The “square kagome” quantum antiferromagnet and the eight vertex model

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We introduce a two dimensional network of corner-sharing triangles with square lattice symmetry. Properties of magnetic systems here should be similar to those on the kagome lattice. Focusing on the spin half Heisenberg quantum antiferromagnet, we generalise the spin symmetry group from SU(2) to SU($N$). In the large $N$ limit, we map the model exactly to the eight vertex model, solved by Baxter. We predict an exponential number of low-lying singlet states, a triplet gap, and a two-peak specific heat. In addition, the large $N$ limit suggests a finite temperature phase transition into a phase with ordered “resonance loops” and broken translational symmetry.

Frustrated magnetic systems have been attracting a lot of attention in recent years. One of the more interesting examples is the spin half Heisenberg quantum antiferromagnet (QAF) on the kagome lattice, a two dimensional network of corner-sharing triangles with hexagonal voids. From numerical studies [1] it is known that this model has a gap to magnetic excitations, but this gap is filled with a continuum of singlet excitations. The number of these excitations is estimated to scale exponentially in the number of lattice sites $N_s$, as $1.15^{N_s}$, and therefore there is a significant low temperature entropy in the thermodynamic limit. It is believed that the low-temperature physics would be well described by a resonating valence bond (RVB) picture.

Some insight into this has been gained by generalising the symmetry group to SU($N$) and going to the large $N$ limit with a particle-hole symmetric fermion representation of the spins. It was proved by Rokhsar [2] that for most common lattices, any “fully dimerised” state (in which every site is part of a dimer pair with another site) is a ground-state of the $N = \infty$ model. The ground-state is thus macroscopically degenerate in this limit [3]. Marston and Zeng [4] applied this picture to the kagome lattice. For the physical SU(2) system, superpositions of all such states, with dimers being interpreted as singlet pairings between the respective spins, would be good candidates for the low-lying singlet states. However, it is clear that a further selection of states occurs when going from $N = \infty$ to $N = 2$ since the number of dimer coverings rises with system size as $1.26^{N_s}$ [5] rather than the observed $1.15^{N_s}$.

In this paper we introduce a lattice [6] (figure 1) with square lattice symmetry, on which, we believe, magnetic properties should be similar to those of the kagome lattice. This, too, is a two dimensional network of corner sharing triangles, but the voids in between are alternately squares and octagons, rather than hexagons. We therefore name it the “square kagome” (or “squagome”) lattice. Using the large-$N$ limit as a guidance, we are able to make precise statements on the Heisenberg QAF on this lattice. At $N = \infty$, the ground-state is again exponentially degenerate, corresponding to dimer coverings. We demonstrate that, to next order in the $1/N$ expansion, an exact mapping can be made to the classical eight-vertex model on the square lattice, with an additional two-fold degeneracy per vertex. As a result, a finite-temperature phase transition is found corresponding to the breaking of a discrete symmetry and to the dominance of specific dimer patterns in the low-temperature phase. The ground-state degeneracy is partially lifted to this order, leading to exponentially many excited singlet states below the triplet gap. Further lifting of the ground-state degeneracy is expected to occur at higher orders in the $1/N$ expansion. We fully expect that at least some of these features will persist in the SU(2) model, which will thus have an exponential number of low-lying singlet excitations, a triplet gap, and RVB-like low temperature states, just as in the kagome lattice. Whether a finite-temperature phase transition also applies to the SU(2) case is an intriguing possibility which deserves further investigations.

As in [7,4] we use a particle-hole symmetric fermionic representation of SU($N$) spins, corresponding to the local
constraint \( \sum_\alpha f^\dagger_{i\alpha} f_{i\alpha} = N/2 \) at each lattice site. The Hamiltonian reads:

\[
H = \frac{J}{N} \sum_{\langle ij \rangle} f^\dagger_{i\alpha} f_{i\alpha} f^\dagger_{j\alpha'} f_{j\alpha'}
\]

where \( \alpha, \alpha' \) range from 1 to \( N \), and summations over repeated indices are implied. Introducing a Hubbard-Stratonovich field \( Q_{ij}(\tau) \) on each bond, conjugate to \( \sum_\alpha f^\dagger_{i\alpha} f_{i\alpha} \), and implementing the constraint using a Lagrange multiplier \( \lambda_i(\tau) \) on each site leads to the following imaginary-time effective action, after integrating out the fermions \([7]\):

\[
S_{\text{eff}}/N = \int_0^\beta d\tau \left( \frac{1}{N} \sum_{\langle ij \rangle} |Q_{ij}|^2 - \sum_i \lambda_i \right)
\]

\[
- \text{Tr} \ln \left( \partial_\tau \delta_{ij} + \lambda_i \delta_{ij} + Q_{ij} \right)
\]

At \( N = \infty \), one has to search for saddle-points of this effective action. There are exponentially many saddle points with the lowest energy (as in \([2,4]\)), given by all “dimer coverings” in which every site is paired uniquely with one of its nearest-neighbour and \( Q_{ij} = Q (= J/2 \text{ at } T = 0) \) on dimer bonds and zero otherwise. The \( \lambda_i \)'s are zero at the saddle point. The physical interpretation of a dimer is the formation of a singlet bond between the two sites.

When studying dimer coverings on the squagome lattice, it is useful to look at individual plaquettes of four triangles enclosing a square. The entire lattice can be viewed as a network of such plaquettes joined at corners. One can convince oneself that if each corner of the internal square is to be part of a dimer, then the number of external corners which are parts of dimers in this plaquette will always be even. Moreover, in two such plaquettes joined at a corner, that corner must be part of a dimer in one plaquette and not another plaquette. A consistent scheme for representing this is to draw an arrow pointing out of the plaquette when that corner is part of a dimer, and into the plaquette when the corner is not part of a dimer. It turns out that there are exactly sixteen allowed configurations per plaquette, as illustrated in figure \([3]\).

The remarkable fact is that when we picture the system thus in terms of arrows, \textit{what we have is precisely the eight vertex model on the square lattice} which was solved exactly by Baxter in the 1970s, and discussed in detail in his book \([8]\). There are, however, two possible dimer configurations per vertex, which introduces an extra twofold degeneracy for the original model. In the infinite \( N \) limit (zeroth order in the large \( N \) expansion), all vertices have equal weight; the energy is of order \( NJ \) and so is the “triplet gap”. We now consider the first order corrections to this infinite \( N \) picture, which we expect to lift the degeneracy between different vertices. Read and Sachdev \([9]\) showed that the first correction beyond \( N = \infty \) lowers the energy of configurations in which two dimers sit on the same square plaquette. This leads for example to a columnar dimer order on the square lattice. In the squagome lattice, we find that the same reasoning leads to a lowering of the energy of vertex 8 compared to the others (fig. \([2]\)). To reach this conclusion, we follow \([7]\) and expand around a dimerised saddle-point: \( Q_{ij} = Q D_{ij} + \delta Q_{ij} \). \( D_{ij} \) specifies the dimer pattern \((= 1 \text{ if bond } (ij) \text{ has a dimer, } = 0 \text{ otherwise}) \) and \( \delta Q_{ij}(\tau) \) is a fluctuation. Expanding the effective action to quadratic order in the fluctuations, one finds two types of terms: bond-diagonal terms involving \( Q^2 D_{ij}^2 \delta^2 Q_{ij}^2 \) and off-diagonal terms of the form: \( Q^2 \delta Q_{ij} D_{jk} \delta Q_{kl} D_{li} \). The latter can be non-zero only on a square-plaquette configuration where a pair of opposite sides has dimer bonds and the other two bonds have fluctuations. This first order correction is of order \( 1/N \) in energy, and can be thought of as a ‘resonance’ of the two possible dimer configurations on a square. Only the off-diagonal contributions change the relative energies in our vertex model, hence the lowering of vertex 8 associated with square patterns.

To second and higher order, too, the only off-diagonal contributions come from loops. Thus, the hexagonal dimer configurations in vertices 1–6 will also have a lowering of energy, of order \( J/N \), as pointed out by Marston and Zeng \([4]\) for the kagome lattice. The resonance of an octagonal loop in vertex 7 is at still higher order. So both these can be ignored in the first order approximation. In addition, second order corrections will lift the degeneracy between the two dimer configurations on a square plaquette, favouring a resonating combination. The comparison to the SU(2) case is instructive: for a loop with an even number of sites, the two possible dimerised states are not eigenstates, but superpositions of such states have lower energy expectation values than the pure dimerised states; the energy gain decreases exponentially with increasing loop length. This is the idea behind the “quantum dimer” approach \([10,11]\). The \( 1/N \) expansion is another approach to an expansion in the size of increasingly long resonance loops.

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FIG. 2. The 16 configurations of an individual plaquette, which map onto the 8 allowed vertices in the eight vertex model, with a degeneracy of 2 per vertex.

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1 2 3 4 5 6 7 8
So we have an 8 vertex model with vertex 8 having an energy, of say $-2\varepsilon$, and all other vertices having zero energy. But with periodic boundary conditions, vertices 7 and 8 must occur in equal numbers (because they are respectively “sources” and “sinks”); so it causes no error to assign them equal energies of $-\varepsilon$ each. In this way we have mapped our system to an eight vertex model, with weights of unity for all vertices satisfying the “ice rule” and higher weights for the remaining two vertices, and with an additional “internal” degeneracy of 2 per vertex.

Since vertices 7 and 8 occur in pairs and together contain two defective triangles in eight, and all other vertices contain exactly one defective triangle in four, the total number of defective triangles is always $1/4$ the total number of triangles—just as in the kagome case.

We now draw some conclusions on the physics of the squagome QAF, using the mapping on the eight vertex model. Three properties of the vertex model play an important role in the following. First, its ground state is two-fold degenerate, with the configuration consisting of an alternation of vertices 7 and 8. Second, there are no gapless excitations, but there is a minimum gap of order $\varepsilon$ between any two levels. Excited levels are, in general, degenerate. Third, the vertex model undergoes a phase transition from an ordered state to a disordered, “paramagnetic” state. One should bear in mind, however, that the underlying dimer model has an additional 2-fold degeneracy per plaquette (figure 2). So the ground state has, to this order, a degeneracy of order $2^{N_p}$ with $N_p$ the number of plaquettes, and each excited level has at least this degeneracy too. The spacing between levels is of order $\varepsilon \propto J$, which is much smaller than the triplet gap which is of order $NJ$. So already we have a picture of an exponential number of singlet states below the triplet gap. We expect that the degeneracy $2^{N_p}$ of each excited level will be lifted with further $1/N$ corrections. For finite $N$, each level could then broaden into a band. The exponential ground-state degeneracy (associated with the local twofold degeneracy present at first order) will also be lifted at higher order. So in the SU(2) case, our picture based on this simple mapping is that of a system with a triplet gap and an exponential number of singlet excitations of order $2^{N_p} \approx 1.12^{N_s}$, since $N_p = N_s/6$. This compares well with the commonly accepted picture of the Heisenberg antiferromagnet on the kagome lattice, where the number of singlet states is of the order of $1.15^{N_s}$.

A somewhat different physical picture for this number was recently proposed by Mambrini and Mila, who take as a starting point a lattice of decoupled up-pointing triangles (with internal coupling $J_1$), and show that the degenerate ground state broadens into a band as the inter-triangle coupling $J_2$ is turned on. However, in any dimer covering of the kagome lattice, exactly $1/4$ of the triangles are left without any dimerised side, and it is not clear that when $J_2$ equals $J_1$, it is a good approximation to assume that all these “defective” triangles belong to one sub-lattice—even though that assumption yields the desired number of singlet states. Work on simpler models suggests that, quantitatively, this approximation is not in fact very accurate. The approach has its merits, however, and can also be applied to the squagome lattice; the results, we believe, will be similar.

Using our mapping and Baxter’s results, we can approximate the thermodynamics of the squagome QAF at low temperatures (below the triplet gap). Fig. 3 displays the calculated correlation length and specific heat as a function of temperature. The latter displays a sharp peak near the transition, which takes place on a scale $\varepsilon$ much smaller than the triplet gap. This is reminiscent of the lowest specific-heat peak reported in quantum dimer model based studies of the kagome antiferromagnet. Since the triplet excitations will also contribute a peak at higher energy, we see that this system, too, shows the two-peak feature which was noticed early in the kagome QAF.

An intriguing feature of our results is a hidden ordering in the ground state. At first order beyond $N = \infty$, this ordering corresponds to a staggered pattern in which every other plaquette is in one of the two configurations corresponding to vertex 7, and its neighbors in one of the two configurations corresponding to vertex 8. At higher order, the picture of two equal-energy configurations per vertex will not persist: such configurations will in general mix, leading to a splitting of energies. If the ordering still exists, it would then correspond to a staggered ordering of plaquettes in which the resonating dimers live on the squares on every other plaquette, and on the star-shaped boundary on the neighbouring plaquettes (figure 1). Such an ordering in a real system may manifest itself as an additional electron density along the resonant squares (and octagon stars), much as happens with the hexagonal ring in benzene. This may be detectable via STM experiments. But it is not clear whether this ordering would actually persist in the SU(2) system, or be washed out.
by further $1/N$ corrections. Since the ordering consists of alternate plaquettes having dimer pairs in their central squares, a possible order parameter could be the quantity $(S_1 + S_2 + S_3 + S_4)^2$ where these are the four spins on the square; this is minimised when two opposite sides are paired as singlets. This is not the true SU(2) ground state, but it is possible that such states will dominate a true RVB-like ground state. It is also not clear whether a sharp phase transition will persist in the SU(2) case, but we note that this ordering is not ruled out at finite temperatures by the Mermin-Wagner theorem since it originates from the breaking of a discrete translational symmetry. So the intriguing possibility of such a phase transition in a 2D Heisenberg system exists.

The obvious question at this point is whether such a study can be made of the kagome lattice too. This lattice can be decomposed into star-shaped plaquettes of hexagons bordered by triangles, which sit at the sites of a triangular lattice (figure 5). In each such plaquette, again, the requirement that each internal site must be part of a dimer pair implies that of the six external sites, an even number must be parts of dimers. But to progress beyond that is difficult, for several reasons. First, the underlying lattice is a triangular lattice, with a high coordination number. Second, each vertex has six (rather than four) arms, and the even-number restriction still leads us to 32 kinds of vertices—each being again two-fold degenerate. There is thus no hope of an exact solution. Estimating vertex weights is possible in principle but requires us in this case to go to second order in the $1/N$ expansion. As noted before, hexagons with three dimerised sides will be preferred. This only fixes the weight of one of the 32 vertices, and since every vertex is now a source or a sink, it is impossible to use this statement to fix the weight of any other vertex. Nevertheless, if we assume that such “perfect hexagons” will dominate, one should be able to maximise their number by forming a regular lattice of them, and they can be detected by an order parameter which is the total spin on the six sites of the hexagon, in analogy to the square plaquette order parameter above. Note that there is still a hidden degeneracy of 2 per plaquette which gives rise to $2^{N_p} \approx 1.08^{N_p}$ states, since in this case the number of sites $N_s = 9N_p$. The observed number of low-energy singlets, $1.15^{N_p}$, suggests a significant additional degeneracy from the number of allowed vertex configurations. So even in a large $N$ limit, the kagome ground state may not be as highly ordered as the squagome.

If a hidden ordering does exist in the kagome case, it may correspond to a pattern of hexagon-shaped resonances. However, as described above, our other conclusions about the squagome lattice are very well corroborated by what is known about the kagome lattice, and in general we expect these systems to behave very similarly.

In conclusion, we have displayed a lattice, which we call the squagome lattice, which is conceptually very similar to the kagome lattice, but with square-lattice symmetry. We have argued that physical properties of spin systems should be very similar on this lattice to properties on the usual kagome lattice. We have shown that, to next to leading order in a $1/N$ expansion, an exact mapping exists between the SU($N$) QAF on this lattice and the classical eight-vertex model. This allows to draw several conclusions on the physics of this QAF at large-$N$, some of which are likely to extend to the physical SU(2) case. In particular, we point out the intriguing possibility of a finite-temperature long-range ordering of the resonance loops. Perhaps most notably, we have connected the field of frustrated quantum systems to a classic exactly solved problem of statistical mechanics.

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FIG. 4. The ground state ordering seen in the large $N$ limit may possibly manifest itself in the physical system by increased electron density along the thick grey lines here.

FIG. 5. The kagome lattice divided into star-shaped plaquettes which form a triangular lattice, by analogy with our treatment of the squagome lattice.
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