From frustrated magnetism to spontaneous Chern insulators

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We study the behaviour of electrons interacting with a classical magnetic background via a strong Hund coupling. The magnetic background results from a Hamiltonian which favours at low temperature the emergence of a phase with non-zero scalar chirality. The strong Hund’s coupling combined with the total chirality of the classical spins induces in the electrons an effective flux which results in the realisation of a band structure with non zero Chern number. We study the Density of States (DoS) and Hall conductance as a function of temperature and external magnetic field of the classical spin system in order to analyse the topological transitions. We present the complete phase diagram showing regions where the DoS do has a gap and the Hall conductance is quantised. We also study a similar model in which the Chern number of the filled bands can be “tuned” with the external magnetic field, resulting in a topological insulator in which the direction of the chiral edge mode can be reverted by reversing the orientantion of the magnetic field applied to the classical magnetic system.

Introduction: The discovery of the quantum Hall effect in 1980 [1] opened a new field in condensed matter physics. In this area, topological phases have attracted much interest in the last decade and in particular, the celebrated topological insulator (for a review on the subject see [2]). The first topological insulator correspond to the integer quantum Hall effect where a bidimensional electron gas in a strong magnetic field \( B \) has a Hall conductance with quantised plateaux at \( \sigma_{xy} = \nu e^2/h \) (\( \nu = 1, 2, ... \)) values.

The quantum anomalous Hall insulator is a phenomenon in solids arising from the spin-orbit coupling due to a Hund’s coupling between the electronic spin and spontaneous magnetic moments. It can lead to a topologically non-trivial electronic structure with a quantized Hall effect characterised by the Chern numbers \( C \) of the filled bands and the presence of chiral edge modes. The principal ingredient is a non-collinear spin texture distinguished by a non zero value of the uniform scalar chirality parameter \[3–5\].

In this direction, frustrated systems are good candidates for the emergence of chiral spin textures. Among these, kagome materials \[6\] have been studied both theoretically and experimentally \[7\] due to the possibility for nontrivial spin textures, spin-liquid phases, exotic transport properties, and topologically protected phases (for a recent review see Ref.[8] and references therein). In particular, in a recent paper \[9\] the authors found that a spontaneously broken reflexion symmetry phase with a non zero total chirality can be induced by a magnetic field in the kagome lattice. They found that by decreasing the temperature the system undergoes a phase transition from a normal paramagnet to a chiral state, with either positive or negative total chirality. This opens the possibility of triggering the anomalous Hall effect (AHE) and the emergence of a Chern insulators by just cooling and applying a magnetic field to the magnetic system. While there exist a large number of theoretical studies of AHE at zero temperature, the situation at finite temperature is much less explored.

![Topological Transistor Diagram](image-url)

**FIG. 1:** (Top) Schematic representation of a topological transistor. The spheres represent the sites of a (finite with edges) kagomé lattice under an external magnetic field perpendicular to the kagome layer. Different orientations of the magnetic field up (red) or down (blue) induce opposite mobility of the electrons. (Bottom) The kagomé lattice consisting of three sublattices (red, blue and green spheres) with Bravais vectors \( \vec{e}_1 = (1, 0) \) and \( \vec{e}_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2}) \). Dashed black lines represent the first, second and third nearest neighbors exchange couplings, \( J_1, J_2 \) and \( J_3 \) respectively. \( \vec{D} \) represents the Dzyaloshinskii-Moriya interaction parallel to the external magnetic field.

Motivated by the previous discussion, in this letter we focus on a model described by the Kondo lattice model on the kagome lattice combining electronic and magnetic degrees of freedom. Its first ingredient is given by an electronic term consisting in non-interacting
electrons evolving in a classical magnetic background on
the kagome lattice. There is a Hund’s coupling between
the electronic spin and the local moments on each site
of the lattice. The second ingredient governs the precise
shape of the classical magnetic background, is given
by a pure spin Hamiltonian and we will focus in two
models: an XXZ up to second nearest neighbours and
Heisenberg model with Dzyaloshinskii-Moriya interac-
tion. In the first case, by cooling down the system,
it undergoes a phase transition with a spontaneous
symmetry breaking and an emergent total chirality
that can be either positive or negative. A non-trivial
band structure emerges for the electrons and when
the Fermi energy lies in a gap, the systems becomes a
Chern insulator whose Chern number depends on the
signs of the spontaneous chirality. Note that this is
achieved despite the fact that, as the magnetic system
is bi-dimensional, it does not have a true long-range
magnetic order. The second case, Eq. (4), corresponds
to a system which also shows a non-zero total chirality,
but whose sign is governed by the orientation of the
applied magnetic field. As result, we can easily switch
the Chern number of the filled band by just switching
the orientation of the magnetic field. In both cases,
we numerically investigate the DoS and the value of
the Hall conductivity, and in particular its evolution
with the cooling temperature of the classical background.

Hall conductivity in a chiral background: We consider
a Kondo lattice model on the kagome lattice where
the itinerant electrons are coupled with the classical spins by
a Hund’s coupling as,

\[
H = -t \sum_{\langle (r,r') \rangle, \sigma} (c_{r,\sigma}^\dagger c_{r',\sigma} + H.c.) - J_H \sum_r \mathbf{S}_r \cdot \mathbf{s}_r + H_S
\]

where \( \mathbf{s}_r = \frac{1}{2} \sigma_{\mu \nu} \bar{\sigma}_{\nu \rho} c_{r,\rho} \). Here, the first term is the hopp-
ing of itinerant electrons, where \( c_{r,\sigma} \) (\( c_{r,\sigma}^\dagger \)) is the anni-
hilation (creation) operator of an itinerant electron with
spin \( \sigma \) at \( r \)th site. The sum \( \langle (r,r') \rangle \) is taken over NN sites
on the kagome lattice (see Fig. 1), and \( t \) is the NN trans-
fer integral. The second term is the onsite interaction
between localized spins and itinerant electrons, which
\( \mathbf{S}_r \) and \( \mathbf{s}_r \) represent the localised spin and itinerant electron
spin at \( r \)-th site, respectively (\( \langle \mathbf{S}_r \rangle = 1 \)), and \( J_H \) is the
coupling constant. The last term corresponds to the pure
magnetic Hamiltonian.

We are interested in the limit of strong enough Hund
coupling \( J_H \gg t \). In this limit, although the spin of
the hopping electron \( \mathbf{s}_r \) is not conserved, the electronic
spectrum clearly splits into a low energy and high en-
ergy band set where the spin of the electrons are roughly
aligned parallel and antiparallel, respectively, to the local
moment \( \mathbf{S}_r \). If the magnetic background has non-zero
chirality, this spin-orbit coupling results in an effective
flux acting on the low energy band of the electronic sector
3-5. Therefore, throughout this work we take \( J_H/t = 8 \).

We investigate the transport properties of the model
in Eq. (1) by combining Monte-Carlo simulations for
the classical magnetic sector and exact diagonalization for
the quantum electron gas. In this method, we obtain
the classical magnetic background using the standard
Metropolis algorithm combined with overrelaxation (mi-
crocanonical) updates by studying a pure spin model on
a kagome lattice. Periodic boundary conditions were im-
plemented for a system of \( N = 3 \times L^2 \) sites (\( L = 12-36 \)).
At every magnetic field or temperature we discarded
\( 1 \times 10^5 \) hybrid Monte Carlo steps (MCS) for initial re-
relaxation and spin configurations were collected during
subsequent \( 2 \times 10^5 \) MCS. In all this work all the com-
putations for the itinerant electrons for a given classical
spin configuration are done at zero temperature, which
corresponds to a vast separation between the electronic
(hopping) energy scales and the Heisenberg energy scale
of the classical system. In the following, we show the
results for the largest size with \( N = 3888 \) sites. We have
confirmed that the finite size effects are sufficiently small.
We discuss the effect of thermal disorder in the magnetic
background and we calculate the conductivity by means
of the Kubo formula which, at \( T = 0 \), is reduced to

\[
\sigma_{xy}(\epsilon_F) = \frac{e^2}{hL^2} \sum_{\epsilon_F < \epsilon_F} \sum_{\epsilon_F \geq \epsilon_F} 2\text{Im} \left( \langle v_x^a | v_y | v \rangle \right) \frac{\epsilon_F - \epsilon_F}{(\epsilon_F - \epsilon_F)^2}
\]

where \( \epsilon_F \) is the Fermi energy, \( \epsilon_F \) is the eigenvalue of
the electronic Hamiltonian with the eigenvector \( | \mu \rangle \), \( | v_{\alpha} \rangle \) \( \alpha = x, y \) is the matrix elements of the velocity
operator \( \tilde{v} = \frac{i}{\hbar} \left[ H, \hat{R} \right] \), with the position operator
being \( \hat{R} = \sum_{\sigma} \sum_r c_{r,\sigma} \bar{c}_{r,\sigma} \). When the Fermi energy \( \epsilon_F \) lies
inside the gap, the Hall conductance is quantized as \( \sigma_{xy} = e^2/h \sum_{n} C_n \) where the integers \( C_n \) \( \left[ 10 \right] \) are the so-called Chern numbers connected with the extended
(conducting) states.

Concerning the classical spin sector, the different
phases can be easily identified from the observation of
real-space spin observables, in particular the scalar chi-
rality which is defined as the mixed product of three spins
on a triangular plaquette, \( \chi_{\Delta} = \mathbf{S}_L \cdot (\mathbf{S}_r \times \mathbf{S}_{r'}) \).

Magnetic XXZ model and spontaneous Chern insu-
lator: Our first model consists in an anisotropic XXZ
Hamiltonian with first and second nearest neighbours ex-
change interactions:

\[
H_S = \sum_{a=1}^{2} \sum_{\langle (r,r') \rangle} J_c (\mathbf{S}_r^a \cdot \mathbf{S}_{r'}^a + \Delta_a S_{r}^a S_{r'}^a) - h \sum_r \mathbf{S}_r^a \quad (3)
\]

where \( \langle (r,r') \rangle \) represents the first \( (a = 1) \) and second
\( (a = 2) \) neighbours, with anisotropy \( \Delta_a < 1 \) in the \( z \)
direction, and $S^\perp$ corresponds to the perpendicular ($xy$) component of the spin at site $\mathbf{r}$.

At low temperatures the system undergoes a phase transition in which the reflection symmetry is spontaneously broken. The local magnetic order consists in a $q = 0$ texture with non-zero chirality on each triangle of the kagome lattice. This is precisely the configuration considered in Ref. [3] for the first realization of a Chern insulator due to a strong Hund’s coupling.

In Figs. 2(a) and (b) we show the total chirality (per plaquette) $\chi = \frac{1}{L^2} \sum_{\Delta} \chi_\Delta$ as a function of the magnetic field and temperature, respectively. The appearance of a spontaneous chirality is not necessary related to the emergence of quasi-long-range-order of the magnetic structure which may appear, via a standard Berezinsky-Kosterlitz-Thouless transition, at a lower temperature. Of course, the higher the temperature at which the classical spin system is thermalised, the higher is the disorder felt by the hopping electrons, and the more complicated the resulting spectral structure. This can be clearly seen in Fig. 3(b) where the DoS of the electronic system is plotted. However, at low temperatures ($T/J_1 \lesssim 10^{-1}$) a clear band and gap structure can be identified within the two decoupled Hund sectors. Fig. 3(a) shows the value of the Hall conductivity which clearly takes quantised values when the Fermi energy lies within a gap. A closer look at the transition reveals a very interesting scenario. The emergence of the gap in the electronic sector, and of a non-zero and quantised Hall conductance, seems to immediately appear with the onset of a total chirality of the background, as seen in Fig. 3(d). This seems to indicate that, despite the presence of disorder felt by the electrons because of the thermal fluctuations of the background, the Chern insulator emerges as soon as its “driving force”, the chirality, gets a non-zero value. This makes the situation relatively different to what has been studied in the context of topological insulators in the presence of quenched disorder [12]. In particular, the transition from a topological to a non-topological state may be of a quite different nature.

**Field induced topological transistor:** For our second model we consider for the classical spin sector a Heisenberg Hamiltonian in a magnetic field including an out-of-plane Dzyaloshinskii-Moriya (DM) interaction, in the
same axis as the external magnetic field:

$$H_S = \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} J_1 \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r}'} + \mathbf{D} \cdot (\mathbf{S}_\mathbf{r} \times \mathbf{S}_{\mathbf{r}'}) - \hbar \sum_{\mathbf{r}} \mathbf{S}_\mathbf{r}^2 \quad (4)$$

This system is known to give rise to a $q = 0$ local magnetic order with a non-zero chirality which depends on the sign of the magnetic field $\mathbf{H}$, as can be seen from Figs. 2(c) and (d). For strong enough values of the magnetic field there is band structure with gaps emerging (besides the Hund’s gap) as can be seen in Fig. 4(b). When the Fermi energy is chosen to lie within a gap, the Hall conductivity is clearly quantised, and can be “tuned” with the orientation of the magnetic field (Figs (a) and (c)). It is important to stress that in an experimental context, the magnetic field applied to the magnetic background needed to obtain the desired effect is much lower that the one needed for realizing a genuine quantum Hall effect in the electronic sector.

![Fig. 4: $J_1 = DM$ model ($D/J_1 = 1/2$). Density plot of (a) Hall conductivity (in units of $e^2/h$) and (b) DoS vs external magnetic field (y-axis) and Fermi energy for $T/J_1 = 10^{-2}$. Hall conductivity (c) and DoS (d) vs external magnetic field (at $\varepsilon_F/t = -3.5$) for two temperatures. We observe the integer values for $\sigma_{xy}$ at the zero values of DoS.](image)

Discussion and perspectives: In this work we have studied the interplay between a classical frustrated magnetic system and electronic degrees of freedom that can become, under some circumstances, a Chern insulator. The study of this kind of system dates back to almost twenty years ago [3], but has typically been studied in the presence of a perfect background (what would be equivalent here to the zero temperature configuration) with translation invariance. Here we have taken into account the thermal fluctuations of the magnetic background and we have investigated under which circumstances and range of temperatures one can recover the physics of the perfect background. Moreover, we have studied two models that show an interesting behaviour by tuning either the temperature or the magnetic field of the classical magnetic background. In the first example, we showed that by lowering the temperature we can trigger a phase transition with a spontaneous symmetry breaking and the appearance of a non-zero total scalar chirality, triggering in turn the appearance of an interesting band structure for the coupled electronic system and the presence of a “spontaneous” Chern insulator. The second model we have studied also provides the realisation of a Chern insulator, but in this case the Chern number of the filled bands (and as so the direction of the chiral edge modes) can be switched by inverting the sign of the magnetic field.

Our results open many perspectives in studying this kind of system. First, thermal fluctuations in the classical background play a role of disorder felt by the hopping electrons. As so, tuning the temperature amounts for tuning the degree of disorder in the electronic system, giving rise to the appearance of localised states at the band edges and even closing up the gaps by further increasing the temperature. In fact, the evolution from a topological state to a (non topological) Anderson insulator, as well as the nature of the transitions involved, is a fundamental question for the physics of the quantum Hall effect and has been widely studied [13]. These same questions arise in the study of topological insulators in the presence of impurities, a subject which is actually a very active field of research [12]. The situation in our context is relatively different to what has been studied before, as there is no quenched disorder in the system, but the disorder is induced by the temperature in the magnetic background. Moreover, there appears to be a seemingly simultaneous transition to a chiral state for the spin background and to a Chern insulator for the electronic sector. A more detailed study of the nature of this transition is certainly a very interesting open issue. It would be also interesting to investigate if there are similar systems that would show two well separated transitions, a first one for the emergence of the chirality, and a second one, at a lower temperature, where the electronic sector undergoes a transition to a gapped topological state, which would be a more similar situation to the models studied in the literature [12]. Still concerning disorder, it is possible to generate a classical chiral spin liquid [9], where even the local magnetic order is washed out, but where a total non-zero chirality is present. This system may also present an interesting background for studying the electronic properties.

Another important issue concerns the interplay be-
between the electronic and magnetic degrees of freedom. In this work we have assumed a huge separation of energy scales between the two sector, and as so we have computed all the electronic observable and zero temperature. The next step would of course consist in studying the case where the energy scales of the two sectors are closer. Not only it is possible to compute the electronic observables at non-zero temperature, but it is also possible to implement a feed-back mechanism of the electrons to the magnetic background. This is also a direction that promises a very rich and interesting phenomenology.

Furthermore, our study of the interplay between thermal disorder and AHE on the XXZ and $J_1 - D M$ models opens the door for a deep analysis on others 2D antiferromagnetic lattices with noncoplanar commensurate and incommensurate orders as in FeCrAs [15]. Another possibility is the study of the effect of nonmagnetic impurities on frustrated Kondo-lattice models, since the competition between thermal fluctuations and the site disorder opens the door for a deep analysis on others 2D antiferromagnetic lattices with noncoplanar commensurate and incommensurate orders as in FeCrAs [15]. Another possibility is the study of the effect of nonmagnetic impurities on frustrated Kondo-lattice models, since the competition between thermal fluctuations and the site disorder in pure spin models can stabilize non coplanar states [10]. In all these cases, the perspective of an experimental setup for studying in a controlled way the transition to topological states is a very promising issue.

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