Discontinuous Spontaneous-Symmetry-Breaking in the Microcanonical Ensemble

Hai-Jun Zhou\textsuperscript{1,2} \\
\textsuperscript{1}CAS Key Laboratory for Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China \\
\textsuperscript{2}School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China \\
\textit{(Dated: January 23, 2019)}

Spontaneous-symmetry-breaking (SSB) is a macroscopic collective phenomenon occurring at phase transitions. Although deep understanding of SSB in the canonical statistical ensemble has been achieved, SSB in the microcanonical ensemble (with energy being the control parameter) has rarely been discussed. Here we study microcanonical SSB on the paradigmatic \(Q\)-state Potts model \((Q \geq 3)\). The Bethe-Peierls mean field theory predicts a discontinuous phase transition in regular random graphs as the result of entropy competition at fixed energy between the disordered symmetric phase and the microcanonical polarized phase, with a jump in the density of the dominant color and a jump in the microcanonical temperature. This discontinuous SSB is confirmed by microcanonical Monte Carlo simulations, and our simulation results further suggest that it will also occur in finite-dimensional bond-diluted lattice systems.

Spontaneous-symmetry-breaking (SSB) is a fundamental concept of physics [1]. This intuitive physical picture is underlying 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. In the statistical physics community a widely adopted theoretical paradigm for studying 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 of the Potts model in the canonical ensemble, with the environmental inverse temperature \(\beta\) being the control parameter, has been extensively studied in the literature (see, e.g., Refs. [5][11] for some of the recent interesting results). This transition is driven by competition between energy and entropy. When \(\beta\) is sufficiently low the system is in the disordered phase with all the \(Q\) colors being equally abundant, and entropy wins over energy. At a critical inverse temperature \(\beta_c\), however, energy starts to be more important than entropy and color symmetry breaks spontaneously to reduce energy. This SSB transition is continuous if \(Q = 2\) (the Ising model) or if the graph is a low-dimensional lattice and \(Q\) is small [3][4]. When \(Q\) is moderate or large the SSB transition is a discontinuous phenomenon, characterized by an abrupt increase in the density \(\rho_1\) of the dominant color and an extensive drop in the energy of the system [3].

In the present work we investigate the microcanonical Potts model for which the energy is the control parameter [12][15]. What will happen during the SSB process if the energy of the system is only allowed to fluctuate slightly around certain fixed level? This question has rarely been discussed in the literature. Since the energy density is serving as a continuously changing control parameter, a naïve guess would be a continuous deviation of the order parameter (the dominant color density) \(\rho_1\) from the value \(1/Q\) at certain critical energy density. This simple picture is indeed confirmed by rigorous analytical results in the limiting case of a complete graph, which prove that SSB in the microcanonical ensemble is always a continuous process even though it is generally discontinuous in the canonical ensemble [16]. But for Potts model defined on finite-connectivity random graphs, we find that the Bethe-Peierls mean field theory predicts a discontinuous microcanonical SSB phase transition for any \(Q \geq 3\), with a jump in the density of the dominant color and a drop in the microcanonical inverse temperature. Since energy is fixed at the transition this SSB is driven completely by entropy effect. The partially ordered microcanonical SSB phase starts to have higher entropy than the disordered color-symmetric phase as the energy density decreases from the critical value \(u_{\text{mic}}\). Our microcanonical Monte Carlo simulation results confirm the existence of this discontinuous phase transition in random graphs, and they give strong evidence that the same phenomenon will also occur in finite-dimensional bond-diluted lattice systems. Our work calls for more theoretical efforts on microcanonical SSB.

\textit{Mean field theory}.— Consider a graph \(G\) formed by \(N\) vertices and \(M\) edges between some of these vertices. Each vertex \(i\) has a discrete color \(c_i \in \{1,2,\ldots,Q\}\) and each 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 \(E(c)\) for a color configuration \(c \equiv (c_1,c_2,\ldots,c_N)\) of the graph is simply the summed edge energies, \(E(c) = \sum_{(i,j) \in G} E_{ij}(c_i,c_j)\). This Potts system has \(Q\) degenerate ground states at the minimum energy level \(-M\). The partition function \(Z(\beta)\) at a given inverse temperature \(\beta\) is

\[
Z(\beta) \equiv \sum_c e^{-\beta E(c)} = \sum_c \prod_{(i,j) \in G} \left[1 + (e^\beta - 1)\delta_{c_i c_j}\right]. \tag{1}
\]

We now review the Bethe-Peierls mean field theory for this model [17][18]. For simplicity we describe the theoretical equations for random regular (RR) graphs \(G\),...
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 [18, 19] or through loop expansion of the partition function [20 21].) This mean-field theory is exact for tree graphs, and because random graphs are locally tree-like (loop lengths diverge logarithmically with $N$) and there is no intrinsic frustration in the edge interactions, we expect it to be exact for the RR graph systems as well.

Without loss of generality we assume $c = 1$ to be the dominant (most abundant) color in the system. To compute the marginal probability $\rho_1$ 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 extremely 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 $q (\geq \frac{1}{2})$ 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 ($= \frac{1-q}{Q-1}$) 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

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

This quantity $\rho_1$ is also the dominant color density of the RR graph. A very 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):

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

In the literature this self-consistent expression is referred to as a belief-propagation (BP) equation [22].

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 individual free energies of two vertices) [18 21]. At a BP fixed point the explicit expression of $f$ is

$$f = -\frac{1}{\beta} \ln \left[1 + (e^\beta - 1)q\right]^K + (Q - 1)[1 + (e^\beta - 1)\frac{1-q}{Q-1}]^K$$

$$+ \frac{K}{2\beta} \ln \left[1 + (e^\beta - 1)(q^2 + \frac{(1-q^2)}{Q-1})\right].$$  \hspace{1cm} (4)

It can be checked that $\frac{\partial f}{\partial q} = 0$ when $q = B(q)$. The explicit expression for the mean energy density $u$ is obtained from Eq. (3) as

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

And the entropy density $s$ of the system is computed simply through the expression $s = \beta(u - f)$ [17].

The BP equation (3) always has a trivial fixed point $q = \frac{1}{Q}$, which corresponds to the disordered symmetric (DS) phase in which all the $Q$ colors are equally abundant (Fig. 1(a), but this fixed point becomes unstable with respect to the iteration $q^{t+1} \leftarrow B(q^t)$ when $\beta > \beta_{DS} \equiv \ln(1 + \frac{Q}{Q-1})$. For $K \geq 3$ and $Q \geq 3$, Eq. (3) has a stable fixed point with $q$ strictly larger than $\frac{1}{Q}$ at $\beta > \beta_{CP}$ which corresponds to the canonical polarized (CP) phase of broken color symmetry ($\rho_1$ is much larger than $\frac{1}{Q}$). Here $\beta_{CP} < \beta_{DS}$ is the lowest inverse temperature at which the CP phase becomes possible. The free energy densities of the CP and DS phases become equal at certain critical inverse temperature $\beta_c \in (\beta_{CP}, \beta_{DS})$. 

![FIG. 1: The $Q=6$ Potts model in the canonical ensemble, for $K=4$ regular random graphs. (a) The fixed points of the BP equation (3) are the intersection points of the curve $B(q)$ and the dashed diagonal line. Depending on the inverse temperature $\beta$ there might be one, two, or three fixed points. (b) The 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. (c) The energy density $u(\beta)$, the entropy density $s(\beta)$, the fixed-point value $q(\beta)$ and the density $\rho_1(\beta)$ of the dominant color (inset), for the MP fixed point.](image-url)
so an equilibrium phase transition occurs at $\beta_c$ which is associated with a sudden drop in energy density $u$. For $K = 4$ and $Q = 6$ we have $\beta_{CP} = 1.147$, $\beta_{\Delta S} = 1.174$, $\beta_{DS} = 1.386$ (Fig. 1(b)), and at $\beta_c$ the energy densities of the two phases are $u_{DS} = -0.786$ and $u_{CP} = -1.523$.

Microcanonical SSB.--- For $\beta \in (\beta_{CP}, \beta_{DS})$ the BP equation (3) has also a middle fixed point (Fig. 1(a)). This fixed point is usually neglected as unphysical and irrelevant because it is unstable with respect to the iteration $q^{t+1} \leftarrow B(q^t)$ and its free energy is higher than those of the DS and CP phases (Fig. 1(b)). But it turns out that this fixed point holds the key to understanding SSB in the microcanonical ensemble, and it indeed reveals the existence of a new phase of the configuration space, the microcanonical polarized (MP) phase.

Plotting the predicted thermodynamic values of the MP fixed point in Fig. 1(c) we observe that while $q$ and $\rho_1$ are monotonic functions of $\beta$ as anticipated, the energy density $u$ and entropy density $s$ both are non-monotonic. This surprising feature of $u$ and $s$ is totally unexpected and it leads to the two-branched entropy profile as illustrated in the upper-left inset of Fig. 2(a). These two entropy branches merge and stop at $u_{\text{max}}$, which is the maximal achievable energy density of the MP fixed point ($u_{\text{max}} = -0.861$ for $K = 4, Q = 6$). The entropy of the lower MP branch is 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 the energy density decreases below certain critical value $u_{\text{mic}}$ which is strictly lower than $u_{\text{max}}$ ($u_{\text{mic}} = -0.864$ for $K = 4, Q = 6$), indicating the system will jump from the color-symmetric disordered phase to a color-symmetry-broken MP phase which is stable only in the microcanonical ensemble. The dominant color density $\rho_1 (= 0.293$ for $K = 4, Q = 6$) at $u_{\text{mic}}$ is strictly higher than $u_{\text{mic}}$, so the spontaneous breaking of color symmetry is a discontinuous emerging phenomenon. Notice that at $u$ slightly below $u_{\text{mic}}$ the entropy density of the MP phase is higher than that of the DS phase. In other words, order enhances disorder.

Another major aspect of this SSB transition is that the entropy density function $s(u)$ of the system is continuous but has a kink at $u = u_{\text{mic}}$. This is because the entropy densities of the DS and MP phases are equal at $u = u_{\text{mic}}$ but have different slopes (Fig. 2(a), lower-right inset). Since the microcanonical inverse temperature is equal to the first derivative of the entropy density (i.e., $\beta = \left. \frac{ds}{du} \right|_{u_{\text{mic}}}$) [17], as the system changes from the DS phase to the MP phase at $u_{\text{mic}}$, there will be a sudden drop of the microcanonical inverse temperature and an associated sudden drop of the free energy density $f (= u - \beta s)$. In other words, at $u_{\text{mic}}$ the partially ordered MP phase is strictly hotter than the disordered symmetric phase and has strictly lower free energy density. This peculiar kink feature of the entropy density $s(u)$ is qualitatively different from the recently discussed entropy inflection phenomenon, which is associated with the vanishing of the second-order derivative of $s(u)$ [23]. For the Potts model the entropy inflection point is located at the boundary between the MP and CP phase, at which the microcanonical inverse temperature is equal to $\beta_{CP}$ (Fig. 2(a)).

As long as $Q \geq 3$ the discontinuous SSB phenomenon holds generally for all the RR graph ensembles of degree $K \geq 3$. At each value of $K$ the phase transition point $u_{\text{mic}}$ and the gaps of $\rho_1$ and $\beta$ at $u_{\text{mic}}$ all increase with $Q$, see Table 1. When there are only two colors ($Q = 2$) the microscopic SSB becomes a continuous process and

---

FIG. 2: Entropy density $s$ and dominant color density $\rho_1$ versus energy density $u$, for the disordered symmetric (DS, solid line), microcanonical polarized (MP, dashed line), and canonical polarized (CP, dotted line) BP fixed points. (a) and (b): $K = 4, Q = 6$; (c) $K = 6, Q = 10$. Upper-left and lower-right insets of (a) show an enlarged view of the MP entropy profile and the difference $\Delta s$ between the MP and DS entropy density values. Symbols in (b) and (c) are microcanonical Monte Carlo (MC) simulation results obtained on a single RR graph (circles, $N = 65536$), a bond-diluted eight-dimensional (8D) hypercubic lattice with periodic boundary conditions (diamonds, $N = 4^8 = 65536$), and the full three-dimensional (3D) cubic lattice with periodic boundary conditions (crosses, $N = 40 \times 40 \times 41 = 65600$). The inset of (b) shows the jumping behavior of the densities $\rho_c$ of three colors $c = 1, 2, 3$ with MC evolution time $t$ at fixed energy density $u = -0.870$, obtained on a smaller RR graph of size $N = 10000$ and degree $K = 4$. The dashed vertical lines in (b) and (c) denote the predicted microcanonical phase transition point for RR graphs, and the inset of (c) is an enlarge of the phase transition region.
There are many different microcanonical models on RR graphs of degree $K$. Monte Carlo simulations.— We carry out microcanonical Monte Carlo (MC) simulations to check the theoretical predictions. There are many different microcanonical MC methods (see, e.g., Refs. [12, 14, 15, 21, 20], here we employ a simple single-vertex color flipping MC dynamics to draw a set of independent configurations located on a prescribed objective energy level $E_o$. (The same numerical results are obtained following the more conventional demon method [24].) Starting from an initial color configuration $c$ of energy $E_o$, 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) compare the total energy $E'$ of the resulting new configuration with $E_o$, and with the energy $E$ of the old configuration, and accept the color change $c_i \rightarrow c'_i$ if one of the following conditions is satisfied: (a) $E = E'$ or (b) $E \geq E_o$ and $E' < E_o$ or (c) $E < E_o$ and $E' \geq E_o$, otherwise keep the old color $c_i$; (3) increase the MC evolution time $t$ by a tiny amount $\frac{1}{N}$ (one unit time of this MC dynamics corresponds to $N$ single-flip trials). This MC dynamics only allows the configuration energy to fluctuate very slightly around $E_o$, and it obeys detailed balance so the sampled color configurations are guaranteed to have the same statistical weight.

The simulation results obtained by our MC algorithm on two RR graph instances of size $N = 65536$ are shown in Figs. [2(b)] for $K = 4$, $Q = 6$ and Fig. [2(c)] for $K = 6$, $Q = 10$. We indeed observe a discontinuous phase transition at the predicted critical energy density value $u_{mic}$. The numerical results on the relative abundance $\rho_1$ of the dominant color at $u < u_{mic}$ also agree perfectly with theory. We also observe that if the energy density is only slightly below $u_{mic}$ the dominant color changes with time in a random but collective way (Fig. [2(b) inset), but the waiting time needed for such a spontaneous switch increases quickly with $N$.

We also study finite-dimensional lattice systems by the microcanonical MC algorithm. Some representative simulation results obtained on $D$-dimensional periodic hypercubic lattices are shown in Fig. [2] If $D$ is large (e.g., $D = 8$) and a large fraction of the bonds in the lattice are randomly deleted to reduce the degree of each vertex from $2D$ to $K$, a marked discontinuity in the dominant color density $\rho_1$ is observed as the energy density is decreased to the critical value $u_{mic}$ predicted by the mean field theory. We have checked that the position and the magnitude of the $\rho_1$ jump do not change with the system size $N$, so the discontinuous behavior is unlikely to be a finite-size effect. When the energy density $u$ is further decreased to be considerably below $u_{mic}$, we observe that the dominant color density values $\rho_1$ of the diluted lattice system are almost identical to the corresponding theoretical values in the low-energy region of the MP phase.

For the full hypercubic lattice system without bond dilution (so $K = 2D$), however, our simulation results show that the microcanonical phase transition is continuous (Fig. [2(c)]. This observation is consistent with the droplet theory [27–29] and also with the complete-graph rigorous results (which correspond to $K, D \rightarrow \infty$) [19]. The dominant color density $\rho_1$ increases from $\frac{1}{2}$ almost linearly as the energy density $u$ decreases from the critical value $u_{mic}$, before it finally touches the theoretical CP curve, indicating the coexistence of the DS and CP phases for the intermediate energy density values [12, 27–29].

Outlook.— The Bethe-Peiers mean field theory predicted a discontinuous microcanonical SSB in the random-graph Potts model, and it was confirmed by microcanonical MC simulations. Furthermore, our simulation results suggest that such a discontinuous phase transition will also occur in finite-dimensional diluted lattice systems. Many interesting questions remain to be explored, for example: (1) Why the unstable BP fixed point, corresponding to the canonical free-energy maximum, give physically meaningful results about the microcanonical ensemble? (2) Why and how the color symmetry breaks abruptly at certain critical energy density? Are there precursor community structures similar to those discussed in Refs. [30, 31] hidden in the configuration space before this discontinuous SSB? (3) How to rigorously prove the existence of a discontinuous microcanonical SSB in finite-dimensional diluted lattice systems? And what is the maximum allowed vertex degree $K$ at a given dimensionality $D$? This work may stimulate more theoretical efforts on understanding microcanonical SSB.

The following funding supports are acknowledged: National Natural Science Foundation of China Grants No. 11421063 and No. 11747601; the Chinese Academy of Sciences Grant No. QYZDJ-SSW-SYS018.) Numeri-

| $K$ | $Q$ | $u_{mic}$ | $\Delta \rho_1$ | $\Delta \beta$ |
|-----|-----|---------|-------------|------------|
| 3   | 1   | 0.997   | -0.012      | 0.003      |
| 4   | 1   | 0.929   | -0.035      | 0.040      |
| 5   | 1   | 0.884   | -0.058      | 0.040      |
| 6   | 1   | 0.852   | -0.079      | 0.040      |
| 7   | 1   | 0.827   | -0.009      | 0.076      |
| 8   | 1   | 0.807   | -0.116      | 0.093      |
| 9   | 1   | 0.790   | -0.132      | 0.109      |
| 10  | 1   | 0.776   | -0.146      | 0.124      |

Legend: In the table, $u_{mic}$ denotes the critical energy density, $\Delta \rho_1$ denotes the jump in the dominant color density, and $\Delta \beta$ denotes the drop in the inverse temperature.
tical simulations were carried out at the HPC cluster of ITP-CAS and also at the Tianhe-2 platform of the National Supercomputer Center in Guangzhou. The author thanks Youjin Deng, Gaoke Hu, Hao Hu, Shaomeng Qin, Mutian Shen, and Jinhua Zhao for helpful discussions and/or valuable comments on the manuscript.

[1] K. Brading, E. Castellani, and N. Teh. Symmetry and symmetry breaking. In E. N. Zalta, editor, *The Stanford Encyclopedia of Philosophy*. Metaphysics Research Lab, Stanford University, winter 2017 edition, 2017.

[2] R. B. Potts. Some generalized order-disorder transformations. *Proc. Cambridge Phil. Soc.*, 48:106–109, 1952.

[3] F. Y. Wu. The Potts model. *Rev. Mod. Phys.*, 54:235–286, 1982.

[4] R. J. Baxter. *Exactly Solved Models in Statistical Mechanics*. Academic Press, London, UK, 1982.

[5] V. Gorbenko, S. Rychkov, and B. Zan. Walking, weak first-order transitions, and complex cfts ii. two-dimensional Potts model at q > 4. *SciPost Phys.*, 5:050, 2018.

[6] H. W. J. Blöte, W. Guo, and M. P. Nightingale. Scaling in the vicinity of the four-state Potts fixed point. *J. Phys. A: Math. Theor.*, 50:324001, 2017.

[7] H. Hu and Y. Deng. Universal critical wrapping probabilities in the canonical ensemble. *Nuclear Phys. B*, 898:157–172, 2015.

[8] S. Wang, Z.-Y. Xie, J. Chen, B. Normand, and T. Xiang. Phase transitions of ferromagnetic Potts model on the simple cubic lattice. *Chinese Phys. Lett.*, 31:070503, 2014.

[9] L. Tian, H. Ma, W. Guo, and L.-H. Tang. Phase transitions of the q-state Potts model on multiply-laced sierpinski gaskets. *Eur. Phys. J. B*, 86:197, 2013.

[10] Q. N. Chen, M. P. Qin, J. Chen, Z. C. Wei, H. H. Zhao, B. Normand, and T. Xiang. Partial order and finite-temperature phase transitions in Potts models on irregular lattices. *Phys. Rev. Lett.*, 107:165701, 2011.

[11] Y. Deng, Y. Huang, J. L. Jacobsen, J. Salas, and A. D. Sokal. Finite-temperature phase transition in a class of four-state Potts antiferromagnets. *Phys. Rev. Lett.*, 107:150601, 2011.

[12] D. H. E. Gross, A. Ecker, and X. Z. Zhang. Microcanonical thermodynamics of first order phase transitions studied in the Potts model. *Ann. Physik*, 508:446–452, 1996.

[13] D. H. E. Gross. Microcanonical thermodynamics and statistical fragmentation of dissipative systems: The topological structure of the n-body phase space. *Phys. Reports*, 279:119–201, 1997.

[14] V. Martin-Mayor. Microcanonical approach to the simulation of first-order phase transitions. *Phys. Rev. Lett.*, 98:137207, 2007.

[15] F. Moreno, S. Davis, C. Loyola, and J. Peralta. Ordered metastable states in the Potts model and their connection with the superheated solid state. *Physica A*, 509:361–368, 2018.

[16] Details given in the appendices.

[17] K. Huang. *Statistical Mechanics*. John Wiley, New York, second edition, 1987.

[18] M. Mézard and A. Montanari. *Information, Physics, and Computation*. Oxford Univ. Press, New York, 2009.

[19] M. Mézard, G. Parisi, and M. A. Virasoro. *Spin Glass Theory and Beyond*. World Scientific, Singapore, 1987.

[20] J.-Q. Xiao and H. J. Zhou. Partition function loop series for a general graphical model: free-energy corrections and message-passing equations. *J. Phys. A: Math. Theor.*, 44:425001, 2011.

[21] H. J. Zhou and C. Wang. Region graph partition function expansion and approximate free energy landscapes: Theory and some numerical results. *J. Stat. Phys.*, 148:513–547, 2012.

[22] J. Pearl. *Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference*. Morgan Kaufmann, San Francisco, CA, USA, 1988.

[23] Y.-Z. Xu, C. H. Yeung, H.-J. Zhou, and D. Saad. Entropy inflection and invisible low-energy states: Defensive alliance example. *Phys. Rev. Lett.*, 121:210602, 2018.

[24] M. Creutz. Microcanonical monte carlo simulation. *Phys. Rev. Lett.*, 50:1411–1414, 1983.

[25] K.-C. Lee. Rejection-free monte carlo technique. *J. Phys. A: Math. Gen.*, 28:4835–4842, 1995.

[26] P. Schierz, J. Zierenberg, and W. Janke. First-order phase transitions in the real microcanonical ensemble. *Phys. Rev. E*, 94:021301(R), 2016.

[27] M. Biskup, L. Chayes, and R. Kotecký. On the formation/dissolution of equilibrium droplets. *Europhys. Lett.*, 60:21–27, 2002.

[28] K. Binder. Theory of the evaporation/condensation transition of equilibrium droplets in finite volumes. *Physica A*, 319:99–114, 2003.

[29] T. Nogawa, N. Ito, and H. Watanabe. Evaporation-condensation transition of the two-dimensional Potts model in the microcanonical ensemble. *Phys. Rev. E*, 84:061107, 2011.

[30] H. J. Zhou and H. Ma. Communities of solutions in single solution clusters of a random k-satisfiability formula. *Phys. Rev. E*, 80:066108, 2009.

[31] H. J. Zhou and C. Wang. Ground-state configuration space heterogeneity of random finite-connectivity spin glasses and random constraint satisfaction problems. *J. Stat. Mech.: Theor. Exp.*, page P10010, 2010.
Appendix A: Exact results for complete graphs

Consider a complete graph in which every vertex interacts with every other vertex. The energy of a color configuration \( \mathbf{c} = (c_1, c_2, \ldots, c_N) \) is

\[
E(\mathbf{c}) = -\frac{1}{N} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \delta_{c_i}^c \delta_{c_j}^c, \tag{6}
\]

where the rescaling factor \( \frac{1}{N} \) is introduced to make the total energy an extensive quantity. Suppose there are \( n_c \) vertices of color \( c \in \{1, 2, \ldots, Q\} \) in the configuration \( \mathbf{c} \), then the total energy can be rewritten as

\[
E(\mathbf{c}) = \frac{1}{2} - \frac{N}{2} \sum_{i=1}^{Q} \left( \frac{n_c}{N} \right)^2 = \frac{1}{2} - \frac{N}{2} \sum_{i=1}^{Q} x_c^2, \tag{7}
\]

where \( x_c = \frac{n_c}{N} \) is the density of color \( c \). In the thermodynamic limit of \( N \to \infty \) the energy density \( u \) is simply

\[
u = -\frac{1}{2} \sum_{c=1}^{Q} x_c^2. \tag{8}
\]

The total number of microscopic configurations corresponding to the coarse-grained state \((n_1, n_2, \ldots, n_Q)\) is \( \Omega(n_1, n_2, \ldots, n_Q) = \frac{N!}{n_1! n_2! \cdots n_Q!} \). In the thermodynamic limit then the entropy density \( s \) is

\[
 s = -\sum_{c=1}^{N} x_c \ln x_c. \tag{9}
\]

The task is now to find the values of \((x_1, x_2, \ldots, x_Q)\) which lead to the maximum of \( s \) under the constraints of fixed energy density \( u \) and fixed number \( N \) of vertices. This can be achieved by introducing a function \( z(x_1, \ldots, x_Q) \) with two Lagrange multipliers \( \lambda_1 \) and \( \lambda_2 \):

\[
z = -\sum_{c=1}^{N} x_c \ln x_c + \frac{\lambda_1}{2} \sum_{c=1}^{Q} x_c^2 + \frac{\lambda_2}{2} \sum_{c=1}^{Q} x_c. \tag{10}
\]

The first derivative of this function with \( x_c \) is \( \frac{\partial z}{\partial x_c} = -\ln x_c - 1 + \lambda_1 x_c + \lambda_2 \). Therefore, from the condition \( \frac{\partial z}{\partial x_c} = 0 \) we obtain that

\[
x_c = \frac{e^{\lambda_1 x_c}}{\sum_{c'=1}^{Q} e^{\lambda_1 x_c'}} \quad (c = 1, 2, \ldots, Q). \tag{11}
\]

The color-symmetric fixed-point solution of Eq. (11) is \( x_c = \frac{1}{Q} \) for all colors \( c \). The energy density of this solution is a constant, \( u_{DS} = -\frac{1}{2Q} \), and its entropy density is \( s_{DS} = \ln Q \). If the energy density \( u \) decreases from \( u_{DS} \), then color symmetry has to be broken. Therefore the critical energy density for spontaneous-symmetry-breaking (SSB) is simply \( u_{mic} = -\frac{1}{2Q} \).

The other fixed-point solutions of Eq. (11) can be characterized by two parameters, \( \rho_1 \) and \( m \). The real parameter \( \rho_1 \in \left[ \frac{1}{Q}, 1 \right] \) is the density of a dominant color, and the integer \( m \in \{1, 2, \ldots, Q-1\} \) is the number of dominant colors. Without loss of generality we assume that \( x_i = \rho_1 \) for \( i = 1, 2, \ldots, m \) and \( x_j = \frac{1-m \rho_1}{Q-m} \) for \( j = m+1, m+2, \ldots, Q \). At a fixed integer value of \( m \), the order parameter \( \rho_1 \) is expressed as

\[
 \rho_1 = \frac{1}{Q} + \sqrt{2 \left( \frac{1}{m} - \frac{1}{Q} \right) u_{mic} - u}. \tag{12}
\]

Notice that \( \rho_1 \) is a continuous function of energy density \( u \), so the SSB transition at \( u_{mic} \) must be a continuous phase transition (Fig. 3).

The entropy density \( s \) at the polarized fixed point of Eq. (11) is

\[
 s = -m \rho_1 \ln \rho_1 - (1 - m \rho_1) \ln \frac{1 - m \rho_1}{Q-m}, \tag{13}
\]

where \( \rho_1 \) is determined by Eq. (12). The parameter \( m \) should be set to integer value which maximize \( s \), which turns out to be \( m = 1 \) for all values of \( Q \). Therefore, in the SSB phase there is only one dominant color, and all the other colors are equally abundant in the system. We find that in the general case of \( Q \geq 3 \) the entropy density function \( s(u) \) is convex in the vicinity of \( u_{mic} \) (Fig. 3). This non-convex property means there is a discontinuous SSB phase transition in the canonical ensemble at certain critical value \( \beta \) of the inverse temperature.