Planar pyrochlore, quantum ice and sliding ice

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We study quantum antiferromagnetism on the highly frustrated checkerboard lattice, also known as the square lattice with crossings. The quantum Heisenberg antiferromagnet on this lattice is of interest as a two-dimensional analog of the pyrochlore lattice magnet. By combining several approaches we conclude that this system is most likely ordered for all values of spin, S, with a Néel state for large S giving way to a two-fold degenerate valence-bond solid for smaller S. We show next that the Ising antiferromagnet with a weak four-spin exchange, equivalent to square ice with the leading quantum dynamics, exhibits long range “anti-ferroelectric” order. As a byproduct of this analysis we obtain, in the system of weakly coupled ice planes, a sliding phase with XY symmetry.

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Introduction: On the heels of recent progress in understanding highly frustrated classical magnets, coupled with a substantial experimental effort, renewed attention is now focused on the behaviour of their quantum counterparts. In particular, the Heisenberg pyrochlore antiferromagnet is being studied with view to the question of whether frustration-enhanced quantum fluctuations might lead to unconventional ordering – or complete absence thereof – especially for small values of the quantum spin, S. This model classically is special in that frustration prevents any sort of ordering or dynamical phase transition down to the lowest temperatures, for which reason it is termed a cooperative paramagnet or classical spin liquid.

The challenge of this problem arises from the small energy scale generated by the frustration: in a semiclassical picture, any linear combination of the classically degenerate ground states, the collection of which is of extensive dimensionality, may be selected as the quantum ground state. For the highly frustrated two-dimensional magnet on the related kagome lattice, exact diagonalisations of small clusters have provided crucial benchmarks. This system has turned out to be particularly well suited to this approach as it appears to have a very short correlation length, although one does find a large number of low-lying singlet excitations.

For the pyrochlore magnet, it looks as if such results will elude us for some time to come. The pyrochlore lattice, being three-dimensional, displays a more inclement scaling of the Hilbert space dimension with linear system size. Moreover, its unit cell contains four spins and its structure implies that the smallest system without spurious boundary condition effects contains at least 16 sites.

To evade this, attention has shifted to a system which avoids some of these complications, namely the checkerboard lattice (Fig. 1). It is expected to have similar properties to the pyrochlore as it has the same local structure – both can be thought of as networks of corner-sharing tetrahedra. Further, the size and topology of its ground state manifold for Heisenberg magnets are identical to the pyrochlore case. However, it has a unit cell of only two spins, is two dimensional, and has allowed exact diagonalisations of a good number of finite size systems of up to 36 spins. Such diagonalisations have very recently been carried out by Palmer and Chalker and by Fouet et al. and other workers have also recently studied this system by several techniques.

\[ \text{FIG. 1. Phase diagram of the checkerboard lattice Heisenberg magnet as a function of spin, S. The plaquette (left – fat bonds are those with enhanced probability of singlet formation) and Néel (antiferroelectric) phases. A projection of the 3-d pyrrchlore lattice gives the 2-d checkerboard lattice (middle). A tetrahedron becomes a square with crossings upon projection, all bonds of which have equal strength.} \]

In this paper, we take a somewhat broader view of quantum antiferromagnetism on the checkerboard lattice. For the Heisenberg problem, apart from the small S cases, which we study by a dimer model analysis and an Sp(N) mean field theory, we analyze the large S region, both within Sp(N) – which is also able to treat the intermediate region – and through the semiclassical 1/S expansion. Here we find a strong ordering tendency – into a two-fold degenerate valence bond crystal for small S and a Néel state at large S (Fig. 1). Our predictions find support in the numerical work of Fouet et al. as we discuss further below. The nature of the valence bond order is at odds with other recent work. The S = 1/2 kagome magnet behaves very differently from the checkerboard – and therefore probably the pyrochlore – ones. Details of the ordering, however, depend on properties of the checkerboard lattice (most prominently, the explicit breaking of the symmetry between bonds in a
tetrahedron and the existence of nontrivial closed loops of length four residing on a bipartite lattice) which it does not share with the pyrochlore lattice; there we expect the order to be much more delicate.

In addition we consider the Ising antiferromagnet with a weak four spin exchange dynamics – the Ising ground states are isomorphic to those of square ice and the dynamics represent the shortest ring exchanges in this manifold arising from quantum tunneling – hence “quantum ice”. The resulting state displays long range “antiferroelectric” order in ice terminology, or Néel order in Ising terminology (Fig. 1). A byproduct of this analysis is the state of a stack of weakly coupled ice layers, which is seen to be in a “sliding” phase of the kind discussed in recent work albeit one that is protected by much simpler arrangements.

We turn now to the details of these assertions and sketches of the underlying analyses. We treat the Heisenberg problem first.

**Sp(N) generalization:** The Sp(N) technology for frustrated magnets, a reformulation of Schwinger boson mean field theory controlled by the introduction of 1/N as a small parameter, was introduced and described in detail by Read and Sachdev. One starts by rewriting the SU(2)∼Sp(1) spin operators in terms of bosonic operators, \{b_\uparrow, b_\downarrow\}, with the constraint of \(b_\uparrow b_\downarrow + b_\downarrow b_\uparrow = 2S\) on each site, and \(S^2 = (b_\uparrow b_\downarrow - b_\downarrow b_\uparrow)/2\), \(S^+ = b_\uparrow b_\downarrow\). The antiferromagnetic nearest-neighbour Heisenberg Hamiltonian is rewritten in terms of the bosonic operators (up to a constant): \(H = J \sum_{(ij)} S_i \cdot S_j = (−J/2) \sum_{(ij)} (\epsilon^{\sigma\tau} b^\dagger_\sigma b_\tau)(\epsilon^{\mu\nu} b^\dagger_\mu b_\nu)\). One generalises this expression to Sp(N) by formally introducing \(N\) flavours of bosons, labelled by capital letters, and replacing the antisymmetric tensor in \(H\) by its Sp(N) generalisation \(\mathcal{J}_{\alpha\beta} = \epsilon^{\alpha\beta} \delta_{\alpha\beta}\). In the limit \(N \to \infty\) at a fixed boson number \(N\) per flavour per site, \(S\), one obtains to leading order in \(1/N\) a mean-field theory for spin \(S = \kappa/2\); fluctuations about this give rise to a gauge theory.

Self-consistent solutions to the mean field theory are obtained by minimising with respect to the Hubbard-Stratonovich link fields \(Q_{ij} = \langle \mathcal{J}^{\mu\nu}_{AB} h_\mu^A h^B_{j\nu} \rangle\), subject to a constraint on the boson number \(N\). In the process, one obtains a dispersion relation for the energies \(\omega\) of bosonic spin 1/2 quasiparticles. Within the mean-field theory, there is generically a disordered phase at small \(\kappa\); when one of the bosonic modes goes soft as \(\kappa\) is increased, condensation of these ‘spinons’ occurs, and long-range spin order ensues.

Our results at mean-field level are readily summarised. We find zero expectation value of the diagonal bond variables at all \(\kappa\). On the remaining bonds, long-range Néel order (Fig. 1) develops above \(\kappa_c = 0.393\), exactly as for the simple square lattice. For \(\kappa < \kappa_c\), the Néel correlations are only short-ranged.

Whether or not the spinon excitations in the disordered, small \(\kappa\) phase remain deconfined can only be settled by going beyond mean-field theory. As on the square lattice, one obtains a compact \(U(1)\) gauge theory at \(O(1/N)\), in which instanton tunneling effects lead to the formation of bond (Peierls) order. An analogous calculation is presented by Chung et al. for the Shastry-Sutherland model. Details of the ordering pattern, in particular those due to the inequivalence of the plaquettes with and without crossings, are perhaps most easily studied through a quantum dimer model (QDM).

**Quantum dimer model:** This approach starts from the assumption that the magnet is in a regime where the Néel state is destabilised and the effective degrees of freedom are singlet bonds between neighbouring spins, also called valence bonds, which are represented by dimers. As each spin participates in exactly one singlet bond, the Hilbert space consists of all hardcore dimer coverings. An effective dimer Hamiltonian is obtained by means of an overlap expansion, described in Ref. 22. It is formally perturbative in a small parameter arising from the non-orthogonality of the spin wavefunctions describing the different dimer coverings. To zeroth order, all of the exponentially numerous dimer coverings are degenerate, but at the next order, a resonance term is generated. One obtains a resonance loop of length 4 corresponding to flipping a pair of dimers by 90° (Fig. 2): \(I I \leftrightarrow \Xi\). The question is what kind of quantum dimer state is selected by this resonance move.

The most important difference between the well-studied square lattice QDM and that on the checkerboard lattice is the following. As the overlap expansion is essentially organised by length, \(L\), of the resonance loops, the leading order terms arise from the shortest possible resonance loops, namely those of length four. Carrying out the leading order overlap expansion, we find that all the loops of length four on plaquettes with crossings (the projected tetrahedra) have zero kinetic energy; \(t\), in the dimer model and hence play no role. By contrast, the resonance loops on plaquettes without crossings, have nonzero kinetic energy (Fig. 3). Note that such loops of length four are absent from the pyrochlore lattice, where the shortest loop contacting more than one tetrahedron has length six.

Extending the results from the square lattice QDM, one therefore expects the resulting state to be a valence-bond crystal; the staggering of \(t\) strongly favours the plaquette crystal, with the dimers resonating on one of two sublattices of plaquettes without crossings (Fig. 1). Note that the degeneracy of this state is two rather than four, as would be the case for the plaquette state on the square lattice, because of the explicit symmetry breaking introduced by the presence of the plaquettes with crossing interactions.

**Semiclassics:** We now consider the case of large spin \(S\) and large \(\kappa\) for SU(2) and Sp(N), respectively. In either case, one compares the zero-point energy due of the excitations (spin waves and spinons, respectively) of different, classically degenerate ground states. This, in principle, requires evaluating that energy for the entire
ground state manifold, which is of extensive dimensionality.

For $\text{Sp}(N)$, we have compared the zero-point energies of all four-sublattice states, as well as of eight-sublattice coplanar states, and found that the Néel state selected at $\kappa_c$ is also favoured in this limit, which suggests its stability for all $\kappa > \kappa_c$.

For large $S$, we have computed the zero-point energy of all four-sublattice states. We find good qualitative agreement with Henley’s suggestion of an effective energy functional of the biquadratic type, $-\sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2$, in that it correctly reproduces the location of the maximum and the minima. There remains a degeneracy between some inequivalent collinear states. One of the remaining degenerate states is indeed the Néel state, but other states, disfavoured at $O(1/\kappa)$, still have exactly the same energy of zero-point fluctuations at $O(1/S)$.

**Implications for the 3-d pyrochlore magnet:** The actual ordering behaviour of the pyrochlore is still far from settled. At this stage it appears to be somewhat closer to that of the checkerboard lattice than either of the two is to the kagome case, where there has so far been no strong indication of long-range order of any kind for $S = 1/2$, and where the large-$S$ state is necessarily non-collinear. We emphasize, however, that details of the ordering we find, such as the pattern of the bond solid or the size of the unit cell, crucially depend on differences between the two lattices -- such as spatial dimensionality, the presence of inequivalent links, and short closed loops linking different tetrahedra. Moreover, we remark that most approaches employed so far for $d = 3$ pyrochlore explicitly remove the equivalence of all tetrahedra by weakening the bonds on half of them; from such a starting point, it would would seem rather difficult to restore this equivalence, which is necessary for obtaining the plaquette ordering we find.

**Finite-size diagonalisations:** The agreement of the above calculations on a number of central points is reassuring. Most importantly, they all predict ordered states with translational symmetry breaking and a two-fold degeneracy. For small $S$, they lead us to expect dimer order of the plaquette flavour, which gives way to a Néel state at intermediate $S$. How does this compare to exact diagonalisations of $S = 1/2$ Heisenberg magnets?

Palmer and Chalker, who have studied systems containing up to 24 spins, find no clearly identifiable degeneracy. Rather, there appears to be a large number of low-lying singlet states with a small gap and a much larger gap to triplet excitations. They rule out Néel order but are inconclusive about translational symmetry breaking. Fouet *et al.* agree with their results, but have in addition studied a system with 36 sites. There, they find a particularly low ground state energy, suggesting that the boundary conditions for this system size accommodate well the quantum ground state. For this system, there does appear a two-fold near degeneracy of the ground state, with the states being described by the wavevectors expected for our dimer crystal.

**Quantum ice and sliding ice:** We turn next to the Ising problem. The ground states of the Ising antiferromagnet on the checkerboard lattice require two up and two down spins on each tetrahedron (square with crossings). The six such possible configurations on each tetrahedron can be identified with the allowed vertices of the six-vertex model as follows. Divide the square lattice consisting of the crossings at the centres of the tetrahedra into sublattices A and B in the usual fashion. Orient the links coming out of sublattice A(B) inwards if the spin sitting on that link is up(down) and outswards if the spin in down(up) (Fig. 1). As all weights are vertically equal, the ground state manifold has the extensive entropy, $(3/4) \ln(4/3)$ per spin, of square ice. We will shortly find it useful that the ice problem also has a height representation in which an integer valued height living on the dual lattice steps up(down) by one on crossing an in(out) arrow clockwise around any vertex.

As a matter of principle, the degeneracy of the ice manifold will be lifted by quantum effects which will involve (in six vertex language) closed loops of arrows that will reverse direction. Here we study the ordering produced by this dynamics. The simplest such process for square ice involves a loop around a single plaquette. Translated into the Ising spin representation on the checkerboard lattice it gives rise to a Hamiltonian, $H_Q$, acting between ground states of the classical Ising model,

$$H_Q = -\Gamma \sum_p (\sigma^+ \sigma^- + \text{h.c.})$$

where $p$ denotes a sum over non-crossed plaquettes of the lattice, and $\sigma^+(-)$ are the raising(lowering) operators of the Ising spins $\sigma^z = \pm 1$. To study this Hamiltonian it is convenient to use an imaginary time discrete representation of the path integral via the standard Trotter-Suzuki procedure -- in this case it yields a set of ferromagnetically stacked planes of the checkerboard lattice, with an implicit time continuum limit at large ferromagnetic coupling, $K^c \sum_n \sigma^z_n \sigma^z_{n+1}$, between neighbouring sites in adjacent layers, labeled by $n$.

We digress briefly to study the imaginary time representation at weak coupling, $K^c \ll 1$, which could be interpreted as the classical statistical mechanics of a set of square ice planes with a potential interaction between the planes. In this limit the interaction competes with the entropy of the planes and we may as it prevails despite its weakness. To answer this we switch to the height representation description of the ice problem. Herein the coarse grained heights in a given plane are weighted by the pseudo-Boltzmann factor

$$\rho(h(x)) \propto e^{-\frac{1}{\Gamma^2} \int d^2x (\nabla h)^2}$$

while the spins (arrows) are represented by $\nabla \times h$ for their small momentum components and by $e^{i m h}$ for momenta in the vicinity of $(\pi, \pi)$. For uncoupled planes,
the distribution $\prod_n \rho[h_n(x)]$ is a fixed point of a two-dimensional renormalization group (RG) transformation in the standard fashion. The coupling between the planes induces two perturbations in the height language: the first of these, $\phi_1 = \sum_n \int d^2 x (\nabla h_n) \cdot (\nabla h_{n+1})$, is exactly marginal under the RG while the second $\phi_2 = \sum_n \int d^2 x \cos[\pi(h_{n+1} - h_n)]$ is irrelevant as is readily verified. It follows then that the system exhibits a sliding phase at weak coupling, whence sliding ice.

FIG. 2. Spin correlations on sublattice 1 in the x-direction from Monte Carlo on 48 × 48 × 16 plaquettes. The classical curve, $K^\tau = 0$, and $K^\tau = 0.1$ coincide. Néel long-range order, albeit weak, obtains for $K^\tau = 0.2$. Inset: Numbers label sublattices, arrow translation vectors. In the QDM, one type of resonance move has zero kinetic energy, $t = 0$.

Returning to the strong coupling problem, it is clear that we need to look for a phase transition out of the sliding phase into a flat phase where the layers lock. To this end we have carried out a Monte Carlo simulation whose results confirm the existence of the sliding phase as well as of the flat phase (Fig. 2). From our RG analysis, this should happen via a second order transition driven by $\phi_2$ becoming relevant, although we have not explored this in detail. Translated back the quantum ice problem our results indicate that the system exhibits long range order of the antiferroelectric (or F model) kind (Fig. 2), in which it maximizes the density of flippable plaquettes.

For the spins on the checkerboard lattice this is Néel order. The quantum dynamics is the leading order effect of either a transverse field (in which context the Néel phase was conjectured by us previously) or an XY exchange of either sign. One may wonder whether this conflicts with our previous analysis in suggesting Néel order at the Heisenberg point. However it has been shown within spin wave theory that the Néel state on the checkerboard lattice is unstable for $S \leq 1$ so there is every reason to expect a phase transition en route. For such order by disorder phenomena this is by no means exceptional; one generically finds that fluctuations generate an ordered state out of a disordered ensemble, which they then in turn destroy as their strength increases.

In summary, we have explored quantum frustrated antiferromagnetism on the checkerboard lattice. Despite an enormous classical ($S = \infty$) degeneracy, we find a robust ordering tendency for Heisenberg magnets of any spin; for stacked square ice (Ising spins), a sliding phase precedes an antiferroelectric ordering transition.

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One also has to worry about whether all the dimer states are linearly independent as the derivation of the QDM involves inverting their overlap matrix. However, our final result is unaltered if one includes the diagonal bonds in the derivation of the dimer Hamiltonian without allowing dimers to be placed on them, for which case linear independence is assured.

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