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Emergence of loop structure in scale-free networks and dynamical consequences

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Previous work has revealed that the synchronizability of a scale-free network tends to be suppressed when its clustering coefficient is increased. We present a theory to explain this phenomenon. Our proposition is that, as the network becomes more strongly clustered, topological loop structure can emerge, generating a set of eigenvalues that are close to zero. As a result, the dynamics of synchronization tends to be dominated by the loop structure. As the clustering coefficient is increased, the size of the dominant loop increases, leading to continuous degradation of the network synchronizability. We provide analysis and numerical evidence to support the proposition and we speculate that the loop structure can provide a platform for controlling dynamical processes on scale-free networks with high clustering coefficients.

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I. INTRODUCTION

The effect of the topology of a complex network on various dynamical processes taking place on it is a fundamental issue in statistical and nonlinear physics. Two types of network topologies, namely, small-world [1] and scale-free [2], are topics of tremendous recent interest. Briefly, a small-world network is characterized by a high clustering coefficient, the probability that two nodes are connected provided that they are both linked to a common third node, and a small network diameter, which is the average number of links connecting two arbitrary nodes in the network. The defining trait of a scale-free network is a power-law distribution in the number of links that a node possesses, or the node degree. For dynamics on networks, representative processes of recent interest include synchronization [3–6], information or virus spreading [7], and transport [8]. In terms of the interplay between network topology and dynamics, scale-free networks have been studied extensively due to their relevance to a large variety of real-world networked systems [9].

Most existing works on dynamics on scale-free networks concern about the effect of the power-law degree distribution [3–8], which naturally implies a small network diameter. In particular, a distinct feature of a scale-free network is the existence of a small set of hub nodes, nodes of unusually large degrees. The hub nodes are responsible for the long tail of the power-law degree distribution, and they typically lead to a small network diameter. Indeed, works addressing the effect of network diameter on dynamical processes were among the first in the area of complex-network dynamics [3–5]. More recently, the effect of clustering on dynamics in scale-free networks has been studied [10], with the result that networks with high clustering coefficients tend to have low synchronizability.

In this paper, we present a physical theory to explain the finding [10] that synchronization is generally suppressed in strongly clustered scale-free networks. Our central idea is to search for some dominant *loop structure* embedded in a large scale-free network. Here, a loop structure is defined as a subset of nodes that are connected with each other as if they were located on a part of a ring, where any node is connected with two nodes, one on each side. Among all possible loops on the network, the dominant loop has the largest number of nodes. Our purpose is to consider the shortest loop passing through a node, which is different from those of existing works [11] on loops in complex networks that focus on the scaling behavior of number of loops with the network size. We find that when the clustering coefficient c increases, obvious loop structure emerges (which may contain several large size loops) and we hypothesize that, if the network is sparse, the loop structure will play a determining role in shaping the network dynamics. Among these loops, we define the largest one as the dominant loop and let n be the size of the largest loop. Intuitively, as the clustering coefficient c is increased, n is increased too. Deeming the largest loop as an isolated loop then the key eigenvalues of it can be calculated, which determine the dynamics on the loops. It is possible to obtain analytic insight into how the dynamics change as c is varied. Because of the dominant role played by the loop in network dynamics, the effect of varying c on the global network dynamics can then be inferred. We will show that for sparse scale-free networks with high clustering coefficients, key eigenvalues calculated from the dominant loop agree reasonably well with the respective eigenvalues of the whole network, indicating that for such networks, the dominant loop structure can be used to serve as a predictive tool for the network synchronizability.

In Sec. II, we characterize the network synchronizability as a function of the clustering coefficient c and demonstrate the emergence of the loop structure for scale-free networks with high values of c. In Sec. III, we obtain formulas for the eigenvalues of the loop structure and present evidence that the formulas can be used to explain the suppression of the network synchronizability by strong clustering. Brief conclusion and discussion are presented in Sec. IV.

II. EMERGENCE OF LOOP STRUCTURE IN SCALE-FREE NETWORKS

In this paper, we mainly focus on the sparse scale-free networks. To have scale-free networks with systematically varying value of the clustering coefficient c, we use a stochastic rewiring algorithm. Specifically, we first generate a scale-free network using, for example, the standard preferential-attachment rule [2]. We then rewire the links randomly [12] to vary the clustering coefficient but without changing the degrees of the nodes. In particular, we first randomly pick up two edges, say (A,B) and (C,D). We then compare the numbers of local triangular structures associated with all three configurations [(A,B),(C,D)], [(A,C),(B,D)] and [(A,D),(B,C)], and select the one with most triangles and connect the nodes accordingly, where duplicated links are avoided. Note that, in this process, if a link from a given node is detached, a different link is immediately attached to this node. The process continues until a desirable value of c is attained. In this way the degree distribution and the degree sequence of the network are fixed, and the only topological property changed is c.

Synchronization of the network is determined by the spectral property of the coupling (Laplacian) matrix. Given a network of N nodes, its Laplacian matrix $L := (L_{i,j})_{N\times N}$ is defined as $L_{i,i}=k_i$, where k_i is the degree (number of edges) of node i; $L_{i,j}=-1$ if i and j are connected; and $L_{i,j}=0$ otherwise. The matrix L satisfies $\Sigma_{j=1}^{N} L_{i,j}=0$ for $i=1,\ldots,N$, which ensures the existence of synchronization states. In particular, previous works have established that the synchronizability of a network can be characterized by the largest eigenvalue λ_N and the smallest nontrivial eigenvalue λ_2 of the Laplacian matrix [3–6]. The eigenratio defined by $R \equiv \lambda_N/\lambda_2$ determines the ability of the network to have synchronous dynamics: the smaller the value of R, the more probable that the network can be synchronized. To have reasonably robust power-law degree distribution whose degree variation extends over several orders of magnitude, the underlying network must be relatively large and sparse. In this case, the largest eigenvalue λ_N is approximately given by [13]

$$\lambda_N \approx k_{\max} + 1, \tag{1}$$

where $k_{\max}$ is the maximum degree of the network. Since for our model network, the degree sequence is fixed when c is varied, $k_{\max}$ is independent of c, so is λ_N. Thus, to assess the effect of varying c on the network synchronizability, it suffices to focus on the dependence of λ_2 on c. Numerically, we find that, indeed, λ_N remains constant as c is increased from near-zero value. A typical result is shown in Fig. 1(a). The variation of λ_2 with c is shown in Fig. 1(b). We observe that λ_2 tends to decrease as c is increased, which is consistent with the previous finding that scale-free networks with relatively larger values of c have weaker synchronizability [10].

Based on the behavior of the eigenvalues of the Laplacian matrix, we can now argue that, as c is increased from a near-zero value, it is possible for some dominant loop structure to emerge in the network. As shown in Fig. 1(b), as c is increased, λ_2 decreases toward zero. In fact, a number of eigenvalues that are slightly larger than λ_2 exhibit the same tendency. Since zero is the natural minimum eigenvalue of the Laplacian matrix, the set of decreasing eigenvalues tend to cluster near but larger than zero as c is increased. What is the consequence of having a small set of near-zero eigenvalues? To gain insight, we imagine a set of isolated subnetworks, say q of them. Viewing the set of subnetworks as comprising a single network, we see that it must have q eigenvalues that are exactly zero. The intuition is then that, if a connected network possesses a number of near-zero eigenvalues, it must be quite fragile in the sense that the probability for a small perturbation to its connecting topology, such as removing a single node or a few rewirings, to disconnect the network is high. The natural and perhaps the simplest topological structure that satisfies this requirement is loops, where a set of nodes are uniformly connected by approximately the same number of links. It should be noted that the loop structure is a topological concept. For example, one can replace each node in a loop by a subnetwork, and the resulting network still satisfies the requirement that a small structural perturbation is likely to disconnect the network. Such a network actually possesses a clustered or a community structure. In this case, the presence of a set of eigenvalues close to zero indicates that the network may have a strong community structure [10]. Actually, algorithm based on spectral methods is an effective way to detect communities in large networks [14].

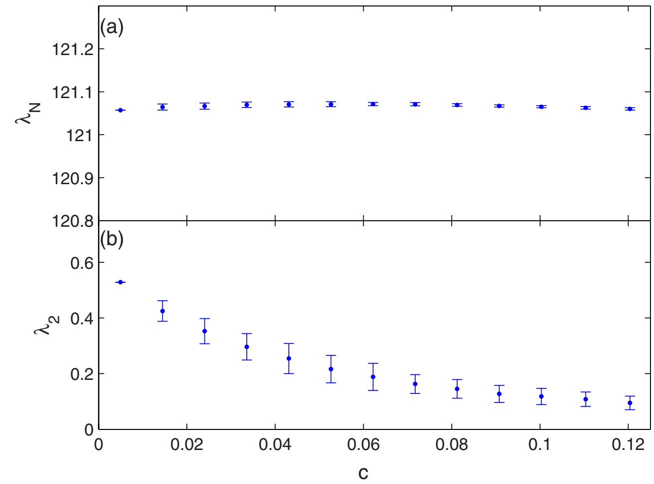

FIG. 1. (Color online) For a scale-free network of $N=2000$ nodes and average degree $\langle k\rangle=4$, the largest and the smallest nontrivial eigenvalues of the Laplacian matrix, λ_N (a) and λ_2 (b), respectively, versus the clustering coefficient c. Each data is obtained from 50 random realizations from a given initial scale-free network and both the average values and standard deviations are given.

An example of the emergence of some distinct loop structure is shown in Fig. 2 where, to facilitate visualization, we have used a relatively small scale-free network of $N=100$ nodes and average degree $\langle k\rangle=4$. We see that, for the small value of c in Fig. 2(a), there is no apparent, large-scale loop structure. However, for the relatively large value of c in Fig. 2(b), loop structures on a global scale exist.

The above argument and the numerical observation in Fig. 2 lead us to hypothesize that it is the emergence of the loop structure which causes λ_2 to decrease. To provide support, our strategy is then to calculate the smallest nontrivial eigenvalue from a topological loop, which can be done analytically, and to compare the result with the actual value of λ_2 from the network.

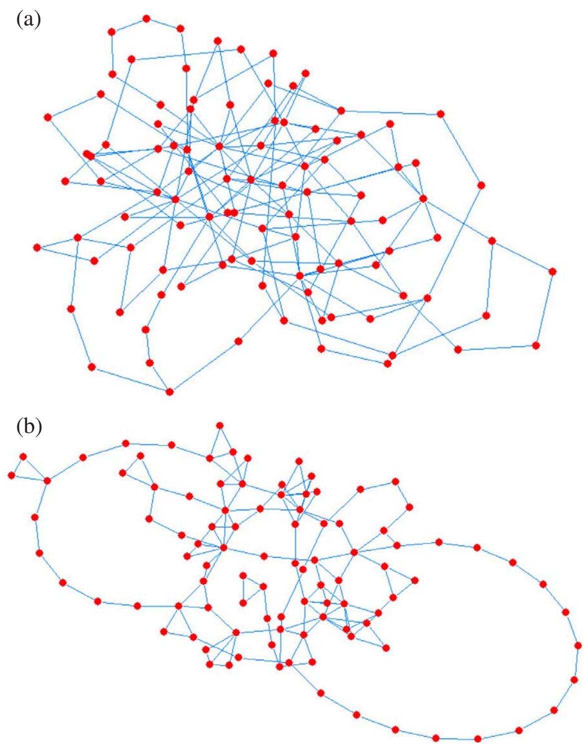

FIG. 2. (Color online) Visualizing a scale-free network ($N=100$ and $\langle k\rangle=4$): (a) absence of distinct loop structure for $c=0.02$ and (b) emergence of apparent loop structure for $c=0.32$. The graph is generated by the PAJEK software [15] using an iterative method that avoids link intersection and keeps neighboring nodes in the network as neighbors in the visualization plane.

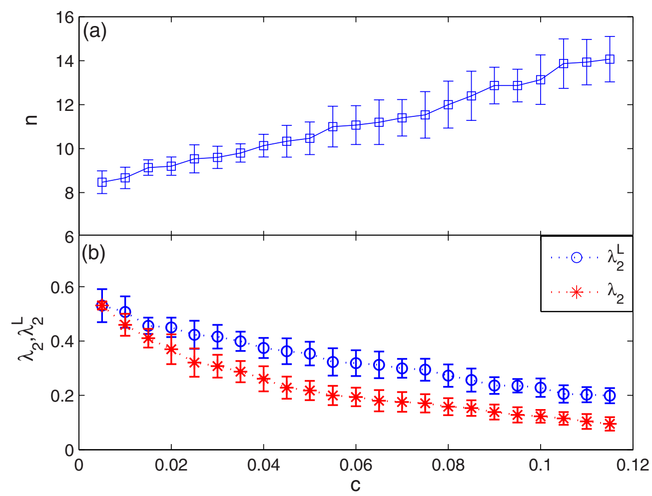

FIG. 3. (Color online) For a sparse scale-free network of $N=2000$ nodes and average degree $\langle k\rangle=4$. (a) The size of the largest loop in the network versus the clustering coefficient c and (b) the smallest nontrivial eigenvalues λ_2^L and λ_2 of the closed loop and of the whole network versus c. Each data is obtained from 50 random realizations and both the average values and standard deviations are given. The closeness of the two eigenvalues indicates the dominant role of the loop structure in network dynamics.

III. EIGENVALUES OF LOOP STRUCTURE

The purpose is to provide quantitative support for our proposition that the set of near-zero eigenvalues is dominated by the loop structure in the network. For an idealized "ring" network where each node is connected with $2m$ neighboring nodes, the eigenvalue spectrum $\{\mu_f\}$ of the Laplacian matrix is given by

$$\mu_f = 2m + 1 - \frac{\sin[(2m+1)f\pi/n]}{\sin(f\pi/n)}, \tag{2}$$

where $f=0,1,\ldots,n-1$. The eigenvalues can be ordered in an ascending sequence, and we write $0=\lambda_1^L<\lambda_2^L\leq\ldots\lambda_N^L$. We have $\lambda_2^L=\mu_1$ or μ_{n-1}. For the simple dominant loop structure as in Fig. 2(b), we have $m=1$ and, hence,

$$\lambda_2^L = 3 - \frac{\sin(3\pi/n)}{\sin(\pi/n)}. \tag{3}$$

To calculate λ_2^L for any given value of c, it is necessary to compute n, the number of nodes involved in the dominant loop structure, which can be done numerically. Figure 3 shows one such example, where the sparse scale-free network has $N=2000$ nodes and average degree $\langle k\rangle=4$. To numerically find the largest loop, we use the following procedure. For each pair of connected nodes (i,j), we first remove the link between them and then calculate their shortest path l_{ij}. The process is repeated for all links in the network, yielding max l_{ij}, the maximum of such shortest paths. The size n of the dominant loop is given by max $l_{ij}+1$. If there are more than one largest loops, we pick one randomly. From Fig. 3(a), we observe that, as c is increased, n also increases. Then we deem this loop as an isolated one and calculate the eigenvalues of the resulting coupling matrix. The loop eigenvalue λ_2^L and the counterpart λ_2 for the whole network versus c are shown in Fig. 3(b). The two eigenvalues are reasonably close to each other, suggesting that the network dynamic is dominated by the loop structure.

Equation (3) and Fig. 3 provide a plausible explanation to the decrease in λ_2 as c is increased. From Eq. (3), we see that $\partial\lambda_2^L/\partial n<0$ for $n>2$, indicating that for any nontrivial loop structure (say $n\gg 2$), λ_2^L is a decreasing function of n. This fact, in combination with the result in Figs. 3(a) and 3(b), suggests that λ_2 be a decreasing function of c. For the specific case of synchronous dynamics, this means that, as nodes in the network become more strongly clustered, its synchronizability deteriorates. This provides a physical explanation to the recent finding in [10]. A few remarks are in order.

A. Relative smallness of the dominant loop structure

The scale-free network used in Fig. 3 has $N=2000$ nodes. However, the number of nodes contained in the dominant loop is 2 orders of magnitude smaller. It thus appears surprising that such a small substructure embedded in the network can have a significant effect on the network dynamics. Indeed, the key eigenvalue λ_2 calculated from the entire network and λ_2^L calculated from the loop are approximately equal, insofar as the number of nodes constituting the loop exceeds a few, as we have observed numerically. The dominant role played by the loop structure in synchronization can be understood, heuristically, as follows. When there is a

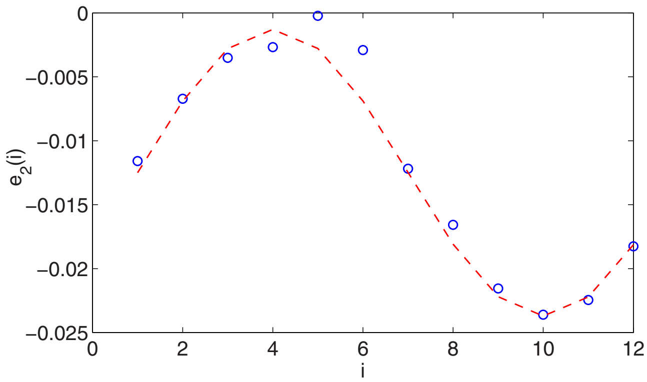

FIG. 4. (Color online) For a scale-free network of $N=1000$ nodes and average degree $\langle k \rangle = 4$, the components of the eigenvector $\mathbf{e}_2$ of the network with respect to the dominant loop.

dominant loop, the whole network can be regarded as the combination of the loop and its complementary network. The smallest nontrivial eigenvalue of the Laplacian matrix of the rest of the network can be much larger than that of the loop. If the coupling parameter is not so large, the loop is not synchronized, while the complementary network can be synchronized by itself if it is isolated from the loop. While the dynamical effect of the loop on the complementary network can be regarded as perturbations, the dynamics on the loop and on the complementary network are not synchronized, leading to a lack of global synchronization for the whole network.

B. Eigenvector associated with the dominant loop structure

To provide further evidence for the existence of a dominant loop structure, we examine the components of the eigenvectors. The idea is that, if such a structure is embedded in the network, the components of the eigenvector associated with λ_2 (not λ_2^L) from the whole network will exhibit an approximately sinusoidal structure on the subset of nodes constituting the dominant loop, due to the ringlike topology on the loop. In particular, for a ring network of n nodes, the ith component of the jth normalized eigenvector $\mathbf{e}_j$ is

$$e_j^L(i) = \sqrt{\frac{2}{n}}\sin\left(\frac{2\pi f i}{n} + \phi_j\right), \tag{4}$$

for $i,j=1,\ldots,n$, where f is the corresponding spatial frequency, and ϕ_j is the phase shift associated with the jth eigenvector. While Eq. (4) indicates a perfect sinusoidal dependence of the loop eigenvector on i, the surprising phenomenon is that the eigenvectors for the full network exhibits a nearly sinusoidal structure on the dominant loop. An example is shown in Fig. 4, where the components of the eigenvector $\mathbf{e}_2$ on the nodes in the dominant loop are plotted against the node index.

C. Sparsity of the network

The example in Fig. 3 is for a quite sparse scale-free network ($N=2000$ and $\langle k \rangle = 4$) where we observe that λ_2^L and λ_2 are approximately equal. What if the network becomes less sparse? To address this question, we have analyzed a scale-free network whose average degree doubled ($N=2000$ and $\langle k \rangle = 8$). The resulting eigenvalues λ_2^L and λ_2 versus c are shown in Fig. 5(b). We observe relatively large discrepancies between the two eigenvalues for small values of c, but as c becomes larger, the difference decreases and nearly diminishes for $c > 0.32$. This indicates that, insofar as the network is reasonably sparse, the loop structure becomes more influential on dynamics for locally more clustered networks. Heuristically, the difference between the two eigenvalues in the small c regime can be understood, as follows. For a fixed value of c, as the average degree is increased, the size of the dominant loop does not tend to increase (as we have observed numerically), thereby weakening the influence of the loop structure on the network dynamics. In Ref. [16], Samukhin *et al.* found that the Laplacian spectra of complex networks are mainly determined by the minimum degree, and the position of the lower edge of the Laplacian spectrum and the limiting behavior of the density of eigenvalues as approaching this lower edge are quite different for the case where the minimum degree is greater than 2 and the case where the minimum degree is less than or equal to 2. This result seems to be correlated with our results that the dominant loop approach agrees with the real situation better when the average degree is small. However, Ref. [16] assumes the thermodynamic limit, i.e., almost all finite subgraphs are trees, while in this paper, our concern is the effect of loop structures in finite networks. Intuitively, the large loops occur more easily in sparse networks. As for dense networks, connection probability is higher between any pair of nodes, thus the large loops, even if they exist, are more probable to be destructed by some shortcuts, lowering the order of the loops.

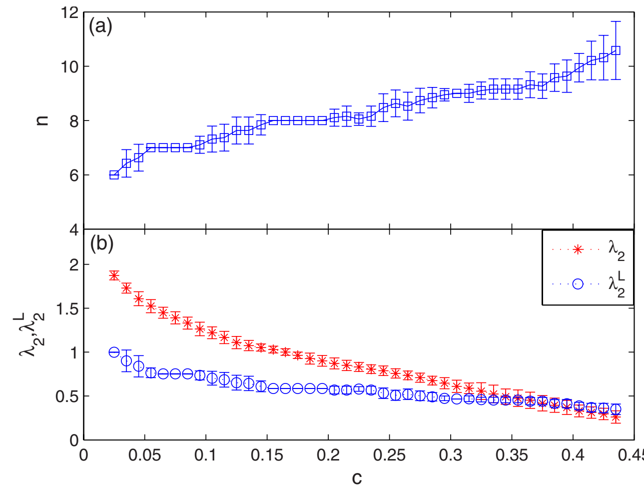

FIG. 5. (Color online) For a sparse scale-free network of $N=2000$ nodes and average degree $\langle k \rangle = 8$. (a) The size of the largest loop in the network during the realizations and (b) the smallest nontrivial eigenvalues λ_2^L and λ_2 of the closed loop and of the whole network versus c. An ensemble statistic of 50 random realizations has been carried out. The two eigenvalues agree well for relatively large values of c.

D. Minimum degree of the network

The average degree of nodes in a loop structure embedded in the network is typically 2. Thus the minimum degree of the network becomes a relevant issue. In our discussion, the scale-free network, by construction, has the minimum degree of $m > 1$. In realistic situations a scale-free network may contain a number of "leaf" nodes with degree 1. The existence of these leaves affects many aspects of the network properties such eigenvalue spectrum [16] and random walk processes [17]. Thus a concern is that are the leaf nodes influential on synchronization dynamics when clustering coefficient c increases? To address this question, we have modified the construction of the scale-free network by including a small number of leaf nodes. In particular, at each time step in the construction, we generate a leaf node with a small probability p. We find that, insofar as p is small (say $p < 0.1$, which means that less than 10% of the nodes in the network are leaf nodes), our proposition that $\lambda_2^L \approx \lambda_2$ is still valid. However, large values of p can cause significant difference between the two eigenvalues. Our assessment is that the large p cases are not as important, for the following two reasons: (1) realistic scale-free networks usually have small p values, and (2) networks with large p values usually cannot be strongly clustered (we find in numerical experiments that it becomes more and more difficult to achieve high values of c as p is increased). Thus, for scale-free networks with significant number of leaf nodes, the issue of the effect of high clustering coefficient on network dynamics is less relevant.

E. Random networks

Our result $\lambda_2^L \approx \lambda_2$ holds for scale-free networks. For a random network, the degree distribution is homogeneous, preventing the formation of relatively large loops [18]. While small loops can still emerge and their associated eigenvalues can be computed, usually they do not dominate the synchronization dynamics of the whole network. In general the emergence of a dominant loop structure with significant influence on network dynamics is more probable in networks with heterogeneous degree distributions. Despite of synchronization, the presence or lack of loop structure also has influence on other dynamical processes taking place on networks. For example, for random walks, it has been found that looped networks induce a faster dynamics, compared to complex trees, for both the coverage and the mean topological displacement problems [17].

IV. CONCLUSION

In conclusion, to account for the recent finding that strong local clustering in scale-free networks tend to suppress the network synchronizability, we have theorized the formation of loop structures that arise as the clustering coefficient of the network is increased. We have provided heuristic analysis and evidence, lending credence to our proposition that, as soon as an obvious loop structure emerges, it exerts a significant influence on the network dynamics. For sparse networks with high clustering coefficients, the largest loop can practically dominate the network dynamics. As a practical utility, we conceive that the dominant loop structure can be used as a platform for controlling the network dynamics. For example, one can add or remove nodes and links in those large loops to alter the synchronizability of the whole network. Since the size of the dominant loop is typically orders of magnitude smaller than that of the network, any modifications to the loop structure are effectively perturbations of negligible influence on the network structure, yet such small perturbations can have drastic impact on the network dynamics. Our work can be useful to real-world networks that are sparse and locally clustered.

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