Two-Dimensional Periodic Frustrated Ising Models in a Transverse Field

R. Moessner,[1] S. L. Sondhi,[1] and P. Chandra[2]

[1]*Department of Physics, Jadwin Hall, Princeton University, Princeton, New Jersey 08544*
[2]*NEC Research Institute, 4 Independence Way, Princeton, New Jersey 08540*
(Received 1 November 1999)

We investigate the interplay of classical degeneracy and quantum dynamics in a range of periodic frustrated transverse field Ising systems at zero temperature. We find that such dynamics can lead to unusual ordered phases and phase transitions or to a quantum spin liquid (cooperative paramagnetic) phase as in the triangular and kagome lattice antiferromagnets, respectively. For the latter, we further predict passage to a bond-ordered phase followed by a critical phase as the field is tilted. These systems also provide exact realizations of quantum dimer models introduced in studies of high temperature superconductivity.

The introduction of quantum fluctuations to a frustrated system with a large ground-state degeneracy can lead to a multitude of new quantum phases and transitions. This occurs because the set of degenerate states provides no energy scale and hence all perturbations are *singular*. Any linear combination of the classically degenerate states is a candidate quantum ground state. The most celebrated instance of such behavior is the quantum Hall problem, where the degeneracy induced by a frustrated kinetic energy leads to a plethora of strongly correlated states when lifted by interactions and disorder.

In this Letter we report results from the first systematic study of a series of simple spin models which have the potential for such behavior. These are geometrically frustrated transverse field Ising models. The frustrated nature of the exchanges leads to an extensive zero-point entropy, S, in the classical (zero-field) case (for a review, see Ref. [1]), and they are not ordered even at $T = 0$. The quantum dynamics is provided by the application of a magnetic field transverse to the couplings.

These models are interesting as they are the simplest possible frustrated quantum magnets, containing the minimal ingredients required for a nontrivial quantum dynamics; this simplicity allows considerable progress towards their solution. Further, in addition to the encouraging likelihood of direct experimental realization in highly anisotropic magnetic systems, we expect that they will serve as effective theories in other frustrated systems where a local Ising degree of freedom can be identified. Indeed, there is intense current interest in these models in the context of *Heisenberg* systems: the square lattice fully frustrated Ising model arises in a group of theories of the cuprate superconductors [2].

Specifically, we study Hamiltonians of the form [3]

$$H = \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z + \Gamma \sum_i S_i^x + h \sum_i S_i^z, \qquad (1)$$

where the J_{ij} are the nearest-neighbor exchange couplings with $|J_{ij}| = J$ and $\prod_{\text{plaquette}} (J_{ij}/J) = -1$, Γ is the strength of the transverse field, the S^a are the Pauli spin

operators, and h is the strength of a (classical) longitudinal, Ising symmetry breaking field.

Counterintuitively, but commonly, there is an Ising version of "order by disorder" *à la* Villain *et al.* [4], in which configurations with long-range order allow the softest fluctuations and hence minimize the entropy/zero-point energy; in the Ising case it is fluctuations *into* the ground-state manifold that matter. In the complementary "disorder by disorder" scenario, suggested by Fazekas and Anderson [5], a disordered classical manifold continues into a disordered quantum phase. To our knowledge, no such disorder-free Ising spin liquid was known to exist previous to the work described here.

To make progress in this strongly interacting problem, we have developed or adapted a number of approaches—variational, weak-coupling, and strong-coupling ones, as well as mappings to other models. From our systematic study, we present three models realizing different connections between classical and quantum ordering and, among others, unconventional critical and spin liquid phases. A more complete account of this study, including a wider range of lattices and finite-temperature properties, will follow this Letter [6].

Among our results, we derive a sufficient condition for quantum ordering, which is fulfilled by a class of models, critical at $T = 0$, including the triangular lattice Ising (IAFM) antiferromagnet and the square fully frustrated Ising magnet (FFIM). The kagome IAFM and the hexagonal fully frustrated Ising magnets, both exhibiting exponential correlations in the ground-state manifold [1], do not fulfill this criterion and yet lead to different quantum states: the latter orders thus ruling out a strict connection between classical and quantum disorder. By contrast, the former is a rare example of a *quantum spin liquid* in $d = 2 + 1$, as it remains disordered at all couplings. In the kagome problem there is a particularly interesting twist in which a purely longitudinal field, $0 < |h| < 4J$, can be used to produce a critical classical finite-entropy phase which then orders in a further transverse field. Interesting by-products of the analyses include unusual phase transitions, such as an $O(4)$ transition for the hexagonal FFIM.

General considerations.—Before discussing specific lattices, we sketch three general approaches. At small Γ, there is an Ising analog of the saddle-point method to identify instances of order by disorder. In this limit we need to diagonalize the transverse field term within the subspace of the classical ground states. Note that this will lead to a discontinuous change in the ground-state properties, even though the energy levels are set by Γ, and hence evolve continuously. As the quantum ground state is not perturbatively constructible, it is useful to think variationally about different configurations. Evidently, spins able to orient in the x direction can gain energy from the transverse field. Such spins are "flippable" in the z representation, being connected to their neighbors by equal numbers of satisfied and unsatisfied bonds (see Fig. 1). An intuitive variational candidate for the ground state is thus constructed from the classical ground states which maximize the number of flippable spins; the privileging of these configurations, which are typically more regular, is the quantum mechanism of order by disorder. While this kind of semiclassical argument is suggestive, it leaves open the possibility that the true wave function has the bulk of its support elsewhere in configuration space. Note that in either case there are fluctuations in the ground state.

A very useful feature of the transverse field problem is that at *large* Γ, there is a unique paramagnetic ground state (polarized along x) separated by a gap $\Delta = \Gamma$ from the lowest excited states, independent of wave vector. This degeneracy is lifted in an expansion in J/Γ: to first order, there appears a dispersion $\epsilon(\mathbf{k}) \sim \Delta + \sum_{\mathbf{j}} e^{i\mathbf{k}\cdot\mathbf{j}} J_{0\mathbf{j}}$, which softens with reduced coupling. Even without high-order computations, one can identify soft wave vectors. Following Ref. [7], these can be used together with lattice symmetry considerations to guess at the Landau-Ginzburg-
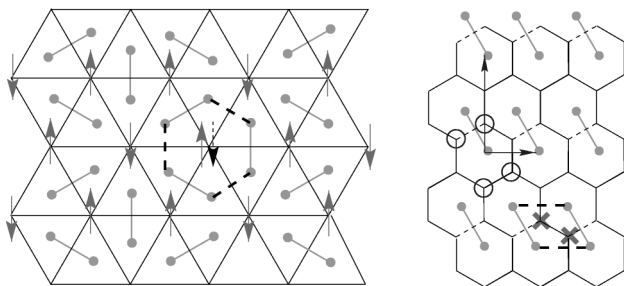
Wilson (LGW) action governing the transition and the symmetry-breaking pattern of the putative weak-coupling ordered phase. This possibility does *not* always exist; e.g., an XY magnet is a nontrivial problem on its own, which frustrates attempts to perturb in the Ising exchange.

Finally, we derive an ordering criterion based on the mapping of the d-dimensional transverse field Ising model onto a ferromagnetically stacked model in $d + 1$. This follows from the Euclidean path integral representation, $Z = \mathrm{Tr}e^{-H}$, of the problem governed by the 3D classical Hamiltonian, $H = \sum_{\langle ij\rangle, n} K_{ij}^s S_i^z(na_\tau)S_j^z(na_\tau) + \sum_{i,n} K_\tau S_i^z(na_\tau)S_i^z((n+1)a_\tau)$, where a_τ is the imaginary time step introduced to obtain a discrete representation, $K_{ij}^s \propto J_{ij}$, and the $K_\tau > 0$ are ferromagnetic. Time continuum quantum evolution corresponds to the double limit, $a_\tau \rightarrow 0$, $K_\tau \rightarrow \infty$ with $a_\tau e^{K_\tau}/2 = \Gamma$ held fixed. For *small* K_τ, the specific free energy, F, of this model is given by $-\beta F = S + (K_\tau^2/2)\sum_i \langle S_i(0)S_j(0)\rangle^2 + O(K_\tau^4)$, with $|K^s| = \infty$ enforcing the ground-state constraint.

If the integral $I = \int d^2r \langle S_0 S_r\rangle^2$ diverges, the free energy above is *nonanalytic* as $K_\tau \rightarrow 0$, implying that the quantum ($K_\tau \rightarrow \infty$) and classical points ($K_\tau = 0$) are in different phases. For classically disordered antiferromagnets with exponentially decaying spin correlations at $T = 0$ even though no single term in the series expansion becomes unbounded, the whole series may diverge when K_τ is beyond the radius of convergence, and hence both ordered and disordered quantum states are allowed. In the following we demonstrate that all three possibilities are realized in practice by presenting an example for each one.

Triangular IAFM: Order from criticality.—Because this lattice is bond sharing, the ground states of the triangular IAFM can be mapped onto hard-core dimer coverings of its dual hexagonal lattice (Fig. 1); furthermore, since the latter is bipartite, the ground-state manifold of this spin model admits a height representation, which, under reasonable assumptions, implies that the classical correlations are critical [8]. We have a diverging $I_{\mathrm{tri}} = \int d^2r/r$ [1]. Our above argument thence implies a transition separating the classical and the quantum models.

More directly, we study the effect of small Γ ($h = 0$) for this problem by noting that, in dimer language, states connected by the action of the resulting Hamiltonian [Eq. (1)] differ by a 60° rotation of a triplet of dimers (Fig. 1). The degenerate problem is *exactly* the hexagonal-lattice version of the Rokshar-Kivelson quantum dimer model [9]

FIG. 1. Left: Maximally flippable spin configuration of the triangular IAFM. Dimers mark the frustrated bonds, covering the dual lattice. Flipping the spin in the center, which experiences zero net exchange field, yields the indicated dimer plaquette move. Right: The FFIM on the hexagonal lattice, which can be thought of as a rectangular lattice (with vectors indicated by arrows) with a basis of four (encircled) sites. Broken lines represent antiferromagnetic bonds, solid lines ferromagnetic ones. The dimer configuration for the maximally flippable state with all spins aligned is shown. The elementary dimer move corresponds to flipping the two spins indicated by crosses.

$$H_{\mathrm{QDM}} = -t\left(|\rangle\langle\,| + \mathrm{H.c.}\right) + v\left(|\rangle\langle\,| + |\rangle\langle\,|\right)$$

at the point $t = \Gamma$ and $v = 0$ [10]. The ground state of H_{QDM} at $v = t$ is known to be an equal-amplitude superposition of all dimer coverings [11]. As the diagonal equal-time correlations at this point are exactly those of the classical problem, the question of fluctuation selection reduces to determining if the point $v = 0$ lies in the same phase. From an exact diagonalization study of clusters of

this extended problem with up to 18 spins [6], we find that the point $v = 0$ lies in a hexagonal dimer phase which terminates at $v = t$. This is also the phase identified by our heuristic semiclassical analysis (Fig. 1).

Such hexagonal correlations were previously found by an LGW analysis of ferromagnetically stacked triangular lattices [7], which in the proper limit can be carried over to our model [12]. This analysis suggests that the paramagnetic phase orders via a 3D XY transition.

We note that the presence of an XY transition should manifest itself in a finite-temperature critical phase where Γ acts as a locking field to suppress defect production [6]. Finally, we remark that these results apply, *mutatis mutandis,* to the square lattice FFIM.

Kagome IAFM: Disorder from disorder.—The kagome IAFM has short-ranged correlations in the classical limit, with a ground-state entropy per site of $0.502k_B$, in excess of the triangular lattice value of $0.323k_B$ [1]. Its ground states map onto neither a height nor a dimer model.

Interestingly, a longitudinal field $|h| < 4J$ does not fully eliminate this extensive entropy but reduces it to precisely the triangular lattice result even as it creates a net ferromagnetic moment. Most remarkably, it simultaneously induces critical (connected) spin correlators. To see this, note that maximizing the polarization requires that every elementary triangle of the lattice contain two up and one down spin. By placing dimers on the dual lattice defined by the triangles such that one dimer is centered on each down spin (Fig. 2), one obtains dimer coverings of a hexagonal lattice precisely as in the triangular lattice problem in zero field, from which the above results follow.

Next, consider the effect of tilting the field somewhat, i.e., of adding a small transverse component $\Gamma \ll h$. At the first five orders in Γ/h there is no mixing between the polarized states and no lifting of their degeneracy. At sixth order they mix, and the degenerate manifold Hamiltonian

is precisely given by H_{QDM} with $t \propto \Gamma(\Gamma/h)^5$ and $v = 0$. Hence we find that long-range bond order of the hexagonal kind considered previously sets in immediately.

Consider now the problem with the transverse field alone. A low-order LGW analysis as described above fails to predict an ordering pattern: an entire dispersionless branch of excitations [13] goes soft, rather than only excitations at a small number of wave vectors. Following our previous strategy we can alternatively attempt to identify candidate orderings by finding the maximally flippable states. These states are precisely the "dimer states" selected by a longitudinal field (and their Ising reversed counterparts) since only they saturate the upper bound of two flippable spins in each triangle. A significant restriction to this dimer manifold should manifest itself in correlations reminiscent of the bond-ordered phase.

To test this possibility we have carried out Monte Carlo (MC) simulations on the Euclidean 3D path integral representation. As we expect any order to be strongest at small Γ, we have primarily simulated the problem with the spatial couplings made very large, in effect requiring that all time slices remain in the ground-state manifold. In order to explore large K_τ without freezing, we use a cluster algorithm [14] in the time direction so that it is the exponential growth of the correlation length in the time direction that limits our simulations in practice. The largest system we simulated is a stack of height 512 and the maximal coupling was chosen such that a typical cluster size is around 50. Each slice contains 432 spins.

Figure 3 shows the spin-spin correlation function of this system, which is evidently tiny beyond the first few neighbors, in stark contrast to the models known to order; e.g., in the triangular case, the saturated correlation function reaches well above 0.5 at the largest distances.
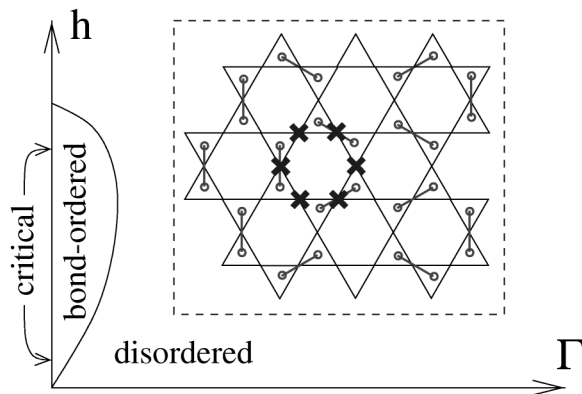

FIG. 2. Phase diagram for the kagome Ising antiferromagnet in a field. Inset: Mapping of the kagome IAFM in a longitudinal field onto the hexagonal lattice dimer model. The down spins are marked by dimers. The nontrivial move to sixth order in perturbation theory corresponds to flipping all the spins marked by crosses.
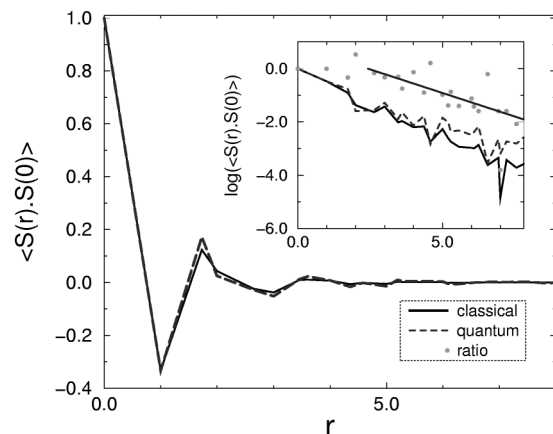

FIG. 3. Angularly averaged correlation functions (classical and quantum) for the kagome lattice from MC simulations. Inset: The logarithm of the absolute value of the same functions. In addition, the points denote the logarithm of the ratio of the classical and the quantum correlation functions. The straight line is a guide to the eye.

Note that the shape of the quantum correlation function mirrors that of the classical one: their signs are the same at all points in the region plotted. Since the classical correlations are known to decay exponentially, and since the ratio of the two also appears to do so but with a smaller slope (Fig. 3 inset), we conclude that the quantum correlations, although enhanced over the classical ones, still decay exponentially to zero with distance.

In addition, we have checked that relaxing the spatial couplings leads to a further weakening of the correlations of the stacked model. We have also simulated the effect of a weak longitudinal field added to the transverse field and find that, while it induces a magnetization per site $m \propto h$, the connected correlations appear to remain short ranged. At short distances, we observe incipient correlations characteristic of the hexagonal dimer state described above for $\Gamma \ll h$. This leads us to conjecture that, as the field is tilted farther, there is likely a continuous quantum phase transition to the hexagonal phase. For larger h, diverging equilibration times prevent us from exploring this portion of the phase diagram numerically. The simplest phase diagram incorporating all these facts within the framework discussed here is depicted in Fig. 2; evidently, this is a fruitful topic for future work.

Hexagonal lattice FFIM: Order from disorder.— As an example of another classically disordered model, we consider the FFIM on the hexagonal lattice. This model, which maps onto a dimer but not a height model, is obtained from a ferromagnet by changing the sign of the exchange interaction of one bond in each hexagon, as displayed in Fig. 1. As the coordination of the lattice is odd, the transverse field does not lift the degeneracy until second order in Γ; this corresponds to flipping not an individual spin but a pair of neighboring spins (Fig. 1). Whereas the entropy of the ground states is extensive, at $0.214 k_B$ per spin [1], the number of maximally flippable states (for an example, see Fig. 1), is exponential only in the linear size of the system.

We have carried out a LGW analysis as described above and found that there are four soft modes, at wave vectors $\pm(\pi/6, \pi/2), \pm(5\pi/6, \pi/2)$, with a surprisingly large unit cell of 48 spins. The resulting LGW Hamiltonian [6] is $O(4)$ symmetric up to sixth order, where a (in $d = 2 + 1$, dangerously irrelevant) 48-fold symmetry breaking term appears.

Our MC simulations of the stacked model clearly display the pattern predicted by the LGW analysis, indicating the presence of an ordering transition as Γ is lowered [15]. The connection of this ordering pattern with the variational analysis is rather involved [6]; here we note that the fairly nontrivial ordering pattern is remarkable both as

an instance of order by disorder and of ordering in a quantum dimer model where the classical correlations are short ranged.

In summary, we have found a rich variety of behavior in frustrated transverse field Ising models. The exciting possibility here is that it should be possible to approximate the triangular and kagome IAFMs fairly well not only in real, highly anisotropic magnets but also in more general quantum frustrated systems.

[1] R. Liebmann, *Statistical Mechanics of Periodic Frustrated Ising Systems* (Springer, Berlin, 1986), and references therein.

[2] S. Sachdev and M. Vojta, cond-mat/9910231; T. Senthil and M. P. A. Fisher, cond-mat/9910224.

[3] For work on one-dimensional models, see B. K. Chakrabati *et al., Quantum Ising Phases and Transitions in Tranverse Ising Models* (Springer-Verlag, Berlin, 1996).

[4] J. Villain *et al.,* J. Phys. (Paris) **41**, 1263 (1980); E. F. Shender, Sov. Phys. JETP **56**, 178 (1982).

[5] P. Fazekas and P. W. Anderson, Philos. Mag. **30**, 23 (1974).

[6] R. Moessner, S. Sondhi, and P. Chandra (to be published).

[7] D. Blankschtein *et al.,* Phys. Rev. B **29**, 5250 (1984).

[8] B. Nienhuis *et al.,* J. Phys. A **17**, 3559 (1984).

[9] D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. **61**, 2376 (1998).

[10] This mapping was also noted independently by C. L. Henley, in *Book of Abstracts of STATPHYS 20,* edited by A. Gervois, M. Gingold, and D. Iagolnitzer (IUPAP Commission on Statistical Physics, Paris, 1998).

[11] M. E. Fisher and J. Stephenson, Phys. Rev. **132**, 1411 (1963).

[12] Alternatively, the quantum problem can be mapped onto a 3D height model; there, only smooth surfaces are expected, which in turn suggests the observed ordering. We are grateful to S. Sachdev for explaining this to us.

[13] J. N. Reimers *et al.,* Phys. Rev. B **43**, 865 (1991).

[14] R. H. Swendsen *et al.,* Top. Appl. Phys. **71**, 75 (1992).

[15] This ordering pattern is already present for only 30 stacks of 1152 spins each. While our numerics are highly suggestive, a definitive finite-size scaling study is out of the reach of our current workstation due to the large size of the unit cell.