be computed from the dispersion relation (2). For the strongly disordered case at $p = 0.5$ we find an almost four-fold symmetry, whereas the ordered triangulated structure only has a reflection symmetry with respect to the line $k_x = -k_y$. This is to be expected because for $p = 0.5$ both orientations for the diagonals (cp. Fig. 1) are equally probable. Thus the four-fold symmetry of the square lattice is restored on average. Similar results hold for the mosaic structures.

6 Conclusions

We have considered the spectral properties of a TB Hamiltonian defined on certain 2D random graphs. Although the systems are not energetically disordered, the LSD exhibits level repulsion much as for the energetically disordered Anderson model of

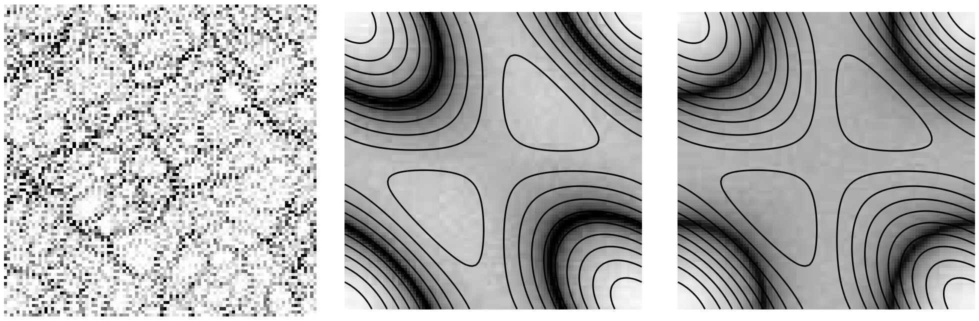

Fig. 4 Left: Probability amplitude of a typical eigenstate at $E \approx 1.5$ in the random triangulation with $p = 0.5$ and $N = 100 \times 100$. Dark regions correspond to high probability amplitudes. Center: Averaged probability amplitude of Fourier-transformed eigenstates at $p = 0.01$ with E and N as in the left panel. The lines indicate the Fermi surfaces of the ordered structure. Right: Same as in the center but with $p = 0.5$.

localization in the metallic regime [8] and also for TB models defined on quasiperiodic tilings [9]. However, more evidence, such as the spectral rigidity mentioned above, is needed before we can conclusively decide whether the level repulsion is indeed identical to the behavior of GOE. We remark that preliminary results for eigenfunction statistics may indicate systematic deviations from the GOE results for the most disordered mosaic structures.

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