Structural control of reaction-diffusion networks

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Recent studies revealed that reaction-diffusion (RD) dynamics can be significantly influenced by the structure of the underlying network. In this paper, a framework is established to study a closely related problem, i.e., to control the proportion of active particles in an RD process by adjusting the structure of the underlying diffusion network. Both distributed and centralized rewiring and reweighting control schemes are proposed for unweighted and weighted networks, respectively. Simulations show that the proportion of active particles can indeed be controlled to a certain extent even when the distributed control mechanism is totally random, while quite high precision can be achieved by centralized control schemes. More interestingly, it is found that the reactants in heterogeneous networks have wider controllable ranges than those in homogeneous networks with similar numbers of nodes and links, if only the weights of links are changed with a fixed bound. Therefore, it is believed that heterogeneous networks fit the changeable environment better, which provides another explanation for some common observations on many heterogeneous real-world networks.

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I. INTRODUCTION

The term "reaction-diffusion (RD) process" refers to a group of particles which locally react with each other and globally diffuse in space. The RD process was first introduced by Turing [1] to account for the main phenomena of morphogenesis. In fact, many dynamics, such as chemical reactions [2], population evolution [3], biological pattern formation [4], epidemics [5], and computer virus spreading [6], can be modeled by RD processes, where the particles are molecules, organisms, cells, people, or documents, and spaces are normal Euclidean spaces or discrete network spaces. Since a discrete Euclidean space can always be represented by a lattice of the same dimension [7,8], it is quite useful for studying RD processes in complex networks especially for computer simulations.

Recall that many real-world biological [9], social [10], and technological [11] networks possess heterogeneous structures. Because such structures can be characterized by a power-law degree distribution, this type of network is classified as scale-free (SF), as introduced by Barabási and Albert (BA) in their pioneering work [12]. The study of RD processes in SF networks provides many interesting results. For example, in studying annihilation reactions, Gallos and Argyrakis [13] found that the generation of a depletion zone and the segregation of the reactants formed in a normal Euclidean space did not occur in SF networks; in studying susceptible-infected-susceptible (SIS) dynamics, Colizza *et al.* [14] found that in SF networks the reaction activity was still sustained even in the limit of a vanishing density of particles, which had not been investigated in normal Euclidean spaces before. These results suggest that the spatial distributions of different kinds of particles produced by RD processes are not only determined by the reaction equations but also significantly influenced by the topological structures of the underlying networks in which the diffusion takes place.

Generally, an RD process is controlled by tuning the rates of the reactions involved. For example, in consideration of reversible chemical reactions, the forward and reverse reactions are competing with each other and they differ in reaction rates, and therefore, in some situations the equilibrium point can be shifted to a desired side by changing temperature or pressure; when epidemic spreading is considered, the infected rate can be decreased by encouraging people to receive vaccination or wear respirators. However, far less attention has been paid to another control mechanism: control of the RD processes by adjusting the structures of the underlying diffusion networks, which may be especially useful in situations where some macroscopic measurements, such as temperature and pressure, must remain unchanged throughout the process. This is partly attributed to the lack of knowledge about the structure and functioning of complex networks.

This control mechanism seems feasible today. In fact, as nano-technologies have developed [15,16], physical chemists are now able to build nanofluidic devices such as lipid nanotube-vesicle networks using soft-matter materials, where transport, mixing, and shape changes can be achieved at or near thermal energy levels, and their kinetics can be controlled by shape and volume changes [17]. In addition, with the current advance in complex networks theory, our recent work [18] also proved that, by adopting the SIS model, epidemics can be statistically controlled by a distributed random rewiring process in the diffusion network. Here, "distributed control" [19] means that each node is a subsystem with a controller to partly control its own state by changing its local structure with or without communication with others, while "centralized control" [20] means that the overall system has only one controller (like the brain) to control the state of the system by changing the global structure of the network. Since these two different control schemes each have advantages in different situations, both of them will be adopted here to control RD processes.

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In this paper, a theoretical framework is introduced for controlling RD processes by adjusting the structures of the underlying networks, where a network structural property, i.e., heterogeneity, is correlated to the steady-state density of active particles. In order to be self-contained, part of our earlier work [18] will be reviewed. In this framework, by considering each node as an agent [21,22], which can rearrange its neighbors when it senses differences between its own state and the external requirement, statistically distributed rewiring and reweighting schemes are proposed for unweighted and weighted diffusion networks, respectively. It is found that the RD dynamics can be controlled to a certain extent via a local and random mechanism, as reflected by the proportion of active particles existing in the network nodes. Moreover, this study suggests that the emergence of common heterogeneous structures of many biological networks [9,23] may be attributed to their interior microscopic dynamics rather than the ordinary connecting rules. On the other hand, in situations where the proportion of active particles in a network can be estimated in real time, some centralized control schemes are proposed, which turn out to be far more efficient than the distributed ones, and thus may be more useful in future microfabrication industries [24,25], wherever global control is feasible. Interestingly, when the network topology is fixed and only the weights of links can be changed with a fixed bound, it is found that the proportion of active particles in heterogeneous networks can be controlled in wider ranges than those in homogeneous ones with similar numbers of nodes and links. In other words, by comparison, heterogeneous networks have stronger plasticity and thus are more likely to survive in cruel natural competitions.

The rest of the paper is organized as follows. In Sec. II, some theoretical analysis is reviewed for the SIS model on a network, and the structural control framework for RD processes is formulated. In Sec. III, some distributed rewiring and reweighting control schemes are introduced, for unweighted and weighted networks, respectively, while some centralized control schemes are presented in Sec. IV. The work is finally concluded in Sec. V.

II. THEORETICAL FRAMEWORK

Throughout this paper, the diffusion space is represented by a network where different kinds of particles in each node react with each other, while they diffuse to neighboring nodes simultaneously.

In this section, first, the micromechanism of the well-known SIS model, which has been studied in physics [26] and mathematical epidemiology [27], is investigated, and then the relationship between structural properties of the diffusion network and the outputs of the SIS model is discussed by adopting the mean-field (MF) theory [14,18]. Finally, a feedback structural control scheme is proposed.

The micromechanism of the SIS model on a network of V nodes is composed of the following two reactions:

$$\beta \rightarrow \alpha, \tag{1}$$

$$\alpha + \beta \rightarrow 2\beta. \tag{2}$$

Eqs. (1) and (2) ensure that the total number of particles does not change in the process. Here, β particles are identified as active particles because α particles cannot spontaneously generate β particles [14]. Next, the parameters involved are introduced before the theoretical analysis is provided. The reaction rates of Eqs. (1) and (2) are denoted by μ_1 and μ_2, and the diffusion rates of α and β particles are denoted by η_α and η_β, respectively. For each node i, $i = 1,2,\ldots,V$, in the network, its neighbor set and degree are denoted by π_i and k_i, respectively. Moreover, if weighted networks are considered, its weighted degree is denoted by $\omega_i = \sum_{j\in\pi_i} \omega_{ij}$, where ω_{ij} is the weight of the link connecting nodes i and j. At the same time, the weighted degree distribution is denoted by $P(\omega)$, and the average degree and average weighted degree are represented by $\langle k\rangle$ and $\langle\omega\rangle$, respectively. In addition, the numbers of α and β particles in the network are denoted by N_α and N_β, respectively, and thus the total number of particles is $N = N_\alpha + N_\beta$. Then, the densities of α, β, and total particles are defined by $\rho_\alpha = N_\alpha/V$, $\rho_\beta = N_\beta/V$, and $\rho = N/V$, respectively.

Based on these parameters and supposing that there are $n_{\alpha,i}(t)$ α particles and $n_{\beta,i}(t)$ β particles in node i at present, after reactions, the numbers of α and β particles in node i are changed to

$$\widetilde{n}_{\alpha,i}(t) = n_{\alpha,i}(t) + \mu_1 n_{\beta,i}(t) - \mu_2\Gamma_i(t), \tag{3}$$

$$\widetilde{n}_{\beta,i}(t) = (1-\mu_1)n_{\beta,i}(t) + \mu_2\Gamma_i(t), \tag{4}$$

where the reaction kernel $\Gamma_i(t)$ takes the form of $\Gamma_i(t) = n_{\alpha,i}(t)n_{\beta,i}(t)$. Then, in the diffusion process, differing from [14,18], when weighted networks are considered, with probability $\eta_\alpha\omega_{ij}/\omega_i$ or $\eta_\beta\omega_{ij}/\omega_i$, an α or a β particle in node i jumps to one of its neighbors j. That is, the diffusion process is determined not only by the diffusion rates by also by the weighted links. As a result, after one round of the RD process, the total numbers of α and β particles in node i are statistically recalculated as

$$n_{\alpha,i}(t+1) = (1-\eta_\alpha)\widetilde{n}_{\alpha,i}(t) + \eta_\alpha \sum_{j\in\pi_i} \frac{\omega_{ij}\widetilde{n}_{\alpha,j}(t)}{\omega_j}, \tag{5}$$

$$n_{\beta,i}(t+1) = (1-\eta_\beta)\widetilde{n}_{\beta,i}(t) + \eta_\beta \sum_{j\in\pi_i} \frac{\omega_{ij}\widetilde{n}_{\beta,j}(t)}{\omega_j}, \tag{6}$$

respectively. From Eqs. (3)–(6), it follows that the dynamical RD equations in each node i can be represented by

$$\frac{\partial n_{\alpha,i}}{\partial t} = -n_{\alpha,i} + (1-\eta_\alpha)[\mu_1 n_{\beta,i} + n_{\alpha,i} - \mu_2\Gamma_i] + \eta_\alpha\left[\sum_{j\in\pi_i}\frac{\omega_{ij}(\mu_1 n_{\beta,j} + n_{\alpha,j} - \mu_2\Gamma_j)}{\omega_j}\right], \tag{7}$$

$$\frac{\partial n_{\beta,i}}{\partial t} = -n_{\beta,i} + (1-\eta_\beta)[(1-\mu_1)n_{\beta,i} + \mu_2\Gamma_i] + \eta_\beta\left[\sum_{j\in\pi_i}\frac{\omega_{ij}[(1-\mu_1)n_{\beta,j} + \mu_2\Gamma_j]}{\omega_j}\right], \tag{8}$$

where the time indices t are dropped for simplicity. Supposing $\eta_\alpha = \eta_\beta = \eta$, denoting the total number of particles in node i by $n_i = n_{\alpha,i} + n_{\beta,i}$, and summing Eqs. (7) and (8), one has

$$\frac{\partial n_i}{\partial t} = \eta \left(\sum_{j\in\pi_i} \frac{\omega_{ij} n_j}{\omega_j} - n_i \right). \tag{9}$$

Denoting $\phi_i = n_i/\omega_i$, Eq. (9) becomes

$$\omega_i \frac{\partial \phi_i}{\partial t} = \eta \left(\sum_{j\in\pi_i} \omega_{ij}\phi_j - \omega_i\phi_i \right). \tag{10}$$

Assume that the RD process takes place in the SIS model on a connected network of V nodes, defined by a weighted adjacency matrix W with elements having values ω_{ij} if nodes i and j are connected or 0 otherwise. Then, Eq. (10) can be put in the matrix form

$$\frac{\partial \phi}{\partial t} = -\eta\Lambda^{-1}L\phi, \tag{11}$$

where $\phi = [\phi_1,\phi_2,\ldots,\phi_V]^T$, $\Lambda = \mathrm{diag}(\omega_1,\omega_2,\ldots,\omega_V)$, and $L = \Lambda - W$ is the Laplacian matrix of the weighted network [28]. Equation (11) has a steady solution $\phi = [c,c,\ldots,c]^T$ under the condition $\sum_{i=1}^V \omega_i\phi_i = cV\langle\omega\rangle = N$. Then one has $c = \rho/\langle\omega\rangle$, so that a steady solution of Eq. (9) can be obtained as

$$n_i = \frac{\omega_i}{\langle\omega\rangle}\rho. \tag{12}$$

This means that a node of a larger weighted degree always attracts more particles to pass through it.

Suppose that there are V_ω nodes possessing a weighted degree ω in the network, and denote by $N_{\alpha,\omega}$ and $N_{\beta,\omega}$ the numbers of α and β particles, respectively, located in these nodes. Then the quantities

$$\rho_{\alpha,\omega} = \frac{N_{\alpha,\omega}}{V_\omega}, \quad \rho_{\beta,\omega} = \frac{N_{\beta,\omega}}{V_\omega} \tag{13}$$

represent the densities of α and β particles, respectively, in each node with weighted degree ω. Then, by the MF theory and under the assumption of having no weighted degree correlation between any two linked nodes [14,18], Eqs. (7) and (8) become

$$\frac{\partial \rho_{\alpha,\omega}}{\partial t} = -\rho_{\alpha,\omega} + (1-\eta_\alpha)[\mu_1\rho_{\beta,\omega} + \rho_{\alpha,\omega} - \mu_2\Omega_\omega] + \frac{\eta_\alpha\omega}{\langle\omega\rangle}[\mu_1\rho_\beta + \rho_\alpha - \mu_2\Omega], \tag{14}$$

$$\frac{\partial \rho_{\beta,\omega}}{\partial t} = -\rho_{\beta,\omega} + (1-\eta_\beta)[(1-\mu_1)\rho_{\beta,\omega} + \mu_2\Omega_\omega] + \frac{\eta_\beta\omega}{\langle\omega\rangle}[(1-\mu_1)\rho_\beta + \mu_2\Omega], \tag{15}$$

with $\rho_\alpha = \sum_\omega P(\omega)\rho_{\alpha,\omega}$, $\rho_\beta = \sum_\omega P(\omega)\rho_{\beta,\omega}$, and $\Omega = \sum_\omega P(\omega)\Omega_\omega$, where the reaction kernel now takes the form of $\Omega_\omega = \rho_{\alpha,\omega}\rho_{\beta,\omega}$.

When $\eta_\alpha = \eta_\beta = 1$, which means that all the particles in a node at time $t-1$ will jump to its neighbors at time t, the stationary states can be obtained by considering $\partial_t\rho_{\alpha,\omega} = 0$ and $\partial_t\rho_{\beta,\omega} = 0$, resulting in the following equations:

$$\rho_{\alpha,\omega} = \frac{\omega}{\langle\omega\rangle}[\mu_1\rho_\beta + \rho_\alpha - \mu_2\Omega], \tag{16}$$

$$\rho_{\beta,\omega} = \frac{\omega}{\langle\omega\rangle}[(1-\mu_1)\rho_\beta + \mu_2\Omega]. \tag{17}$$

Multiplying Eq. (17) by $P(\omega)$ and then summing it over ω, one gets

$$\rho_\beta = \frac{\mu_2}{\mu_1}\Omega. \tag{18}$$

Then, by using Eq. (18), Eqs. (16) and (17) can be further simplified to

$$\rho_{\alpha,\omega} = \frac{\omega}{\langle\omega\rangle}\rho_\alpha, \quad \rho_{\beta,\omega} = \frac{\omega}{\langle\omega\rangle}\rho_\beta, \tag{19}$$

with

$$\rho_\alpha = \rho - \frac{\mu_2}{\mu_1}\Omega, \quad \rho_\beta = \frac{\mu_2}{\mu_1}\Omega. \tag{20}$$

From Eqs. (19) and (20) and the definition of Ω, when the dynamics are statistically steady, one can get the average densities of α and β particles in the network, respectively, as

$$\rho_\alpha = \frac{\mu_1}{\mu_2}\frac{\langle\omega\rangle^2}{\langle\omega^2\rangle}, \quad \rho_\beta = \rho - \frac{\mu_1}{\mu_2}\frac{\langle\omega\rangle^2}{\langle\omega^2\rangle}, \tag{21}$$

where $\langle\omega^2\rangle = \sum_{i=1}^V \omega_i^2/V$. It should be noted here that, when different kinds of particles have different diffusion rates, i.e., $\eta_\beta = 1$ and $0 < \eta_\alpha < 1$, a similar result can be obtained; the RD results for more values of the diffusion rates were introduced in [14]. In the rest of this paper, however, we will only focus on the situation when $\eta_\alpha = \eta_\beta = 1$ for simplicity. In Eq. (21), one can see that the steady-state density of α or β particles in the network is not only determined by the reaction parameters, such as μ_1 and μ_2, but also influenced by a weighted-degree-related structural property of the network, $\langle\omega\rangle^2/\langle\omega^2\rangle$, the value of which is typically used to define the heterogeneity of a weighted network, i.e.,

$$H = \frac{\langle\omega^2\rangle}{\langle\omega\rangle^2}. \tag{22}$$

In particular, when considering an unweighted diffusion network, i.e., there is no difference in diffusion rates between any two links, Eq. (21) becomes

$$\rho_\alpha = \frac{\mu_1}{\mu_2}\frac{\langle k\rangle^2}{\langle k^2\rangle}, \quad \rho_\beta = \rho - \frac{\mu_1}{\mu_2}\frac{\langle k\rangle^2}{\langle k^2\rangle}, \tag{23}$$

with $\langle k^2\rangle = \sum_{i=1}^V k_i^2/V$. Accordingly the heterogeneity of the unweighted diffusion network is calculated by

$$H = \frac{\langle k^2\rangle}{\langle k\rangle^2}. \tag{24}$$

Since the final density of α or β particles is directly associated with the heterogeneity of the diffusion network, as represented by Eqs. (21)–(24), it is possible to control the RD process by adjusting the structure of the diffusion network dynamically. In the following, two distinct control themes are proposed based on distributed [19] and centralized [20] structural controls, by rewiring and reweighting processes for

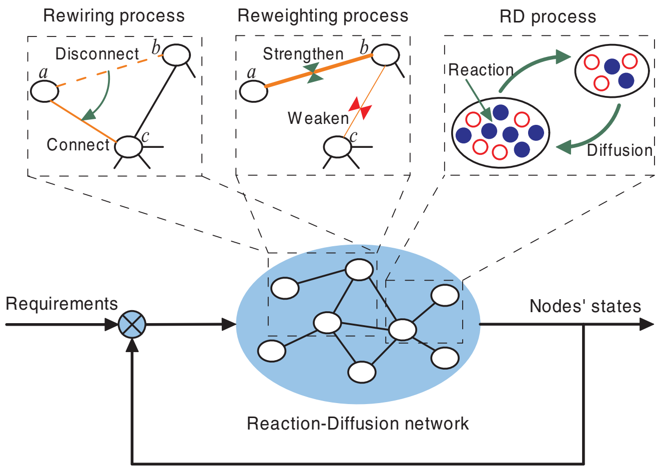

FIG. 1. (Color online) The structural control framework of the RD process with the SIS model. Here, α and β particles diffuse between neighboring nodes, and inside each node they react with each other. For distributed structural control, once a node senses that the ratio of α to β particles in it does not meet the external (natural or artificial) requirement, it rearranges its neighbors immediately by a rewiring or reweighting process for unweighted and weighted diffusion networks. Thus, the network evolves adaptively as the external requirements change. For centralized structural control, it is supposed that the overall proportion of α or β particles in the whole network can be estimated. Thus, the network undergos a centralized rewiring or reweighting process when the density does not meet the external requirement.

unweighted and weighted networks, respectively, as shown in Fig. 1.

III. DISTRIBUTED STRUCTURAL CONTROL

For natural systems, nodes in a network are often considered as selfish agents. That is, once a node senses the difference between its state and the external requirement, it rearranges its associations with neighbors immediately without much consultation with the others, so as to increase its own advantages and benefit in natural competitions. It is quite interesting to study whether a heterogeneous structure can emerge from the external requirement that encourages more α or β particles, through a random rewiring or reweighting strategy, such that the differences between the states of nodes and the external requirement are gradually eliminated. In the following, two distributed structural control mechanisms, i.e., distributed rewiring and reweighting strategies, are proposed for unweighted and weighted networks respectively, which will be applied totally at random.

A. Distributed rewiring control

Without loss of generality, suppose that the external condition or requirement for each node i is set to be the same, to encourage the active particles β, as formulated by

$$\sigma_{\beta,i} = \frac{n_{\beta,i}}{n_i} > \theta, \tag{25}$$

with $\theta \in [0,1)$. When the initial diffusion network is set to be a two-dimensional unweighted lattice, the distributed structural control scheme is implemented by a random local rewiring process consisting of the following five steps [18]:

(1) *Initialization*. Numbers $N_\alpha(0)$ of α particles and $N_\beta(0)$ of β particles are randomly distributed in an $L \times L$ two-dimensional lattice containing $V = L^2$ nodes. Set $\gamma = 0$; this will be used to judge whether the network structure is statistically stable and thus the rewiring process can be terminated.

(2) *Reaction*. At each time t, numbers $n_{\alpha,i}(t-1)$ of α particles and $n_{\beta,i}(t-1)$ of β particles in each node i react with each other according to Eqs. (1) and (2). That is, each β particle in a node is transformed to α particle with probability μ_1 and the reverse takes place with probability $1-(1-\mu_2)^{n_{\beta,i}(t-1)}$ [14]. Here, $n_{\alpha,i}(t-1)$ and $n_{\beta,i}(t-1)$ can be any nonnegative integers including zero whena bosonic RD process is considered [29].

(3) *Diffusion*. After reactions, the particles diffuse in the network by random walks. That is, every particle in each node of degree k jumps into one of its neighbors with the same probability $1/k$. It should be noted that, when $\eta_\alpha < 1$ or $\eta_\beta < 1$, every α or β particle is selected with probability η_α or η_β to perform the above diffusion operation. Then, after a round of the RD process, the numbers of α particles and β particles in node i are updated to be $n_{\alpha,i}(t)$ and $n_{\beta,i}(t)$, respectively.

(4) *Rewiring*. When the RD process in the network is relatively steady, i.e., $t > T_s$ (T_s is a large number), in every τ ($\tau \gg 1$) time steps, denote by τ_i^f the total times that the state of each node i fails to meet the external condition. If node i always fails, i.e., $\tau_i^f/\tau > \xi$ with ξ being the tolerance degree, it seeks structural changes and is added into a rewiring candidate set R. And if none of the nodes seeks structural changes in these τ rounds of RD processes, i.e., $R = \emptyset$, set $\gamma = \gamma + 1$; otherwise, randomly select a candidate from the set R, denoted by a, and let it undergo local structural changes by a rewiring step as follows: Select one of its neighbors, denoted by b, release the link between them, and then create a new link between node a and one randomly chosen neighbor of node b, denoted by c, as shown in Fig. 1, “Rewiring process.” It should be noted that self-loops and multiple edges are not allowed, that is, the network remains unchanged and the rewiring operation is canceled if node a and node c were already connected. Set $R = \emptyset$, $\gamma = 0$, and turn to step 2. This local rewiring strategy can ensure network connectivity and retain the average degree of the network.

(5) *Termination*. If none of the nodes in the network seeks structural changes in $T_1 \times \tau$ successive rounds of RD processes, i.e., $\gamma = T_1$, we consider that the network structure is statistically stable and the rewiring process is terminated. It should be noted that if the above condition cannot be achieved, the program is also stopped when $t = T_2$. In this case, we think that the network structure cannot be stable under such a rigorous external requirement.

When the parameters are set to be $\mu_1 = 0.2$, $\mu_2 = 0.05$, $\rho = 5$ with $\rho_\alpha(0)/\rho_\beta(0) = N_\alpha(0)/N_\beta(0) = 1$, $V = L^2 = 625$, $\xi = 0.9$, $T_s = 10^6$, $\tau = 100$, $T_1 = 200$, and $T_2 = 10^7$, examples of the diffusion network at different stages with different values of θ are shown in Fig. 2. Note that, based on Eq. (23), the reaction rates must satisfy $\mu_1/\mu_2 < \rho$ in order to produce β particles in a two-dimensional lattice where $\langle k^2\rangle \approx \langle k\rangle^2$.

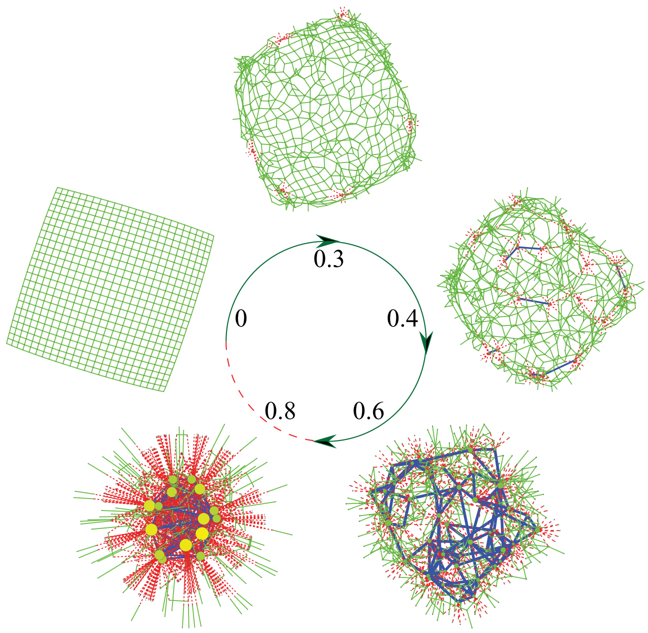

FIG. 2. (Color online) The initial two-dimensional lattice as well as some examples of the diffusion network in different stages with $\theta = 0.3, 0.4, 0.6, 0.8$, under distributed rewiring control. In each scene, the node size is proportional to the node degree; the links between the nodes with degree not smaller than 10 are plotted by thick blue lines, while those between the nodes with degree smaller than 10 are plotted by solid green lines, and the remaining links are plotted by dashed red lines.

Here, we set $\mu_1/\mu_2 = 4$, a little smaller than ρ; thus we can investigate the change of the proportion of β particles in a wide interval in the rewiring process. Next, the RD process in different network scenarios obtained under different external conditions is reconsidered. Define the average ratio of β particles over all the nodes and the proportion of β particles in the whole network by

$$\sigma_\beta = \frac{1}{V} \Sigma_{i=1}^{V} \sigma_{\beta,i}, \tag{26}$$

$$\chi_\beta = \frac{\rho_\beta}{\rho}, \tag{27}$$

respectively. It is found that, with the values chosen for the reaction rates, the proportion of α or β particles in the whole network changes steadily in a large range as the network evolves, as shown in Fig. 3. Intuitively, when θ increases, the adaptive network is becoming more and more heterogeneous, so that most nodes in the network possess relatively higher ratios of active particles β. Moreover, from Eqs. (23), (24), and (27), one can get the theoretical average proportion of β particles in the whole network, as follows:

$$\chi_\beta = 1 - \frac{\mu_1}{\rho\mu_2} \frac{1}{H}. \tag{28}$$

When the parameters are set to be $\rho = 5$, $\mu_1 = 0.2$, and $\mu_2 = 0.05$, Eq. (28) can be simplified to $\chi_\beta = 1 - 0.8/H$. Then, for each network scenario with fixed structure, we calculate the analytic χ_β, which is also shown in Fig. 3 for comparison. The difference between the controlled and analytic χ_β may be attributed to the degree correlations between pairwise-linked nodes in the diffusion network, which violates the assumption in adopting the MF theory, as was carefully discussed in our previous work [18]. In addition, in the rewiring process introduced here, a node seeks structural changes only when it fails 90 times to meet the external condition in 100 time steps, i.e., $\xi = 0.9$; as a result, the average proportions of β particles in the network scenarios (controlled results) are a little smaller than the expected values denoted by $\chi_\beta(\theta) > \theta$, as is shown in Fig. 3, although the network structure is stable, i.e., the rewiring process is terminated when $\gamma = T_1$, in most cases (the only exception is when $\theta = 0.8$). Certainly, one can reduce these gaps by simply increasing the value of the tolerance degree ξ, but (every coin has two sides) it may also produce with a higher probability an unstable network structure in the process.

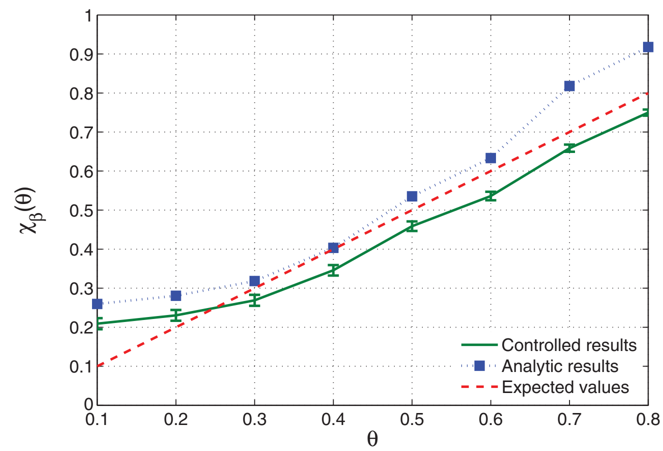

FIG. 3. (Color online) The controlled and analytic proportions of particles in the network as well as the expected values at different stages of evolution under distributed rewiring control. In each network stage, the RD process is parallel implemented 10^4 times after the early time transients and then the corresponding results are recorded (the same method is used for the figures below).

B. Distributed reweighting control

The RD process can also be controlled, to a certain extent, by adjusting the flows through the links, as described by Eqs. (21) and (22). Naturally, it seems much easier to redistribute the weights of links than to make a topological change. Here, distributed reweighting control is studied on a two-dimensional lattice and a BA SF network, respectively, with the topological structures of the networks being kept unchanged. The reweighting process also consists of five steps:

(1) *Initialization.* Numbers $N_\alpha(0)$ of α particles and $N_\beta(0)$ of β particles are randomly distributed in a weighted network with V nodes. The weights of all links are set to be the same, denoted by ω. Set $\gamma = 0$.

(2) *Reaction.* At each time t, each β particle in a node is transformed to an α particle with probability μ_1 and the reverse takes place with probability $1 - (1 - \mu_2)^{n_{\beta,i}(t-1)}$.

(3) *Diffusion.* After reactions, every particle in each node i with weighted degree ω_i jumps to one of its neighbors, node j, with probability ω_{ij}/ω_i, proportional to the weight of the

link between them. Then the numbers of α and β particles in each node i are updated to $n_{\alpha,i}(t)$ and $n_{\beta,i}(t)$, respectively.

(4) *Reweighting*. Similarly, when the RD process in the network is relatively steady, i.e., $t > T_s$ for a large T_s, in every τ ($\tau \gg 1$) time steps, count the total times τ_i^f that the state of each node i does not meet the external condition. Once $\tau_i^f/\tau > \xi$, node i is added into a reweighting candidate set R. If $R = \emptyset$, set $\gamma = \gamma + 1$; otherwise, randomly select a candidate from the set R, denoted by b, and let it undergo local structural changes by a reweighting step as follows: Select one of its neighbors, denoted by a, increase the weight of the link between them by $\Delta\omega_{bc}(t)$, and then decrease the weight of the link between node b and another randomly chosen neighbor c, by $\Delta\omega_{bc}(t)$, as shown in Fig. 1 "Reweighting process." Here, if node b has only one neighbor, a, the network remains unchanged and the reweighting operation is canceled. At the same time, in order to ensure that the weight of each link is larger than 0, it is necessary that $0 \leqslant \Delta\omega_{bc}(t) < \omega_{bc}(t)$, where $\omega_{bc}(t)$ is the weight of the link between nodes b and c at present. Set $R = \emptyset$, $\gamma = 0$, and turn to step 2. Such a local reweighting strategy can ensure the network connectivity and retain the average weighted degree of the network. The external requirement is set to be the same, i.e., to encourage the active particles β, as formulated by Eq. (25).

(5) *Termination*. When $\gamma = T_1$ or $t = T_2$, the process is terminated.

When the parameters are set to be $\mu_1 = 0.5$, $\mu_2 = 0.05$, $\rho = 20$ with $\rho_\alpha(0)/\rho_\beta(0) = N_\alpha(0)/N_\beta(0) = 1$, $V = 64$, $\omega = 10$, $\xi = 0.9$, $T_s = 10^5$, $\tau = 100$, $T_1 = 200$, $T_2 = 10^7$, and $\Delta\omega_{bc}(t) = \lfloor 0.5\delta\omega_{bc}(t)\rfloor$ with $\delta \in (0,1)$ being a random value, and at each time a newly added node is linked to two different existing nodes in the BA SF network, the scenarios for the two-dimensional lattice and the BA SF network in different stages with different values of θ are shown in Fig. 4, top and bottom, respectively. Here, $\Delta\omega_{bc}(t) \geqslant 0$ is an integer, which means that the weight of each link can only be adjusted

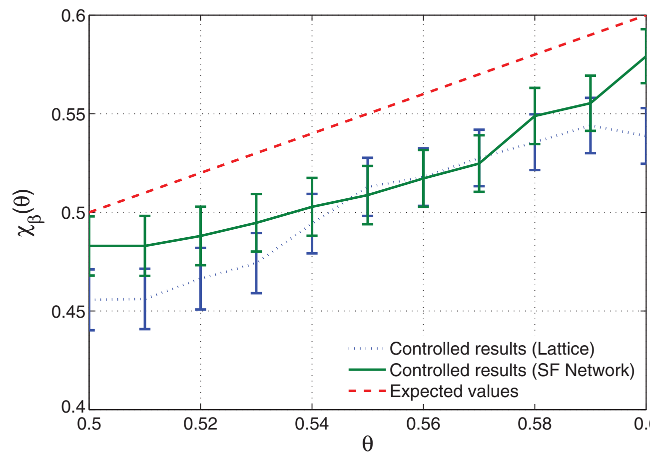

FIG. 5. (Color online) The controlled proportions of particles in the lattice and SF networks as well as the expected values at different stages of evolution under distributed reweighting control.

discretely. Intuitively, in order to produce more active particles, the weights of most links associated with the nodes of large degree are strengthened while those associated with the nodes of small degree are weakened, all by self-organization. The controlled χ_β in the scenarios of a two-dimensional lattice and a BA SF network are shown in Fig. 5. As can be seen, the average proportions of β particles in the network scenarios are also a little smaller than the expected values under a relatively large tolerance degree, i.e., $\xi = 0.9$.

Note that here the analytic χ_β for each network scene can also be calculated by Eq. (28) with $H = \langle\omega^2\rangle/\langle\omega\rangle^2$, which is found to be larger than 0.8 in most cases, and thus the gaps between the analytic and controlled results or the expected values are much larger than those of the rewiring scheme shown in Fig. 3. The reasons may be that, on one hand, the smaller network size produces a larger variance in predicting the values of χ_β by the MF theory, while on the other hand,

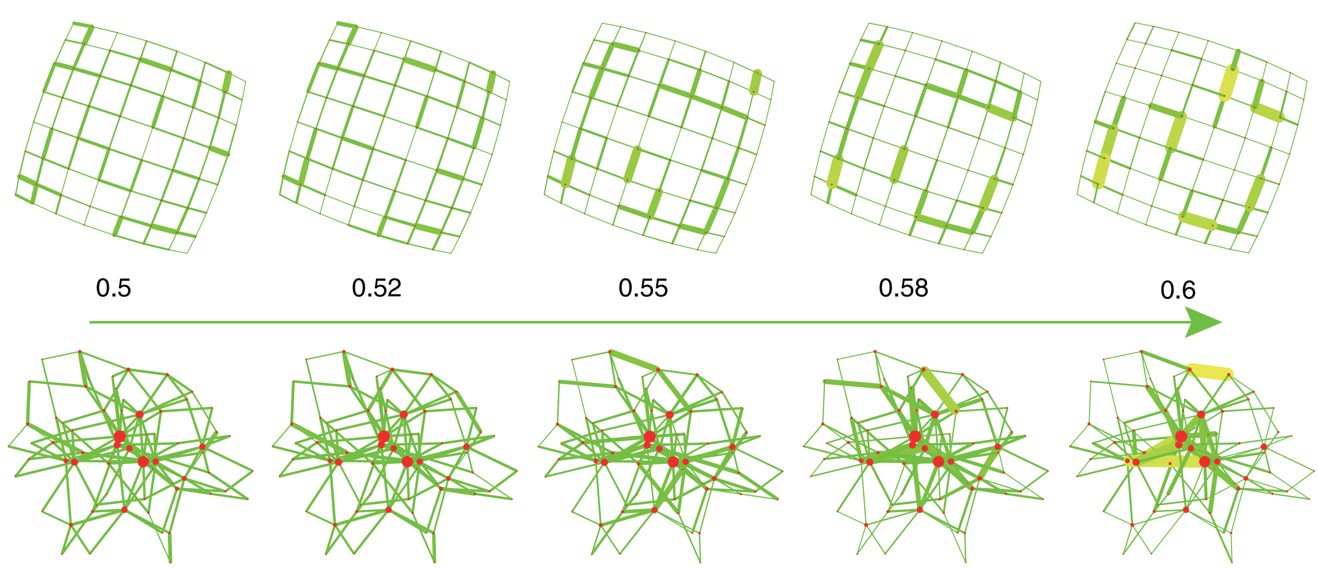

FIG. 4. (Color online) Different scenarios in two diffusion networks, i.e., two-dimensional lattice (above) and BA SF network (below), at different stages with $\theta = 0.5, 0.52, 0.55, 0.58, 0.6$, under distributed reweighting control. In each scenario, the node size is proportional to its degree, and the link width is proportional to its weight.

the weighted degrees of two linked nodes are more likely to be correlated with each other because they increase or decrease synchronously when the weight of the link between them increases or decreases. In fact, a similar deviation was reported by Baronchelli and Pastor-Satorras [30] when they studied diffusive dynamics on weighted networks using the MF theory. They found that the deviation is further strengthened if the weights of links are positively correlated with their associated nodes, which suggests a positive correlation between weighted degrees of linked nodes introduced here, as is shown in Fig. 4 (later evolving stages). Due to this limitation of the MF theory, we create a feedback, rather than open-loop, framework to control the proportions of reactants in RD networks, which can guarantee control performance even with model uncertainties [31]. Here, such model uncertainty is reflected by the deviation of analytic results, described by Eq. (28), from real RD dynamics.

IV. CENTRALIZED STRUCTURAL CONTROL

For artificial systems, when the state of the whole network, here the proportion of β particles, can be estimated in real time, no doubt it can be controlled more efficiently by tuning the structure of network in a centralized fashion if the structure can be changed at will. Here, the external requirement is formulated by

$$\chi_\beta = \theta, \tag{29}$$

rather than encouraging more β particles as represented by Eq. (25). Obviously, the external requirement Eq. (29) is far more difficult to achieve than Eq. (25), and is almost impossible by the two distributed control schemes introduced above. Accordingly, two different centralized control strategies, i.e., centralized rewiring and reweighting controls, are introduced below for unweighted and weighted diffusion networks, respectively.

A. Centralized rewiring control

When an unweighted diffusion network is considered, on average the proportion of β particles can be estimated by Eq. (28), with $H = \langle k^2\rangle/\langle k\rangle^2$. Consequently,

$$\Delta\chi_\beta = \frac{\mu_1}{\mu_2\rho}\frac{\Delta H}{H^2}, \tag{30}$$

where $\Delta H \ll H$. Considering the same rewiring process as shown in Fig. 1 and denoting by k_a, k_b, and k_c the degrees of nodes a, b, and c, respectively, the variation of the heterogeneity after a rewiring step can be calculated by

$$\Delta H = \frac{(k_b-1)^2+(k_c+1)^2-k_b^2-k_c^2}{V\langle k\rangle^2} = \frac{2(\Delta k+1)}{V\langle k\rangle^2}, \tag{31}$$

where $\Delta k = k_c - k_b$, since the average degree $\langle k\rangle$ of the network remains unchanged through the entire rewiring process. Then, the relationship between $\Delta\chi_\beta$ and Δk can be established as

$$\Delta\chi_\beta = \frac{2\mu_1(\Delta k+1)}{\mu_2\rho V H^2\langle k\rangle^2}. \tag{32}$$

Based on Eq. (32), the above distributed rewiring control scheme can be improved by changing the neighbors of nodes with proper degrees, assuming that the difference between the expected and the current steady proportions of β particles, denoted by $\Delta\chi_\beta = \theta - \overline{\chi}_\beta$, can be estimated.

Specifically, the centralized rewiring control scheme is composed of the following five steps:

(1) *Initialization*. Numbers $N_\alpha(0)$ of α particles and $N_\beta(0)$ of β particles are randomly distributed in an $L\times L$ two-dimensional lattice containing $V = L^2$ nodes.

(2) *Estimation*. After the RD process reaches its steady state, the process is repeated τ more times, and the average proportion in these τ rounds is calculated as an acceptable estimation of the current steady proportion of β particles. Then, the difference between the expected and estimated proportions of β particles is calculated by

$$\Delta\chi_\beta = \theta - \frac{\sum_{t=T_s+1}^{\tau}\chi_\beta(t)}{\tau}. \tag{33}$$

The heterogeneity H given by Eq. (24) and the average degree $\langle k\rangle$ of the current network structure are calculated. Then, the needed variation of the node degree can be inferred from Eq. (32) by

$$\Delta k_T = \frac{\mu_2\rho V H^2\langle k\rangle^2}{2\mu_1}\Delta\chi_\beta - 1. \tag{34}$$

(3) *Candidate selection*. For each pair of linked nodes, if $\Delta k_T \geqslant 0$, which means that a node of larger degree gains a neighbor from a node of smaller degree in order to decrease the absolute value of $\Delta\chi_\beta$, denote by b_i the node of smaller degree and by c_i the other node; otherwise, denote by b_i the node of larger degree and by c_i the other one. When b_i has another neighbor which is not linked to c_i, the pair of nodes b_i and c_i are included in the candidate set ψ of rewiring node pairs.

(4) *Rewiring*. Select a pair of nodes from ψ with the closest difference in their degrees compared to the theoretical $|\Delta k_T|$, still denoted by b_i and c_i, respectively. Randomly select another neighbor of b_i, denoted by a_i, release the link between a_i and b_i, and then create a new link between a_i and c_i.

(5) *Termination*. When the relative difference between the expected and the estimated proportions of β particles satisfies $|\Delta\chi_\beta/\theta| < \epsilon$, the rewiring process is terminated. Here, ϵ is a relatively small positive number. Similarly, if the above condition cannot be achieved, the program is also stopped when $t = T_2$.

It should be noted that when $\Delta k_T \in (-1.5,-0.5)$, the heterogeneity of the network will not be changed any further by the rewiring process. Consequently, there is a theoretical upper bound of the control error calculated by

$$E_U = \frac{\mu_1}{\mu_2\rho V H^2\langle k\rangle^2}, \tag{35}$$

which can be inferred from Eq. (34) and suggests that higher control accuracy can be expected in a diffusion network with a larger average degree and a higher heterogeneity.

When the parameters are set to be $\mu_1 = 0.2$, $\mu_2 = 0.05$, $\rho = 5$ with $\rho_\alpha(0)/\rho_\beta(0) = N_\alpha(0)/N_\beta(0) = 1$, $V = L^2 = 625$, $\tau = 10^3$, $\epsilon = 10^{-4}$, $T_s = 10^5$, and $T_2 = 10^7$, the scenes of the diffusion network at different stages with different values of θ

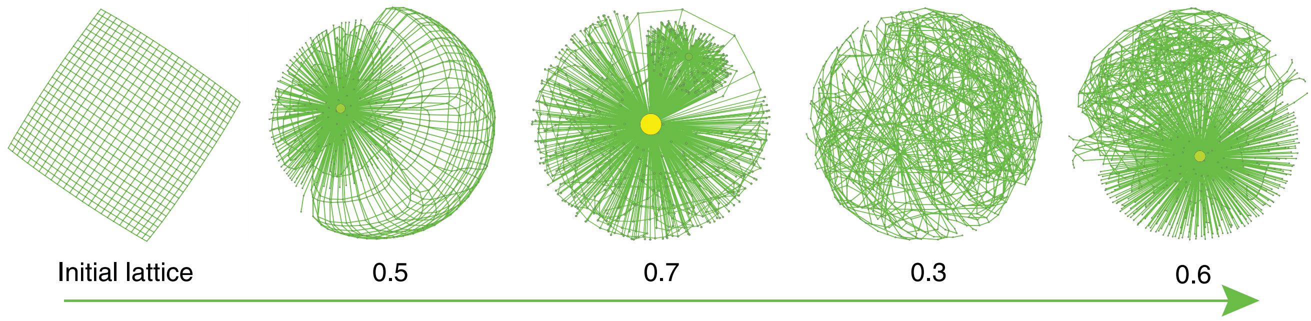

FIG. 6. (Color online) The initial two-dimensional lattice as well as some scenarios of the diffusion network in different stages with $\theta = 0.5,0.7,0.3,0.6$, under centralized rewiring control. In each scenario, the node size is proportional to the node degree.

are shown in Fig. 6. Moreover, the controlled and analytic proportions of β particles in different network scenes are shown in Fig. 7. Interestingly, it is found that χ_β can be controlled to different points in a certain range with quite high accuracy by the proposed centralized rewiring mechanism, although the theoretical results still largely deviate from the set points. This is because, as formulated by Eq. (12), the emergence of hub nodes in heterogeneous networks provides a chance for α particles to meet more β particles in a local world so as to be infected with a higher probability. Therefore, the heterogeneity of a network is indeed statistically related to the proportions of different reactants in it. This is the basis of the feedback centralized control method introduced above, where the heterogeneity is increased if the density of β particles is lower than the expected value and is decreased otherwise. However, since the analytic results are obtained by the MF theory under the assumption of having no weighted degree correlation between any two linked nodes, it is not strange that they deviate from the real results when the assumption cannot be guaranteed in the control process.

B. Centralized reweighting control

When a weighted diffusion network is considered, the only difference from an unweighted one is that here $H = \langle\omega^2\rangle/\langle\omega\rangle^2$.

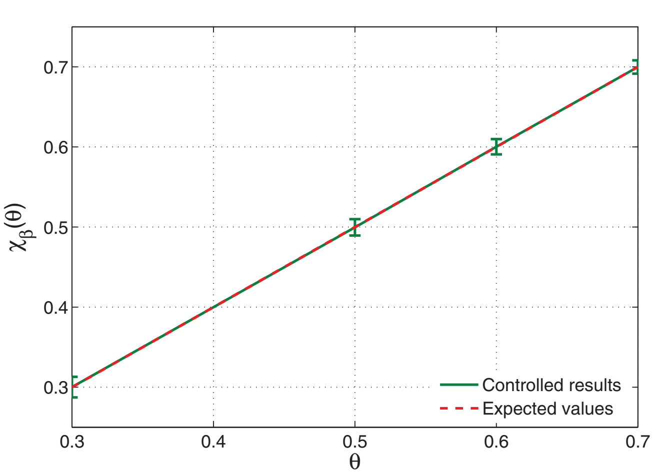

FIG. 7. (Color online) The controlled and analytic proportions of particles in the network as well as the expected values at different stages of evolution under centralized rewiring control.

Consider the same reweighting process shown in Fig. 1 and denote by ω_a, ω_b, and ω_c the weighted degrees of nodes a, b, and c, respectively. The variation of the heterogeneity after a reweighting step, where the weight of the link between a and b increases by δ and that between b and c decreases by δ, respectively, is calculated by

$$\Delta H = \frac{(\omega_a+\delta)^2 + (\omega_c-\delta)^2 - \omega_a^2 - k_c^2}{V\langle\omega\rangle^2} = \frac{2(\delta\Delta\omega+\delta^2)}{V\langle\omega\rangle^2}, \tag{36}$$

where $\Delta\omega = \omega_a - \omega_c$, because the average weighted degree $\langle\omega\rangle$ of the network remains unchanged through the entire reweighting process. Here, it is supposed that the weights of links belong to a common range, denoted by $[\omega_{\min},\omega_{\max}]$, with $\omega_{\min} > 0$, in order to keep the connectivity of the weighted network. Therefore, it is required that

$$0 \leqslant \delta \leqslant \min(\omega_{bc} - \omega_{\min}, \omega_{\max} - \omega_{ab}). \tag{37}$$

Denoting $\Delta\zeta = \delta(\Delta\omega + \delta)$, the relationship between $\Delta\chi_\beta$ and $\Delta\zeta$ can be established as

$$\Delta\chi_\beta = \frac{2\mu_1\Delta\zeta}{\mu_2\rho V H^2\langle\omega\rangle^2}. \tag{38}$$

Based on Eq. (38), the centralized reweighting control scheme is composed of the following five steps:

(1) *Initialization*. Numbers $N_\alpha(0)$ of α particles and $N_\beta(0)$ of β particles are randomly distributed in a network of N nodes. The weights of all links are set to be the same, denoted by ω.

(2) *Estimation*. Estimate the difference between the expected and the current steady densities of β particles by Eq. (33). Calculate the heterogeneity H by Eq. (22) and the average weighted degree $\langle\omega\rangle$ of the current weighted network structure. Then, from Eq. (38), one gets

$$\Delta\zeta_T = \frac{\mu_2\rho V H^2\langle\omega\rangle^2}{2\mu_1}\Delta\chi_\beta. \tag{39}$$

(3) *Candidate selection*. For each ordered node triple $[a_i,b_i,c_i]$, where b_i is a common neighbor of a_i and c_i, calculate the minimum value of $\varepsilon_i = |\delta_i(\Delta\omega_i+\delta_i) - \Delta\zeta_T|$ for $\Delta\omega_i = \omega_{a_i} - \omega_{c_i}$ and $\delta_i \in [0, \min(\omega_{b_ic_i} - \omega_{\min}, \omega_{\max} - \omega_{a_ib_i})]$. Denote by ε_i^ϕ the minimum value of ε_i, which is

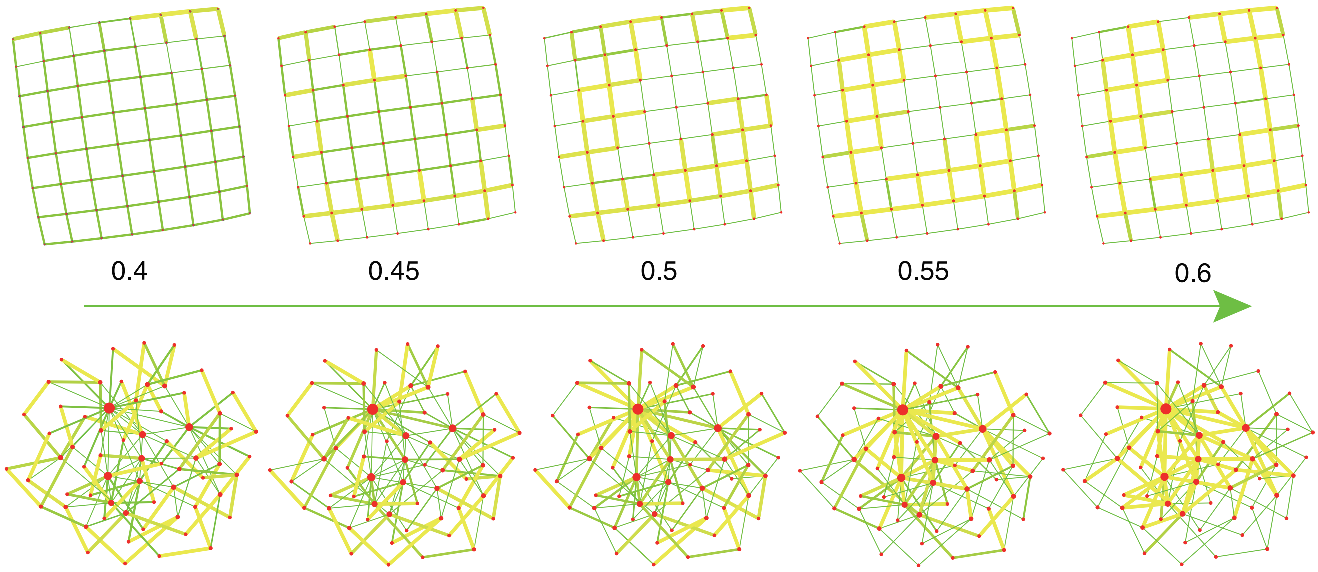

FIG. 8. (Color online) Different scenarios in two diffusion networks, i.e., a two-dimensional lattice (above) and a BA SF network (below) at different stages with $\theta = 0.4, 0.45, 0.5, 0.55, 0.6$, under centralized reweighting control. In each scenario, the node size is proportional to the node degree and the link width is proportional to its weight. Note that, this figure as well as Figs. 2, 4, 6 are all ploted by Cytoscape [32].

obtained when $\delta_i = \delta_i^{\phi}$. Then include the ordered node triple $[a_i, b_i, c_i]$ in the candidate set ψ of ordered reweighting nodes.

(4) *Reweighting*. Select the ordered node triple in ψ with a minimum ε_i^{ϕ}, still denoted by $[a_i, b_i, c_i]$. Increase the weight of the link between a_i and b_i by δ_i^{ϕ} and decrease that between b_i and c_i by δ_i^{ϕ}.

(5) *Termination*. When $|\Delta\chi_\beta/\theta| < \epsilon$ or $t = T_2$, the reweighting process is terminated.

When the parameters are set to be $\mu_1 = 0.5$, $\mu_2 = 0.05$, $\rho = 20$ with $\rho_\alpha(0)/\rho_\beta(0) = N_\alpha(0)/N_\beta(0) = 1$, $V = 64$, $\omega = 10$, $\omega_{\text{min}} = 1$, $\omega_{\text{max}} = 20$, $\tau = 10^3$, $\epsilon = 10^{-4}$, $T_s = 10^5$, and $T_2 = 10^7$, and each time a newly added node is linked to two different existing nodes in the BA SF network, the scenarios of diffusion networks at different stages with different values of θ are shown in Fig. 8. The controlled and analytic proportions of β particles in the scenarios of the two-dimensional lattice and the BA SF network are shown in Fig. 9. As expected, the centralized reweighting control scheme gives better results than the distributed one. More interestingly, by comparison, it is found that the proportion of α or β particles in heterogeneous networks can be controlled through the reweighting processes in wider ranges than in homogeneous networks with similar numbers of nodes and links, if the weights of links have the same bound. Generally, a system with stronger plasticity can fit a changeable environment better, which may explain why heterogeneous networks are so common in nature.

V. CONCLUSION

By designing distributed rewiring and reweighting control schemes for unweighted and weighted networks, respectively, it is found that the networks evolve to be more and more heterogeneous in a self-organized fashion in order to satisfy the external requirements which encourage more active particles in the networks. Based on the relationship between the heterogeneity of a diffusion network and the proportion of active particles, if the proportion of active particles can be estimated in real time, it is possible to propose more efficient centralized control schemes. More interestingly, it is revealed that the proportions of active particles in heterogeneous networks can be controlled in wider ranges than those in homogeneous networks with similar numbers of nodes and links, under the assumption that only the weights of links can be changed within a fixed bound. Consistent with the natural law "the fittest survives," this finding may provide another explanation for the common heterogeneous structures existing in many real-world networks.

In the future, the work presented here can be expanded regarding the following three issues. First, different kinds of

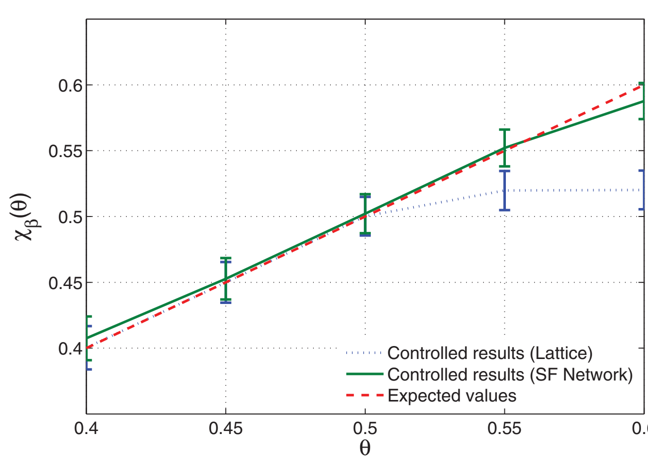

FIG. 9. (Color online) The controlled and analytic proportions of particles in the networks as well as the expected values at different stages of evolution under centralized rewiring control.

RD process may be considered under the same framework to examine whether they can be controlled by similar methods. Second, more precise relationships between structural properties and the RD results should be established. Finally, more effective control schemes might be developed to improve the control efficiency.

ACKNOWLEDGMENTS

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