Ab initio method for spin excitations in noncollinear spin textures

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Noncollinear spin structures are promising platforms for non-volatile information storage. Controlling these textures through spin excitations enables ultrafast and low-dissipation signal processing, offering a route toward next-generation spintronic technology. To simulate the interplay between excited state and spin structure, in this work we develop a first-principles approach for computing spin waves in magnetic systems with noncollinear spin textures, based on density functional theory and many-body perturbation theory [1]. The computational challenges posed by nanoscale spin configurations—often tens to thousands of times larger than a primitive unit cell—are overcome through a Wannier-basis representation [2] and a data-driven ansatz potential method [3], enabling parameter-free simulations of systems containing $O(10^2)$ spins, in stark contrast with $O(10^0)$ spins of typical collinear cases. We adopt this new method to the spin-helix state of type-II multiferroic $LiCu_2O_2$ successfully capturing its steady-state spin-rotation pitch and resolving the characteristic magnon dispersion in agreement with the experimental measurements. We further analyze the interplay between the spiral spin structure and the spin-exchange splitting, elucidating the crucial role of magnetic dipoles on ligand ions in mediating effective ferromagnetic interaction among the primary spins on Cu^{2+} ions. Overall, this work establishes a general and computationally efficient framework for simulating collective spin dynamics in large-scale noncollinear magnetic systems from first principles.

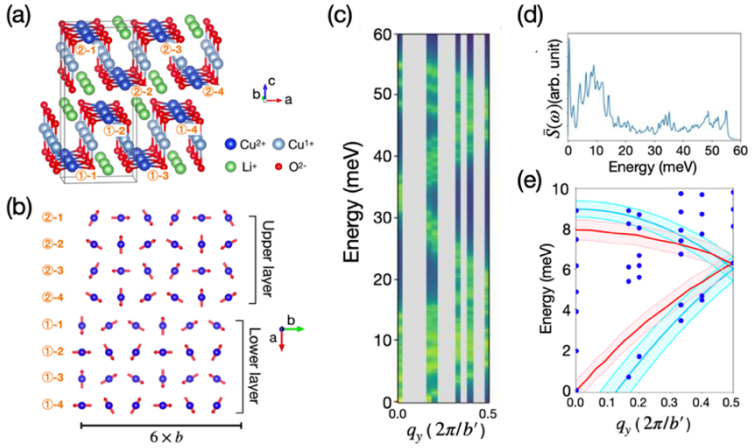

Figure 1. Physical properties of type-II multiferroic $LiCu_2O_2$: (a) Crystal structure. (b) Ground state helical spin texture. (c) Computed magnetic response spectrum. (d) Computed magnon density of state. (e) Comparison of magnon dispersion between experimental measurement (red line) and theoretical prediction (blue line).

[1] H.-Y. Chen, et. al., First-principles approach to spin excitations in noncollinear magnetic systems, *npj* Comput. Mater. **12**, 237 (2026)
[2] E. Sasioglu, et. al., Wannier-function approach to spin excitations in solids, Phys. Rev. B **81** 054434 (2010).
[3] H.-Y. Chen, et. al., Topological Hall Effect of Skyrmions from first Principles, Phys. Rev. X **15** 011054 (2025)