

FORMULAS

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From: September 3, 2024

1 Theory

The exchange interactions in DFT were estimated by magnetic force theorem (MFT) approach [1, 2] using electron Green's functions, calculated in Wannier basis

$$G_{rr',\sigma}^{mm'}(\mathbf{k}, i\nu_n) = \left[(i\nu_n + \mu)I - H_{\mathbf{k},\sigma}^{rm,r'm'} \right]_{rm,r'm'}^{-1} \quad (1)$$

where I is the identity matrix, $H_{\mathbf{k},\sigma}^{rm,r'm'}$ is the Wannier Hamiltonian,

$$H_{\mathbf{k},\sigma}^{rm,r'm'} = \langle \psi_{\mathbf{k}\sigma rm}^W | H | \psi_{\mathbf{k}\sigma r'm'}^W \rangle = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \langle 0\sigma rm | H | \mathbf{R}\sigma r'm' \rangle$$

and the inversion is performed in the site- and orbital space. To obtain $H_{\mathbf{k},\sigma}^{rm,r'm'}$ wannier transformation was performed on both spin components separately relying on that $|\mathbf{R}\sigma rm\rangle$ would be independent on spin $|\mathbf{R}rm\rangle$ so that we would have common basis for both components.

$$J_{\mathbf{q}}^{rr'} = -\frac{2T}{\mathbf{m}_r \mathbf{m}_{r'}} \sum_{\mathbf{k}, i\nu_n} \text{Tr} \left[\Delta_r \tilde{G}_{rr',\downarrow}(\mathbf{k} + \mathbf{q}, i\nu_n) \times \Delta_{r'} \tilde{G}_{r'r,\uparrow}(\mathbf{k}, i\nu_n) \right] \quad (2)$$

where $\Delta_r^{mm'} = \sum_{\mathbf{k}} (H_{\mathbf{k},\uparrow}^{rm,rm'} - H_{\mathbf{k},\downarrow}^{rm,rm'})$ is spin splitting and $\tilde{G}_{rr',\sigma}^{mm'}(\mathbf{k}, i\nu_n) = G_{rr',\sigma}^{mm'}(\mathbf{k}, i\nu_n) - \sum_{\mathbf{k}'} G_{rr',\sigma}^{mm'}(\mathbf{k}', i\nu_n)$, the trace is taken over orbital indexes, and \mathbf{m}_r is the magnetic moment at the r -th atom (in units of Bohr magneton μ_B). Equivalently we calculate

$$J_{\mathbf{q}}^{rr'} = -\frac{2T}{\mathbf{m}_r \mathbf{m}_{r'}} \sum_{\mathbf{k}, i\nu_n} \text{Tr} [\Delta_r G_{rr',\downarrow}(\mathbf{k} + \mathbf{q}, i\nu_n) \times \Delta_{r'} G_{r'r,\uparrow}(\mathbf{k}, i\nu_n)] - J_{\text{self}} \delta_{rr'} \quad (3)$$

where J_{self} is self exchange that can be found as $J_{\text{self}} = -\frac{2T}{\mathbf{m}_r \mathbf{m}_{r'}} \sum_{\mathbf{k}, i\nu_n} \text{Tr} [\Delta_r G_{\text{loc},\downarrow}(i\nu_n) \times \Delta_{r'} G_{\text{loc},\uparrow}(i\nu_n)]$ with $G_{\text{loc},\sigma} = \frac{1}{V_{BZ}} \int_{BZ} G_{ii,\sigma}^{mm'}(i\nu_n, \mathbf{k}) d\mathbf{k}$.

1.1 1 atom per cell

In case of one magnetic atom in unit cell we calculate $G_{0j,\sigma}^{mm'}(i\nu_n) = \frac{1}{V_{BZ}} \int_{BZ} G_{\sigma}^{mm'}(i\nu_n, \mathbf{k}) e^{2\pi i \mathbf{k} \mathbf{R}_j} d\mathbf{k}$ and $G_{j0,\sigma}^{mm'}(i\nu_n) = \frac{1}{V_{BZ}} \int_{BZ} G_{\sigma}^{mm'}(i\nu_n, \mathbf{k}) e^{-2\pi i \mathbf{k} \mathbf{R}_j} d\mathbf{k}$ where k is in range $[0, 1] \otimes [0, 1]$ and \mathbf{R}_j is integer vector, $\Delta^{mm'} = \frac{1}{V_{BZ}} \int_{BZ} (H_{\uparrow}^{mm'}(\mathbf{k}) - H_{\downarrow}^{mm'}(\mathbf{k})) d\mathbf{k}$

$$J_{0j} = -\frac{2T}{\mathbf{m} \mathbf{m}} \sum_{i\nu_n} \sum_{\substack{mm' \\ m''m'''}} \left(\Delta^{mm'} G_{0j,\downarrow}^{m'm''}(i\nu_n) \Delta^{m''m'''} G_{j0,\uparrow}^{m'''m}(i\nu_n) \right) = \\ -\frac{2T}{\mathbf{m} \mathbf{m}} \sum_{i\nu_n} \text{Tr} [\Delta G_{0j,\downarrow}(i\nu_n) \Delta G_{j0,\uparrow}(i\nu_n)]$$

$$J_q = -\frac{2T}{\mathbf{m}^2 V_{BZ}} \sum_{i\nu_n} \int_{1BZ} dk \sum_{\substack{mm' \\ m''m'''}} \left(\Delta^{mm'} G_{k+q,\downarrow}^{m'm''}(i\nu_n) \Delta^{m''m'''} G_{k,\uparrow}^{m'''m}(i\nu_n) \right) =$$

$$-\frac{2T}{\mathbf{m}^2 V_{BZ}} \sum_{i\nu_n} \int_{1BZ} dk \text{Tr} [\Delta G_{k+q,\downarrow}(i\nu_n) \Delta G_{k,\uparrow}(i\nu_n)]$$

Tips to check

$$G_{0j,\sigma}^{mm'}(-i\omega_n)^\dagger = \frac{1}{V_{BZ}} \int_{BZ} G_\sigma^{mm'}(-i\omega_n, \mathbf{k})^\dagger e^{-2\pi i \mathbf{k} \mathbf{R}_j} d\mathbf{k} =$$

$$\frac{1}{V_{BZ}} \int_{BZ} G_\sigma^{mm'}(i\omega_n, \mathbf{k}) e^{-2\pi i \mathbf{k} \mathbf{R}_j} d\mathbf{k} = G_{j0,\sigma}^{mm'}(i\omega_n)$$

$$0 = \int dq J_q$$

Magnon dispersion in Heisenberg model

$$E(\mathbf{q}) = \frac{4\mu_B}{\mathbf{m}} [J(\mathbf{0}) - J(\mathbf{q})]$$

1.2 2 atoms per cell

In case of 2 (magnetic) atoms in unit cell we add indices i, j that number these atoms

$$G_{ij,\sigma}^{mm'}(i\nu_n, \mathbf{k}) = (i\nu_n + E_F - H_{mm',ij,\sigma}^{WF}(\mathbf{k}))^{-1}$$

$$G_{00,\sigma}^{mm'}(i\nu_n, \mathbf{R}_l) = \frac{1}{V_{BZ}} \int_{BZ} G_{\sigma 00}^{mm'}(i\nu_n, \mathbf{k}) e^{2\pi i \mathbf{k} \mathbf{R}_l} d\mathbf{k}$$

$$G_{01,\sigma}^{mm'}(i\nu_n, \mathbf{R}_l) = \frac{1}{V_{BZ}} \int_{BZ} G_{\sigma 01}^{mm'}(i\nu_n, \mathbf{k}) e^{2\pi i \mathbf{k} \mathbf{R}_l} d\mathbf{k}$$

where \mathbf{R}_l is translation vector (in our case both atoms are in G so \mathbf{R}_l is integer vector)

$$\Delta_{ii}^{mm'} = \frac{1}{V_{BZ}} \int_{BZ} \left(H_{\uparrow ii}^{mm'}(\mathbf{k}) - H_{\downarrow ii}^{mm'}(\mathbf{k}) \right) d\mathbf{k}. \quad (4)$$

$$J_{ij}(\mathbf{R}_l) = \frac{T}{4} \sum_{i\nu_n} \text{Tr} [\Delta_{ii} G_{ij,\downarrow}(i\nu_n, \mathbf{R}_l) \Delta_{jj} G_{ji,\uparrow}(i\nu_n, -\mathbf{R}_l)] \quad (5)$$

$$J_{ij}(q) = \frac{T}{4V_{BZ}} \sum_{i\nu_n} \int_{1BZ} dk \text{Tr} [\Delta_{ii} G_{ij,\downarrow}(i\nu_n, k+q) \Delta_{jj} G_{ji,\uparrow}(i\nu_n, k)] \quad (6)$$

from $J_{ij}(\mathbf{q})$ we can also get $J_{ij}(\mathbf{R}_l)$ via

$$J_{ij}(\mathbf{R}_l) = \frac{1}{V_{BZ}} \int_{BZ} J_{ij}(\mathbf{q}) e^{2\pi i \mathbf{q} \mathbf{R}_l} d\mathbf{q} \quad (7)$$

References

- [1] D. M. Korotin, V. V. Mazurenko, V. I. Anisimov, and S. V. Streltsov, “Calculation of the exchange constants of the Heisenberg model in the plane-wave based methods using the Green’s function approach,” *Physical Review B*, vol. 91, p. 224405, June 2015. arXiv:1411.4169 [cond-mat].
- [2] A. I. Liechtenstein, M. I. Katsnelson, V. P. Antropov, and V. A. Gubanov, “Local spin density functional approach to the theory of exchange interactions in ferromagnetic metals and alloys,” *Journal of Magnetism and Magnetic Materials*, vol. 67, pp. 65–74, May 1987.