

In conclusion, by combining our recursive calculation of partition functions of finite disordered systems with simulations, we have separated equilibrium from nonequilibrium effects. From the size dependence we conclude that there is no nonzero order parameter for  $d=2$  Ising  $\pm J$  spin-glasses, although there are strong spin correlations over large distances at low temperatures. Applications of our method to  $c \neq \frac{1}{2}$  and Ising systems with random fields are in progress.<sup>22</sup> Clearly, this method should yield useful results for a large class of models for disordered materials. In addition, investigating a possible power-law decay of correlations theoretically from the point of view of frustration and gauge invariance<sup>12,14</sup> would be very interesting.

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<sup>13</sup>To reduce fluctuations going from one realization  $\{J_{ij}\}$  to another one, we furthermore require (at  $c = \frac{1}{2}$ ), for each individual realization, that  $\sum_{\langle i,j \rangle} J_{ij} = 0$ , and that the concentration of frustrated plaquettes [G. Toulouse, Commun. Phys. **2**, 115 (1977)] exactly equals  $\frac{1}{2}$ . These conditions follow from  $P(J_{ij})$  for  $N \rightarrow \infty$  but would hold only approximately for finite  $N$ . This "restricted"  $P(J_{ij})$  is also a valid distribution for a spin-glass, of course.

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## Frustration Effect in Quantum Spin Systems

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We have calculated the ground-state properties of the  $s = \frac{1}{2}$  XY and Heisenberg models on finite triangular and square lattices with competing interactions which would lead to frustrated classical spin models. The evidence favors the hypothesis that quantum spin models on infinite two-dimensional lattices experience no frustration.

The concept of the *frustration* effect in spin systems with competing interactions has been elaborated especially for the  $s = \frac{1}{2}$  Ising model<sup>1,2</sup> and for the planar model.<sup>3</sup> The assignment of the signs of the interactions to bonds of the lattice is such that the ground state of these classical systems is highly degenerate. A motivation for such studies is the elucidation of the nature of spin-glasses.<sup>4</sup> The first frustrated system studied was the Ising antiferromagnet on the triangular lattice.<sup>5</sup>

Frustrated spin models are usually characterized by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \sum_{\alpha=1}^n S_i^\alpha S_j^\alpha. \quad (1)$$

The first sum is over nearest-neighbor pairs of sites on a lattice.  $n = 1, 2,$  and  $3$  correspond to the Ising, XY, and Heisenberg models, respectively. In the classical ( $S = \infty$ ) limit,  $S_i^\alpha$  is a Cartesian component of a unit vector; in the ex-

tre quantum ( $S = \frac{1}{2}$ ) limit,  $S_i^\alpha = \sigma_i^\alpha$ , a Pauli matrix. All previous studies of frustration have considered explicitly only the classical models or the quasiclassical  $S = \frac{1}{2}$  Ising model. Here we investigate the frustration concept for fully quantum mechanical models, making explicit calculations for the  $S = \frac{1}{2}$  XY and Heisenberg models. We study both models with all interactions antiferromagnetic on the triangular lattice and with both one quarter and three quarters of the interactions antiferromagnetic on the square lattice in two different patterns.

For the even- $N$ , purely ferromagnetic XY model the ground state is nondegenerate,<sup>6</sup> belongs to the identity representation of the space group of the lattice and has

$$M_z \equiv \sum_{i=1}^N S_i^z = 0.$$

(For odd  $N$  the ground state is doubly degenerate.) The Heisenberg antiferromagnet on bipartite lattices also has a nondegenerate ground state<sup>7</sup> and has  $\vec{M} = 0$ . For either of the antiferromagnets on the triangular lattice or for mixed ferromagnetic and antiferromagnetic interaction models no exact results for general  $N$  are known.

Below we calculate the properties of the  $S = \frac{1}{2}$  XY and Heisenberg models with competing interactions on *finite* ( $N \leq 12$ ) triangular and square lattices (or cells) with periodic boundary conditions. We extrapolate from the results for finite lattices to form a hypothesis on the frustration effect for quantum spin models on infinite two-dimensional lattices. The infinite square lattice can be tiled with squares of  $N = l^2 + m^2$  sites, where  $l, m = 0, 1, 2, \dots$ . The triangular lattice can be tiled with  $60^\circ$  equilateral parallelograms of  $N = l^2 + m^2 + lm$  sites. Betts and Oitmaa<sup>8</sup> have estimated the ground-state properties of the  $S = \frac{1}{2}$  XY and Heisenberg ferromagnets on infinite two-dimensional lattices by calculating exactly the properties of interest on finite  $N$  lattices with periodic boundary conditions and extrapolating against  $1/N$ . Exploitation of symmetries permitted completion of calculations for all  $N < 20$ . All intensive properties of interest such as the ground-state energy per spin or the root-mean-square magnetization per spin vary quite linearly with  $1/N$  for  $N > 4$  thus allowing precise estimates for the infinite lattice.

Local or *plaquette* frustration was discussed by Toulouse<sup>1</sup> and others, but two-dimensional spin systems can also suffer from a global type of frustration induced by periodic boundary condi-

tions which we call *toroidal* frustration. For example, the Ising antiferromagnet on the square lattice does not suffer plaquette frustration. However, for odd  $N$ , if *periodic* boundary conditions are applied, the model is frustrated and the ground state becomes highly degenerate. For a  $3 \times 3$  square with periodic boundary conditions the ground-state degeneracy of the  $S = \frac{1}{2}$  model,  $g_9 = 102$ .

The Ising antiferromagnet on the triangular lattice may suffer both types of frustration. On an infinite lattice this model suffers only plaquette frustrations, and in the (highly degenerate) ground state each frustrated bond is shared between two plaquettes. On a finite triangular lattice with free boundary conditions the Ising antiferromagnet has only the Kramers degeneracy in the ground state because frustrated bonds do not occur on the boundary. On a finite lattice with periodic boundary conditions the Ising antiferromagnet will suffer toroidal frustration for certain cell sizes. If toroidal frustration is present, then the dimensionless ground-state energy per site,  $E_0/N|J| > -\frac{1}{2}$ .

Table I reveals that the seven-spin cell suffers toroidal frustration while the nine- and twelve-spin cells do not. Toroidal frustration adds nearly 50% to the ground-state entropy of the seven-spin cell expected if plaquette frustration alone were present. A two-point extrapolation against  $1/N$  of the ground-state entropy per site with use of the nine- and twelve-spin results yields  $S_0/Nk_B \approx 0.35$  for the infinite lattice, about 10% above the exact results,<sup>5</sup> indicating the level of confidence for similar extrapolations.

For the  $S = \frac{1}{2}$  XY and Heisenberg uniform antiferromagnets ( $J_{ij} = J < 0$ ) we present the ground-

TABLE I. Ground-state properties of  $S = \frac{1}{2}$  antiferromagnets on triangular lattices of  $N$  spins.

| $N$                  | 7      | 9      | 12     | $\infty$ |
|----------------------|--------|--------|--------|----------|
| (a) Ising model      |        |        |        |          |
| $E_0/3NJ$            | 0.2143 | 1/6    | 1/6    | 1/6      |
| $g$                  | 70     | 42     | 120    |          |
| $S_0/Nk_B$           | 0.6069 | 0.4153 | 0.3990 | 0.3231   |
| (b) XY model         |        |        |        |          |
| $E_0/3NJ$            | 0.1429 | 0.2827 | 0.2861 | 0.30     |
| $g$                  | 28     | 4      | 1      |          |
| (c) Heisenberg model |        |        |        |          |
| $E_0/3NJ$            | 0.2143 | 0.3829 | 0.4069 | 0.46     |
| $g$                  | 28     | 4      | 1      |          |

state energy and degeneracy of triangular lattices of seven, nine, and twelve sites with periodic boundary conditions. The seven-site lattice is highly frustrating to both models. The ground-state energy per bond has almost the same value for the nine- and the twelve-site lattices and permits a meaningful extrapolation to the infinite lattice. For both models the ground state on the twelve-site lattice is nondegenerate; plaquette frustration is absent!

One might wonder why  $g_9 = 4$  and not 2 (Kramers degeneracy). Additional insight into the properties of frustrated quantum mechanical spin models is afforded by the antiferromagnetic planar model on the triangular lattice. For an equilateral triangle of spins there are two types of antiferromagnetic ground state, the vortex and antivortex types, in each of which each spin makes an angle of  $\pm 2\pi/3$  with its neighbors, and the whole pattern may be rotated through an arbitrary angle. Ground states of the triangular lattice consist of states in which every triangular plaquette is in a ground state. If we start to construct a ground state of the entire lattice by orienting the spins to achieve a ground state of an arbitrary plaquette, the remainder of the construction is seen to be unique. Thus the ground state has the same degeneracy and symmetry,  $O(2)$ , as a single plaquette. The ground state is illustrated in Fig. 1. The ground-state energy  $E_0 = -3N|J|/4$ . There are only two inequivalent spin-spin correlations; for nearest neighbors  $\langle \vec{S}_0 \cdot \vec{S}_1 \rangle = 2 \langle S_0^x S_1^x \rangle = -\frac{1}{2}$ , and the second neighbor correlation  $\langle \vec{S}_0 \cdot \vec{S}_2 \rangle = 1$ . The ground state is completely "full" of vortices and antivortices. The planar antiferromagnet on a finite triangular lattice will clearly

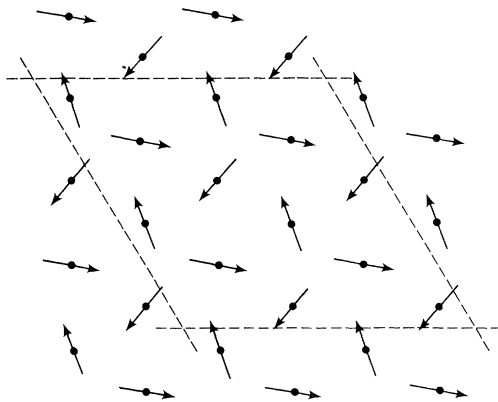


FIG. 1. Ground-state configuration of the planar antiferromagnet on the triangular lattice. The dashed lines outline a twelve spin cell.

TABLE II. Ground-state correlations on the twelve-site and nine-site triangular lattice for  $S = \frac{1}{2}$  antiferromagnets.

| $j$      | XY model                                |   | Heisenberg model                                      |   |
|----------|---|---|---|---|
|          | $\langle \sigma_0^x \sigma_j^x \rangle$ | $\langle \sigma_0^z \sigma_j^z \rangle$ | $\langle \vec{\sigma}_0 \cdot \vec{\sigma}_j \rangle$ | $\langle \vec{\sigma}_0 \cdot \vec{\sigma}_j \rangle$ |
| $N = 12$ |   |   |   |   |
| 1        | -0.2861                                 | -0.1951                                 | -0.7673   | -0.8136   |
| 2        | 0.3878                                  | 0.0806                                  | 0.8562  | 0.7719  |
| 3        | -0.1570                                 | -0.0356                                 | -0.3495   | -0.2169   |
| $N = 9$  |   |   |   |   |
| 1        | -0.2828                                 | -0.1551                                 | -0.7205   | -0.7778   |
| 2        | 0.4897                                  | 0.0207                                  | 1.0000  | 1.0000  |

suffer toroidal frustration unless the number,  $N$ , of sites is a multiple of 3.

For the two quantum models the ground-state correlations are listed in Table II for the nine- and twelve-site triangular lattices. Qualitatively the corresponding correlations in the two models are similar. The nearest-neighbor  $x-x$  correlations for the  $S = \frac{1}{2}$  XY model is only 10% greater than that for the planar model. The fairly strong negative nearest-neighbor  $z-z$  correlation in both quantum models indicates why a lattice with an odd number of spins imposes a degree of toroidal frustration on quantum models (e.g.,  $g_9 = 4$ ) as opposed to the planar model.

Now we turn to square lattices which are of maximum plaquette frustration for classical models. In pattern I, all bonds in every second horizontal row are distinguished by having the sign of the interaction opposite to that of the remaining three quarters of the bonds. Pattern II of distinguished bonds is illustrated in Fig. 2. For both patterns it is possible to construct an

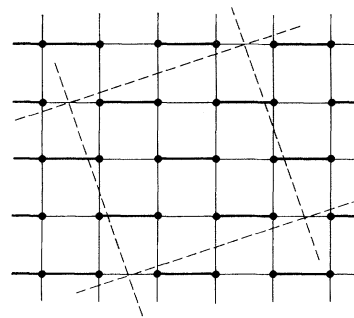


FIG. 2. Square lattice with pattern-II maximal plaquette frustration. Heavy and light bonds represent interactions of opposite sign. Dashed lines outline a ten-site cell.

TABLE III. Ground-state energies per bond,  $-E_0/2N|J|$ , of the  $S = \frac{1}{2}$  XY and ferromagnetic (HF) and antiferromagnetic (HA) Heisenberg models on frustrated square lattices.

| Model | Pattern I |         | Pattern II |              |
|-------|-----------|---------|------------|--------------|
|       | $N = 8$   | $N = 8$ | $N = 10$   | $N = \infty$ |
| XY    | 0.4330    | 0.3953  | 0.3889     | 0.36         |
| HF    | 0.4373    | 0.4781  | 0.4772     | 0.47         |
| HA    | 0.5354    | 0.5500  | 0.5423     | 0.51         |

$N = 8$  square with periodic boundary conditions; for pattern II, it is also possible to construct an  $N = 10$  square as illustrated in Fig. 2.

For the Heisenberg model the case (F) of three-quarters of the bonds (in either pattern) ferromagnetic and one-quarter antiferromagnetic is distinct from the case (A) of three-quarters of the bonds antiferromagnetic. For the XY model the two cases are equivalent. The ground-state energies of all three models on the three finite lattices mentioned above are listed in Table III. In seven of the nine cases the ground state is nondegenerate and  $M_z = 0$ . In contrast, on the  $N = 8$  pattern-I square lattice the Heisenberg ferromagnet is *quintuply degenerate* with  $M_z = 0, \pm 1, \pm 2$  and the antiferromagnet is triply degenerate with  $M_z = 0, \pm 1$ . It is plausible that a larger pattern-I lattice, say of  $N = 16$ , would have a nondegenerate ground state, but it is beyond our present computational power to check this conjecture.

In summary, we have studied the ground state of quantum XY and Heisenberg models on finite two-dimensional lattices on which classical spin models would be highly frustrated. The lattices considered include the triangular lattice with all bonds antiferromagnetic and the square lattice with one-quarter or with three-quarters of the bonds antiferromagnetic in two different patterns. On some of the smaller finite lattices the ground state of the quantum models is degenerate; i.e., the models are frustrated. We attribute such degeneracy not to the plaquette frustration experienced by classical models but to toroidal frustration associated with the size of the lattice. The overall evidence is in favor of the hypothesis that *quantum spin models on infinite two-dimensional lattices experience no frustration for any configuration of antiferromagnetic bonds.*

TABLE IV. Ratio of ground-state energy of spin models with competing interactions to the energy of the same model with purely ferromagnetic interactions on infinite two-dimensional lattices.

| Lattice              | Model  |        |      |      |      |
|----------------------|--------|--------|------|------|------|
|                      | Ising  | Planar | XY   | HF   | HA   |
| Triangular           | 0.3333 | 0.5000 | 0.56 |      | 0.86 |
| Square<br>pattern II | 0.5000 | 0.7071 | 0.67 | 0.94 | 1.02 |

Although quantum spin systems on lattices with competing interactions appear not to be frustrated in that the ground-state entropy is zero, the competition might be expected to affect the ground-state energy. Table IV lists the ratio of the ground-state energy of each model with competing interactions to the corresponding pure ferromagnet for two classical and two quantum models.<sup>8</sup> Competing interactions raise the ground-state energy of the  $S = \frac{1}{2}$  XY model by approximately the same amount as in the planar model. However the  $S = \frac{1}{2}$  Heisenberg-model energy is almost unaffected by the competition among the interactions in all three cases.

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