Approximate calculation of the ground-state energy for Potts spin-glass models

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We consider the q-state Potts spin-glass model, with quenched couplings taking two different values only. As an approximation for this model a proper generalization of the random energy model is derived. Formulas of the resulting diluted generalized random energy model (DGREM) are applied to calculate the ground-state energy for the two-dimensional Potts spin-glass model. The semianalytical results are compared with numerical determinations of the ground-state energy, using multicanonical, random cost, and simulated annealing techniques.

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I. INTRODUCTION

Spin-glass models are used to describe quenched, disordered materials with randomly distributed, competing interactions [1–4]. Due to the latter property, being the characteristic feature of all spin glasses, numerical investigations of this class of models are among the computationally hard problems. An important example is the exact calculation of spin-glass ground states which, in greater than two dimensions or generally in the presence of a magnetic field as well as with periodic boundary conditions, is known to belong to the class of nonpolynomial NP-hard problems [5]. Despite many recent quite elaborate studies, even for seemingly simple cases such as the Edwards-Anderson Ising spin-glass model in two [6] and three [7–9] dimensions, the behavior in the spin-glass phase (at zero temperature [6,7], for low temperatures [8] and around the freezing point [9]) is still not fully understood. In such a situation it is interesting to look for alternative methods, even if their accuracy is somewhat limited. Making use of numerical data for the corresponding *ferromagnetic* model on the same lattice, we shall calculate in this paper approximate properties of *spin-glass* models via an analogy with random energy model-like systems.

The random energy model (REM) [10] and its generalizations [11–16] have a variety of applications in modern physics. In Ref. [15] the diluted generalized random energy model (DGREM) has been suggested and applied to an approximate calculation of the ground-state energy of the two-dimensional (2D) Edwards-Anderson Ising spin-glass model, where each spin can only take on the two different values $s_i = \pm 1$.

The purpose of this work is to generalize these ideas to the q-state Potts spin-glass model, where the spins can be in one of the q discrete states $s_i \in \{1, \ldots, q\}$ [17–22]. This type of models is suitable for the description of anisotropic orientational glasses [23], which can arise from random dilution of molecular crystals such as N_2 diluted with Ar [24]. In such materials the model parameter q is associated with the q orientations of the uniaxial molecule in the crystal. Typical cases are $q=3$, when the molecules can align only along the x, y, and z axes of a cubic crystal and $q=6$, when the face diagonals are the preferred directions.

We thus consider a model of N integer valued Potts spins $s_i \in \{1, \ldots, q\}$ interacting via quenched, random ± 1 nearest-neighbor couplings J_{ik} on a d-dimensional hypercubic lattice with Hamiltonian

$$H_1 = -\sum_{\langle ik \rangle} J_{ik}[q\,\delta_{s_i,s_k} - 1]\frac{1}{q-1}. \tag{1}$$

In the case where the couplings J_{ik} are drawn from a symmetric distribution, one can rewrite Eq. (1) into the equivalent form

$$H_2 = -\sum_{\langle ik \rangle} J_{ik}\left[\frac{q}{q-1}\,\delta_{s_i,s_k} - \frac{q}{2(q-1)}\right]. \tag{2}$$

Of course, for a symmetric distribution of the couplings, the two Hamiltonians are completely equivalent, but the second form is more convenient for our purposes. The reason is that in H_2 the local contributions to the total energy are also symmetrically distributed, taking on the two possible values $\pm[q/2(q-1)]$.

In the following section, we derive the DGREM scheme for general q-state Potts spin-glass models (2) and apply this semianalytical approximation to the determination of the ground-state energy of the two-dimensional models with $q=2$, 3, and 4. In Sec. III, our results are compared with numerical estimates obtained with three different techniques: multicanonical simulations, the random-cost algorithm, and the standard simulated annealing method. Finally, in Sec. IV, we close with our conclusions and an outlook to future applications.

II. THE DGREM APPROXIMATION

The basic idea of the DGREM scheme is to approximate the system (2) with another (simpler and analytically solvable) model with the same number of configurations q^N as well as the same one- and two-energy level distributions. It is easy to calculate the energy distribution for one spin configuration as well as for two configurations. If we consider the energy distribution for any given spin configuration, in representation (2) the energy is a sum of $z=Nd$ random num-

bers $\pm[q/2(q-1)]$ with symmetric distribution. The symmetric distribution of couplings J_{ik} clears the bias of $[q/(q-1)\delta_{s_i,s_k}-q/2(q-1)]$ and the terms of our sum are independent. Hence, we have

$$\rho_1(E,z)\equiv\langle\delta[H_2(s)-E]\rangle_J=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}dk\exp\left[-kE+z\ln\cosh\left(\frac{kq}{2(q-1)}\right)\right], \tag{3}$$

where in Eq. (3) the average is taken over all possible choices of the couplings J_{ik}. Note that the right-hand side of Eq. (3) does *not* depend on the given spin configuration $s\equiv\{s_i\}$, $i=1,\ldots,N$. One has a simple formula for the superposition of two distributions (3)

$$\int dE_1dE_2\rho_1(E_1,z_1)\rho_1(E-E_2,z_2)=\rho_1(E,z_1+z_2). \tag{4}$$

Let us now consider two spin configurations $s^{(1)}$ and $s^{(2)}$, i.e.,

$$\rho_2(E)\equiv\langle\delta[H_2(s^{(1)})-H_2(s^{(2)})-E]\rangle_{J,s^{(1)},s^{(2)}}, \tag{5}$$

and let us look at $H_2(s^{(1)})-H_2(s^{(2)})$, which may be expressed as

$$H_2(s^{(1)})-H_2(s^{(2)})=-\sum_{\langle ik\rangle=1}^{z(1-v_0)}J_{ik}\frac{q}{q-1}[\delta_{s_i^{(1)},s_k^{(1)}}-\delta_{s_i^{(2)},s_k^{(2)}}]. \tag{6}$$

Here, $z=Nd$ is again the total number of bonds and v_0 is the fraction of bonds with identical products $S_iS_k^*$ of complex valued spins $S_i\equiv\exp(i2\pi s_i/q)$ in the two configurations, or in terms of the integer valued spins of Eqs. (1) and (2): $s_i^{(1)}-s_k^{(1)}+q,\mathrm{mod}(q)=s_i^{(2)}-s_k^{(2)}+q,\mathrm{mod}(q)$.

To calculate the distribution of v_0 for different realizations $s^{(1)},s^{(2)}$ one should consider the *ferromagnetic* Potts model with Hamiltonian

$$H_f=-\sum_{\langle ik\rangle}\left[\frac{q}{(q-1)}\delta_{s_i,s_k}-\frac{1}{(q-1)}\right], \tag{7}$$

where, $s_i=s_i^{(1)}-s_i^{(2)}+q,\mathrm{mod}(q)$. With this normalization the ferromagnetic energy varies between $-Nd$ for $T=0$ and 0 in the limit $T\to\infty$, and for $q=2$ all expressions reduce smoothly to the standard Ising model notation (with $2\delta_{s_i,s_j}-1$ replaced by $\sigma_i\sigma_j$ and $\sigma_i=\pm1$). For the Hamiltonian (7), we can express the energy via the fraction v_0 of ''active'' bonds $[\delta_{s_i,s_k}\equiv\delta([s_i-s_k+q,\mathrm{mod}(q)],0)=1]$ as

$$E_f(v_0)=-\left[\frac{q}{q-1}v_0-\frac{1}{q-1}\right]z. \tag{8}$$

So, we derive the number of situations with v_0 for a choice of all different configurations $s^{(1)},s^{(2)}$,

$$\mathcal{N}(v_0)=q^N\Omega(v_0)\equiv q^N\exp(S[E_f(v_0)]), \tag{9}$$

where $\Omega(v_0)$ is a number of configurations with a fraction v_0 of active bonds and $S(E_f)$ is the associated microcanonical entropy of the ferromagnetic model (7).

Let us calculate $\rho_2(E)$ in Eq. (5) at a *fixed* value of v_0. As products of spins $s_i^{(1)}$ are different, we should consider $q(q-1)$ different situations when considering Eq. (6). We then have

$$\rho_{2,v_0}(E)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}dk\exp\left[-kE+z(1-v_0)\ln\frac{q-2+2\cosh\left(\frac{kq}{q-1}\right)}{q}\right]. \tag{10}$$

For small energies ($E\sim\sqrt{N}$) this expression simplifies to a Gaussian distribution,

$$\rho_{2,v_0}(E)\sim\exp\left[-\frac{(q-1)^2}{4q(1-v_0)z}E^2\right]. \tag{11}$$

Recall that $\rho_{2,v_0}(E)$ is the density of energy differences for two configurations with a fixed fraction v_0 of equal bonds. The relation with the density $\rho_2(E)$ in Eq. (5) is obviously

$$\rho_2(E)=\int_0^1dv_0\mathcal{N}(v_0)\rho_{2,v_0}(E). \tag{12}$$

We thus know the one-energy level distribution for our system and the distribution for the difference of two levels. There is some ambiguity in the choice of the one level distribution. The Hamiltonian H_2 is a peculiar choice due to its symmetry properties; that is why we have chosen it and its corresponding distribution (3).

Let us now construct a simple REM approximation for our case without going too much into the details. We consider q^N energy levels with independent distributions (3)

$$\rho(E_1,E_2)\equiv\langle\delta[H_2(s^{(1)})-E_1]\delta[H_2(s^{(2)})-E_2]\rangle_J=\rho_1(E_1,z)\rho_1(E_2,z). \tag{13}$$

Here, one has for the partition function Z an expression

$$Z=\sum_{i=1}^{q^N}\exp(-\beta E_i), \tag{14}$$

where $\beta=1/T$ is the inverse temperature. If $N\equiv\ln(q^N)/\ln(q)$ is the number of Potts spins [in the original model (2) formulated via spin-spin interactions], then the REM approximation has a free parameter

$$\alpha=\frac{z}{N}. \tag{15}$$

Following Refs. [11,12], we note that at high temperatures the system is in the paramagnetic phase, and in this phase quenched and annealed expressions for the free energy are the same,

$$\langle \ln Z(\beta)\rangle = \ln\langle Z(\beta)\rangle = \alpha N \ln\cosh\left(\frac{\beta q}{2(q-1)}\right) + N\ln q, \tag{16}$$

where the average is now taken over the energy distribution (3), with the number of couplings $z=Nd$ replaced by $N\alpha$. To obtain Eq. (16), we used the identity

$$\int_{-\infty}^{\infty} dE\,\exp(-\beta E)\rho(E) = \exp[f(\beta)],$$
$$\rho(E) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} dk \exp[-kE + f(k)]. \tag{17}$$

The solution (16) is correct at high temperatures. At some finite temperature $T_c = 1/\beta_c$ the entropy $\langle \ln Z(\beta)\rangle - \beta(d\langle \ln Z\rangle/d\beta)$ vanishes,

$$\alpha N\left[\ln\cosh\left(\frac{\beta_c q}{2(q-1)}\right) - \frac{\beta_c q}{2(q-1)}\tanh\left(\frac{\beta_c q}{2(q-1)}\right)\right] + N\ln q = 0. \tag{18}$$

This is the main peculiar feature of REM. While in usual physical systems the entropy vanishes at zero temperature, here it happens already at a finite temperature. At this temperature the system is frozen in the spin-glass phase with $\langle \ln Z(\beta_c)\rangle$ given by Eq. (16). If we assume that the system is frozen into some low-level energy configuration with zero entropy, then below that freezing temperature $\langle \ln Z(\beta)\rangle$ should be proportional to β. Since the free energy is a continuous function of temperature, we thus have in the low-temperature phase

$$-\beta F = \langle \ln Z(\beta)\rangle = \frac{\langle \ln Z(\beta_c)\rangle}{\beta_c}\beta = \beta\alpha N \frac{q}{2(q-1)}\tanh\left(\frac{\beta_c q}{2(q-1)}\right). \tag{19}$$

To derive the last expression, we made use of Eq. (18).

The spin-glass phase exists only for large connectivity $\alpha > \alpha_c$. The critical value α_c can be obtained by considering the limit $T_c \to 0$, $\beta_c \to \infty$ in Eq. (18), leading to

$$\alpha_c = \frac{\ln q}{\ln 2}. \tag{20}$$

For the case $q=4$ this estimate gives $\alpha_c = 2$, i.e., the bound $d \geqslant 2$ for $q=4$ or $q \leqslant 4$ in $d=2$ for the existence of a spin-glass phase. It is unlikely that a spin-glass phase exists at finite temperatures.

So far, we have only considered the one-energy distribution. In the REM approach all energy configurations decouple and, thus, there are no nontrivial two-point correlator functions to simulate those of the model (2). To succeed with nontrivial expressions we have to introduce DGREM, a generalized version of REM. As before one can define DGREM with the one-energy distribution (3). In addition there is now a K level hierarchical structure (later, we will take the limit $K\to\infty$) with a parameter v for the ith hierarchy level $v \equiv i/K$, $0 \leqslant v \leqslant 1$. If we denote the branching number at level i by f_i, the total number of branches at level $i \equiv Kv$ is given by $\Pi_{i=1}^{K} f_i \equiv \exp[s(v)]$. At the last level of the hierarchy, we require for the total number of end points

$$\exp[s(1)] = q^N. \tag{21}$$

Let us put random variables ψ_l at each branch l with the distribution

$$\rho_1\left(\psi, \frac{z}{K}\right). \tag{22}$$

We put our energy configurations at the end points of the tree. Every end point has a single path, connecting it with the origin of the tree. One defines an energy of a given configuration, located at the point x as

$$E_x = \sum_l \psi_l. \tag{23}$$

According to the property (4) all the energy configurations have again the energy distribution

$$\rho(E) = \rho_1(E,z). \tag{24}$$

Before deriving an expression for the two-point correlator, let us first give expressions for the free energy $\langle \ln Z\rangle_\psi$, where the average is now over distributions of all ψ. Thermodynamically DGREM is equivalent to a chain of REM's having z/K couplings and $[s'(v)/\ln q](z/K)$ spins (q valued). In the limit of large K one can consider $1/K$ as differential dv. We have that $s(v)$ is a monotonic function with $s(0)=0$ and $s(1) = N\ln q$. The part of hierarchy from $v=0$ up to v_c is frozen in the spin-glass phase, and $v_c < v < 1$ holds in the paramagnetic phase. We calculate the free energy of our system as a sum of the paramagnetic part with $(1-v_c)z$ couplings and $s(v_c)/\ln q$ spins [14,15] and the spin-glass part

$$\langle \ln Z(\beta)\rangle = (1-v_c)z\ln\cosh\left(\frac{\beta q}{2(q-1)}\right) + s(v_c) + \frac{z\beta q}{2(q-1)}\int_0^{v_c} dv_1 \tanh\left(\frac{\beta_0(v_1)q}{2(q-1)}\right), \tag{25}$$

where the function $\beta_0(v_1)$ is defined as the solution of the equation

$$\ln\cosh\left(\frac{\beta_0 q}{2(q-1)}\right) - \frac{\beta_0 q}{2(q-1)}\tanh\left(\frac{\beta_0 q}{2(q-1)}\right) = -\frac{s'(v_1)}{z}, \tag{26}$$

which is identical to Eq. (18) for β_c with $\alpha = z\ln q/s'(v_1)$. At the critical value v_c, we have the relation

$$\beta_0(v_c)=\beta, \tag{27}$$

which can be derived from the extremum condition of Eq. (25) with respect to v_c.

We should next construct a DGREM, which has the same distribution [with Hamiltonian (2)] for one-energy as well as for two-energy levels. To have a correct one-energy distribution it is sufficient to take $z=dN$, i.e., $\alpha=d$. Let us now consider the distribution for the difference of two-energy levels. The difference between energies of two configurations comes from the ψ_l at higher levels of the hierarchy. If two configurations one and two meet at level v of the hierarchy, then their difference is defined as

$$E_1-E_2=\sum_{v_1=v}^{1}\psi_{v_1,l_1}-\sum_{v_2=v}^{1}\psi_{v_2,l_2}, \tag{28}$$

where v_1,l_1 and v_2,l_2 identify the branches at the hierarchy levels v_1 and v_2, respectively. The label l_1 corresponds to the branch on the path connecting the end point 1 with the origin of the tree and l_2 to the path connecting the end point 2. Let us calculate the distribution for E_1-E_2 by analogy with Eq. (10) (the distribution (3) is equivalent to the distribution of the sum of z independent variables $\pm[q/2(q-1)]$). Only when calculating Eq. (10), we were limited by the constraint $\psi_{l_1}\neq\psi_{l_2}$; now those are independent and we obtain

$$\hat{\rho}_{2,v}(E)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}dk\exp\left[-kE+z(1-v)\ln\frac{q^2-2q+2+2(q-1)\cosh\left(\frac{kq}{q-1}\right)}{q^2}\right],$$

$$\hat{\rho}_2(E)=\sum\hat{\rho}_{2,v_i}(E)(f_i-1)\prod_{j=i+1}^{K}f_j \approx\int_0^1 dv\,\hat{\rho}_{2,v_i}(E)e^{[s(1)-s(v)]}s'(v). \tag{29}$$

Here, $\hat{\rho}_{2,v}(E)$ is the energy distribution for two configurations with a crossing point at hierarchy level v. By comparing Eq. (29) with Eq. (10) for small values of energies, we find (ignoring the prefactors) that

$$\frac{q(1-v_0)}{q-1}=(1-v),\quad v=-\frac{E_f}{Nd},$$

$$s(v)=N\ln q-S(-vNd), \tag{30}$$

where E_f is the energy (8) and $S(E_f)$ the microcanonical entropy in Eq. (9) of the ferromagnetic model. For our proper choice of the ferromagnetic Hamiltonian (7) the parameter v, thus, indeed, varies in the interval $0\leqslant v\equiv-(E_f/Nd)\leqslant 1$.

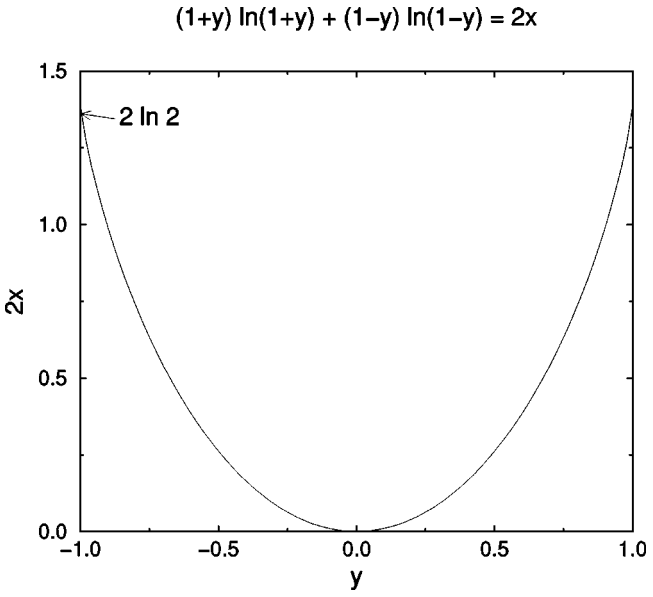

FIG. 1. Graphical representation of Eq. (32) for $y(x)$, illustrating that for $x\to\ln 2$ the solution y approaches ± 1, the limits of the allowed range for real values of x.

There is an important principal aspect here. When considering Eq. (9) one observes that $\mathcal{N}(v_0)$ is monotonic in the region $1/q<v_0<1$, then it falls off after the point $v_0=1/q$. On the other hand, on hierarchical lattices we have that the equivalent of $\mathcal{N}(v_0)$ (the number of all branches between levels of hierarchy i and $i+1$) grows all the time. In formula (30), we constructed the DGREM scheme, which imitates our finite-dimensional model for the values of v_0 in the region $1/q<v_0<1$.

Next, we rewrite Eq. (25) via integrating by parts in the limit $\beta\to\infty$. To this end, we first introduce the abbreviation

$$y=\tanh\left(\frac{\beta_0 q}{2(q-1)}\right). \tag{31}$$

It is then tedious but straightforward to show that the self-consistency Eq. (26) can be rewritten as

$$(1+y)\ln(1+y)+(1-y)\ln(1-y)=2x, \tag{32}$$

with $x\equiv s'(v_1)/z$. For a graphical illustration see Fig. 1.

Using the identity $S'(E_f)=\beta_1$ (inverse temperature of the ferromagnetic model (7), that is, H_1 in Eq. (1) with $J_{ik}\equiv 1$), and inserting $\beta_1=x=s'(v_1)/z$ into Eq. (26) we rewrite Eq. (25) as

$$\langle\ln Z(\beta)\rangle=\frac{z\beta q}{2(q-1)}\left[1-v_c+\int_0^{v_c}dv_1 y\left(\frac{s'(v_1)}{z}\right)\right]$$

$$=\frac{z\beta q}{2(q-1)}\left[1-v_c+v_c y\left(\frac{s'(v_c)}{z}\right)-\int_0^{v_c}dv_1 v_1\frac{dy\left(\frac{s'(v_1)}{z}\right)}{dv_1}\right]. \tag{33}$$

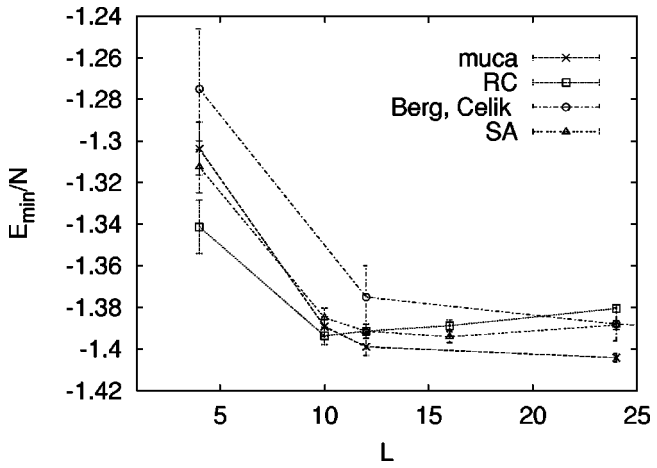

FIG. 2. Finite-size scaling of the ground-state energy results for the 2D EAI spin-glass model using multicanonical simulations (muca), the random-cost algorithm (RC), and simulated annealing techniques (SA). For comparison also the multicanonical data of Berg and Celik [26] are shown.

Changing the integration variable, $v_1 \rightarrow \beta_1(v_1)=s'(v_1)/z$, using the identities $v_1=-E_f(\beta_1)/Nd$, $y(s'(v_1)/z)=y(\beta_1)$, and considering the limit $\beta\rightarrow\infty$, $y(s'(v_c)/z)\rightarrow 1$ and in this limit $s'(v_c)/z=\ln 2$, we transform Eq. (33) into

$$-E_{\min}=\frac{qNd}{2(q-1)}\left[1-\int_0^{\ln 2} d\beta_1 \frac{-E_f(\beta_1)}{Nd}\frac{dy(\beta_1)}{d\beta_1}\right]$$
$$=\frac{qNd}{2(q-1)}\left[1-\int_0^{\ln 2} d\beta_1 \frac{-E_f(\beta_1)}{Nd}\frac{2}{\ln\frac{1+y(\beta_1)}{1-y(\beta_1)}}\right]. \quad (34)$$

The lower bound $\beta_1(v=0)=0$ follows because the energy of Hamiltonian (2) is zero at zero inverse temperature and the last fraction in the second line is just $dy(\beta_1)/d\beta_1$ as calculated from Eq. (32). This is the central result of the DGREM approximation.

It is interesting to compare this result with the REM estimate for the energy of REM with Nd couplings, $\alpha=d$. Recalling Eq. (31), the solution β_c of Eq. (18) can then be expressed as

$$\tanh\left(\frac{\beta_c q}{2(q-1)}\right)=y\left(\frac{\ln q}{d}\right), \quad (35)$$

and from Eq. (19), we obtain the purely analytical expression

$$-E_{\min}=\frac{qNd}{2(q-1)}y\left(\frac{\ln q}{d}\right), \quad (36)$$

with $y(\ln q/d)$ determined as solution of Eq. (32).

As an example, for the case $d=2$, $q=3$, we obtain from Eq. (36) by solving Eq. (32) numerically

$$E_{\min}/N\approx -1.4020 \quad \text{(REM)}, \quad (37)$$

while, upon inserting into Eq. (34) the numerically determined energy of the ferromagnetic model as a function of temperature (for more details see below), our DGREM approach gives

$$E_{\min}/N\approx -1.3156 \quad \text{(DGREM)}. \quad (38)$$

In the following section, these values will be compared with numerically determined estimates of the ground-state energy using Monte Carlo minimization methods.

In two dimensions, another interesting phenomenon should happen at $q=4$. Here at $T=0$, if the spin-glass phase does exist, is a multicritical point or the edge of the spin-glass phase. Let as assume, that there exists some spin-glass phase with some frozen spins. Such spins carry information $N\ln 4$. On the other hand, our couplings carry an information $2N\ln 2$. So in some sense the information content of the random couplings equals that of the spins in vacuum configurations. Such qualitative arguments show that the spin-glass transition point is improbable for $d=2$, $q\geqslant 4$.

III. NUMERICAL RESULTS

To judge the quality of the approximate calculations based on the DGREM approach, we have performed a direct ground-state energy computation for the models at hand using three different methods: the multicanonical algorithm [25,26], the random-cost algorithm [27], and the simulated annealing technique [28].

TABLE I. Results for the ground-state energy of the 2D EAI spin-glass model from our multicanonical simulations (muca) in comparison with those by Berg and Celik [26]. Also shown are the results from the random cost and simulated annealing studies.

L	Muca	Berg and Celik	Random cost	Simulated annealing
4	-1.304 ± 0.013	-1.275 ± 0.029	-1.341 ± 0.013	-1.312 ± 0.013
10	-1.389 ± 0.005	–	-1.393 ± 0.004	-1.385 ± 0.005
12	-1.399 ± 0.005	-1.375 ± 0.015	-1.391 ± 0.004	-1.391 ± 0.004
16	–	–	-1.389 ± 0.003	-1.394 ± 0.003
24	-1.404 ± 0.002	-1.388 ± 0.008	-1.381 ± 0.002	-1.388 ± 0.002
∞	-1.407 ± 0.002	-1.394 ± 0.007	-1.386 ± 0.002	-1.395 ± 0.002

TABLE II. Ground-state energy $E'_{\min}/N$ of the 2D three-state Potts spin-glass model.

L	Muca	Random cost
4	-0.754 ± 0.014	-0.781 ± 0.015
8	-0.820 ± 0.007	-0.822 ± 0.007
10	-0.822 ± 0.007	-0.822 ± 0.006
16	-0.830 ± 0.003	-0.828 ± 0.004
20	-0.830 ± 0.003	-0.819 ± 0.003
24	-0.827 ± 0.003	-0.816 ± 0.002
∞	-0.832 ± 0.002	-0.821 ± 0.002

A. 2D Edwards-Anderson Ising spin glass

As a benchmark case let us first consider the Edwards-Anderson Ising (EAI) spin-glass model with Hamiltonian [29]

$$H_2=-\sum_{\langle ik\rangle} J_{ik}\sigma_i\sigma_k, \tag{39}$$

where $\sigma_i=\pm1$ and $J_{ik}=\pm1$ are quenched, random couplings which are drawn with equal probability. We always assume periodic boundary conditions. The (total) energy is given as $E(\beta)=[\langle H_2\rangle]_{\rm av}=[\langle-\Sigma_{\langle ik\rangle}J_{ik}\sigma_i\sigma_k\rangle]_{\rm av}$, where $\langle\cdots\rangle$ is the usual thermodynamic expectation value and $[\cdots]_{\rm av}$ denotes the average over the quenched disorder.

On two-dimensional lattices of size $N=L^2$ with $L=4,10,12$, and 24 we performed multicanonical simulations, studying 100 different realizations per lattice size. We used these results to check our codes on results in the literature [26], see Fig. 2 and Table I. For the estimate of the infinite-volume ground-state energy per spin, $e_{\min}=E_{\min}/N$, we used a finite-size scaling (FSS) fit of the form $e_{\min}(L)=e_{\min}+c/L^2$. Applied to our multicanonical (muca) data in Table I this ansatz works perfectly with a χ^2 per degree of freedom of 0.7.

For the 2D Ising spin-glass model much more accurate estimates are available in the literature for further comparison. Using a combinatoric matching method to find for a given disorder realization the *exact* ground-state energy on lattices as big as 1800×1800, Palmer and Adler [30] recently extrapolated [31] an infinite-volume limit of [32] $e_{\min}=-1.40193(2)$. Other recent estimates include $e_{\min}=-1.4015(8)$ (Ref. [33], using similar methods), $e_{\min}=-1.400(5)$ (Ref. [34], pure cluster exact approximation),

TABLE III. Ground-state energy $E'_{\min}/N$ of the 2D four-state Potts spin-glass model.

L	Muca	Random cost
4	-0.796 ± 0.015	-0.791 ± 0.014
8	-0.831 ± 0.007	-0.832 ± 0.007
10	-0.832 ± 0.006	-0.832 ± 0.006
16	-0.834 ± 0.004	-0.838 ± 0.004
24	-0.834 ± 0.003	-0.833 ± 0.003
∞	-0.836 ± 0.002	-0.836 ± 0.003

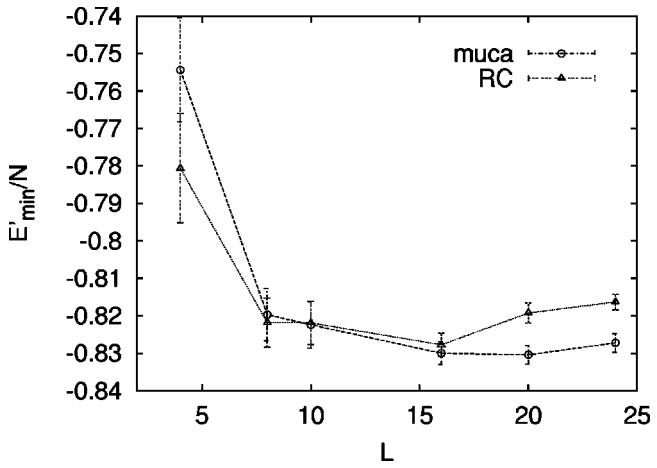

FIG. 3. Finite-size scaling of the ground-state energies $E'_{\min}/N$ of the 2D three-state Potts spin-glass model using multicanonical (muca) and random-cost (RC) simulations.

$e_{\min}=-1.4015(3)$ (Ref. [35], mixed genetic and cluster exact approximation), $e_{\min}=-1.4024(12)$ (Ref. [36], transfer-matrix calculations), and $e_{\min}=-1.407(8)$ (Ref. [37], replica Monte Carlo). There is a clear consensus amongst these results of a central value between -1.401 and -1.402, which is compatible with our multicanonical estimates.

After this test, we turned to the random-cost (RC) algorithm and simulated annealing (SA) runs. On lattices of size $L=4,10,12,16$, and 24, we considered again 100 different realizations per lattice size and used the same FSS ansatz for the infinite-volume extrapolations as in the multicanonical simulations. All our results for the ground-state energy are collected in Table I, see also Fig. 2.

Our combined ground-state estimate $e_{\min}=-1.397\pm0.002$ (using an average over the three methods used) is thus consistent with previous estimates [26,30,33–37].

B. 2D q-state Potts spin glass with $q=3$ and 4

Next, we considered the 2D q-state Potts spin-glass model with $q=3$ and 4 states per spin where no (quasi-) exact ground-state energies are available. Here, we thus relied on the Monte Carlo procedures tested in the Ising case. In the numerical work it was more convenient to work with the Hamiltonian

$$H'_2=-\sum_{\langle ik\rangle} J_{ik}\delta_{s_i,s_k}, \tag{40}$$

instead of H_1 or H_2 of Eq. (1) or (2). Again, $s_i=1,\ldots,q$, and $J_{ik}=\pm1$ are quenched, random couplings which are drawn with equal probability. The (total) energy is, thus, given as $E'(\beta)=[\langle H'_2\rangle]_{\rm av}=[\langle-\Sigma_{\langle ik\rangle}J_{ik}\delta_{s_i,s_k}\rangle]_{\rm av}$, such that, recalling the normalization of H_2, $E_{\min}=[q/(q-1)]E'_{\min}$.

For both values of q, we used the multicanonical algorithm and investigated 100 different realizations for the lattice sizes $L=4,8,10,16,20$, and 24. We also performed random-cost simulations and investigated another 100 different realizations for the same lattices sizes. For the larger

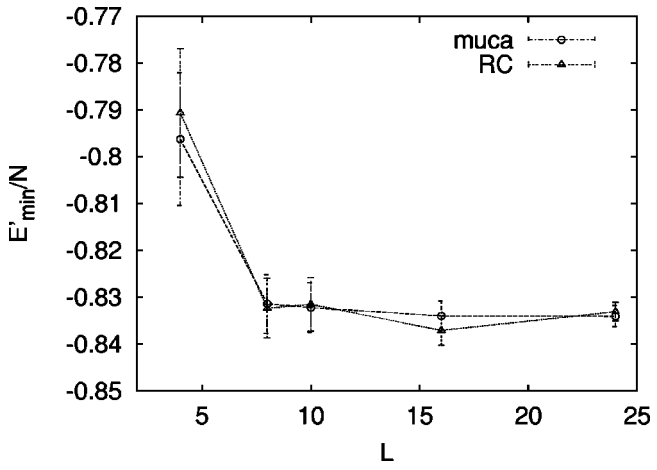

FIG. 4. Finite-size scaling of the ground-state energies $E'_{\min}/N$ of the 2D four-state Potts spin-glass model using multicanonical (muca) and random-cost (RC) simulations.

lattices the random-cost algorithm turned out to be ill behaved, and by closer inspection (e.g., much longer runs in some cases), we convinced ourselves that it is difficult to find reliable ground-state configuration with this method. As our final estimate for the ground-state energy, we therefore take the infinite-volume extrapolation (again in $1/L^2$) of the multicanonical data, i.e., $e'_{\min}(q=3)=-0.832\pm0.002$ and $e'_{\min}(q=4)=-0.836\pm0.002$. All results are collected in Tables II and III, see also Figs. 3 and 4.

C. Comparison with the DGREM approximation

For the evaluation of the DGREM approximation (34), we need the energy of the corresponding ferromagnetic model as a function of temperature. To this, end we performed Monte Carlo (MC) simulations of the two-dimensional ferromagnetic models in the relevant β-range. Since here one may employ a cluster algorithm for updating the Potts spins, we could easily simulate sufficiently large lattices and thus avoid finite-size effects, at least for all practical purposes. This is illustrated in Fig. 5, where the MC data of a 100×100 lattice for the three-state Potts model are compared with low- and (dual) high-temperature series expansions [38] to very high order. By using the ferromagnetic energies as obtained in the MC simulations and performing the integration in Eq. (34) numerically, we arrived at the numbers for $q=2$, 3, and 4 given in the third column of Table IV. For comparison the numerically determined ground-state energies $E_{\min}/N=[q/(q-1)]E'_{\min}/N$ are compiled in the fourth column, and the last column showing the ratio of the DGREM and MC estimates indicates the relative accuracy of the DGREM approximation which turns out to be about 5%–10%.

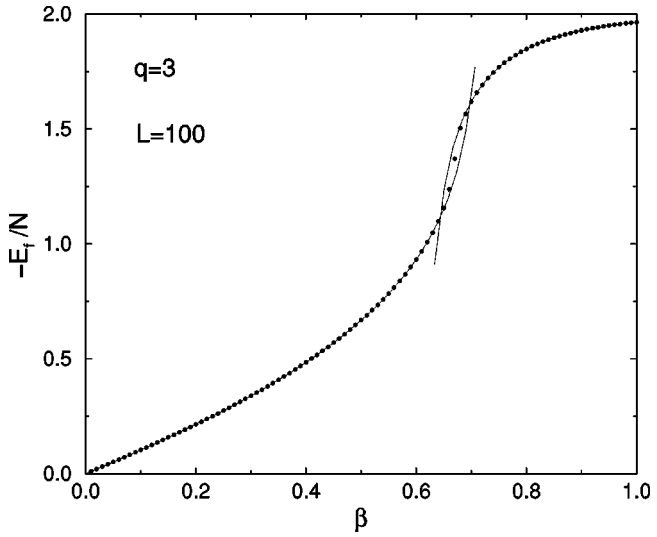

FIG. 5. The energy of the 2D three-state Potts ferromagnet as a function of inverse temperature as obtained from Monte Carlo simulations on a 100×100 lattice with periodic boundary conditions (filled circles). The two solid lines show for comparison low- and (dual) high-temperature series expansions [38] up to order 45 in the respective variables.

TABLE IV. Ground-state energies $E_{\min}/N$ of 2D q-state Potts spin-glass models with $q=2$, 3, and 4 as obtained from the REM scheme, the semianalytical DGREM approximation, and Monte Carlo (MC) minimization methods.

q	REM	DGREM	MC	DGREM/MC
2	−1.5599	−1.4758	−1.40193(2)	1.0527
3	−1.4020	−1.3156	−1.248(3)	1.054
4	−1.3333	−1.2297	−1.115(3)	1.103

Let us finally mention an upper bound for $E_{\min}(q)$ with $q\geqslant3$, which follows from the trivial inequality

$$-E_{\min}(q)=\frac{q}{q-1}\left[\left(\sum_{\langle ik\rangle}J_{ik}\delta_{s_is_k}\right)_{\max\{s_i=1,\ldots,q\}}\right]_{\mathrm{av}}$$

$$\geqslant\frac{q}{q-1}\left[\left(\sum_{\langle ik\rangle}J_{ik}\delta_{s_is_k}\right)_{\max\{s_i=1,2\}}\right]_{\mathrm{av}}$$

$$=\frac{q}{2(q-1)}[-E_{\min}(q=2)]. \tag{41}$$

Inserting the (almost) exact result for the ground-state energy of the Ising ($q=2$) spin-glass model, we obtain the (almost) exact bounds

$$E_{\min}(q=3)/N\leqslant-1.0510, \tag{42}$$

$$E_{\min}(q=4)/N\leqslant-0.9343. \tag{43}$$

IV. CONCLUSIONS

From Monte Carlo data for the energy as a function of temperature of the q-state Potts *ferromagnet*, we give an approximate expression for the ground-state energy of the q-state Potts *spin-glass* model by using the analogy with the DGREM scheme. The accuracy in two dimensions is about 5%–10%. The suggested method can be applied to other situations when graph theoretical or direct Monte Carlo investigations of the ground-state energy are too complicated.

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