Chiral phase transition and thermal Hall effect in the anisotropic kagome lattice

F.A. Gómez Albarracín,1,2 H. D. Rosales,1,2 and P. Pujo1,3

1Instituto de Física de Líquidos y Sistemas Biológicos (IFLYSIB), UNLP-CONICET, La Plata, Argentina and Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, c.c. 16, suc. 4, 1900 La Plata, Argentina.
2Departamento de Ciencias Básicas, Facultad de Ingeniería, UNLP, La Plata, Argentina.
3Laboratoire de Physique Théorique-IRSAMC, CNRS and Université de Toulouse, UPS, Toulouse, F-31062, France.

We present a study of the thermal Hall effect in the extended Heisenberg model with XXZ anisotropy in the kagome lattice. This model has the particularity that, in the classical case, and for a broad region in parameter space, an external magnetic field induces a chiral symmetry breaking: the ground state is a doubly degenerate $q = 0$ order with either positive or negative net chirality. Here, we focus on the effect of this chiral phase transition in the thermal Hall conductivity using Linear-Spin-Waves theory. We explore the topology and calculate the Chern numbers of the magnonic bands, obtaining a variety of topological phase transitions. We also compute the quantum corrections to the critical temperature associated with the chiral phase transition ($T_{c}^{SW}$). Our main result is that, the thermal Hall conductivity, which is nul for $T > T_{c}^{SW}$, becomes non-zero as a consequence of the spontaneous chiral symmetry breaking at low temperatures. Therefore, we present a simple model where it is possible to “switch” on/off the thermal transport properties introducing a magnetic field and heating or cooling the system.

Introduction– One of the most significant current discussions in condensed matter physics concerns the connection between non-trivial topological properties and transport phenomena in insulating magnets. It has been at the heart of numerous experimental and theoretical studies, mainly because these types of materials are candidates for carriers of the spin information without dissipation from Joule heating but with good transport coherence. Recently, particular attention has been brought upon the magnon thermal Hall effect (THE) where the transverse heat current induced by introducing a longitudinal thermal gradient is carried by magnonic excitations.

The magnon THE was predicted theoretically and observed experimentally in materials such as the insulating ferromagnet Ln$_2$V$_2$O$_7$, which has a pyrochlore lattice and out of plane antisymmetric Dzyaloshinskii-Moriya (DM) interactions. Other ferromagnetic pyrochlore insulators include Ho$_2$V$_2$O$_7$, and In$_2$Mn$_2$O$_6$. It has also been measured in perovskites La$_3$NiMnO$_9$ and YTiO$_3$ and kagome magnets Cu$_{1-3}$bdc$_2$, [CaCu$_3$(OH)$_6$Cl$_2$-0.6H$_2$O]. Magnon transport has also been theoretically studied in different topological structures and models, which include both chiral and coplanar systems. Furthermore, this transport phenomena has even lead to the proposition of devices to manipulate the spin wave current in what is called “topological magnonics”.

A previous work (Ref. [20]), we presented an extended XXZ antiferromagnetic model in the kagome lattice with an emergent “spontaneous” Chern insulator, where the net chirality can be controlled by an external magnetic field. There is a hidden phase transition in terms of the scalar chirality that separates the high-temperature phase from the chiral low-temperature phase holding two $q = 0$ ground states with opposite net scalar chirality. In this paper, we explore the consequences of this chiral phase transition in the thermal Hall conductivity. Using the Linear-Spin-Waves (LSW) theory approach, we first calculate the Chern numbers of the magnonic bands, obtaining a variety of topological phase transitions. We also compute the quantum corrections to the classical critical temperature ($T_{c}^{SW}$). Finally, we present the effects of the chiral phase transition and the associated symmetry breaking in the thermal conductivity: a nul contribution for $T > T_{c}^{SW}$. We close with discussion and conclusions.

Model and Non-interacting Magnons– We consider the extended antiferromagnetic Heisenberg model in the kagome lattice up to third nearest-neighbor interactions, taking only third nearest neighbors interactions across the hexagons (see Fig. 1).

\[
H = \sum_{n=1}^{3} \sum_{(i,j)_{n}} J_{n} \left( S_{i}^{x} S_{j}^{x} + S_{i}^{y} S_{j}^{y} + \Delta S_{i}^{z} S_{j}^{z} \right) - h \sum_{n} S_{n}^{z}
\]

where $n$ indicates the $n$-th nearest neighbor (as shown in Fig. 1), $\Delta < 1$ is the XXZ anisotropy parameter and $h$ is the external magnetic field along the $z$ direction. For simplicity, we set $J_{1} = 1$. In the SO(3) invariant $\Delta = 1$ case, the classical $T = 0$ phase diagram of this model is well known: it presents the so called “cubic” phases (with spontaneous and alternate scalar chirality), and a $q = 0$ phase for $J_{3} < J_{2} < J_{1}$. At the special line $J_{2} = J_{3} < J_{1}$, the ground state has a semi-extensive degeneracy where lines of spins from the $q = 0$ order can be “swapped”. For practical reasons, we will take $J_{1} = 1$ for the rest of the manuscript.

The combination of the XXZ anisotropy and an external magnetic field induces a $q = 0$ “umbrella” order with spontaneous non-zero net chirality. The emergence
of scalar chirality in this simple model is quite remarkable, with a rich potential for unconventional phenomena. The $xy$ projections of these two possible plaquette orders with opposite scalar chirality are shown in Fig. 1(b) and (c), where the three spins have the same projection along the field.

In these two possible ground states, the classical order is a cant$120^\circ$ plaquette. The state shown in Fig. 1(b) can be described (minus a global rotation around the $z$ axis) as: $\vec{S}_1 = S \left( -\frac{\sqrt{3}}{2} \sin \theta, -\frac{1}{2} \sin \theta, \cos \theta \right)$, $\vec{S}_2 = S \left( \frac{\sqrt{3}}{2} \sin \theta, -\frac{1}{2} \sin \theta, \cos \theta \right)$ and $\vec{S}_3 = S (0, \sin \theta, \cos \theta)$ where $S$ is the spin length and $\theta$ is the angle measured from the $z$ axis. As it is well known, the scalar chirality in a plaquette is defined as the triple product of the three spins $\chi_\Delta = \vec{S}_1 \cdot (\vec{S}_2 \times \vec{S}_3)$ which is a measure of the solid angle formed by them ($\chi_\Delta^0 = S^3 3/2\sqrt{3} \cos \theta \sin^2 \theta$ for this configuration).

In a recent work[20], we focused on the special case $J_1 = 1$, $J_2 = 1/2$, $J_3 = 0$, $\Delta = 0.9$ and showed that at low temperature the system undergoes a phase transition where the reflection symmetry is spontaneously broken, and most importantly the relevant order parameter is in fact the total scalar chirality (per plaquette) $\chi_{tot} = \frac{1}{N^2} \sum_\Delta \chi_\Delta^0$ where the sum involves all the triangular plaquettes $N_\Delta$. This will allow us to study the effect of quantum fluctuations in the critical temperature, defining the chirality operator, as we will show later.

In order to introduce quantum spin fluctuations and characterize the transport properties of the magnon excitations of this model, we resort to a linear spin wave (LSW) analysis[23]. Following the standard approach, we employ a three sublattice Holstein-Primakoff (HP) mapping with the bosonic operators (see Supplemental Material for details).

Even though classically, there are only two types of solutions with opposite chirality, quantum fluctuations show a rich phenomenology in the magnon spectrum. To characterize the bands of the spectrum, we calculate the Chern number $C_n$ for each $n$-th band, defined as $C_n = \frac{1}{2\pi} \int_{BZ} \Omega_n^2(k) dk^2$, where $\Omega_n^2(k)$ is the Berry curvature, $\Omega_n^2(k) = i \left\langle \frac{\partial u_n}{\partial k} \times \frac{\partial u_n}{\partial k} \right\rangle$ being $|u_n(k)\rangle$ the Bloch waves in the $n$-th band. To calculate this quantity numerically, we resorted to the efficient method detailed in Ref.[25], taking up to $10000 \times 10000$ points in discretized Brillouin Zone (BZ). As we describe in the next subsection, depending on the microscopic parameters, even for small modifications of the classical solution, the associated magnonic bands present different $C_n$, which leads to several interesting phenomena.

**Topological magnonic bands and Topological Phase Transitions**– In order to discuss the magnon band structure, we choose as the classical groundstate one of the two $q = 0$ states, shown in Fig. 1(b). From a general analysis, i.e. setting $h \sim 0.6$ ($\theta \sim 1.5$), we find that there are regions in the parameter space $(J_2, J_3, \Delta)$ with topologically non-trivial band structure with different $C_n$. These regions are divided by topological transitions, that occur when the magnon bands touch, and the “local” gap between them closes. For a representative case of this situation we fix $J_2 = 0.8$ and $J_3 = 0.2$ with $\Delta \in [0, 0.9]$. The band structure for $\Delta = 0.7$ is depicted in Fig. 2(a), where there are local gaps between all the bands. In Fig. 2(b) we plot the Chern number of each band as a function of $\Delta$. The $C_n$ appear as steps in the constructed curve, and there are at least four topological transitions at different values of the anisotropy parameter. The sets of $C_n$ (from the lowest $(w_{0,1})$ to the top $(w_{0,3})$ band) go as $(-3,3,0) \rightarrow (3,-3,0) \rightarrow (5,-5,0) \rightarrow (5,-7,2) \rightarrow (-1,-1,2)$. As $\Delta$ increases, the topology of the bands change. For stronger XXZ anisotropy, the lower bands have opposite $C_n$ and the top band has a trivial topology ($C_n = 0$). For higher $\Delta \gtrsim 0.65$ the top band gets a non-trivial $C_n$. In Fig. 2(c) we show the gap between successive bands as a function of $\Delta$ for specific points in the BZ. As expected, there is a perfect correspondence between the values of $\Delta$ where there is a topological transition and the values of the anisotropy parameter where two of the bands touch.

Another interesting issue is the role that the magnetic field plays on the topological transitions, even though classically the magnetic field just changes the canting angle of the spins. Varying the field triggers a series of topological transitions, that are reflected in the change of the $C_n$. We show this for $\Delta = 0.7$ in Fig. 2(d), where the $C_n$ go $(5,-7,2) \rightarrow (-1,1,0) \rightarrow (-3,3,0) \rightarrow (5,-5,0)$. As above, the surprisingly large values of the obtained $C_n$ are also remarkable. A similar feature was discussed in Ref.[17], where this was attributed to an in-plane DM interaction. In our work, there are no antisymmetric interactions; the distinctive feature is the XXZ anisotropy and the antiferromagnetic nature of the couplings.

**Chirality and Phase Transition**– A key question in this work is the effect of quantum fluctuations in the classical
Monte-Carlo (MC) simulations in Fig. 3(c), as the system approaches the $J_2 = J_3$ line, where the classical model has a semieextensive degeneracy. For the MC simulations, we resort to the Metropolis algorithm combined with overrelaxation (microcanonical) updates in system size of $3L^2$ sites ($L = 30$). The estimated $T_c^{SW}$, even within the LSW approximation, seems to be of the same order of magnitude as the one obtained form MC, a situation which contrasts with 3D systems with long range magnetic order, and for which in general LSW gives an huge overestimation of the critical

phase transition and the consequences on the thermal transport properties. The relevant order parameter in this case, since we are dealing with a 2D system, is not the magnetization but the scalar chirality which allows to detect the spontaneous symmetry breaking at low temperature. To this end, we compute the quantum version of the scalar chirality $\chi_{tot}$ using HP tranformation and retaining terms up to quadratic order obtaining,

$$\langle \chi_{tot} \rangle = \left( 1 + \frac{3}{2S} \right) \lambda^0_{SW} + S^2 \sum_{k,\alpha=1}^{|S|} \left[ \tilde{Q}_{k,\alpha} g(S w_{k,\alpha}) + \tilde{Q}_{k,\alpha} + 3 \alpha + 3 (1 + g(S w_{k,\alpha})) \right]$$  \hspace{0.5cm} (2)

where $N_k$ is the number of points in the Brillouin zone, $\lambda^0_{SW}$ is the classical scalar chirality for one triangular plaquette, $g(S w_{k,\alpha})$ is the Bose-Einstein distribution and $\tilde{Q}_{k,\alpha}$ is the chirality operator matrix in the diagonal basis (explicit expressions in Supplemental Material).

Let us first explore the dependence of critical temperature $T_c^{SW}$ in terms of the spin length $S$ taking $J_2 = 0.8$, $J_3 = 0.2$, $\Delta = 0.7$, $h/J_1 = 0.6$. From Fig. 3(a) we observe that the chiral phase is stable up to the point $\langle \chi_{tot} \rangle / S^3 = 0$ which defines the critical temperature $T_c^{SW}$. For every $S$, as the spin increases, the curves tend to collapse around $T_c^{SW} / S^3 \sim 0.34$. We show $\langle \chi_{tot} \rangle / S^3$ for $S = 1$ as a function of temperature for different values of $\Delta$ (fixing $\theta = 1.5$, Fig. 3(b)) and external magnetic field (fixing $\Delta = 0.7$, Fig. 3(c)), where we can see that the behavior is robust.

By Eq. (2), we can compute $T_c^{SW,\infty}$ in the classical limit $S \to \infty$ defined by the condition $\langle \chi_{tot} \rangle = 0$. After a simple analysis we obtain

$$T_c^{SW,\infty} = -\frac{\lambda^0_{SW} S^3}{\sum_{k} \sum_{\alpha=1,2,3} \tilde{Q}_{k,\alpha} + 3 \alpha + 3 (1 + g(S w_{k,\alpha}))}$$  \hspace{0.5cm} (3)

Therefore, Eq. (3) allows us to compare $T_c^{SW}$ with Monte-Carlo (MC) simulations in Fig. 3(c), as the

\[\text{FIG. 2: Fixing } J_2 = 0.8, J_3 = 0.2 \text{ (a) Magnon spectrum for } h = 0.6, \Delta = 0.7. \text{ The bands do not touch at any point in the BZ. (b)} \ C_n \text{ for each magnon band as a function of } \Delta, \text{ for } \theta = 1.5. \text{ (c) Distance between magnon bands at different points in the BZ as a function of } \Delta. \text{ When the distance is zero, we identify a closing of the local gap between bands. (d) } C_n \text{ as a function of external magnetic field, } \Delta = 0.7.\]
temperature \( T \). The reason for the good estimation of the critical temperature with LSW is likely to rely on the low value (compared to the microscopic parameters) of it, implying a low contribution of the high energy levels to the magnon spectrum necessary for the validity of the LSW approximation. The most important feature of our results is that lowering the temperature from the paramagnetic phase, the quantum version of the model in Eq.(1) undergoes a phase transition in which the reflection symmetry is spontaneously broken. This has relevant consequences in the transport properties and the thermal Hall conductivity, which we will discuss below.

**Spontaneous Thermal Hall Conductivity**– The presence of a nontrivial Berry curvature in the magnon bands implies the existence of a thermal Hall signature provided that the Berry curvature is not odd in momentum. The thermal Hall conductivity \( \kappa_{xy} \) may be calculated as:

\[
\kappa_{xy} = -\frac{k_B^2 T}{(2\pi)^2 h} \sum_n \int_{BZ} \left[ c_2(g(2SW_{\alpha}(k))) - \frac{\pi^2}{3} \right] \Omega_n(\mathbf{k}) d^2k
\]

where \( k_B \) is the Boltzmann constant, \( g(2w_{\alpha}(k)) \) is the Bose-Einstein distribution and \( c_2 \) is defined as:

\[
c_2(x) = (1 + x) \left[ \ln \left( \frac{1 + x}{x} \right) \right]^2 - (\ln x)^2 - 2\text{Li}_2(-x)
\]

where \( \text{Li}_2(x) \) is the dilogarithm.

**Discussion and Conclusions**– The purpose of the present work was to study a chiral phase transition in an anisotropic Heisenberg model in the kagome lattice, in which the reflection symmetry is spontaneously broken, and where the low temperature phase shows a thermal Hall effect.

To this end, using the Linear-Spin-Waves theory approach, we have studied numerically the topology of the magnonic bands and their Chern numbers. We have shown that there are several topological transitions driven by the magnetic field and the microscopic parameters. We have also studied the effect of quantum fluctuations in the chiral phase transition in terms of these parameters. We have paid a particular attention to the dependence of the critical temperature with the magnitude of the spins and obtained an interesting result comparing the value obtained taking the classical limit \((S \to \infty)\) with Monte Carlo simulations.

Finally, we calculate the thermal Hall conductivity as a function of temperature showing that effectively its sign is “spontaneous”. Therefore, we show with this simple model that it is possible to “switch” on the thermal transport properties by manipulation of the external parameters.

A unique feature of this work resides in the chiral phase transition. Previous works have established that a nonzero scalar chirality in the ground state could lead to THE. Here, the chirality serves as an order parameter associated with a spontaneous broken symmetry, and thus allows us to conjecture the behaviour of the thermal Hall conductivity with temperature and define a critical temperature above which the thermal Hall conductivity is suppressed. In addition, we have shown that this conductivity can be tuned by the external magnetic field and the XXZ anisotropy.

Following the previous discussion, it would be interesting to consider magnon interactions going beyond LSW theory including three and four bosonic terms to obtain a more accurate estimation of the conductivity near the

---

**FIG. 4:** For \( S = 1, J_2 = 0.8, J_3 = 0.2 \) (a) Thermal conductivity \( \kappa_{xy} \) as a function of temperature for different values of \( \Delta \), for \( \theta = 1.5 \) \( \kappa_{xy} \) as a function of \( h \) taking \( \Delta = 0.7 \), and \( T \approx 0.6 \); (c) \( \kappa_{xy} \) as a function of temperature obtained from the magnon spectrum of the two possible classical ground states with opposite scalar chirality for \( \Delta = 0.7, h = 0.6 \).

In Fig.4(a) we show \( \kappa_{xy} \) (in units of \( k_B^2/(2\pi h) \)) for \( S = 1 \) as a function of the temperature for different \( \Delta \), corresponding to different regions marked by the topological transitions in Fig.4(b). In Fig.4(b) we show \( \kappa_{xy} \) as a function of the external field for \( T < T_{SW} \).

The most important feature of this study is shown in Fig.4(c). This figure shows that the sign of \( \kappa_{xy} \) depends on the sign of the scalar chirality from the classical ground state. This suggests that \( \kappa_{xy} \) will have a spontaneous sign for \( T < T_{SW} \). However, because \( \langle x_{tot} \rangle = 0 \) for \( T > T_{SW} \), \( \kappa_{xy} \) must vanish for \( T > T_{SW} \), implying a “switchable” THE. Unfortunately, this suppression of the \( \kappa_{xy} \) is not completely captured by LSW. We expect magnon interactions, not included at this stage, to establish the cancelation of \( \kappa_{xy} \) for \( T > T_{SW} \). This requires a higher order spin wave calculation (in powers of \( 1/\alpha \)) which is beyond the scope of this paper. Nonetheless, given the previous discussion, we propose a cutoff in \( \kappa_{xy} \) as represented in Fig.4(c) with a dashed black line.
chiral phase transition. We defer this for future investigations.

Acknowledgments- We would like to thank the “Laboratoire International Associé” LIA LICOQ for support and Mike Zhitomirsky for very fruitful discussions. H.D.R. and F.A.G.A. acknowledge the Laboratoire de Physique Théorique (LPT) in Toulouse for their hospitality during their 2019 visits. H.D.R. and F.A.G.A. are partially supported by PIP 2015-0813 CONICET and SECyT-UNLP. H.D.R. acknowledges support from PICT 2016-4083 and F.A.G.A. from PICT 2018-02968.

1. Tokura, Y., Yasuda, K. and Tsukazaki, A. Nat Rev Phys 1, 126 (2019).

2. Hosho Katsura, Naoto Nagaosa, and Patrick A. Lee, Phys. Rev. Lett. 104, 066403 (2010).

3. Y. Onose, T. Ideue, H. Katsura, Y. Shiomi, N. Nagaosa, and Y. Tokura, Science 329, 297 (2010).

4. R. Matsumoto and S. Murakami, Phys. Rev. Lett. 106, 197202 (2011).

5. R. Matsumoto and S. Murakami, Phys. Rev. B 84, 184406 (2011).

6. S. Murakami and A. Okamoto, J. Phys. Soc. Jap. 86, 011010 (2017).

7. Y. Onose, T. Ideue, H. Katsura, Y. Shiomi, N. Nagaosa, and Y. Tokura, Science 329, 297 (2010).

8. T. Ideue, Y. Onose, H. Katsura, Y. Shiomi, S. Ishiwata, N. Nagaosa, and Y. Tokura, Phys. Rev. B 85, 134411 (2012).

9. M. Hirschberger, R. Chisnell, Y. S. Lee, and N. P. Ong, Phys. Rev. Lett. 115, 106603 (2015); R. Chisnell, J. S. Helton, D. E. Freedman, D. K. Singh, R. I. Bewley, D. G. Nocera, and Y. S. Lee, Phys. Rev. Lett. 115, 147201 (2015).

10. H. Doki, M. Akazawa, H.Y. Lee, J. H. Han, K. Sugii, M. Shimozawa, N. Kawashima, M. Oda, H. Yoshida, and M. Yamashita, Phys. Rev. Lett. 121, 097203 (2018).

11. P. Laurell and G. A. Fiete, Phys. Rev. Lett. 118, 177201 (2017).

12. A. Mook, J. Henk, and I. Mertig, Phys. Rev. B 90, 024412 (2014).

13. A. Mook, J. Henk, and I. Mertig, Phys. Rev. B 91, 224411 (2015).

14. X. S. Wang, Ying Su, and X. R. Wang, Phys. Rev. B 95, 014435 (2017).

15. Kyusung Hwang, Nandini Trivedi, Mohit Randeria, arXiv:1712.08170

16. Masataka Kawano and Chisa Hotta, Phys. Rev. B 99, 054422 (2019).

17. P. Laurell and G. A. Fiete, Phys. Rev. B 98, 094419 (2018).

18. Alexander Mook, Jrgen Henk, and Ingrid Mertig, Phys. Rev. B 99 014427 (2019).

19. X.S. Wang, H.W. Zhang, and X.R. Wang Phys. Rev. Applied 9, 024029 (2019).

20. H. D. Rosales, F. A. Gómez Albarracín and P. Pujol, Phys. Rev. B 97, 054422 (2019).

21. F. A. Gómez Albarracín and P. Pujol, Phys. Rev. B 97, 104419 (2018).

22. L. Messio, C. Lhuillier, and G. Misguich, Phys. Rev. B 83, 184401 (2011).

23. A. Auerbach, Interacting Electrons and Quantum Magnetism (Springer-Verlag, New York, 1994).

24. J. Colpa, Phys. A: Stat. Mech. App. 93, 327 (1978).

25. T. Fukui, Y. Hatsugai, and H. Suzuki, J. Phys. Soc. Jap. 74, 1674 (2005).

26. Z. Li, T. Cao, S. G. Louie, Journal of Magnetism and Magnetic Materials 463, 28-35 (2018).

27. Ryo Matsumoto, Ryuichi Shindou, and Shuichi Murakami Phys. Rev. B 89, 054420 (2014).

28. A. Mook, J. Henk, and I. Mertig, Phys. Rev. B 89, 134409 (2014).

29. A. L. Chernyshev and M. E. Zhitomirsky, Phys. Rev. Lett. 113, 237202 (2014); A. L. Chernyshev and M. E. Zhitomirsky Phys. Rev. B 79, 144416 (2009); Erratum Phys. Rev. B 91, 219905 (2015).