Kinked Entropy and Discontinuous Microcanonical Spontaneous Symmetry Breaking

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Spontaneous symmetry breaking (SSB) in statistical physics is a macroscopic collective phenomenon. For the paradigmatic Q-state Potts model it means a transition from the disordered color-symmetric phase to an ordered phase in which one color dominates. Existing mean field theories imply that SSB in the microcanonical statistical ensemble (with energy being the control parameter) should be a continuous process. Here we study microcanonical SSB on the random-graph Potts model and discover that the entropy is a kinked function of energy. This kink leads to a discontinuous phase transition at certain energy density value, characterized by a jump in the density of the dominant color and a jump in the microcanonical temperature. This discontinuous SSB in random graphs is confirmed by microcanonical Monte Carlo simulations, and it is also observed in bond-diluted finite-size lattice systems.

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Spontaneous symmetry breaking (SSB) is a fundamental concept of physics and is tightly linked to the origin of mass in particle physics, the emergence of superconductivity in condensed-matter system, and the ferromagnetic phase transition in statistical mechanics, to name just a few eminent examples [1]. In statistical physics a theoretical paradigm for SSB is the Potts model, a simple two-body interaction graphical system in which each vertex has Q discrete color states [2–4]. The equilibrium SSB transition of the Potts model in the canonical ensemble, where inverse temperature β is the control parameter, has been extensively investigated (see Refs. [5–12] for some of the recent results). Driven by energy-entropy competitions, this transition is a discontinuous phenomenon when Q is sufficiently large, with the density ρ_1 of the dominant color jumps from $1/Q$ to a much larger value at the critical inverse temperature β_c. To compensate for the extensive loss of entropy, such a discontinuous transition is always accompanied by a discontinuous decrease of the system's energy density u [3,4].

When the system is isolated and cannot exchange energy with the environment (the microcanonincal ensemble [13–16]), it is generally believed that the SSB transition will occur gradually, with the dominant color density ρ_1 deviating from $1/Q$ continuously at certain critical energy density $u_{\rm mic}$. Indeed if the microscopic entropy density $s(u)$ is a C^1-continuous function of energy density u [i.e., both $s(u)$ and its first derivative are continuous], there is no reason to expect a discontinuity of the order parameter ρ_1. The C^1 continuity of $s(u)$ can be easily verified for the mean field Potts model on a complete graph [17]. For finite-dimensional lattices the phase separation mechanism (the nucleation and expansion of droplets [18–21]) will guarantee a C^1-continuous entropy profile in the thermodynamic limit. For random graph systems one would naïvely expect $u_{\rm mic}$ to be an inflection point of $s(u)$ [22], which ensures C^1 continuity.

In this Letter we investigate the microcanonical Potts model on random graphs using the Bethe-Peierls mean field theory and discover that the entropy density $s(u)$ is actually not C^1 continuous but is kinked at $u = u_{\rm mic}$ for any $Q \geq 3$ (Fig. 1). Consequently, there is a discontinuous microcanonical phase transition at $u_{\rm mic}$, with a jump in the dominant density ρ_1 and a drop in the microcanonical inverse temperature. This SSB transition is driven completely by entropy competitions between the microcanonical polarized (MP) phase and the disordered symmetric (DS) phase, and at $u_{\rm mic}$ the MP phase is hotter than the DS phase. These theoretical predictions for random graphs are verified by microcanonical Monte Carlo simulations. The

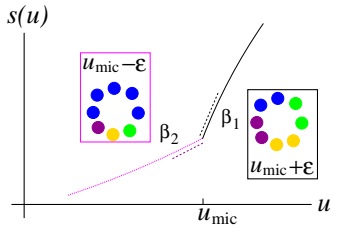

FIG. 1. Schematic drawing of kinked entropy density $s(u)$. As the energy density u of the Q-state Potts model decreases to $u_{\rm mic}$, $s(u)$ changes from concave to convex and its slope drops from β_1 to β_2. The system is color-symmetric at $u_{\rm mic} + \varepsilon$ ($\varepsilon \to 0$) with a lower microcanonical temperature $1/\beta_1$, but at $u_{\rm mic} - \varepsilon$ it has a highly dominant color and a higher microcanonical temperature $1/\beta_2$.

discontinuous SSB transition is also observed in three- and higher-dimensional bond-diluted lattices, but only for system sizes not too large [17]. The phenomenon of kinked entropy may persist in other multiple-state spin glass systems or combinatorial optimization problems [23]. Our work also adds new insight on the debate about ensemble inequivalence [24–27].

Mean field theory.—Consider a graph G formed by N vertices and M edges. Each vertex i has a discrete color $c_i \in \{1, 2, \ldots, Q\}$ and an edge (i, j) between vertices i and j has a ferromagnetic interaction energy $E_{ij}(c_i, c_j) = -\delta_{c_i}^{c_j}$, where $\delta_{c_i}^{c_j} = 1(0)$ if $c_i = c_j$ ($c_i \neq c_j$). The total energy of a color configuration $\boldsymbol{c} \equiv (c_1, c_2, \ldots, c_N)$ is the summed edge energies, $E(\boldsymbol{c}) = \sum_{(i,j)\in G} E_{ij}(c_i, c_j)$, which is symmetric with respect to color permutations. The partition function $Z(\beta)$ at a given inverse temperature β is

$$Z(\beta) \equiv \sum_{\boldsymbol{c}} e^{-\beta E(\boldsymbol{c})} = \sum_{\boldsymbol{c}} \prod_{(i,j)\in G} [1 + (e^{\beta} - 1)\delta_{c_i}^{c_j}]. \quad (1)$$

We now review the Bethe-Peierls theory for this model [23,28]. For simplicity we describe the theoretical equations for random regular (RR) graphs, which are maximally random except that every vertex has exactly K attached edges. (The mean field theory for general graphs can easily be derived following the cavity method of statistical physics [23,29] or through loop expansion of the partition function [30,31].) This theory is exact for tree graphs, and because random graphs are locally treelike (loop lengths diverge logarithmically with N) and there is no intrinsic frustration in the edge interactions, we expect it to be exact for RR graphs as well.

Without loss of generality we assume $c = 1$ to be the dominant (most abundant) color. To compute the marginal probability ρ_1 of this color state for a randomly chosen vertex i we first delete i and all its attached edges from the graph. Because short loops are rather rare in the graph, the K nearest neighbors of i will now be far separated in the perturbed cavity graph and consequently their color states will be independent. We denote by q ($\geq 1/Q$) the probability of such a neighboring vertex j to be in state $c_j = 1$ in the perturbed graph, and assume that vertex j has equal probability $(1 - q)/(Q - 1)$ to be in any of the other color states. When vertex i and its K edges are added back to the graph, its probability of being in state $c_i = 1$ is then

$$\rho_1 = \left[1 + (Q-1)\left(\frac{1 + (e^{\beta} - 1)\frac{1-q}{Q-1}}{1 + (e^{\beta} - 1)q}\right)^{K}\right]^{-1}. \quad (2)$$

This quantity ρ_1 is also the dominant color density of the RR graph. A similar expression for the cavity probability q of the neighboring vertex j can be written down (j has $K - 1$ edges in the cavity graph):

$$q = B(q) \equiv \left[1 + (Q-1)\left(\frac{1 + (e^{\beta} - 1)\frac{1-q}{Q-1}}{1 + (e^{\beta} - 1)q}\right)^{K-1}\right]^{-1}. \quad (3)$$

This self-consistent expression is referred to as a belief-propagation (BP) equation [32].

The free energy density $f \equiv -(1/N\beta)\ln Z(\beta)$ of the system can be computed by first summarizing the individual contributions of all the vertices, and then subtracting the individual contributions of all the edges (because each edge contributes to the free energies of two vertices) [23,29–31]. At a BP fixed point the explicit expression of f is

$$\begin{aligned} f = -\frac{1}{\beta}\ln\Bigg\{ & [1 + (e^{\beta} - 1)q]^{K} \\ & + (Q-1)\left[1 + (e^{\beta} - 1)\frac{1-q}{Q-1}\right]^{K}\Bigg\} \\ & + \frac{K}{2\beta}\ln\left[1 + (e^{\beta} - 1)\left(q^2 + \frac{(1-q)^2}{Q-1}\right)\right]. \end{aligned} \quad (4)$$

One can verify that $(\partial f/\partial q) = 0$ when $q = B(q)$. The mean energy density u is obtained from Eq. (4) as

$$u \equiv \frac{\partial(\beta f)}{\partial \beta} = -\frac{K}{2}\frac{e^{\beta}(q^2 + \frac{(1-q)^2}{Q-1})}{1 + (e^{\beta} - 1)(q^2 + \frac{(1-q)^2}{Q-1})}. \quad (5)$$

The entropy density s of the system is then determined by $s = \beta(u - f)$ [28].

The BP equation (3) always has a trivial fixed point $q = 1/Q$ which corresponds to the disordered symmetric phase with all the colors being equally abundant [17]. This fixed point becomes unstable with respect to the iteration $q^{t+1} \leftarrow B(q^t)$ when $\beta > \beta_{\mathrm{DS}} \equiv \ln[1 + Q/(K - 2)]$. For $K \geq 3$ and $Q \geq 3$, Eq. (3) has a stable fixed point with q and ρ_1 strictly larger than $1/Q$ at $\beta > \beta_{\mathrm{CP}}$, which corresponds to the canonical polarized phase of broken color symmetry. Here β_{CP} ($< \beta_{\mathrm{DS}}$) is the lowest inverse temperature at which the *CP* phase becomes possible. The *CP* and DS phases have equal free energy density at a critical inverse temperature $\beta_{\mathrm{c}} \in (\beta_{\mathrm{CP}}, \beta_{\mathrm{DS}})$, so an equilibrium phase transition occurs at β_{c}, with a sudden drop in energy density u [17].

Microcanonical SSB.—For $\beta \in (\beta_{\mathrm{CP}}, \beta_{\mathrm{DS}})$ the BP equation (3) has another fixed point which is unstable with respect to $q^{t+1} \leftarrow B(q^t)$ [17]. This fixed point is usually neglected because its free energy is higher than those of the DS and *CP* phases [Fig. 2(a)]. But we find that it reveals a discontinuous microcanonical phase transition between the DS phase and a new microcanonical polarized phase of the configuration space.

Plotting the predicted thermodynamic values of the MP fixed point [Fig. 2(b)], we observe that while q and ρ_1 are monotonic functions of β as anticipated, the energy density u and entropy density s both are nonmonotonic. This

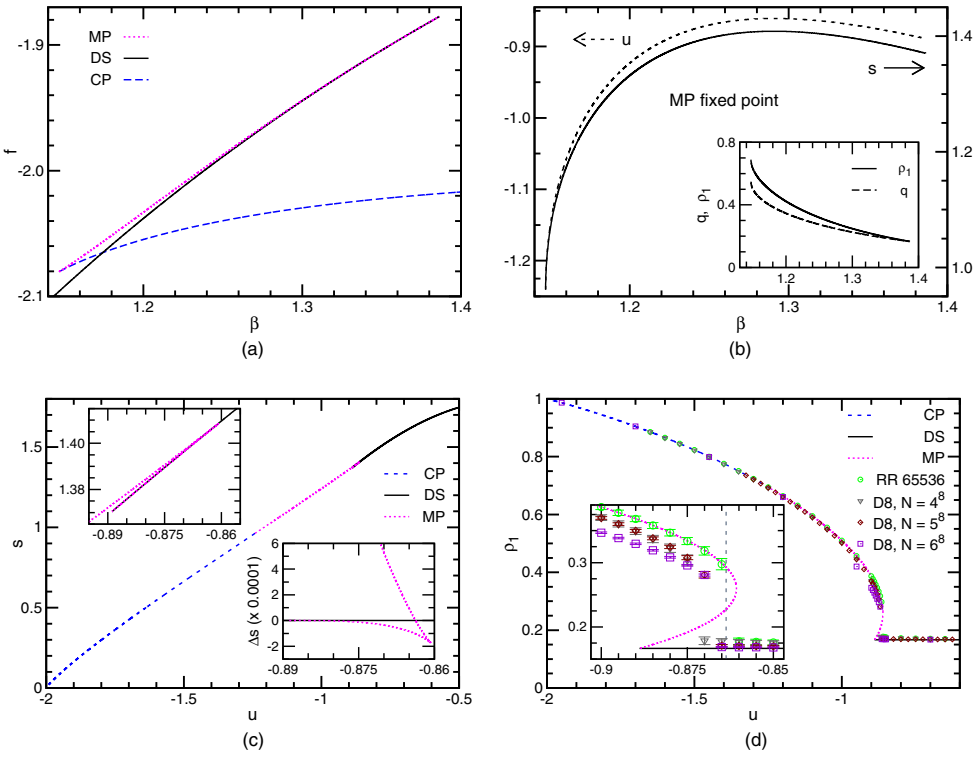

FIG. 2. Potts model on regular random graphs, $K = 4$ and $Q = 6$. (a) Free-energy densities $f(\beta)$ for the disordered symmetric (DS, solid line), the canonical polarized (CP, dashed line), and the microcanonical polarized (MP, dotted line) fixed points of the BP equation. The DS solution is stable at inverse temperature $\beta < \beta_{\rm DS} = 1.386$, the CP solution exists for $\beta \geq \beta_{\rm CP} = 1.147$, and the DS-CP phase transition occurs at $\beta_{\rm c} = 1.174$ with the energy density u dropping from -0.786 to -1.523. (b) Energy density $u(\beta)$, entropy density $s(\beta)$, fixed-point value $q(\beta)$, and density $\rho_1(\beta)$ of the dominant color (inset), for the MP fixed point. The maximal achievable MP energy density is $u_{\rm max} = -0.861$. (c),(d) Entropy density s and dominant color density ρ_1 vs energy density u for the DS (solid line), MP (dashed line), and CP (dotted line) fixed points. Upper-left and lower-right insets of (c) show an enlarged view of the MP entropy profile and the difference Δs between the MP and DS entropy density values ($\Delta s = 0$ at energy density $u_{\rm mic} = -0.864$). Symbols in (d) are microcanonical Monte Carlo simulation results obtained on a single RR graph ($N = 65536$) and several bond-diluted eight-dimensional periodic hypercubic lattices of side length $L = 4, 5, 6$ (D8, $N = L^8$), degree $K = 4$ and $Q = 6$. The inset of (d) is an enlarged view of the transition region, and the phase transition point $u_{\rm mic}$ for RR graphs is marked by the vertical dashed line, at which ρ_1 jumps from $1/6$ to 0.293.

surprising feature of u and s leads to the two-branched entropy profile shown in the upper-left inset of Fig. 2(c). These two entropy branches merge and stop at $u_{\rm max}$, which is the maximal achievable energy density of the MP phase. The entropy of the lower MP branch is slightly lower than that of the DS phase so this branch has no physical significance. On the other hand, the entropy of the upper MP branch exceeds that of the DS phase as u decreases below certain critical value $u_{\rm mic}$ which is strictly lower than $u_{\rm max}$, indicating the system will jump from the color-symmetric phase to a color-symmetry-broken MP phase which is stable only in the microcanonical ensemble. The dominant color density ρ_1 at $u_{\rm mic}$ is strictly higher than $1/Q$, so the spontaneous breaking of color symmetry is a discontinuous emerging phenomenon. Notice that at u slightly below $u_{\rm mic}$ the entropy density of the MP phase is higher than that of the DS phase.

Because the entropy densities of the DS and MP phases are equal at $u = u_{\rm mic}$ but have different slopes [Fig. 2(c)], the system's entropy density function $s(u)$ is not C^1 continuous but is kinked at $u_{\rm mic}$ [17]. Since the microcanonical inverse temperature is equal to the first derivative of $s(u)$, $\beta \equiv [{\rm d}s(u)/{\rm d}u]$ [28], there will be a sudden drop of the microcanonical β and an associated sudden drop of the free energy density f ($=u - \beta s$) as the system changes from the DS to the MP phase at $u_{\rm mic}$. In other words, at $u_{\rm mic}$ the partially ordered MP phase is hotter than the disordered symmetric phase and has a lower free energy density. This peculiar feature of $s(u)$ is qualitatively different from the recently discussed entropy inflection phenomenon, which is associated with the vanishing of the second-order derivative of $s(u)$ [22].

We have checked that as long as $Q \geq 3$, the discontinuous SSB phenomenon holds for all the RR graph ensembles of degree $K \geq 3$. As demonstrated in Table I, at each fixed value of Q the ρ_1 and β gaps at $u_{\rm mic}$ both decrease with degree K (and vanish gradually as $K \to \infty$ [17]). The discontinuous microcanonical phase transition will also

TABLE I. The critical energy density $u_{\rm mic}$, the jump $\Delta\rho_1$ of the dominant color density, and the drop $\Delta\beta$ of the microcanonical inverse temperature at $u_{\rm mic}$, for the Q-state Potts model on RR graphs of degree K.

K	Q	$u_{\rm mic}$	$\Delta\rho_1$	$\Delta\beta$	K	Q	$u_{\rm mic}$	$\Delta\rho_1$	$\Delta\beta$
3	3	−0.997	0.065	−0.012	5	3	−1.248	0.040	−0.007
	4	−0.929	0.109	−0.035		4	−1.085	0.071	−0.022
	5	−0.884	0.138	−0.058		5	−0.984	0.092	−0.040
	6	−0.852	0.158	−0.079		6	−0.913	0.108	−0.059
	7	−0.827	0.171	−0.099		7	−0.860	0.119	−0.076
	8	−0.807	0.182	−0.116		8	−0.819	0.127	−0.093
	9	−0.790	0.189	−0.132		9	−0.785	0.133	−0.109
	10	−0.776	0.195	−0.146		10	−0.757	0.138	−0.124
4	3	−1.108	0.049	−0.009	6	3	−1.398	0.033	−0.005
	4	−0.991	0.085	−0.028		4	−1.192	0.061	−0.018
	5	−0.916	0.110	−0.048		5	−1.065	0.081	−0.034
	6	−0.864	0.126	−0.069		6	−0.977	0.095	−0.050
	7	−0.824	0.139	−0.088		7	−0.911	0.105	−0.067
	8	−0.792	0.147	−0.105		8	−0.861	0.113	−0.083
	9	−0.766	0.154	−0.121		9	−0.820	0.119	−0.098
	10	−0.745	0.159	−0.136		10	−0.786	0.124	−0.112

occur in an extended Potts model with additional kinetic energies [17].

Monte Carlo simulations.—We carry out microcanonical Monte Carlo (MC) simulations to check the theoretical predictions. There are many discussions on microcanonical MC methods [13,15,16,33–35], and here we employ the simple demon method [33] to draw a set of independent configurations which are located slightly below a prescribed objective energy level $E_{\rm o}$. Starting from an initial configuration $\boldsymbol{c}$ of energy $E \le E_{\rm o}$, an elementary MC step unfolds as follows: (1) pick a vertex i uniformly at random and change its color c_i to a uniformly random new value c_i' ($\neq c_i$); (2) accept this color change if the energy E' of the resulting new configuration satisfies $E' \le E_{\rm o}$, otherwise keep the old color c_i; (3) increase the evolution time t by a tiny amount $1/N$ (one unit time therefore corresponds to N single-flip trials). This MC dynamics obeys detailed balance, so the sampled color configurations all have the same statistical weight. The simulation results obtained on a large RR graph instance are shown in Fig. 2(d) ($K = 4$, $Q = 6$). We indeed observe a discontinuous transition at the predicted critical energy density $u_{\rm mic}$. The numerical results on the dominant color density ρ_1 also agree perfectly with theory. The predicted inverse temperature gap $\Delta\beta$ is also quantitatively confirmed by computer simulations [17].

We also consider bond-diluted D-dimensional hypercubic lattices of side length L with periodic boundary conditions ($N = L^D$). By keeping only K bonds in a maximally random manner for every vertex (see [17] for construction details), the shortest loops passing through the vertices rapidly increase their lengths as K decreases and D increases, and the diluted lattice is locally resembling a random graph [36]. A discontinuous SSB transition is observed in the MC dynamics for such bond-diluted lattice systems at high dimensions [e.g., $D = 8$, Fig. 2(d)] and also at the physical dimension $D = 3$ [17]. However, unlike the case of truly random graphs, we expect that the SSB transition in these lattice systems will become continuous in the thermodynamic limit [17], because phase separation is deemed to occur as the system size L becomes sufficiently large [18–21].

Conclusion.—In summary, we predicted and confirmed a discontinuous microcanonical SSB phase transition in the Q-state Potts model on random graphs. Such a discontinuous transition was also observed in bond-diluted finite-size lattice systems (even down to three dimensions [17]). In the future we need to investigate the geometric property of the configurations in the MP phase (e.g., the possibility of a percolating cluster of connected same-color vertices) [20], and possible latent structures prior to the microcanonical transition [37,38], and to study systematically the microcanonical SSB transition in finite-dimensional finite-size systems and the associated inequivalence between the microcanonical and the canonical ensembles [24–27]. The discovered property of kinked entropy may be a general feature of random graphical models with a canonical discontinuous phase transition, and it may have important computational consequences in optimization tasks [23].

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