

Analytical study of the Berry curvature and the band orbital angular momentum for tight binding models

Vittorio Basso,¹ Adriano Di Pietro,¹ and Alessandro Sola¹

¹*Istituto Nazionale di Ricerca Metrologica,
Strada delle Cacce 91, 10135, Torino, Italy*

The Berry curvature of Bloch bands is an intrinsic property of metallic and insulating systems that has recently emerged as the key factor determining several physical effects of ferromagnets such as: the spontaneous (also called anomalous) Hall and Nernst effects [1,2], the quantum spontaneous Hall effect [3] and the orbital contribution to the magnetization [4]. The results obtained by computing the anomalous Hall and Nernst conductivity by DFT are in good agreement with experiments [1,2], however the general trends of the behavior and the possible directions for the optimization of the effects by electronic band structure tailoring are still missing [5]. The open point is the lack of the comprehension of the delicate interplay between spin orbit interaction and bonding geometry that give rise to a non zero Berry curvature and possibly to a topological band structure. To get some insights into this interplay we present a tight binding model using two d orbitals both with $m_s = -1/2$ (majority electrons d_{zx} and d_{yz}) giving rise to an unquenched atomic orbital angular momentum along z . By computing bcc, fcc and hcp structures we are able to derive analytic expressions for the Berry curvature and to the orbital angular momentum [5,6,7]. We evidence the presence of the band orbital angular momentum in the same regions of the Brillouin zone in which the atomic (unquenched) contribution is found. This fact can be the basis of recipes for the possible maximization of the transverse transport effects by electronic band structure tailoring.

References:

- [1] H. Kontani, T. Tanaka and K. Yamada Phys. Rev. B 75 (2007) 184416
- [2] J. Weischenberg, F. Freimuth, S. Blugel and Y. Mokrousov, Phys. Rev. B 87 (2013) 060406
- [3] C. Z. Chang, C. X. Liu and A. H. MacDonald, Rev. Mod. Phys. 95 (2023) 011002.
- [4] J. Shi, G. Vignale, D. Xiao and Q. Niu, Phys. Rev. Lett. 99 (2007) 197202
- [5] V. Basso, A. Di Pietro and A. Sola, arXiv:2508.08756
- [6] R. B. Atencia, A. Agarwal and D. Culcer, Adv. Phys. X 9 (2024) 2371972.
- [7] A. Graf and F. Piechon, Phys. Rev. B, 104 (2021) 085114

Research Projects of Relevant National Interest (PRIN project Xverse T.E.C “Transverse thermoelectric energy conversion”: Grant No. 2022LLWM5F).