PAPER: DISORDERED SYSTEMS, CLASSICAL AND QUANTUM

Path counting on simple graphs: from escape to localization

To cite this article: S K Nechaev *et al J. Stat. Mech.* (2017) 053301

View the article online for updates and enhancements.

Related content

Recent citations

Path counting on simple graphs: from escape to localization

S K Nechaev[1], M V Tamm[2,3] and O V Valba[3,4]

[1] J.-V Poncelet Laboratory, CNRS, UMI 2615, 11 Bolshoy Vlasievski, 119002 Moscow, Russia
[2] Physics Department, Moscow State University, 119992, Moscow, Russia
[3] Department of Applied Mathematics, National Research University Higher School of Economics, 101000, Moscow, Russia
[4] N N Semenov Institute of Chemical Physics RAS, 119991, Moscow, Russia
E-mail: tamm@polly.phys.msu.ru

Abstract. We study the asymptotic behavior of the number of paths of length N on several classes of infinite graphs with a single special vertex. This vertex can work as an 'entropic trap' for the path, i.e. under certain conditions the dominant part of long paths becomes localized in the vicinity of the special point instead of spreading to infinity. We study the conditions for such localization on decorated star graphs, regular trees and regular hyperbolic graphs as a function of the functionality of the special vertex. In all cases the localization occurs for large enough functionality. The particular value of the transition point depends on the large-scale topology of the graph. The emergence of localization is supported by analysis of the spectra of the adjacency matrices of corresponding finite graphs.

J. Stat. Mech. (2017) 053301

Contents

1. Introduction

In this paper we study the asymptotic behavior of the total number of paths of length N on several classes of regular graphs. We call this a 'path counting' (PC) problem, as opposed to the more usual 'random walk' (RW) problem, which studies the distribution of the end points of symmetric random walks on graphs. The difference between PC and RW problems lies in the different normalizations of the elementary step: for the former all steps enter in the partition function with the weight one, while for symmetric RW problems, the step probability depends on the vertex degree, p: the probability to move along each graph bond equals p^{-1}. For graphs with a fixed vertex degree, the PC partition function and the RW probability distribution only differ by the global normalization constant, and the corresponding averages are indistinguishable. However, for inhomogeneous graphs the distinction between PC and RW problems is crucial: in the former 'entropic' localization of the paths may occur, while it never happens for the latter. The distinction between PC and RW problems, and the entropic localization phenomenon were first reported for self-similar structures in [1] and later were rediscovered for star graphs in [2]. More recently, this phenomenon was studied for regular lattices with defects in [3], where the authors introduced the notion of the 'maximal entropy random walk', which is essentially identical to our PC problem.

Following [2], we begin with star-like discrete graphs, $\mathcal{G}$, i.e. a union of p discrete half-lines joined together in one point (the root), see figure 1(a). This model was discussed in [2]. Regard all N-step discrete trajectories on $\mathcal{G}$, and define $Z_N(x)$, the total number of trajectories starting from the root of the graph and ending at distance $x = 0$, 1, 2,... from the root (regardless of which branch the path ends at). One can consider $Z_N(x)$ as the partition function of an ideal polymer chain with N links and one end fixed in the root of the graph $\mathcal{G}$ and the other end anywhere. Given the partition function $Z_N(x)$, one can define the corresponding averages:
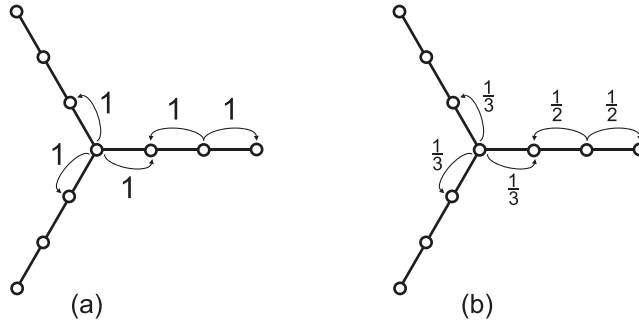
Figure 1. Star-like graph with $p = 3$ branches. In panel (a) we enumerate the trajectories and each step carries a weight 1. In panel (b) the local transition probabilities satisfy the conservation condition in each vertex.

$$\left\langle x^2(N|\,p)\right\rangle = \frac{\sum\limits_{x=0}^{\infty} x^2 Z_N(x|\,p)}{\sum\limits_{x=0}^{\infty} Z_N(x|\,p)}. \tag{1}$$

Straightforward computations [2] show that the asymptotic behavior of $\left\langle x^2(N|\,p)\right\rangle$ at $N \to \infty$ for large N depends drastically on the number of branches, p, in the star-like graph $\mathcal{G}$. Indeed,

$$\left\langle x^2(N|\,p)\right\rangle_{N\to\infty} \to f(p) \times \begin{cases} O(N), & p = 1, 2; \\ O(1), & p = 3, 4, \dots \end{cases} \tag{2}$$

where $f(p)$ is some positive function that depends solely on p and does not depend on N. In other words, for $p = 1, 2$ (the half-line and the full line) the trajectories on average diverge from the origin with a typical distance that is proportional to $\sqrt{N}$, as one would naturally expect for a regular RW. Further, for $p > 2$ the trajectories on average stay localized in the vicinity of the junction point.

To understand this behavior qualitatively, note that the recursion relation connecting $Z_N(x|\,p)$ with $Z_{N+1}(x|\,p)$ depends crucially on whether x is the root point ($x = 0$). Indeed, for each trajectory of length N ending at a point $x \geqslant 1$ there are exactly two possible ways to add the $(N + 1)$th step, and thus each such path 'gives birth' to two paths of length $(N + 1)$. In contrast to that, for each N-step path which ends at $x = 0$, there are p different ways of adding a new step. Therefore, $p > 2$ passing to $x = 0$ becomes entropically favorable, and the root point plays the role of an effective 'entropic trap' for trajectories.

Let us emphasize that this peculiar behavior of the partition function (as a function of p) is specific to the *path-counting* problem, and manifests itself in the *equilibrium* (combinatoric) computations of ideal polymer conformational statistics. In contrast to this, one can think of a closely related *non-equilibrium* problem, namely the calculation of a probability distribution, $P_N(x|\,p)$, for the end-to-end distance of an N-step RW on the star graph of p branches. In this case, the probability distribution, due to the normalization condition, should be integrated into 1 on each step, which leads to the obvious normalization of $P_N(x,p)$:

$$\sum_{x=0}^{\infty} P_N(x \,|\, p) = 1 \text{ for any } N. \tag{3}$$

Therefore, the entropic advantage of staying at the origin is compensated by the fact that the possible steps from the origin have probability p^{-1} instead of $1/2$. In other words, if in the PC problem all trajectories have equal weights 1, in the RW problem the trajectories have weights $2^{-(N-n)} p^{-n}$, where n is the number of returns to the point $x = 0$, varying from path to path. It is easy to see that in the RW problem

$$\lim_{N \to \infty} \frac{\langle x^2(N \,|\, p) \rangle}{N} = \lim_{N \to \infty} \frac{1}{N} \sum_{x=0}^{\infty} x^2 P_N(x \,|\, p) = \text{const} > 0, \tag{4}$$

regardless of the value of p.

Qualitative arguments supported by exact computations for specific models demonstrate that entropic localization occurs in PC in inhomogeneous systems with broken translational invariance. On uniform trees there are no entropically favorable vertices and PC does not exhibit any localization transitions [4]. However, as we shall see below, localization is a topology-dependent phenomenon and occurs in decorated graphs.

This paper is organized as follows. In section 2 we consider finite tree-like regular graphs with a special vertex (entropic trap) at the origin, and compute the asymptotics of the partition function based on the spectral properties of the graph adjacency matrix. We show, however, that this approach has some limitations: even if we increase the size of the tree to infinity we cannot capture a non-localized solution properly. This is not surprising: a finite tree of any size has a non-vanishing fraction of nodes with the degree '1' (terminal 'leaves'). In turn, an infinitely large tree does not have such vertices, and therefore not all of its properties can be recovered by studying the sequence of increasing finite graphs. To resolve this problem, in section 3 (which plays the central role in this paper) we study infinite tree-like graphs with a special vertex, and show that, depending on the functionality of the vertex, a transition between the localized and delocalized states does indeed exist. In section 4, we generalize the results for two other families of graphs with a special entropically attractive point (we call these two families 'decorated star graphs' and 'regular hyperbolic graphs'). In the final section we summarize and discuss the obtained results and formulate some open questions.

2. Path counting on finite tree-like graphs

Consider an arbitrary graph $\mathcal{G}$ with the adjacency matrix $B_{\mathcal{G}}$. It is easy to see that the partition function Z_N described above can easily be expressed in terms of $B_{\mathcal{G}}$. Indeed, the matrix elements of $B_{\mathcal{G}}^N$

$$\langle i | B_G^N | j \rangle \tag{5}$$

enumerate walks of length N starting in vertex j and ending in vertex i. Therefore, e.g., the total number of paths starting at the ith vertex and ending at a distance x from it, $Z_N^{(i)}(x)$, equals the sum of the matrix elements over all j with a given distance x from i

$$Z_N^{(i)}(x) = \sum_{j:\text{dist}\,(i,j)=x} \left\langle i | B_G^N | j \right\rangle. \tag{6}$$

Clearly, this means that the asymptotic behavior of Z_N is controlled by the largest eigenvalue of $B_{\mathcal{G}}$, $\lambda_{\max}(\mathcal{G})$. More precisely, in the large N limit

$$\log Z_N(x) \approx N \log \lambda_{\max}(\mathcal{G}) + o(N). \tag{7}$$

Note that for bimodal graphs there is always a symmetrical pair of the largest eigenvalues $\pm\lambda_{\max}(\mathcal{G})$, and as a result $Z_N(x)$ alternates between the value prescribed by (7) for even $(N+x)$ and 0 for odd $(N+x)$. In what follows this trivial alternating behavior will appear recurrently and will not be mentioned specifically.

As a particular example of $\mathcal{G}$, consider a regular branching tree-like graph with p_0 branches coming out of the origin, and p branches coming out of any other vertex (as we are interested in a possible localization at the origin, we suppose $p_0 \geqslant p$). The maximum number of generations is n. The number of vertices in such a graph grows exponentially with n, so direct analysis of its spectrum might seem challenging. However, it turns out that one can simplify the problem drastically by exploiting the symmetries of $\mathcal{G}$. Indeed, according to [5, 6] the set of eigenvalues of $B_{\mathcal{G}}$ coincides with the set of eigenvalues of a tri-diagonal symmetric matrix A_n with elements $a_{ij}^{(n)}$, which are defined as follows:

$$\begin{cases} a_{i,i}^{(n)} = 0 \\ a_{n,n-1}^{(n)} = a_{n-1,n}^{(n)} = \sqrt{p_0} \\ a_{i,i-1}^{(n)} = a_{i-1,i}^{(n)} = \sqrt{p-1}; \qquad (i = 2, ..., n-1). \end{cases} \tag{8}$$

The eigenvalues of $j \times j$ submatrices correspond to multiply degenerated eigenvalues of $B_{\mathcal{G}}$ (the multiplicity of eigenvalues equals the number of vertices at the generation $n-j$ of the tree from the root point). The corresponding eigenvectors are localized on the outer branches, vanishing exactly at the lowest $n-j$ generations, and take alternating values at the adjacent outer sub-branches. The eigenvalues of the whole matrix A_n are non-degenerate and their eigenvectors span the whole tree. It follows immediately that the largest eigenvalue of $B_{\mathcal{G}}$, which is of crucial importance for estimating the asymptotics of Z_N, is an eigenvalue of the matrix A_n itself: indeed, its eigenvector should be positively defined. Thus, studying the spectrum of an exponentially large matrix $B_{\mathcal{G}}$ is reduced to studying a similar small and simple matrix A_n, which can easily be treated both numerically (see figure 3) and analytically.

The characteristic polynomial $P_n(p_0, p)$ for the matrix A_n satisfies the recursion relation [7]:

$$\begin{cases} P_n(p_0, p) = \lambda P_{n-1}(p_0, p) - (p-1) P_{n-2}(p_0, p); \\ P_0(p_0, p) = \frac{p_0}{p-1}; \\ P_1(p_0, p) = \lambda. \end{cases} \tag{9}$$

This system is easy to solve if one looks for $P_n(p_0, p)$ in the form

$$P_n(p_0, p) = C_+ \mu_+^n + C_- \mu_-^n, \tag{10}$$

giving

$$\mu_{\pm} = \frac{\lambda \pm \sqrt{\lambda^2 - 4(p-1)}}{2}, \tag{11}$$

and

$$C_{\pm} = \frac{p_0}{2(p-1)} \mp \frac{\lambda(p_0 - 2(p-1))}{2(p-1)\sqrt{\lambda^2 - 4(p-1)}}. \tag{12}$$

It is easy to see that the resulting equation $P_n(p_0, p) = 0$ is even with respect to λ. To solve it, define a new variable ϕ by

$$\lambda = \pm 2\sqrt{p-1}\cosh\phi, \tag{13}$$

where $|\lambda| \geqslant 2\sqrt{p-1}$ corresponds to real ϕ and $\lambda < 2\sqrt{p-1}$—to purely imaginary ϕ. Then

$$\mu_{\pm} = \sqrt{p-1}\,e^{\pm\phi},$$
$$C_{\pm} = \frac{p_0}{2(p-1)} \pm \frac{p_0 - 2(p-1)}{2(p-1)\tanh\phi}, \tag{14}$$

and the equation $P_n(p_0, p) = 0$ becomes

$$\tanh n\phi = \frac{p_0}{p_0 - 2(p-1)}\tanh\phi, \tag{15}$$

which for any n has many imaginary solutions and a single real one, which corresponds to $\lambda_{\max}^{(n)}$. The limit of this solution for $n \to \infty$ is

$$\lambda_{\max} = \lim_{n \to \infty} \lambda_{\max}^{(n)} = \frac{p_0}{\sqrt{p_0 - p + 1}}. \tag{16}$$

Therefore, we conclude that on any large but finite tree the number of trajectories in the $N \to \infty$ limit behaves asymptotically as (see equation (7))

$$Z_N(x, p, p_0, n) \sim (\lambda_{\max})^N = \left(\frac{p_0}{\sqrt{p_0 - p + 1}}\right)^N. \tag{17}$$

This result, however, looks a bit strange after close examination: for a partition function on an *infinite* tree there is (for $p_0 \geqslant p$) a lower bound

$$Z_N(x, p, p_0, n = \infty) \geqslant p^N. \tag{18}$$

Indeed, at each step there are at least p different directions to go in, which seems to contradict (17) for $p < p_0 < \bar{p}_0 = p^2 - p$. This apparent discrepancy is, of course, due to the order of taking limits $n \to \infty$ and $N \to \infty$. In a system with large but finite n there is always a finite fraction of terminal nodes ('leaves' of the tree) with degree '1', violating the reasoning behind (18). In turn, in a system with infinite n, as we show in the next section, there exists an additional eigenvalue of the adjacency matrix equal to p, corresponding to a density wave spreading with finite velocity from the root point to infinity. Depending on which of the two eigenvalues—the one given by (16), or this new one, $\lambda = p$—is maximal, the partition function of the infinitely large system is either localized or delocalized, respectively.
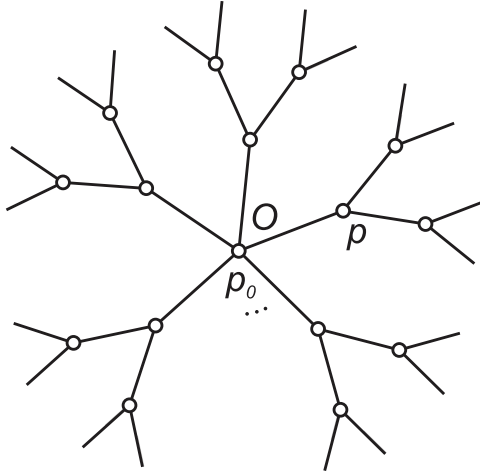
Figure 2. Image of a regular p-branching Cayley tree with p_0 branches at the origin $x = 0$. The particular case of a tree with $p = 3, n = 3$ is shown.

3. Localization of trajectories on an infinite tree with a 'heavy' root

Consider the same graph $\mathcal{G}$ that is defined above (see figure 2), but with an infinitely large number of generations n. We begin by writing the explicit recursion relation for the partition function, $Z_N(x)$, enumerating all N-step paths on $\mathcal{G}$, starting at the origin and ending at some distance x from it:

$$\begin{cases} Z_{N+1}(x) & = & (p-1)Z_N(x-1) + Z_N(x+1), & x \geqslant 2 \\ Z_{N+1}(x) & = & p_0 Z_N(x-1) + Z_N(x+1), & x = 1 \\ Z_{N+1}(x) & = & Z_N(x+1), & x = 0 \\ Z_N(x) & = & 0, & x \leqslant -1 \\ Z_{N=0}(x) & = & \delta_{x,0}, \end{cases} \tag{19}$$

where x is the distance from the root of the Cayley graph $\mathcal{G}$, measured in the number of generations of the tree.

In order to solve this set of equations [8, 9] we make a shift $x \to x + 1$, and substitute

$$Z_N(x) = A^N B^x W_N(x). \tag{20}$$

with $A = B = \sqrt{p-1}$. This substitution allows us to symmetrize the original equation, which in terms of W now takes the form

$$\begin{cases} W_{N+1}(x) & = & W_N(x-1) + W_N(x+1) + \frac{p_0-p+1}{p-1}\delta_{x,2} W_N(x-1), & x \geqslant 1 \\ W_N(x) & = & 0, & x = 0 \\ W_{N=0}(x) & = & \frac{\delta_{x,1}}{\sqrt{p-1}}. \end{cases} \tag{21}$$

Note that this equation can be written in matrix form,

$$\mathbf{W}_{N+1} = T\,\mathbf{W}_N; \qquad \mathbf{W}_0 = ((p-1)^{-1/2}, 0, \dots)^{\intercal}, \tag{22}$$

where the transfer matrix T is an infinite tri-diagonal matrix

$$T = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ \frac{p_0}{p-1} & 0 & 1 & 0 & \dots \\ 0 & 1 & 0 & 1 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

(23)

whose nth main minors are almost equal to $\sqrt{p-1}A_n$.

Introducing the generating function

$$\mathcal{W}(s,x) = \sum_{N=0}^{\infty} W_N(x)s^N \qquad \left(W_N(x) = \frac{1}{2\pi i} \oint \mathcal{W}(s,x)s^{-N-1}\, ds \right)$$

(24)

and its sine Fourier transform

$$\tilde{\mathcal{W}}(s,q) = \sum_{x=0}^{\infty} \mathcal{W}(s,x)\sin qx \qquad \left(\mathcal{W}(s,x) = \frac{2}{\pi} \int_0^\pi \tilde{\mathcal{W}}(s,q)\sin qx\, dq \right),$$

(25)

one obtains from (21)

$$\frac{\tilde{\mathcal{W}}(s,q)}{s} - \frac{\sin q}{s\sqrt{p-1}} = 2\cos q\, \tilde{\mathcal{W}}(s,q) + \frac{2}{\pi}\frac{p_0 - p + 1}{p-1}\sin 2q \int_0^\pi \tilde{\mathcal{W}}(s,q)\sin q\, dq.$$

(26)

Rewriting (26) as

$$\tilde{\mathcal{W}}(s,q) = \frac{1}{\sqrt{p-1}}\frac{\sin q}{1 - 2s\cos q} + \frac{2s(p_0 - p + 1)}{\pi(p-1)}\frac{\sin 2q}{1 - 2s\cos q} \int_0^\pi \tilde{\mathcal{W}}(s,q)\sin q\, dq,$$

(27)

and multiplying both sides of (27) by $\sin q$ and integrating over q, $q \in [0, \pi]$, one arrives at an algebraic equation for

$$I(s) = \int_0^\pi \tilde{\mathcal{W}}(s,q)\sin q\, dq,$$

(28)

namely

$$I(s) = \frac{1}{\sqrt{p-1}} \int_0^\pi \frac{\sin^2 q}{1 - 2s\cos q}\, dq + I(s)\frac{2s(p_0 - p + 1)}{\pi(p-1)} \int_0^\pi \frac{\sin q\,\sin 2q}{1 - 2s\cos q}\, dq.$$

(29)

The solution of this equation reads

$$I(s) = \frac{\frac{1}{\sqrt{p-1}}\int_0^\pi \frac{\sin^2 q}{1 - 2s\cos q}\, dq}{1 - \frac{2s(p_0 - p + 1)}{\pi(p-1)}\int_0^\pi \frac{\sin q\,\sin 2q}{1 - 2s\cos q}\, dq} = \frac{\pi\sqrt{p-1}\left(1 - \sqrt{1 - 4s^2}\right)}{4s^2(p-1) - (p_0 - p + 1)\left(1 - \sqrt{1 - 4s^2}\right)^2}.$$

(30)

Substituting $I(s)$ into (27), and performing the inverse Fourier transform, we arrive at the following explicit expression for the generating function $\mathcal{W}(s,x)$:

$$\mathcal{W}(s,x) = \frac{2}{\pi} \int_0^\pi \tilde{\mathcal{W}}(s,q)\sin qx\, dq$$

$$= \frac{1}{s\sqrt{p-1}}\left(\frac{1 - \sqrt{1 - 4s^2}}{2s}\right)^x \left(1 + \frac{2(p_0 - p + 1)\left(1 - \sqrt{1 - 4s^2}\right)}{4s^2(p-1) - (p_0 - p + 1)\left(1 - \sqrt{1 - 4s^2}\right)^2}\right).$$

(31)

8

Since, by definition, $Z_N(x) = A^N B^x W_N(x)$ (see (20)), we can write down the relation between the generating functions of $Z_N(x)$ and of $W_N(x)$:

$$\mathcal{Z}(\sigma, x) = \sum_{N=0}^{\infty} Z_N(x)\sigma^N = \sum_{N=0}^{\infty} A^N B^x W_N(x)\sigma^N = B^x \mathcal{W}(\sigma A, x). \tag{32}$$

Thus,

$$\mathcal{Z}(\sigma, x | p, p_0) = (p-1)^{x/2} \mathcal{W}(\sigma\sqrt{p-1}, x), \tag{33}$$

where $\mathcal{W}(\sigma\sqrt{p-1}, x)$ is given by (31), where we should substitute $\sigma\sqrt{p-1}$ for s. Thus, the grand partition function, $\mathcal{Z}(\sigma, x | p, p_0)$, of the initial PC problem reads

$$\mathcal{Z}(\sigma, x | p, p_0) = \frac{2p_0\sigma \left(\frac{1-\sqrt{1-4\sigma^2(p-1)}}{2\sigma}\right)^x}{2\sigma^2 p_0(p-1) - (p_0 - p + 1)\left(1 - \sqrt{1-4\sigma^2(p-1)}\right)}. \tag{34}$$

The partition function, $\bar{Z}(N | p, p_0)$, of all paths starting at the origin, can be obtained by the summation over x:

$$\bar{\mathcal{Z}}(\sigma | p, p_0) = \sum_{x=0}^{\infty} \mathcal{Z}(\sigma, x | p, p_0). \tag{35}$$

Straightforward computations lead us to the following result

$$\bar{\mathcal{Z}}(\sigma | p, p_0) = \frac{4p_0\sigma^2 \left(1 - \sqrt{1-4\sigma^2(p-1)}\right)}{\left[2\sigma - 1 + \sqrt{1-4\sigma^2(p-1)}\right]\left[2\sigma^2 p_0(p-1) - (p_0 - p + 1)\left(1 - \sqrt{1-4\sigma^2(p-1)}\right)\right]}. \tag{36}$$

To extract the asymptotic behavior of the partition function

$$\bar{Z}_N(p, p_0) = \frac{1}{2\pi i} \oint \bar{\mathcal{Z}}(\sigma | p, p_0)\sigma^{-N-1}\mathrm{d}\sigma \tag{37}$$

as a function of N, one should analyze the behavior of $\bar{\mathcal{Z}}(\sigma | p, p_0)$ (see equation (36)) at its singularities. There are three of them, namely

$$\sigma_1 = \frac{1}{2\sqrt{p-1}} \tag{38}$$

for a branching point of the square root, and

$$\sigma_2 = \frac{1}{p}, \quad \sigma_3 = \frac{\sqrt{p_0 - p + 1}}{p_0} \tag{39}$$

for zeroes of the first and second factors in the denominator of (36), respectively. The asymptotic behavior is governed by the dominant singularity, i.e. the one with the smallest absolute value. It is instrumental to compare these singularities with the eigenvalues of the corresponding finite-size problem discussed in the previous section. Indeed, σ_3 is nothing but the $\lambda_{\max}^{-1}$ given by equation (16), while σ_1 corresponds to the border of the quasi-continuous spectrum shown in figure 3, and σ_2 is, as discussed at
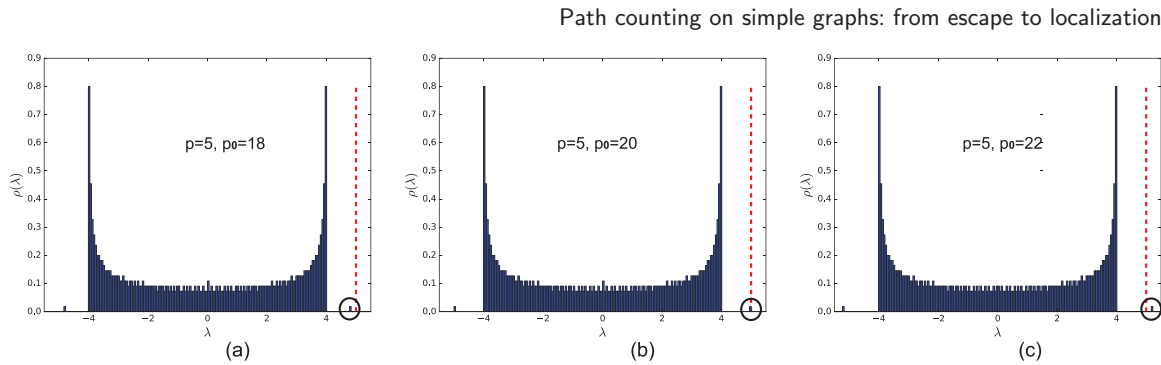
Figure 3. Spectral density of the matrix A_{1000} (a) the localization transition, (b) at the transition point and (c) in the localized phase. The red line indicates $\lambda = p$.

the end of the previous section, the solution that runs away from the origin, and is therefore unavailable in the finite-system case.

Since $\sigma_1 > \sigma_2$ for any $p \geqslant 3$ regardless of the value of p_0, the square-root singularity never dominates. In turn, σ_3 equals σ_2 at the critical value p_0 defined by the equation:

$$\bar{p}_0 = p^2 - p. \tag{40}$$

For $p_0 < \bar{p}_0$ the singularity at σ_2 gives the dominant contribution to the partition function and in the large N limit the total number of paths scales as

$$\bar{Z}(N|\,p, p_0)\big|_{N \gg 1} \approx \sigma_2^{-N} = c(p, p_0)\, p^N, \tag{41}$$

where $c(p, p_0)$ is N-independent. The behavior of $\bar{Z}(N \gg 1|\,p, p_0)$ in equation (41) should be compared to that for $p_0 = p$, where $\bar{Z}(N|\,p, p_0 = p) = p^N$ for any N (for $p_0 = p$ there are always exactly p different ways to add an Nth step to any $(N-1)$-step trajectory). We see that in this regime the root essentially has no influence on the asymptotics of a partition function, and any typical N-step trajectory ends at a distance $\bar{x} = \frac{p-2}{p}N$ from the origin. Since there are always more possibilities to go away from the origin than to go back to it, there is a finite drift, with Gaussian fluctuations of order $\Delta x \sim \sqrt{N}$ around the mean value of $\bar{x}$. We refer the reader to [4], where the statistics of the trajectories on regular Cayley trees are discussed in detail.

In contrast to this, for $p_0 > \bar{p}_0$ the large-N scaling of the number of paths depends significantly on p_0:

$$\bar{Z}(N|\,p, p_0) \approx \sigma_3^{-N} \sim \left(\frac{p_0}{\sqrt{p_0 - p + 1}}\right)^N, \tag{42}$$

which is a signature of localization. Indeed, the very fact that the partition function depends on p_0 for any N indicates that typical trajectories return to the origin for any N. To obtain a better understanding of the typical behavior of trajectories, we insert the critical value σ_3 into (34), which results in the following x-dependence of the partition function

$$Z(N, x|\,p, p_0) \approx \sigma_3^{-N} \sim \left(\frac{p_0}{\sqrt{p_0 - p + 1}}\right)^N \left(\frac{p-1}{\sqrt{p_0 - p}}\right)^x. \tag{43}$$
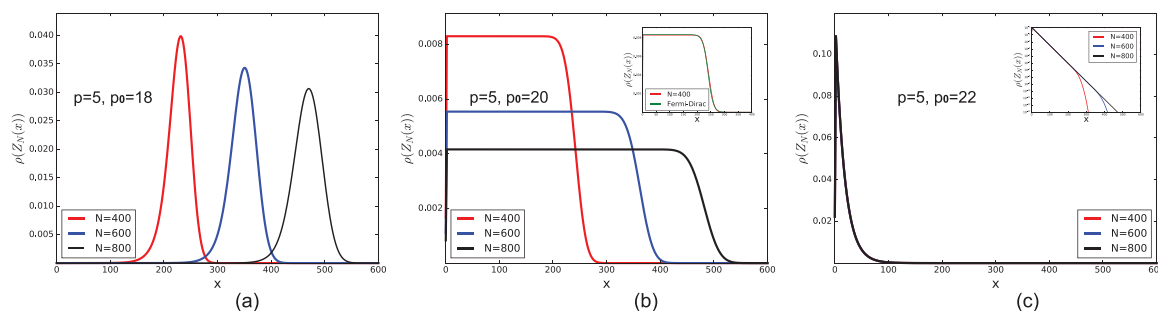
Figure 4. The distribution of the the trajectory endpoint $\rho(Z_N(x)) = Z(N, x | p, p_0) \left[\bar{Z}(N | p, p_0) \right]^{-1}$ as a function of x (a) below the localization transition, (b) at the transition point (inset: the numerical results are fitted by the Fermi–Dirac distribution with the Fermi energy $e_\mathrm{F} = \bar{x} = \frac{p-2}{p} N$) and (c) in the localized phase (inset: in the logarithmic scale).
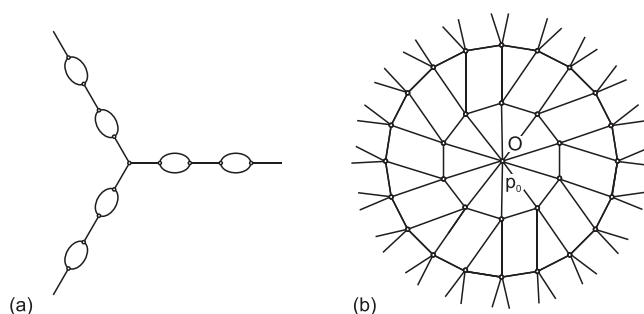

Figure 5. Decorated star graphs. (a) Simplest decorated star graph with $p_0 = p = 3$. (b) Generic decorated graph with $p_0 = 10$, $p = 5$ and $b = 2$.

Equation (43) indicates the exponential decay of $Z(N, x | p, p_0)$ as a function of x. That behavior (as well as equation (40)) is confirmed by direct iterations of equation (19) for $p = 5$ and $p_0 = 17$ (below the localization transition point), and $p_0 = 20$ (at the transition point) and $p_0 = 22$ (in the localized phase), see figure 4. Note that exactly at the transition point $p_0 = \bar{p}_0$ the distribution of the the trajectory endpoint is approximated nicely by the Fermi–Dirac distribution.

4. Path counting on decorated star graphs and regular hyperbolic graphs

Here we aim to generalize the above results for two classes of more general graphs. One class, called a 'decorated star graph', is shown in figure 5(a), it consists of p_0 bundles, such that each bundle has an overall linear topology, but all vertices in the bundle have functionality p. The second class is a class of 'regular hyperbolic graphs' with a special point at the origin (see figure 5(b)). Here, once again, p_0 bonds originate from the root and each vertex except the root has functionality p. However, among p bonds originating from a node at distance x from the root, one bond is going 'down' to a point at distance $(x - 1)$, $(p - b - 1)$ are going 'up' to points at distance $(x + 1)$ and b 'horizontal' bonds connect the node with others at the same distance x from the origin.
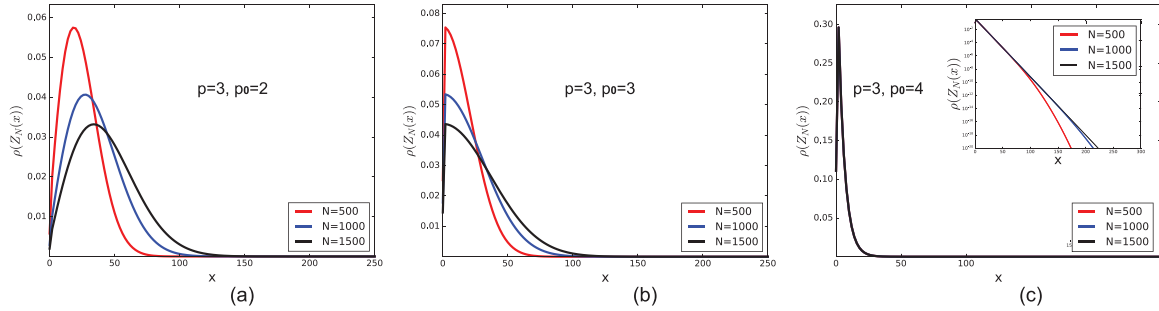
Figure 6. The distribution of the the trajectory endpoint $\rho(Z_N(x)) = Z(N, x \,|\, p, p_0) \left[\bar{Z}(N \,|\, p, p_0) \right]^{-1}$ as a function of x (a) below the localization transition, (b) at the transition point and (c) in the localized phase (inset: in the logarithmic scale).

Clearly, the star graphs considered in the introduction are decorated stars with $p = 2$, while the regular trees with heavy roots considered in sections 2 and 3 are regular hyperbolic graphs with $b = 0$. In this section we aim to understand how the additional parameters—p in the first case and b in the second one—influence the position of the localization transition. Since the mathematical structure of these two problems is extremely similar, we discuss them in parallel.

First consider a decorated star graph. For such a graph, the partition function, $Z_N(x)$, of all N-step paths starting at the origin and ending at some distance x from the root (regardless of which branch it is on), satisfies the recursion (compare with (19)):

$$\begin{cases} Z_{N+1}(x) &= Z_N(x-1) + (p-1)Z_N(x+1), & x = 2k+1 \ (k \geqslant 1) \\ Z_{N+1}(x) &= (p-1)Z_N(x-1) + Z_N(x+1), & x = 2k \ (k \geqslant 1) \\ Z_{N+1}(x) &= p_0 Z_N(x-1) + (p-1)Z_N(x+1), & x = 1 \\ Z_{N+1}(x) &= Z_N(x+1), & x = 0 \\ Z_N(x) &= 0, & x \leqslant -1 \\ Z_{N=0}(x) &= \delta_{x,0}. \end{cases} \tag{44}$$

The results of the direct iterations of (44) presented in figure 6 show that, depending on the values of the vertex degrees, p and p_0, localization of the trajectories may or may not exist: one clearly sees a different behavior of $Z(N, x \,|\, p, p_0)$ as a function of x for a few values of p_0 above and below the transition point, $\bar{p}_0 = p$.

As previously discussed in section 2, half of the values of the partition function $Z_N(x)$ (those corresponding to odd values of $(N + x)$) equal zero. Therefore, without loss of information, one can replace $Z_N(x)$ by $V_N(y)$, defined as follows:

$$\begin{cases} V_N(y) &= Z_N(2y-1) + Z_N(2y), & k \geqslant 1 \\ V_N(0) &= Z_N(0). \end{cases} \tag{45}$$

This new partition function $V_N(k)$ satisfies

$$\begin{cases} V_{N+1}(k) &= V_N(k-1) + (p-2)V_N(k) + V_N(k+1), & k > 1 \\ V_{N+1}(k) &= p_0 V_N(k-1) + (p-2)V_N(k) + V_N(k-1), & k = 1 \\ V_{N+1}(k) &= V_N(k+1), & k = 0 \\ V_N(k) &= 0, & k \leqslant -1 \\ V_{N=0}(k) &= \delta_{k,0}. \end{cases} \tag{46}$$

It turns out that this set of equations is nothing but the set of equations describing the PC problem on regular hyperbolic graphs, as defined above for the particular case of $b = p - 2$.

Indeed, writing the recursion relation for a regular hyperbolic graph explicitly, one obtains:

$$
\begin{cases}
Z_{N+1}(x) = (p - b - 1)Z_N(x-1) + bZ_N(x) + Z_N(x+1), & x > 1 \\
Z_{N+1}(x) = p_0 Z_N(x-1) + bZ_N(x) + Z_N(x-1), & x = 1 \\
Z_{N+1}(x) = Z_N(x+1), & x = 0 \\
Z_N(x) = 0, & x \leqslant -1 \\
Z_{N=0}(x) = \delta_{x,0}.
\end{cases}
\tag{47}
$$

In what follows we solve the more general case of equation (47), and then obtain the result for decorated star graphs when substituting $b = p - 2$ in the final expression. The solution below is completely analogous to what is presented above in section 3. Making a shift $x \to x + 1$ and symmetrizing (47) by substitution:

$$
Z_N(x) = (p - b - 1)^{N/2}(p - b - 1)^{x/2}W_N(x)
\tag{48}
$$

results in

$$
\begin{cases}
W_{N+1}(x) = W_N(x-1) + W_N(x+1)\frac{b}{\sqrt{p-b-1}}W_N(x) \\
\qquad + \frac{p_0 - (p-b-1)}{p-b-1}\delta_{x,2}W_N(x-1) - \frac{b}{\sqrt{p-b-1}}\delta_{x,1}W_N(x), & x \geqslant 1 \\
W_N(x) = 0, & x = 0 \\
W_{N=0}(x) = \frac{\delta_{x,1}}{\sqrt{p-b-1}}.
\end{cases}
\tag{49}
$$

Performing the sine Fourier transform for the generating function (similarly to (24) and (25)), we obtain an integral equation

$$
\frac{\tilde{\mathcal{W}}(s,q)}{s} - \frac{\sin q}{s\sqrt{p-b-1}} = (2\cos q + B)\tilde{\mathcal{W}}(s,q) + \frac{2}{\pi}[A\sin 2q - B\sin q]\int_0^\pi \tilde{\mathcal{W}}(s,q), \sin q \, \mathrm{d}q
\tag{50}
$$

where

$$
\tilde{\mathcal{W}}(s,q) = \sum_{x=0}^\infty \mathcal{W}(s,x)\sin qx, \qquad \mathcal{W}(s,x) = \sum_{N=0}^\infty W_N(x)s^N
\tag{51}
$$

and

$$
A = \frac{p_0 - (p-b-1)}{p-b-1}, \qquad B = \frac{b}{\sqrt{p-b-1}}.
\tag{52}
$$

Expressing $\tilde{\mathcal{W}}$ from (50) and integrating over q, $q \in [0, \pi]$ with the weight $\sin q$, we obtain

$$
I(s) = \int_0^\pi \tilde{\mathcal{W}}(s,q)\sin q \, \mathrm{d}q = \frac{1}{\sqrt{p-b-1}}\int_0^\pi \frac{\sin^2 q}{1 - 2s\cos q - Bs} \, \mathrm{d}q
$$
$$
+ \frac{2s}{\pi}I(s)\left[A\int_0^\pi \frac{\sin q \sin 2q}{1 - 2s\cos q - Bs} \, \mathrm{d}q - B\int_0^\pi \frac{\sin^2 q}{1 - 2s\cos q - Bs} \, \mathrm{d}q\right].
\tag{53}
$$

The solution of (53) reads

$$I(s) = \frac{\pi\sqrt{p-b-1}\left(1 - Bs - \sqrt{(1-Bs)^2 - 4s^2}\right)}{4s^2 - A\left(1 - Bs - \sqrt{(1-Bs)^2 - 4s^2}\right)^2 + 2Bs\left(1 - Bs - \sqrt{(1-Bs)^2 - 4s^2}\right)}. \tag{54}$$

Performing the inverse Fourier transform, one obtains an explicit expression for the generating function $\mathcal{W}(s,x)$:

$$\mathcal{W}(s,x) = \frac{2}{\pi}\int_0^\pi \tilde{\mathcal{W}}(s,q)\sin qx\,\mathrm{d}q$$
$$= \frac{1}{s^2\sqrt{p-b-1}}\left(\frac{1 - Bs - \sqrt{(1-Bs)^2 - 4s^2}}{2s}\right)^x\left[1 + \frac{2}{\pi}\sqrt{p-b-1}\,I(s)(2A - Bs)\right]. \tag{55}$$

Finally, continuing in a way that is analogous to the procedure in section 3, we obtain an explicit expression for the generating function $Z(\sigma|p,p_0)$ of all paths of length N:

$$\bar{\mathcal{Z}}(\sigma|p,p_0) \equiv \sum_{x=0}^{\infty}(p-b-1)^{x/2}\mathcal{W}(\sigma\sqrt{p-b-1},x)$$
$$= \frac{1}{\sigma(p-b-1)}\frac{1}{2\sigma - 1 + b\sigma + \sqrt{(1-b\sigma)^2 - 4\sigma^2(p-b-1)}}$$
$$\times\left[1 + \frac{2}{\pi}I(\sigma\sqrt{p-b-1})\left(2\frac{p_0 - (p-b-1)}{p-b-1} - b\right)\right]. \tag{56}$$

This function once again has three singularities: the branching point of the square root (56):

$$\sigma_1 = \frac{1}{b + 2\sqrt{p-b-1}}, \tag{57}$$

corresponding to the border of the continuous spectrum, the zero of the denominator of (56)

$$\sigma_2 = \frac{1}{p}, \tag{58}$$

corresponding to the spreading wave solution, and the third singularity, σ_3, corresponding to the zero of the denominator of $I(\sigma\sqrt{p-b-1})$ (see (54)), which corresponds to the localized solution. Substituting σ_2 into equation for σ_3 provides the condition for a critical value of p_0 that separates the localized and delocalized regimes for regular hyperbolic graphs, which is

$$\bar{p}_0 = p(p-b-1) \tag{59}$$

for decorated star graphs $b = p - 2$, and this condition reduces to a simple $\bar{p}_0 = p$, in full agreement with the numerical simulations presented above, while for a tree-like graph (G) with $b = 0$, (59) reduces to (40).

It seems interesting to compare the statistics for the trajectories on the simplest star-like graph, G, shown in the figure 1(a) with those for the trajectories on the decorated one, G_d, depicted in the figure 5(a). The mean-square displacement of the end of the N-step path on a *single branch* of G and of G_d scales as $\sqrt{N}$ in both cases (with different numeric coefficients). Further, the trajectories on the graph G are localized for $p_0 \geqslant 3$, and on the decorated graph G_d the localization occurs at $p_0 \geqslant 4$ (for $p_0 = 3$ the paths on G_d are delocalized).

5. Discussion

In this paper we study the localization properties for a PC problem for several classes of regular graphs with a single special vertex (trees with a 'heavy' root, decorated stars and regular hyperbolic graphs). Generalizing the argument of [2], we show that in all these cases a special vertex with a functionality that is larger than that of the regular ones works as an entropic trap for the paths on the graph, and may lead, if the trap is strong enough, to *path localization.*

We use two different techniques, studying the spectral properties of the graph adjacency matrix for finite graphs and the singularities of the grand canonical partition function for infinite graphs. In our opinion, parallel consideration of these two approaches has significant methodological value in itself, allowing the reader to see the similarity of these methods, and the ways in which the same values can be interpreted in two different languages.

To the best of our knowledge, the results presented in this paper add some new flavor to path localization on inhomogeneous graphs and networks, and they are certainly an addition to the long-standing theory of localization in disordered systems, whose development goes all the way back to the works of I M Lifhsitz [10, 11].

There are a variety of problems in the physics of disordered systems and inhomogeneous media whose solutions (e.g. the solutions of corresponding hyperbolic or parabolic equations, or the leading eigenvectors of corresponding operators, etc) are localized in the vicinity of some spatial regions. Similar localization problems are often studied in polymer physics, where they correspond to a polymer chain being adsorbed at some specific location in space, e.g. point-like defects of texture within some particular region of space, or in the vicinity of interfaces. Most commonly, the reason for such localization is energetic: it is due to some attractive force between a localized particle or polymer chain and the absorbing substrate.

The situation described in this paper belongs to a class of problems for which the origin of localization is purely *entropic*, with its cause being exclusively geometric. Among similar problems discussed in the literature are, first of all, the localization of ideal polymer chains on regular lattices with defects, as discussed in [3], and the trapping of RWs in inhomogenious media [12, 13]. Similar situations are also widely discussed in spectral geometry, where the solutions of Laplace or Helmholtz equations in regions of complex shape (e.g. obtained by gluing together several simple shapes) are studied. The principal question there involves determining the conditions on the localization of wavefunctions in these complex regions [14].

Although it has a slightly different probabilistic setting, the phase transition on regular graphs was discussed recently in [15], where the authors described the exit boundary of RWs on homogeneous trees exhaustively. They showed that the model exhibits a phase transition, manifested in the loss of ergodicity of a family of Markov measures, as a function of the parameter, which controls the local transition probabilities on the tree. We plan to analyze whether the transition found in [15] has a direct relation to the transition described in our paper.

We would like to make one last remark concerning the results obtained above. It can be seen from our results that the conditions for localization to occur depend significantly on the overall geometry of the graph. Indeed, on decorated star graphs it is sufficient to have $p_0 > p$ to obtain localization, while on tree-like graphs one needs $p_0 > p(p-1) \sim p^2$ in order for trajectories to be localized. Accordingly, it remains unclear whether it is possible to push the transition value $\bar{p}_0$ below p by changing the graph geometry, so that localization will even occur on a graph where all the vertices have the same degree, p. One possible candidate for such a localization might be a regular random graph (i.e. a random graph whose vertices all have the same degree, p); by chance, on such graphs there is a small (order one) number of short cycles. In principle, it is conceivable that these cycles work as entropic traps in a similar way to that discussed here. The localization on a family of specially prepared random regular graphs with an enriched fraction of short loops was recently studied in [16, 17].

Acknowledgments

Note added in proof. Z Burda pointed out that in [18] the system very similar to the one described in our section 2, have been discussed. However, the authors of [18] considered finite tree-like graphs where there is no localizatfion transition.

References

[1] Maritan A 1989 Random walk and the ideal chain problem on self-similar structures *Phys. Rev. Lett.* **62** 2845–8

[2] Ternovsky F F, Nyrkova I A and Khokhlov A R 1992 Statistics of an ideal polymer chain near the bifurcation region of a narrow tube *Physica* A **184** 342–53

[3] Burda Z, Duda J, Luck J-M and Waclaw B 2009 Localization of the maximal entropy random walk *Phys. Rev. Lett.* **102** 160602

[4] Monthus C and Texier C 1996 Random walk on the Bethe lattice and hyperbolic Brownian motion *J. Phys. A: Math. Gen.* **29** 2399–409

[5] Rojo O and Soto R 2005 The spectra of the adjacency matrix and Laplacian matrix for some balanced trees *Linear Algebra and its Applications* vol 403 (Amsterdam: Elsevier) pp 97–117

[6] Rojo O and Robbiano M 2007 An explicit formula for eigenvalues of Bethe trees and upper bounds on the largest eigenvalue of any tree *Linear Algebra and its Applications* vol 427 (Amsterdam: Elsevier) pp 138–50

[7] Kovaleva V, Maximov Yu, Nechaev S and Valba O 2016 Peculiar spectral statistics of ensembles of trees and star-like graphs (arXiv:1612.01002)

[8] Nechaev S K, Semenov A N and Koleva M K 1987 Dynamics of polymer chain in an array of obstacles *Physica* A **140** 506–20

[9] Gangardt D M and Nechaev S K 2008 Wetting transition on a one-dimensional disorder *J. Stat. Phys.* **130** 483–502

[10] Lifshitz I M 1968 Theory of fluctuation levels in disordered systems *Sov. Phys.—JETP* **26** 462

[11] Lifshitz I M, Gredeskul S A and Pastur L A 1988 *Introduction to the Theory of Disordered Systems* (New York: Wiley)

[12] Balagurov B Y and Vaks V G 1974 Random walks of a particle on lattices with traps *Sov. Phys.—JETP* **38** 968

[13] Donsker M D and Varadhan S R S 1975 Asymptotic evaluation of certain Markov process expectations for large time, I *Commun. Pure Appl. Math.* **28** 525

[14] Delitsyn A L, Nguyen B T and Grebenkov D S 2012 Exponential decay of Laplacian eigenfunctions in domains with branches of variable cross-sectional profiles *Eur. Phys. J.* B **85** 371
Grebenkov D S and Nguyen B T 2013 Geometrical structure of Laplacian eigenfunctions *SIAM Rev.* **55** 601–7

[15] Vershik A M and Malyutin A V 2015 Phase transition in the exit boundary problem for random walks on groups *Funct. Anal. Appl.* **49** 86–96

[16] Avetisov V, Hovhannisyan M, Gorsky A, Nechaev S, Tamm M and Valba O 2016 Eigenvalue tunneling and decay of quenched random network *Phys. Rev.* E **94** 062313

[17] Avetisov V, Gorsky A, Nechaev S and Valba O 2016 Many-body localization and new critical phenomena in regular random graphs and constrained Erdos–Renyi networks (arXiv:1611.08531)

[18] Ochab J K and Burda Z 2012 Exact solution for statics and dynamics of maximal entropy random walk on Cayley trees *Phys. Rev.* E **85** 021145