Partially frustrated Ising models in two dimensions

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We examine ordered, periodic, Ising models on a sq lattice at varying levels x of frustration. The thermodynamic singularity of the *fully* frustrated model ($x=1$) is at $T=0$ while those of *partially* frustrated lattices ($0<x\leqslant 1$) occur at finite T_c. The critical indices in the *partially* frustrated lattices that we consider—including the logarithmic specific heat—are all identical to those in the ferromagnet ($x=0$.) We display exact values of T_c and of ground-state energy and entropy E_o and $\boldsymbol{S}_o$, at $x=1$, 2/3, 1/2, 2/5,...,0.

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INTRODUCTION

This work discusses the phenomenon of partial ''frustration.'' [1] Interest in systems with ''frozen-in'' randomness, commonly denoted ''spin glasses,'' has continued unabated since the 1970s.[2] The only statistical systems with any chance of being solved in closed form are Ising-model spin glasses. These come in at least two varieties: site-centered random *gauge glasses* that can be analyzed completely and sometimes even solved exactly,[3] and those with competing $\pm J$ interactions that are *both* random *and* frustrated and generally cannot be solved at all. Toulouse identified *frustration* as the result of competing interactions.[4] The unit of frustration is a plaquette in which the product of J's around the perimeter has a negative sign.[5] Frustration increases both the ground-state energy and the ground-state entropy over their values in the ferromagnet. Ramirez[6,7] identified ''*geometrical* frustration'' as the disorder inherent in the correlation functions of what are frustrated but otherwise *structurally perfectly ordered* materials. (The prototype is the Ising antiferromagnet on a regular, triangular lattice, about which more will be said later. Other well-known examples include *ice* at 0 °C and the *pyrochlores*.[5,6]) Still, in the words of Ramirez,[6] ''... there is comparatively little known about [such] materials,'' although, at first blush, geometrically frustrated materials seem to share many properties with *structurally random* glassy materials having random bonds and/or fields at every site.

The present work sets out to distinguish between the two. It is introductory and admittedly incomplete, but because our results are exact they may serve as markers in a field that is not fully understood. We show that under certain circumstances a sharp distinction can be drawn between *partially frustrated* systems (the usual case) and the *disordered* systems they superficially resemble. We display exact values of ground-state entropy $\boldsymbol{S}_o$, ground-state energy E_o, critical temperature T_c, and quasiparticle dispersion calculated at some discrete values of x (where x is the fraction of frustrated plaquettes). We also indicate possible directions for future investigations.

As a brief example of how much disordered and frustrated systems can resemble one another, consider the apparently random Edwards-Anderson-Ising spin ladder in Fig. 1, containing nearest-neighbor bonds $J_{i,j}=\pm J$ in $H=-\Sigma_{(i,j)}J_{i,j}S_iS_j$. By gauge transformations $S\rightarrow -S$ on just 2 sites (1 and 2), it transforms into a *regular array* in which the antiferromagnetic (AF) bonds are all on the left vertical riser and all other bonds are ferromagnetic. Among the many ground states[8] of this configuration one finds two ferromagnetic states (all spins up or all down) and a ground-state energy $E_0=-4|J|$. Except in its response to an external field, this model is an example of perfect geometrical frustration (i.e., $x=1$) and *not* of disorder! Later we shall see that merely specifying the extent of frustration x in the range $0<x<1$ is *also* generally *insufficient* to determine whether this model or material can support an ordered phase.

In trying to understand and systematize the distinction between random and geometrically frustrated systems, we propose a classification scheme. Type A is representative of pure geometrical frustration, such as the nearest-neighbor Ising model on a triangular lattice with *all* equal antiferromagnetic (AF) bonds in which *all* plaquettes are frustrated ($x=1$.) The thermodynamic properties of this model are known:[9] it has no ordered phase at $T>0$. Geometrically frustrated systems such as this can only sustain disordered phases at finite T while others (frustrated chessboard or frustrated hexagonal lattices) maintain a finite correlation length even at $T=0$ and thus possess no critical exponents whatever.[9]

Type B: the Edwards-Anderson (E-A) model[1] on the two-dimensional sq lattice is a prime example of a magnetically amorphous material in which spin-glass behavior is *caused* by the *randomness*. In it, Ising spins $S_i=\pm 1$ are subject to randomly frozen-in nearest-neighbor (NN) bonds $J_{i,j}=\pm J$. The prototype E-A model consists of a sq lattice with a fraction $p=\frac{1}{2}$ of antiferromagnetic ($J<0$) bonds located at random. This causes half the plaquettes, on average, to become frustrated, i.e., $x=\frac{1}{2}$. The location of the frustrated plaquettes is random. In two dimensions this model does not exhibit a phase transition at any finite T (although it may in higher dimensions.)

The Hamiltonian in the E-A model is $H=-\Sigma_{(ij)}J_{i,j}S_iS_j$, the sum being over NN's. Its partition function is $Z=\mathrm{Tr}\{\exp-\beta H\}$. But it is the free energy, $F=-k_BT\ln Z$ and not Z that needs be averaged over the random variables. In addition to the temperature $T=1/k_B\beta$ one needs consider at least one supplementary material parameter.[10] This extra parameter is frequently taken to be p, the fraction of AF (–) bonds.[11]

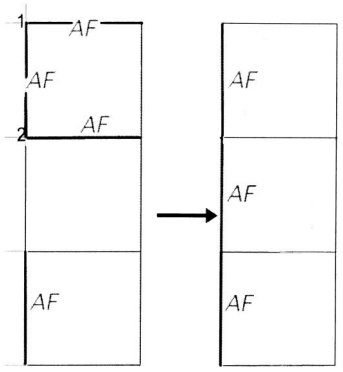

FIG. 1. Random, or ''ordered but geometrically frustrated?'' Heavy lines are AF bonds, light lines are ferrmagnetic. The apparently disordered ladder on the left turns into an ordered (but equally frustrated!) ladder after two spins are ''flipped'' by a gauge transformation: $S_1 \rightarrow -S_1$ and $S_2 \rightarrow -S_2$.

The *fully frustrated Ising model* (FFIM), illustrated in Fig. 2(a),[11] has $p=\frac{1}{4}$ and $x=1$. Any additional, or any fewer, antiferromagnetic bonds necessarily decrease the fraction x of frustrated plaquettes. As illustrated, this model does not exhibit any structural randomness. Taking the unit cell to consist of two neighboring columns, this model exhibits translational periodicity—no less so than does the triangular lattice with all antiferromagnetic bonds. It is therefore of type A. By trivial gauge transformations it can be made to *look* perfectly random and seemingly impossible to solve by the ordinary methods of statistical mechanics! Yet it has been known[11] to be solvable since 1977.

The FFIM has already been the subject of several investigations, including a mapping onto eight-vertex models, renormalization-group (RG) studies, etc.,[12,13] that revealed a sort of ''phase transition'' at $T_c=0$ with a power-law correlation function $\propto 1/r^{\eta}$, exponent $\eta=\frac{1}{2}$. The divergent $T=0$ paramagnetic susceptibility calculated by Kandel, Ben-Av, and Domany,[12] $\chi \propto L^{2-\eta}$, with $\eta=0.507\pm0.009$, confirms this unusual value of η that is shared with the triangular AF lattice,the prototype of species A.[13] Both have $T_c=0$ and comparable ground-state entropies *per* site. Additional symmetries, including some form of *duality*, have been uncovered in other fully frustrated models and may exist here also.[14,1]

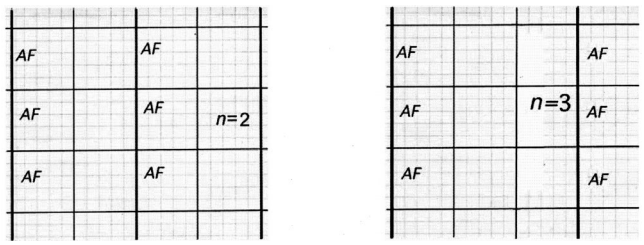

FIG. 2. The frustrated 2D Ising model on a sq lattice. (a) FFIM: special case of n (number of columns in a unit cell)$=2$. Spins $S=\pm1$ live at each vertex, with nearest neighbors connected by ferromagnetic (light lines) or antiferromagnetic bonds (heavy lines.) A unit cell consists of 2 vertical lines (one of antiferromagnetic bonds and one of ferromagnetic bonds.) Horizontal lines contain only ferromagnetic bonds. (b) Illustrating the periodic, *partly* ($x=2/3$) frustrated, 2D Ising model for $n=3$.

Type C: Regular, homogeneous, systems with partial frozen-in frustration. The Ising versions have finite values of T_c, hence an ordered low-temperature phase (and $\eta=\frac{1}{4}$ in two dimensions). This is the category denoted ''*partially frustrated*,'' that is studied below.

DISTINCTION BETWEEN TYPES

Type-C systems exhibit *some* geometrical frustration and their ground states are typically degenerate. But unlike type A, they support an ordered phase and unlike type B they are not random (although the unit cell may be large). By an obvious gauge symmetry of the sq lattice, or of bipartite lattices in general, $F(1-p)=F(p)$ in the absence of finite external fields. Hence we can (and shall) limit our studies to $0<p\leqslant\frac{1}{2}$.

At the upper limit of $p=\frac{1}{2}$ one uncovers a fundamental difference between types C and B in two dimensions. Consider the following type-C model on a sq lattice: all vertical bonds are antiferromagnetic $(-)$ and all horizontal bonds are ferromagnetic $(+)$. Not a single plaquette is frustrated and there is a phase transition from disorder to an ordered phase as one lowers T below a critical temperature. This is to be contrasted with the E-A model at $p=\frac{1}{2}$ on the same lattice, which is of type B. As we have already noted, in the latter case half the plaquettes are frustrated on average and $T_c=0$. So just specifying the fraction p of antiferromagnetic bonds does not tell us what thermodynamic phase diagram can be expected.

But then, neither is the fraction x of frustrated plaquettes indicative of the thermodynamic properties that are to be expected! For example, the thermodynamic behavior of the above-mentioned two-dimensional E-A model ($x=\frac{1}{2}$) differs completely from that of the $n=4$ model of type C investigated below (in which $x=\frac{1}{2}$ also). Unlike the former, the latter has a second-order phase transition and supports an ordered low-temperature phase.

THIS WORK

We investigate the range $p=1/(2n)=\frac{1}{4}, \frac{1}{6}, \frac{1}{8}, \ldots,$ all $\leqslant\frac{1}{4}$, where n $(n\geqslant2)$ is the number of columns in the unit cell.[15] In the regular example illustrated in Fig. 2(b), each unit cell of n columns contains one AF vertical and two ferromagnetic vertical lines and corresponds to $x=\frac{2}{3}$. (All horizontal bonds are ferromagnetic.) In general, for $n-1$ ferromagnetic vertical lines the fraction of frustrated plaquettes is $x=2/n=4p=1, \frac{2}{3}, \frac{1}{2}, \ldots$. Geometrical regularity, such as it is, allows us to calculate the free energy using an (exact) transfer-matrix approach. Unfortunately this method does not easily extend to higher p where the system is *also* partially frustrated. Clearly the range $\frac{1}{4}\leqslant p<\frac{1}{2}$ is complementary to what we cover on the present work and represents an important area of investigation for the future, whether studied by exact methods, numerical methods or RG.

In the present work, we find that—with the singular ex-

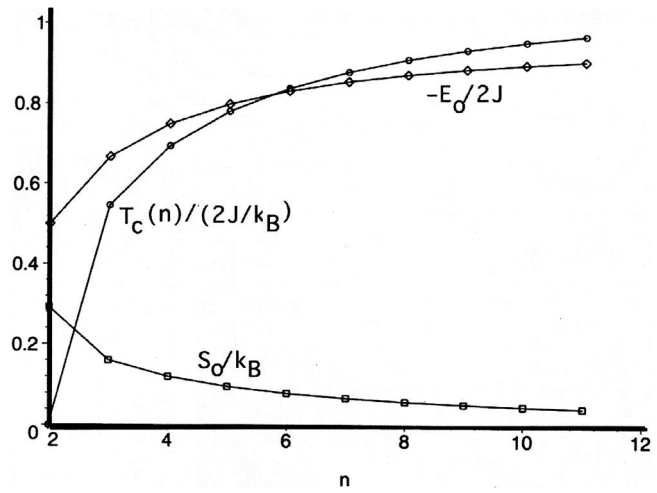

FIG. 3. Calculated ground-state energy (times -1): $-E_o(n)$ ($\diamond$), ground-state entropy $S_0(n)$ ($\square$), and critical temperature of the order-disorder phase $T_c(n)$ ($\bigcirc$), as functions of n, for $n=2$ (i.e., FFIM) and $n=3$, 4,.... (Lines connecting points are just a visual aid.) Note: $x=2/n$, the fraction of frustrated squares, ranges from 1 to 0.

ception of $n=2$ (for which $x=1$, the FFIM which is actually of type A)—the columnar models of type C for $n>2$ all have an order-disorder phase transition at finite $T_c(n)$ and share *all* critical exponents at T_c with those in the limit $n=\infty$, i.e., with the ferromagnetic two-dimensional (2D) Ising model.

The precise value of T_c increases with n. This is shown in Fig. 3 at the discrete values of $n=2,3,4,5,...$, i.e., for $x=1$, $\frac{2}{3}$, $\frac{1}{2}$, $\frac{2}{5}$,.... For $n\gg 1$, we obtain the asymptotic dependence of $T_c(n)$ on n,

$$\sinh 2J/kT_c = 1 + \frac{1.2465}{n} + o(1/n). \tag{1}$$

This formula agrees with the classic result in $\lim n\to\infty$. Our solution is obtained by transforming the transfer matrix into an exponential form in free fermions, following Onsager's procedure (cf. the detailed review).[16] The dispersion of the free fermions exhibits a mass gap at all T except precisely *at* T_c. At all values of $n>2$ the appearance of the mass gap, both above and below T_c, and its disappearance *at* T_c, parallels the behavior in the two-dimensional Ising ferromagnet. Minor discrepancies manifest themselves only at the Brillouin-zone boundaries.

DETAILS

Here we outline details of the calculations. The partition function is given by the largest value of the transfer matrix, evaluated along the horizontal direction, in which all the bonds are ferromagnetic (in order to avoid imaginary terms that occur in the exponent of the *vertical* transfer matrix). In its Hermitean representation, our transfer matrix consists of three factors for each unit cell. These have to be combined and Fourier transformed, following the Jordan-Wigner transformation to fermion operators labeled by q. The largest eigenvalue of this transfer operator then takes the form $Z=\Pi_{q>0}Z_q$, where

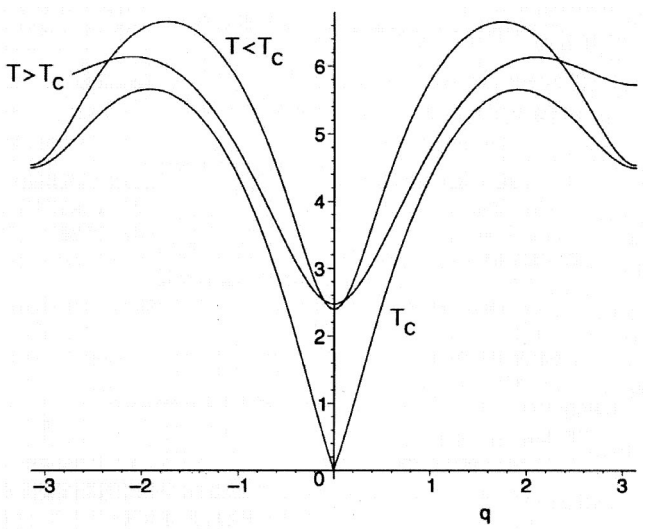

FIG. 4. $\varepsilon(q)$ vs q below, at, and above T_c. This figure illustrates the quasiparticle spectrum of the transfer matrix at three temperatures. In this example calculated at $n=3$, they are T_c (given by $\sinh 2J/kT_c=2$) and T substantially below or above T_c (as given by $\sinh 2J/kT=5$ or 1.) One notes the appearance and disappearance of the mass gap and the apearance (albeit irrelevant to the critical-point thermodynamics) of novel structure near the Brillouin-zone boundaries at $q=\pm\pi$.

$$Z_q=[A^2(T)]^n e^{\varepsilon_q(T)}, \tag{2}$$

in which $A^2(T)=2\sinh 2J/kT$ and $\varepsilon_q(T)$, defined in terms of q, f_q, and ϑ_q, describe the quasiparticle dispersion. It is the largest real solution of the following set of equations:[17]

$$\cosh\varepsilon_q(T)\equiv\cosh nf_q\cosh 4J/kT - \sinh nf_q\sinh 4J/kT\sin\vartheta_q, \tag{3a}$$

$$\cosh f_q(T)\equiv\frac{\cosh^2 2J/kT}{\sinh 2J/kT}-\cos q, \tag{3b}$$

and

$$\sinh f_q(T)\sinh\vartheta_q(T)\equiv\cosh 2J/kT-\coth 2J/kT\cos q. \tag{3c}$$

Thanks to some additional symmetries, the result for $n=2$ can be simplified and agrees with that given explicitly by Villain.[11,18] It is the only instance in which $T_c=0$.

Generally, Eqs. (3) have to be solved numerically, as we have done at various values of n. Choosing a typical value, $n=3$, in Fig. 4, we display the calculated dispersion in the free fermion spectrum $\varepsilon(q)$ at three different temperatures: T lower than, equal toand higher than $T_c(n)$, this last being the temperature at which the gap disappears. Based on the premise that *all* critical thermodynamic quantities are func-

tionals of the dispersion relations at small q (long wavelengths) we are now able to conclude that all systems of type C ($n>2$) belong to the same universality class as the ferromagnet ($n\to\infty$.)

The ground-state energy is found by inspection,[19] but the ground-state entropy $\boldsymbol{S}_o$ requires more study. For $n=2$ is it easily computed by differentiating the free energy at $T=0$; this yields:[20] $\boldsymbol{S}_o/k_B=0.2916...$. At larger n a similar procedure could be used, although the formulas are enormously more complicated.

It is more practical to calculate $\boldsymbol{S}_o$ as follows: starting from the fully ferromagnetic state, one counts the degenerate configurations created by flipping any number of spins on any AF column, subject to the rule: *no two flipped spins are nearest neighbors*. For all $n\geqslant 3$, neighboring AF columns constitute domain walls that are statistically independent in the ground state. A one-dimensional calculation yields the exact ground-state degeneracy and ground-state entropy *per spin*.[21] After some algebra we obtain $\boldsymbol{S}_o$ in terms of the golden mean. It vanishes as $1/n$, i.e., as $\propto x$ in $\lim x\to 0$:

$$\frac{1}{n}\ln\frac{1+\sqrt{5}}{2}\approx\frac{0.4812}{n}=\boldsymbol{S}_o/k_B \quad (n\geqslant 3). \tag{4}$$

CONCLUSION

Frustration promotes violation of Nernst's ''third law'' (the presumption that the ground-state entropy *per* particle vanishes). In the presence of finite ground-state entropy the critical temperature for the order-disorder phase transition is lower than it might otherwise be. We have determined for a class of partly frustrated, geometrically ordered models, that once the amount of frustration is insufficient to suppress a phase transition at finite T the critical indices at T_c revert to those of the pure ferromagnet. These are exact results in our model, yet they do not speak to models of type B in which ''percolation'' and disorder may be playing an additional role. To finally close this chapter it will be necessary to find a convenient way to introduce a controlled amount of disorder and to extend the analysis into a region $\frac{1}{4}\leqslant p\leqslant\frac{1}{2}$ that remains inaccessible by present means.

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[1] Basically, extending R. Liebmann's treatise *Statistical Mechanics of Periodic Frustrated Ising Systems* (Springer-Verlag, Berlin, New York, 1986).

[2] Ising spins with random nearest-neighbor interactions were introduced by S. F. Edwards and P. W. Anderson, J. Phys. F: Met. Phys. **5**, 965 (1975), and with long-range interactions, by D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1792 (1975); see also D. Chowdhury and A. Mookerjee, Phys. Rep. **114**, 1 (1984).

[3] For example, the model of Ising or X-Y glass in which the two-spin interaction parameters are $J_{i,j}=J\varepsilon_i\varepsilon_j$, in which each of N parameters $\varepsilon_i=\pm 1$ is frozen in at random, as in D. C. Mattis, Phys. Lett. **A56**, 421 (1976); The case of a gauge glass with infinite-ranged interactions (mean-field limit) was recently solved in some detail by P. Sollich, H. Nishimori, A. Coolen, and A. van der Sijs, J. Phys. Soc. Jpn. **69**, 3200 (2000).

[4] G. Toulouse, Commun. Phys. (London) **2**, 115 (1977).

[5] Upon defining $J>0$ for ferromagnetic and <0 for antiferromagnetic interactions.

[6] A. P. Ramirez, in Annu. Rev. Mater. Sci. **24**, 453–480 (1994).

[7] A. P. Ramirez, in *Handbook of Magnetic Materials*, edited by K. Buschow (Elsevier, Amsterdam, 2001), Vol. 13, Chap. 4.

[8] Exercise for the reader: how *many* ground states are there in this simple example? Note: if *all* the bonds had been *ferromagnetic* (or all antiferromagnetic) the two ground states would have had energy $E_0=-10|J|$ and *all remaining* 254 configurations would have been higher.

[9] G. Wannier, Phys. Rev. **79**, 357 (1950); and R. Houtappel, Physica (Amsterdam) **16**, 425 (1950) studied the frustrated triangular lattice; several more sophisticated models introduced subsequently, notably by W. F. Wolff and J. Zittartz, Z. Phys. B: Condens. Matter **47**, 341 (1982); **49**, 229 (1982); **50**, 131 (1983), are reviewed in Ref. 1, p. 68 ff. These include some that have no phase transition and maintain a finite correlation length even at $T=0$, such as the frustrated chessboard and hexagonal lattices; [these have been denoted ''superfrustrated'' by A. Süto, *ibid.* **44**, 121 (1981).]

[10] We restrict ourselves to zero fields (hence to zero-field susceptibility) in order to be able to solve the various models explicitly.

[11] This model is the creation of J. Villain, J. Phys. C **10**, 1717 (1977), see also G. Forgacs, Phys. Rev. B **22**, 4473 (1980). The ground-state analysis was extended by E. H. Lieb and P. Schupp, Phys. Rev. Lett. **83**, 5362 (1999) to the Heisenberg model, in the case of the geometrically frustrated pyrochlore checkerboard lattice.

[12] D. Kandel, R. Ben-Av, and E. Domany, Phys. Rev. Lett. **65**, 941 (1990); Phys. Rev. B **45**, 4700 (1992).

[13] J. Stephenson, J. Math. Phys. **11**, 420 (1970).

[14] H. Nishimori and K. Nemoto, J. Phys. Soc. Jpn. **71**, 1198 (2002); H. Nishimori, *Statistical Physics of Spin Glasses and Information Processing*, (Oxford University Press, Oxford, 2001).

[15] We do not treat $n=1$, as we have already seen it to be trivial.

[16] T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964).

[17] The actual derivation of Eqs. (3) is too lengthy to show here, but it will be detailed elsewhere.

[18] See also D. C. Mattis, *Statistical Mechanics Made Simple* (World Scientific, Singapore, 2003), Chap. 8.

[19] Because the ferromagnetic state is among the ground states, the ground-state energy (in units of J) is just $E_0/J=-2N+2N_{AF}$, where $2N$ is the total number of bonds and N_{AF} is the total number of AF bonds.

[20] I. Guim, T. Burkhardt, and T. Xue, Phys. Rev. B **42**, 10 298 (1990) find this number to be G/π, where $G=$Catalan's constant$=0.915\,966...$, and we confirm this result. When evaluated, the formula in Villain's original work (Ref. 11) appears to give a value twice as large.

[21] At $n=2$ the columns *do* interact and Eq. (4) is just a lower bound to the FFIM entropy (yet remains remarkably close to the exact value 0.2916).