Theory

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1 Heisenberg model

Heisenberg model reads here

$$\hat{H} = -\sum_{i \neq j} J_{ij} \vec{e}_i \cdot \vec{e}_j$$

so positive exchanges mean FM state. In this convention (omiting details in expression on the right)

$$(-1)^P J_{ij} \propto -\sum_{i\nu_n} \mathrm{Tr}\left[\Delta_i G_{ij}\left(i\nu_n\right) \Delta_j G_{ji}\left(i\nu_n\right)\right],$$

where ν_n denotes the Matsubara frequency. Here we set $P = 0$ (1) when the spins at i and j sites are aligned parallel (antiparallel) to each other depending on the state in which Δ was calculated. Practically depending on the configuration in DFT.

2 All in all

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

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

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

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

and the inversion is performed in the site- and orbital space. To obtain $H^{rm,r'm'}_{\mathbf{k},\sigma}$ 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.

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

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

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

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

3 Single atom per cell

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

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

$$J_q = -\frac{2T}{\mathfrak{m}^2 V_{BZ}}\sum_{i\nu_n}\int_{1BZ}\mathrm{d}k\sum_{\substack{mm'\\m''m'''}}\left(\Delta^{mm'}G^{m'm''}_{k+q,\downarrow}(i\nu_n)\Delta^{m''m'''}G^{m'''m}_{k,\uparrow}(i\nu_n)\right) = \\ -\frac{2T}{\mathfrak{m}^2 V_{BZ}}\sum_{i\nu_n}\int_{1BZ}\mathrm{d}k\,\mathrm{Tr}\left[\Delta G_{k+q,\downarrow}(i\nu_n)\Delta G_{k,\uparrow}(i\nu_n)\right]$$

Tips to check

$$G^{mm'}_{0j,\sigma}(-i\omega_n)^{\dagger} = \frac{1}{V_{BZ}}\int_{BZ} G^{mm'}_{\sigma}(-i\omega_n,\mathbf{k})^{\dagger}e^{-2\pi i\mathbf{k}\mathbf{R}_j}d\mathbf{k} = \\ \frac{1}{V_{BZ}}\int_{BZ} G^{mm'}_{\sigma}(i\omega_n,\mathbf{k})e^{-2\pi i\mathbf{k}\mathbf{R}_j}d\mathbf{k} = G^{mm'}_{j0,\sigma}(i\omega_n)$$

$$0 = \int \mathrm{d}q J_q$$

Magnon dispersion in Heisenberg model

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

4 Several types of atoms per cell

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

$$G^{mm'}_{ij,\sigma}(i\nu_n,\mathbf{k}) = \left(i\nu_n + E_F - H^{WF}_{mm',ij,\sigma}(\mathbf{k})\right)^{-1}$$

here matrix is inverted in full basis. Then intersite Green's function is

$$G^{mm'}_{i'j',\sigma}(i\nu_n) = \frac{1}{V_{BZ}}\int_{BZ} G^{mm'}_{ij,\sigma}(i\nu_n,\mathbf{k})e^{2\pi i\mathbf{k}\left((\mathbf{R}_{i'}-\mathbf{R}^0_i)-(\mathbf{R}_{j'}-\mathbf{R}^0_j)\right)}d\mathbf{k}$$

where $G^{mm'}_{ij,\sigma}(i\nu_n,\mathbf{k})$ is the inter-site Green's function of the primitive cell for given $\mathbf{k}$ point, $\mathbf{R_{i'}}$ - is the position of atom i' in the lattice, and $\mathbf{R^0_i}$ is the position of the same atom within the primitive cell. This means integer vectors (in crystal coordinates) in the exponent for interatomic exchanges. $\mathbf{k}$-vectors should be in fractional coordinates here.

Δ matrix is also block-diagonal and we need only blocks on its diagonal.

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

Using this we ge

$$J_{ij} = -\frac{2T}{\mathfrak{mm}} \sum_{i\nu_n} \mathrm{Tr} \left[\Delta_{ii} G_{ij,\downarrow}(i\nu_n) \Delta_{jj} G_{ji,\uparrow}(i\nu_n) \right] \tag{5}$$

where J_{ij} is exchange between particular pair of atoms. Normally it should be identical for all representatives of neighbours order.

In momentum space between types of atoms i and j (not particular pairs of them) we get

$$J_{ij}(q) = -\frac{2T}{\mathfrak{mm}} \sum_{i\nu_n} \int_{1BZ} \mathrm{d}k \, \mathrm{Tr} \left[\Delta_{ii} G_{ij,\downarrow}(i\nu_n, k+q) \Delta_{jj} G_{ji,\uparrow}(i\nu_n, k) \right] \tag{6}$$

and from this $J_{ij}(\mathbf{q})$ we can also get $J_{ij}(\mathbf{R}_l)$ where $\mathbf{R}_l$ is vector connecting particular pair of atoms, via

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

and vice versa.

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.