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Cyclic Heating-Annealing and Boltzmann Distribution of Free Energies in a Spin-Glass System

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Abstract *Ergodicity of a spin-glass is broken at low temperatures; the system is trapped in one of many ergodic configurational domains. Transitions between different ergodic domains are achievable through a heating-annealing procedure. If this experiment is repeated infinite times, all ergodic configurational domains will be visited with frequences that decreasing exponentially with their free energies. The mean free energy density of a spin-glass system on a random graph is calculated based on this free energy Boltzmann distribution in the present work, by means of the cavity approach.*

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Spin-glasses are simple models of complex frustrated systems. In a spin-glass, there exist both ferromagnetic and antiferromagnetic spin-spin interactions, which are distributed randomly in the system.[1] Because different spins of the system face different local environments, at low temperatures their spontaneous magnetizations will be different. Some spins have positive magnetic moments and others have negative ones, while the system as a whole has no spontaneous magnetization. More significantly, at low temperatures ergodicity is broken in a spin-glass. The configurational space of the system is split into many ergodic domains. Due to the existence of extremely high free energy barriers, the system can never spontaneously jump from one configurational domain to another different domain. (Hereafter, an ergodic configurational domain is referred to as a *macroscopic state* or *thermodynamic state*).

The existence of (infinitely) many order parameters and broken ergodicity make theoretical studies of spin-glasses very challenging. Concerning equilibrium properties, so far there are two major theoretical frameworks, the replica-symmetry-breaking (RSB) theory,[2,3] which is most suitable for studying infinite-connectivity models, and the cavity approach.[4,5] The later approach at the moment is equivalent to the first-step RSB theory,[5] it is still under development. Important issues include possible spin correlations among different vertices[6−8] and possible higher-level organizations of the configurational space.

In this paper, we study the low-temperature properties of spin-glasses from the angle of temperature heating and annealing. Although a spin-glass at low temperatures is not ergodic, when the system is first heated and then annealed to the original low temperature, it may escape from the old thermodynamic state and drop to another different state. If this heating-annealing experiment is repeated an infinite number of times, we anticipate that all macroscopic states will be visited by the system (albeit with different frequences). In other words, ergodicity at the macroscopic states level is recovered by this cyclic heating-annealing. This picture, in combination with the usual cavity approach of Mézard and Parisi,[5] enables us to calculate the mean free energy density of a spin-glass on a random graph; and we also discuss some possible extensions of the present work.

Heating-Aneaing At temperature T lower than the spin-glass transition temperature $T_{\rm sg}$, a spin-glass is in an ergodicity-broken phase. Each macroscopic state α of the system contains a set of microscopic spin configurations; its free energy F_α is defined through the following fundamental formula:

$$F_\alpha(N,\beta) = -\frac{1}{\beta}\ln\Big(\sum_{\vec{\sigma}\in\alpha} {\rm e}^{-\beta E(\vec{\sigma})}\Big)\,, \tag{1}$$

where N is the total number of spins in the system; $\beta = 1/T$ is the inverse temperature (Boltzmann's constant is set to unity); $\vec{\sigma} \equiv \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ denotes a microscopic configuration, and $E(\vec{\sigma})$ is the configurational energy. The total partition function by definition is $\mathcal{Z}(N,\beta) = \sum_{\vec{\sigma}} \exp\big(-\beta E(\vec{\sigma})\big)$. It can be expressed as a summation over all the macroscopic states α,

$$\mathcal{Z}(N,\beta) = \sum_\alpha \exp\big(-\beta F_\alpha(N,\beta)\big)\,. \tag{2}$$

Each macroscopic state α contributes a term ${\rm e}^{-\beta F_\alpha(N,\beta)}$ to the total partition function.

We need to explore different macroscopic states to fully characterize a spin-glass system. For the system to escape from a single macroscopic state α, we can first increase the temperature to be well above $T_{\rm sg}$. After the system has reached equilibrium at the ergodic high-temperature paramagnetic phase, we then decrease the temperature *extremely slowly* until the original low temperature T is reached again. During this annealing process, the system may relax to another different macroscopic state. If this heating-annealing cycle runs again and again, all the macroscopic states of the system at T will be visited many times. What is the probability that the system drops to a particular macroscopic state α in one round of the annealing experiment? Since ergodicity is recovered at the macroscopic states level through repeated heating-annealing, and since the system is in equilibrium at T, we conclude from Eq. (2) that macroscopic state α will be visited with frequence proportional to $\exp(-\beta F_\alpha)$. This is a

Boltzmann distribution of free energies over all the macroscopic states. In what follows, we will understand the total partition function of a spin-glass from this heating-annealing perspective.

At this point, we generalize Eq. (2) by defining a new partition function $\mathcal{Z}(N,\beta;y)$ through

$$\mathcal{Z}(N,\beta;y) \equiv \mathrm{e}^{-yG(N,\beta;y)} = \sum_{\alpha} \exp\bigl(-yF_{\alpha}(N,\beta)\bigr)\,, \quad (3)$$

where y is an artificial inverse temperature for the level of macroscopic states, and the grand free energy is $G(N,\beta;y) \equiv -(1/y)\ln\mathcal{Z}(N,\beta;y)$. (A re-weighting parameter y was previously introduced in Ref. [9] for spin-glasses at exactly zero temperature). The probability of staying in macroscopic state α is then

$$p_{\alpha}(\beta;y) = \frac{\mathrm{e}^{-yF_{\alpha}(N,\beta)}}{\sum_{\alpha}\mathrm{e}^{-yF_{\alpha}(N,\beta)}}\,. \quad (4)$$

When y is set to $y=\beta$, $\mathcal{Z}(N,\beta;y)$ reduces to $\mathcal{Z}(N,\beta)$ of the physical system. $\mathcal{Z}(N,\beta;y)$ can be re-written as

$$\mathcal{Z}(N,\beta;y) = \int \mathrm{d}f \exp\bigl[N(\Sigma(f)-yf)\bigr]\,. \quad (5)$$

In Eq. (5), $f=F/N$ is the free energy density of a macroscopic state; the function $\Sigma(f)$ is called the complexity,[5,9] which is related to the total number $\Omega_{\rm mac}(F)$ of macroscopic states by

$$\Sigma(f) = \Bigl(\frac{1}{N}\Bigr)\ln\Omega_{\rm mac}(Nf)\,. \quad (6)$$

The complexity $\Sigma(f)\geq 0$ is a measure of the total number of macroscopic states with free energy density f. When $N\gg 1$, $\mathcal{Z}(N,\beta;y)$ is contributed only by those macroscopic states whose free energy density f satisfies $\partial\Sigma(f)/\partial f = y$. The parameter y is eventually set to $y=\beta$ if the corresponding complexity Σ is non-negative.

In Ref. [5] it was assumed that the total number $\Omega_{\rm mac}(F)$ of macroscopic states diverges exponentially with F according to

$$\Omega_{\rm mac}(F) \propto \exp\bigl(x\beta F\bigr)\,, \quad (7)$$

where $0<x<1$ is a dimensionless constant to be determined self-consistently. This might be a rather strong assumption. It may not hold for some spin-glass models. For systems with many-body interactions, even if the exponential form of Eq. (7) might be valid in certain range of free energy values, the parameter x may exceed unity. The original cavity iterative equations of Ref. [5] is not well defined for $x\geq 1$. The present effort is instead developed on the free energy Boltzmann distribution (4), without the need of assuming Eq. (7). It has the same mathematic format both for non-zero and for zero temperature.[9] In addition, it can be easily extended to include the possibility of further clustering of macroscopic states.

Cavity Magnetization and Free Energy Density The free energies of macroscopic states are calculated with the inverse temperature β, while the grand free energy G is calculated with the inverse temperature y. As the "community structure" of the configurational space is *a priori* unknown, a direct application of Eqs. (1) and (3) is impossible. This difficulty is partially circumvented by the iterative cavity approach,[4,5] which combines the Bethe–Peierls approximation[10] with the proliferation of thermodynamic states. Here we demonstrate how to combine the free energy Boltzmann distribution (4) with the cavity approach. To be concrete, we first work on the $\pm J$ spin-glass model[11] on a random regular graph $G_K(N)$ of degree K.[12] The configurational energy is

$$E(\sigma_1,\sigma_2,\ldots,\sigma_N) = -\sum_{(i,j)\in G_K} J_{ij}\sigma_i\sigma_j\,, \quad (8)$$

where $\sigma_i\in\pm 1$ is the spin of vertex i; J_{ij} ($=\pm J$ with equal probability) is quenched compling between neighboring vertices of the graph $G_K(N)$. We also need to introduce the concept of cavity random graphs $G_K(N;m)$.[5,9] In $G_K(N;m)$ only $N-m$ vertices have degree K; the remaining ones have degree $K-1$, they are called cavity vertices. A spin-glass system on $G_K(N;m)$ is referred to as a cavity system.

In a macroscopic state α of the cavity system on $G_K(N;m)$, each cavity vertex j has a cavity magnetization m_j due to the influences of its $K-1$ neighbors, and its marginal spin value distribution is $\rho_j(\sigma_j) = [(1+m_j)/2]\delta^{+1}_{\sigma_j} + [(1-m_j)/2]\delta^{-1}_{\sigma_j}$. In a random cavity graph $G_K(N;m)$ the typical shortest-path length between two cavity vertices diverges logarithmically with size N,[12] therefore when $N\gg 1$ the spins on different cavity vertices may fluctuate independently of each other. Under this assumption of mutual-independence, the joint distribution $\rho_{j,k,\ldots}(\sigma_j,\sigma_k,\ldots)$ of spin values on a group of cavity vertices can be factorized as

$$\rho_{j,k,\ldots}(\sigma_j,\sigma_k,\ldots) = \rho_j(\sigma_j)\rho_k(\sigma_k)\ldots \quad (9)$$

A cavity graph $G_K(N+1;1)$ can be generated by connecting a new vertex i to the $K-1$ cavity vertices of the graph $G_K(N;K-1)$. The configurational energy difference between the two corresponding cavity systems is $\Delta E^{(i)} = -\sum_{j\in\partial i} J_{ij}\sigma_i\sigma_j$, where ∂i denotes the set of neighbors of vertex i in $G_K(N+1;1)$. By assuming Eq. (9), we can obtain an iterative equation for the cavity magnetization m_i of vertex i: $m_i = (z^{(i)}_+ - z^{(i)}_-)/(z^{(i)}_+ + z^{(i)}_-)$, where $z^{(i)}_{\pm} = \prod_{j\in\partial i}(1\pm v_{ij}m_j)$ with $v_{ij}\equiv\tanh\beta J_{ij}$.[5] Based on Eqs. (1) and (9), the free energy difference between the macroscopic state α of the enlarged system and that of the old system is calculated to be $\Delta F^{(i)} = (1/2\beta)\sum_{j\in\partial i}\ln(1-v^2_{ij}) - (1/\beta)\ln(z^{(i)}_+ + z^{(i)}_-)$.

The cavity magnetization m_i of vertex i depends on the macroscopic state α. Its value may be different in different macroscopic states. We denote $P_i(m_i)$ as the probability of *observing* a macroscopic state in which vertex i has cavity magnetization m_i. As we mentioned before, a macroscopic state is visited with probability (4). Therefore, in going from the macroscopic state α of the cavity system on $G_K(N;K-1)$ to that of the system on $G_K(N+1;1)$, the statistical weight of the later is multiplied with an additional factor $\mathrm{e}^{-y\Delta F^{(i)}}$. We then obtain the following self-consistent equation:

$$P_i(m_i) \propto \int \prod_{j\in\partial i} \mathrm{d}m_j P_j(m_j)\, \mathrm{e}^{-y\Delta F^{(i)}} \delta\left(m_i - \frac{z_+^{(i)} - z_-^{(i)}}{z_+^{(i)} + z_-^{(i)}}\right). \quad (10)$$

In deriving Eq. (10) we have extended the Bethe–Peierls approximation to the level of macroscopic states by assuming

$$P_{j,k,\ldots}(m_j, m_k, \ldots) = P_j(m_j)P_k(m_k)\ldots, \quad (11)$$

which is equivalent to saying that, the fluctuations of the cavity magnetizations of different cavity vertices are mutually independent. From Eq. (3) and using the statistical independence assumption Eq. (11), we can derive that the grand free energy difference $\Delta G^{(i)}$ between the cavity systems $G_K(N+1;1)$ and $G_K(N;K-1)$ is

$$\Delta G^{(i)} = -\frac{1}{y}\ln\Big[\int \prod_{j\in\partial i} \mathrm{d}m_j P_j(m_j)\, \mathrm{e}^{-y\Delta F^{(i)}}\Big]. \quad (12)$$

At this point, we have illustrated the essential ideas of the present cavity approach. The grand free energy density $g(\beta; f)$ of the spin glass system can be obtained from the same line of reasoning: First we calculate the grand free energy difference ΔG_1 (ΔG_2) between the system on the graph $G_K(N)$ ($G_K(N+2)$) and the cavity system on the cavity graph $G_K(N, 2(K-1))$; and then

$$g(\beta; f) = \lim_{N\to\infty} \frac{1}{N} G(N, \beta; y) = \frac{1}{2}(\overline{\Delta G_2} - \overline{\Delta G_1}), \quad (13)$$

where the overline indicates averaging over the random graphs and the quenched randomness in the coupling constants J_{ij}. From Eq. (5) we know that, the mean free energy density of a macroscopic state is $\bar{f} = \partial(yg)/\partial y$, and the complexity is $\Sigma = y^2 \partial g/\partial y$.

We have performed population dynamics simulation[5] to find the steady-state solution of Eq. (10) for the $\pm J$ spin-glass model of $K = 6$ and $T = 0.8J$. A population of $\mathcal{N} = 1000$ densities $P_i(m_i)$ is stored in an array and is updated using Eq. (10). At $y = \beta$, the above mean-field theory reports a negative complexity, indicating that the equilibrium properties of the system at this temperature are determined by the thermodynamic states of the minimal free energy density. The complexity $\Sigma(y)$ decreases to zero at $y/\beta = 0.23(1)$. At this y value, we obtain that the mean free energy density, energy density (both in units of J), and entropy density of a macroscopic state is, respectively, $\bar{f} = -1.859\ 33(7)$, $\epsilon = -1.800\ 7(2)$ and $s = 0.073\ 2(5)$. These results remain almost unchanged when we increase the population size to $\mathcal{N} = 6000$; they are consistent with earlier numerical predictions, indicating the feasibility of the present approach. To make a quantitative comparison, we notice that the mean energy density as estimated by the Monte Carlo simulation of Carrus, Marinari and Zuliani (cited in Ref. [5]) is $\epsilon = -1.799(1)$; and the population dynamics of Ref. [5] reported a mean free energy density $\bar{f} = -1.858(2)$ and an entropy density $s = 0.074(4)$.

Clustering of Macroscopic States The macroscopic states of a spin-glass system may not distribute uniformly in the configurational space of the system. They may further organize into clusters of macroscopic states. If this further clustering occurs, the magnetization distribution $P_i(m_i)$ of a cavity vertex will be different in different clusters. To describe this situation we can introduce a functional probability distribution $\mathcal{P}_i[P_i(m_i)]$ for vertex i, which characterizes the distribution of the probability function $P_i(m_i)$ among all the clusters of macroscopic states. Under the same assumption of mutual independence of different cavity vertices, the cavity method of the preceding section can be easily extended. For example, when the functional probability distribution $\mathcal{P}_i[P_i(m_i)]$ is introduced, the grand free energy increase Eq. (12) is revised into

$$\Delta G^{(i)} = -\frac{1}{y}\ln\Big[\int \prod_{j\in\partial i} \mathcal{P}_j[P_j]\mathcal{D}P_j \int \prod_{k\in\partial i} \mathrm{d}m_k P_k(m_k)\, \mathrm{e}^{-y\Delta F^{(i)}}\Big]. \quad (14)$$

Notice that we do *not* introduce an additional inverse temperature at the level of clusters. The spin-glass system is already ergodic at the level of macroscopic states, it can jump between different clusters of macroscopic states through the heating-annealing process. Therefore a cluster does not correspond to a higher-level thermodynamic state. We group macroscopic states into different clusters so that possible structural similarities among different macroscopic states can be partially taken into account in the cavity approach.

Although an iterative equation for the functional distribution $\mathcal{P}_i[P_i(m_i)]$ is very easy to write down, the steady-state solution of this equation is difficult to determine with high precision. The situation becomes easier at the limit of zero temperature. At $T = 0$, $P_i(m_i)$ reduces to a δ-function and can be represented by just one variable m_i. To demonstrate this more clearly, we study possible clustering of macroscopic states in the minimal vertex-cover problem on a random Poissonian graph.[13] The minimal vertex-cover problem consists in covering vertices in a graph with as few "markers" as possible such that for each edge (i, j) in the graph, at least one of its two end vertices i or j is covered.[13] This problem was studied in Ref. [14] without including the possibility of clustering of macroscopic states.

In each macroscopic state α of minimal vertex-covers, a vertex i is either always uncovered ($S_i = 0$) or always covered ($S_i = 1$) or being unfrozen ($S_i = *$).[6,14] We denote $\pi_i^{(c)}$ as the probability that vertex i has $S_i = 0$ in macroscopic states of cluster c; and denote $\mathcal{P}_i[\pi_i]$ as the probability of finding $\pi_i^{(c)} = \pi_i$ for a cluster of macroscopic states. For a random graph with mean vertex degree $\gamma = 10$ we have performed extensive population dy-

namics to find a steady distributions of the $\mathcal{P}_i$ probabilities. For $y < y^* \approx 3.06$, the steady-state distribution of $\mathcal{P}_i[\pi]$ approaches a δ-function, i.e., $\mathcal{P}_i[\pi] = \delta(\pi - r_i)$ with r_i being different for different vertices. This δ-form of the probability distributions suggests that, when $y < y^*$ all macroscopic states can be grouped into one single cluster; in other words, the macroscopic states of the system do not further cluster into higher-level groups. However, when $y > y^*$, the steady-state distribution for $\mathcal{P}_i[\pi]$ is $\mathcal{P}_i[\pi] = r_i\delta^1_\pi + (1 - r_i)\delta^0_\pi$. In other words, when $y > y^*$ macroscopic states do cluster into different clusters, but in each cluster of macroscopic states, a vertex i either always takes the value $S_i = 0$ ($\pi_i = 1$) or never ($\pi_i = 0$). This condition can be satisfied if each cluster is composed of just one macroscopic state. It is unexpected for us to find that, the "phase-transition" point $y = y^*$ is also the point where the complexity of this vertex-cover system transit from being positive to being negative. Further work is needed to fully understand this coincidence.

For the minimal vertex-cover problem, further clustering of macroscopic states therefore cannot make the complexity $\Sigma(y)$ be non-negative for $y > y^*$. Another possible cause of this negative complexity will be discussed below.

Conclusion and Discussion In this paper the issue of ergodicity in low-temperature spin-glasses was discussed. When ergodicity is broken, the physical meaning of the total partition function of a spin-glass system is interpreted in terms of a gedanken experiment of cyclic heating and annealing. We argued that all macroscopic states of the spin-glass are visited under repeated heating-annealing, and that the frequency of visiting a particular macroscopic state follows the Boltzmann distribution of free energies. The mean free energy density and other thermodynamic densities of a given spin-glass model on a finite-connectivity random graph was calculated by combining the Boltzmann distribution of macroscopic state free energies (4) with the cavity idea of Mézard and Parisi.[5] The present theoretical framework was validated in the case of the $\pm J$ spin-glass model on a random regular graph. We have also extended the analytical approach to the case when macroscopic states of a spin-glass system further organize into different clusters.

For the two spin-glass systems with two-body interactions studied in this paper, the mean-field calculation reports a negative complexity when the artificial inverse temperature y approaches the true inverse temperature β. This is related to the fact that, $\Sigma'(f_{\min}) < \beta$, i.e., the first derivative of the complexity at the minimal free energy density $f_{\min}$ is less than β. Consequently, the equilibrium properties of the system are contributed by those thermodynamic states whose free energy density is equal to the minimal free energy density $f_{\min}$. The optimal reweighting parameter y^* then actually equals $\Sigma'(f_{\min})$. For spin-glass systems with many-body interactions, the situation is more complex, in that the thermodynamic properties of the system might be determined by those "excited" macroscopic states. More thorough discussion of this point will be reported in a later publication.

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