Microcanonical Analysis of Spin Glasses Using Gauge Symmetry

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We apply the method of gauge transformation to spin glasses under the microcanonical ensemble to study the possibility of ensemble inequivalence in systems with long-range interactions and quenched disorder. It is proved that all the results derived under the canonical ensemble on the Nishimori line (NL) can be reproduced by the microcanonical ensemble irrespective of the range of interactions. This establishes that ensemble inequivalence should take place away from the NL if it happens in spin glasses. It is also proved on the NL that the microcanonical configurational average of the energy as a function of temperature is exactly equal to the average energy in the canonical ensemble for any finite-size systems with Gaussian disorder. In this sense, ensembles are equivalent even for finite systems.

KEYWORDS: microcanonical ensemble, ensemble inequivalence, spin glass, gauge symmetry

Equivalence of canonical and microcanonical ensembles is well established for systems with short-range interactions.[1,2] It is not necessarily the case in the presence of long-range interactions because of the absence of additivity:[3] If two independent systems with long-range interactions are put together, the total energy is not equal to the sum of the energies of two separate systems, and thus the standard derivation of the canonical ensemble from the microcanonical ensemble breaks down. One of the prominent consequences is the emergence of negative specific heat in the microcanonical ensemble, which has long been discussed in the astrophysical context[4–6] and has been observed in condensed matter of small size where the range of interactions is comparable to the system size.[7] Ensemble inequivalence has also been discussed in spin systems with long-range interactions with[8] and without[9–12] quenched disorder. It is therefore important to establish exact/rigorous results on ensemble equivalence and inequivalence that are applicable generically to a class of problems. The present contribution represents a step toward this goal.

More specifically, we develop a general theory of spin glasses using gauge symmetry in the microcanonical ensemble, which should be compared with the corresponding theoretical framework in the conventional canonical ensemble, in particular on the so-called Nishimori line (NL).[13,14] The results agree with those from the canonical ensemble, whenever comparison is possible, irrespective of the range of interactions including the infinite-range case. It is therefore concluded that canonical and microcanonical ensembles are equivalent in spin glasses on the NL as long as physical quantities that can be analyzed by gauge symmetry are concerned.

Let us study the Edwards-Anderson model of spin glasses,[15)]

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i S_j, \tag{1}$$

where the J_{ij} are quenched random interactions and the $S_i (= \pm 1)$ are Ising spins. The range of interactions is arbitrary and includes the infinite-range Sherrington-Kirkpatrick model.[16)] The lattice structure and spatial dimensionality are also arbitrary. The present theory is thus very general.

We first discuss the Gaussian distribution of J_{ij} implemented in the microcanonical context. Our microcanonical analysis starts from the entropy for a given energy, averaged over disorder,

$$S(E) = \frac{1}{C_J} \int \mathrm{D}J\, \delta\big(N_B J_0 - \sum_{\langle ij \rangle} J_{ij}\big) \log \sum_S \delta(E - H), \tag{2}$$

where C_J is the normalization factor of the configurational average

$$C_J = \int \mathrm{D}J\, \delta\big(N_B J_0 - \sum_{\langle ij \rangle} J_{ij}\big) \tag{3}$$

with N_B being the number of bonds, and $\mathrm{D}J$ is the Gaussian integral kernel

$$\mathrm{D}J = \prod_{\langle ij \rangle} \frac{\mathrm{d}J_{ij}}{\sqrt{2\pi}} \exp(-J_{ij}^2/2). \tag{4}$$

In eq. (2), the configurational average is taken under the condition $\sum J_{ij} = N_B J_0$. This is the microcanonical version of the Gaussian distribution with average J_0, which corresponds to the standard (canonical) weight,

$$\exp\Big(-\frac{1}{2}\sum_{\langle ij \rangle}(J_{ij} - J_0)^2\Big) = \exp\Big(-\frac{1}{2}\sum_{\langle ij \rangle}(J_{ij}^2 + J_0^2)\Big) \exp\Big(J_0 \sum_{\langle ij \rangle} J_{ij}\Big). \tag{5}$$

The final factor in the above equation indicates that the value of the sum $\sum J_{ij}$ can fluctuate according to the probability weight $\exp(J_0 \sum J_{ij})$. The microcanonical version of eq. (2) strictly enforces the value of $\sum J_{ij}$ to $N_B J_0$.

It is convenient to evaluate here the normalization factor C_J using the condition $E = -N_B J_0$ that will be explained later,

$$C_J(E) \;=\; \frac{1}{2\pi} \int \mathrm{d}\lambda\, \exp(-i\lambda E) \int \mathrm{D}J\, \exp(-i\lambda \sum J_{ij})$$

$$= \frac{1}{2\pi}\int \mathrm{d}\lambda\, \exp(-i\lambda E - N_B\lambda^2/2) = \frac{1}{\sqrt{2\pi N_B}}\exp\big(-E^2/(2N_B)\big). \qquad (6)$$

Let us apply the gauge transformation $J_{ij} \to J_{ij}\sigma_i\sigma_j,\ S_i \to S_i\sigma_i\ (\forall i,j)$, where the $\sigma_i = \pm 1$ are gauge variables. Following the prescription established in the canonical ensemble,[13,14] we sum the result over all configurations of the gauge variables to have

$$S(E) = \frac{1}{2^N C_J}\int \mathrm{D}J \sum_{\sigma}\delta\big(N_B J_0 - \sum_{\langle ij\rangle} J_{ij}\sigma_i\sigma_j\big)\log\sum_S \delta\big(E + \sum_{\langle ij\rangle} J_{ij}S_iS_j\big), \qquad (7)$$

where N is the number of sites. The basic strategy of microcanonical calculations is to take the derivative of the entropy with respect to the energy and equate the result to the inverse temperature β. If we carefully look at the expression of this derivative,

$$\beta = \frac{\partial S}{\partial E} = \frac{1}{2^N C_J}\int \mathrm{D}J \sum_{\sigma}\delta\big(N_B J_0 - \sum_{\langle ij\rangle} J_{ij}\sigma_i\sigma_j\big)\frac{\partial_E \sum_S \delta\big(E + \sum_{\langle ij\rangle} J_{ij}S_iS_j\big)\big)}{\sum_S \delta\big(E + \sum_{\langle ij\rangle} J_{ij}S_iS_j\big)\big)}, \qquad (8)$$

we notice that the summation over σ in the configurational average cancels with the summation over S in the denominator when $E = -N_B J_0$. This is the microcanonical condition for the NL. Then the above expression reduces to

$$\begin{aligned}
\beta &= \frac{\partial S}{\partial E} = \frac{1}{2^N C_J(E)}\partial_E \sum_S \int \mathrm{D}J\, \delta\big(E + \sum_{\langle ij\rangle} J_{ij}S_iS_j\big) \\
&= \frac{1}{C_J(E)}\partial_E \int \mathrm{D}J\, \delta\big(E + \sum_{\langle ij\rangle} J_{ij}\big) \\
&= \frac{\partial_E C_J(E)}{C_J(E)} = -\frac{E}{N_B},
\end{aligned} \qquad (9)$$

where we have used eq. (6). The second line has been derived by the gauge transformation $J_{ij} \to J_{ij}S_iS_j$. Thus we have

$$E = -N_B\beta \qquad (10)$$

in precise agreement with the canonical case.[13,14] The NL condition in the canonical ensemble $\beta = J_0$ also follows from the condition $E = -N_B J_0$ in conjunction with eq. (10). It is remarkable that both ensembles give the same exact energy as a function of temperature for any finite-size system, any dimension, and any range of interactions. Usually, the results of two ensembles agree only in the thermodynamic limit.

Upper and lower bounds for the specific heat C for $E = -N_B J_0$ can also be estimated as shown below, and the results agree with the corresponding canonical inequalities,

$$0 \le C \le \frac{N_B}{T^2}. \qquad (11)$$

Since the specific heat is non-negative and upper-bounded by the same expression as in the canonical ensemble, there exists no ensemble inequivalence under the NL condition at least as long as the energy and bounds on the specific heat are concerned.

To prove eq. (11), we evaluate the second derivative of the entropy with respect to the energy, using the notation $\Omega(E) = \sum_S \delta(E - H)$,

$$\frac{\partial^2 S}{\partial E^2} = \frac{1}{2^N C_J} \int \mathrm{D}J \sum_{\sigma} \delta\big(N_B J_0 - \sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j\big) \left\{ \frac{\partial_E^2 \Omega(E)}{\Omega(E)} - \left(\frac{\partial_E \Omega(E)}{\Omega(E)} \right)^2 \right\}$$

$$\leq \frac{1}{2^N C_J} \int \mathrm{D}J \sum_{\sigma} \delta\big(N_B J_0 - \sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j\big) \frac{\partial_E^2 \Omega(E)}{\Omega(E)}$$

$$- \left(\frac{1}{2^N C_J} \int \mathrm{D}J \sum_{\sigma} \delta\big(N_B J_0 - \sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j\big) \frac{\partial_E \Omega(E)}{\Omega(E)} \right)^2$$

$$= \frac{\partial_E^2 C_J(E)}{C_J(E)} - \left(\frac{\partial_E C_J(E)}{C_J(E)} \right)^2 = -\frac{1}{N_B}. \tag{12}$$

If we remember the relation

$$-\frac{1}{CT^2} = \frac{\partial \beta}{\partial E}, \tag{13}$$

it follows

$$-\frac{1}{CT^2} \leq -\frac{1}{N_B}, \tag{14}$$

which is the desired inequality (11).

The same analysis applies to the $\pm J$ model, where $J_{ij} = 1$ with probability p and $J_{ij} = -1$ with probability $1 - p$. We have set $J(= |J_{ij}|) = 1$ for simplicity without losing generality. The points to be modified from the Gaussian case are (i) to replace the integral over J_{ij} with the summation over $J_{ij} = \pm 1$, (ii) to replace the normalization C_J with C_p, where

$$C_p = \sum_{\{J_{ij}\}} \delta\big(N_B(2p-1) - \sum_{\langle ij \rangle} J_{ij}\big), \tag{15}$$

and (iii) to replace the condition $E = -N_B J_0$ with $E = -N_B(2p - 1)$. The resulting relation corresponding to eq. (9) is

$$\beta = \frac{\partial_E C_p(E)}{C_p(E)}, \tag{16}$$

where

$$C_p(E) = \int \mathrm{d}\mu \, \exp(\mu E + N_B \log 2\cosh\mu). \tag{17}$$

Here we have omitted the factor $1/2\pi$ since it plays no role in the following. The integral variable μ corresponds to $i\lambda$ in eq. (6). For finite N_B, it is impossible to evaluate the integral explicitly, which is a difference from the Gaussian case. In the thermodynamic limit, the saddle-point method yields $\beta = \mu_0$ from eq. (16), where μ_0 is the saddle point specified by

$$E + N_B \tanh \mu_0 = 0. \tag{18}$$

In combination with $\beta = \mu_0$ and $E = -N_B(2p-1)$, we conclude $E = -N_B \tanh \beta$ under the condition $\tanh \beta = 2p - 1$. This is in perfect agreement with the canonical analysis.[13,14] Complete ensemble equivalence holds only in the thermodynamic limit in the $\pm J$ model.

Upper and lower bounds for the specific heat on the NL can also be estimated as in the Gaussian model. The central inequality is

$$\frac{\partial \beta}{\partial E} \le \frac{\partial_E^2 C_p(E)}{C_p(E)} - \left(\frac{\partial_E C_p(E)}{C_p(E)}\right)^2. \tag{19}$$

If we naively apply the saddle-point method and take only the leading term, the right-hand side reduces $\mu_0^2 - \mu_0^2 = 0$, leading to

$$-\frac{1}{CT^2} \le 0 \tag{20}$$

or $C \ge 0$. This positivity of the specific heat is non-trivial in the microcanonical ensemble but is not very exciting. A better inequality is obtained from the leading correction to the saddle point. The normalization factor $C_p(E)$ is written as, to the leading correction to the saddle point, with the notation $f(\mu) = \mu E + N_B \log 2 \cosh \mu$,

$$C_p(E) = \exp\big(f(\mu_0)\big) \int \mathrm{d}\mu \, \exp\big((\mu - \mu_0)^2/2\sigma^2\big), \tag{21}$$

where $1/\sigma^2$ is the second derivative $\partial^2 f(\mu)/\partial \mu^2|_{\mu_0} = N_B \mathrm{sech}^2 \mu_0$. The integral converges because it runs from $-i\infty$ to $i\infty$ through the saddle point μ_0 on the real axis. Similarly, we have

$$\partial_E^2 C_p(E) = \exp\big(f(\mu_0)\big) \int \mathrm{d}\mu \, \mu^2 \, \exp\big((\mu - \mu_0)^2/2\sigma^2\big). \tag{22}$$

Then the right-hand side of eq. (19) is

$$\frac{\displaystyle\int \mathrm{d}\mu \, \mu^2 \exp\big((\mu - \mu_0)^2/2\sigma^2\big)}{\displaystyle\int \mathrm{d}\mu \, \exp\big((\mu - \mu_0)^2/2\sigma^2\big)} - \mu_0^2 = (-\sigma^2 + \mu_0^2) - \mu_0^2 = -\sigma^2. \tag{23}$$

It is therefore concluded that

$$-\frac{1}{CT^2} \le -\frac{1}{N_B \mathrm{sech}^2 \mu_0}, \tag{24}$$

which leads to the bounds for the specific heat $0 \le CT^2 \le N_B \mathrm{sech}^2 \beta$ as is already known in the canonical ensemble.[13,14]

Identities and inequalities for correlation functions can also be established. Let us realize that the microcanonical delta constraint $\delta(E - H)$ with E being the control parameter plays a very similar role as the canonical Boltzmann factor $\exp(-\beta H)$ with β the control parameter. It is then straightforward to apply the same argument as in the canonical case to derive identities and inequalities for correlation functions. If we take the example of the Gaussian disorder and use the notation $E_J \equiv -N_B J_0$ (the NL conditions is $E = E_J$), the results are

$$[(\langle S_i S_j\rangle_E)^n] = [\langle S_i S_j\rangle_{E_J}(\langle S_i S_j\rangle_E)^n] \quad (n = 1, 3, 5, \cdots) \tag{25}$$

$$[P(m)] = [P(q)] \quad (E = E_J) \tag{26}$$

$$|[\langle S_i S_j\rangle_E]| \leq [|\langle S_i S_j\rangle_{E_J}|] \tag{27}$$

$$[\mathrm{sgn}\langle S_i S_j\rangle_E] \leq [\mathrm{sgn}\langle S_i S_j\rangle_{E_J}]\,, \tag{28}$$

where the suffix of the angular brackets specifies the value of the microcanonical energy. The square brackets denote the configurational average. The first relation (25) with $n = 1$ shows that the ferromagnetic correlation on the left-hand side is equal to the spin glass correlation on the right-hand side if the system is on the NL. The limit $|i - j| \to \infty$ yields $m = q$, where m and q are the ferromagnetic and spin glass (Edwards-Anderson) order parameters, respectively. The second identity (26) restates this fact from the perspective of the distribution functions of the magnetization and the spin glass order parameter,

$$P(m) = \frac{\sum_S \delta(Nm - \sum_i S_i)\delta(E - H)}{\sum_S \delta(E - H)} \tag{29}$$

$$P(q) = \frac{\sum_{S^{(1)},S^{(2)}} \delta(Nq - \sum_i S_i^{(1)} S_i^{(2)})\delta(E - H^{(1)})\delta(E - H^{(2)})}{\sum_{S^{(1)},S^{(2)}} \delta(E - H^{(1)})\delta(E - H^{(2)})}, \tag{30}$$

where $H^{(k)}$ is the Hamiltonian with the spins S_i in eq. (1) replaced by the spins $S_i^{(k)}$ of the $k(= 1, 2)$th replica. This identity (26) proves that there is no replica symmetry breaking on the NL in the sense of non-trivial distribution $[P(q)]$ because the distribution of magnetization $[P(m)]$ is always trivial. The third relation (27) proves that the phase boundary between the ferromagnetic and non-ferromagnetic phases below the multicritical point should be either vertical or reentrant in the phase diagram. The final inequality (28) implies that the number of mutually parallel spin pairs takes its maximum value on the NL when we change the energy (and consequently the temperature). The system is thus in its most ordered state on the NL if we focus ourselves to the spin orientation, ignoring the magnitude, as indicated by the signum function. All these results are shared by the canonical ensemble.

The distribution of a local energy $-J_{12}S_1S_2$ can be calculated similarly on the NL using its gauge invariance. The strategy is exactly the same as in the derivation of eq. (9). The result is

$$[\langle\delta(\epsilon + J_{12}S_1S_2)\rangle_{E_J}] = c\,\exp\left(-\frac{N_B}{2(N_B-1)}(\epsilon - J_0)^2\right), \tag{31}$$

where c is the normalization constant. The local energy naturally distributes in a Gaussian form around its mean J_0.

A different viewpoint can be introduced if we apply random fields and impose a microcanonical constraint that the 'staggered magnetization' along the random fields has a specific value. For the Gaussian distribution of disorder, the entropy is

$$\begin{aligned} S(E) &= \frac{1}{C_J}\int \mathrm{D}J\,\mathrm{D}h\,\delta\big(N_BJ_0 - \sum_{\langle ij\rangle} J_{ij}\big)\delta\big(Nh - \sum_i h_i\big) \\ &\quad \cdot \log\sum_S \delta\big(E + \sum_{\langle ij\rangle} J_{ij}S_iS_j\big)\delta\big(Nm - \sum_i h_iS_j\big). \end{aligned} \tag{32}$$

The normalization is now

$$C_J = \int \mathrm{D}J\,\mathrm{D}h\,\delta\big(N_BJ_0 - \sum_{\langle ij\rangle} J_{ij}\big)\delta\big(Nh - \sum_i h_i\big), \tag{33}$$

which can be evaluated as in eq. (6) under the generalized NL condition $E = -N_BJ_0$ and $h = m$ to give

$$C_J(E,m) = \frac{1}{2\pi\sqrt{NN_B}}\,\exp\big(-E^2/(2N_B) - Nm^2/2\big). \tag{34}$$

Then, when $E = -N_BJ_0$ and $h = m$, the first and second derivatives of S with respect to m are evaluated as before,

$$\frac{\partial S}{\partial m} = \partial_m \log C_J(E,m) = -mN, \tag{35}$$

$$\frac{\partial^2 S}{\partial m^2} = \frac{\partial_m^2 C_J(E,m)}{C_J(E,m)} - \left(\frac{\partial_m C_J(E,m)}{C_J(E,m)}\right)^2 = -N. \tag{36}$$

Thus, for $m = h > 0$, the entropy is a decreasing concave function of the staggered magnetization on the NL ($E = -N_BJ_0$). In particular, for $m = h = 0$, the vanishing value of the staggered magnetization is thermodynamically stable in the sense that the entropy is maximum. This is natural because the system is not in the spin glass phase ($q > 0, m = 0$) on the NL ($q = m$) and thus cannot be staggered-magnetized along a given unbiased random field (unbiased in the sense $h = 0$). For a finite value of $h(> 0)$, the stable value of the staggered magnetization is closer to zero than $m = h$ since the entropy will be larger for smaller m according to eq. (35).

In summary, we have shown that all the results obtained from gauge symmetry in spin glasses in the canonical ensemble can be reproduced in the microcanonical formulation of the same problem. In particular, the microcanonical configurational average of the energy for the Gaussian distribution agrees exactly with the corresponding canonical energy for any finite-size systems. This implies complete ensemble equivalence for finite-size systems, an unusual phenomenon. These results are valid for a generic system with arbitrary range of interactions in arbitrary dimension including the infinite-range limit as long as the system is on the NL. We have proved that there are no anomalies such as multiple values of the temperature for a given energy or negative specific heat as observed in certain systems with long-range interactions.[3–6, 9–12] If ensemble inequivalence exists in spin glasses with long-range interactions, it should happen away from the NL. Preliminary calculations indeed suggest possible ensemble inequivalence away from the NL, and the results will be reported in a forthcoming publication.

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