Block spins and chirality in the frustrated Heisenberg model on *kagomé* and triangular lattices

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The spin-$\frac{1}{2}$ frustrated Heisenberg Model (HM) is investigated using a block-spin perturbation approach on *kagomé* and triangular lattices. In both cases, after coarse graining the triangles on the original lattice and truncation of the Hilbert space to the triangular ground-state subspace, HM reduces to an effective model on a triangular lattice in terms of the triangular-block degrees of freedom, viz. the spin and the chirality quantum numbers. The chirality part of the effective Hamiltonian captures the essential difference between the two lattices. It is seen that chiral-ordered variational states have high energies compared to the other variational states.

Antiferromagnetism (AF) in frustrated lattice systems is known to display some physically striking features, for instance a finite ground-state entropy.[1] Heisenberg spin systems on frustrated lattices have been investigated extensively using diverse methods,[2–4] and ground states with novel structures have been proposed.[5,6] Many authors have addressed the question of a chiral long-range order, especially after the suggestion of its possible connection with the high-T_c superconductors.[5,7,8] Here we investigate Heisenberg spin systems using a block-spin perturbation theory scheme on lattices whose basic unit is a triangle, which is the smallest system with frustration and a chirality. After coarse graining the triangles on the original lattice we derive an effective Hamiltonian which explicitly shows the form of the chiral interactions between the blocks.

We consider a spin-1/2 Heisenberg antiferromanget on triangular and *kagomé* lattices. The Hamiltonian is given by

$$\mathcal{H} = J \sum_{ij} \vec{s}_i \cdot \vec{s}_j, \tag{1}$$

where the sum is over all the bonds on the *kagomé* lattice (KAF) or triangular lattice (TAF), $\vec{s}_i$ is a spin-1/2 operator at site i, and J is the exchange interaction strength. The classical states (which correspond to the limit $s \to \infty$) are known for both lattices, where the angle between any pair of spins is $2\pi/3$, and all the spins on a triangle are coplanar. In contrast, in the spin-1/2 ground state on a triangle the spins are not on a plane, and the chirality is a measure of this noncoplanarity.

We are interested in developing a systematic coarse-graining procedure capturing the essentials of frustration, and finding explicitly the block-spin effective interaction. Also we can see the difference between the effective triangular interaction on the *kagomé* and the triangular lattices, as the amount of frustration is different in the two cases. We start with blocking the original lattice into independent triangular blocks. Using the eigenfunctions of the triangles we derive a block-spin Hamiltonian in terms of the block degrees of freedom, namely, the total spin and the chirality. This procedure will be an exact transformation if all the eight states per triangular block are kept. However, we will effect a truncation of the Hilbert space at the block level by keeping only half the number of states, i.e., restricting the Hilbert space to the block ground-state subspace, as is explained below. This procedure is equivalent to doing a perturbation theory on the interblock interaction. A similar scheme was implemented for coupled Heisenberg chains recently.[9,10] For KAF we block all the triangles standing upright (as shown in Fig. 1), and in the case of TAF we use the blocking scheme used by Niemeijer and van Leeuven for the Ising problem[11] (here one-third of the triangles standing upright are blocked). In both cases the interactions between the blocks is mediated by the inverted triangles (i.e., triangles standing on one vertex). The new interblock Hamiltonian after coarse graining is defined on a triangular lattice with the total number of sites a third of the original lattice.

The Heisenberg model on a triangle has two fourfold degenerate energy levels with total spin $S = 1/2$ and $3/2$. The ground state with $S = 1/2$ has an energy $-\frac{3}{4}J$, and the $S = 3/2$ excited states are $1.5J$ above the ground state, which we will drop by halving the Hilbert space. A twofold Kramers degeneracy in the ground state is implied as we have an odd number of spins. The extra degeneracy comes from the chirality of the triangle. The chirality operator for a triangle is defined[7] through $\chi = \frac{2}{\sqrt{3}} \vec{s}_1 \cdot \vec{s}_2 \times \vec{s}_3$. We have inserted a numerical factor along with the box product of spins so as to make the chirality operator a spin-1/2 operator. The above operator can be chosen to be the z component of the chirality operator $\vec{\chi}$. It is not usual in the literature to treat the chirality as a spin-1/2 operator. However, within the ground-state subspace for a triangle the twofold degenerate ground state in both the spin sectors can be thought of as a chiral spin-1/2 system.[9,10] Interblock interactions cause transitions between the two chiral states; thus lowering and raising chiral operators naturally arise, which we write in terms of the original spin operators later. To be consistent with labeling as the chirality changes sign under odd permutation of spin labels, chirality always refers to the chirality of a triangle standing upright with the first spin at the vertex and the second spin at the left

corner of the base. Let us label the four ground states using the two block quantum numbers $S^z = \pm 1/2$, and the chirality $\chi^z = \pm 1/2$. The state with $S^z = 1/2, \chi^z = 1/2$ denoted by $|++\rangle$ is given in the s^z basis as

$$|++\rangle = \frac{1}{\sqrt{3}}|\uparrow\uparrow\downarrow\rangle + \frac{\omega}{\sqrt{3}}|\uparrow\downarrow\uparrow\rangle + \frac{\omega^2}{\sqrt{3}}|\downarrow\uparrow\uparrow\rangle, \quad (2)$$

where ω is the cube root of unity. The other states can be generated by interchanging ω and ω^2 (this changes the chirality from + to − with S^z fixed), and by operating with the total spin-lowering operator (this changes S^z from 1/2 to −1/2 with the chirality fixed). Let us construct the chiral-raising operator and its Hermitian conjugate by defining $\chi^+|+\rangle = 0$ and $\chi^+|-\rangle = |+\rangle$ in both spin sectors. It should be noted that there is local degree of freedom for each triangle; that is, we can choose any arbitrary linear combinations of the two chiral states, as the Hamiltonian does not have explicit chirality terms. This can be used to advantage in the effective Hamiltonian we derive below.

We would like to write an effective Hamiltonian between the blocks in terms of the total block spin $\vec{S}_i$ and the chirality $\vec{\chi}_i$ of the blocks. Since the original Hamiltonian has only pairwise interactions, the problem reduces to a two-triangle problem (with a 16-dimensional Hilbert space) which can be done analytically. That is, we express $\langle\psi_l|\vec{s}_i(T1)\cdot\vec{s}_j(T2)|\psi_m\rangle$ as an operator, where l and m are labels of the wave functions of the two-block system, viz., direct products of eigenfunctions of two triangles $T1$ and $T2$, which are connected through the spins s_i and s_j. To accomplish this we need to know the action of original spin operators on the triangle eigenfunctions; i.e., for instance, for a given triangle we have

$$s_1^z|++\rangle = 1/2|++\rangle - \frac{\omega^2}{\sqrt{3}}|\downarrow\uparrow\uparrow\rangle,$$

$$s_1^z|+-\rangle = 1/2|+-\rangle - \frac{\omega}{\sqrt{3}}|\downarrow\uparrow\uparrow\rangle,$$

and similar relations involving the other states and operators. We can anticipate that the effective interaction between the block spins will be isotropic, as we have not broken the rotational symmetry in spin space by our blocking procedure. The spin part of the operator factors, and we are left with a four-state problem. We can explicitly carry out the evaluation of the above matrix elements and write the effective interaction between two triangles as a product of spin and chiral interactions. The details of the calculation will not be given here. The effective Hamiltonian is given as

$$\mathcal{H}_{\text{eff}} = -\frac{NJ}{4} + \frac{J}{3}\sum \vec{S}_i \cdot \vec{S}_j \frac{16}{9}(H_{ij} + U_{ij} + D_{ij}), \quad (3)$$

where the operators H, D, and U are nonzero on horizontal, upward, and downward bonds, respectively, on a triangular lattice as shown in Fig. 2. The constant term shown above is the energy of the unperturbed ground states, and we have included a denominate factor of 3 as the number of sites of the new lattice has come down by the same factor. The explicit form of these bond operators will be given below. It is interesting to see that bonds now carry arrows as shown, and all the bonds in one direction have the arrow in the same direction. Inside a triangle the arrow is in one direction only. If we assign a new chiral variable to the direction of the arrow for a given triangle, two neighboring touching triangles have opposite chirality. Let us define the operators T^A, T^B, T^C for every block in terms of the raising and lowering chiral operators through $T^A = \chi^+ + \chi^-/2$, $T^B = \omega\chi^+ + \omega^2\chi^-/2$, $T^C = \omega^2\chi^+ + \omega\chi^-/2$. In terms of these operators, the bond interactions in Eq. (3) are given as

$$H_{ij} = (\tfrac{1}{4} - T_i^A)(\tfrac{1}{4} - T_j^C), \quad U_{ij} = (\tfrac{1}{4} - T_i^B)(\tfrac{1}{4} - T_j^A), \quad D_{ij} = (\tfrac{1}{4} - T_i^C)(\tfrac{1}{4} - T_j^B) \text{ for KAF}, \quad (4)$$

$$H_{ij} = (\tfrac{1}{2} + T_i^A)(\tfrac{1}{4} - T_j^A), \quad U_{ij} = (\tfrac{1}{2} + T_i^B)(\tfrac{1}{4} - T_j^B), \quad D_{ij} = (\tfrac{1}{2} + T_i^C)(\tfrac{1}{4} - T_j^C) \text{ for TAF}. \quad (5)$$

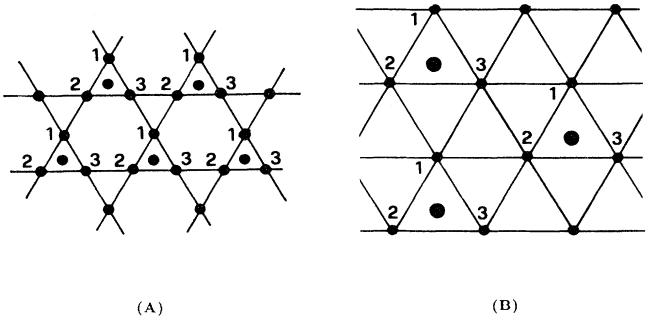

FIG. 1. A part of the original (A) *kagomé* and (B) triangular lattices. The blocked triangles are indicated with dots. The effective model is defined on a new triangular lattice with the number of sites reduced to a third of the original lattice.

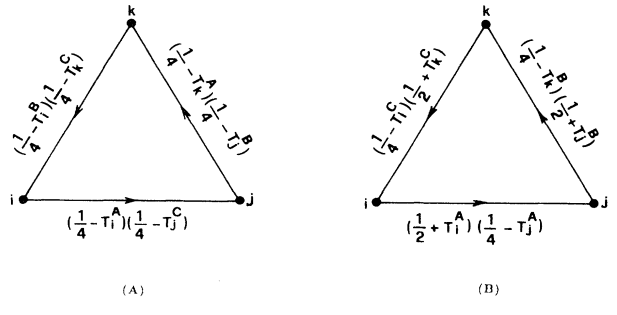

FIG. 2. The effective block-spin interactions for (A) *kagomé* and (B) triangular lattices. The arrows carry the information of the relative orientation of the blocks on the original lattices. All the horizontal bonds have arrows in one direction only, and similarly the other bonds.

As we can see from the above the chirality part of the effective Hamiltonian is very different for the two lattices. Also it is peculiar that there are no terms involving χ^z operators, and the interaction in the x and y directions is anisotropic and not very intuitive. In both cases the bonds are directional, though the way the bonds become directional in the two cases is different. For the *kagomé* lattice the orientation of a given block with respect its nearest neighbor blocks gives directionality to the effective bond strength. There is an additional source of directionality for the triangular lattice; there are two bonds from a single site of one block going to two different sites of another block. It is interesting to see, though the effective model on a triangular lattice is also frustrated, if the block spin and the chirality can conspire so as to cancel some of the frustration effects, which we investigate later.

The T operators are linearly dependent $T^A + T^B + T^C = 0$, and we will see below that these are related to the permutation operators of the triangular block. The eigenfunctions of the operator T^A in the χ^z basis are $|+\rangle \pm |-\rangle/\sqrt{2}$. The operators T^B and T^C have the expectation values $\pm 1/4$ in eigenstates of T^A with eigenvalues $\mp 1/2$. By choosing a given linear combination of the twofold degenerate chiral states for a given block we can monitor the bond strength for the block spins. Thus we have a variety of variational wave functions that can be constructed for the effective model with the bond strengths transferred to the desired singlet valence bonds. Let the ith block be in state $\phi_i = a_i|+\rangle + b_i|-\rangle$, where the kets denote the chiral states. Then the T operators have the expectation values $T^A = 2c_i$, $T^B = -c_i + \frac{\sqrt{3}}{2}d_i$, $T^C = -c_i - \frac{\sqrt{3}}{2}d_i$, where $c_i = \mathrm{Re}(a_i^* b_i)$ and $d_i = \mathrm{Im}(a_i^* b_i)$. Now we have variational parameters a_i explicitly in the Hamiltonian itself, which can be chosen to minimize the energy. Let us try a simple choice ϕ_i such that $T_i^A = -1/2$, $T_i^B = 1/4$, $T_i^C = 1/4$ and $T_i^A = 1/4$, $T_i^B = 1/4$, $T_i^C = -1/2$ at alternate sites for KAF. This makes all the bond strengths zero except half the horizontal bonds (with bond strength J). The ground-state is just a singlet spin state on these bonds. This gives us a bound on the ground-state energy per site for KAF, $E_{\mathrm{g.s.}}(\mathrm{KAF}) \leq -3/8J$. We expect that with a careful choice of ϕ_i one can get a better bound. For the triangular lattice problem a choice of $T^A = 1/2$ and $T^A = -1/2$ at alternate sites along with spin singlets on horizontal bonds of strength $\frac{4}{3}J$ yields a bound $E_{\mathrm{g.s.}} \leq -\frac{5}{12}J$.

Let us consider the effective Hamiltonian of KAF and TAF on a triangle. Since the effective bond interaction is directional (see Fig. 2), we have to examine two types of triangles, viz., a triangle standing upright and a triangle standing on a vertex. For the KAF effective model the maximum strength of any bond is J in any variational state. In contrast for TAF we can have bonds of strength $\frac{4}{3}J$. This means the valence bond state has an energy of $-3/4$ and -1 for KAF and TAF, respectively, in units of J, which is also the energy for a bare Heisenberg Hamiltonian on a triangle. But we can do better than this by taking advantage of the larger number of states we have in the case of the effective model (64 states). In fact it is borne out by the exact diagonalization we have done numerically. The ground state is in the $S = 1/2$ sector with fourfold degeneracy, implying a new chirality. The energy is -0.987 for an upright triangle (more than 30% lower than a valence bond state) and $-3/4$ for the upside down triangle for KAF, where as for TAF both triangles have an energy -1. It is tempting to carry out further levels of blocking. However, the next level of blocking would make sense only if the excited states above the fourfold ground state are spaced in energy farther than the coupling energy of the blocks. The excited states for both KAF and TAF are very close to the ground state at this level of blocking; the nearest excited state (spin 3/2) for KAF is only about 0.1 away in units of the coupling strength (also there are nearby spin-1/2 excited states). This is becuase we have 64 states per block, which is responsible in the first place for a lowering of energy (as opposed to 8 states per block at the first level). This would seriously limit any perturbation-theoretic basis for further blocking, indicating that one should resort to variational methods.

We would like to see the effect of inclusion of the spin-3/2 states that are dropped in our truncation scheme at the first level of blocking. This is achieved by using second-order perturbation theory for the triangular blocks. The effective interaction A_{ij}^{eff} between two blocks i and j within the spin-1/2 ground-state subspace (the spin-3/2 excited states being $\frac{3}{2}J$ away) to second order in the interblock coupling is given by $\langle G'|A_{ij}^{\mathrm{eff}}|G\rangle = -\frac{3}{2}J + \langle G'|A_{ij}|G\rangle + \sum\langle G'|A_{ij}|X\rangle\langle X|A_{ij}|G\rangle/(E_G - E_X)$. The first term is just the energy of the two blocks in the ground state and the second term gives the interaction given in Eq. (3). The third term includes the effect of the virtual transitions to the excited states of the blocks. Here $G = G_1G_2$, $X = G_1X_2$, X_1G_2, X_1X_2, denoting the ground state and the excited states of a block by G_1 and X_1, respectively, and E_G and E_X represent the energies of ground state and excited states, respectively, of the two-block system. The sum is over all the excited states (there are 48 of them). The operator A_{ij} is given in terms of the original spin operators; for KAF it is just a bond operator connecting the two blocks and for TAF it is a sum of the two-bond operator that connect two blocks. The sum over the excited states in the above can be analytically carried out and we can rewrite the effective interactions in terms of the block spin and chirality quantum numbers [as given in Eq. (3)]. The effective interaction is again directional and is given as (for the horizontal bonds of the new lattice) for KAF as

$$\mathcal{H}_{\mathrm{eff}}^{\mathrm{KAF}} = -\frac{35}{108}NJ + \frac{J}{3}\sum_{ij}\vec{S}_i\cdot\vec{S}_j\left\{\frac{200}{189}\left(\frac{3}{10} - \frac{7}{5}T_i^A\right)\left(\frac{3}{10} - \frac{7}{5}T_j^C\right) - \frac{11}{189} + \frac{4}{27}T_i^AT_j^C\right\} + \frac{4J}{81}\sum_{ij}T_i^AT_j^C. \quad (6)$$

Note that for the other bonds a similar interaction obtains, except that suitable T operators should be used [as given in Eq. (4)]. For TAF the effective interaction is given to second order by

$$\mathcal{H}_{\text{eff}}^{\text{TAF}} = -0.343NJ + \frac{J}{3}\sum_{ij}\vec{S}_i\cdot\vec{S}_j\left\{\left(\frac{5}{27}-\frac{38}{27}T_i^A\right)\left(\frac{2}{3}+\frac{4}{3}T_j^A\right)+\frac{4}{27}T_i^AT_j^A\right\}-\frac{4J}{81}\sum_{ij}T_i^AT_j^A. \quad (7)$$

As can be seen from Eqs. (4)-(7)—the effective interaction between the first-order perturbation and that of the second-order theory—the effective interaction is not changed in the form though the coupling constants have changed significantly (which will change the ground-state energy estimate considerably). For TAF, one can get an estimate of the ground-state energy $E_{\text{g.s.}}$ from (7); $E_{\text{g.s.}} = -0.343NJ + e_{\text{g.s.}}^{\text{cs}}NJ/3$, where $e_{\text{g.s.}}^{\text{cs}}$ is the ground-state energy in units of the coupling constant per site of the chiral-spin Hamiltonian given above [i.e., the ground-state energy per site of $3(\mathcal{H}_{\text{eff}}^{\text{KAF}} - \frac{35}{108}NJ)/J$]. Finite-cluster diagonalizations show that the ground-state energy of the simple Heisenberg Hamiltonian is higher than that of the chiral-spin Hamiltonian given above, i.e., $e_{\text{g.s.}} \geq e_{\text{g.s.}}^{\text{cs}}$ (for a six-site cluster the energies are -3.4 and -4.3, respectively, for Heisenberg and chiral-spin models). This gives an estimate, for TAF, of $E_{\text{g.s.}} = -0.5145NJ$. For KAF the estimate for the ground-state energy from a six-site cluster diagonalization of the effective Hamiltonian given in Eq. (6) (there are 1280 states in the $S^z = 0$ sector in this case) is $E_{\text{g.s.}} = -(\frac{35}{108} + \frac{0.414}{3})NJ = -0.426NJ$. However, these estimates for the ground-state energies cannot be used as variational estimates as we have used a second-order perturbation theory for calculating the effective Hamiltonian. For investigating variational trial wave functions one should use the effective Hamiltonian from perturbation theory, as we discuss below.

Now we will rewrite the effective Hamiltonian from first-order perturbation theory given in (3) in a more transparent form. First, we note that the interblock interactions are causing transitions between the two chiral states of a block, as is clear from the appearance of the χ^+ operators. The chirality of a block is changed by a permutation of the spin labels. This implies that one can explicitly construct the chirality operators using the permutation operators. Let us define a permutation operator P_1, which permutes spins 123–132 of a given block, and similarly P_2 and P_3 exchange spins 1,3 and 1,2, respectively. The P operators can be written in terms of the spin operators,[1] for instance $P_1 = 2(\vec{s}_2\cdot\vec{s}_3+1/4)$. The action of the permutation operators on the chiral states is seen explicitly, $P_1|+\rangle = \omega|-\rangle$ and $P_1|-\rangle = \omega^2|+\rangle$. Let us denote by e_i the operator of a bond opposite to site i in a block. We have $\langle e_1+e_2+e_3\rangle = -3/4$ and $-3/4 \leq \langle e_i\rangle \leq 1/4$. The chirality operator χ^z is defined as a commutator of P operators through

$$\chi^z \equiv \frac{i}{2\sqrt{3}}[P_2,P_1] = \frac{2i}{\sqrt{3}}(e_2e_1 - e_1e_2), \quad (8)$$

and the operator χ^x is just half of P_3. It is interesting to note that a similar construction can be used to construct the chirality operators in terms of the spin operators directly even in a general case of more than three spins,[10] in contrast with the usual practice of defining χ^z in terms of fermion operators.[7]

It is easy to check that the T operators appearing in the effective Hamiltonian are related to the permutation operators through $T^A = P_3/2$, $T^B = P_2/2$, and $T^C = P_1/2$. The effective Hamiltonian has a very simple form in terms of the bond operators. For instance two blocks l and m on a *kagomé* lattice, with block spins $\vec{S}_l$ and $\vec{S}_m$, connected at sites $i(l)$ and $j(m)$, have the effective interaction

$$\frac{16}{9}J\vec{S}_l\cdot\vec{S}_m e_i(l)e_j(m).$$

This has a physical significance, in terms of a valence bond trial wave function, that the block spins prefer that the bonds opposite to the connecting sites to be in singlet so that the block spins can form a singlet too. The frustration of the original lattice translates into frustration for the block spin bonds. For TAF the scenario is different, as a pair of blocks standing upright are connected by two bonds of the original lattice, between the vertex of the lth block [vertex site $i(l)$] and the base of the mth block with [vertex site $i(m)$]. The interaction between the block spins is $-16/9J\vec{S}_l\cdot\vec{S}_m e_i(l)[3/4+e_i(m)]$.

With the effective bond strengths expressed in terms of the original bond operators, we can now investigate chiral-ordered states of the original lattice. Let us try a trial wave function $|\psi\rangle$ with chiral ordering on the original lattice, which implies for each block that we choose one of the chiral states. In any of the four chiral states of a given block, all the bond operators have an expectation value $e_i = -1/4$. This means that the block spins interact with a strength of $2/9J$ for TAF, and $1/9J$ for KAF for this trial state. This gives us a bound $E_{\text{TAF}}(\psi) \leq -\frac{1}{4} + \frac{2}{27}E_{\text{TAF}}$, implying $E_{\text{TAF}}(\psi) \leq -0.27$, which is significantly larger than the energy of the valence bond state we discussed above. Similarly for the case of KAF, one can see that chiral-ordered variational states have energies well above the other variational states. However, one can try other variational states, particularly the resonating-valence-bond-type states are very convenient to work with in this respect. If a triangle has a singlet valence bond, it implies that one of the e_i is equal to $-3/4$ and the others vanish. That is, four out of the six bonds incident on a particular site on the effective lattice have an exchange strength of zero. And the expectation values are calculated straightforwardly, as the effective model decomposes into cluster Hamiltonians. An investigation of various variational trial states on the effective model is in progress.

In summary, we have established an effective Hamiltonian in terms of block spins and chirality for both *kagomé* and triangular lattices, using a block-spin perturbation theory approach. A further level of blocking is not suit-

able because of the existence of low-lying excited states. The effective model has a simple physical way of understanding in terms of the permutation and bond operators of the triangular blocks of the original lattices. The bond operator expectation values of the blocks can be effectively used in variational valence bond wave functions. Chiral-ordered wave functions are seen to be high in energy compared to other simple trial wave functions.

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