Eigenvalue crossing in principal eigenvector localized networks

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(Dated: June 28, 2019)

Investigation of eigenvectors localization of complex networks is important to get insight into various structural and dynamical properties of the corresponding systems. Ref. [1] has demonstrated that the highly localized network posses a typical structure composed of two subgraphs accompanied with a sensitivity of principal eigenvector (PEV). Here, we investigate origin of the occurrence of the sensitivity of PEV in highly localized networks and show that the high localization of PEV is related with the behavior of the largest eigenvalue of the subgraph components. In particular, we find evidences of eigenvalue crossing in the networks having highly localized PEV, which in turn, provides an explanation of the origin of the sensitivity of PEV. Taking a clue from the eigenvalue crossing phenomenon, we develop an analytical treatment for direct construction of highly localized networks without performing any optimization scheme. We substantiate the eigenvalue crossing phenomenon by using the RNA neutral network population dynamical model. Our analysis provides insight into the structural and spectral properties of networks from the perspective of PEV localization.

PACS numbers: 89.75.Hc, 02.10.Yn, 5.40.-a

I. INTRODUCTION

The graph isomorphism has applications in many areas of science, including Feynman diagrams, biometrics, molecular modeling, and cryptography [2-5]. It is well known that a pair of isomorphic graphs are isocpectral. However, the existence of non-isomorphic cospectral graphs follows that eigenvalues of the adjacency matrices are not enough for characterizing the corresponding graphs, addition information of the eigenspace is necessary to find the isomorphism pairs in cospectral graphs [6]. In addition to the graph isomorphism, there exists other problems in network science which includes ranking of vertices [7], detection of communities [8, 9], perturbation analysis [10-12], vibration confinement [13], identification of important genes [14] where investigations of eigenvectors provide understanding to the behaviors of the underlying systems. Particularly, the eigenvector corresponding to the largest eigenvalue, referred as the principal eigenvector, is known to play a crucial role in the characterization of various structural as well as dynamical properties of the underlying graphs [15-17]. For instance, a connected non-bipartite graph having the largest eigenvalue $\lambda_1$ and principal eigenvector $x_1 = ((x_1)_1, (x_1)_2, \ldots, (x_1)_n)^T$, the number of walks of length $k$ between a pair of vertices $i$ and $j$ is asymptotic to $\lambda_1^k (x_1)_i (x_1)_j$, as $k \to \infty$ (see Theorem 2.2.5 of Ref. [6]). Further, localization of PEV is related to the epidemic spreading [18, 19] as well as is used to detect criticality in the brain network dynamics. [20, 21]. Further, localized eigenvectors are successful in the identification of microscopic functional units in the neural networks. [22, 23]. Furthermore, bistable activities of signaling in the biological networks have been examined through the localization of PEV of the corresponding adjacency matrices. [24]. Recently, PEV localization has been examined in multilayer networks demonstrating the impact of structural properties of one layer on the localization behavior of the entire multilayer networks [25]. An eigenvector with one entry taking value 1 and rest of the entries taking values zero, such as $x = (1, 0, \ldots, 0)^T$, is referred to as the most localized eigenvector. Similarly, an eigenvector represented by $x = (1/\sqrt{n}, 1/\sqrt{n}, \ldots, 1/\sqrt{n})^T$ corresponds to a delocalized state [17, 26]. Roots of the eigenvector localization trace back to the Anderson localization which describes the diffusion of electrons in a random, disordered medium [27]. Later on, Anderson model was used in various scientific disciplines and received remarkable success in understanding behaviors of many complex systems [28-33].

Motivated from the success of the Anderson localization in understanding behavior of complex systems, we focus on exploring eigenvector localization to gain insight into the behavior of corresponding complex systems of network's adjacency matrices. One of the previous study [1] had presented an optimized edge rewiring algorithm to construct networks having highly localized PEV’s (Fig. 1). The optimized network was shown to consist subgraphs connected via a node (Fig. 1b)). Furthermore, the optimized networks were shown to have largest two eigenvalues being very close to each other. Importantly, the optimized network was shown to contain few special edges, rewiring one of them leads to a delocalization of the PEV from a highly localized state which was referred as sensitivity of PEV [1].

In the present study, we focus on identifying the origin of sensitivity behavior of PEV localization as well as devise a method based on an analytical derivation of network parameters for a direct construction of a highly

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localized network without using any evolution scheme. The current investigation can be summarized as follows: First, we show that the eigenvalue crossing phenomenon which takes place when an edge is rewired in the localized network structure is an essence of the sensitivity behavior of PEV localization. Second, taking a clue from this eigenvalue crossing phenomenon, we establish a relationship between the largest eigenvalues of the individual subgraph of the optimized network structure. Using this relation, we analytically derive the network parameters required for a direct construction of the PEV localized networks. Ergo, our investigation identifies the necessary structural and spectral properties for highly localized networks. Third, we substantiate the eigenvalue crossing phenomenon by using the RNA neutral network population dynamical model.

The entire article is designed as follows: Section II describes the notations and definitions of the mathematical terms. It also contains a brief explanation of the network evolution method. Section III illustrates the numerical results demonstrating the relationships between the PEV localization and the second largest eigenvector which is required for eigenvalue crossing. The analytical treatment given in subsection B provides us a method for direct construction of PEV localized network without performing a network evolution method. Subsection C describe the results for the steady-state behavior of the RNA model networks. Finally, section IV summarizes our work and discusses various open problems for further investigations.

II. THEORETICAL FRAMEWORK

We represent a finite graph, \( G = \langle V, E \rangle \), where \( V = \{v_1, v_2, \ldots, v_n \} \) is the set of vertices and \( E = \{e_1, e_2, \ldots, e_m \} \) \( e_p = (v_i, v_j), p = 1, 2, \ldots, m \) is the set of edges. We define the universal set \( U = V \times V = \{(v_i, v_j) | v_i, v_j \in V \text{ and } i \neq j \} \) which contains all possible ordered pairs of vertices excluding the self-loops. The complementary set of the edges can be defined as \( E^c = U - E = \{(v_i, v_j) | v_i, v_j \in U \text{ and } (v_i, v_j) \notin E \} \) i.e., \( E \cap E^c = \emptyset \) and \( E \cup E^c = U \). We denote the adjacency matrix corresponding to \( G \) as \( A \in \mathbb{R}^{n \times n} \) which can be defined as

\[
a_{ij} = \begin{cases} 
1 & \text{if nodes } i \text{ and } j \text{ are connected} \\
0 & \text{Otherwise}
\end{cases}
\]

The \( |V| = n \) and \( |E| = m \) represent the number of nodes and number of edges in \( G \), respectively, and thus \( |E^c| = \frac{n(n-1)}{2} - m \). Here, \( A \) is a real symmetric matrix, hence, it has a set of orthonormal eigenvectors \( \{x_1, x_2, \ldots, x_n \} \) corresponding to the real eigenvalues \( \{\lambda_1, \lambda_2, \ldots, \lambda_n \} \). Moreover, the edge weights of \( A \) are non-negative \( (a_{ij} \geq 0) \), and in our current study network is always connected. Thus, \( A \) is a non-negative and irreducible matrix. Hence, we know from the Perron-Frobenius theorem that all the entries in PEV of \( A \) are positive and \( \lambda_1 > |\lambda_i|, \forall i \neq 1 \geq 34 \).

The inverse participation ratio (IPR) quantifies the localization as well as delocalization behavior of eigenvectors in complex networks \[10, 17, 21\]. We calculate the IPR value \( (Y_{\pi_j}) \) of an orthonormal eigenvector \( (x_j)_1, (x_j)_2, \ldots, (x_j)_n \) \( \text{ and } (x_j)_n \) of \( A \) as follows:

\[
Y_{\pi_j} = \sum_{l=1}^{n} (x_j)_l^4
\]

where \( (x_j)_l \) is the \( l^th \) component of \( x_j \). A delocalized eigenvector has \( Y_{\pi_j} = \frac{1}{n} \) and which can be obtained from a regular network (every node having the same degree), whereas the most localized eigenvector yields an IPR value equal to \( Y_{\pi_j} = 1 \) and can be obtained from a disconnected network. For a connected network, the IPR values lies between \( 1/n \leq Y_{\pi_j} < 1 \). In general, for a network, PEV is said to be localized if \( Y_{\pi_j} = 1 \) and delocalized if \( Y_{\pi_j} = 0 \) as \( n \to \infty \)

The PEV of an adjacency matrix approximate the steady-state vector of many linear dynamical systems. For instance, epidemic spreading model, RNA neutral networks model, rumor spreading models, brain network dynamical model \[13, 18, 21\]. By optimizing the IPR of PEV as an objective function, we obtain a network structure which has a few nodes contributing more in the dynamical process with the rest of the nodes having...
a tiny contribution. Scrutiny of structural and spectral properties of the optimized network structure can help us in reverse engineering the system design [11].

Next, we summarize the network evolution process [1]. Starting from an Erdös-Rényi (ER) random connected network, we obtain the optimized network structure through a network evolution process (Fig. 2). The ER random network is generated with an edge probability \( (k/n) \), where \( (k) \) is the average degree of the network [35]. We denote the initial random network as \( G_{init} \) (Fig. 1(a)) and the optimized network as \( G_{opt} \) (Fig. 1(b)). For an evolution step, we choose an edge \( e_p \in E \) (\( p = 1, 2, \ldots, |E| \)) uniformly at random from \( G_i \) and remove it. At the same time, we introduce an edge uniformly at random in \( G_j \) from \( e_q \in E^c \) (\( q = 1, 2, \ldots, |E^c| \)). The new network and the corresponding adjacency matrix are denoted as \( G_{i+1} \) and \( A_{i+1} \), respectively. We calculate the IPR value of the PEV from \( A_i \) and \( A_{i+1} \). If \( Y_{x_1^{i+1}} > Y_{x_1^i} \), \( A_i \) is replaced with \( A_{i+1} \) for the next evolution step (Fig. 2). On the otherhand, if \( Y_{x_1^{i+1}} < Y_{x_1^i} \), we keep \( A_i \) as it is and perform another edge rewiring on \( A_i \) which is denoted as \( A_{i+2} \). This step is repeated until we obtain \( A_{i+\tau} \) which yields to the next evolution step satisfying \( Y_{x_1^{i+\tau}} > Y_{x_1^{i}} \). Hence, each evolution step requires several trials (\( t = 1, 2, \ldots \)) of edge rewirings. We repeat the above evolution step until the IPR saturates to a very high value. The evolution process yields a sequence of networks \( G_1, G_2, \ldots, G_i, G_{i+1}, \ldots, G_\tau \) and the corresponding adjacency matrices as

\[
A_1, A_2, \ldots, A_i, A_{i+1}, \ldots, A_\tau
\]  

where \( \tau \) is the total number of edge rewiring performs during the network evolution process. Notably, during an edge rewiring, there is a possibility that network becomes disconnected. However, we allow only those edge rewirings which yield a connected network through the depth first search algorithm [35]. The network evolution process is performed with the assistance of the Monte Carlo algorithm [1].

III. RESULTS

A. Analysis of eigenvectors angles: signature of eigenvalue crossing

To capture the sensitive behavior of PEV in the optimized network structure, we consider rewiring of all the edges (trials) during the network evolution without paying attention if a rewiring leads to an increase in the IPR value or not (Appendix A). Starting from a random connected network, the optimized edge rewiring process segregates the evolution steps into three different regions referred to as \( r_1 \), \( r_2 \) and \( r_3 \) as depicted in Fig. 3(a). The regions are categorized based on the nature of changes in the IPR value of the PEV (small increment, fast increment, and saturation). To check the robustness of our results, we consider power-law degree distributed networks as the initial networks [35]. We find that the behavior of the IPR evolution remain the same irrespective of the type of initial network chosen (Fig. 3(b)).

The adjacency matrices during the network evolution process can be denoted as mentioned in (2) and the corresponding eigenvectors and IPR values can be represented as follows

\[
x_1^i, x_2^i, \ldots, x_i^i, x_{i+1}^i, \ldots, x_{\tau}^i
\]

\[
Y_{x_1^i}, Y_{x_2^i}, \ldots, Y_{x_i^i}, Y_{x_{i+1}^i}, \ldots, Y_{x_{\tau}^i}
\]

for \( j = 1, 2, \ldots, n \) and \( i = 1, 2, \ldots, \tau \)

where each \( A_i \) matrix contains a set of eigenvectors as \( \{x_1^i, x_2^i, \ldots, x_i^i\} \) with corresponding IPR values as \( \{Y_{x_1^i}, Y_{x_2^i}, \ldots, Y_{x_i^i}\} \). One can observe that due to single edge rewiring there are changes in the IPR of PEV. Next, we focus on those edge rewirings which bring IPR value of PEV from a highly localized to a delocalized state. As evident from Fig. 3 in the \( r_3 \) region, there exists abrupt
changes in the $Y_{x_1}$ and $Y_{x_2}$ values due to a single edge rewiring. Note that in the $r_1$ and $r_2$ regions none of the edge rewirings leads to such abrupt changes in the IPR values of largest two eigenvectors (Fig. 3). In other words, PEV is not sensitive in the $r_1$ and $r_2$ region to a single edge rewiring.

To elaborate this aspect of the abrupt changes in the IPR value in $r_3$ region, as a consequence of a single edge rewiring, we focus on two consecutive networks in the $r_3$ region, say, $A_i$ and $A_{i+1}$ such that $A_{i+1}$ is achieved after a single edge rewiring on $A_i$. We observe that $x_i^{1+1}$ reaches to a delocalized state, from a highly localized state, at $(i + 1)^{th}$ time step (Fig. 4 (a)). This abrupt changes in IPR value of $x_i^{1+1}$ is accompanied with a high localization of $x_2^{1+1}$ from a delocalized state ($x_2^1$) (Fig. 4 (a)). Scrutinizing the entries of the largest and the second largest eigenvectors in this two consecutive steps and comparing them with those of the initial networks, we show that there exist radical changes in the eigenvector entries (Fig. 4). In the $r_3$ region, $x_1^i$ is highly localized with maximum entry value residing to the hub node (marked with a circle in Fig. 5 (b)). However, after a single edge rewiring on $A_i$, though $A_{i+1}$ has almost the same structure, $x_1^{i+1}$ becomes delocalized (Fig. 4 (a)). The entry corresponding to the hub node for this delocalized $x_1^{i+1}$ takes a very small value (Fig. 5 (c)). Surprisingly, for $x_2^{i+1}$, the entry corresponding to the hub node takes the same value as that of the $x_1^i$ (Fig. 4 (b) and (f)). The entries in the largest two eigenvectors show a clear flip thereby affecting the IPR values of both the $x_1^{i+1}$ and $x_2^{i+1}$ in $A_{i+1}$. It is worth noting here that the delocalized PEV of $A_{i+1}$ in the $r_3$ region is very much different from the delocalized PEV of $A_i$ in the $r_1$ region (Fig. 5 (a) and 5 (c)).

An examination of relative positions of the two largest eigenvectors provide insight into the sensitive behavior of the PEV in the $r_3$ region. To trace the relative position of the largest two eigenvectors in the vector space, we track the angle by computing

$$(x_1^i)^T x_1^{i+1} \quad \text{and} \quad (x_2^i)^T x_2^{i+1} \quad \text{for} \quad i = 1, 2, \ldots, \tau$$

during the edge rewiring process in the $r_3$ region. One can see that in the $r_3$ region, presence of the flips in IPR values (Fig. 4 (a)) are reflected in similar abrupt changes in the dot product values (Fig. 4 (b))). These abrupt changes in $(x_1^1)^T x_1^{i+1}$ and $(x_2^1)^T x_2^{i+1}$ manifest a signature of the eigenvalue crossing. In the $r_3$ region, the rewiring of an edge connected to the hub node leads to rotation of $x_1$ and $x_2$ by approx. 90° (Fig. 4 (b)). It has already been reported that abrupt changes in the eigenvector entries carry information of the eigenvalue crossing [33, 34]. Moreover, it has also been noted that just after the crossing, the eigenvector becomes orthogonal to the eigenvector before the crossing. The largest two eigenvectors in the $r_3$ region satisfy these two criteria mentioned above during the flipping of the IPR values.

Further, to confirm the eigenvalue crossing phenomenon, we perform the following experiments. We separate two graph components ($C_1^i$ and $C_2^i$) of $G_i$ corresponding to $A_i$ (Fig. 4(b)) by breaking the existing connection between them, and record the largest two eigenvalues. We observe that the largest two eigenvalues of the $G_i$ remain almost the same as of the largest eigenvalue of the two graph components separately (Table I).

$$\lambda_1^{C_1^i} \approx \lambda_1^G, \lambda_2^{C_1^i} \approx \lambda_2^G$$

Further, one can also notice that

$$\lambda_1^{C_1^i} > \lambda_1^{C_2^i} \quad (3)$$

In an another experiment, if we remove an edge from $G_i$, which is connected to the hub node in $C_1^i$, and add it between a randomly selected pair of nodes in $C_2^i$, there exists a an abrupt change in the localization behavior of PEV. The modified network is denoted as $\tilde{G}_{i+1}$. This reshuffling of an edge makes $x_1^{i+1}$ to be in a delocalized and $x_2^{i+1}$ to be in a highly localized state (Fig. 4 (a)). Next, if we separate two components of $\tilde{G}_{i+1}$, we observe (Table I) that

$$\lambda_1^{C_2^{i+1}} \approx \lambda_1^{\tilde{G}_{i+1}}, \lambda_1^{C_1^{i+1}} \approx \lambda_2^{\tilde{G}_{i+1}}$$

The transition between localized and delocalized state for $x_1^{i+1}$ and $x_2^{i+1}$ respectively in $\tilde{G}_{i+1}$ is accompanied with a change in the $\lambda_1^{C_1^{i+1}}$ value leading to

$$\lambda_1^{C_1^{i+1}} < \lambda_1^{C_2^{i+1}} \quad (4)$$

For both the experiments, the largest eigenvalues of $G_i$ and $\tilde{G}_{i+1}$ are always greater than the corresponding sec-
TABLE I. Largest three eigenvalues and IPR values of two largest eigenvectors of the optimized networks (G_i) in the r_3 region as well as its two components (C_1 and C_2). After rewiring of an edge connected to the hub node in G_i, the new network is denoted as G_{i+1} and its two components are denoted with C_{i+1} and C_{i+1}.

| Networks | n  | k_{max} | m   | Y_\cdot_{x1} | Y_\cdot_{x2} | \lambda_1 | \lambda_2 | \lambda_3 |
|----------|----|---------|-----|-------------|-------------|-----------|-----------|-----------|
| G_i      | 500| 101     | 2512| 0.19059     | 0.00253     | 11.48807  | 11.47669  | 6.28379   |
| C_1      | 102| 101     | 236 | 0.19075     | 0.02251     | 11.48764  | 2.65329   | 2.63804   |
| C_2      | 397| 12      | 2274| 0.00253     | 0.00657     | 11.47660  | 6.28334   | 6.10097   |
| G_{i+1}  | 500| 100     | 2512| 0.00253     | 0.19084     | 11.48227  | 11.42444  | 6.29319   |
| C_{i+1}  | 102| 100     | 235 | 0.19075     | 0.02251     | 11.42401  | 2.65315   | 2.63839   |
| C_{i+1}  | 397| 13      | 2275| 0.00253     | 0.00643     | 11.48217  | 6.29273   | 6.11759   |

TABLE II. Various structural and spectral properties of two components (C_1 and C_2), and the one achieved by connecting them through a link. We consider ER random graph, Scale-free (SF), wheel (W), and random regular (R) networks as individual component. Satisfying \lambda_1^{C_1} > \lambda_2^{C_2} leads to a localized PEV and for \lambda_1^{C_1} < \lambda_2^{C_2} yields delocalized PEV of the combined graph.

| No. | G    | n_1 | n_2 | | | | | |
|-----|------|-----|-----|-----|-----|-----|-----|-----|
| 1   | ER-SF| 500 | 500 | | | | | |
| 2   | R-W  | 500 | 24  | | | | | |
| 3   | ER-SF| 500 | 500 | | | | | |
| 4   | R-W  | 500 | 26  | | | | | |

TABLE III. Largest three eigenvalues and IPR values of two largest eigenvectors of the optimized networks (G_i) in the r_3 region as well as its two components (C_1 and C_2). After rewiring of an edge connected to the hub node in G_i, the new network is denoted as G_{i+1} and its two components are denoted with C_{i+1} and C_{i+1}.

\[
\lambda_1^{G_i} > \lambda_2^{G_i} \quad \text{and} \quad \lambda_1^{G_{i+1}} > \lambda_2^{G_{i+1}} \\
\lambda_1^{C_1} > \lambda_2^{C_1} \quad \text{and} \quad \lambda_1^{C_{i+1}} < \lambda_2^{C_{i+1}} \\
\]

which also satisfy the primitivity property of Perron-Frobenius theorem \cite{34}. However, changes occur in the largest eigenvalue of the individual components in G_i and G_{i+1} (Eqs. 33 and 34) occurs due to the eigenvalue crossing. In other words, for the case of the highly localized PEV the component containing the hub node has prime contribution in the largest eigenvalue.

To summarize, the optimized network evolution process acts as a black box which takes a given network of size n and m as input and produces an optimized structure (G_i) having two components (C_1 and C_2) connected via a node, where C_1 contains a hub node, and C_2 has almost a regular structure. Additionally, \lambda_1^{G_i} > \lambda_2^{G_i} and \lambda_1^{C_1} > \lambda_2^{C_1}.

On the other hand, for delocalized PEV \lambda_1^{G_{i+1}} > \lambda_2^{G_{i+1}} and \lambda_1^{C_{i+1}} < \lambda_2^{C_{i+1}}. In other words, optimization process provides a partition to a given network of n number of nodes and m number of edges into two components such that \( n = n_1 + n_2 + 1, m = m_1 + m_2 + 2 \) and \( \lambda_1^{C_1} > \lambda_2^{C_2} \) where \(|E_{C_1}| = m_1 \) and \(|E_{C_2}| = m_2 \). Next, we ask a question that can be use one or all of these pieces of information to directly construct a network, without performing the network evolution process. Note that, combining any two components with one of them containing a hub node and another having a regular structure, does not produce a localized PEV, thereby making the problem more challenging. For instance, by combining two components where one of them contains a hub node and another has a regular structure, one can bring the largest two eigenvalues of G close enough (e.g., ER random and scalefree (SF) networks). However, this way of the network construction while yields close enough \lambda_1^{G} and \lambda_2^{G}, may not lead to a localized PEV (Table II (No. 1, 2)) indicating that closeness of largest two eigenvalues is a necessary but not a sufficient condition. It turns out, for a localized PEV a particular eigenvalue relation \( \lambda_1^{C_1} > \lambda_2^{C_2} \) between the individual component should hold true (Table II (No. 3, 4)). In the following we analytically calculate the subgraph component size which satisfy the particular eigenvalue relation.

B. Analytical method for direct construction of localized network using wheel graph

From the numerical simulations, we learn that in the optimized networks, C_1 contains a hub node while C_2 has almost a regular structure. Hence, we choose structures which resemble to C_1 and C_2 components. The closest structures corresponds to C_1 is a star or wheel graph (Fig. II (b)). For C_2 component, we choose a random regular structure.

It turns out that one can recreate the spectral properties of the optimized network by replacing C_1 with a wheel graph and C_2 with a random regular network. A wheel graph is denoted as W = \{V_W, E_W\} where |V_W| = n_1 is the number of nodes and |E_W| = 2(n_1 - 1) is the number of edges in W. Further, the random regular graph is denoted as R = \{V_R, E_R\} where |V_R| = n_2 is the number of nodes and |E_R| = \( \frac{3n_2}{2} \) is the number of edges with each node having degree 3 \( \leq \kappa \leq n_2 - 2 \). We generate the random regular graph using the algorithm in \cite{40}. Further, it is known that for a wheel and random regular graph, the largest eigenvalues are as follows \cite{41}

\[
\lambda_1^{W} = 1 + \sqrt{n_1} \quad \text{and} \quad \lambda_1^{R} = \kappa \\
\]

Interestingly, to connect a wheel graph with a random regular network such that \( \lambda_1^{W} > \lambda_1^{R} \), we need the information about the size of the individual component (n_1, n_2 and \kappa) of the combined network (G_{new}). By using the
relation $\lambda^W_1 > \lambda^R_1$, we consider,

$$\lambda^W_1 = \lambda^R_1 + \epsilon \text{ where } 0 < \epsilon < 1 \quad (6)$$

and from Eqs. (5) and (6), we obtain the size of the wheel graph as follows

$$n_1 = \lceil (\kappa - 1 + \epsilon)^2 \rceil \quad (7)$$

where $\lceil \cdot \rceil$ is the ceiling function and Eq. (7) tells that for a particular value of $\kappa$ if we take $[(\kappa - 1 + \epsilon)^2]$ as a number of nodes for the wheel graph, then combined graph will satisfy Eq. (6).

Importantly, in Eq. (7) the number of nodes in the $W$ component of $G_{new}$ depends on the average degree of the $R$ component in $G_{new}$. Therefore, to construct $G_{new}$, we are free to choose any arbitrary number for the nodes and for the average degree $(3 \leq \kappa \leq n_2 - 2)$ of the random regular component such that $\kappa n_2$ is even.

From the above investigation, we learn that we can construct a PEV localized network without having any restriction on $\kappa$ and $n_2$. However, to avoid the rewiring process, the partition of a given set of $n$ and $m$ should be such that it satisfies Eq. (7) as well as the following two relations

$$n = n_1 + n_2 + 1 \quad (8)$$

and

$$m = |E_W| + |E_R| + 2 = \frac{4n_1 + n_2\kappa}{2} \quad (9)$$

simultaneously. From Eqs. (7) and (8) we know that

$$n_2 = n - \lceil (\kappa - 1 + \epsilon)^2 \rceil - 1 \quad (10)$$

To find a $\kappa$ value for any given set of $n$ and $m$ such that they satisfy Eqs. (7), (8) and (9), we rearrange Eq. (9) with the help of Eqs. (7) and (10), and reach to a cubic equation of the form

$$\kappa^3 + b\kappa^2 + c\kappa + d = 0 \quad (11)$$

where $b = (-4 - 2(1 - \epsilon))$, $c = ((1 - \epsilon)^2 + 8(1 - \epsilon) + 1 - n)$, and $d = (2m - 4(1 - \epsilon)^2)$ are the coefficient of the cubic equation. Next, roots of the cubic equation can be written from the Cardano’s formula as follows,

$$\kappa_1 = \frac{1}{2}(\Delta_1 + \Delta_2) - \frac{b}{3} \quad (12)$$

$$\kappa_2 = -\frac{1}{2}(\Delta_1 + \Delta_2) + \frac{i\sqrt{3}}{2}(\Delta_1 - \Delta_2) - \frac{b}{3}$$

$$\kappa_3 = -\frac{1}{2}(\Delta_1 + \Delta_2) - \frac{i\sqrt{3}}{2}(\Delta_1 - \Delta_2) - \frac{b}{3}$$

such that

$$\Delta_1 = \sqrt{-\beta/2 + \sqrt{\Delta}} \text{ and } \Delta_2 = \sqrt{-\beta/2 - \sqrt{\Delta}} \quad (13)$$

where $\Delta = \frac{-b^2}{4} + \frac{c^2}{4}$, $\alpha = \frac{1}{3}(3c - b^2)$, $\beta = \frac{1}{9}(2b^3 - 9bc + 27d)$ and $i^2 = -1$. Therefore, given a set of $n$ and $m$, we obtain three different possible values for $\kappa$ to partition $n$ and $m$ between two subgraphs. There is a possibility to get complex values for $\kappa$. The following analysis present bounds to avoid complex numbers as well as other unnecessary situation.

We know that for a given $n$, value of $m$ can vary between $n - 1$ to $n(n - 1)/2$. It turns out that as $m$ varies, nature of the roots changes yielding real or complex values for $\kappa$’s. We know that behavior of the discriminant ($\Delta$) leads to a change in the nature of the roots. However, we donot know the exact relation between $m$ and $\Delta$. It is known that (a) $\Delta = 0$ yields three real roots in which at least two are equal, (b) $\Delta > 0$ gives one real root and other two complex conjugate roots, (c) $\Delta < 0$ yields three unequal real roots [12]. To know the behavior of the discriminant as $m$ changes for a particular value of $n$, we analyze $\Delta$ in Eq. (13) of the cubic equation as;

$$\Delta = (m - n\sigma - p)^2 - \left(\frac{n}{3} + q\right)^3 \quad (14)$$

where $\sigma = (1 - \frac{\epsilon}{\sqrt{3}})$, $p = \frac{c^2 + 9\epsilon^2 + 36\epsilon}{27}$, $q = \frac{c^2 + 6\epsilon + 6}{9}$ and we consider $n \geq 49$ (Appendix B). Analyzing the discriminant reveals that for

$$m = (n\sigma + p) + \frac{(n + 3q)\sqrt{3(n + 3q)}}{9} \quad (15)$$
(a) $\Delta = 0$ (see Appendix [13]). Further, from the above equation, we find the lower and upper bounds of $m$ for which $\Delta < 0$ and $\Delta > 0$ as follows

$$n + 1 \leq m \leq \left[ (n\sigma + p - 1) + \frac{(n + 3q)\sqrt{3(n + 3q)}}{9} \right]$$

$$\left[ (n\sigma + p + 1) + \frac{(n + 3q)\sqrt{3(n + 3q)}}{9} \right] \leq m \leq \frac{n(n - 1)}{2}$$

The ranges of $m$ illustrates that as network becomes dense, $\Delta$ becomes greater or equal to zero (Fig. 5). From Eq. (13), one can see that $\Delta = 0$ appears when $m$ is a real with fractional part (Eq. (15)). However, in our case, $m$ represents the number of edges in $G_{new}$ and is a positive integer. Hence, $\Delta = 0$ can never appear. Further analysis of the discriminant reveals that for (b) $\Delta > 0$, $n_1$ calculated from $\kappa_1$ (in Eq. (7)) is always larger than the given value of $n$. Hence, we can not use $\kappa_1$ to find $n_1$ and $n_2$ in Eqs. (7) and (10) for the construction of $G_{new}$ (see Appendix [13]). Finally, we investigate the case (c) which corresponds to three unequal real roots in Eq. (12) (see Appendix [13]). We have achieved two different ways to divide the number of nodes in two different groups such that the entire network has a localized PEV. The first way is that we consider a sparse regular structure with a smaller size wheel graph, and the second way is to consider a dense regular structure with a larger size wheel graph. Similar to the network evolution process, coefficients of the cubic equation take $n$, $m$ and $\epsilon$ as the input parameter and produce the subgraph parameters for a direct construction of the PEV localized network (Fig. 7).

Table [11] verifies the theoretical approach of arranging the graph components into two different ways. For a given value of $n$ and $m$, we calculate average degree of regular graph ($\kappa_1$) from Eq. (12). Next, from Eqs. (7) and (10), we calculate $n_1$ and $n_2$ values which in turn provide us the size of the wheel and the random regular graphs while satisfying Eq. (6). This combined graph has a localized $x_1$ and a delocalized $x_2$. Similarly, the root $\kappa_2$ can be calculated by the same procedure and we can calculate $n_1$ and $n_2$. The $Y_{x_1}$ value obtained from the analysis come out to be the same as the value obtained from the optimized edge rewiring process (Table [11]).

The method simplifies our understanding to the origin of peculiar spectral properties of the optimized structure, as well as provides us a simple method to achieve a large size PEV localized network without performing any optimized edge rewiring process. To conclude, investigation of an optimized network structure obtained through the network evolution reveals that the high localization of the PEV is accompanied by holding the eigenvalue relation between the individual components ($\lambda_1^W > \lambda_1^R$). The analysis presented in this section is an attempt to solve the problem in a reverse manner. It shows that by considering $\lambda_1^W > \lambda_1^R$, one can produce a network structure having a highly localized as well as sensitive PEV.

### C. Localization behavior on RNA dynamical model

In the previous part, we investigate eigenvalue crossing and its relation with the sensitivity behavior of PEV corresponding to the adjacency matrices. Next, we turn our attention to show the impact of eigenvalue crossing phenomenon, caused by single edge rewiring, on the steady-state behavior of a dynamical system. We consider RNA neutral network population linear dynamical model [16, 14, 10] and is given by

$$M = f(1 - \mu)I + \frac{f\mu}{3L}A$$

where $M$, $I$, and $A$ are the transition, identity, and adjacency matrices respectively. The transition matrix $M$ models a process in which for each timestep a population replicates at each node at a rate $f > 1$, and each daughter sequence leaves the node with a probability $\mu$ and survives with a probability $1 - \mu$ where $L$ is the sequence length and $0 < \mu < 1$. For the above model, the steady-state vector is obtained from the PEV of the transition matrix. Importantly, for the above model, all the eigenvectors of $A$ and $M$ are the same which can easily be shown from Eq. (16) as follows

$$Mx_i^A = f(1 - \mu)Ix_i^A + \frac{f\mu}{3L}Ax_i^A$$

$$= f(1 - \mu)x_i^A + \frac{f\mu}{3L}\lambda_i^A x_i^A$$

$$= \lambda_i^M x_i^A$$

where $\lambda_i^M = f(1 - \mu) + \frac{f\mu}{3L}\lambda_i^A$, $\lambda_i^M$ and $\lambda_i^A$ denotes the eigenvalues and $x_i^M$ and $x_i^A$ are the eigenvectors of $M$ and $A$ respectively. Further, $\lambda_i^M$ is the asymptotic growth rate of the population and from Eq. (17) one can observe that limit distribution of population or the steady-state vector of the transition matrix is solely determined by the PEV of the adjacency matrix [16, 12].

| $n$ | $m$ | $\kappa_1$ | $n_1$ | $n_2$ | $Y_{x_1}$ | $\kappa_2$ | $n_1$ | $n_2$ | $Y_{x_1}$ |
|-----|-----|-----------|------|------|----------|-----------|------|------|----------|
| 500 | 2512 | 18        | 290  | 209  | 0.22     | 13        | 145  | 354  | 0.21     |
| 520 | 2630 | 19        | 325  | 194  | 0.22     | 13        | 145  | 374  | 0.21     |
| 2448| 14806| 46        | 2027 | 420  | 0.23     | 13        | 145  | 2302| 0.21     |
| 4720| 13712| 69        | 4627 | 92   | 0.24     | 6         | 26   | 4693| 0.17     |
| 10498| 52490| 101       | 10005| 492  | 0.24     | 11        | 101  | 10396| 0.20     |
| 20422| 163376| 138      | 18775| 1646 | 0.24     | 17        | 257 | 20164| 0.22     |
One can observe (Figs. 8 and 9) drastic changes in the steady-state vector of the RNA model arising due to the eigenvalue crossing phenomenon. The two largest eigenvalues of the network remain close to each other, but there exist changes in the individual eigenvalue relation leading to change in the behavior of the steady-state. To avoid this sensitive dependence of the steady-state arising due to a single edge rewiring, we either increase the largest eigenvalue of the wheel graph component by increasing the size, or we can increase the average degree of the regular graph component which we learned from the analytical approach discussed in subsection B. Although the wheel-random structure is quite special, it provides us an understanding of the localization behavior observed for the networks evolved through the optimized evolution process. Note that the dynamical system used here is a simplified and discrete-time version of the Eigen’s molecular-evolution model [44]. All the data and codes used in this paper are available at GitHub repository [47].

We perform the power iteration method on $M$ with an initial population distribution vector having all the entries same. Considering $A$ as the adjacency matrix corresponding to the wheel-random structure with $\lambda_1^W > \lambda_1^R$, maximum contribution to the dynamical process comes from a single node (Fig. 8). In the wheel-random network, we rewire an edge connected to the hub node and add it to the random regular structure, and the new transition matrix is denoted by $M'$. We again perform the power iteration method on $M'$ with the initial population distribution vector which has all the entries same.

Our investigation reveals that the eigenvalue crossing along with the presence of a hub node is the prime reason behind the sensitivity of the PEV in the optimized network. We found that single edge rewiring in the optimized network structure leads to an eigenvalue crossing which is detected through the dot product of the two largest eigenvectors. We show that the eigenvalue crossing leads to a change in the eigenvalue relation of the individual components and in turn, governs the sensitivity of the PEV localization. To check the robustness of our results, we have considered power-law degree distributed networks as the initial networks and find that behavior of the IPR values remains the same irrespective of the type of initial network chosen.

From the observation of the eigenvalue crossing phenomenon, we obtain a method for the direct construction of a network structure which has a highly localized as well as sensitive PEV. Importantly, this structure is obtained without performing an optimization scheme. In other words, we use the information of spectral properties of the optimized network to perform reverse engineering to construct a network structure having a highly localized PEV. By mapping the eigenvalue relation of the individual components to a cubic equation and solving it analytically, we find the component size for direct construction of PEV localized networks.

Although the structure of the wheel-random network is far from those of the real-world networks, few unique properties (localized PEV, existence of sensitivity, presence of a hub node with size related to largest eigenvalues of the individual component) of the networks can act as a benchmark for further applications and theoretical analysis in the future. Note that instead of using a wheel graph, we can also use a star graph to construct $G_{new}$ having the localized PEV. Additionally, we show that

IV. CONCLUSION
the eigenvalue crossing phenomenon exists for the RNA neutral network population dynamical model as well as is sensitive to the dynamical behavior on the wheel-random network structure due to single edge rewiring. Here, we have focused only on adjacency matrices with binary entries which are different from the matrices used in the Anderson localization and several other matrix representations of networks (e.g., Laplacian, Jacobian, Hessian, etc.) [48–51]. It will be interesting to use the framework developed here to analyze other matrix representations of complex networks.

ACKNOWLEDGMENTS

SJ acknowledges CSIR, Govt. of India grant (25(0293)/18/EMR-II) and DAE, Govt. of India grant (37(3)/14/11/2018-BRNS/37131) for financial support. PP acknowledges CSIR, Govt. of India grant (09/1022(0070)/19-EMR-I) for SRF fellowship. We are indebted to Manavendra Mahato (IIT Indore) for useful discussions on the eigenvalue crossing phenomenon and are thankful to members of CSL at IIT Indore for discussions.

Appendix A: Behavior of all IPR values

The appendix revolves around explaining the behavior of all the IPR and eigenvalues during the optimization process. During the evolution, by considering only those edge rewirings which perform increments in the IPR value of PEV, we observe that the localization of PEV leads to a complete delocalization of the second largest eigenvector as well as localization of the lowest eigenvector. Whereas, IPR values of rest of the eigenvectors fluctuate around almost a constant value without noticeable changes (Fig. 10). Further, one can observe from the eigenvalue behavior, in the $r_3$ region, the second largest ($\lambda_2$) and the lowest eigenvalues ($\lambda_n$) start drifting away from the bulk part of the eigenvalues, whereas rest of the eigenvalues does not show significant changes (Fig. 11). It is known that localization of PEV leads to a localization of the lowest eigenvector [24]; however, the behavior of the second largest eigenvector, and moreover, its relation with the PEV localization have so far not been explored. Our analysis reveals that the localization behavior of the second largest eigenvector is related to the sensitive behavior of PEV in the $r_3$ region. To check the robustness of our results, we have considered power-law degree distributed networks as the initial networks (Figs. 12 and 13) and find that the behavior of the network evolution remains the same irrespective of the type of initial network chosen.

Appendix B: Discriminant analysis

The section analyzes the discriminant of Eq. (13) and provides the bounds for the wheel graph size ($n_1$) as a function of $n$. To achieve, we first find the range of $m$ values and their relations with the behavior of discriminant ($\Delta$). Then, we calculate the bounds for the roots and calculate the bounds for $n_1$. We rewrite the discriminant in Eq. (13)

$$
\Delta = \frac{\beta^2}{4} + \frac{\alpha^3}{27} = (m - n\sigma - p)^2 - \left(\frac{n}{3} + q\right)^3
\tag{B1}
$$

where $\sigma = (1 - \frac{1}{4})$, $p = \frac{e^3 + 9e^2 + 36e}{27}$, and $q = \frac{e^2 - 6e + 6}{9}$. We consider connected network and choose $m$ in between $n + 1$ to $n(n - 1)/2$ where $n \geq 49$. 
Case (i) [$\Delta = 0$]: To find out the value of $m$ for which $\Delta = 0$, we solve,

$$
(m - n\sigma - p)^2 - \left(\frac{n}{3} + q\right)^3 = 0 \quad (B2)
$$

Solving the quadratic equation for $m$, we get $m = (n\sigma + p) \pm \frac{(n+3)\sqrt{3(n+3q)}}{9}$ for which $\Delta = 0$. We know that $m$ should always be a positive quantity, hence we consider

$$
m = (n\sigma + p) + \frac{(n+3)\sqrt{3(n+3q)}}{9} \quad (B3)
$$

Moreover, in our case, $m$ is always a positive integer but from Eq. $(B3)$, $m$ is a real value with fractional part. Hence, $\Delta = 0$ can never appear for our case.

Case (ii) [$\Delta > 0$]: Now, as $m$ should be a positive integer we add 1 to Eq. $(B3)$ and get the lower bound for $m$ value as follows

$$
\left[(n\sigma+p+1) + \frac{(n+3q)\sqrt{3(n+3q)}}{9}\right] \leq m \leq \frac{n(n-1)}{2} \quad (B4)
$$

for which $\Delta > 0$. Now, we substitute Eq. $(B1)$ in Eq. $(B4)$, and we have

$$
\Delta_1 = \left[-(m - n\sigma - p) + \sqrt{(m - n\sigma - p)^2 - \left(\frac{n}{3} + q\right)^3}\right]^{1/3}
$$

$$
\Delta_2 = \left[-(m - n\sigma - p) - \sqrt{(m - n\sigma - p)^2 - \left(\frac{n}{3} + q\right)^3}\right]^{1/3}
$$

Further, for the range of $m$ values mentioned in Eq. $(B4)$, $(m - n\sigma - p) > \sqrt{(m - n\sigma - p)^2 - \left(\frac{n}{3} + q\right)^3}$, thus

$$
\frac{\sqrt{(m - n\sigma - p)^2 - \left(\frac{n}{3} + q\right)^3}}{m - n\sigma - p} < 1 \quad \text{and hence using bionomial ap-}
$$

proximation we get

$$
\Delta_1 \approx -(m - n\sigma - p)^{1/3} \left[1 - \frac{\sqrt{3(n+3q)}}{3(m - n\sigma - p)} \right]
$$

$$
\Delta_2 \approx -(m - n\sigma - p)^{1/3} \left[1 + \frac{\sqrt{3(n+3q)}}{3(m - n\sigma - p)} \right]
$$

Therefore, from Eq. $(12)$ and using the above two relations we get,

$$
\kappa_1 = -2(m - n\sigma - p)^{1/3} + \frac{6 - 2\epsilon}{3} \quad (B5)
$$

Further, from Eq. $(B5)$ with the help of inequality in Eq. $(B1)$, we get lower bound for $\kappa_1$ using the bionomial approximation as follows

$$
\kappa_1 > -2\left(\frac{n(n-1)}{2} - n\sigma - p\right)^{1/3} + \frac{6 - 2\epsilon}{3}
$$

$$
= -2\left(\frac{n^2}{2} - \frac{n(9 - 2\epsilon - p)}{6}\right)^{1/3} + \frac{6 - 2\epsilon}{3}
$$

for $0 < \epsilon \ll 1$

$$
\approx -2^{2/3}n^{2/3}\left(1 - \frac{1}{n}\right) + 2
$$

for $n \to \infty$

$$
\approx -(2n)^{2/3} + 2
$$

Similarly, we calculate the upper bound for $\kappa_1$ from Eqs. $(B4)$ and $(B5)$ as follows

$$
\kappa_1 < -\frac{2}{\sqrt[3]{n}} + 2
$$

Hence, combining the above two cases for $\Delta > 0$ we have

$$
(2n)^{2/3} + 2 < \kappa_1 < -\frac{2}{\sqrt[3]{n}} + 2
$$
and finally from Eq. (7), we get bounds for \( n_1 \) as follows
\[
\frac{4}{3} n^{\frac{1}{3}} - \frac{4}{\sqrt[3]{n}} < n_1^{\kappa_1} < (2n)^{4/3} - 4n^{2/3}
\]
From the above, we conclude that for a given \( n \) value as \( m \) varies in the range given in Eq. (B4), size of the wheel graph varies in the above range. Finally, we show that \( \frac{4}{3} n^{\frac{1}{3}} - \frac{4}{\sqrt[3]{n}} > n \) for \( n \geq 49 \) and \( (2n)^{4/3} - 4n^{2/3} > n \) for \( n \geq 4 \). Hence, for \( n \geq 49 \), size of the wheel graph exceeds the given \( n \). Thus, we can not use \( \kappa_1 \) for the wheel graph size calculation from Eq. (7).

**Case (iii) \( \Delta < 0 \):** Subtracting 1 from Eq. (B3), we get upper bound for \( m \)
\[
n + 1 \leq m \leq \left( (n\sigma + p - 1) + \frac{(n + 3q)\sqrt{3(n + 3q)}}{9} \right)
\]
for which \( \Delta < 0 \). Now, following the inequality in Eq. (B7), from Eq. (13) we get
\[
\Delta_1 = z_1^{1/3} \quad \text{and} \quad \Delta_2 = z_2^{1/3}
\]
where
\[
z_1 = \left[ -(m - n\sigma - p) + i\sqrt{\left(\frac{n}{3} + q\right)^3 - (m - n\sigma - p)^2} \right], \quad z_2 = \left[ -(m - n\sigma - p) - i\sqrt{\left(\frac{n}{3} + q\right)^3 - (m - n\sigma - p)^2} \right]
\]
Hence, \( \Delta_1 \) and \( \Delta_2 \) are the cubic roots of complex numbers \( z_1 \) and \( z_2 \) respectively. Therefore, in the polar form
\[
z_1 = r_1 \cos \theta_1 + i \sin \theta_1, \quad z_2 = r_2 \cos \theta_2 + i \sin \theta_2
\]
and the cubic roots of \( z_1 \) and \( z_2 \) can be calculated as
\[
\Delta^s_1 = \sqrt[s]{r_1} \left[ \cos \left( \frac{2\pi s + \theta_1}{3} \right) + i \sin \left( \frac{2\pi s + \theta_1}{3} \right) \right], \quad s = 0, 1, 2
\]
\[
\Delta^s_2 = \sqrt[s]{r_2} \left[ \cos \left( \frac{2\pi s + \theta_2}{3} + i \sin \left( \frac{2\pi s + \theta_2}{3} \right) \right), \quad s = 0, 1, 2
\]
and hence from Eq. (12) we get
\[
\kappa_1 = \Delta^1_1 + \Delta^1_2 - \frac{b}{3}
\]
\[
= \sqrt[r_1]{\cos \left( \frac{2\pi s + \theta_1}{3} \right) + i \sin \left( \frac{2\pi s + \theta_1}{3} \right) + \left( \frac{2\pi s + \theta_2}{3} \right) + i \sin \left( \frac{2\pi s + \theta_2}{3} \right) - \frac{b}{3}
\]
To simplify the above equation, we perform the following steps. From Eq. (B8), we calculate
\[
r_{z_1} = \sqrt{\left( -(m - n\sigma - p) \right)^2 + \left( \sqrt{\left(\frac{n}{3} + q\right)^3 - (m - n\sigma - p)^2} \right)^2} = \left( \frac{n}{3} + q \right)^{\frac{2}{3}}
\]
Similarly, from Eq. (B8) we also get, \( r_{z_2} = \left( \frac{n}{3} + q \right)^{\frac{2}{3}} \).

\[
\text{Hence,} \quad r_{z_1} = r_{z_2} = \left( \frac{n}{3} + q \right)^{\frac{2}{3}}
\]
Now, one can see that for the range of \( m \) value in Eq. (B7), \( (m - n\sigma - p) > 0 \) and \( \sqrt{\left(\frac{n}{3} + q\right)^3 - (m - n\sigma - p)^2} \)
implies that \( \frac{\pi}{6} < \theta_1 < \pi \), \( \frac{\pi}{6} < \theta_2 < \pi \), and \( \frac{\pi}{2} < \theta_3 < \pi \). Finally, \( \frac{\pi}{6} < \theta_1 < \pi \), \( \frac{\pi}{6} < \theta_2 < \pi \), and \( \frac{\pi}{2} < \theta_3 < \pi \).

Further, it is known \( \Delta < 0 \) provides three unequal real roots, hence, \( \kappa_1 \) should be a real value \[42\]. One can see that we get a real value for \( s = 0 \) and complex number for other \( s \) values. Finally, for \( s = 0 \), from Eq. (B12) we get
\[
\kappa_1 = 2 \left( \frac{n}{3} + q \right)^{\frac{2}{3}} \cos \frac{\theta_1}{3} + \frac{6 - 2\epsilon}{3}
\]
and similarly from Eq. (12) by using the relation in Eqs. (B10), (B11) we get
\[
\kappa_1 = \frac{2\sqrt{r_1} \cos \frac{\theta_1}{3} + \frac{6 - 2\epsilon}{3}}{3}
\]
and for \( s = 0 \), we get
\[
\kappa_2 = 2 \left( \frac{n}{3} + q \right)^{\frac{2}{3}} \sin \frac{\theta_2}{3} + \frac{6 - 2\epsilon}{3}
\]
and which is positive. Further, \( 0 < \theta_1 < \pi \), \( \frac{\pi}{6} < \theta_2 < \frac{\pi}{2} \) implies that \( 0 < \sin \left( \frac{\theta_1}{3} - \frac{\pi}{6} \right) < \frac{1}{2} \). Finally, \( \frac{\pi}{3} < \theta_1 < \frac{\pi}{2} \) implies that \( \frac{\pi}{2} < \sin \left( \frac{\theta_1}{3} + \frac{\pi}{6} \right) < 1 \). Further, we find the
lower and upper bound for the roots from Eqs. [113] and [114] using the binomial approximation for $0 < \epsilon \ll 1$ and $n \to \infty$ as follows

$$\frac{1}{\sqrt{3}} \sqrt{n} + 2 < \kappa_1 < \sqrt{n} + 2$$

$$2 < \kappa_2 < \frac{1}{\sqrt{3}} \sqrt{n} + 2$$

$$\frac{2}{\sqrt{3}} \sqrt{n} + 2 < \kappa_3 < -\sqrt{n} + 2$$

Finally, use the lower and upper bounds of $\kappa_1$ and calculate the bounds of $n_1$ in Eq. (7) as follows

$$\frac{1}{3} n + \frac{2}{\sqrt{3}} \sqrt{n} < n_1^\kappa_1 < n + 2 \sqrt{n}$$

$$1 < n_1^\kappa_2 < \frac{1}{3} n + \frac{2}{\sqrt{3}} \sqrt{n}$$

$$n - 2 \sqrt{n} < n_1^\kappa_3 < \frac{4}{3} n - \frac{4}{\sqrt{3}} \sqrt{n}$$

From the above $\frac{1}{3} n + \frac{2}{\sqrt{3}} \sqrt{n} > n$ for $n < 3$, $n + 2 \sqrt{n} > n$ for $n > 0$, and finally $\frac{4}{3} n - \frac{4}{\sqrt{3}} \sqrt{n} > n$, $n \geq 48$. Hence, if we choose $n \geq 49$, $n_1^\kappa_2$ will always be less than $n$.

We numerically vary $m$ in the range in Eq. (17) and examine the behavior of three different roots (Fig. 14(a)) and their corresponding $n_1$ values (Fig. 14(b)). One can observe that for a small region, size of $n_1^\kappa_1$ and $n_1^\kappa_3$ exceeds the given $n$ (depicted by a horizontal dotted line in Fig. 14(b)). Importantly, the bounds obtained from the analysis are in good agreement with the numerical results and indicate that for sparse networks small portion of the $\kappa_1$ cannot be used to find wheel graph size (Fig. 14(a) marked with an ellipse). Consequently, for dense networks, $\kappa_3$ can not be used for the wheel graph size calculation (Fig. 14(a) marked with an ellipse) and $\kappa_2$ always works well. Hence, we use $\kappa_1$ and $\kappa_2$ to calculate the wheel and random regular component size to construct $G_{new}$.

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Our codes and data are available at the following link: 
https://github.com/priodyuti/pev_loc_eigval_crossing

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