Spin Orbit Coupling Contribution to Anisotropic Magnetic Interaction

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Anisotropic magnetic exchange interactions lead to a surprisingly rich variety of the magnetic properties. Considering the spin orbit coupling (SOC) as perturbation, we extract the general expression of a bilinear spin Hamiltonian, including isotropic exchange interaction, antisymmetric Dzyaloshinskii-Moriya (DM) interaction and symmetric Γ term. Though it is commonly believed that the magnitude of the DM and Γ interaction correspond to the first and second order of SOC strength respectively, we clarify that the term proportional to λ^2 also has contribution to DM interaction. Based on combining magnetic force theorem and linear-response approach, we have presented the method of calculating anisotropic magnetic interactions, which now has been implemented in the open source software WienJ. Furthermore, we introduce another method which could calculate the first and second order SOC contribution to the DM interaction separately, and overcome some shortcomings of previous methods. Our methods are successfully applied to several typical weak ferromagnets for 3d, 4d and 5d transition metal oxides. We also predict the conditions where the DM interactions proportional to λ are symmetrically forbidden while the DM interactions proportional to λ^2 are nonzero, and believe that it is widespread in certain magnetic materials..

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[1] Di Wang, Xiangyan Bo, Feng Tang, Xiangang Wan, Phys. Rev. B 108, 085140 (2023).