Ground-state energy of the q-state Potts model: The minimum modularity

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(Received 23 March 2014; revised manuscript received 9 September 2014; published 19 November 2014)

A wide range of interacting systems can be described by complex networks. A common feature of such networks is that they consist of several communities or modules, the degree of which may quantified as the *modularity*. However, even a random uncorrelated network, which has no obvious modular structure, has a finite modularity due to the quenched disorder. For this reason, the modularity of a given network is meaningful only when it is compared with that of a randomized network with the same degree distribution. In this context, it is important to calculate the modularity of a random uncorrelated network with an arbitrary degree distribution. The modularity of a random network has been calculated [Reichardt and Bornholdt, Phys. Rev. E **76**, 015102 (2007)]; however, this was limited to the case whereby the network was assumed to have only two communities, and it is evident that the modularity should be calculated in general with $q(\geqslant 2)$ communities. Here we calculate the modularity for q communities by evaluating the ground-state energy of the q-state Potts Hamiltonian, based on replica symmetric solutions assuming that the mean degree is large. We found that the modularity is proportional to $\langle\sqrt{k}\rangle/\langle k\rangle$ regardless of q and that only the coefficient depends on q. In particular, when the degree distribution follows a power law, the modularity is proportional to $\langle k\rangle^{-1/2}$. Our analytical results are confirmed by comparison with numerical simulations. Therefore, our results can be used as reference values for real-world networks.

DOI: 10.1103/PhysRevE.90.052140 PACS number(s): 05.50.+q, 89.75.−k

I. INTRODUCTION

A wide range of networks, including, for example, the Internet, the world wide web, social relationships, and biological systems [1–4], may appear unrelated to each other. However, it has recently been shown that there exist several common features in such networks, including the existence of hub and fat-tailed degree distributions [5–7]. In particular, one important common feature is that a network consists of several *communities*, which are densely connected subnetworks compared with other parts of the network.

Understanding the community structure of a given network is of practical importance. A set of nodes in the same community typically has similar properties or functions. For example, nodes belonging to the same community found in the world wide web [8] and social networks [9] have similar topics and identities, respectively. In addition, nodes in the same community of a metabolic network have been shown to have similar metabolic functions [4,10]. Therefore, identifying the community structure provides information that aids in the understanding of the role of a specific node in a network. Moreover, the analysis of community structures of gene-disease and metabolite-disease networks may provide a method to predict complications associated with diseases [11].

Motivated by such practical importance, many authors have attempted to identify the optimal community structure of a given network, and a number of sophisticated algorithms to detect the possible optimal community structure have been reported [12–23]. Most of these algorithms make use of the *property* that the link density within a community is much larger than the intercommunity link density. Therefore, it is crucial for community-detection algorithms to employ a suitable function to quantify such a *property*. A widely used function for this purpose is the *modularity*, introduced by Newman and Girvan [12]. The modularity function takes a community configuration as its argument and returns a value between 0 and 1. The modularity represents how modular a given network is, i.e., a larger modularity corresponds to a network that is more modularized or has a richer community structure.

The absolute value of the modularity, however, is not necessarily helpful in discerning how modular a network is. In other words, a finite modularity does not guarantee a truly modular structure of a network. In Ref. [24], Guimerà *et al.* showed that even a random uncorrelated network, which presumably does not have a modular structure, has a finite modularity because of the presence of quenched disorder. For example, Fig. 1(a) shows a random uncorrelated network generated using a static model [25]. Despite the lack of any obvious community structure, the modularity of this network is 0.51, which may be considered to be a relatively large value of the modularity in the usual sense. Figure 1(b) shows another network with the same size and the same degree distribution. In this case we can see a clear community structure, and the modularity is 0.72, which is larger than that of the first example.

It follows that the modularity is meaningful only when compared with a random uncorrelated network with the same degree distribution. Therefore, calculating the modularity of random uncorrelated networks with an arbitrary degree distribution is important to determine a reference modularity. Reichardt *et al.* [26] found that calculating the ground-state energy of an Ising model of a network is equivalent to finding the modularity of the network if the network has

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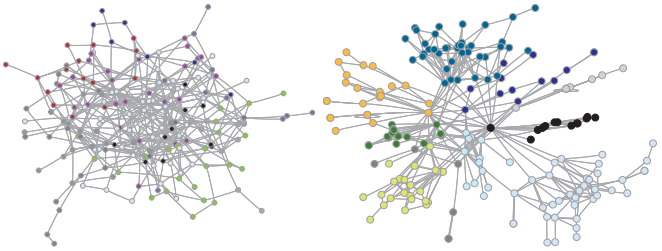

(a) (b)

FIG. 1. (Color online) Examples of a random uncorrelated and a modular network. Each color represents a different community, as identified by the q-state Potts model. (a) A static model with a modularity of 0.51. (b) A modular network with a modularity of 0.72.

two communities. Using this equivalence, they calculated the modularity of a random uncorrelated network with an arbitrary degree distribution assuming that the network had only two communities.

In general, however, it is clear that the modularity should be calculated with an arbitrary number of communities. Here we denote the number of communities as $q(\geqslant 2)$, and we calculate the modularity of networks with q communities. To achieve this, we map the modularity function for a network with q communities onto the ground-state energy of the q-state Potts model. We then calculate the energy of the Potts model for a random uncorrelated network with an arbitrary degree distribution in the large mean-degree limit. Our main result is that the ground-state energy is given by $-C(q)\langle\sqrt{k}\rangle/\langle k\rangle$, Eq. (45), where $\langle k\rangle$ is the mean degree of the network. The coefficient $C(q)$ is an increasing function of q for $q \leqslant 5$ and $C(q) = C(5)$ for $q > 5$. For a scale-free network, $\langle\sqrt{k}\rangle/\langle k\rangle \propto \langle k\rangle^{-1/2}$.

The remainder of this paper is organized as follows. In Sec. II we first describe how the problem of finding a community structure can be mapped to that of finding the ground state of the q-state Potts model. This is achieved by comparing the modularity function with the Hamiltonian of the q-state Potts model. We then derive the replica-symmetric solutions for the free energy and energy of the Hamiltonian. In Sec. III we give analytic expressions for the energy, especially the ground-state energy, for general q. In Sec. IV we compare the analytical results with numerical simulations.

II. ANALYTIC SOLUTIONS FOR THE q-STATE POTTS MODEL

A. Hamiltonian of the q-state Potts model

We begin by describing the modularity and discussing how it is related to the q-state Potts model. Consider a network composed of N nodes, L edges, and q communities. The degree distribution of the network is p_k. Let us arbitrarily assign a unique integer in the range from 1 to q to each community. Then let σ_i denote the number of communities assigned to a node i. The modularity $Q_{\rm MOD}$ [27] is defined as the difference between the proportion of the intracommunity edges of a given network and the expected proportion of such edges in a random uncorrelated network with the same degree distribution. That is, $Q_{\rm MOD}$ is given by

$$\begin{aligned} Q_{\rm MOD} &= \frac{1}{L}(\text{number of intracommunity edges}) \\ &\quad - \frac{1}{L}(\text{expected number of such edges}) \\ &= \frac{1}{L}\sum_{i<j}\left(A_{ij} - \frac{k_i k_j}{\langle k\rangle N}\right)\delta(\sigma_i,\sigma_j), \end{aligned} \tag{1}$$

where the adjacency matrix element $A_{ij} = 1$ if there is an edge between two distinct nodes i and j; otherwise, $A_{ij} = 0$. Here k_i denotes the degree of node i, i.e., $k_i = \sum_j A_{ij}$, and $\langle k\rangle$ is the mean degree of the network. Note that the term $k_i k_j/(\langle k\rangle N) \equiv f_{ij}$ in the above expression is the connection probability between nodes i and j in a random uncorrelated network.

If a specific community structure $\{\sigma_1,\ldots,\sigma_N\}$ is initially given, the calculation of the modularity is straightforward. However, in most cases, this information is not known *a priori*; rather, the optimal community structure is determined as the one that maximizes the modularity, which is chosen from all possible configurations of $\{\sigma_1,\ldots,\sigma_N\}$. This maximum modularity will be denoted by $Q^*_{\rm MOD}$. Therefore, a major task for community detection is finding the community configuration that maximizes the modularity. However, since the number of all possible configurations increases exponentially with N ($\sim q^N$), it is not generally feasible to enumerate and test all of them for a network with large N.

To avoid such difficulties, several *feasible* algorithms [24,28,29] have been proposed. One particularly interesting approach is to use the q-state Potts model, the Hamiltonian of which is given by [26]

$$\mathcal{H} = -\frac{1}{\langle k\rangle}\sum_{i<j}(A_{ij} - \eta f_{ij})\delta(\sigma_i,\sigma_j) \quad \left(f_{ij} = \frac{k_i k_j}{\langle k\rangle N}\right), \tag{2}$$

where σ_i denotes the spin state of node i of q possible spin states and η is a control parameter. Note that the connection probability f_{ij} is typically very small, i.e., $f_{ij} \ll 1$. Therefore, when $A_{ij} = 1$ ($A_{ij} = 0$), the coupling constant between nodes i and j becomes positive (negative); thus, two spins, σ_i and σ_j, tend to be in the same (different) spin state(s) in order to lower the energy E of the Hamiltonian. The ground-state energy E_g of this model can be obtained from the spin configuration by minimizing the Hamiltonian. When $\eta = 1$, the ground-state energy is proportional to the maximized modularity $Q^*_{\rm MOD}$, i.e.,

$$Q^*_{\rm MOD} = -2E_g/N. \tag{3}$$

Therefore, finding the community structure of a network now becomes a problem of searching for the ground-state of the q-state Potts model Hamiltonian.

B. Free energy

In this section we describe the calculation of the free energy of the q-state Potts model Hamiltonian (2) for an uncorrelated random network with an arbitrary degree distribution p_k as a reference value for the modularity. We assume that the typical free energy of Eq. (2) is the same as the quenched average of

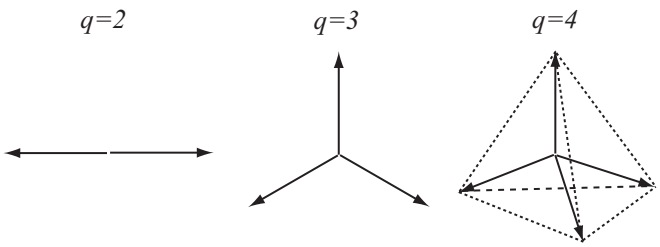

FIG. 2. Potts spin vector. q-state Potts spin can be mapped into vertices of a $r(=q-1)$-dimensional simplex.

the free energy over the network configurations $\{A_{ij}\}$. Using the replica method, the configuration-averaged free energy is given by

$$[\ln Z]_c = \lim_{n\to 0} \frac{[Z^n]_c - 1}{n}, \tag{4}$$

where Z is the partition function of the Hamiltonian for a one-network configuration and $[\cdots]_c$ denotes the configuration-ensemble average [30,31]. In the context of the replica method, n is assumed to be a nonzero integer, prior to discussing the limit $n = 0$. For any integer n, we can write the above expression as

$$[Z^n]_c = [(\mathrm{Tr}_i e^{-\beta\mathcal{H}})^n]_c = \int \prod_{i<j} dJ_{ij}\, P(J_{ij}) \mathrm{Tr}_{i,\alpha} \exp\left[\frac{\beta}{\langle k\rangle} \sum_{\substack{i<j \\ \alpha}} J_{ij}\delta\left(\sigma_i^\alpha,\sigma_j^\alpha\right)\right],$$

where β is the inverse temperature, $J_{ij} \equiv (A_{ij} - \eta f_{ij})$, and $\mathrm{Tr}_{i,\alpha}$ denotes the sum of all possible spin states σ_i^α over all nodes in all the replicas. Using $P(J_{ij}) = f_{ij}\delta(J_{ij} - 1 + \eta f_{ij}) + (1 - f_{ij})\delta(J_{ij} + \eta f_{ij})$, $[Z^n]_c$ becomes

$$[Z^n]_c = \mathrm{Tr}_{i,\alpha} \exp\left(-\frac{\beta}{\langle k\rangle}\sum_{i<j}\sum_{\alpha}\eta f_{ij}\delta\left(\sigma_i^\alpha,\sigma_j^\alpha\right)\right) \exp\left[\sum_{i<j}\ln\left(1 + f_{ij}\left\{\exp\left[\frac{\beta}{\langle k\rangle}\sum_{\alpha}\delta\left(\sigma_i^\alpha,\sigma_j^\alpha\right)\right] - 1\right\}\right)\right]. \tag{5}$$

Now we use an approximation

$$\sum_{i<j}\ln(1 + f_{ij}D_{ij}) \approx \sum_{i<j} f_{ij}D_{ij} = \sum_{i<j}\frac{k_i k_j}{\langle k\rangle N}D_{ij}, \tag{6}$$

which is valid in the thermodynamic limit for a wide range of uncorrelated ensembles [32]. Then, $[Z^n]_c$ becomes

$$[Z^n]_c = \mathrm{Tr}_{i,\alpha} \exp\left[\sum_{i<j}\frac{k_i k_j}{\langle k\rangle N}\left(-\frac{\beta\eta}{\langle k\rangle}\sum_{\alpha}\delta\left(\sigma_i^\alpha,\sigma_j^\alpha\right) + \exp\left(\frac{\beta}{\langle k\rangle}\sum_{\alpha}\delta\left(\sigma_i^\alpha,\sigma_j^\alpha\right)\right) - 1\right)\right]. \tag{7}$$

To manipulate the Kronecker δ function, it is convenient to adopt the vector representation for q-state Potts spins [33,34]. As shown in Fig. 2, each q-state Potts spin σ_i can be mapped to a $q-1$ dimensional vector $\vec{S}_i$. The angle between any two vectors is identical. Then, the Kronecker δ function can be written as

$$\delta(\sigma_i,\sigma_j) = \frac{1}{q}(r\vec{S}_i\cdot\vec{S}_j + 1) = \frac{1}{q}\left(r\sum_{\mu} S_{i\mu}S_{j\mu} + 1\right), \tag{8}$$

where

$$r \equiv q - 1. \tag{9}$$

The vector-component index μ varies from 1 to r.

In this work we consider the densely connected limit [35], i.e., $\beta \ll \langle k\rangle$ for fixed β, which was also used in Reichardt *et al.* [26]. Then, by expanding the exponential term $\exp(\frac{\beta}{\langle k\rangle}\sum_\alpha \delta(\sigma_i^\alpha,\sigma_j^\alpha))$ in Eq. (7) up to the second order in $\frac{\beta}{\langle k\rangle}$ and by using Eq. (8), Eq. (7) can be written as

$$[Z^n]_c = \exp\left(\frac{n\beta(1-\eta)N}{2q}\right)\Lambda, \tag{10}$$

with

$$\Lambda = \mathrm{Tr}_{i,\alpha}\exp\left[\frac{C_1 N}{2}\sum_{\alpha,\mu}\left(\sum_i\frac{k_i}{\langle k\rangle N}S_{i\mu}^\alpha\right)^2 + \frac{C_2 N}{2}\sum_{\alpha\neq\beta,\mu\nu}\left(\sum_i\frac{k_i}{\langle k\rangle N}S_{i\mu}^\alpha S_{iv}^\beta\right)^2 + \frac{C_2 N}{2}\sum_{\alpha,\mu\nu}\left(\sum_i\frac{k_i}{\langle k\rangle N}S_{i\mu}^\alpha S_{iv}^\alpha\right)^2\right], \tag{11}$$

where

$$C_1 = \frac{\beta(1-\eta)r}{q}, \quad C_2 = \frac{\beta^2 r^2}{2\langle k\rangle q^2}. \tag{12}$$

Note that the terms which are higher order than n are ignored in the above derivation since they will vanish as $n \to 0$.

Now, performing the Hubbard-Stratonovich transform on each quadratic term in Λ and applying the saddle point method subsequently, Λ becomes

$$\Lambda = \exp\left[-\frac{C_1 N}{2}\sum_{\alpha\mu}\left(\overline{M}_\mu^\alpha\right)^2 - \sum_{\alpha\neq\beta,\mu\nu}\frac{C_2 N}{2}\left(\overline{Q}_{\mu\nu}^{\alpha\beta}\right)^2 - \sum_{\alpha,\mu\nu}\frac{C_2 N}{2}\left(\overline{L}_{\mu\nu}^\alpha\right)^2 + N\sum_k p_k \ln \mathrm{Tr}_\alpha \exp\mathcal{H}^{(k)}\right], \tag{13}$$

where p_k is the degree distribution of a given network and $\mathcal{H}^{(k)}$ is given by

$$\mathcal{H}^{(k)} = \frac{k}{\langle k\rangle}\left(C_1\sum_{\alpha\mu} S_\mu^\alpha \overline{M}_\mu^\alpha + C_2\sum_{\alpha\neq\beta,\mu\nu} S_\mu^\alpha S_\nu^\beta \overline{Q}_{\mu\nu}^{\alpha\beta} + C_2\sum_{\alpha,\mu\nu} S_\mu^\alpha S_\nu^\alpha \overline{L}_{\mu\nu}^\alpha\right). \tag{14}$$

Here $\overline{M}_\mu^\alpha$, $\overline{Q}_{\mu\nu}^{\alpha\beta}$, and $\overline{L}_{\mu\nu}^\alpha$ are chosen to satisfy the saddle point condition. Their explicit replica-symmetric forms will be shown later in Eqs. (20) to (22).

At this stage we seek a replica symmetric solution so that we assume $\overline{M}_\mu^\alpha \to M_\mu$, $\overline{Q}_{\mu\nu}^{\alpha\beta} \to Q_{\mu\nu}$, and $\overline{L}_{\mu\nu}^\alpha \to L_{\mu\nu}$. Then, Λ and $\mathcal{H}^{(k)}$ can be simplified as

$$\Lambda = \exp\left[-\frac{NC_1 n}{2}\sum_\mu (M_\mu)^2 - \frac{NC_2 n(n-1)}{2}\sum_{\mu\nu}(Q_{\mu\nu})^2 - \frac{NC_2 n}{2}\sum_{\mu\nu}(L_{\mu\nu})^2 + N\sum_k p_k \ln \mathrm{Tr}_\alpha \exp\mathcal{H}^{(k)}\right] \tag{15}$$

and

$$\frac{\langle k\rangle}{k}\mathcal{H}^{(k)} = C_1\sum_{\alpha\mu} S_\mu^\alpha M_\mu + C_2\sum_\alpha\sum_{\mu\nu} S_\mu^\alpha S_\nu^\alpha (L_{\mu\nu} - Q_{\mu\nu}) + C_2\sum_{\mu\nu} Q_{\mu\nu}\left(\sum_\alpha S_\mu^\alpha\right)\left(\sum_\beta S_\nu^\beta\right). \tag{16}$$

The quadratic nature of the last term in Eq. (16) allows us to perform the modified Hubbard-Stratonovich transform. In Appendix A it is shown that

$$\ln \mathrm{Tr}_\alpha \exp\mathcal{H}^{(k)} = n\iint \mathcal{D}z\mathcal{D}w\ \ln \mathrm{Tr}\exp h^{(k)} + O(n^2), \tag{17}$$

where $\mathcal{D}z = \prod_{\mu\nu}\frac{dz_{\mu\nu}}{\sqrt{2\pi}}\exp(-\frac{z_{\mu\nu}^2}{2})$ and $\mathcal{D}w = \prod_{\mu\nu}\frac{dw_{\mu\nu}}{\sqrt{2\pi}}\exp(-\frac{w_{\mu\nu}^2}{2})$ and $h^{(k)}$ is defined as

$$h^{(k)} \equiv \frac{kC_1}{\langle k\rangle}\sum_\mu S_\mu M_\mu + \frac{kC_2}{\langle k\rangle}\sum_{\mu\nu} S_\mu S_\nu (L_{\mu\nu} - Q_{\mu\nu}) + \sum_{\mu\nu}\sqrt{\frac{2kC_2 Q_{\mu\nu}}{\langle k\rangle}}(\mathcal{S}_{\mu\nu} z_{\mu\nu} + \mathcal{A}_{\mu\nu} w_{\mu\nu}), \tag{18}$$

with $\mathcal{S}_{\mu\nu} \equiv \frac{1}{2}(S_\mu + S_\nu)$ and $\mathcal{A}_{\mu\nu} \equiv \frac{i}{2}(S_\mu - S_\nu)$.

From Eqs. (10), (15), and (17) the free energy density is given by

$$\begin{aligned} f &= -\frac{1}{\beta}\lim_{n\to 0}\frac{[Z^n]-1}{nN} \\ &= -\frac{(1-\eta)}{2q} + \frac{C_1}{2\beta}\sum_\mu M_\mu^2 + \frac{C_2}{2\beta}\sum_{\mu\nu}\left(L_{\mu\nu}^2 - Q_{\mu\nu}^2\right) - \frac{1}{\beta}\sum_k p_k \iint \mathcal{D}z\mathcal{D}w\ \ln(\mathrm{Tr}\exp h^{(k)}). \end{aligned} \tag{19}$$

Here M_μ, $L_{\mu\nu}$, and $Q_{\mu\nu}$ are determined by minimization of the free energy. For M_μ, the condition $\frac{\partial f}{\partial M_\mu} = 0$ gives

$$M_\mu = \sum_k \frac{p_k k}{\langle k\rangle}\iint \mathcal{D}z\mathcal{D}w\ \langle S_\mu\rangle_{h^{(k)}}, \tag{20}$$

where $\langle(\bullet)\rangle_{h^{(k)}}$ denotes the expectation value with respect to $h^{(k)}$, namely, $\langle(\bullet)\rangle_{h^{(k)}} \equiv \frac{\mathrm{Tr}(\bullet)\exp h^{(k)}}{\mathrm{Tr}\exp h^{(k)}}$. Similarly, one can find

$$L_{\mu\nu} = \sum_k \frac{p_k k}{\langle k\rangle}\iint \mathcal{D}z\mathcal{D}w\ \langle S_\mu S_\nu\rangle_{h^{(k)}} \tag{21}$$

and

$$\begin{aligned} Q_{\mu\nu} &= L_{\mu\nu} - \sum_k p_k\sqrt{\frac{k}{2\langle k\rangle C_2 Q_{\mu\nu}}}\iint \mathcal{D}z\mathcal{D}w\ \langle \mathcal{S}_{\mu\nu} z_{\mu\nu} + \mathcal{A}_{\mu\nu} w_{\mu\nu}\rangle_{h^{(k)}} \\ &= \sum_k \frac{p_k k}{\langle k\rangle}\iint \mathcal{D}z\mathcal{D}w\ \langle S_\mu\rangle_{h^{(k)}}\langle S_\nu\rangle_{h^{(k)}}, \end{aligned} \tag{22}$$

where the last equality in Eq. (22) is obtained by integration by parts. From Eqs. (21) and (22), one can easily check that $L_{\mu\nu} = L_{\nu\mu}$ and $Q_{\mu\nu} = Q_{\nu\mu}$. By a proper rotation of r-dimensional space, any r-dimensional vector $(M_1, M_2, \ldots, M_r)$ can be transformed into one satisfying the following condition:

$$M_\mu = M_1 \delta_{\mu 1}. \tag{23}$$

In this coordinate setting, one can prove some important identities for $Q_{\mu\nu}$ and $L_{\mu\nu}$ such as $Q_{\mu\nu} = L_{\mu\nu} = 0$ for $\mu \neq \nu$, $L_{\mu\mu} = L_{\nu\nu}$ and $Q_{\mu\mu} = Q_{\nu\nu}$ for $\mu > 1$ and $\nu > 1$, and $\sum_{\mu=1}^{q} L_{\mu\mu} = 1$, which are derived in Appendix C. Using them, we finally obtain

$$f = -\frac{(1-\eta)}{2q} + \frac{C_1}{2\beta} M_1^2 + \frac{C_2}{2\beta} \sum_\mu \left(L_{\mu\mu}^2 - Q_{\mu\mu}^2\right) - \frac{1}{\beta} \sum_k p_k \int \mathcal{D}z \, \ln(\mathrm{Tr} \exp h^{(k)}), \tag{24}$$

where $h^{(k)}$ is now simplified as Eq. (C11). Note that in the above equation the integral with respect to $\int \mathcal{D}w$ disappears and $\mathcal{D}z$ is reduced to $\prod_\mu \frac{dz_{\mu\mu}}{\sqrt{2\pi}} \exp(-\frac{z_{\mu\mu}^2}{2})$ (see Appendix C). From now on $\int \mathcal{D}z$ means the product of integrals with respect to only the diagonal integral variables $z_{\mu\mu}$ if there is no other comment.

C. Energy

From Eq. (24) the energy E is given by

$$E/N = \frac{\partial(\beta f)}{\partial \beta} = -\frac{(1-\eta)}{2q} + \frac{C_1}{2\beta} M_1^2 + \frac{C_2}{\beta} \sum_\mu \left(L_{\mu\mu}^2 - Q_{\mu\mu}^2\right) - \sum_k p_k \int \mathcal{D}z \times \left\langle \frac{kC_1}{\beta \langle k \rangle} S_1 M_1 + \frac{2kC_2}{\beta \langle k \rangle} \sum_\mu S_\mu^2 (L_{\mu\mu} - Q_{\mu\mu}) + \sum_\mu \sqrt{\frac{2kC_2 Q_{\mu\mu}}{\beta^2 \langle k \rangle}} S_\mu z_{\mu\mu} \right\rangle_{h^{(k)}}. \tag{25}$$

Using Eqs. (20) to (22), the three terms in the average $\langle(\bullet)\rangle_{h^{(k)}}$ in Eq. (25) can be reduced to

$$\sum_k \frac{p_k k}{\langle k \rangle} \int \mathcal{D}z \, \langle S_1 \rangle_{h^{(k)}} = M_1, \tag{26a}$$

$$\sum_k \frac{p_k k}{\langle k \rangle} \int \mathcal{D}z \, \langle S_\mu^2 \rangle_{h^{(k)}} = L_{\mu\mu}, \tag{26b}$$

$$\sum_k p_k \int \mathcal{D}z \left\langle \frac{\sqrt{k} S_\mu z_{\mu\mu}}{\sqrt{\beta^2 \langle k \rangle}} \right\rangle_{h^{(k)}} = \frac{\sqrt{2C_2 Q_{\mu\mu}}}{\beta} (L_{\mu\mu} - Q_{\mu\mu}). \tag{26c}$$

With these equations, one can simplify Eq. (25) as

$$E/N = -\frac{(1-\eta)}{2q} - \frac{C_1}{2\beta} M_1^2 - \frac{C_2}{\beta} \sum_\mu \left(L_{\mu\mu}^2 - Q_{\mu\mu}^2\right). \tag{27}$$

Using Eqs. (C9b), (C18), and (26c), Eq. (27) becomes

$$E/N = -\frac{(1-\eta)}{2q} - \frac{C_1}{2\beta} M_1^2 - \frac{1}{\langle k \rangle} \sum_k p_k \sqrt{k} C(q,k), \tag{28}$$

where

$$C(q,k) = \frac{r\sqrt{r}}{2q} \Big[(L_{11} + Q_{11}) \int \mathcal{D}z \, z_{11} \langle S_1 \rangle_{h^{(k)}} + (L_{22} + Q_{22})(r-1) \int \mathcal{D}z \, z_{22} \langle S_2 \rangle_{h^{(k)}} \Big]. \tag{29}$$

By plugging the solutions of the self-consistent equations (26) into Eq. (28), we can calculate the energy for any β and η.

III. GROUND-STATE ENERGY FOR EACH q

A. $q = 2$

In this case, Potts spins become one-dimensional vectors, which greatly simplifies the trace with respect to $h^{(k)}$ as follows:

$$\mathrm{Tr} \exp h^{(k)} = \exp\left(\frac{\beta^2 k}{8\langle k \rangle^2}(1 - Q_{11})\right) 2\cosh(\beta h(z)) \tag{30}$$

and

$$\mathrm{Tr} S_1 \exp h^{(k)} = \exp\left(\frac{\beta^2 k}{8\langle k \rangle^2}(1 - Q_{11})\right) 2\sinh(\beta h(z)), \tag{31}$$

where $z = z_{11}$ and $\beta h(z) = \frac{\beta(1-\eta)}{2\langle k \rangle} M_1 + \frac{\beta\sqrt{k}}{2\langle k \rangle} \sqrt{Q_{11}} z$. Using Eqs. (30) and (31), the self-consistent equations (20)–(22) become

$$M_1 = \sum_k \frac{p_k k}{\langle k \rangle} \int \mathcal{D}z \, \tanh(\beta h(z)), \tag{32a}$$

$$Q_{11} = \sum_k \frac{p_k k}{\langle k \rangle} \int \mathcal{D}z \, \tanh^2(\beta h(z)), \tag{32b}$$

and

$$L_{11} = \sum_k \frac{p_k k}{\langle k \rangle} \int \mathcal{D}z \, 1 = 1, \tag{32c}$$

where $\mathcal{D}z = \frac{dz}{\sqrt{2\pi}} \exp(-\frac{z^2}{2})$.

Finally, the free energy [Eq. (24)] and the energy [Eq. (28)] become

$$f = -\frac{1-\eta}{4}\left(1-M_1^2\right) - \frac{\beta}{16\langle k\rangle}(Q_{11}-1)^2 - \frac{1}{\beta}\sum_k p_k \int \mathcal{D}z\ \ln 2\cosh\left(\beta h(z)\right) \tag{33a}$$

and

$$E/N = -\frac{1-\eta}{4}\left(1+M_1^2\right) - \frac{\beta}{8\langle k\rangle}\left(1-Q_{11}^2\right) = -\frac{1-\eta}{4}\left(1+M_1^2\right) - \frac{\beta(1+Q_{11})}{8\langle k\rangle}\frac{q}{\beta r\sqrt{Q_{11}}} \times \sum_k p_k\sqrt{k}\int \mathcal{D}z\, z\tanh\left(\beta h(z)\right), \tag{33b}$$

respectively. Equation (22) is used for deriving the last equality in the above equation. We are interested in the modularity which is proportional to the ground-state energy with $\eta = 1$. Therefore, setting $\eta = 1$ and taking the $\beta \to \infty$ limit, the ground-state energy is given by

$$E_g/N = -\frac{1}{2\langle k\rangle}\sum_k p_k\sqrt{k}\int_{-\infty}^{\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)|z| = -\frac{1}{\sqrt{2\pi}}\frac{\langle\sqrt{k}\rangle}{\langle k\rangle}. \tag{34}$$

Strictly speaking, the large β limit in this study should be taken with maintaining the condition $\beta/\langle k\rangle \ll 1$ (see more discussion on the $\beta \to \infty$ limit in Appendix E). Note that Eq. (34) is in agreement with the result presented in Ref. [26].

B. q = 3

For the $q = 3$ case, $h_t^{(k)}$ in Eq. (C11) for each Potts spin vector can be written as

$$h_1^{(k)} = \frac{\beta(1-\eta)rk}{q\langle k\rangle}M_1 + \frac{\beta^2r^2k}{2\langle k\rangle^2q^2}(L_{11}-Q_{11}) + \frac{\beta r}{\langle k\rangle q}\sqrt{kQ_{11}}z_{11}, \tag{35a}$$

$$h_2^{(k)} = -\frac{\beta(1-\eta)rk}{2q\langle k\rangle}M_1 + \frac{\beta^2r^2k}{2\langle k\rangle^2q^2}\left[\frac{(L_{11}-Q_{11})}{4} + \frac{3(L_{22}-Q_{22})}{4}\right] + \frac{\beta r}{\langle k\rangle q}\left[\frac{-\sqrt{kQ_{11}}z_{11}}{2} + \frac{\sqrt{3kQ_{22}}z_{22}}{2}\right], \tag{35b}$$

$$h_3^{(k)} = -\frac{\beta(1-\eta)rk}{2q\langle k\rangle}M_1 + \frac{\beta^2r^2k}{2\langle k\rangle^2q^2}\left[\frac{(L_{11}-Q_{11})}{4} + \frac{3(L_{22}-Q_{22})}{4}\right] + \frac{\beta r}{\langle k\rangle q}\left[\frac{-\sqrt{kQ_{11}}z_{11}}{2} - \frac{\sqrt{3kQ_{22}}z_{22}}{2}\right]. \tag{35c}$$

Note that $\langle S_\mu\rangle_{h^{(k)}} = \sum_{t=1}^q S_{t,\mu}\exp h_t^{(k)}/\sum_{t=1}^q \exp h_t^{(k)}$, where $S_{t,\mu}$ is the μth component of $\vec{S}_t^{(q)}$ (see Appendix B). As $\beta \to \infty$, the largest term in the summation dominates among $\exp h_1^{(k)}$, $\exp h_2^{(k)}$, and $\exp h_3^{(k)}$. Now let us define

(1) $\ell_1 \equiv z_{22} - \sqrt{\frac{3Q_{11}}{Q_{22}}}z_{11} - G$,
(2) $\ell_2 \equiv z_{22} + \sqrt{\frac{3Q_{11}}{Q_{22}}}z_{11} + G$,
(3) $\ell_3 \equiv z_{22}$,

where

$$G = \frac{\sqrt{3k}(1-\eta)}{\sqrt{Q_{22}}}M_1 + \frac{\sqrt{3k}r}{4\langle k\rangle q\sqrt{Q_{22}}}[\beta(L_{11}-Q_{11}) - \beta(L_{22}-Q_{22})]. \tag{36}$$

Note that the three lines $\ell_1 = 0$, $\ell_2 = 0$, and $\ell_3 = 0$ meet at one point $(-G\sqrt{\frac{Q_{22}}{3Q_{11}}},0)$ in a two-dimensional plane (z_{11},z_{22}) and divide a whole plane into three regions A, B, and C as follows:

(1) $A : \ell_1 < 0$ and $\ell_2 > 0$,
(2) $B : \ell_1 > 0$ and $\ell_3 > 0$,
(3) $C : \ell_2 < 0$ and $\ell_3 < 0$.

Then, one can show that $h_1^{(k)}$, $h_2^{(k)}$, and $h_3^{(k)}$ dominate in A, B, and C, respectively. On these divided regions, in the $\beta \to \infty$ limit, the self-consistent equation for M_1, Eq. (26a), can be written in terms of the regions as

$$M_1 = 1 - 3D, \tag{37}$$

where

$$D \equiv \sum_k \frac{p_k k}{\langle k\rangle}\iint_B \mathcal{D}z = \frac{1}{2} - \frac{1}{2}\sum_k \frac{p_k k}{\langle k\rangle}\iint_A \mathcal{D}z\,. \tag{38}$$

Other self-consistent equations in Eqs. (26b) and (26c) can also be written in terms of the regions in the similar way. Calculation details are presented in Appendix D. Collecting all the new self-consistent equations written in terms of the regions A, B, and C, the ground-state energy [Eq. (28)] can now be calculated as

$$E_g/N = -\frac{1-\eta}{2}(1-4D+6D^2) - \frac{1}{\langle k\rangle}\left(-2\sqrt{1-\frac{3}{2}D}X + \sqrt{2D}Y\right), \tag{39}$$

where

$$X = \sum_k p_k\sqrt{k}\iint_B \mathcal{D}z\, z_{11}$$

and

$$Y = \sum_k p_k\sqrt{k}\iint_B \mathcal{D}z\, z_{22}.$$

Here X and Y are the self-consistently determined quantities (see Appendix D). In the case of $\eta = 1$, D becomes $\frac{1}{3}$ and thus

$$E_g/N = -\frac{1}{\langle k\rangle}\left(-\sqrt{2}X + \sqrt{\frac{2}{3}}Y\right) = -\sqrt{\frac{\frac{3}{2}}{2\pi}}\frac{\langle\sqrt{k}\rangle}{\langle k\rangle}. \quad (40)$$

C. q = 4

For $q = 4$, calculation of the ground-state energy is rather complicated and tedious, but proceeds in a similar way as the previous section; in this case, the three-dimensional plane (z_{11}, z_{22}, z_{33}) is divided into four regions and the self-consistent equations are written as the integral over the divided regions. Here we present only the final result for the ground-state energy when $\eta = 1$ as below:

$$E/N = -\frac{3\sqrt{3}}{4\langle k\rangle}\sum_k p_k\sqrt{k}\int \mathcal{D}z\, z_{\mu\mu}\frac{\mathrm{Tr}S_\mu \exp h^{(k)}}{\mathrm{Tr}\exp h^{(k)}} \quad \text{(for any } \mu)$$

where

$$\int \mathcal{D}z\, z_{\mu\mu}\frac{\mathrm{Tr}S_\mu \exp h^{(k)}}{\mathrm{Tr}\exp h^{(k)}}$$
$$\xrightarrow{\beta\to\infty} \frac{2\sqrt{6}}{3}\int_0^\infty dz_{33}\int_{-\infty}^{\frac{z_{33}}{\sqrt{3}}} dz_{22}\int_{-\infty}^{\frac{\sqrt{6}z_{33}-\sqrt{2}z_{22}}{4}} dz_{11}\frac{z_{33}}{(2\pi)^{\frac{3}{2}}}$$
$$\times \exp\left(-\frac{\sum_{\mu=1}^3 z_{\mu\mu}^2}{2}\right) \approx 0.243, \quad (41)$$

Where $\mathcal{D}z = \prod_{\mu=1}^3 \frac{dz_{\mu\mu}}{\sqrt{2\pi}}\exp(-\frac{z_{\mu\mu}^2}{2})$. Then,

$$E_g/N \approx -\frac{3\sqrt{2}}{2}\times 0.243\sum_k p_k\sqrt{k}$$
$$\approx -\sqrt{\frac{\frac{5}{3}}{2\pi}}\frac{\langle\sqrt{k}\rangle}{\langle k\rangle}. \quad (42)$$

D. Modularity for q > 4

For $q > 4$ case, the calculation of the ground-state energy becomes much more complex for general η. Therefore, in this section, we focus on the $\eta = 1$ case only, where the ground-state energy is proportional to the modularity as explained in Sec. II A. To go further, we tentatively assume that M_1, defined as Eq. (26a), will be zero in the ground state as is the case with $q \leqslant 4$. This assumption, $M_1 = 0$, implies that all q spin states are equally distributed to all nodes in the ground state; if not, M_1 would not be zero. The validity of this assumption will be discussed later.

The assumption $M_1 = 0$ greatly simplifies the calculation. When $M_1 = 0$, $L_{\mu\mu} = \frac{1}{r}$ for all μ as shown in Eqs. (C9a) and (C9b), and $Q_{\mu\mu} = Q_{\nu\nu}$ for any μ and ν as shown in Eq. (C20). Then, in the $\beta \to \infty$ limit Eq. (28) becomes

$$E_g/N = -\frac{1}{\langle k\rangle}\sum_k p_k\sqrt{k}C_0(q) = -C_0(q)\frac{\langle\sqrt{k}\rangle}{\langle k\rangle}, \quad (43)$$

where

$$C_0(q) = \frac{r\sqrt{r}}{q}\int \mathcal{D}z\, z_{11}\langle S_1\rangle_{h^{(k)}}. \quad (44)$$

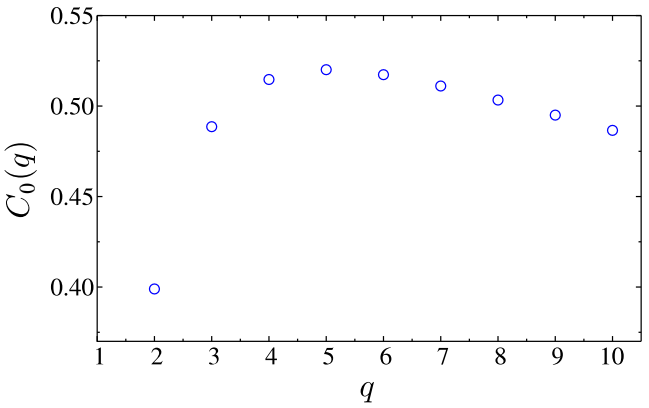

FIG. 3. (Color online) $C_0(q)$ as defined in Eq. (44) for various q.

A more explicit integral form of $C_0(q)$ is presented in Appendix F.

We numerically evaluate $C_0(q)$ up to $q = 10$ as shown in Fig. 3. Interestingly, $C_0(q)$ becomes maximum at $q = 5$. This indicates that, within the assumption $M_1 = 0$, the ground-state energy becomes minimum at $q = 5$. However, the decreasing behavior of $C_0(q)$ for $q > 5$ is problematic because it should satisfy the relation $E_g(q) \geqslant E_g(q+1)$, where $E_g(q)$ is the ground-state energy with q-possible spin states. If we denote a spin configuration of N nodes with q-possible spin states as $\{\sigma_1, \ldots, \sigma_N\}_q$, all possible spin configurations of $\{\sigma_1, \ldots, \sigma_N\}_q$ are included in those of $\{\sigma_1, \ldots, \sigma_N\}_{q+1}$. Therefore, $E_g(q+1)$ should be smaller than or equal to $E_g(q)$. We attribute this contradiction to the assumption $M_1 = 0$.

Through numerical simulations for scale-free networks as described in Sec. IV, we checked when this assumption is valid. As seen in Table I, we found $M_1 = 0$ for $q \leqslant 5$. However, for $q > 5$ we found that the ground-state spin configuration is the same as that of $q = 5$. In other words, in the ground state only five spin states are equally distributed to all nodes even for $q > 5$ case. Thus, we conclude that the proportionality coefficient $C(q)$, defined in Eq. (46), is

TABLE I. Ground-state spin configuration data for a network with 10^4 nodes, $\langle k\rangle = 128$, and $\gamma = 3.5$ obtained from the numerical simulations described in Sec. IV. A number in the table denotes the number of nodes having the same spin state. Up to $q = 5$, all q spin states are almost equally distributed to all nodes, which implies $M_1 = 0$. For $q > 5$, ground-state spin configurations are the same as that of $q = 5$; only five spin states are used.

$q=2$	$q=3$	$q=4$	$q=5$	$q=6$	$q=7$	$q=8$	$q=9$	State index
5024	3369	2503	2017	2017	2017	2017	2017	1
4976	3317	2474	1981	1981	1981	1981	1981	2
	3314	2517	2084	2084	2084	2084	2084	3
		2506	1950	1950	1950	1950	1950	4
			1968	1968	1968	1968	1968	5
				0	0	0	0	6
					0	0	0	7
						0	0	8
							0	9

independent of q for $q > 5$. Therefore, we finally come to the conclusion that the ground-state energy is given by

$$E_g/N = -C(q)\frac{\langle\sqrt{k}\rangle}{\langle k\rangle}, \tag{45}$$

where

$$C(q) = \begin{cases} C_0(q) & \text{for } q \leqslant 5 \\ C_0(5) & \text{for } q > 5. \end{cases} \tag{46}$$

This expression is verified by the simulation in Sec. IV. Equation (45) is one of our main results.

From Eq. (3) the modularity of a random uncorrelated network with arbitrary degree distribution based on q communities becomes

$$[Q^*_{\rm MOD}]_c = 2C(q)\frac{\langle\sqrt{k}\rangle}{\langle k\rangle}. \tag{47}$$

Note that for the ER network with $\langle k\rangle = c$, $[Q^*_{\rm MOD}]_{c,\rm ER} = 2C(q)\sum_0^\infty \sqrt{k}c^{k-1}e^{-c}/k!$ and for a regular random network with a fixed degree c, $[Q^*_{\rm MOD}]_{c,\rm regular} = 2C(q)/\sqrt{c}$.

IV. NUMERICAL SIMULATIONS

Here we describe the results of numerical simulations and compare them with the analytical expressions derived in the previous sections. We used the static model introduced by Goh *et al.* [25] to generate an ensemble of random networks. The term "static" originates from the fact that the number of vertices N of a network is fixed while constructing a network sample. In this model, a normalized weight P_i ($\sum_i P_i = 1$) is assigned to each vertex i. We consider the case whereby P_i follows a power-law form, i.e., $P_i = i^{-\alpha}/\sum_j j^{-\alpha}$. A network is constructed via the following process. In each time step, the two vertices i and j are selected with probabilities P_i and P_j, respectively. If $i = j$ or an edge connecting i and j already exists, we do nothing; otherwise, an edge is added between vertices i and j. We repeat this step NK times. The probability that a given pair of vertices i and $j (i \neq j)$ are not connected by an edge following this process is given by $(1 - 2P_iP_j)^{NK} \simeq e^{-2NKP_iP_j}$. Thus, the connection probability for nodes i and j is $1 - e^{2NKP_iP_j}$. Here we used the condition $P_i \ll 1$. The factor 2 in the exponent comes from the equivalence of (ij) and (ji). The connection probability f_{ij} can thus be approximated as $f_{ij} \approx 2NKP_iP_j \approx \langle k_i\rangle\langle k_j\rangle/(\langle k\rangle N)$ in the thermodynamic limit, where we used the fact $\langle k_i\rangle = 2KNP_i$ in this limit [36]. The resulting network is scale-free and has a degree exponent γ given by

$$\gamma = 1 + \frac{1}{\alpha}. \tag{48}$$

Note that a network generated by the static model becomes uncorrelated when $\gamma \geqslant 3$ [36]. Therefore, we performed the simulation on a network with $\gamma \geqslant 3$. For this scale-free network, the Eq. (47) becomes

$$[Q^*_{\rm MOD}]_c = 2C(q)\frac{\sqrt{(\gamma-1)(\gamma-2)}}{\left(\gamma-\frac{3}{2}\right)}\langle k\rangle^{-1/2}. \tag{49}$$

The size of the networks N used in this study was 10 000, and the exponents of the degree distributions were 3.0, 3.5, 4.0, and 4.5. As $\gamma \to \infty$ limit, we also performed the same numerical simulations for the Erdős-Rényi (ER) network [37] of the same size.

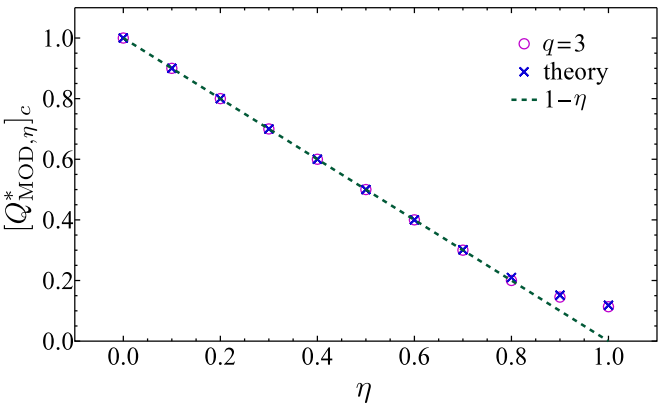

FIG. 4. (Color online) Plot of $[Q^*_{\rm MOD},\eta]_c$ against η for $q = 3$, $N = 10\,000$, $\langle k\rangle = 64$, and $\gamma = 3.5$. The red open circles represent the data calculated using the simulated annealing method. The cross symbols indicate the solutions of Eq. (39) obtained by solving the self-consistent equations (36), (D2), (D7), and (D9) numerically. For small η, D is expected to be small, and thus $[Q^*_{\rm MOD},\eta]_c$ is very close to $1 - \eta$ (the blue dashed curve), which can be seen in Eq. (39).

Since finding the ground state of the Potts model Hamiltonian is an NP-hard problem, it is practically impossible to do so for very large networks. Instead, we used the simulated annealing method [38] to obtain an approximate solution. Initially, one of the q possible spins was randomly assigned to each node in the network. The initial temperature was set to be sufficiently high. In the Monte Carlo simulation we chose one spin at random, and determined whether the spin state was changed according to the Metropolis algorithm. This procedure was repeated until the system reached a stationary state at a fixed temperature. The temperature was then reduced according to a predefined schedule, and the simulation was repeated until it reached a stationary state for this new temperature. The final state, i.e., the stationary state at zero temperature, was assumed to be the ground state of the system.

Figure 4 shows a plot of $[Q^*_{\rm MOD},\eta]_c$ versus η for $q = 3$, $\langle k\rangle = 64$, and $\gamma = 3.5$. The analytical results were in very good agreement with the simulated data. As η approached 0, the interaction between Potts spins became more ferromagnetic and $M_1 \to 1$. We then found that $D \to 0$ from Eq. (D3), which made $[Q^*_{\rm MOD},\eta]_c \approx 1 - \eta$, from Eq. (39).

Figure 5(a) shows $[Q^*_{\rm MOD}]_c$ as a function of $\langle k\rangle$ for various γ with $\eta = 1.0$ and $q = 3$. Note that $[Q^*_{\rm MOD}]_c$ is rescaled by $\mathcal{G}(\gamma) \equiv \frac{\sqrt{(\gamma-1)(\gamma-2)}}{(\gamma-3/2)}$ in order to observe the collapsing behavior. As expected from the analytical results, all the simulated data collapsed onto the curve given by Eq. (49). Figure 5(b) shows $[Q^*_{\rm MOD}]_c$ as a function of $\langle k\rangle$ for various q with $\eta = 1.0$ and $\gamma = 3.5$. In this case, $[Q^*_{\rm MOD}]_c$ is rescaled by $C(q)$. As seen in the figure, the data collapses well with the theoretical line for all q. By carefully investigating the ground-state spin configurations obtained from the simulations, we confirmed that the assumption $M_1 = 0$ used in Sec. III D is valid for $q \leqslant 5$. We also checked that the ground-state spin

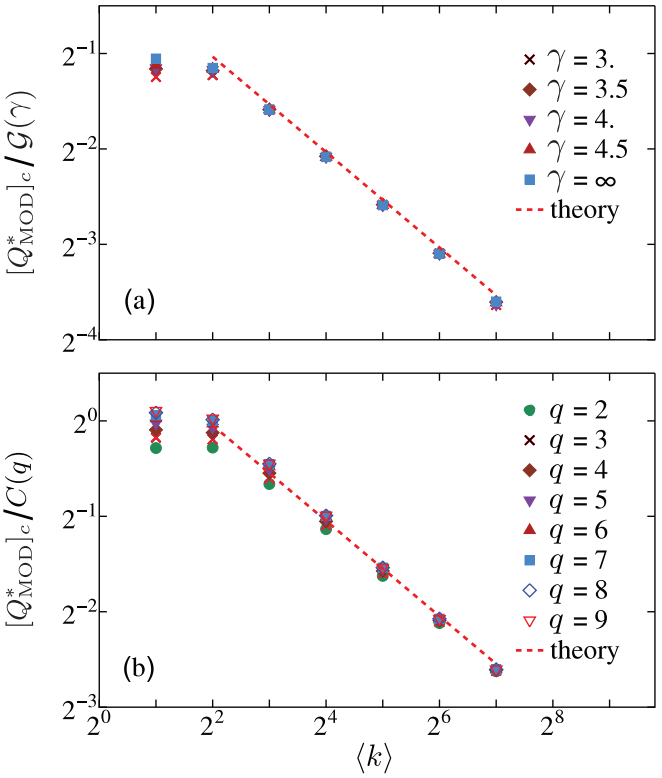

FIG. 5. (Color online) (a) Plot of $[Q^*_{\rm MOD}]_c$ rescaled by $\mathcal{G}(\gamma)$ as a function of $\langle k \rangle$ for $\gamma = 3, 3.5, 4, 4.5$, and ER ($\gamma \to \infty$), with $\eta = 1.0$ and $q = 3$. The red dashed curve shows the result of Eq. (49). The gradient of the curve in the double logarithmic scale is -0.5. (b) Plot of $[Q^*_{\rm MOD}]_c$ rescaled by $C(q)$ as a function of $\langle k \rangle$ for eight values of q up to $q = 9$ with $\eta = 1.0$ and $\gamma = 3.5$. The red dashed curve shows the theoretical curve from Eq. (49).

configuration for $q > 5$ are essentially the same as that for $q = 5$. However, we note that if the simulation starts with very large q, it will take too long time to reach the optimal spin configuration consisting of only five communities.

The correspondence between our theoretical and simulated data indicates that the replica symmetric (RS) solution is valid for calculating the energy of the Potts model. We also note that the analytical results can be improved by taking into account the replica symmetry breaking (RSB) solutions. For example, as stated in Ref. [26], for $q = 2$, the modularity obtained from the RSB solution is more accurate. The difference in modularity between RS and RSB was approximately 6%. However, this small difference is not significant in the logarithmic scale, as can be seen from Fig. 5.

V. CONCLUSION

We have described a community detection method based on maximizing the modularity function, which is equivalent to finding a ground-state energy of the q-state Potts model Hamiltonian, Eq. (2), when $\eta = 1$. Because a random uncorrelated network has a finite modularity due to quenched disorder, the modularity of a given network is meaningful only when it is compared with that of a random network. Therefore, we analytically calculated the modularity of a random uncorrelated network as a reference by finding the ground-state energy of the q-state Potts model. We used the replica method to find a replica symmetric solution. We also studied the densely connected regime where $\beta \ll \langle k \rangle$, even if we take the limit $\beta \to \infty$, which is described formally at the later stages of the calculation.

We showed that, for an arbitrary q, the modularity is proportional to $\langle \sqrt{k} \rangle / \langle k \rangle$ when $\eta = 1$. Especially for a scale-free network, it is proportional to $\langle k \rangle^{-0.5}$. The q dependence is included only in the coefficient $C(q)$, which increases as q increases up to $q = 5$ and becomes constant for $q \geqslant 5$. Surprisingly, this "critical" value, $q = 5$, is universal for any random-uncorrelated complex networks. In this context, it would be mathematically interesting to extend the results for noninteger q and check whether the maximum value of $C_0(q)$ is obtained at noninteger q.

We also performed simulations using the simulated annealing method to find the ground state of the q-state Potts model and showed that our analytical results were in good agreement with the simulated data. Our results provide a theoretical minimum value over which the modularity of a network becomes meaningful. In addition, our calculation method may be applicable to evaluating the energy of a similar type of q-state Potts model.

ACKNOWLEDGMENT

This research was supported by the National Research Foundation (NRF) of Korea, Grant No. 2011-35B-C00014 (J.S.L.) and No. 2010-0015066 (B.K.).

APPENDIX A: LINEARIZATION OF QUADRATIC SPIN PRODUCT

We begin by introducing the modified Hubbard-Stratonovich transform as follows:

$$\exp(2\lambda^2 ab) = \iint \frac{dz}{\sqrt{2\pi}} \frac{dw}{\sqrt{2\pi}} \times \exp\left(-\frac{1}{2}z^2 - \frac{1}{2}w^2 + \lambda(a+b)z + i\lambda(a-b)w\right). \tag{A1}$$

Using the above transformation, the last term of the exponent in Eq. (16) becomes

$$\exp\left[\frac{kC_2}{\langle k \rangle}\sum_{\mu\nu} Q_{\mu\nu}\left(\sum_\alpha S^\alpha_\mu\right)\left(\sum_\beta S^\beta_\nu\right)\right] = \iint \mathcal{D}z\mathcal{D}w \exp\left[\sum_{\mu\nu}\sum_\alpha \sqrt{\frac{kC_2Q_{\mu\nu}}{2\langle k \rangle}}\left\{\left(S^\alpha_\mu + S^\alpha_\nu\right)z_{\mu\nu} + i\left(S^\alpha_\mu - S^\alpha_\nu\right)w_{\mu\nu}\right\}\right], \tag{A2}$$

where $\mathcal{D}z\mathcal{D}w = \prod_{\mu\nu} \frac{dz_{\mu\nu}}{\sqrt{2\pi}} \frac{dw_{\mu\nu}}{\sqrt{2\pi}} \exp(-\frac{z^2_{\mu\nu}}{2} - \frac{w^2_{\mu\nu}}{2})$. Note that the term quadratically coupled by two replica indices is now linearized in the final expression. Then, the trace of $\exp \mathcal{H}^{(k)}$

of Eq. (16) can be evaluated as

$$\mathrm{Tr}_\alpha \exp \mathcal{H}^{(k)} = \iint \mathcal{D}z\mathcal{D}w\, (\mathrm{Tr} \exp h^{(k)})^n, \tag{A3}$$

where $h^{(k)}$ is defined in Eq. (18).

APPENDIX B: VECTOR REPRESENTATION OF q-STATES POTTS MODEL

Consider a r-dimensional simplex with q vertices whose center of mass is located at the origin. If we define θ_q to be the angle between any two vectors pointing from the origin to the vertices of the simplex, it satisfies $\cos\theta_q = -\frac{1}{q-1}$. Because Potts spin vectors can be identically mapped to the vectors of the simplex [39], r-dimensional Potts vector can be expressed by θ_q. For $q=2$, $\vec{S}_1^{(2)} = (1)$ and $\vec{S}_2^{(2)} = (\cos\theta_2)$. For $q=3$, $\vec{S}_1^{(3)} = (1,0)$, $\vec{S}_2^{(3)} = (\cos\theta_3, \sin\theta_3)$, and $\vec{S}_3^{(3)} = (\cos\theta_3, \sin\theta_3\cos\theta_2)$. Apart from $\vec{S}_1^{(3)}$, the other two vectors can be written as $\vec{S}_2^{(3)} = \cos\theta_3 || \sin\theta_3 \vec{S}_1^{(2)}$ and $\vec{S}_3^{(3)} = \cos\theta_3 || \sin\theta_3 \vec{S}_2^{(2)}$, where the concatenation operator $||$ is defined as $a||(b_1,b_2,\ldots,b_\ell) \equiv (a,b_1,b_2,\ldots,b_\ell)$. With this operator, the q-states Potts spin vectors can be written as $\vec{S}_1^{(q)} = (1,0,\ldots,0)$ and $\vec{S}_\ell^{(q)} = \cos\theta_q || \sin\theta_q \vec{S}_{\ell-1}^{(q-1)}$ for $\ell = 2,\ldots,q$. By construction, one can prove the several identities stated below. Let $S_{t,\mu}$ be the μth element of $\vec{S}_t^{(q)}$. Then, one can verify

$$S_{t,\mu} = 0, \tag{B1}$$

for $1 \leqslant t \leqslant \mu - 1$ and

$$S_{t,\nu} = S_{\nu+1,\nu}, \tag{B2}$$

for $\nu < t$. It can also be shown that

$$\sum_{\mu=1}^{q-1} S_{t,\mu} S_{u,\mu} = 1 - (1-\delta_{tu})(1-\cos\theta_q), \tag{B3a}$$

$$\sum_{t=1}^{q} (S_{t,\mu})^2 = \frac{q}{q-1}, \tag{B3b}$$

$$\sum_{t=1}^{q} S_{t,\mu} = 0. \tag{B3c}$$

APPENDIX C: PROPERTIES OF $L_{\mu\nu}$ AND $Q_{\mu\nu}$

In Eq. (21) the expression $\langle S_\mu S_\nu \rangle_{h^{(k)}}$ for $\mu > \nu$ can be simplified as

$$\begin{aligned}\langle S_\mu S_\nu \rangle_{h^{(k)}} &= \frac{\mathrm{Tr} S_\mu S_\nu \exp h^{(k)}}{\mathrm{Tr} \exp h^{(k)}} \\ &= \sum_{t=1}^{q} \frac{S_{t,\mu} S_{t,\nu} \exp h_t^{(k)}}{\mathrm{Tr} \exp h^{(k)}} \\ &= \sum_{t=\mu}^{q} \frac{S_{t,\mu} S_{t,\nu} \exp h_t^{(k)}}{\mathrm{Tr} \exp h^{(k)}} \\ &= S_{\mu,\nu} \sum_{t=\mu}^{q} \frac{S_{t,\mu} \exp h_t^{(k)}}{\mathrm{Tr} \exp h^{(k)}} = S_{\mu,\nu} \langle S_\mu \rangle_{h^{(k)}},\end{aligned} \tag{C1}$$

where $h_t^{(k)}$ denotes a $h^{(k)}$ calculated at $\vec{S}_t^{(q)}$. Note that Eqs. (B1) and (B2) are used for the third and fourth equalities, respectively, in the above equation. Using the facts that $\sum_k \frac{p_k k}{\langle k \rangle} \iint \mathcal{D}z\mathcal{D}w \langle S_\mu \rangle_{h^{(k)}} = M_\mu = 0$ for $\mu > 1$ and $L_{\mu\nu} = L_{\nu\mu}$, we have

$$L_{\mu\nu} = 0 \tag{C2}$$

for $\mu \neq \nu$.

Next, we will show that $L_{\mu\mu} = L_{\nu\nu}$ for $\mu > 1$ and $\nu > 1$. First, it is useful to consider the sum of $L_{\mu\mu}$:

$$\begin{aligned}\sum_{\mu=1}^{q} L_{\mu\mu} &= \sum_{\mu=1}^{q} \sum_k \frac{p_k k}{\langle k \rangle} \iint \mathcal{D}z\mathcal{D}w \langle S_\mu^2 \rangle_{h^{(k)}} \\ &= \sum_k \frac{p_k k}{\langle k \rangle} \iint \mathcal{D}z\mathcal{D}w \left\langle \sum_{\mu=1}^{q} S_\mu^2 \right\rangle_{h^{(k)}} = 1,\end{aligned} \tag{C3}$$

where Eq. (B3a) is used for the last equality. Here $\mathcal{D}z\mathcal{D}w = \prod_{\mu\nu} \frac{dz_{\mu\nu}}{\sqrt{2\pi}} \frac{dw_{\mu\nu}}{\sqrt{2\pi}} \exp(-\frac{z_{\mu\nu}^2}{2} - \frac{w_{\mu\nu}^2}{2})$. To proceed further, we define a quantity

$$V_t \equiv \sum_k \frac{p_k k}{\langle k \rangle} \iint \mathcal{D}z\mathcal{D}w \frac{\exp h_t^{(k)}}{\mathrm{Tr} \exp h^{(k)}}. \tag{C4}$$

Then, M_μ can be written as the sum of V_t and $S_{t,\mu}$, i.e.,

$$M_\mu = \sum_{t=1}^{q} V_t S_{t,\mu}, \tag{C5}$$

for $\mu = 1,\ldots,q-1$. The set of linear equations, Eq. (C5), can be solved and the solution is

$$V_m = V_2, \tag{C6}$$

for $m = 3,\ldots,q$ and $V_1 = M_1 + V_2$. Thus, one finds that for $\mu > 1$,

$$\begin{aligned}L_{\mu\mu} &= \sum_k \frac{p_k k}{\langle k \rangle} \iint \mathcal{D}z\mathcal{D}w \langle S_\mu^2 \rangle_{h^{(k)}} \\ &= \sum_{t=1}^{q} V_t S_{t,\mu}^2 = \sum_{t=\mu}^{q} V_t S_{t,\mu}^2 \\ &= V_2 \sum_{t=\mu}^{q} S_{t,\mu}^2 = V_2 \frac{q}{q-1},\end{aligned} \tag{C7}$$

where Eqs. (B1), (B3b), and (C6) are used for the third, last, and fourth equalities, respectively. Similarly, we obtain

$$L_{11} = V_1 + \frac{V_2}{q-1}. \tag{C8}$$

Plugging Eqs. (C7) and (C8) into Eq. (C3), $L_{\mu\mu}$ is given by

$$L_{11} = \frac{1 + (q-2)M_1}{q-1} \tag{C9a}$$

and

$$L_{22} = \frac{1 - M_1}{q-1} = L_{\nu\nu} \quad \text{for } \nu > 1. \tag{C9b}$$

Next, let us examine the properties of $Q_{\mu\nu}$. We will show that there exist nontrivial solutions for the self-consistent Eq. (22) satisfying the following conditions:

$$Q_{\mu\nu} = 0 \tag{C10a}$$

for $\mu \neq \nu$ and

$$Q_{\mu\mu} = Q_{\nu\nu} \tag{C10b}$$

for $\mu > 1$ and $\nu > 1$. With these conditions, $h_t^{(k)}$ in Eq. (18) can be written as

$$\begin{aligned} h_t^{(k)} \equiv{}& \frac{kC_1}{\langle k\rangle} S_{t,1} M_1 \\ &+ \frac{kC_2}{\langle k\rangle} S_{t,1}^2 (L_{11} - Q_{11}) + \frac{kC_2}{\langle k\rangle}(L_{22} - Q_{22}) \sum_{\mu=2}^{r} S_{t,\mu}^2 \\ &+ \sqrt{\frac{2kC_2 Q_{11}}{\langle k\rangle}} S_{t,1} z_{11} + \sqrt{\frac{2kC_2 Q_{22}}{\langle k\rangle}} \sum_{\mu=2}^{r} S_{t,\mu} z_{\mu\mu}. \end{aligned} \tag{C11}$$

If we define $\widetilde{Q}_{11} = \sqrt{\frac{2kC_2 Q_{11}}{\langle k\rangle}}$ and $\widetilde{Q}_{22} = \sqrt{\frac{2kC_2 Q_{22}}{\langle k\rangle}}$, $h_t^{(k)}$ for $t = 1$ and $t = w > 1$ can be written as

$$\begin{aligned} h_1^{(k)} &= \mathcal{B}_1 + \widetilde{Q}_{11} z_{11}, \quad \text{and} \\ h_w^{(k)} &= \mathcal{B}_2 - \widetilde{Q}_{11} \frac{z_{11}}{r} + \widetilde{Q}_{22} \vec{S}_w^{(q)} \cdot \vec{z}', \end{aligned} \tag{C12}$$

respectively, where

$$\begin{aligned} \mathcal{B}_1 &= \frac{kC_1}{\langle k\rangle} M_1 + \frac{kC_2}{\langle k\rangle}(L_{11} - Q_{11}), \\ \mathcal{B}_2 &= -\frac{kC_1}{\langle k\rangle}\frac{M_1}{r} + \frac{kC_2}{r^2\langle k\rangle}(L_{11} - Q_{11}) \\ &\quad + \frac{kC_2(r^2-1)}{\langle k\rangle r^2}(L_{22} - Q_{22}), \\ \vec{S}_t^{(q)} &= (S_{t,1}, S_{t,2}, \ldots, S_{t,r}), \\ \vec{z}' &= (0, z_{22}, z_{33}, \ldots, z_{rr}). \end{aligned} \tag{C13}$$

Note that $\mathcal{B}_1$ and $\mathcal{B}_2$ have nothing to do with the auxiliary integration variables $z_{\mu\mu}$.

From Eq. (22), $Q_{\mu\mu}$ can be written as

$$\begin{aligned} Q_{\mu\mu} &= \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\left(\sum_{t=1}^q S_{t,\mu} \exp h_t^{(k)}\right)^2}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} \\ &= \sum_{u,v} S_{u,\mu} S_{v,\mu} \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\exp h_u^{(k)} \exp h_v^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2}. \end{aligned} \tag{C14}$$

Note that in the above equation the integral with respect to $\int \mathcal{D}w$ disappears because $\mathcal{A}_{\mu\nu} = 0$ for $\nu = \mu$ and $Q_{\mu\nu} = 0$ for $\nu \neq \mu$, thus, all the integration variables $w_{\mu\nu}$ in $h^{(k)}$ in Eq. (18) vanish. In addition, now $\mathcal{D}z = \prod_\mu \frac{dz_{\mu\mu}}{\sqrt{2\pi}} \exp(-\frac{z_{\mu\mu}^2}{2})$ because the off-diagonal terms of $z_{\mu\nu}$ also vanish by Eq. (C10a). Then, the integral in Eq. (C14) can be categorized into the following four cases:

$$\begin{aligned} &\int \mathcal{D}z \frac{\exp h_u^{(k)} \exp h_v^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} \\ &= \begin{cases} \int \mathcal{D}z \frac{\exp h_1^{(k)} \exp h_1^{(k)}}{(\sum_{t=1}^q \exp h_t^{(k)})^2}, & \text{for} \quad u = v = 1 \\ \int \mathcal{D}z \frac{\exp h_1^{(k)} \exp h_2^{(k)}}{(\sum_{t=1}^q \exp h_t^{(k)})^2}, & \text{for} \quad u = 1 \text{ and } v > 1 \\ \int \mathcal{D}z \frac{\exp h_2^{(k)} \exp h_2^{(k)}}{(\sum_{t=1}^q \exp h_t^{(k)})^2}, & \text{for} \quad u = v > 1 \\ \int \mathcal{D}z \frac{\exp h_2^{(k)} \exp h_3^{(k)}}{(\sum_{t=1}^q \exp h_t^{(k)})^2}. & \text{for} \quad u, v > 1 \text{ and } u \neq v. \end{cases} \end{aligned} \tag{C15}$$

The derivation for the above equation is straightforward. For example, for $u = 1$ and $v > 1$ (the second case), using Eq. (C12), the integral becomes

$$\int \mathcal{D}z \frac{e^{h_1^{(k)} + \mathcal{B}_2 - \widetilde{Q}_{11}\frac{z_{11}}{r}} e^{\widetilde{Q}_{22} \vec{S}_v^{(q)} \cdot \vec{z}'}}{\left(e^{h_1^{(k)}} + e^{\mathcal{B}_2 - \widetilde{Q}_{11}\frac{z_{11}}{r}} \sum_{t=2}^q e^{\widetilde{Q}_{22} \vec{S}_t^{(q)} \cdot \vec{z}'}\right)^2}. \tag{C16}$$

Because $\vec{S}_t^{(q)}$ for $t > 1$ possesses rotational symmetry in the subspace spanned by z_{22}, z_{33}, ..., and z_{rr}, Eq. (C16) is invariant under the exchange of different $v(>1)$. Therefore, the integral is the same as the integral for $u = 1$ and $v = 2$. The other cases can be derived in the similar way.

From Eqs. (C14) and (C15), Q_{11} becomes

$$\begin{aligned} Q_{11} &= \sum_u S_{u,1}^2 \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\exp 2h_u^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} + \sum_{u\neq v} S_{u,1} S_{v,1} \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\exp h_u^{(k)} \exp h_v^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} \\ &= S_{1,1}^2 \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\exp 2h_1^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} + \sum_{u=2}^{q} S_{u,1}^2 \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\exp 2h_2^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} \\ &\quad + 2\sum_{v=2}^{q} S_{1,1} S_{v,1} \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\exp h_1^{(k)} \exp h_2^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} + \left[\left(\sum_{u=2} S_{u,1}\right)^2 - \sum_{u=2}^{q} S_{u,1}^2\right] \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \frac{\exp h_2^{(k)} \exp h_3^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} \\ &= \sum_k \frac{p_k k}{\langle k\rangle} \int \mathcal{D}z \left[\frac{\exp 2h_1^{(k)} + \frac{1}{r} \exp 2h_2^{(k)} - 2\exp h_1^{(k)} \exp h_2^{(k)} - \left(1 - \frac{1}{r}\right) \exp h_2^{(k)} \exp h_3^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2}\right]. \end{aligned} \tag{C17}$$

For the third equality, we used Eqs. (B3b) and (B3c). Using the similar way, we can find $Q_{\mu\mu}$ as

$$Q_{\mu\mu} = \frac{r+1}{r}\sum_k \frac{p_k k}{\langle k\rangle}\int \mathcal{D}z \left(\frac{\exp h_2^{(k)}\exp h_2^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} - \frac{\exp h_2^{(k)}\exp h_3^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2}\right) = Q_{\nu\nu}, \tag{C18}$$

for all $\mu,\nu > 1$. Finally, we can also check that

$$Q_{\mu\nu} = \sum_k \frac{p_k k}{\langle k\rangle}\int \mathcal{D}z \,\langle S_\mu\rangle_{h^{(k)}}\langle S_\nu\rangle_{h^{(k)}} = 0 \tag{C19}$$

for all $\mu \neq \nu$ pairs. Equations (C18) and (C19) consistently satisfy the initially imposed conditions, Eqs. (C10a) and (C10b). Even though it is not clear whether there exist other solutions for $Q_{\mu\nu}$ from the self-consistent equations which do not satisfy Eq. (C10b), these imposed conditions must be satisfied in the $\beta\to\infty$ limit. From Eq. (22) we can see that $\beta(L_{\mu\nu}-Q_{\mu\nu})$ remains finite as $\beta\to\infty$, which indicates $Q_{\mu\nu}\to L_{\mu\nu}$ in the zero temperature limit. Note that $L_{\mu\nu}$ satisfies $L_{\mu\nu}=0$ for $\mu\neq\nu$ and $L_{\mu\mu}=L_{\nu\nu}$ for $\mu,\nu>1$ [see Eqs. (C2) and (C9b)]. Therefore, it is reasonable to impose the same conditions for $Q_{\mu\nu}$ at least in the large β limit.

Finally, we briefly discuss the properties of $Q_{\mu\nu}$ when $\eta = 1$. In this case, using the similar method presented above, we can show that there exist nontrivial solutions for the self-consistent equations (22) satisfying (C10a) for $\mu\neq\nu$ and

$$\begin{aligned} Q_{\mu\mu} &= \frac{r+1}{r}\sum_k \frac{p_k k}{\langle k\rangle} \\ &\quad\times \int \mathcal{D}z \left(\frac{\exp h_1^{(k)}\exp h_1^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2} - \frac{\exp h_1^{(k)}\exp h_2^{(k)}}{\left(\sum_{t=1}^q \exp h_t^{(k)}\right)^2}\right) \\ &= Q_{\nu\nu}, \end{aligned} \tag{C20}$$

for all μ and ν.

APPENDIX D: CALCULATION DETAILS FOR THE GROUND-STATE ENERGY WITH $q = 3$

Since $\exp h_1^{(k)}$, $\exp h_2^{(k)}$, and $\exp h_3^{(k)}$ dominate in the regions A, B, and C (defined in Sec. III B), respectively, in the $\beta\to\infty$ limit, the self-consistent equation for M_1, Eq. (26a), can be written as

$$M_1 = \sum_k \frac{p_k k}{\langle k\rangle}\left[\iint_A \mathcal{D}z + \iint_B \mathcal{D}z\left(-\frac{1}{2}\right) + \iint_C \mathcal{D}z\left(-\frac{1}{2}\right)\right], \tag{D1}$$

where $\iint_R \mathcal{D}z$ denotes the integral over the domain R and $\mathcal{D}z = \prod_{\mu=1}^2 \frac{dz_{\mu\mu}}{\sqrt{2\pi}}\exp(-\frac{z_{\mu\mu}^2}{2})$. Note that $\iint_B \mathcal{D}z = \iint_C \mathcal{D}z$ by symmetry and $\iint_{A\cup B\cup C}\mathcal{D}z = 1$. From these identities one can show that

$$D \equiv \sum_k \frac{p_k k}{\langle k\rangle}\iint_B \mathcal{D}z = \frac{1}{2} - \frac{1}{2}\sum_k \frac{p_k k}{\langle k\rangle}\iint_A \mathcal{D}z\,. \tag{D2}$$

The magnetization M_1, thus, can be written in terms of D as

$$M_1 = 1 - 3D. \tag{D3}$$

Similarly, from Eqs. (26b) and (26c), one can find

$$L_{11} = Q_{11} = 1 - \tfrac{3}{2}D \tag{D4}$$

and

$$L_{22} = Q_{22} = \tfrac{3}{2}D. \tag{D5}$$

To obtain the ground-state energy, we should calculate $\beta(L_{\mu\mu}-Q_{\mu\mu})$ in the $\beta\to\infty$ limit. From the first equality in Eq. (26c), one can obtain

$$\beta\,(L_{11}-Q_{11}) = \frac{-3q}{r\sqrt{Q_{11}}}X, \tag{D6}$$

where

$$X \equiv \sum_k p_k\sqrt{k}\iint_B \mathcal{D}z\, z_{11}. \tag{D7}$$

For the derivation of the above equation, we used the facts $\iint_{A\cup B\cup C}\mathcal{D}z\, z_{11} = 0$ and $\iint_B \mathcal{D}z\, z_{11} = \iint_C \mathcal{D}z\, z_{11}$. Similarly, one can show that

$$\beta\,(L_{22}-Q_{22}) = \frac{\sqrt{3}q}{r\sqrt{Q_{22}}}Y, \tag{D8}$$

where

$$Y \equiv \sum_k p_k\sqrt{k}\iint_B \mathcal{D}z\, z_{22} \tag{D9}$$

using the identity $\iint_B \mathcal{D}z\, z_{22} = -\iint_C \mathcal{D}z\, z_{22}$.

Note the following three facts: (i) D, X, and Y are determined by the region B, (ii) the region B depends on G, and (iii) G is evaluated from D, X, and Y. Therefore, Eq. (36) and the set of equations (D2), (D7), and (D9) form self-consistent equations.

APPENDIX E: DISCUSSION ON THE $\beta\to\infty$ LIMIT IN THIS STUDY

Our theory was developed under the condition $\beta/\langle k\rangle \ll 1$ to expand the exponential term in Eq. (7) up to the second order. Therefore, in this study the large β limit should be taken with maintaining the condition $\beta/\langle k\rangle \ll 1$. For a given $\langle k\rangle$, one can estimate a valid range of β satisfying this condition. Define the energy evaluated at the maximum value of β in the valid range as $E_{\beta_{\max}}$. We also define the energy at $\beta=\infty$ limit as E_g. Then, their difference $E_g - E_{\beta_{\max}}$ decreases exponentially on β as $e^{-\beta a}$, where a is some positive number and $O(a) \geqslant O(\langle\sqrt{k}\rangle/\langle k\rangle)$. [This exponential dependence on β comes from the calculation of $\langle S_\mu\rangle_{h^{(k)}} = \sum_{t=1}^q S_{t,\mu}\exp h_t^{(k)}/\sum_{t=1}^q \exp h_t^{(k)}$; a dominant term among all Boltzmann factors is exponentially larger than the second largest term. For example, see Eqs. (35a) to (35c).] Since the maximum value of β in the valid range can become sufficiently

large for a large $\langle k\rangle$, $E_{\beta_{\max}}$ can become approximately the same as E_g. In this sense, the limit $\beta\to\infty$ can be justified.

APPENDIX F: EXPLICIT INTEGRAL FORM OF $C_0(q)$

Here we will show that $C_0(q)$ defined in Eq. (44) can be explicitly written in the following form:

$$C_0(q)=\frac{\sqrt{r}}{(2\pi)^{\frac{q-1}{2}}}\int_0^\infty dz_1 z_1 e^{-\frac{1}{2}z_1^2}\int\cdots\int_{\Delta^{q-2}(\sqrt{2qr}z_1)} \times dz_2\cdots dz_{q-1}e^{-\frac{1}{2}(z_2^2+z_3^2+\cdots+z_{q-1}^2)}, \tag{F1}$$

where the integral range $\Delta^d(x)$ denotes a volume inside a regular d-dimensional simplex whose center is located at the origin in d-dimensional space and whose side length is x. To derive the above equation, let us first examine the integrand $\langle S_1\rangle_{h^{(k)}}$ in Eq. (44). In the limit of $\beta\to\infty$, this term can be simplified as

$$\langle S_1\rangle_{h^{(k)}}=\sum_{t=1}^q S_{t,1}\exp h_t^{(k)}\Big/\sum_{t=1}^q\exp h_t^{(k)} =\begin{cases}1, & \vec{z}\in\mathcal{A}\\ -\frac{1}{r}, & \vec{z}\notin\mathcal{A},\end{cases} \tag{F2}$$

where $\mathcal{A}$ is a region in the r-dimensional space defined as $\mathcal{A}=\{\,\vec{z}\mid\vec{z}\cdot(\vec{S}_1^{(q)}-\vec{S}_t^{(q)})\geqslant 0$ for all $t\in\{2,\ldots,q\}\}$. The region $\mathcal{A}$ can be derived from the condition $h_1^{(k)}\geqslant h_t^{(k)}$ for all $t=2,\ldots,q$ when $M_1=0$, where $h_t^{(k)}$ is defined in Eq. (C11). Then, noting that $\int\mathcal{D}z\,z_1=0$, Eq. (44) can be written as

$$C_0(q)=\sqrt{r}\int\cdots\int_{\mathcal{A}}\mathcal{D}zz_1. \tag{F3}$$

If we define $\mathcal{A}_x$ as the region satisfying $z_1=x$ in $\mathcal{A}$, then $\mathcal{A}_x=\{(x,z_2,\ldots,z_q)|x(1+\cos\theta_q)\geqslant(z_2,\ldots,z_q)\sin\theta_q\vec{S}_t^{(q-1)}$ for all $t\in\{2,\ldots,q\}\}$, where $\cos\theta_q$ and $\sin\theta_q$ are defined in Appendix B. Then Eq. (F1) becomes

$$C_0(q)=\frac{\sqrt{r}}{(2\pi)^{\frac{q-1}{2}}}\int_0^\infty dz_1 z_1 e^{-\frac{1}{2}z_1^2} \times\int\cdots\int_{\mathcal{A}_x}dz_2\cdots dz_{q-1}e^{-\frac{1}{2}(z_2^2+z_3^2+\cdots+z_{q-1}^2)}. \tag{F4}$$

Note that the set $(z_2,\ldots,z_q)$ belonging to $\mathcal{A}_x$ is the volume inside the regular $(q-2)$-dimensional simplex whose center is located at the origin and whose side length is $\sqrt{2qr}x$. Thus, Eq. (F4) can be written as Eq. (F1).

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