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 a kagome lattice. Focusing on the spin-1/2 Heisenberg quantum antiferromagnet, we generalize 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.

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Frustrated magnetic systems have been attracting a lot of attention in recent years. One of the more interesting examples is the spin-1/2 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 generalizing 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 dimerized'' 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 a 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 the system size as 1.26^{N_s},[5] rather than the observed 1.15^{N_s}.

In this paper we introduce a lattice[6] (Fig. 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 call it a ''square kagome'' lattice. Using the large-N limit as a guide, 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 twofold 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. A 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 investigation.

As in the kagome lattice, an attempted ''full dimerization'' leaves (as we show) 1/4 of triangles without dimerized sides, which suggests, even without large-N arguments, that the RVB picture is equally valid here. The approach of Mambrini and Mila,[11] who decoupled the kagome lattice into disjoint sets of isolated upward- and downward-pointing triangles, is also applicable to the square kagome lattice, which also can be decoupled into two disjoint sets of isolated triangles. (Note in passing that the well-known features of the classical kagome Heisenberg antiferromagnet—macroscopic

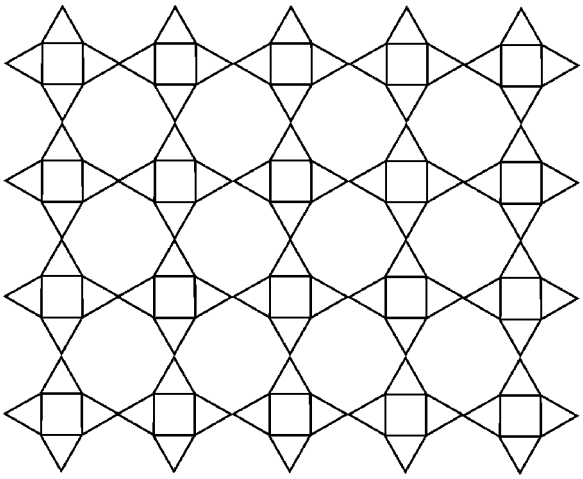

FIG. 1. The ''square kagome'' lattice introduced in this paper.

degeneracy of planar ground states, with additionally several nonplanar ground states obtained by rotating groups of spins without an energy cost—also persist in the square kagome lattice.)

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

$$H = \frac{J}{N} \sum_{\langle ij \rangle} f^\dagger_{i\alpha} f_{i\alpha'} f^\dagger_{j\alpha'} f_{j\alpha}, \tag{1}$$

where α and α' 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 $\Sigma_\alpha f^\dagger_{i\alpha} f_{j\alpha}$, 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]

$$S_{\rm eff}/N = \int_0^\beta d\tau \Bigg[\frac{1}{J} \sum_{\langle ij \rangle} |Q_{ij}|^2 - \sum_i \lambda_i - \mathrm{Tr} \ln(\partial_\tau \delta_{ij} + \lambda_i \delta_{ij} + Q_{ij}) \Bigg]. \tag{2}$$

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 Refs. 2 and 4), given by all ''dimer coverings'' in which every site is paired uniquely with one of its nearest neighbors, and $Q_{ij} = Q$ ($= J/2$ at $T=0$) on dimer bonds and zero otherwise. The λ_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 square kagome 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 16 allowed configurations per plaquette, as illustrated in Fig. 2.

The remarkable fact is that when we picture the system thus in terms of arrows, *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 first-order corrections to this infinite N picture,

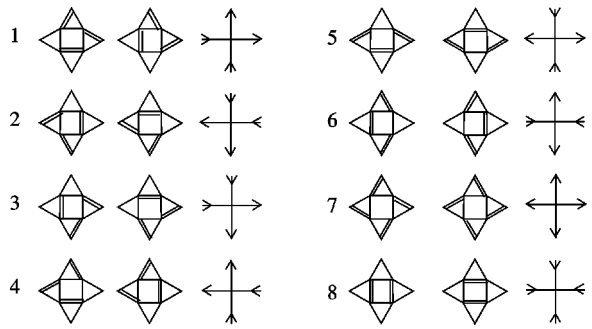

FIG. 2. The 16 configurations of an individual plaquette, which map onto the eight allowed vertices in the eight-vertex model, with a degeneracy of 2 per vertex.

which we expect to lift the degeneracy between different vertices. Read and Sachdev[7] 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 square kagome 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 Ref. 7 and expand around a dimerized saddle point: $Q_{ij} = Q D_{ij} + \delta Q_{ij}$. D_{ij} specifies the dimer pattern [$=1$ if bond (ij) has a dimer, $=0$ 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 $Q^2 D_{ij}^2 \delta Q_{ij}^2$, and off-diagonal terms of the form $Q^2 \delta Q_{ij} D_{jk} \delta Q_{kl} D_{li}$. The latter can be nonzero 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 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 orders, 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 of 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, favoring a resonating combination. The comparison to the SU(2) case is instructive: for a loop with an even number of sites, the two possible dimerized states are not eigenstates, but superpositions of such states have lower-energy expectation values than the pure dimerized states; the energy gain decreases exponentially with increasing loop length. This is the idea behind the ''quantum dimer'' approach.[9,10] The $1/N$ expansion is another approach to an expansion in the size of increasingly long resonance loops.

So we have an eight-vertex model with vertex 8 having an energy, of say -2ϵ, 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''); thus it causes no error to assign them equal energies of $-\epsilon$ 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 $\frac{1}{4}$, the total number of triangles—just as in the kagome case.[5]

We now draw some conclusions on the physics of the square kagome 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 twofold 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 ϵ 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. Since each vertex configuration can correspond to two plaquette dimer configurations, the degeneracy of the ground state, and of every other vertex configuration, is in fact of order 2^{N_p} where N_p is the number of plaquettes. If we assume that the low-lying singlet states in the SU(2) case originate from a mixing of dimer configurations which correspond to the (nonmacroscopic number of) low-lying states of the vertex model, then we expect these low-lying singlets to be macroscopic in number, of order $2^{N_p}=1.12^{N_s}$ where $N_s=6N_p$ is the number of sites. 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}. In the kagome case, the total number of dimerized states is 1.26^{N_s}; the large N approach suggests a reason why not all of these states contribute to the low-lying singlets.[12]

Using our mapping and Baxter's results,[8] we can approximate the thermodynamics of the square kagome QAF at low temperatures (below the triplet gap). Figure 3 displays the calculated correlation length and specific heat as functions of temperature. The latter displays a sharp peak near the transition, which takes place on a scale ϵ 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.[10] In addition, the triplet excitations will contribute a peak at higher energy. A two-peak feature was earlier suggested for the kagome QAF.[5]

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 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 alternate plaquettes, and on the star-shaped boundary on the remaining plaquettes (Fig. 4). It is not clear whether this ordering would actually persist in a SU(2) system, or be washed out by further $1/N$ corrections; in any case, such states are not a true SU(2) groundstate (GS), but may dominate a true RVB-type GS. For instance, in Fig. 4, one can think of having a strong coupling (J_1) along the gray lines and a weak coupling (J_2) along the black lines; for $J_1>J_2$ such an ordering is quite reasonable, and if the ground state has a breaking of the translational symmetry (driven by the desire to maximize the number of resonating square plaquettes), this order may persist up to the $J_1=J_2$ point.

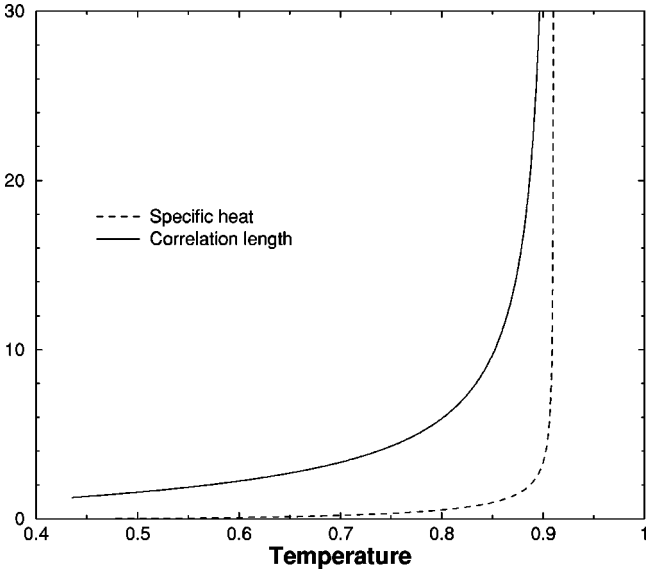

FIG. 3. The specific heat, and correlation length, of the eight-vertex model approximation to the lattice (temperature in units of ϵ).

A possible order parameter could be the quantity $(\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4)^2$, where these are the four spins on the

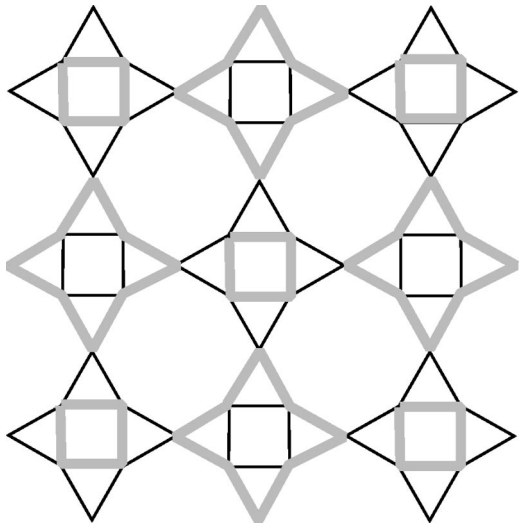

FIG. 4. The ground-state ordering seen in the large-N limit may possibly manifest itself in the physical system by an increased electron density along the thick gray lines here.

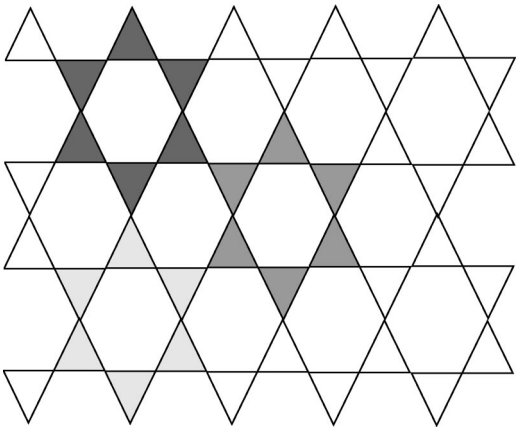

FIG. 5. The kagome lattice divided into star-shaped plaquettes which form a triangular lattice, by analogy with our treatment of the square kagome lattice.

square; this is minimized when two opposite sides are paired as singlets. 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 scanning tunneling microscopy experiments. Whether the large-N phase transition will persist is hard to say, but such 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 two-dimensional Heisenberg system exists.

The obvious question at this point is whether such a study can also be made of the kagome lattice. This lattice can be decomposed into star-shaped plaquettes of hexagons bordered by triangles, which sit at the sites of a triangular lattice (Fig. 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 twofold 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,[4] hexagons with three dimerized sides will be preferred (also see Ref. 13). 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 maximize 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 $2^{N_p} \approx 1.08^{N_s}$ states, since in this case the number of sites $N_s = 9N_p$. The observed number of low-energy singlets, 1.15^{N_s}, 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 square kagome.

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 square kagome 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 square kagome 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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