In classical spin systems, competing interactions commonly frustrate the conventional \((\pi, \pi)\) Néel order, possibly leading to more exotic arrangements of the local spins. Prominent examples include helicoidal configurations, \([1, 2, 3]\) which usually break space inversion and time reversal. Noticeably, such spin chirality is a sufficient condition for multiferroic behavior, i.e., non-zero coupling between magnetization and electric polarization\([1, 5]\).

However it is not uncommon that non-planar magnetic orders relieve the frustration even more effectively than helicoidal configurations do. The associated magnetic order parameter is then three-dimensional, hence also chiral. To date, two such orders have been exhibited, both on triangular-based lattices with competing interactions: a 4-sublattice tetrahedral order was found on the triangular lattice\([6]\) while a 12-sublattice cuboctahedral order was found more recently on the kagomé lattice.\([7]\)

In two dimensions, complex magnetic orders might seem of purely theoretical interest since gapless spin-waves destroy the spin long-range order at arbitrarily low temperatures. However, this disordering process is soft, in the sense that at low but finite temperature, the spin-spin correlations remain large enough to sustain emergent long range orders. This is exemplified by the two above-mentioned models where chiral long-range order persists up to finite temperatures, whereas long-range order in the spins is lost. Interestingly, the emergent chiral order parameter is Ising-like, and in a straightforward extrapolation one expects that these chiral phases will disappear through a critical transition in the 2D Ising universality class. However, Momoi and Kubo showed that in the case of the tetrahedral order, this is true only in the “weak universality” sense.\([6]\)

We point out that such three-dimensional magnetic orders completely break the \(SO(3)\) symmetry of Heisenberg interactions. Hence the order parameter space is \(SO(3)\) which supports point defects, namely vortices in two dimensions, around which the order parameter is rotated by \(2\pi\). However, note that rotation of \(4\pi\) is equivalent to the identity, so that the order parameter may only wind by \(\pm 2\pi\), as can be more formally deduced from \(\Pi_1 = Z_2\). This evidences the peculiar topology of \(SO(3)\) vortices compared to the well known \(SO(2)\) vortices involved in the Berezinski.-Kosterlitz-Thouless (BKT) transition. In particular, since \(SO(3)\) rotations of \(4\pi\) are equivalent to the identity, \(SO(3)\) only supports vortices with unit “winding number”, as can be deduced more formally through \(\Pi_1(SO(3)) = Z_2\). These \(Z_2\) vortices were first exhibited in an early numerical work by Kawamura and Miyashita\([8]\) on the antiferromagnetic Heisenberg model on the triangular lattice, where the defects were shown to proliferate rather abruptly at finite temperature. To date, however, there is still no conclusive evidence that a genuine phase transition indeed takes place in this model. On the experimental front, the proof of existence of the \(Z_2\) vortices remains rather elusive, although they may have been probed indirectly in recent NMR experiments on \(\text{NaCr}_2\text{O}_3\).\([9]\)

In this letter we exhibit \(Z_2\) vortices in the \(J_1 - J_2\) model on the kagomé lattice and show that they are responsible for the first order nature of the chiral transition and we study the effects of frustration on the core energy of these defects.

The Hamiltonian of this model reads:

\[
\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,k \rangle\rangle} \vec{S}_i \cdot \vec{S}_k
\]  

(1)

where the first sum runs over pairs of nearest neighbors (at distance 1 on the kagomé lattice) and the second sum over pairs of second nearest neighbors (at distance \(\sqrt{3}\)).

We are interested in the 12-sublattice antiferromagnetic ground state obtained for \(J_1 < 0\) and \(J_2 > |J_1|/3\).\([7]\). The associated order parameter has the symmetry of a cuboctahedron, with scalar chirality \(\sigma_{ijk} = \sqrt{2} \vec{S}_i \cdot \vec{S}_j \times \vec{S}_k\) either +1 or −1, where \((i, j, k)\)
chiral phase increases with increasing antiferromagnetic

ods. We simulated samples of linear size

suitable to overcome the free energy barriers encountered

parallel tempering algorithm. This method is indeed

results of the simulations are collected in Fig. 2. Start-

largest samples the number of Monte Carlo steps needs

an "effective critical" slowing-down. Therefore, for the

existence of a large spin-spin correlation length drives

down associated to the crossing of free energy barriers,

The two degenerate ground states differ only by their scalar chirality, namely

the triple product of 3 spins on a (shaded) triangle.

\[ C = \frac{3}{2N} \sum_{ijk} (-1)^{sijb} \sigma_{ijk} \]  

where the sum runs over all 2N/3 triangles of the kagomé lattice with \( \sigma_{ijk} = 0 \) (1) for triangles pointing up (down).

To investigate the finite-temperature phase diagram of this model, we perform Monte Carlo simulations using a parallel tempering algorithm. This method is indeed suitable to overcome the free energy barriers encountered at first-order phase transitions, as we will show is the case for the chiral transition in this model. Further, this algorithm is easy to parallelize and yields thermodynamic quantities over a large range of temperatures in a single run, once combined with reweighting methods. We simulated samples of linear size \( L \) ranging from 12 to 64, with up to \( N = 3L^2 \leq 12288 \) spins. Although the tempering method suppresses the slowing-down associated to the crossing of free energy barriers, the existence of a large spin-spin correlation length drives an “effective critical” slowing-down. Therefore, for the largest samples the number of Monte Carlo steps needs to be increased up to \( 2^{22} \) steps per spin. The first results of the simulations are collected in Fig. 2. Starting from \( J_2/J_1 = 1/3 \), the temperature extent of the chiral phase increases with increasing antiferromagnetic

\( J_2 \). We have monitored several thermodynamic quantities, namely the averaged value of the energy per spin \( \langle e \rangle \), the specific heat, \( C_v/k_B = \frac{N}{k_B T^2} \langle (\varepsilon^2) - \langle \varepsilon \rangle^2 \rangle \), the staggered chirality \( \langle |C| \rangle \) and the associated susceptibility

\[ k_B \chi_C = \frac{2N}{k_B T^2} \left( \langle C^2 \rangle - \langle |C| \rangle^2 \right) \]  

Figure 3 shows the rapid destruction of the chiral long-range order at the transition (note the very small temperature scale) for \( J_2/J_1 = 0.38 \).

To characterize the chiral transition we use standard finite-size scaling analysis. For \( 1/3 < J_2/J_1 < 0.45 \), the energy distribution becomes bimodal in the neighborhood of the transition, and its maxima become more pronounced with increasing sample sizes. Both the maximum of the specific heat \( C_v^{\text{max}}(L) \) and of the chiral susceptibility \( \chi_C^{\text{max}}(L) \) increase algebraically with \( L \) with exponents within \( 2.0 \pm 0.15 \) for \( J_2/J_1 \leq 0.38 \).

For \( J_2/J_1 = 0.39 \) and 0.40, the scaling regime is reached only for the largest samples. In addition, denoting \( T_{C_v}(L) \) and \( T_{\chi_C}(L) \) the temperatures of the maximum of \( C_v(L) \) and \( \chi_C(L) \) one obtains \( 1/T_{C_v,\chi_C}(\infty) - 1/T_{C_v,\chi_C}(L) \sim 1/L^2 \) for \( J_2/J_1 \leq 0.38 \). The above analysis shows that the transition does not belong to the expected Ising universality class, but is first-order, although the increasing difficulty to reach the scaling regime, when increasing \( J_2/J_1 \), evidences the concomitant growth of a correlation length. This is consistent with the continuous decrease of the latent heat with increasing \( J_2/J_1 \) \( (0.034, 0.028, 0.012 \) for \( J_2/J_1 = 0.36, 0.38, 0.45 \) )

To account for the discontinuous nature of the chiral transition a thermally activated mechanism was looked for: proliferation of point defects is an obvious candidate, and we now proceed to compute the \( \mathbb{Z}_2 \) vortices of
The chirality (otherwise). We computed the vortex density $C_v$ is maximum. Finally we define the $Z_2$ vorticity inside an elementary (triangular) contour by

$$V_\Delta = \frac{1}{2} \left( 1 - \frac{1}{2} Tr \left( \prod_{j \in \Delta} U(\hat{n}_j, \theta_j) \right) \right)$$

where $V_\Delta = 1(0)$ when the loop $\Delta$ encloses a singularity (otherwise). We computed the vortex density $\langle n_v \rangle = 6/N \sum_{\Delta} V_\Delta$, where the sum runs over all $N/6$ triangles of the super-lattice. The results are displayed in Fig. 3 versus $(T - T^*)/T^*$, where $T^*(L)$ is the temperature of the maximum of $C_v(L)$. They clearly show that the chiral transition is concomitant with the proliferation of vortices.

The behavior of the spin-spin correlation length $\xi_{spin}$ close to the transition evidences that vortex proliferation drastically decreases the magnetic short range order as well as it kills the emergent chiral order, far before the expected critical regime of the chiral phase is attained. Hence the Ising chiral transition is avoided simply because the vortex proliferation triggers a first-order phase transition that preempts the critical regime. We emphasize that the disordering effect of the $Z_2$ defects is much stronger than that of $Z$ vortices at the BKT transition. Fig. 3 indeed shows that $\xi_{spin}$ is divided by three in a temperature range $\sim 10^{-3} T^*$, and this brutal decrease may even be smoothed by the finite size of the sample.

The chiral correlation length $\xi_{chiral}$, as computed from the structure factor of the chirality $C$ at the transition, measures the discontinuity of the chiral transition. For $J_2/J_1 = 0.38$ we find $\xi_{chiral} = 6$, while it exceeds the largest available lattice size ($\xi_{chiral} > 64$) already for $J_2/J_1 = 0.40$. Consistently, the vortex proliferation smoothes upon increasing $J_2/J_1$ (Fig. 3) and for large enough $J_2/J_1 = 0.45$, the number of vortices at the transition is clearly seen to decrease. Although this is not the core of our study, note that the fast growth of $\xi_{chiral}$ with increasing $J_2/J_1$ makes it particularly delicate to identify a possible critical end point to the line of first order chiral transitions shown in Figure 2.

Discussion: The chiral transition in the present $J_1 - J_2$ model may be typical of many frustrated magnets. Indeed, as emphasized above, as long as the ground state completely breaks the $O(3)$ symmetry of the Heisenberg Hamiltonian, as is the case for non-planar Néel orders, both chirality and $Z_2$ vortices exist. The complete breaking of $SO(3)$ induces $Z_2$ point defects, while the breaking of time reversal (the discrete part of $O(3)$) leads to chiral degenerate ground-states. Hence we expect very similar features for the chiral transition in the present model and that observed on the triangular lattice by Momoi et al.: in a posterior study, these authors indeed noticed that the chiral transition may be weakly discontinuous.

However, the nature of the chiral transition cannot be deduced from symmetry arguments alone and will ultimately depend on the energetics of the two competing mechanisms that suppress chiral order: formation of chiral domain walls versus creation of $Z_2$ vortices.

In this respect, the case of the $J_1 - J_3$ model on the square lattice is interesting. Capriotti and Sachdev have shown that in this model, the doubly degenerate helicoidal ground-state results in a finite temperature chiral phase. Although $Z_2$ vortices are allowed by symmetry, the chiral transition at finite temperature clearly falls in the 2D-Ising universality class. Consistently, we understand that in a problem dominated by antiferromagnetic long-wavelength fluctuations, forming a chiral domain wall is much less costly than creating a $Z_2$ vortex.

Correspondingly, in the $J_1 - J_2$ model under study, we expect that competing ferromagnetic and antiferromagnetic interactions will enhance the short-range fluc-
tensions, hereby decreasing the core energy of $Z_2$ vortices. This qualitative argument is supported by the observation that the discontinuity of the chiral transition is maximal when the competition of interactions is highest, i.e. close to $J_2/|J_1| = 1/3$: there the chiral transition is clearly triggered by the proliferation of defects.

Note also that the decrease of the transition temperature as $J_2/|J_1| \to 1/3$ suggests that the core energy of the $Z_2$ vortices vanishes at the $T = 0$ phase boundary, i.e. $J_2/|J_1| = 1/3$.

However, in this very low temperature regime quantum fluctuations are expected to play a significant role. The $T = 0$ quantum problem was actually studied previously by three of us: [7] using exact diagonalizations for spins 1/2 as well as spin-wave expansions, it was shown that both classical ground states, ferromagnetic and 12-sublattice antiferromagnetic, survive quantum fluctuations with a quantum phase transition located at $J_2/|J_1| \approx 1/3$. Hence, although the present study is purely classical, it yields the promising prospect that additional excitations become gapless exactly at the quantum phase transition, supplementing the usual gapless magnons that exist in either of two neighboring phases. This is highly reminiscent of the breakdown of the Landau paradigm in quantum spin systems, [12] although the route from classical $Z_2$ vortices to some fractionalized “spinon” excitations for spins 1/2 remains a totally open problem.

Experimentally, a large number of magnets on the kagomé lattice have been synthetized up to now, and it has been a long route to arrive at the Herbertsmithite $Z_n\text{CuO}$, which remains an antiferromagnetic spin liquid down to 50 mK. [13] [14] with a dominant antiferromagnetic interaction of about 190 K. Amongst other difficulties, the sign of the nearest neighbor coupling is a pending problem: Atacamite, parent both of Paratacamite and Herbertsmithite, becomes ferromagnetic around 10 K. Similarly, Cutitmb, the organic compound at the origin of our interest in the present model, [15] [16] was recently shown to experience a transition to three dimensional ferromagnetic order around 500 mK [17]: this tendency to ferromagnetism is deeply rooted in the geometry of the exchange paths between nearest neighbor Cu ions on the kagomé lattice. If the malediction of such low-temperature ferromagnetic orderings can somehow be avoided, possibly through a decrease of the inter-layer couplings, the present study would be of direct experimental interest, beyond its initial theoretical motivation.

In this letter, we showed that in the $J_1 - J_2$ model on the kagomé lattice, chiral order is wiped out at finite temperature by the first-order proliferation of $Z_2$ vortices. In the region of extreme frustration $J_2/|J_1| \approx 1/3$ the core energy of the defects decreases and appears to vanish exactly at the $T = 0$ phase boundary. This behavior is probably common to frustrated spin systems in which competing interactions lead to three-dimensional antiferromagnetic order parameters.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{vortex_density_vs_temperature}
\caption{(Color online) Evolution of the vortex density $\langle n_v \rangle$ around the transition temperature $T^*$ as a function of $J_2/|J_1|$.}
\end{figure}