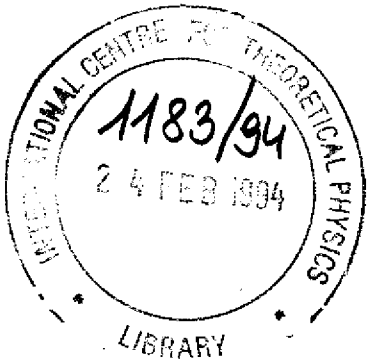

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ABSTRACT

The spin-$\frac{1}{2}$ Heisenberg model (HM) is investigated using a block-spin renormalization approach on Kagome and triangular lattices. In both cases, after coarse graining the triangles on 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 simple eigenstates can be constructed for the effective model whose energies serve as upper bounds on the exact ground state energy of HM, and chiral-ordered variational states have high energies compared to the other variational states.

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Antiferromagnetism 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 has been investigated extensively using diverse methods [2, 3, 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 a suggestion of its possible connection with the high-T_c superconductors[5, 7, 8]. In this letter we investigate Heisenberg spin systems using a block-spin renormalization 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 Kagome lattices. The Hamiltonian is given by

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

where the sum is over all the bonds on the Kagome 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 corresponds to the limit $s \to \infty$) are known for both the 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 Kagome 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 8 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 inter-block interaction. A similar scheme has been implemented for the Heisenberg model on C_{60} recently[9]. 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 inter-block 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 four-fold degenerate energy levels with the 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 two-fold 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 $\chi = \frac{2}{\sqrt{3}}\vec{s}_1.\vec{s}_2 \times \vec{s}_3$. 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 abvoe operator can be chosen to be the $z-$component of the chiratlity operator $\vec{\chi}$. It is not usual in the literature to treat the chirality as a spin-half operator. However, within the ground state subspace for a triangle the two-fold degenerate ground state in both the spin sectors can be thought of as a chiral spin-1/2 system[10]. Inter-block interactions cause transitions between the two chiral states, thus the lowering and raising chiral operators naturally arise, which we write in terms of the 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 $|++>$ is given in the s^z basis as

$$|++> = \frac{1}{\sqrt{3}}|\uparrow\uparrow\downarrow> + \frac{\omega}{\sqrt{3}}|\uparrow\downarrow\uparrow> + \frac{\omega^2}{\sqrt{3}}|\downarrow\uparrow\uparrow>, \tag{2}$$

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 the 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 its hermitian conjugate by defining $\chi^+|+>= 0$, and $\chi^+|->= |+>$ in both the 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 pair-wise interactions, the problem reduces to a two-triangle problem (with a 16-dimensional Hilbert space) which can be done analytically. That is we express $< \psi_l|\vec{s}_i(T1).\vec{s}_j(T2)|\psi_m >$ as an operator, where l and m are labels on the wavefunctions of 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

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

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

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

$$\mathcal{H}_{eff} = \frac{16}{9} J \sum \vec{S}_i . \vec{S}_j (H_{ij} + U_{ij} + D_{ij}) \tag{3}$$

where the operators H, D, U are nonzero on horizontal, upward and downward bonds respectively on a triangular lattice as shown in Fig.2. 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

$$H_{ij} = (\frac{1}{4} - T_i^A)(\frac{1}{4} - T_j^C),\ U_{ij} = (\frac{1}{4} - T_i^B)(\frac{1}{4} - T_j^A),\ D_{ij} = (\frac{1}{4} - T_i^C)(\frac{1}{4} - T_j^B) \text{ forKAF},$$

$$H_{ij} = (\frac{1}{2} + T_i^A)(\frac{1}{4} - T_j^A),\ U_{ij} = (\frac{1}{2} + T_i^B)(\frac{1}{4} - T_j^B),\ D_{ij} = (\frac{1}{2} + T_i^C)(\frac{1}{4} - T_j^C) \text{ forTAF}.$$

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 x and y directions is anistropic 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 Kagome lattice the orientation of a given block with respect its nearest neighbor blocks gives the 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 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 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 χ^z basis are $|+> \pm |-> /\sqrt{2}$. The operators T^B and T^C have expectation values $\pm 1/4$ in eigenstates of T^A with eigenvalues $\mp 1/2$. By choosing a given linear combination of the two-fold degenerate chiral states for a given block we can monitor the bond strength for the block spins! Thus we have a variety of variational wavefunctions that can be constructed for the effective model with the bond strengths transfered to the desired singlet valence bonds. Let i'th block be in state $\phi_i = a_i|+> + b_i|->$, 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 $c_i = Re(a_i^* b_i)$ and $d_i = Im(a_i^* b_i)$. 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, $E_{gs}(KAF) \leq -3/8J$. We expect that a careful choice of ϕ_i one can get a better bound. For the triangular lattice problem a choice with $T^A = 1/2$ and $T^A = -1/2$ at alternate sites along with spin singlets on horizontal bonds of strength $\frac{4}{3}J$ yields a bound $E_{gs} \leq -\frac{5}{12}J$.

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 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 more 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 $S = 1/2$ sector with four-fold 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. This gives an indication that for KAF the frustration is reduced considerably at the first level of blocking, and presumably it should get better on further blocking (for instance blocking the less-frustrated triangles at the second level). Let us write the ground state energy per site of KAF as $E_{gs}(KAF)/J = \sum_{i=1}^{\infty} x_i/3^i$, where x_i is the energy of a triangular unit at i'th blocking. We have the first two terms of the series, $x_1 = -3/4$, and $x_2 = -0.987$. Let $y_i = x_i/x_{i-1}$ be the ratio of the energies of the basic unit at successive blockings. If we assume that after each blocking y_i does not decrease, *i.e.* $y_i \leq y_2 = 1.316$, which is supported by the fact that the frustration effects are not as strong after blocking as discussed above, we can get a bound on the ground state energy, $E_{gs} \leq x_1/(3 - y_2) = -0.445$. We need at least a few more x_i (which could be computed numerically) to support this estimate, but indication is in favor of this. Similarly for TAF we have $x_1 = 3/4, x_2 = 1$, $y_2 = 4/3$, this gives us a bound $E_{gs}(TAF) \leq -9/20$. In this case, it may be a good idea to try variational valence bond wavefunctions with the effective Hamiltonian. This is because of the lack of indication of frustration growing less at this first level of blocking and the Hamiltonian is difficult to carry out the next level blocking analytically. The valence bond variational states can exploit the ablility of turning off or on of bonds, and can give better upperbounds.

Now we will rewrite the effective Hamiltonian in a more transparent form. Firstly, we note that the inter-block interactions are causing transitions between the two chiral states of a block, as it is clear from the appearance of χ^+ operators. The chirality of a block is changed by a permutation of the spin labels. This implies one can explicitly construct the chirality operators using the permutation operators. Let us define permutation operator $P1$, which permutes the spins 123 to 132 of a given block, and similarly P_2, and P_3 exchange spins 1 and 3, and 1 and 2 respectively. The P operators can be written in terms of the spin operators[1], for instance $P_1 = 2(\vec{s}_2.\vec{s}_3 + 1/4)$. The action of the permutation operators on the chiral states is seen explicitly, $P_1|+> = \omega|->$, and $P_1|-> = \omega^2|+>$. Let us denote by

e_i the operator of a bond opposite to site i in a block. We have $< e_1 + e_2 + e_3 > = -3/4$, and $-3/4 \leq < e_i > \leq 1/4$. The chirality operator χ^z is defined as a commutator of P operators through

$$\chi^z \equiv \frac{i}{2\sqrt{3}}[P_2, P_1] = \frac{2i}{\sqrt{3}}(e_2 e_1 - e_1 e_2), \tag{4}$$

and the operator χ^z 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 Kagome lattice, with block spins $\vec{S}_l$ and $\vec{S}_m$, connected at sites $i(l)$ and $j(m)$ have the effective interaction

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

This has a physical significance, in terms of a valence bond trial wavefunction, 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 l'th block (vertex site $i(l)$) and the base of m'th block with (vertex site i(m)). The interaction between the block spins is $-16/9 J \vec{S}_l.\vec{S}_m e_i(l)(3/4 + e_i(m))$.

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 wavefunction $|\psi>$ with chiral ordering on the original lattice, which implies for each block 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 $E_{TAF}(\psi) \leq -\frac{1}{4} + \frac{2}{27} E_{TAF}$, implying $E_{TAF}(\psi) \leq -0.27$, 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 RVB-type states are very convenient to work 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 exchange strength 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.

We would like to add that this procedure is also equivalent to using the real-space renormalization prescription in terms of the density matrix of the block given by White[12]. This is because the density matrix does not mix states with different spin, though it mixes the excited states with the same spin as that of the ground state. However, in the case of a bigger block, for instance a pentagon, with spin-1/2 excited states the two procedure are not equivalent. We would also like to point out that one can in fact include all the 8 states of a triangle. The effective model would be similar, except that it is difficult to work with due to the appearance of spin-3/2 projection operators.

In summary, we have established an effective Hamiltonian in terms of block spins and chirality for both Kagome and triangular lattices, using a block-spin renormalization approach. The frustration effects are seen to reduce considerably for the Kagome lattice. 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 wavefunctions.

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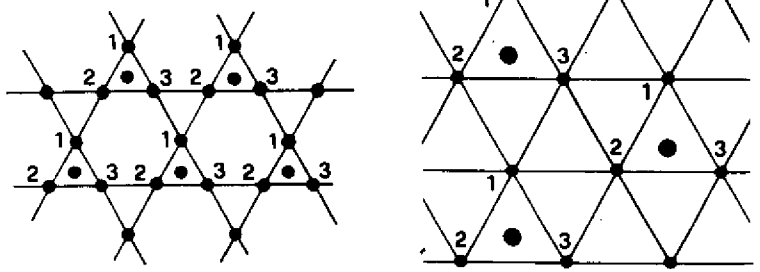

Figure 1: A part of the original (A) Kagome (B) triangular lattices. The blocked triangles are indicated with dots. The effective model is defined on a new triangular lattice with the number of sites reduced to a third of the original lattice.

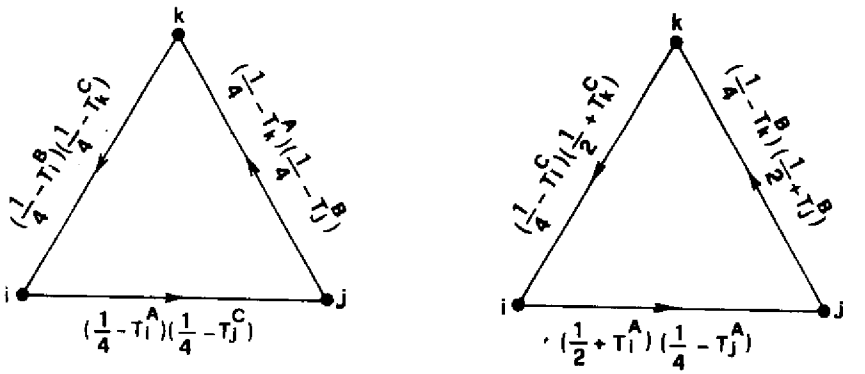

Figure 2: The effective block-spin interactions for (A) Kagome (B) triangular lattices. The arrows carry the information of the relative orientation of the blocks on the orignial lattices. All the horizontal bonds have arrows in one direction only, and similarly the other bonds.