Exchange parameters from first principles in noncollinear magnets

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Interatomic exchange interactions in non-collinear magnets

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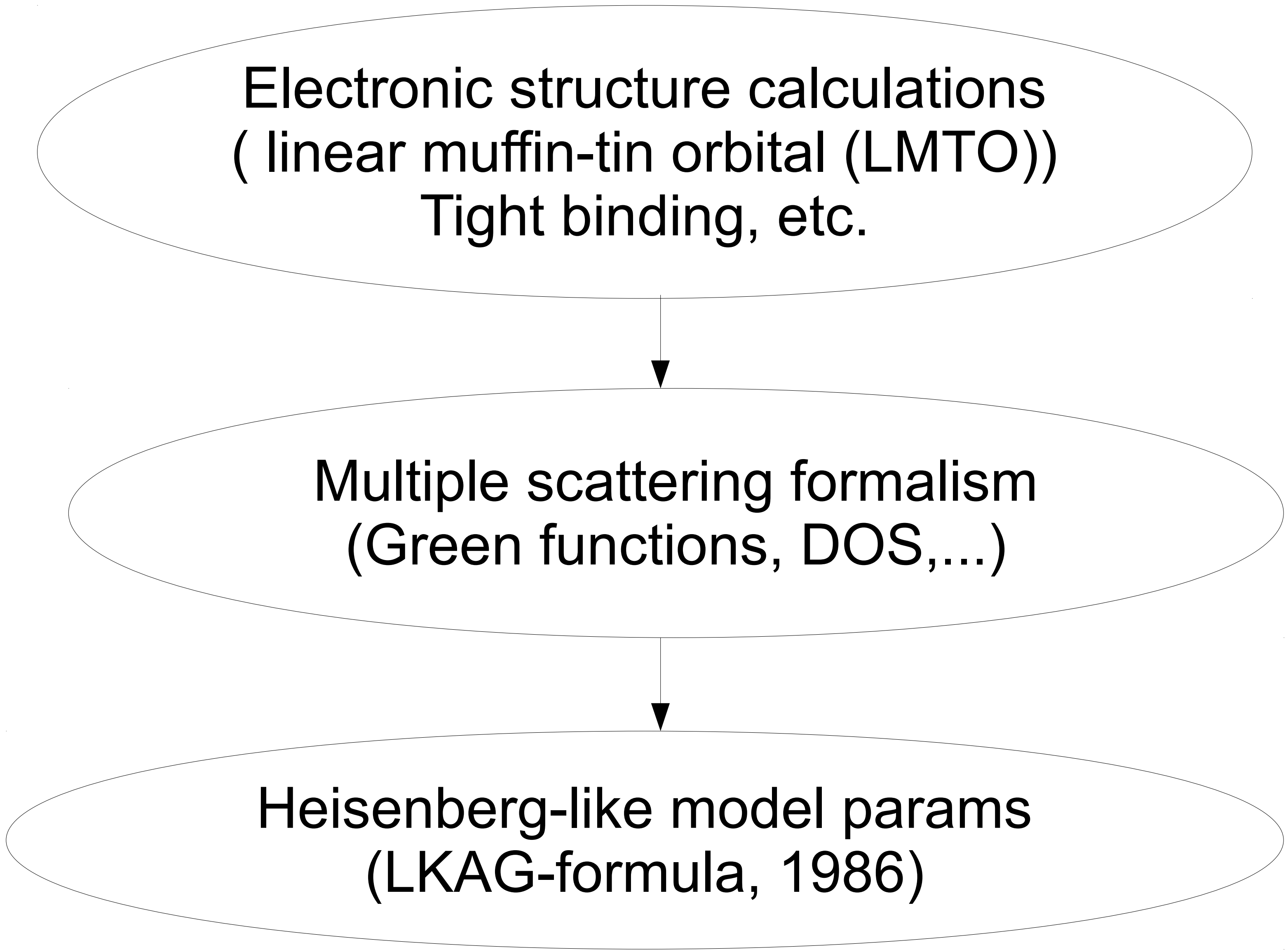
Summary

- Intro
- Methods
- Results: ferromagnetism of Fe (Ni)
- Outro

Intro

- Goal: derive simple, effective (uderstandable) spin models from electronic structure (Hubbard-> AFM Heisenberg//FM?)
- Calculate the effective parameters
- Alternative route: use sophisticated elect. struct. calculations->derive magn. Models
- Examples: **Fe, Ni**
- (Remember Krisztián Palotás's talk!)



A. I. Liechtenstein, M. I. Katsnelson, V.P. Antropov, V.A. Gubanov, J. Magn. Magn. Mater. **67** 65 (1987)

- Band struct. calc. highly technical, not understandable by simple means
- Soph. numerical tech., few params (lattice constant, 137, self-consistent potential,...)
- MST: -”- (a 2 semester course...)
- Heisenberg:
- Classical Heisenberg:
- Bilinear-tensorial:
- Biquadratic:

$$H_{eff} = -\sum_{l \neq k} J_{ij} \vec{S}_i \vec{S}_j$$

$$\mathcal{H}^L = -\sum_{l \neq k} J_{lk} \overrightarrow{n}_l \overrightarrow{n}_k$$

$$\mathcal{H}^T = -\sum_{i \neq j} \overrightarrow{n}_i \mathbf{J}_{ij} \overrightarrow{n}_j$$

$$\mathcal{H}^Q = -\sum_{i \neq j} J'_{ij} \overrightarrow{n}_i \overrightarrow{n}_j - \sum_{i \neq j} B_{ij} \left(\overrightarrow{n}_i \overrightarrow{n}_j \right)^2$$

$$J^L_{ij} = A^{00}_{ij} - A^{zz}_{ij} \qquad J'_{ij} = A^{00}_{ij} - 3A^{zz}_{ij} \qquad B_{ij} = A^{zz}_{ij}$$

- Q: What kind of interactions are present? (All!<=>LKAG->J^L)
- Q: Parameter values?
- Q: Measurable quantities?

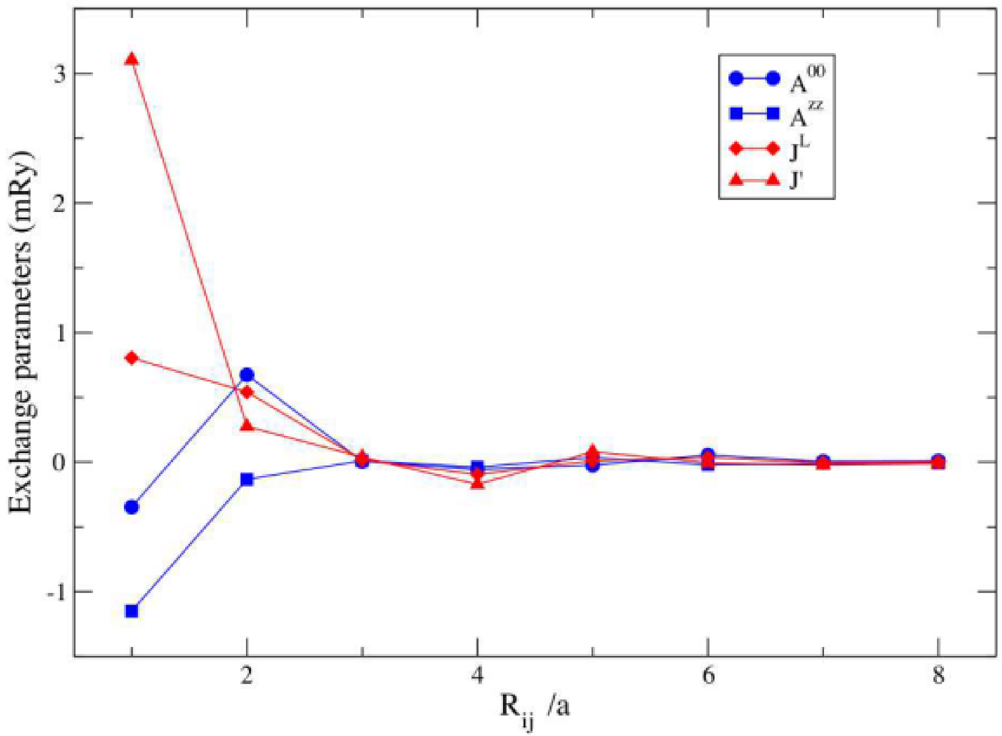


FIG. 1: Collinear exchange parameters (A^{00} and A^{zz}) between the first eight neighbors in bcc Fe. J^{L}, see Eq. (7) and J', see Eq. (18) are derived parameters for the bilinear and biquadratic spin Hamiltonians, the biquadratic B equals A^{zz}, which is rather large for nearest neighbors.

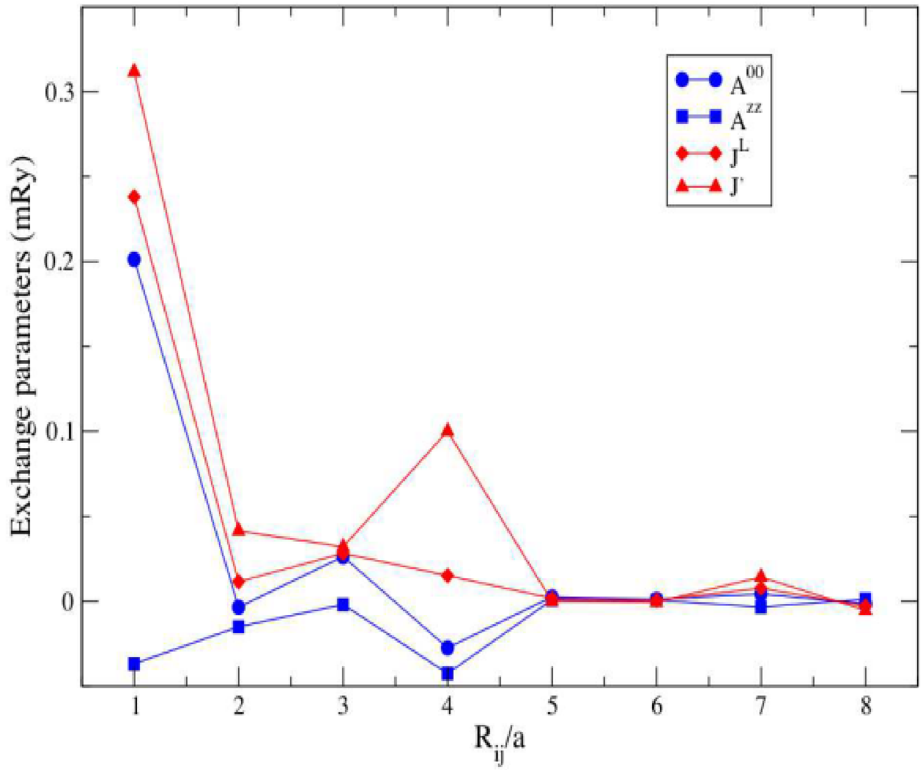


FIG. 2: Collinear exchange parameters between the first eight neighbors in fcc Ni. The bilinear parameter of bilinear model, J^{L}, and the bilinear parameter of biquadratic model, J', are very close to each other in fcc Ni. $A^{zz} \ll A^{00}$.

Ferromagnon spectra

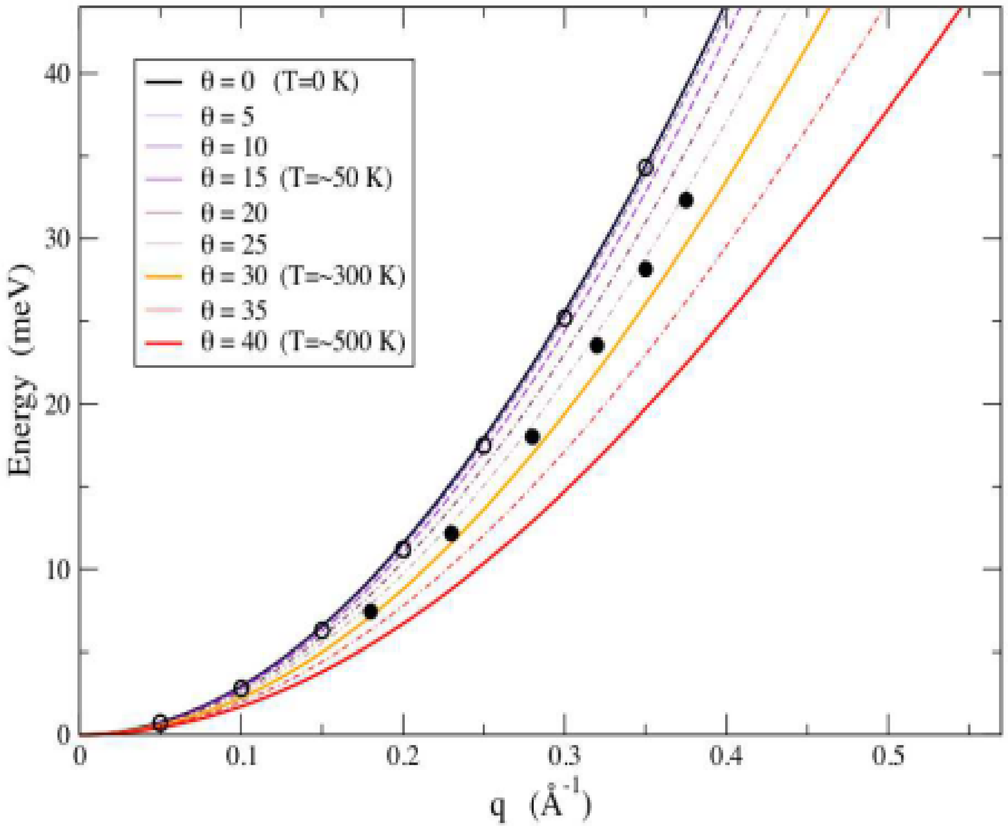


FIG. 4: Spin-wave dispersion relation calculated at different temperatures along the Γ-H direction. The top thick (black) line shows the calculated spectrum from collinear LKAG exchange parameters, open circles come from magnetization measurement at 4.2 K [15] The middle thick (yellow) line corresponds to the calculated spectrum at 300 K and the filled circles refer to the room temperature neutron scattering measurement data[14].

- Stiffness (T=0K): 287 meVÅ^2
- Exp. (4.2K): $D_{\mathrm{exp}} = 280\text{-}330$ meVÅ^2
- 300K: 219 meVÅ^2
- Exp (300K): 230
- T-dependent J_ij(T)->e.g. Deviatons from Bloch's law

Outro: can we use this formalism in nanophysics?

- Definitely yes
- Similar models for magnetic single-ion anisotropy in gold nanoparticles
- Magnetic impurities in the vicinity of noble metal surfaces (incl. RKKY)
- Magnetic nanoparticle simulations

Conclusions

- Truly ab initio calculations of effective model parameters
- Higher order interactions present
- Temperature dependent parameters

Thank you for your attention!