Theoretical Study of the Magnetoelectric Effect in Ba_2CuGe_2O7

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Ba_2CuGe_2O7 is a multiferroic material exhibiting a magnetoelectric response, where an applied magnetic field modifies the electric polarization[1]. Understanding the microscopic mechanism underlying this coupling is essential for controlling functionalities and guiding materials design. Previous studies have proposed that the magnetoelectric effect originates from spin-direction-dependent Cu (3d)–O (2p) hybridization (d–p model) in the crystal [2,3]. However, those analyses rely on phenomenologically derived polarization formulas, leaving the quantitative evaluation of polarization and the role of individual interaction terms insufficiently validated.

In this work, we re-examine the d–p model using a quantum-mechanical theoretical framework. We construct a model based on a CuO_4 building block in the crystal and evaluate the electric polarization under external magnetic fields by combining first-principles-based parameterization with model calculations. Specifically, we formulate a matrix Hamiltonian $H = H_0 + H_{\mathrm{Zeeman}} + H_{\mathrm{soc}}$, where H_0 contains on-site and hopping terms, H_{Zeeman} describes the magnetic-field-induced modification of electronic states, and H_{soc} accounts for spin–orbit coupling. From the eigenstates, we compute the wave functions within a tight-binding approximation and derive the electric polarization from the resulting charge density.

Our calculations reproduce the characteristic angular dependence of the polarization with respect to the magnetic-field direction in the single-CuO_4 model, consistent with the experimentally reported periodic response in Ba_2CuGe_2O7. Because our approach evaluates polarization without relying on phenomenological rules, it enables quantitative validation and decomposition of contributions from different interaction terms. These results provide independent theoretical support for the picture that Cu–O d–p hybridization plays a primary role in the magnetoelectric effect. As a next step, we will extend the present single-CuO_4 model to the full unit cell and achieve a more accurate reproduction.

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