Statistical Transfer Matrix of a Spin-Glass Ladder

Daniel C. Mattis* and Prabasaj Paul

Department of Physics, University of Utah, 115 S 1400 East, #201, Salt Lake City, Utah 84112

(Received 9 April 1999)

This work concerns the Edwards-Anderson Ising model of a spin ladder, in which random bonds $\pm J$ connect nearest-neighbor Ising spins. We calculate the exact free energy of the quenched, frustrated, spin-glass-like ladder as an integral over a probability distribution $P(x)$, the eigenfunction of a statistical transfer matrix. Our approach takes advantage of the *statistical* homogeneity of the spin glass.

PACS numbers: 75.10.Jm, 05.50.+q, 75.10.Nr

In the present Letter we obtain an exact, closed-form expression for the thermodynamic properties of the Edwards-Anderson (EA) model of an Ising spin glass [1] in the simplest geometry to exhibit frustration, i.e., the simple ladder of two linear chains connected by transverse bonds. In this geometry each new rung of the ladder brings in two spins and three new nearest-neighbor bonds, each of strength $\pm J$ with equal and independent probability.

We now distinguish two out of the many possibilities. In the *completely annealed* "bond-liquid" phase the bonds rearrange themselves to optimize the free energy; in this phase all thermodynamic properties are easy to calculate. In the *spin-glass* phase (SG) the same bonds are *quenched*—i.e., their $(\pm)$ signs are assigned at random and fixed ("frozen-in") at all temperatures. The thermodynamic properties in the SG phase are comparatively difficult to obtain. Indeed, the search for closed-form solutions of model spin glasses over the two decades spanning 1974 to 1994 introduced the replica method, ultrametricity, and other arcane procedures into the vocabulary of statistical physics [2]. A high-temperature series expansion has been carried out to the 15th order in $d \geq 3$ dimensions [3]. Yet, to date no method has been totally successful in clarifying the issues and there still does not exist a simple theory of the spin-glass problem comparable to the transfer matrix solution [4] of the ordinary two-dimensional Ising model, although some numerical studies do come close to it in spirit. For example, Morgenstern and Binder [5] performed a row-by-row evaluation of the partition function and claimed excellent results as compared with the usual Monte Carlo approach. Saul and Kardar [6] reduce a finite-sized strip to a sum over closed random walks of fixed length, each to be averaged over random configurations. Our procedure systematizes their approaches and makes a transparent, closed-form solution possible in the ladder geometry. It also allows for a coherent formulation of glassy models in 2D and 3D, even if the solution does become vastly more complex with increasing numbers of degrees of freedom.

Each of N spins is allowed two values, $S_n = \pm 1$. In the EA version of the Ising model, each nearest-neighbor bond J_{ij} is allowed just two values, $J_{ij} = \pm J$. (A bond $-J$ promotes parallel nearest-neighbor spins whereas $+J$ promotes antiparallel nearest neighbors.) Whether the system is annealed or quenched, the energy H is the sum of all nearest-neighbor interactions $J_{ij}S_iS_j$, with each such term being either $+J$ or $-J$. The free energy is then

$$F = -kT \log Z, \quad \text{where } Z = \mathrm{Tr}\{\exp(-H/kT)\}. \quad (1)$$

The trace is over *both* the 2^N configurations of the N spins *and* the *allowed* subset of $2^{3N/2}$ distinct configurations of the $3N/2$ bonds of the spin ladder. Stipulating this subset defines the type of randomness being imposed. For example, in the bond-liquid version *all* $2^{3N/2}$ possible bond states are allowed with equal weight, whereas in the SG phase, just one is—and it is chosen at random. Thus the entropies of the two phases will be quite different. Assuming $\langle J_{ij}\rangle = 0$, $\langle J_{ij}J_{kl}\rangle = J^2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ and defining $K = J/kT$, the *annealed* bond-liquid partition function is $Z_{\mathrm{anneal}} = 2^N \prod_{(ij)}[2\cosh K]$, with a corresponding free energy

$$F_{\mathrm{anneal}} = -NkT \log 2 - \tfrac{3}{2}NkT \log[2\cosh K]. \quad (2a)$$

We note that at $T = 0$ the limiting value of Eq. (2a) yields a highly degenerate ground state of energy [7] $E_{0,\mathrm{anneal}} = -\frac{3}{2}NJ$ and a ground-state entropy $S_{0,\mathrm{anneal}} = Nk \log 2$ to which both spin and bond degrees of freedom contribute. It is convenient to eliminate the bonds' contribution $3/2Nk \log 2$ and to define a "pseudoannealed" free energy:

$$\begin{aligned} F_{\mathrm{pseudo}} &= F_{\mathrm{anneal}} + (T \times \text{bond entropy}) \\ &= \tfrac{1}{2}NkT \log 2 - \tfrac{3}{2}NkT \log[2\cosh K]. \end{aligned} \quad (2b)$$

This is the quantity most closely comparable to the free energy of the quenched SG.

In the quenched SG phase only *one* configuration of the J_{ij}'s, say $\{J_{ij}\}$, is to be selected. Given this $\{J_{ij}\}$ the partition function $Z(\{J_{ij}\})$ is to be computed as the trace of $\exp(-H\{J_{ij}\}/kT)$ over the 2^N spin configurations. Because translation invariance is broken in the overwhelming majority of configurations the calculation of each $F(\{J_{ij}\}) \equiv -kT \log Z(\{J_{ij}\})$ is a real challenge. Nor is any given $F(\{J_{ij}\})$ representative of the thermodynamic free energy. It is only after an appropriate averaging of all $F(\{J_{ij}\})$'s that one obtains a quantity $\mathcal{F} \equiv -kT\langle \log \mathrm{Tr}_{\mathrm{spins}}\{e^{-H/kT}\}\rangle_{\mathrm{bonds}} = \langle F(\{J_{ij}\})\rangle_{\mathrm{bonds}}$ which is

both homogeneous and extensive and which correctly represents the *thermodynamic* free energy. Identical considerations of course also apply to the two-, three-, and higher-dimensional spin glasses and to other models of disordered spins. This need to average log$Z$ rather than Z is what originally informed the replica method in the study of random systems [2]. However, this need is entirely eliminated in the present approach in which the free energy naturally and conveniently averages itself.

The ladder under consideration is best visualized as a chain of plaquettes laid end to end, as illustrated in Fig. 1. Frustrated plaquettes have one or three antiferromagnetic bonds (of type $+J$) and have a minimum energy $-2J$. Unfrustrated plaquettes have zero, two, or four antiferromagnetic bonds and a minimum energy of $-4J$ [8]. As the probability of any given plaquette being frustrated is 50%, the average ground-state energy in the quenched state lies halfway between that of the totally frustrated case $-\frac{1}{2}NJ$ and the minimum energy $-\frac{3}{2}NJ$ and is therefore $E_{0,\mathrm{SG}} = -NJ$. Thus we find that in an infinite ladder the SG ground-state energy exceeds that of the annealed phase by *precisely* $0.5J$ per spin [9].

With "1" labeling spins on the first chain and "2" on the second and n labeling the distance along the chains, we next introduce variables $L_n = \mathrm{sgn}(J_{1,n,2,n}) \times S_{1,n}S_{2,n} = \pm 1$ with which to replace the $S_{2,n}$. Noting the identity $S_{i,n}^2 = 1$ and making use of gauge transformations $S_{i,n} \to -S_{i,n}$ wherever necessary, we obtain H in canonical form:

$$H = -J\sum_n S_{1,n}S_{1,n+1}(1 + L_nL_{n+1}) + \sum_n J_nL_n, \quad \text{with } J_n = \pm J\,. \tag{3}$$

The transformations were chosen so as to decouple the $S_{1,n}$ spins in the first chain from the new, lumped, random variables $\{J_n\}$. Performing a partial trace over the $S_{1,n}$ results in

$$Z_{\mathrm{SG}} = \lambda^{N/2}\,\mathrm{Tr}'\Big\{\prod_{n=1}^{N/2} e^{(K^*L_nL_{n+1}+K_nL_n)}\Big\} = \lambda^{N/2}\,\mathrm{Tr}'\{V_1 \cdot V_2 \cdots V_n \cdots V_{N/2}\}, \tag{4}$$

in which $\lambda = 2\sqrt{\cosh 2K}$, $\tanh K^* = \tanh^2 K$ and $K_n = J_n/kT = \pm K$ are the new parameters. The prime in Tr' indicates the remaining trace is over the L_n's only. The problem has thus been mapped onto that of a chain of Ising spins L_n in a random external "magnetic field" $\pm J$ and connected by nearest-neighbor bonds $J^* \equiv K^*kT$. Because $J > J^*$ always, the random pseudofield term dominates at all $T > 0$, precluding an order/disorder phase transition at any finite temperature in this particular model.

We identify the factors in (4) as 2×2 matrices $V_n = \begin{bmatrix} e^{K^*+K_n} & e^{-K^*+K_n} \\ e^{-K^*-K_n} & e^{K^*-K_n} \end{bmatrix}$ and Tr' as their inner product. They are of two types: $V(K_n = +K)$ and $V(K_n = -K)$; the two do not commute. The individual K_n are random variables fixed at $\pm K$ with equal probability; the very last trace operation over $\mathbf{V} \equiv V_1 \cdot V_2 \cdots V_n \cdots V_{N/2}$ in (4) sums the *two* eigenvalues of $\mathbf{V}$. However, we note that the ratio of the two eigenvalues of $\mathbf{V}$ is $O(\exp(-\alpha N))$, where α is some function of K, and therefore only the larger of the two eigenvalues survives in the thermodynamic limit $N \to \infty$; it in effect equals the trace to within an exponentially vanishing error. The larger eigenvalue is also the one whose eigenvector has only positive entries, interpretable as probabilities. It is therefore the only physically acceptable solution.

Using a normalization conventional in statistical physics we take for the initial 2-vector $\mathbf{x}_1 \equiv [x_1, (1 - x_1)]$, with x_1 expressing the probability of L_1 pointing "up" (we take it to be in the range $0 < x_1 < 1$) and $(1 - x_1)$ the probability of its pointing "down." We use it to generate the above-mentioned eigenvalue and eigenvector constructively, taking the inner product $\mathbf{x}_1 \cdot V_1 = \chi_1\mathbf{x}_2$ to obtain the resulting probabilities of L_2 being up (x_2) or down $(1 - x_2)$, and iterate the process up to the nth matrix, where n is an arbitrary large number which can be as large as $N/2$. Periodic boundary conditions require setting $\mathbf{x}_{N/2+1} = \mathbf{x}_1$. The unique result is $(\prod_{j=1}^{n}\chi_j)\mathbf{x}_{n+1}$ in which each factor χ_j is >0. Writing y for x_n and x for x_{n+1}, the general recursion relation is, explicitly,

$$[y, 1 - y]V_n = \chi_n[x, 1 - x]. \tag{5}$$

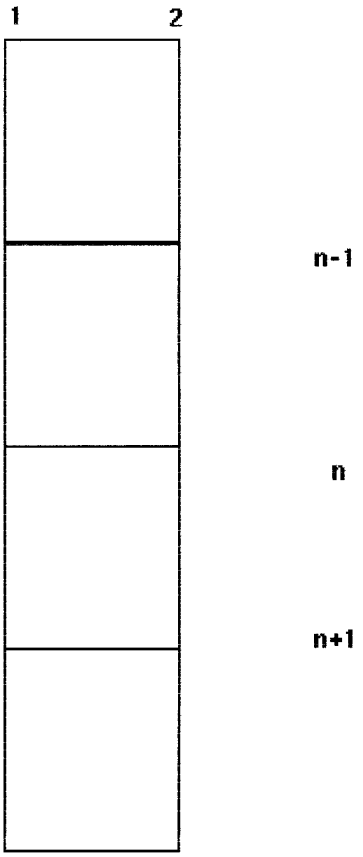

FIG. 1. Illustration of the ladder geometry. The vertices indicate spins $S_{j,n}$ ($j = 1$ or 2 and $n = 1, 2, \ldots, N$), which are connected by nearest-neighbor bonds $\pm J$.

For a given x there are two possible values of y (depending on the two values of K_n) only one of which is realized, at random. At each step two more values are generated, ultimately seeding the entire interval $0 < x < 1$. Thus, the *logarithm* of the resulting partition function $Z_{\mathrm{SG}} = \lambda^{N/2} \prod_{j=1}^{N/2} \chi_j$ is *automatically* self-averaging over the random variables. We find

$$\mathcal{F} = -kT\left\{\frac{N}{2}\log\lambda + \sum_{j=1}^{N/2}\log\chi_j\right\} = -\frac{J}{2K}N\{\log\lambda + \langle\log\chi\rangle\}. \tag{6}$$

At each temperature (or K) we need to evaluate $\langle\log\chi\rangle \equiv \int dx\, P(x)\log\chi(x)$ using an appropriate probability distribution $P(x)$. Equation (5) defines a mapping $x \leftrightarrow y$ remarkably similar to that which governs the distribution ρ of normal modes in a chain of disordered, random masses and springs [10]. The major difference resides in the physical nature of the variables. Here the independent variable is K rather than ω^2, and the dependent variable is $\mathcal{F}(K)$ [from which we can obtain $E(T)$, $S(T)$, or $C(T)$ in the usual way], rather than the density of normal modes $\rho(\omega^2)$. In fact, the exact and novel solution by Fourier transformation derived below can easily be adapted to random chains and complements a large number of attempts to solve that problem, some of which are reviewed in Ref. [10].

Although the *individual* spinors $[x_n, (1 - x_n)]$ *necessarily* vary from site to site, their *probability* distribution $P_n(x_n) = P(x_n)$ does *not.* This invariance is the result of periodic boundary conditions [11] which mandate the *statistical* homogeneity of what is inherently an inhomogeneous medium. From Eq. (5) we deduce that $P(x)$ satisfies the equation

$$P(x) = \left[p_1\frac{dy_1(x)}{dx}P(y_1(x)) + p_2\frac{dy_2(x)}{dx}P(y_2(x))\right]. \tag{7}$$

Setting p_1 and $p_2 = 1 - p_1 = \frac{1}{2}$ reflects equal probabilities of y_1 or y_2 mapping onto x. Here

$$y_1(x) = \frac{e^K}{2\sinh K}\left[\frac{\tanh^2 K + (2x - 1)}{\tanh K + (2x - 1)}\right], \qquad y_2(x) = \frac{e^{-K}}{2\sinh K}\left[\frac{\tanh^2 K + (2x - 1)}{\tanh K - (2x - 1)}\right]. \tag{8}$$

The coefficient in (5) is $\chi_n(y) = (2\cosh K^*)[ye^{K_n} + (1 - y)e^{-K_n}]$. Because y depends only on the set of K_j with $j < n$ but not on K_n, one must average $\log\chi$ separately over K_n and y. There results a translation-invariant free energy density, independent of local details:

$$\mathcal{F}/NJ = -\tfrac{1}{2}K^{-1}\left\{\log\lambda + \log(2\cosh K^*) + \tfrac{1}{2}\int_0^1 dx\, P(x) \times \log[1 + 4x(1 - x)\sinh^2 K]\right\}. \tag{9}$$

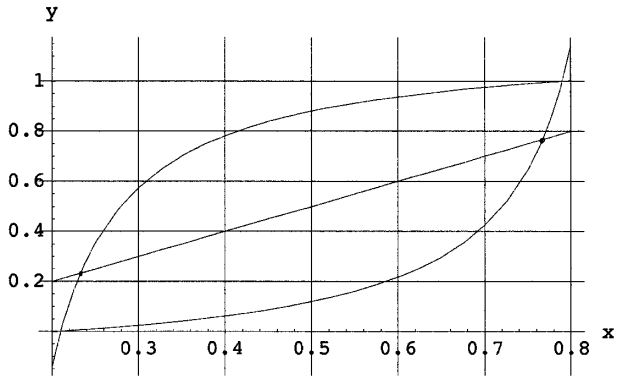

FIG. 2. The mapping: $y_1(x)$ (upper curve), $y_2(x)$, and x plotted vs x for a representative $J/kT \equiv K = 1$. The two critical points $xc[1]$ and $xc[2]$ are the intersections of the y's with x.

For ready comparison we write F_{pseudo} in the same format [12],

$$F_{\mathrm{pseudo}}/NJ = -\tfrac{1}{2}K^{-1}\{\log\lambda + \log(2\cosh K^*) + \log(\cosh K)\}, \tag{10}$$

and define the difference as $\Delta F/N$, the "excess free energy density" stored in the frozen bonds of the SG:

$$\Delta F/N = (\mathcal{F} - F_{\mathrm{pseudo}})/N = -\frac{J}{4K}\int_0^1 dx\, P(x)\log[1 - (1 - 2x)^2\tanh^2 K]. \tag{11}$$

$\Delta F/N$ vanishes at $K \to 0$ and correctly tends to $0.5J$ as $T \to 0$ $(K \to \infty)$.

The form of the solution $P(x)$ of Eq. (7) is analyzed by plotting the target curves $y_i(x)$, illustrated in Fig. 2 for $K = 1$. This plot identifies the two stable fixed points $y_i(x) = x$, denoted $xc[1]$ and $xc[2] = 1 - xc[1]$. In Fig. 3 we plot them as functions of K. Because $p_1 = p_2$, $P(x)$ is symmetric about $x = \frac{1}{2}$. It vanishes outside the range $xc[1] < x < xc[2]$. Inside the range it is discontinuous *everywhere;* the two fixed points are points of accumulation. Its integral, $W(x)$, is a "devil's staircase." The numerical solution of Eq. (7) by iteration is unstable

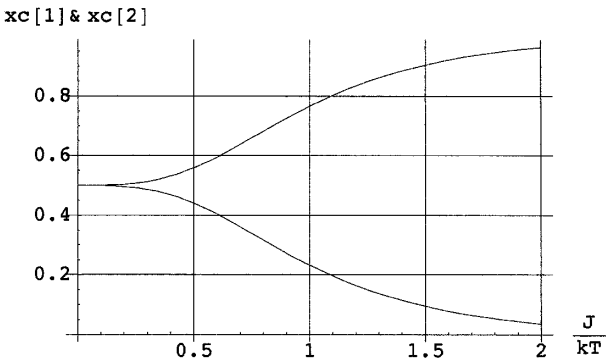

FIG. 3. Critical points $xc[1]$ and $xc[2]$ defined in Fig. 2, plotted as functions of K.

when one uses only a small number of iterations but appears to settle down after seven or more, which corresponds to finite chains of 14 or more spins. Alternatively, we find this equation can be solved *exactly,* in principle, by Fourier transformation. One writes

$$P(x) = \left\{ \sum_{n=0}^{\infty} a_n \cos\left[\pi n \, \frac{1 - 2x}{xc[2] - xc[1]} \right] \right\} \Theta(x), \tag{12}$$

where $\Theta(x) = 1$ in the range $xc[1] < x < xc[2]$ and $= 0$ elsewhere. We set $a_0 = 1/(xc[2] - xc[1])$, as required for normalization. The a_n for $n \neq 0$ are then obtained explicitly as the solution of an *inhomogeneous* set of linear equations $a_n = \sum_m R_{n,m} A_m$, with

$$A_m = \frac{1}{(xc[2] - xc[1])^2} \int dx \cos\left(\pi m \, \frac{1 - 2x}{xc[2] - xc[1]} \right) \times [\Theta(y_1(x)) \, dy_1/dx + \Theta(y_2(x)) \, dy_2/dx]. \tag{13}$$

The relevant matrix is $\mathbf{R} = (\mathbf{1} - \mathbf{M})^{-1}$, where $\mathbf{1}$ is the unit matrix and

$$M_{n,m} = \frac{1}{(xc[2] - xc[1])} \int dx \cos\left(\pi n \, \frac{1 - 2x}{xc[2] - xc[1]} \right) \Theta(x) \times \left[\cos\left(\pi m \, \frac{1 - 2y_1(x)}{xc[2] - xc[1]} \right) \Theta(y_1) \, dy_1/dx + \cos\left(\pi m \, \frac{1 - 2y_2(x)}{xc[2] - xc[1]} \right) \Theta(y_2) \, dy_2/dx \right]. \tag{14}$$

Most of the eigenvalues of $\mathbf{M}$ are zero and the largest does not exceed 0.25 in magnitude at any K. Hence $\mathbf{R}$ is nonsingular. Equations (12), (13), and (14) together yield the exact solution to Eq. (7). With a supercomputer, inversion of 100×100 matrices should not prove too time-consuming and should prove quite accurate over a large range of K.

For this introductory work we have investigated an analytic approach which is easily implemented using a desk computer. It consists of approximating the function $y_1(x)$ by its straight line tangent at $xc[1]$, and similarly for y_2 at $xc[2]$. With $s_1 \equiv dy_1/dx|_{xc[1]}$ and $\xi \equiv x - xc[1] > 0$, the equation $P(\xi) = \frac{1}{2} s_1 P(s_1 \xi)$ has the solution $P \propto 1/\xi^{\alpha}$ near the singularity, with $\alpha = 1 - \log 2 / \log s_1$, and similarly near $xc[2]$. After an appropriate choice of cutoff and normalization this power law yields a useful approximation to P. The free energy is easily calculated as an integral over this function and is exhibited in Fig. 4. We have also obtained a qualitatively similar result (not shown), using the iterative solution of Eq. (7) [13].

We thank Professor Ben Bromley for preliminary discussions concerning the numerical evaluation of Eq. (7).

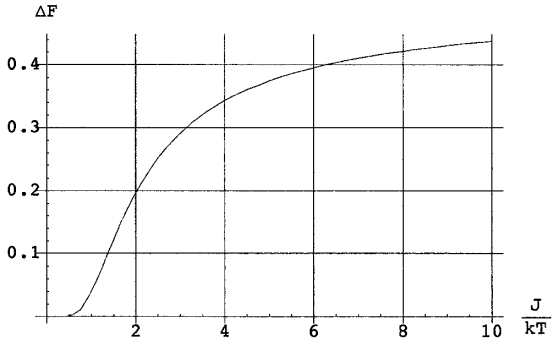

FIG. 4. Excess free energy density $\Delta F(K)/NJ$ as a function of K, calculated using the power-law approximation (see text). The asymptotic approach to the exact ground-state value 0.5 at $K \to \infty$ is observed to be *very* slow.

*Electronic address: mattis@mail.physics.utah.edu

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[7] No arrangement of Ising spins or $\pm J$ bonds can yield an energy lower than this value.
[8] Incidentally, this proves that there is no frustration in the annealed phase which, as shown above, is endowed with the optimal ground-state energy. Nearest-neighbor plaquettes share a bond; hence their thermodynamic functions are not independent and cannot be calculated trivially—making the ladder geometry more interesting than it might otherwise be.
[9] Not very different from the excess energy in 2D, estimated to be $\approx 0.6J$ (see Refs. [2,5,6]). [Remarkably, the ground-state energy of the EA spin glass is still not known exactly for infinite two- or three-dimensional systems, although numerical calculations on large samples are yielding ever smaller error bars; see D. Stauffer, Phys. World **May**, 23 (1999).]
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[11] With periodic boundary conditions all rungs are statistically identical; hence $P(x)$ must be independent of n. This is not affected by the use of different boundary conditions, as they can yield only a surface correction $O(1)$ to the chain's free energy, which is $O(N)$ and is identical to that obtained using periodic boundary conditions.
[12] The reader will verify that Eq. (10) agrees with Eq. (2b).
[13] Starting with a "seed" $P(x) = \delta(x - \frac{1}{2})$ the 7th iteration of Eq. (7) already seems to yield a stable distribution at all $K < 20$.