# Non-perturbative calculation of exchange coupling tensor

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In recent years, spintronics utilizing complex magnetic interactions found in noncollinear magnetic structures has been rapidly advancing. Meanwhile, first-principles evaluation methods for such complex magnetic interactions are still under development. Although several state-of-the-art evaluation methods exist, they are commonly based on perturbation theory, which presents issues regarding quantitative accuracy.

In this project, we first demonstrated that the non-perturbative evaluation of the exchange coupling parameters $J_{ij}$ in the Heisenberg model [1]. Surprisingly, we find that contributions from changes in the electronic structure—which have been ignored in the perturbative methods—are necessary even in relatively small deviations from the ground magnetic state.

Although the exchange coupling parameters in the Heisenberg model remain important, they are insufficient for describing many magnetic orders and textures. Therefore, we believe that non-perturbative methods for evaluating other types of magnetic interactions are also essential. To achieve this, we have developed an efficient implementation of the spin-cluster expansion (SCE) method [2]. While the original SCE formulation theoretically allows for the description of any type of magnetic interaction within the classical spin model, its initial implementation incurred prohibitively high computational costs and was therefore impractical. We overcame this issue by utilizing constraining local magnetic fields [3].

As a demonstration, we applied the spin-cluster expansion method to a relatively simple ferromagnetic system, $L1_0-$FePt. We performed constrained-noncollinear DFT calculations using the GGA-PBE functional implemented in the VASP package. Thirty different spin configurations near the ferromagnetic state were prepared, and the corresponding total energies were collected. The SCE coefficients were then estimated using the least-squares method. For example, the exchange coupling tensor for the first-nearest-neighbor Fe-Fe pair along the $x$-direction, $\mathcal{J}_{1\mathrm{NN}}$, was obtained as

$$\mathcal{J}_{1\mathrm{NN}} = \begin{pmatrix} 17.81 & 0 & 0 \\ 0 & 18.30 & 0 \\ 0 & 0 & 17.67 \end{pmatrix} \mathrm{meV}. \quad (1)$$

This method enables the evaluation of non-diagonal components consisting of symmetric and antisymmetric anisotropic exchange couplings from fully self-consistent DFT calculations. We therefore plan to apply our method to systems exhibiting more complex magnetic textures.

## References

[1] T. Tanaka and Y. Gohda, arXiv:2410.11256.

[2] R. Drautz and M. Fähnle, Phys. Rev. B **69**, 104404 (2004).

[3] T. Tanaka and Y. Gohda, in preparation.