Radboud Universiteit Nijmegen

Exchange interactions and itinerant-electron magnetism

Mikhail Katsnelson

IMM

Institute for Molecules and Materials

Outline

1. Introduction
2. Time-dependent DFT and magnetic susceptibility
3. Exchange interactions from first principles
4. Beyond DFT: correlated systems and LDA+DMFT
5. Itinerant-electron magnets: Fe, Co, Ni
6. Dzyaloshinskii-Moriya interactions
7. Application: Molecular magnets
8. Exchange interactions and bcc-fcc transformation in iron and steel

General formulation

System of interacting electrons (many-body problem) + crystal potential

External strong time-dependent laser field (nonequilibrium problem)

Temperature effects (thermal bath, open system, basic statistical mechanics)

Collect all difficulties of modern theoretical physics

Levels of description

- Macroscopic (LLG equations + temperature balance, etc.)

- Microscopic, classical Heisenberg model

- Microscopic, quantum itinerant-electron model

-Ab initio, time-dependent density functional

Multiscale problem

Time-dependent DFT

SE for many-body wave function in configurational space is replaced by single-particle nonlinear self-consistent equation

Spinor $\Psi = \begin{pmatrix} \Psi_+ \\ \Psi_- \end{pmatrix}$

$$i\frac{\partial \Psi}{\partial t} = [H_L - \hat{\boldsymbol{\sigma}} \cdot \mathbf{B}(\mathbf{r},t)]\Psi$$

B is self-consistent magnetic field

$$H_L = -\nabla_{\mathbf{r}}^2 + \sum_{\mathbf{R}} V_{\mathbf{rR}} + 2\int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + V_{\mathrm{xc}}$$

Simplifications

Adiabatic approx.: V_{xc} and B_{xc} are the same as in the equilibrium + local (spin) density approx.

$$\mathrm{i}\frac{\partial \psi}{\partial t} = H\psi$$

$$H = -\nabla^2 + V(\mathbf{r}) - \tfrac{1}{2}(\mathbf{B}_{\mathrm{xc}}(\mathbf{r}) + \mathbf{B}_{\mathrm{ext}}(\mathbf{r}))\sigma$$

$$V(\mathbf{r}) = V_{\mathrm{ext}}(\mathbf{r}) + \int \mathrm{d}\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\partial}{\partial n}[n\varepsilon_{\mathrm{xc}}]$$

$$\mathbf{B}_{\mathrm{xc}} = -2\frac{\mathbf{m}}{m}\frac{\partial}{\partial m}[n\varepsilon_{\mathrm{xc}}]$$

n,m are charge and spin densities

Linear response: magnetic susceptibility

MIK & Lichtenstein, JPCM 16, 7439 (2004)

$$\mathbf{B}_{\mathrm{ext}}(\mathbf{r}) \rightarrow 0$$

$$\delta B^{\alpha}_{\mathrm{tot}} = \delta B^{\alpha}_{\mathrm{ext}} + \frac{\delta B^{\alpha}_{\mathrm{xc}}}{\delta m^{\beta}} \delta m^{\beta}$$

$$\delta m^{\alpha} = \hat{\chi}^{\alpha\beta} \delta B^{\beta}_{\mathrm{ext}}$$

$$(\hat{\chi}\varphi)(\mathbf{r}) = \int \mathrm{d}\mathbf{r}'\, \chi(\mathbf{r}, \mathbf{r}')\varphi(\mathbf{r}')$$

At the same time (Runge-Gross theorem, 1984) in TD-DFT

$$\delta m^{\alpha} = \hat{\chi}_0^{\alpha\beta} \delta B^{\beta}_{\mathrm{tot}}$$

A response of effective system of noninteracting Kohn-Sham particles (Liu & Vosko 1989 for magnetic case)

Linear response: magnetic susceptibility II

Rigorous exprression

$$\hat{\chi}^{\alpha\beta} = \hat{\chi}_0^{\alpha\beta} + \hat{\chi}_0^{\alpha\gamma} \frac{\delta B_{\mathrm{xc}}^{\gamma}}{\delta m^{\delta}} \hat{\chi}^{\delta\beta}$$

Adiabatic approximation plus LSDA:

$$\frac{\delta B_{\mathrm{xc}}^{\gamma}}{\delta m^{\delta}} = \frac{B_{\mathrm{xc}}}{m} \left(\delta_{\gamma\delta} - \frac{m^{\gamma} m^{\delta}}{m^2} \right) + \frac{m^{\gamma} m^{\delta}}{m^2} \frac{\partial B_{\mathrm{xc}}}{\partial m}$$

Transverse susceptibility is separated from (longitudinal spin + charge) susceptibilities

Transverse susceptibility

$$\chi^{+-}(\mathbf{r},\mathbf{r}',\omega) = \chi_0^{+-}(\mathbf{r},\mathbf{r}',\omega) + \int \mathrm{d}\mathbf{r}''\, \chi_0^{+-}(\mathbf{r},\mathbf{r}'',\omega) I_{\mathrm{xc}}(\mathbf{r}'') \chi^{+-}(\mathbf{r}'',\mathbf{r}',\omega)$$

$$I_{\mathrm{xc}} = \frac{B_{\mathrm{xc}}}{m}$$

Local Stoner parameter

$$m = \sum_{\mu\sigma} \sigma f_{\mu\sigma} |\psi_{\mu\sigma}(\mathbf{r})|^2$$

$$n = \sum_{\mu\sigma} f_{\mu\sigma} |\psi_{\mu\sigma}(\mathbf{r})|^2.$$

$$\chi_0^{+-}(\mathbf{r},\mathbf{r}',\omega) = \sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} \psi^*_{\mu\uparrow}(\mathbf{r}) \psi_{\nu\downarrow}(\mathbf{r}) \psi^*_{\nu\downarrow}(\mathbf{r}') \psi_{\mu\uparrow}(\mathbf{r}')$$

Kohn-Sham states

$$(H_0 - \tfrac{1}{2}\sigma B_{\mathrm{xc}})\psi_{\mu\sigma} = \varepsilon_{\mu\sigma}\psi_{\mu\sigma}$$

$$H_0 = -\nabla^2 + V(\mathbf{r})$$

Longitudinal susceptibility

$$\chi^{zz} = \frac{1}{4}\left(K^{\uparrow\uparrow} + K^{\downarrow\downarrow} - K^{\uparrow\downarrow} - K^{\downarrow\uparrow}\right)$$

$$\begin{aligned}
K^{\uparrow\uparrow} &= X_{\uparrow} + X_{\uparrow}U_{\uparrow\uparrow}K^{\uparrow\uparrow} + X_{\uparrow}U_{\uparrow\downarrow}K^{\downarrow\uparrow} \\
K^{\downarrow\downarrow} &= X_{\downarrow} + X_{\downarrow}U_{\downarrow\downarrow}K^{\downarrow\downarrow} + X_{\downarrow}U_{\downarrow\uparrow}K^{\uparrow\downarrow} \\
K^{\uparrow\downarrow} &= X_{\uparrow}U_{\uparrow\downarrow}K^{\downarrow\downarrow} + X_{\uparrow}U_{\uparrow\uparrow}K^{\uparrow\downarrow} \\
K^{\downarrow\uparrow} &= X_{\downarrow}U_{\downarrow\uparrow}K^{\uparrow\uparrow} + X_{\downarrow}U_{\downarrow\downarrow}K^{\downarrow\uparrow}.
\end{aligned}$$

$$X_{\sigma}\left(\mathbf{r},\mathbf{r}'\right) = \sum_{\mu\nu}\frac{f_{\mu\sigma} - f_{\nu\sigma}}{\omega - \varepsilon_{\mu\sigma} + \varepsilon_{\nu\sigma}}\psi^{*}_{\mu\sigma}(\mathbf{r})\psi_{\nu\sigma}(\mathbf{r})\psi_{\mu\sigma}(\mathbf{r}')\psi^{*}_{\nu\sigma}(\mathbf{r}')$$

$$U_{\sigma\sigma'} = \frac{\partial^2\left(n\varepsilon_{\mathrm{xc}}\right)}{\partial n_{\sigma}\partial n_{\sigma'}}$$

$$n_{\sigma} = \frac{1}{2}\left(n + \sigma m\right)$$

Separation of magnon poles

After rigorous manipulations

$$\hat{\chi}^{+-} = (m + \hat{\Lambda})(\omega - I_{\mathrm{xc}}\hat{\Lambda})^{-1}$$

$$\Lambda(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} \psi^*_{\mu\uparrow}(\mathbf{r})\psi_{\nu\downarrow}(\mathbf{r})\nabla[\psi_{\mu\uparrow}(\mathbf{r}')\nabla\psi^*_{\nu\downarrow}(\mathbf{r}') - \psi^*_{\nu\downarrow}(\mathbf{r}')\nabla\psi_{\mu\uparrow}(\mathbf{r}')]$$

Magnon pole

$$\omega(\mathbf{q}) = \frac{4}{M}\left[J(0) - J(\mathbf{q})\right]$$

$$J(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{4}\sum_{\mu\nu} \frac{f_{\mu\uparrow} - f_{\nu\downarrow}}{\omega - \varepsilon_{\mu\uparrow} + \varepsilon_{\nu\downarrow}} \psi^*_{\mu\uparrow}(\mathbf{r})B_{\mathrm{xc}}(\mathbf{r})\psi_{\nu\downarrow}(\mathbf{r})\psi^*_{\nu\downarrow}(\mathbf{r}')B_{\mathrm{xc}}(\mathbf{r}')\psi_{\mu\uparrow}(\mathbf{r}')$$

Im part corresponds to Stoner damping

Alternative definition of exchanges

Static susceptibility

$$\hat{\chi}^{+-}(0) = m(\hat{\Omega}^{-1} - B_{\mathrm{xc}}^{-1})$$

$$\hat{\tilde{\Omega}} = \hat{\Omega}(1 - B_{\mathrm{xc}}^{-1}\hat{\Omega})^{-1}$$

The first way (poles of susceptibility) corresponds Liechtenstein, MIK & Gubanov, J. Phys. F 1984, the second way (static suscept.) Bruno, PRL 2003. The expressions for stiffness constant coincide and are rigorous within the adiabatic approximation + LSDA

Nonlocal corrections to magnon stiffness

MIK & Antropov, PRB 67, 140406 (2003)

Exchange and correlation in spiral state of homogeneous electron gas

Angular gradient corrections

$$E_{xc} = \int d\mathbf{r}\{n\varepsilon_{xc}(n_\uparrow, n_\downarrow) + \lambda(n_\uparrow, n_\downarrow)D\}$$

$$D = (\nabla_\alpha e_\beta)(\nabla_\alpha e_\beta) = (\nabla\theta)^2 + \sin^2\theta(\nabla\varphi)^2$$

$$\lambda(n_\uparrow, n_\downarrow) = -\frac{e^2}{16\pi^2}\left(\frac{1}{F} - \frac{4}{3}\right)(V_{xc}^\uparrow p_{F\uparrow} + V_{xc}^\downarrow p_{F\downarrow})$$

$$-\frac{e^2}{96\pi^2 F^2}(V_{xc}^\uparrow + V_{xc}^\downarrow)(p_{F\uparrow} + p_{F\downarrow}).$$

Corrections to stiffness constant

$$F = (p_{F\uparrow} + p_{F\downarrow})I(n_\uparrow, n_\downarrow)/2\pi^2$$

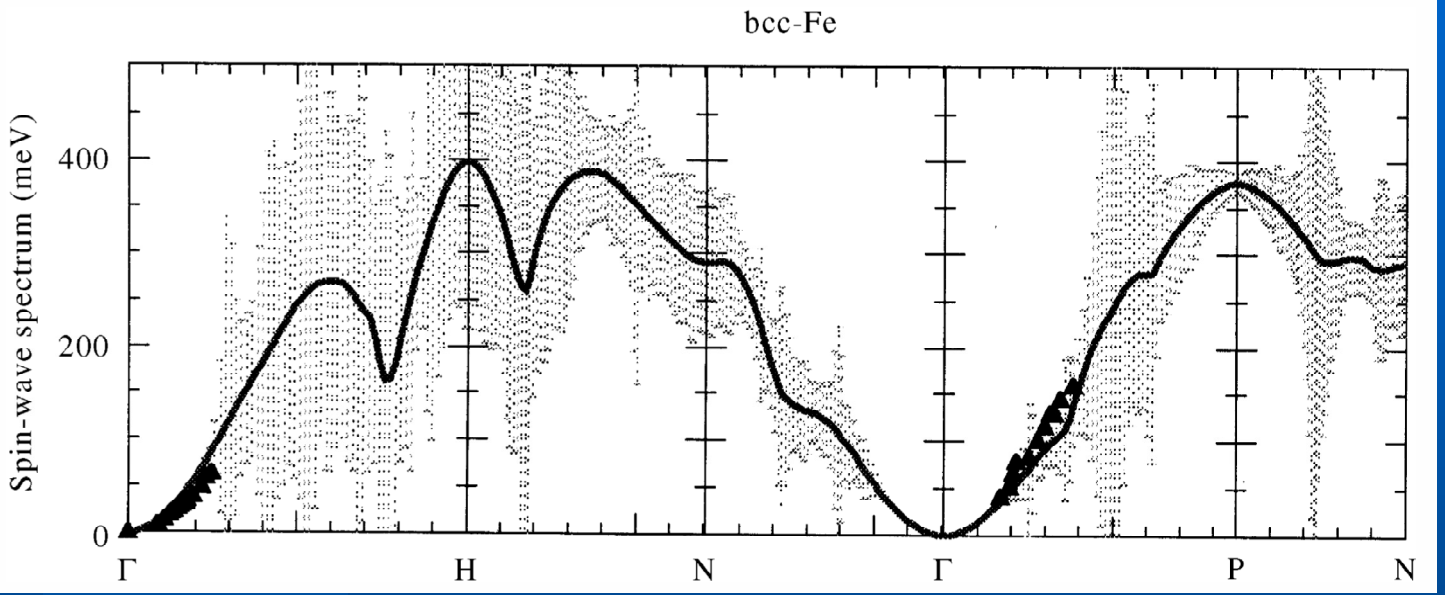
Stiffness constants for Fe and Ni

(in meV/Å^2)

Fe: LSDA	*239*
with gradient corrections	*251*
experiment	*280 - 310*
Ni: LSDA	*692*
with gradient corrections	*735*
experiment	*550-630*

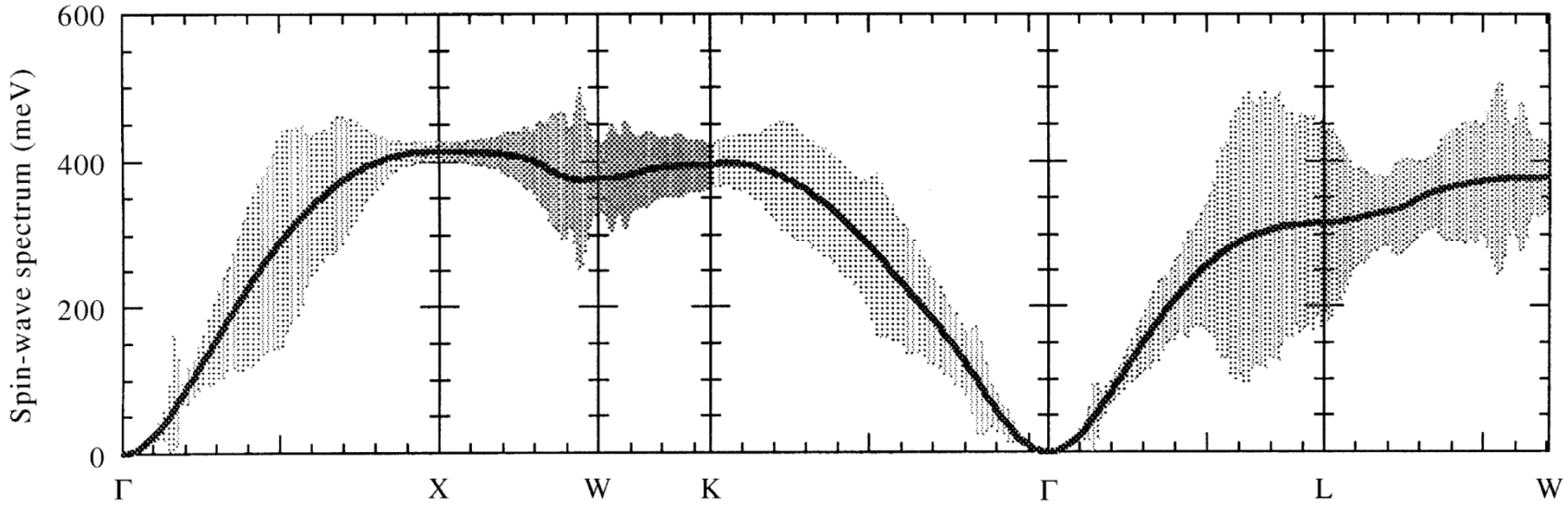
Corrections are quite small

Stoner damping in Fe and Ni



Antropov, Harmon, Smirnov, JMMM 200, 148 (1999)

fcc-Ni



Nonlinear spin dynamics

Rigid spin approximation: slow spin motions, well-defined magnetic moments

Antropov, MIK et al, PRL 75, 729 (1995); PRB 54, 1019 (1996)

1. Start with time-dependent Schroedinger equation

$$i\frac{\partial\Psi}{\partial t}=[H_L-\hat{\boldsymbol{\sigma}}\cdot\mathbf{B}(\mathbf{r},t)]\Psi$$

$$\Psi=\begin{pmatrix}\Psi_+\\ \Psi_-\end{pmatrix}$$

2. Time-dependent unitary transformation tp a coordinate system where spin at given ***rt*** is along *z* axis

$$\Psi=U\chi$$

$$U(\xi)=(1+|\xi|^2)^{-1/2}\begin{pmatrix}1 & \xi\\ -\xi^* & 1\end{pmatrix}$$

$$\xi=-\exp(-i\varphi)\tan\,\theta/2$$

Nonlinear spin dynamics II

In the local coordinate system the Hamiltonian has diagonal part

$$H_{\text{diag}} = -\hat{\sigma}_z B_z - iU^{\dagger}(\xi)\frac{d}{dt}U(\xi)$$

$$U^{\dagger}(\xi)\frac{d}{dt}U(\xi) = \frac{\xi\dot{\xi}^* - \xi^*\dot{\xi}}{1+|\xi|^2}\hat{\sigma}_z = i(1-\cos\theta)\dot{\varphi}\hat{\sigma}_z$$

1. Off-diagonal part can be neglected if local spin splitting is much larger than frequency of rotations (Stoner splitting much larger than typical magnon energy)
Valid for *d(f)* magnets, may be incorrect for *s(p)* magnets (if any)
(Edwards & MIK, JPCM 2006)

2. Rigid rotation within atomic spheres (neglecting terms with gradients of angles)
Valid for well-defined local moments, wrong for weak magnets such as $ZrZn_2$ or Sc_3In

Nonlinear spin dynamics III

$$\dot{\mathbf{e}}_\nu = -\frac{2}{\mu_\nu}[\mathbf{e}_\nu \times \mathbf{I}_\nu]$$

Ab initio SD

$$\mathbf{e} = \left(-\frac{\xi + \xi^*}{1+|\xi|^2},\ i\frac{\xi - \xi^*}{1+|\xi|^2},\ \frac{1-|\xi|^2}{1+|\xi|^2} \right)$$

Magnetic moment direction

$$\mathbf{I}_\nu = \delta E / \delta \mathbf{e}_\nu$$

Torque, *E* is the total energy

Magnetic force theorem

(Lichtenstein & MIK 1984)

Total energy in DF

$$E = E_{sp} - E_{dc}$$

$$E_{sp} = \sum_{\nu}^{occ} \varepsilon_{\nu}$$

$$E_{dc} = E_{Hartree} + \int dr Tr\left[\rho \frac{\delta E_{xc}}{\delta \rho}\right] - E_{xc}$$

Variation

$$\delta E = \delta^* E_{sp} + \delta_1 E_{sp} - \delta E_{dc} = \delta^* E_{sp} = \delta^* \int_{-\infty}^{\varepsilon_F} d\varepsilon \left[\frac{1}{\pi} Tr\, \mathrm{Im}\, \hat{G}(\varepsilon)\right]$$

δ^* at fixed potential

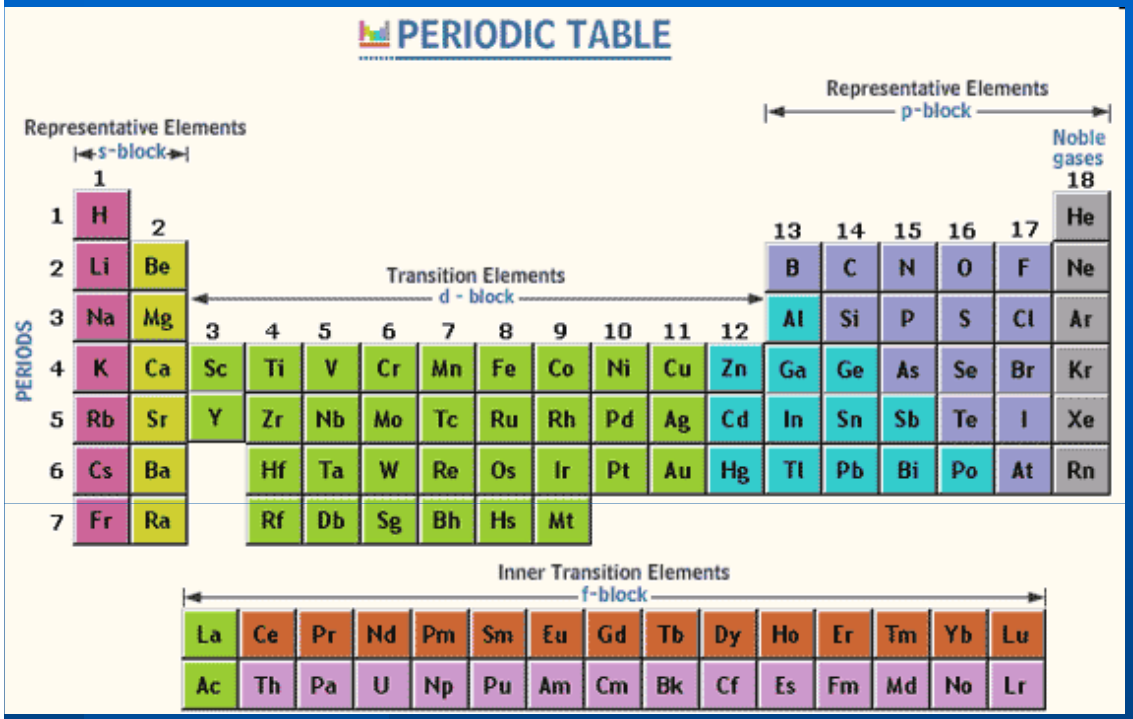
δ_1 due to change of potential

Magnetic force theorem II

- Torque can be written in terms of variation of the density of states
- Decomposition of the torque in pair terms gives exchange integrals (LK)
- These exchange parameters are local (near given magnetic configuration)
- Adding constrain to stabilize rotated configuration gives exchange parameters (Bruno)

Exchange parameters for ***d*** metals are strongly non-Heisenbergian (depend on magnetic configuration) (Turzhevskii, Lichtenstein & MIK, Fiz. Tverd. Tela 1990)

Example: magnetism of Fe, Co, Ni



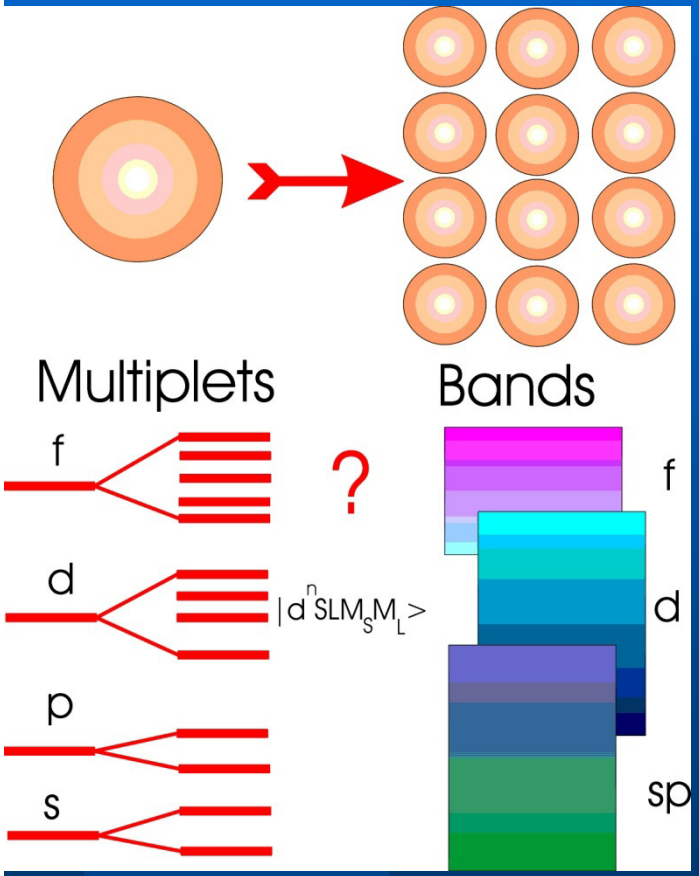
Ferromagnetism of iron is known from ancient times

Iron

Cobalt

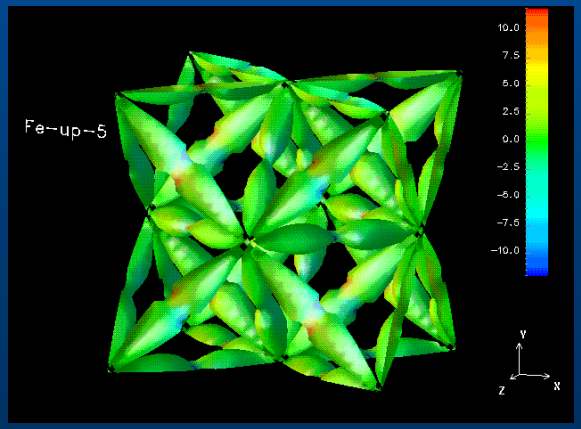
Nickel

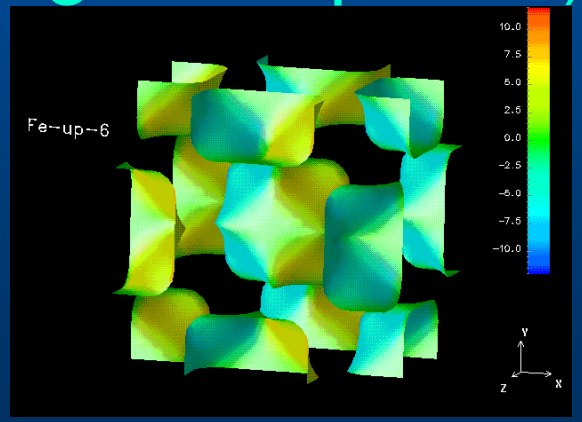
Problem: coexistence of localized and itinerant behavior



Local magnetic moments do exist above T_C (Curie-Weiss law, spectroscopy, neutrons…)

d electrons are itinerant (FS, chemical bonding, transport…)





Iron, majority spin FS

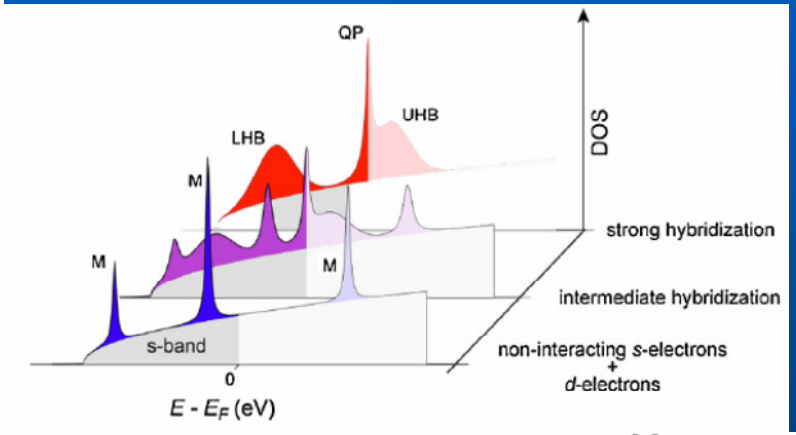
4f electrons are normally pure localized but not 3d

From atomic state to itinerant

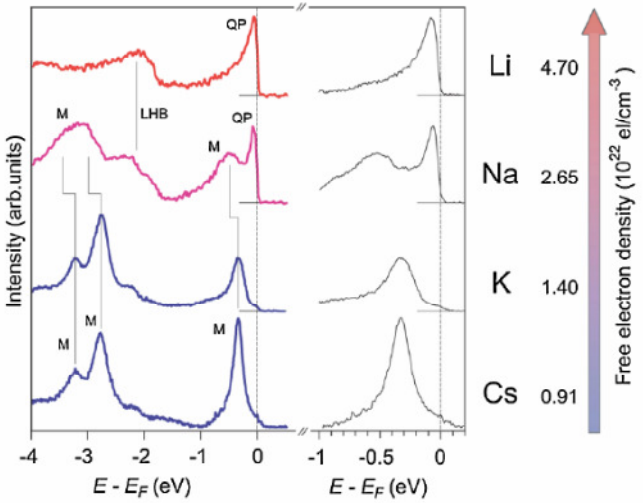
PRL **104,** 117601 (2010) PHYSICAL REVIEW LETTERS week ending 19 MARCH 2010

Correlated Electrons Step by Step: Itinerant-to-Localized Transition of Fe Impurities in Free-Electron Metal Hosts

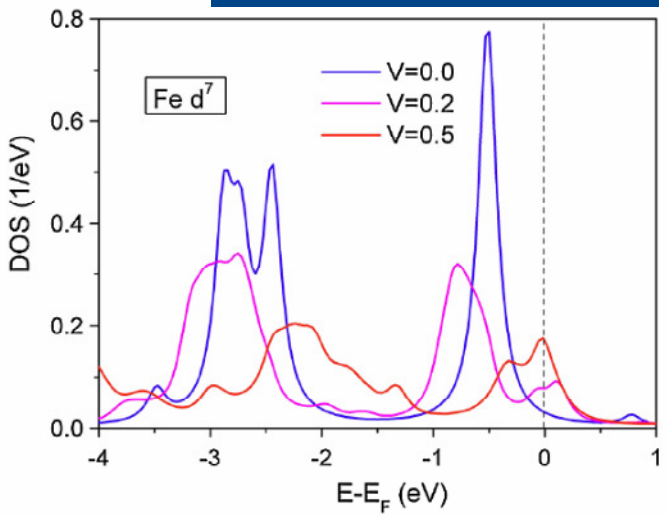
C. Carbone,[1] M. Veronese,[1] P. Moras,[1] S. Gardonio,[1] C. Grazioli,[1] P. H. Zhou,[2] O. Rader,[3] A. Varykhalov,[3] C. Krull,[4] T. Balashov,[4] A. Mugarza,[4] P. Gambardella,[4,5] S. Lebèque,[6] O. Eriksson,[7] M. I. Katsnelson,[8] and A. I. Lichtenstein[9]



Experiment: disappearance of multiplets



Calculations: increase of hybridization



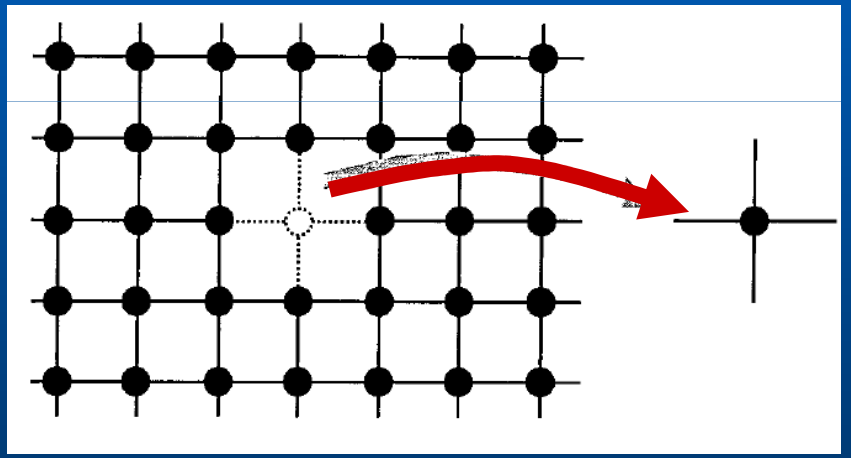
Blue line: exact diagonalization for free atom

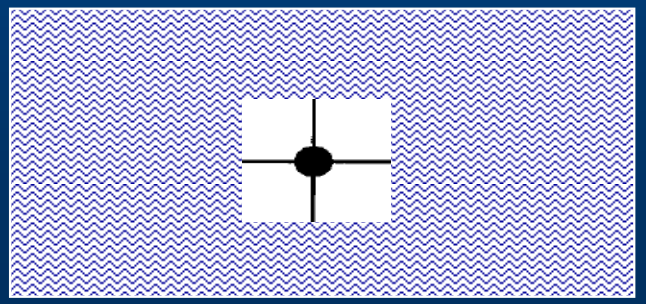
Dynamical Mean Field Theory I

A.Georges, G.Kotliar, W.Krauth and M.Rozenberg, Rev. Mod. Phys. '96

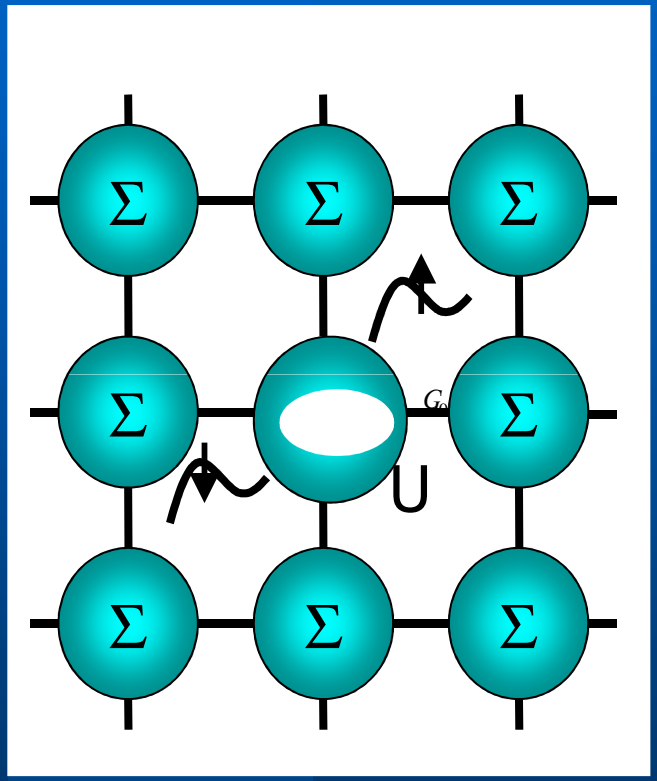
A natural generalization of the familiar MFT
to the problem of electrons in a lattice

Key idea: take one site out of a lattice and embed it in a self-consistent bath = mapping to an effective impurity problem



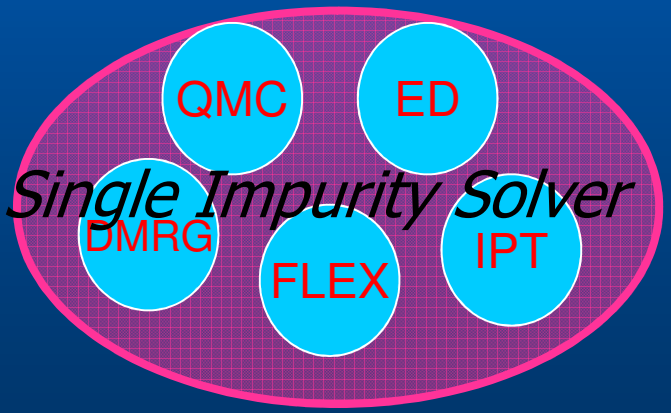


Dynamical Mean Field Theory II



$$\hat{G}(i\omega_n) = \frac{1}{\Omega}\sum_{\vec{k}}^{BZ} \hat{G}(\vec{k}, i\omega_n)$$

$$\hat{\mathcal{G}}_0^{-1}(i\omega_n) = \hat{G}^{-1}(i\omega_n) + \hat{\Sigma}(i\omega_n)$$



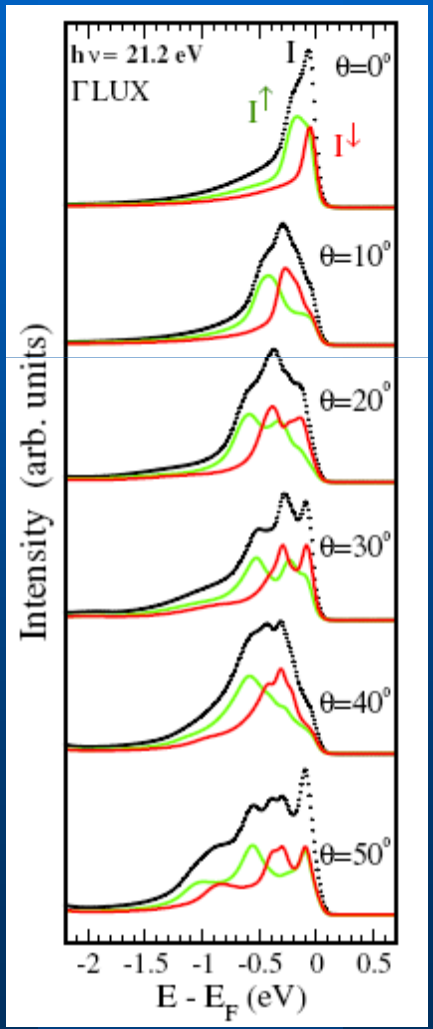
$$\hat{\Sigma}_{new}(i\omega_n) = \hat{\mathcal{G}}_0^{-1}(i\omega_n) - \hat{G}^{-1}(i\omega_n)$$

W. Metzner and D. Vollhardt (1987)
A. Georges and G. Kotliar (1992)

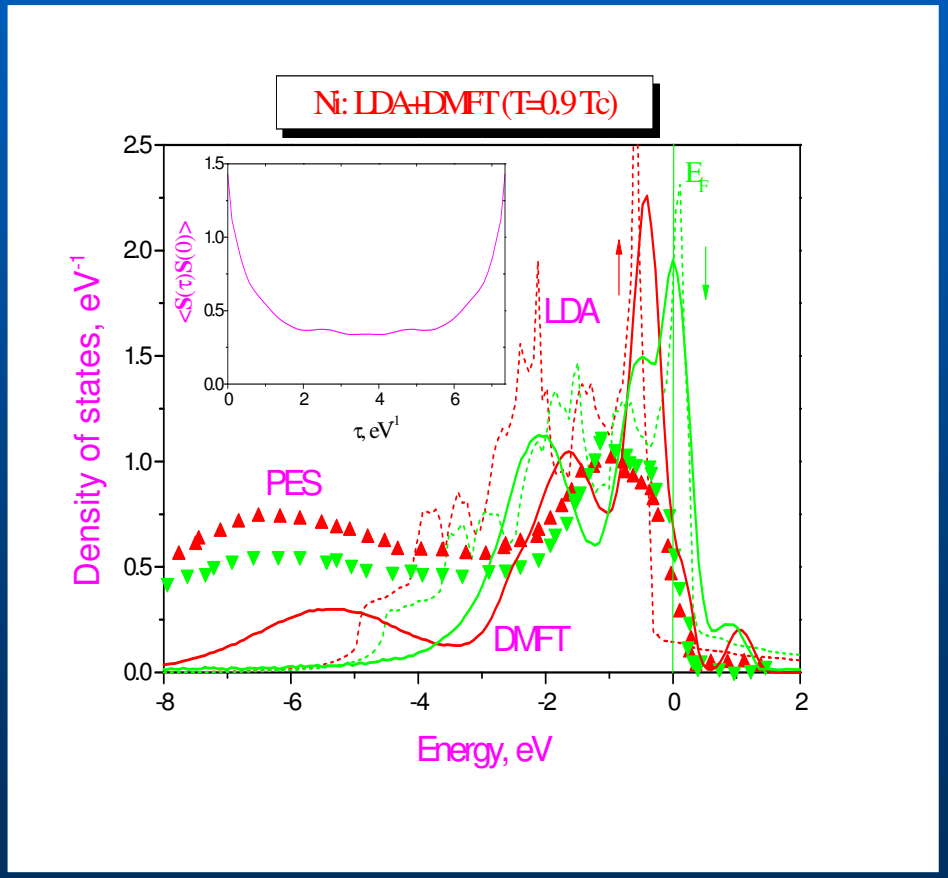
Ferromagnetism of transition metals: LDA+DMFT

Ferromagnetic Ni DMFT vs. LSDA:

- 30% band narrowing
- 50% spin-splitting reduction
- -6 eV sattellite



LDA+DMFT with ME
J. Braun *et al*
PRL (2006)



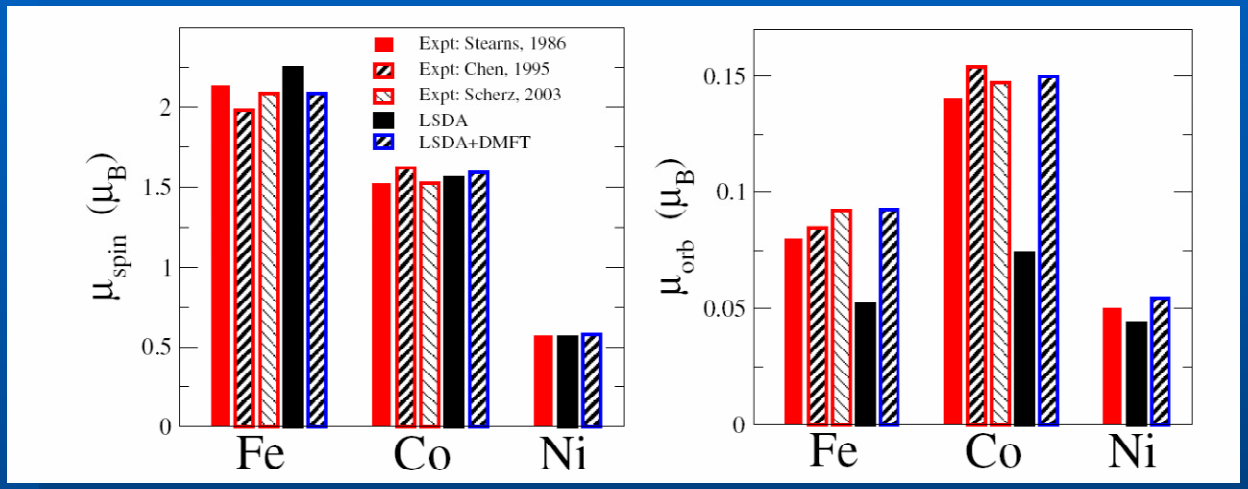
Lichtenstein, MIK, Kotliar, PRL (2001)

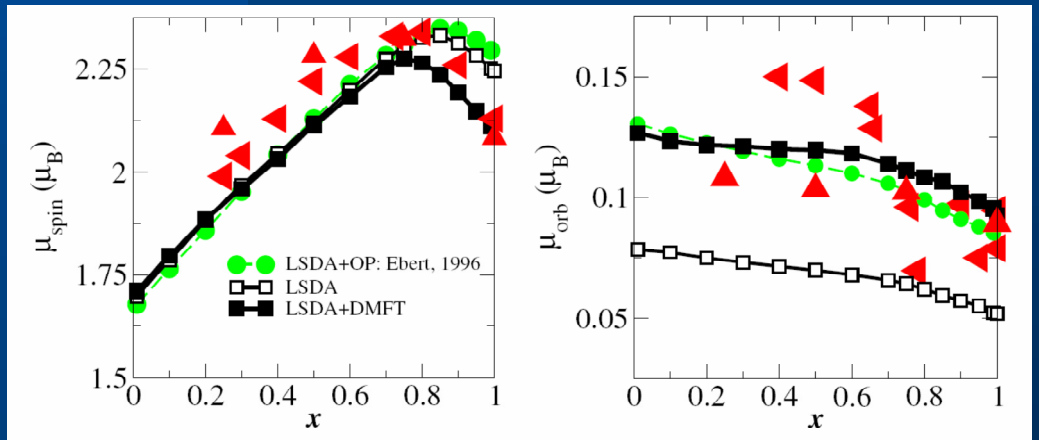
Orbital magnetic moments

Orbital magnetism in transition metal systems: The role of local correlation effects

S. Chadov, J. Minár, M. I. Katsnelson, H. Ebert, D. Ködderitzsch and A. I. Lichtenstein

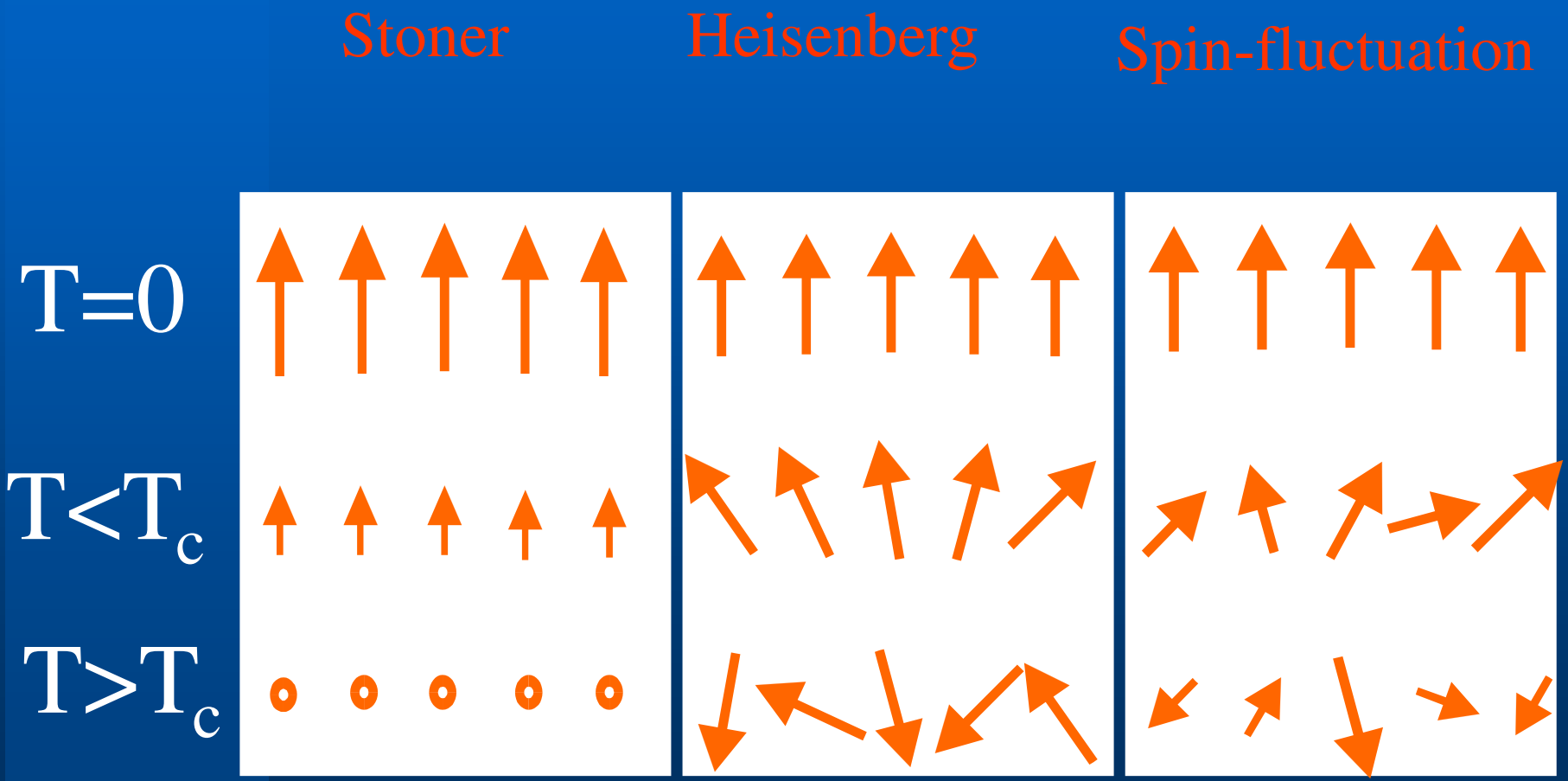
EPL, **82** (2008) 37001





For Fe_xCo_{1-x} alloys

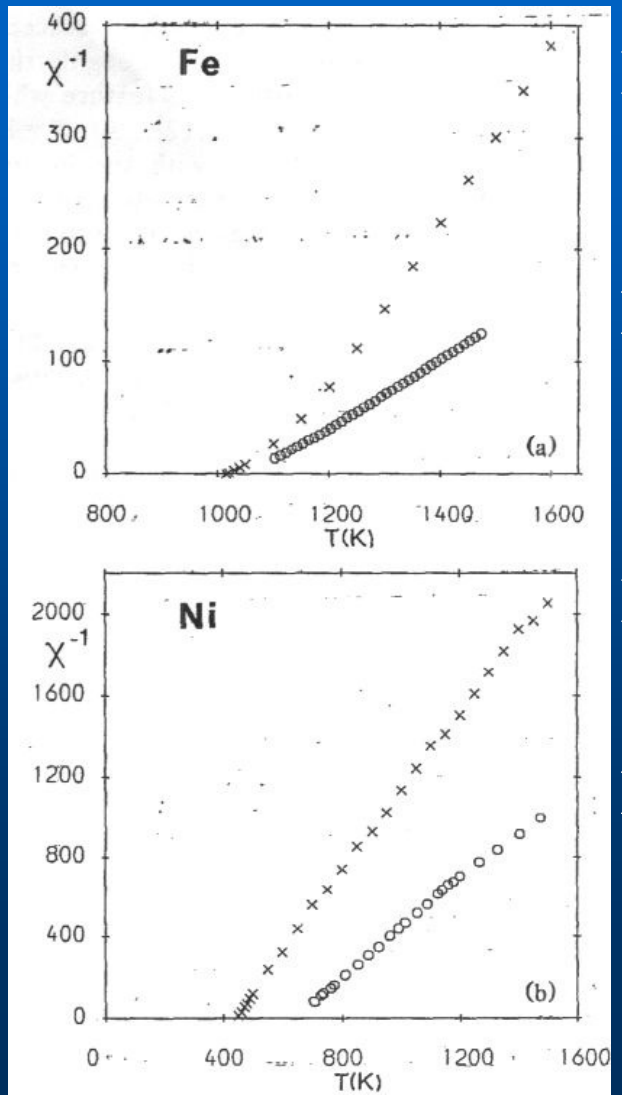
Itinerant-electron ferromagnetism at finite temperatures



LDA+Disordered Local Moments

The best first-principle Spin-fluctuation model with classical moments

J. Staunton and B. Gyorffy
PRL69, 371 (1992)



DLM

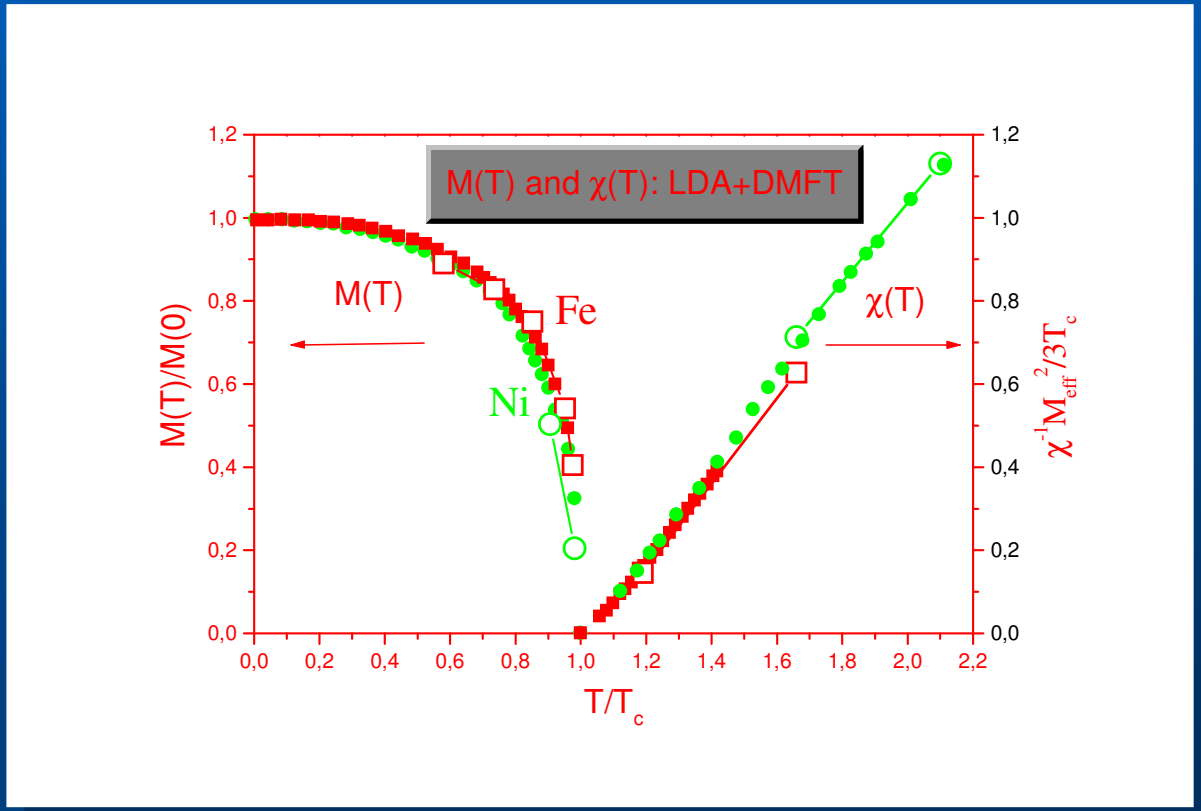
EXP

DLM

EXP

DMFT Effective Magnetic Moments: $T>T_c$

μ	exp	eff	loc	DLM	Tc	exp
Fe	3.13	3.09	2.8	1.96	1900	1043
Ni	1.62	1.5	1.3	1.21	700	631



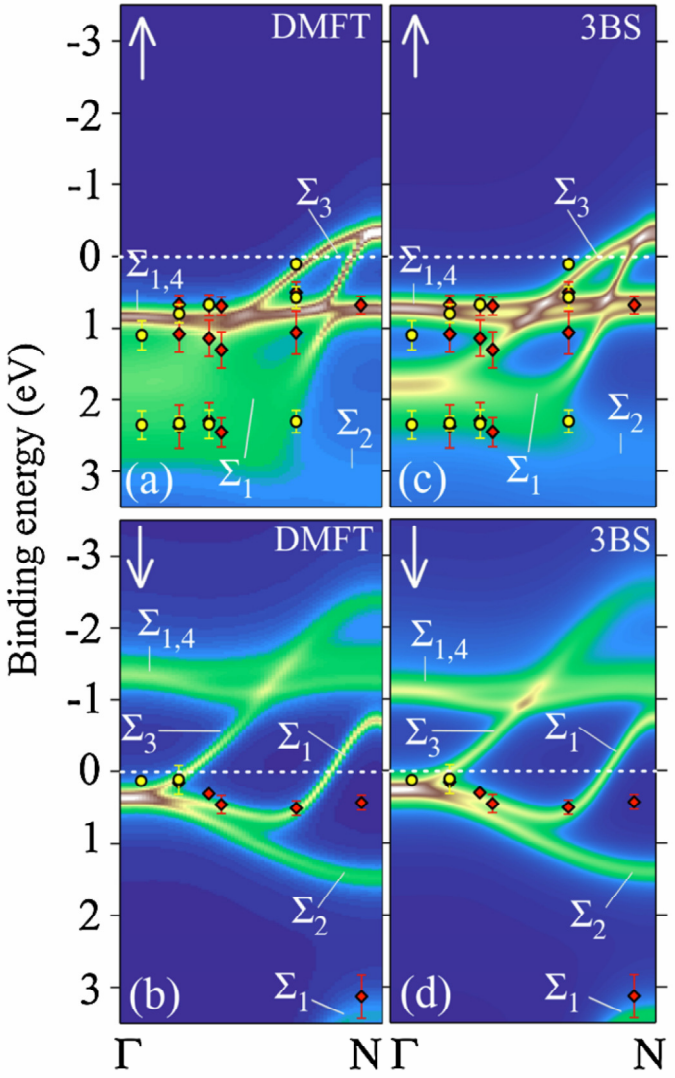
ARPES for iron

PRL **103,** 267203 (2009) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2009

Strength of Correlation Effects in the Electronic Structure of Iron

J. Sánchez-Barriga,[1] J. Fink,[1,2] V. Boni,[3] I. Di Marco,[4,5] J. Braun,[6] J. Minár,[6] A. Varykhalov,[1] O. Rader,[1] V. Bellini,[3] F. Manghi,[3] H. Ebert,[6] M. I. Katsnelson,[5] A. I. Lichtenstein,[7] O. Eriksson,[4] W. Eberhardt,[1] and H. A. Dürr[1]

Agreement is not bad (much better than LDA/GGA) but essentially worse than in nickel. Correlations in iron are not quite local

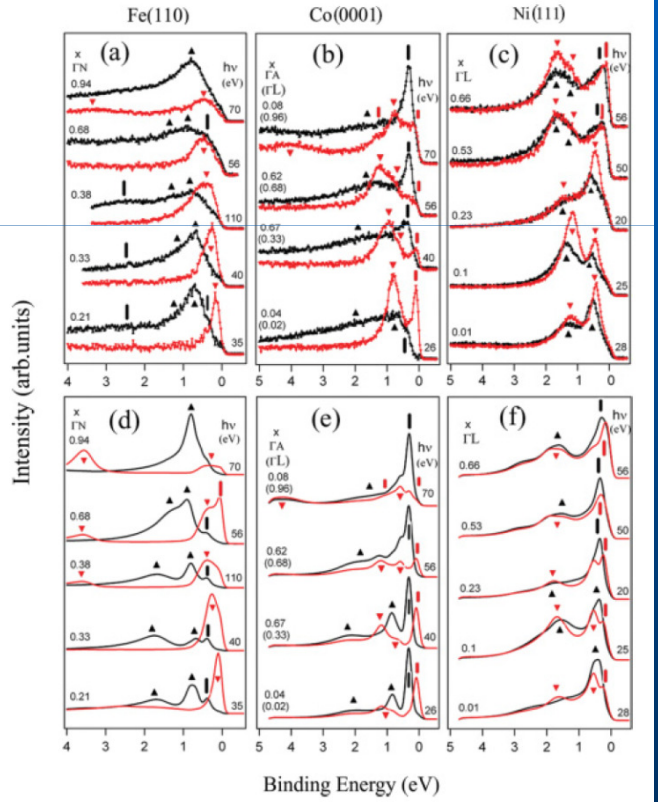


ARPES for 3d metals

PHYSICAL REVIEW B **85**, 205109 (2012)

Effects of spin-dependent quasiparticle renormalization in Fe, Co, and Ni photoemission spectra: An experimental and theoretical study

J. Sánchez-Barriga,[1] J. Braun,[2] J. Minár,[2] I. Di Marco,[3] A. Varykhalov,[1] O. Rader,[1] V. Boni,[4] V. Bellini,[5] F. Manghi,[4] H. Ebert,[2] M. I. Katsnelson,[6] A. I. Lichtenstein,[7] O. Eriksson,[3] W. Eberhardt,[1] H. A. Dürr,[1,8] and J. Fink[1,9]



Variation of U does not help too much for Fe

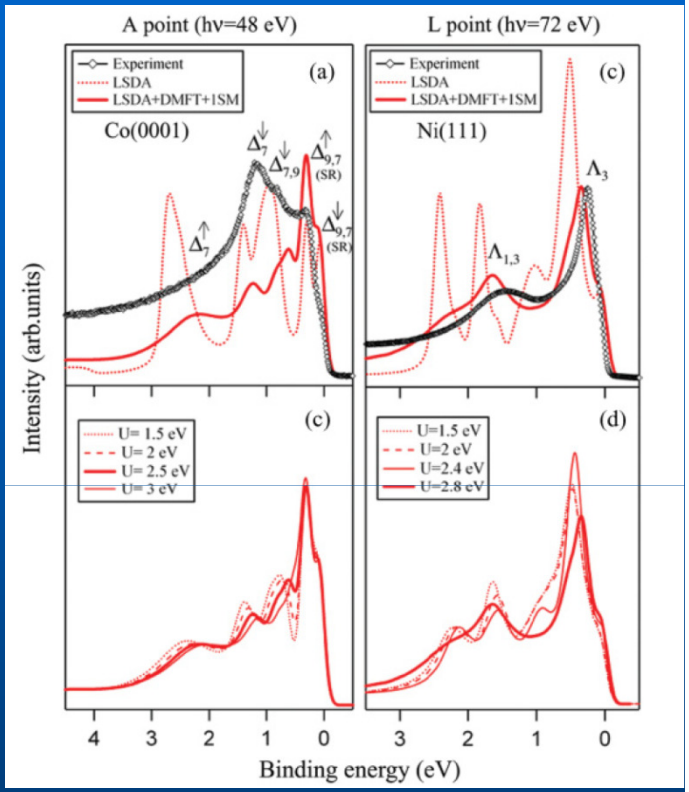
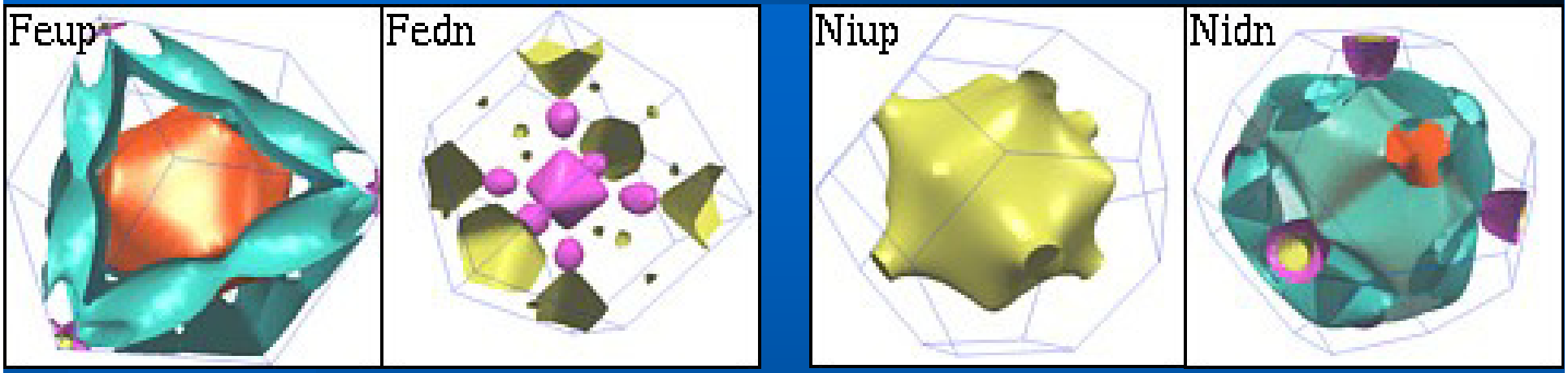


TABLE I. Values of the experimental and theoretical mass enhancement factors m^*/m_0 for majority spin states at high symmetry points of the BBZ of Fe, Co, and Ni, respectively. The theoretical values are derived for $U(\mathrm{Fe}) = 1.5$ eV, $U(\mathrm{Co}) = 2.5$ eV, $U(\mathrm{Ni}) = 2.8$ eV.

Fe			Co			Ni		
	Expt.	Theory		Expt.	Theory		Expt.	Theory
Γ	1.7	1.2	Γ	1.26	1.31	Γ	2.0	1.8
N	1.1	1.2	A	1.29	1.31	Λ	1.9	1.8

Black – spin up, red – spin down
Upper panel – exper,lower - DMFT

Why Ni is more local than Fe?



S. Hershfield ***http://www.phys.ufl.edu/fermisurface***

Nickel is almost half-metallic: majority-spin FS almost coincides with the boundaries of the Brillouin band

But the difference for minority spin is even more dramatic

Occupations for majority (minority) electrons
5 means full occupation

Fe: 4.6 (2.34) *Ni: 4.82 (4.15)*

Why Ni is more local than Fe II

Friedel oscillations originating from FS are much weaker in nickel

PHYSICAL REVIEW B, VOLUME 64, 174402

Ab initio calculations of exchange interactions, spin-wave stiffness constants, and Curie temperatures of Fe, Co, and Ni

M. Pajda,[1] J. Kudrnovský,[2,1] I. Turek,[3,4] V. Drchal,[2] and P. Bruno[1]

TABLE I. Effective Heisenberg exchange parameters J_{0j} for ferromagnetic Fe, Co, and Ni for the first 10 shells. Quantities $\mathbf{R}_{0j}$ and N_s denote, respectively, shell coordinates in units of corresponding lattice constants and the number of equivalent sites in the shell.

Fe (bcc)			Co (fcc)			Ni (fcc)		
$\mathbf{R}_{0j}$	N_s	J_{0j} (mRy)	$\mathbf{R}_{0j}$	N_s	J_{0j} (mRy)	$\mathbf{R}_{0j}$	N_s	J_{0j} (mRy)
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	8	1.432	$(\frac{1}{2}\frac{1}{2}0)$	12	1.085	$(\frac{1}{2}\frac{1}{2}0)$	12	0.206
(100)	6	0.815	(100)	6	0.110	(100)	6	0.006
(110)	12	−0.016	$(1\frac{1}{2}\frac{1}{2})$	24	0.116	$(1\frac{1}{2}\frac{1}{2})$	24	0.026
$(\frac{3}{2}\frac{1}{2}\frac{1}{2})$	24	−0.126	(110)	12	−0.090	(110)	12	0.012
(111)	8	−0.146	$(\frac{3}{2}\frac{1}{2}0)$	24	0.026	$(\frac{3}{2}\frac{1}{2}0)$	24	0.003
(200)	6	0.062	(111)	8	0.043	(111)	8	−0.003
$(\frac{3}{2}\frac{3}{2}\frac{1}{2})$	24	0.001	$(\frac{3}{2}1\frac{1}{2})$	48	−0.024	$(\frac{3}{2}1\frac{1}{2})$	48	0.007
(210)	24	0.015	(200)	6	0.012	(200)	6	−0.001
(211)	24	−0.032	$(\frac{3}{2}\frac{3}{2}0)$	12	0.026	$(\frac{3}{2}\frac{3}{2}0)$	12	−0.011
$(\frac{3}{2}\frac{3}{2}\frac{3}{2})$	8	0.187	$(2\frac{1}{2}\frac{1}{2})$	24	0.006	$(2\frac{1}{2}\frac{1}{2})$	24	0.001

As a result:

Magnons are much softer in Fe than in Ni (Curie temp. Higher but magnon frequencies lower)

	D_{ex} (meV Å^2)	T_C^{ex} (K)
Fe	280,[a] 330[b]	1044–1045
Co	580,[c, a] 510[b]	1388–1398[c]
Ni	555,[d] 422[a]	624–631

The softer magnons the stronger nonlocal e-m intercation

Exchange and Functionals

Magnetic force theorem

$$\begin{aligned} \Omega^d &= \Omega^d_{sp} - \Omega^d_{dc} \\ \Omega^d_{sp} &= -Tr\left\{\ln\left[\Sigma - G_0^{-1}\right]\right\} \\ \Omega^d_{dc} &= Tr\Sigma G - \Phi \end{aligned}$$

$$G^{-1} = G_0^{-1} - \Sigma$$

$$\Sigma = \frac{\delta\Phi}{\delta G}$$

$$\delta\Omega = \delta^*\Omega_{sp} + \delta_1\Omega_{sp} - \delta\Omega_{dc}$$

$$\delta_1\Omega_{sp} = \delta\Omega_{dc} = TrG\delta\Sigma$$

$$\delta\Omega = \delta^*\Omega_{sp} = -\delta^* Tr\ln\left[\Sigma - G_0^{-1}\right]$$

LDA+DMFT

(Lichtenstein & MIK 1997, 1998,1999; Anisimov et al 1997)

LSDA	LDA++
Density functional	Baym-Kadanoff functional
Density $\rho(\mathbf{r})$	Green-Function $G(\mathbf{r},\mathbf{r}',E)$
Potential $V_{xc}(\mathbf{r})$	Self-energy $\Sigma_i(E)$
$E_{tot} = E_{sp} - E_{dc}$	$\Omega = \Omega_{sp} - \Omega_{dc}$
$E_{sp} = \sum_{\lambda<\lambda_F} \varepsilon_\lambda$	$\Omega_{sp} = -Tr\ln[-G^{-1}]$
$E_{dc} = E_H + \int \rho V_{xc} d\mathbf{r} - E_{xc}$	$\Omega_{dc} = Tr\Sigma G - \Phi_{LW}$
Temperature:	Matsubara frequencies: real-T
in the Fermi function	for collective excitations

Exchange interactions from DMFT

Heisenberg exchange:

$$H = -\sum_{ij} J_{ij} S_i S_j$$

$$\delta\Omega = \delta^* \Omega_{sp} = \mathbf{V}_i \delta\varphi_i$$

Magnetic torque:

$$\delta \mathbf{e}_i = \delta\varphi_i \times \mathbf{e}_i$$

$$\mathbf{V}_i = 2Tr_{\omega L}\left[\Sigma_i^s \times \mathbf{G}_{ii}^s\right]$$

Exchange interactions:

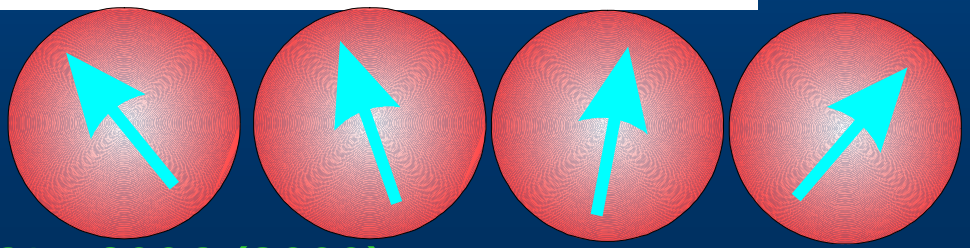
$$J_{ij} = -Tr_{\omega L}\left(\Sigma_i^s G_{ij}^{\uparrow} \Sigma_j^s G_{ji}^{\downarrow}\right)$$

$$\Sigma_i^s = \frac{1}{2}\left(\Sigma_i^{\uparrow} - \Sigma_i^{\downarrow}\right)$$

Spin wave spectrum:

$$\omega_{\mathbf{q}} = \frac{4}{M}\sum_j J_{0j}\left(1 - \cos \mathbf{q}\mathbf{R}_j\right) \equiv \frac{4}{M}[J(0) - J(\mathbf{q})]$$

Non-collinear magnetism :



MIK & Lichtenstein Phys. Rev. B 61, 8906 (2000)

Alternative view

First- and second-order smallness in theta angle!

$$\delta H = \sum_{ij} \mathrm{Tr}_{L\sigma} \left[t_{ij} c_i^+ \left(U_i^+ U_j - 1 \right) c_j \right] = \delta_1 H + \delta_2 H$$

$$\delta_1 H = \sin^2 \frac{\theta}{2} \sum_k \mathrm{Tr}_{L\sigma} \left[\left(t\left(\mathbf{k}+\mathbf{q}\right) - t\left(\mathbf{k}\right) \right) c_{\mathbf{k}}^+ c_{\mathbf{k}} \right]$$

$$\delta_2 H = \frac{1}{2} \sin\theta \sum_{ij} \mathrm{Tr}_L \left[t_{ij} c_{i\downarrow}^+ c_{j\uparrow} \right] \times \left(\exp\left(\mathrm{i}\mathbf{q}\mathbf{R}_i\right) - \exp\left(\mathrm{i}\mathbf{q}\mathbf{R}_j\right) \right).$$

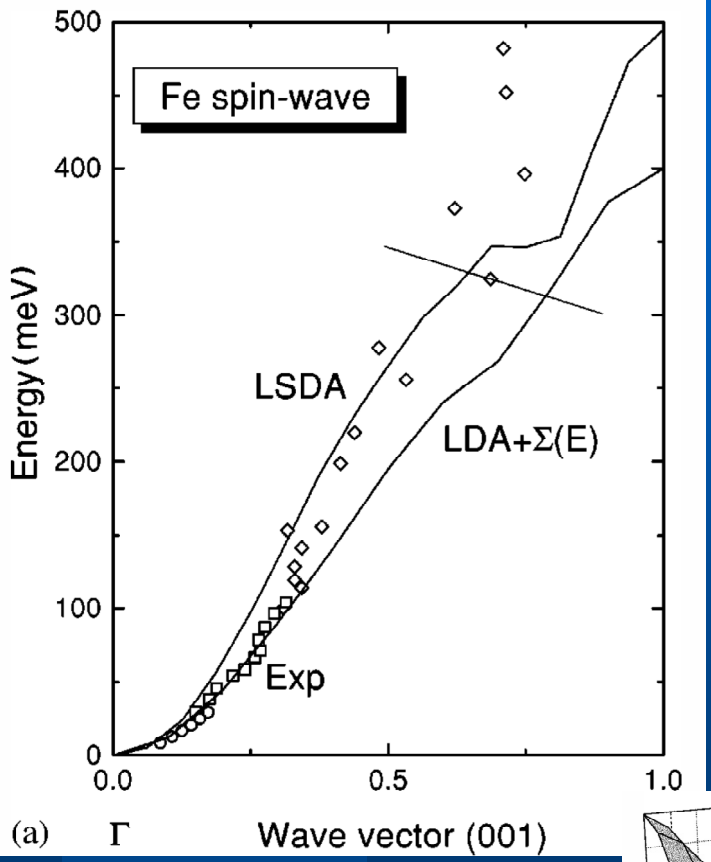
Total energy corrections by diagram technique *neglecting vertex corrections* → our exchanges

$$\omega_{\mathbf{q}} = D_{\alpha\beta} q_\alpha q_\beta, \quad \mathbf{q} \to 0$$

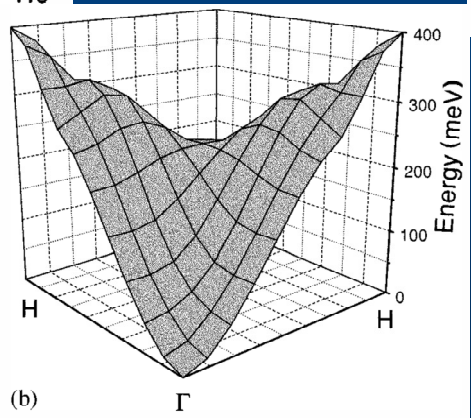
$$D_{\alpha\beta} = -\frac{2}{M} \mathrm{Tr}_{\omega L} \sum_{\mathbf{k}} \left(\Sigma^s \frac{\partial G^\uparrow\left(\mathbf{k}\right)}{\partial k_\alpha} \Sigma^s \frac{\partial G^\downarrow\left(\mathbf{k}\right)}{\partial k_\beta} \right)$$

Exact within DMFT (local self-energy!)

Results for Fe and Ni



bcc Fe



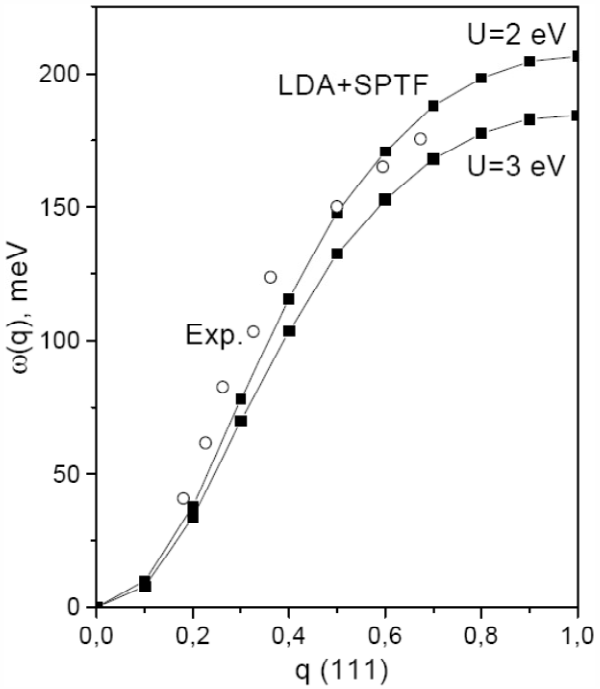


Fig. 2. Spin-wave spectrum for ferromagnetic nickel in LDA+SPTF scheme with different U and $J = 1$ eV in comparison with experimental magnon spectrum (Ref. [36]) in $\Gamma - L$ direction.

Ni

Dzialoshinskii-Moriya interactions

MIK, Kvashnin, Mazurenko & Lichtenstein, PRB 82, 100403 (2010)

LDA+U

$$\begin{aligned}\hat{H} &= \hat{H}_t + \hat{H}_u \\ &= \sum_{12} c_1^+ t_{12} c_2 + \frac{1}{2} \sum_{1234} c_1^+ c_2^+ U_{1234} c_3 c_4\end{aligned}$$

DM interactions (weak FM, etc.)

$$H_{DM} = \sum_{ij} \vec{D}_{ij} [\vec{e}_i \times \vec{e}_j]$$

Small rotations

$$\hat{R}_i = e^{i\delta\vec{\varphi}_i \vec{J}}$$

$$\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$$

Dzialoshinskii-Moriya interactions II

Starting from collinear configuration

$$\delta\hat{H}_t = \sum_{ij} c_i^+(\delta\hat{R}_i^+\hat{t}_{ij} + \hat{t}_{ij}\delta\hat{R}_j)c_j$$

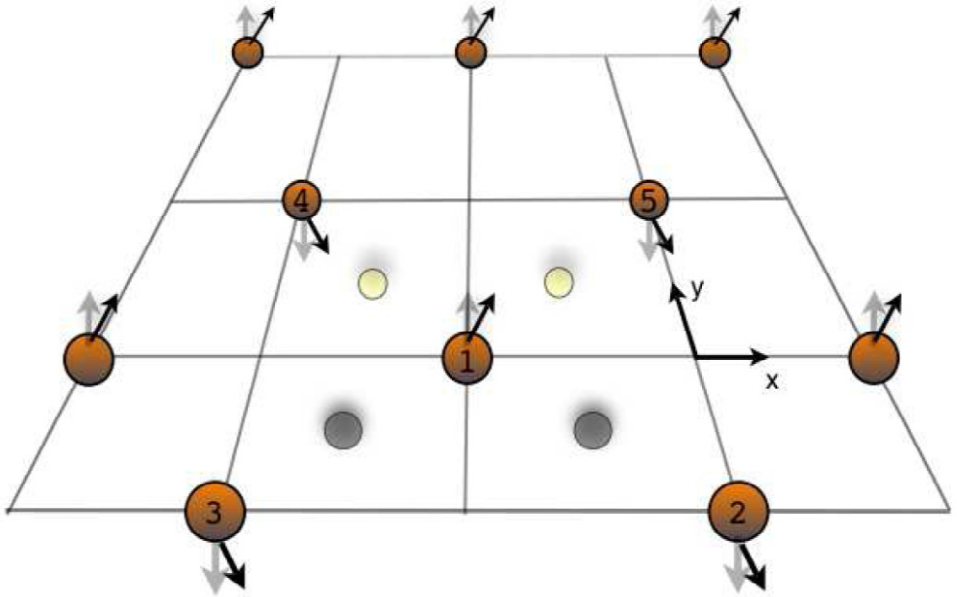
$$= -i\sum_{ij} c_i^+(\delta\vec{\varphi}_i\hat{\vec{J}}\hat{t}_{ij} - \hat{t}_{ij}\hat{\vec{J}}\delta\vec{\varphi}_j)c_j$$

$$= -\frac{i}{2}\sum_{ij} c_i^+(\delta\vec{\varphi}_i - \delta\vec{\varphi}_j)(\hat{\vec{J}}\hat{t}_{ij} + \hat{t}_{ij}\hat{\vec{J}})c_j$$

$$\vec{D}_{ij} = -\frac{i}{2}Tr_{m,\sigma}\langle c_i^+[\hat{\vec{J}}, \hat{t}_{ij}]_+ c_j\rangle = -\frac{i}{2}Tr_{m,\sigma}N_{ji}[\hat{\vec{J}}, \hat{t}_{ij}]_+$$

$$N_{ji} = \langle c_i^+ c_j\rangle = -\frac{1}{\pi}\int_{-\infty}^{E_f} ImG_{ji}(E)dE$$

Applications to La_2CuO_4



Canting angle 0.005
Exper. 0.003

TABLE II: Different contributions to Dzyaloshinskii-Moriya vector (in meV).

$\vec{R}_{1j}$	$\vec{D}_{1j}^{spin}$	$\vec{D}_{1j}^{orb}$
(1,2)	(-0.005;-0.006; 0.0)	(-0.07; -0.03; 0.0)
(1,3)	(-0.005; 0.006; 0.0)	(-0.07;0.03; 0.0)
(1,4)	(-0.005; -0.006; 0.0)	(-0.07;-0.03; 0.0)
(1,5)	(-0.005; 0.006; 0.0)	(-0.07;0.03; 0.0)

$FeBO_3$

LETTERS
PUBLISHED ONLINE: 9 FEBRUARY 2014 | DOI: 10.1038/NPHYS2859
nature physics

Measuring the Dzyaloshinskii–Moriya interaction in a weak ferromagnet

V. E. Dmitrienko[1], E. N. Ovchinnikova[2], S. P. Collins[3]*, G. Nisbet[3], G. Beutier[4], Y. O. Kvashnin[5], V. V. Mazurenko[6], A. I. Lichtenstein[7] and M. I. Katsnelson[6,8]

A novel exper. technique to measure DM vector and not only canting angle (resonant X-ray scattering)

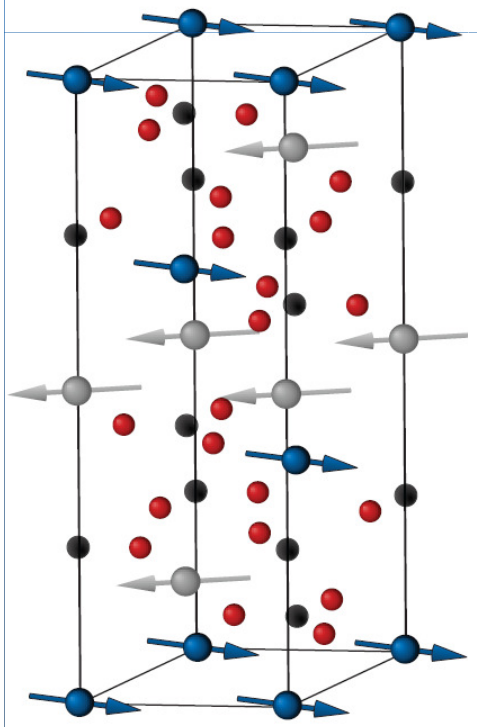


TABLE I. Calculated values of isotropic exchange interactions between magnetic moments in $FeBO_3$ (in meV). The number in parentheses denotes the coordination sphere.

$Fe^{(1)}$	$Fe^{(2)}$	$Fe^{(3)}$	$Fe^{(4)}$	$Fe^{(5)}$	$Fe^{(6)}$	$Fe^{(7)}$
10.28	0.21	0	0.54	-0.08	0	0.02

TABLE III. Parameters of Dzyaloshinskii-Moriya interaction (in meV) calculated by using Eq. (6).

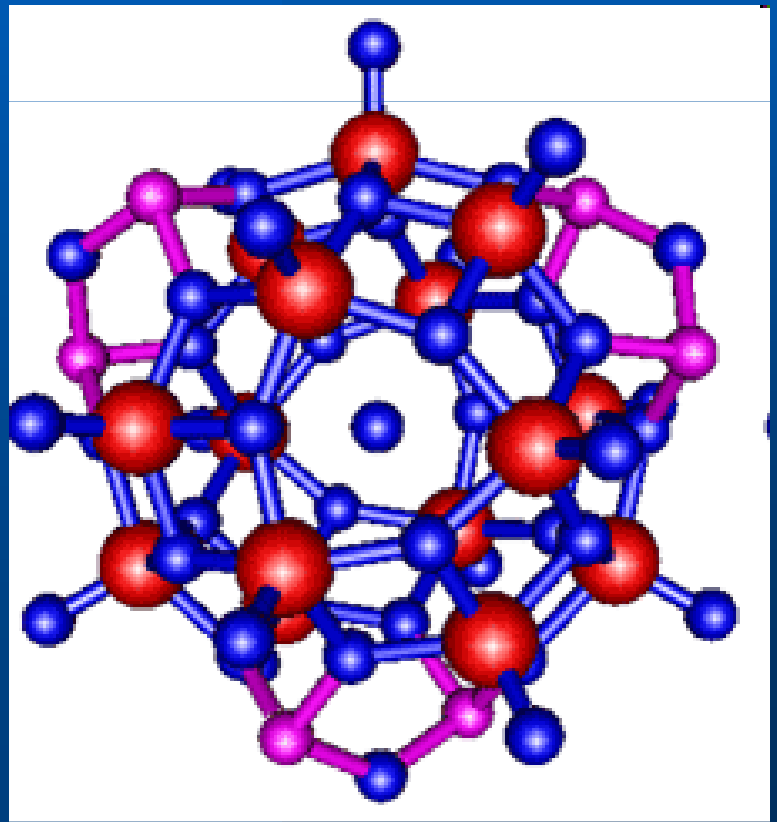
Bond $m-n$	$\mathbf{R}_{mn}$	$\mathbf{D}_{mn}$ (meV)
0-1	(1.0 ; 0.0 ; -0.904)	(-0.25; 0.0; -0.24)
0-2	(-0.5 ; $-\sqrt{3}/2$; -0.904)	(0.12 ; 0.22 ; -0.24)
0-3	(-0.5 ; $\sqrt{3}/2$; -0.904)	(0.12 ; -0.22 ; -0.24)
0-4	(-1.0 ; 0.0 ; 0.904)	(-0.25; 0.0 ; -0.24)
0-5	(0.5 ; $-\sqrt{3}/2$; 0.904)	(0.12 ; -0.22 ; -0.24)
0-6	(0.5 ; $\sqrt{3}/2$; 0.904)	(0.12 ; 0.22 ; -0.24)

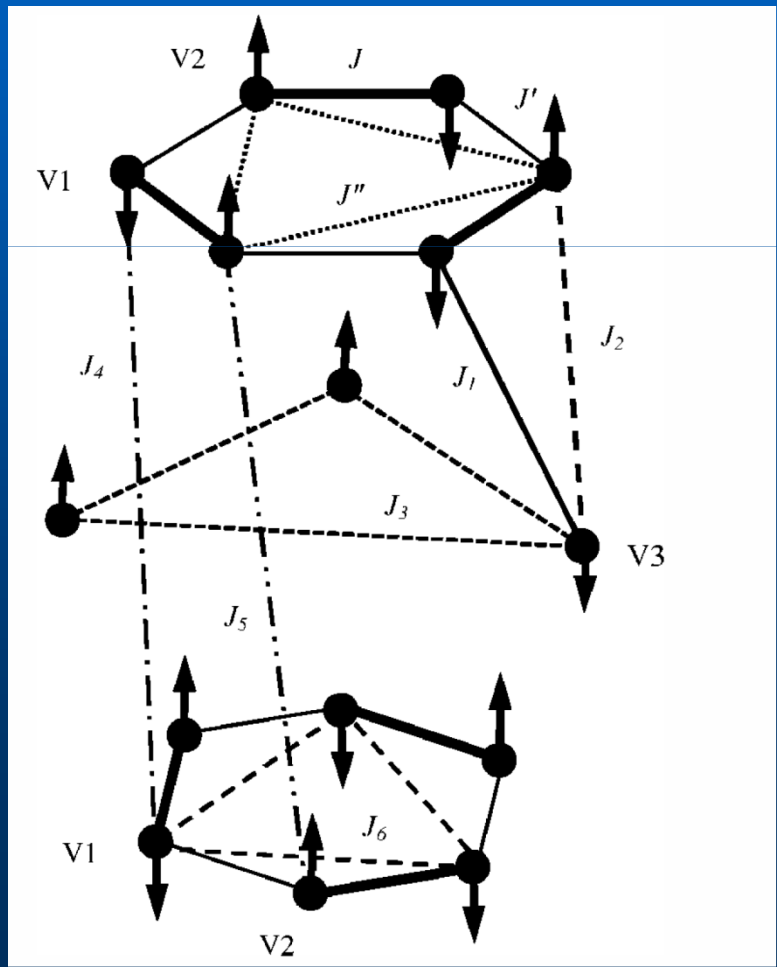
Agrees well with exper.

Molecular magnets

Example: V_{15} AFM ground state *S = 1/2*

$$V_{15}(K_6[V_{15}As_6O_{42}(H_2O)]\cdot 8H_2O)$$





LDA+U calculations

PHYSICAL REVIEW B **70**, 054417 (2004)

Electronic structure and exchange interactions in V_{15} magnetic molecules: LDA+U results

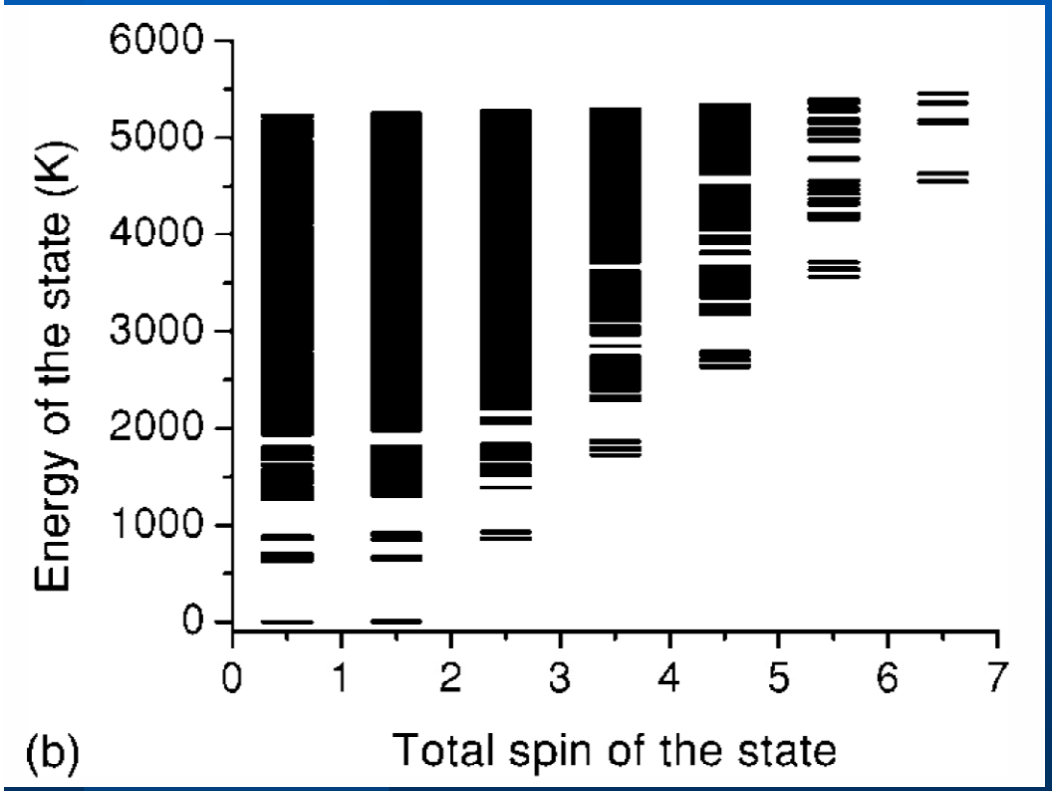
D. W. Boukhvalov,[1,2] V. V. Dobrovitski,[3] M. I. Katsnelson,[2,4] A. I. Lichtenstein,[5] B. N. Harmon,[3] and P. Kögerler[3]

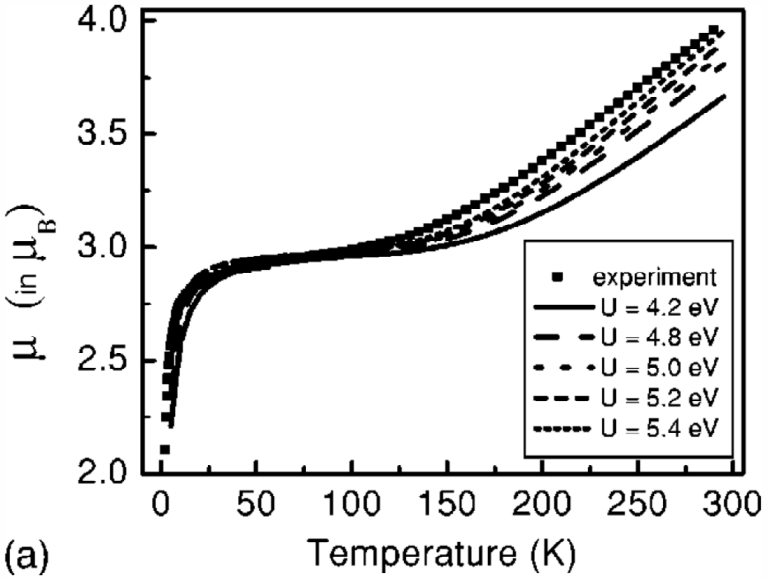
TABLE II. The exchange parameters (in Kelvin), electronic gap, and the magnetic moments of V ions for different magnetic structures of V_{15}. The calculations have been made for U=4 eV, J=0.8 eV.

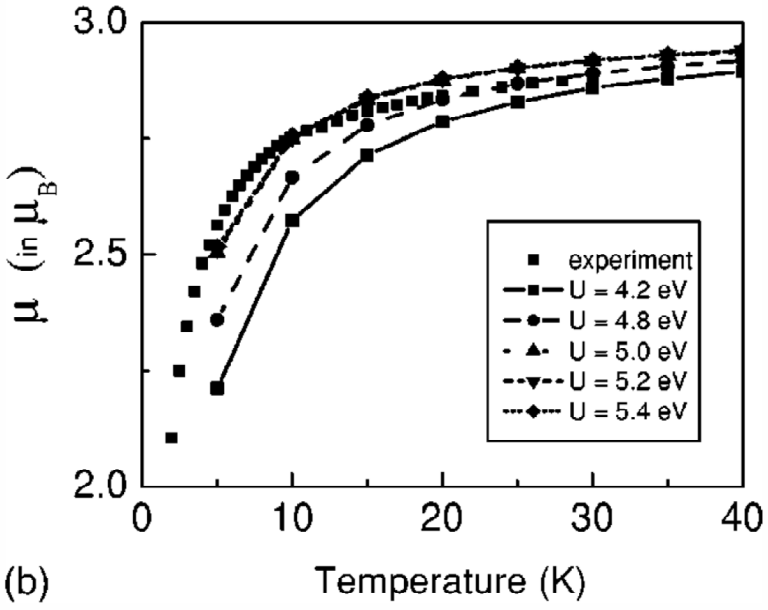
parameter	AFM1	AFM2	FM
J	−910	−905	−942
J'	−45	−46	−53
J''	−136	−139	−156
J_1	−219	−247	−255
J_2	−134	−128	−132
J_3	−5	−5	−6
J_4	−13	−12	−15
J_5	−3	−3	−3
J_6	−3	−3	−3
gap	1.08	1.02	1.16
μ_{V1}	−0.94	−0.93	−0.99
μ_{V2}	+0.91	+0.92	−0.97
μ_{V3}	−1.00	+0.97	−1.00

LDA+U calculations II

Exact diagonalization for Heisenberg model







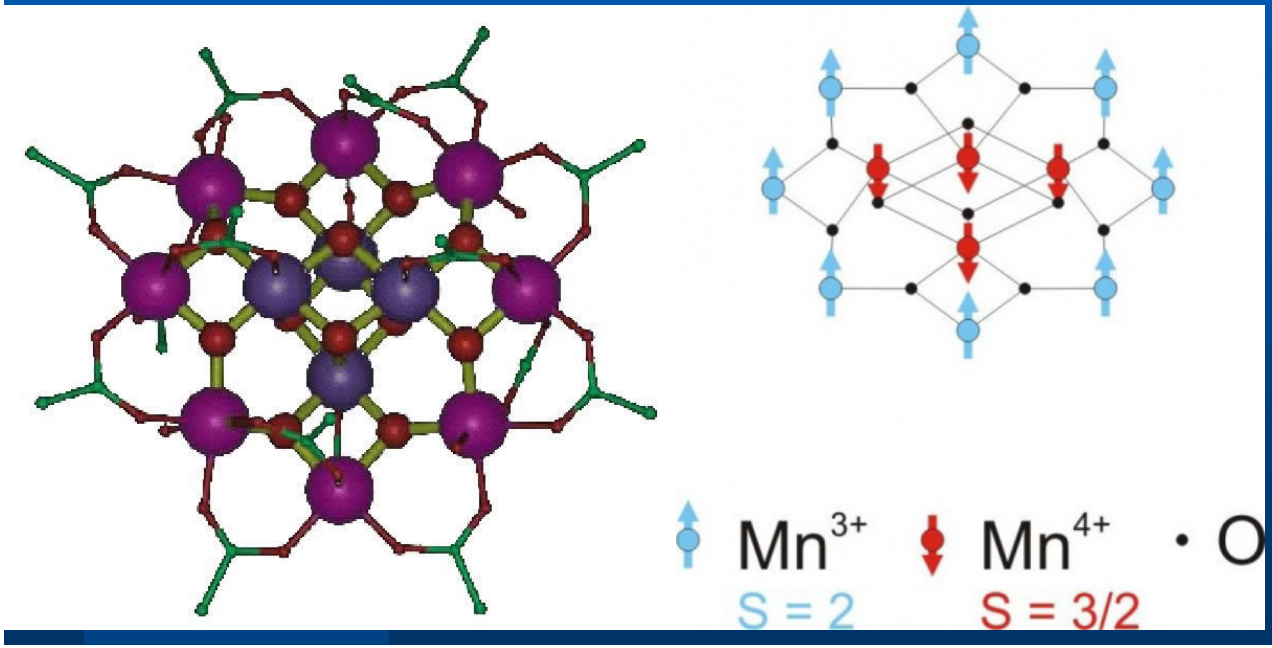
Mn_{12}: full calculations

PHYSICAL REVIEW B **00**, 004400 (2014)

First-principles modeling of magnetic excitations in Mn_{12}

V. V. Mazurenko,[1] Y. O. Kvashnin,[2,3] Fengping Jin,[4] H. A. De Raedt,[5] A. I. Lichtenstein,[6] and M. I. Katsnelson[1,7]

Motivation



The prototype molecular magnet

Dimension of Hilbert space:
$(2^{x}2+1)^{8}(2^{x}3/2+1)^{4}=10^{8}$

A real challenge!

$$[Mn_{12}O_{12}(CH_3COO)_{16}(H_2O)_4]\cdot 2CH_3COOH\cdot 4H_2O$$

Mn_{12}: full calculations II

Inelastic netron scattering data: cannot be explained without strong DM interactions (MIK, Dobrovistki & Harmon, PRB 1999)

Eight-spin model: S = ½ dimers from S=2 and S=3/2
Dimensionality of Hilbert space decreases to 10^4
Cannot be justified quantitatively!

Full LDA+U calculations plus Lanczos ED

$$\hat{H} = \sum_{ij} J_{ij} \hat{\vec{S}}_i \hat{\vec{S}}_j + \sum_{i\mu\nu} \hat{S}_i^{\mu} A_i^{\mu\nu} \hat{S}_i^{\nu} + \sum_{ij} \vec{D}_{ij} [\hat{\vec{S}}_i \times \hat{\vec{S}}_j]$$

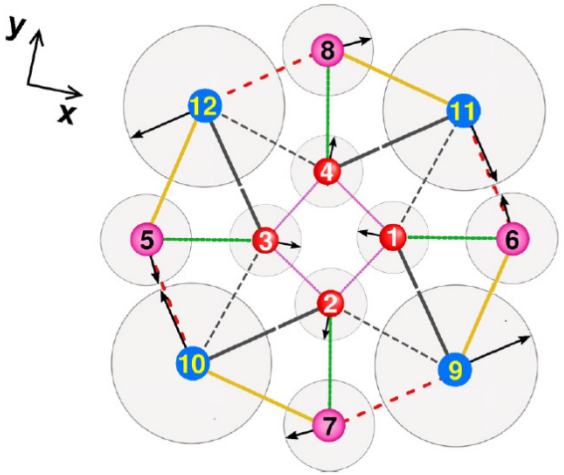


TABLE I. Intramolecular isotropic exchange interaction parameters (in meV) calculated by using the LDA + U approach. Positive sign corresponds to the antiferromagnetic coupling.

Bond (i,j)	1–6	1–11	1–9	6–9	7–9	1–4	1–3
J_{ij} (this work)	4.6	1.0	1.7	−0.45	−0.37	−1.55	−0.5
J_{ij} (Ref. [4])	4.8	1.37	1.37	−0.5	−0.5	−1.6	−0.7
J_{ij} (Ref. [26])	7.4	1.72	1.72			−1.98	

Mn_{12}: full calculations III

TABLE II. Intramolecular anisotropic exchange interaction parameters calculated by using the LDA + U approach. $\vec{R}_{ij}$ is a radius vector connecting ith and jth atoms (in units of $a = 17.31$ Å).

Bond (i, j)	$\vec{R}_{ij}$	$\vec{D}_{ij}$ (meV)
2–7	(0.03; −0.16; 0.0)	(−0.008; −0.013; −0.002)
4–8	(−0.03; 0.16; 0.0)	(0.008; 0.013; −0.002)
1–6	(0.16; 0.03; 0.0)	(−0.013; 0.008; −0.002)
3–5	(−0.16; −0.03; 0.0)	(0.013; −0.008; −0.002)
1–11	(0.06; 0.18; 0.07)	(−0.020; 0.03; −0.055)
3–10	(−0.06; −0.18; 0.07)	(0.020; −0.03; −0.055)
2–9	(0.18; −0.06; −0.07)	(−0.03; −0.020; −0.055)
4–12	(−0.18; 0.06; −0.07)	(0.03; 0.020; −0.055)
1–9	(0.11; −0.16; 0.04)	(0.020; 0.014; 0.03)
3–12	(−0.11; 0.16; 0.04)	(−0.020; −0.014; 0.03)
2–10	(−0.16; −0.11; −0.04)	(−0.014; 0.020; 0.03)
4–11	(0.16; 0.11; −0.04)	(0.014; −0.020; 0.03)
6–9	(−0.04; −0.18; 0.04)	(−0.006; −0.004; −0.012)
5–12	(0.04; 0.18; 0.04)	(0.006; 0.004; −0.012)
7–10	(−0.18; 0.04; −0.04)	(0.004; −0.006; −0.012)
8–11	(0.18; −0.04; −0.04)	(−0.004; 0.006; −0.012)
7–9	(0.15; 0.1; −0.07)	(0.020; −0.004; 0.012)
8–12	(−0.15; −0.1; −0.07)	(−0.020; 0.004; 0.012)
6–11	(−0.1; 0.15; 0.07)	(−0.004; −0.020; 0.012)
5–10	(0.1; −0.15; 0.07)	(0.004; 0.020; 0.012)
4–1	(−0.10; 0.06; 0.11)	(−0.014; 0.005; −0.013)
1–2	(−0.06; −0.10; 0.11)	(−0.005; −0.014; −0.013)
3–4	(0.07; 0.1; 0.11)	(0.005; 0.014; −0.013)
2–3	(−0.10; 0.07; −0.11)	(0.014; −0.005; −0.013)
1–3	(−0.16; −0.03; 0.0)	(−0.006; 0.030; 0)
2–4	(−0.04; 0.17; 0.0)	(−0.030; −0.006; 0)

Plus anisotropy tensors...

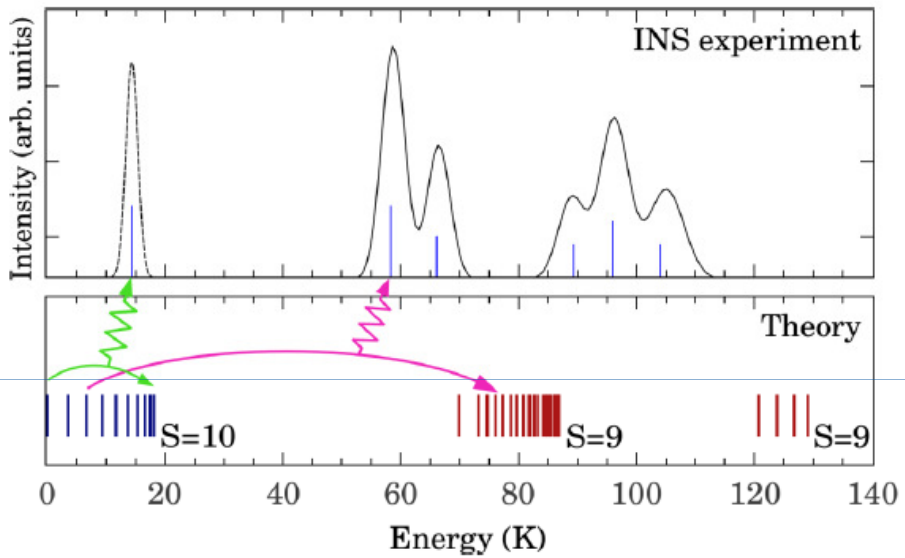


FIG. 2. (Color online) Schematic comparison of the theoretical spectrum obtained by diagonalizing Eq. (1) and INS spectrum taken from Ref. [12] (Figs. 6 and 8 therein). The arrows denote the intra- and interband transitions that correspond to the excitations observed in the INS experiment.

No fitting parameters at all – not so bad!

α-γ transformation in Fe: role of magnetism

Zener: bcc phase of Fe is stabilized by magnetism (DOS peaks destabilizing crystal lattice are moved from the Fermi energy)

SCIENTIFIC REPORTS

OPEN

SUBJECT AREAS:
MAGNETIC PROPERTIES AND MATERIALS
ELECTRONIC PROPERTIES AND MATERIALS

Received
17 March 2014

Accepted
6 June 2014

Published
7 July 2014

Electronic correlations determine the phase stability of iron up to the melting temperature

I. Leonov[1], A. I. Poteryaev[2,3], Yu. N. Gornostyrev[2,3], A. I. Lichtenstein[4], M. I. Katsnelson[5,6], V. I. Anisimov[2,6] & D. Vollhardt[1]

[1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135

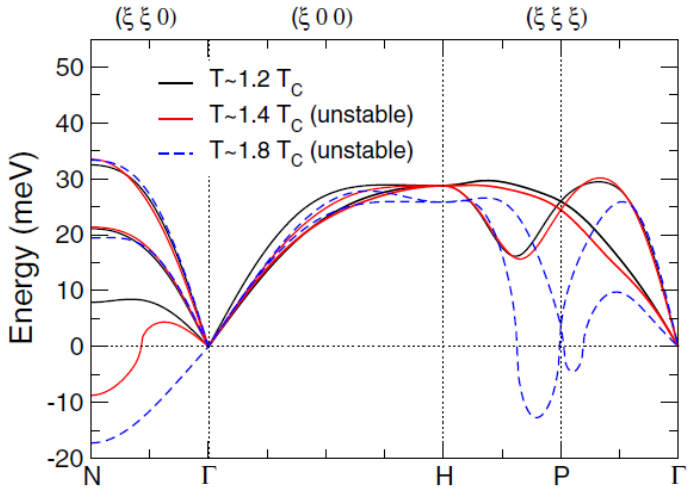


Figure 2 | Calculated phonon dispersions of paramagnetic bcc iron near the α-to-γ and γ-to-δ phase transitions for different temperatures.

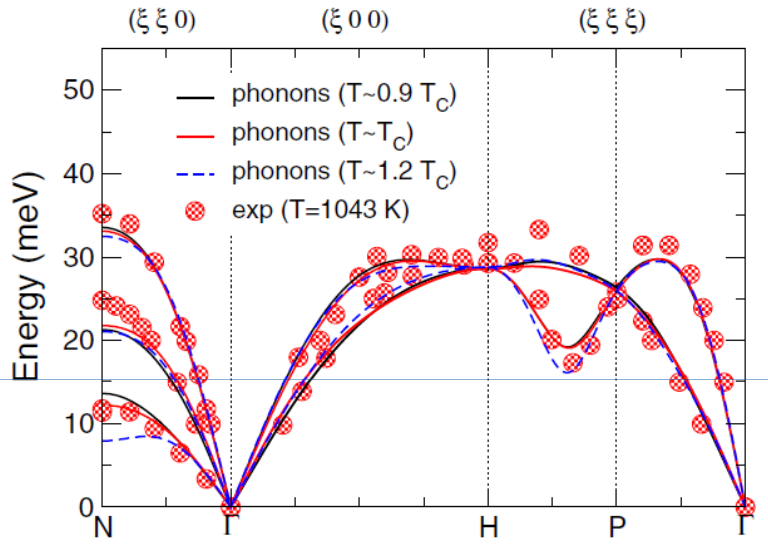


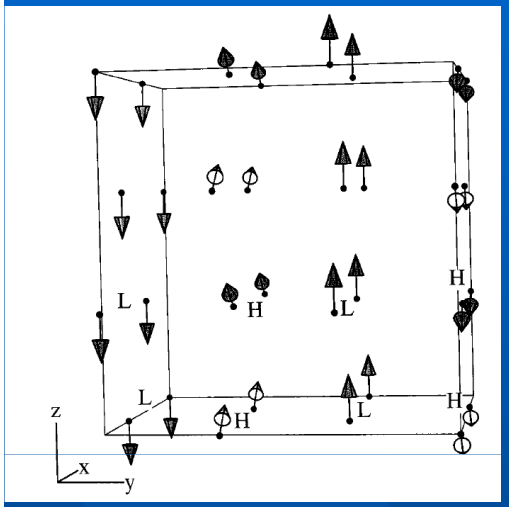
Figure 1 | Calculated phonon dispersion curves for bcc iron near the Curie temperature T_C. The results are compared with neutron inelastic scattering measurements at 1043 K.

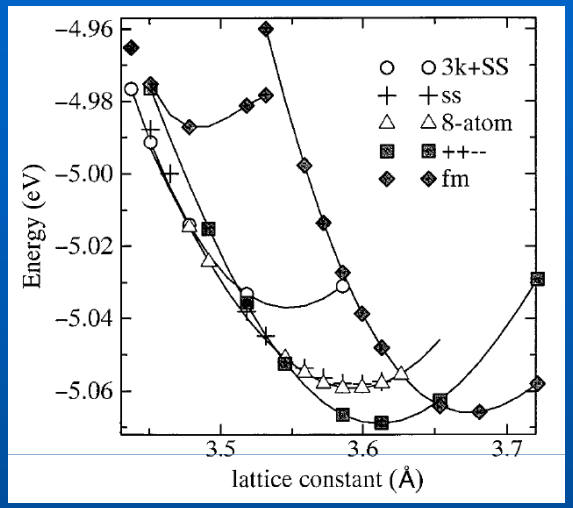
Dynamical instability as a result of disappearance of magnetic moments

DMFT is essential!!!

Frustrated magnetism in γ-Fe

Antropov et al, PRL 1995 - first practical application of ab initio SD





Many magnetic structures with very close energies (frustration); strong dependence on lattice constants

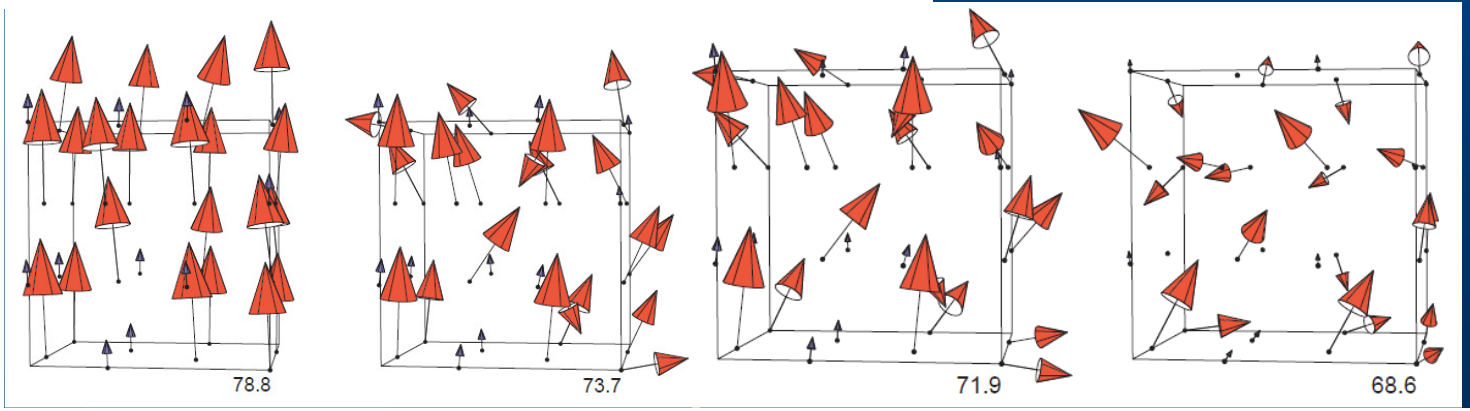
Also in Fe-Ni alloys

Origin of the Invar effect in iron–nickel alloys

NATURE | VOL 400 | 1 JULY 1999

Mark van Schilfgaarde*, I. A. Abrikosov† & B. Johansson†

Application to Invar problem



Fe-Ni

Atomic volumes in a.u.

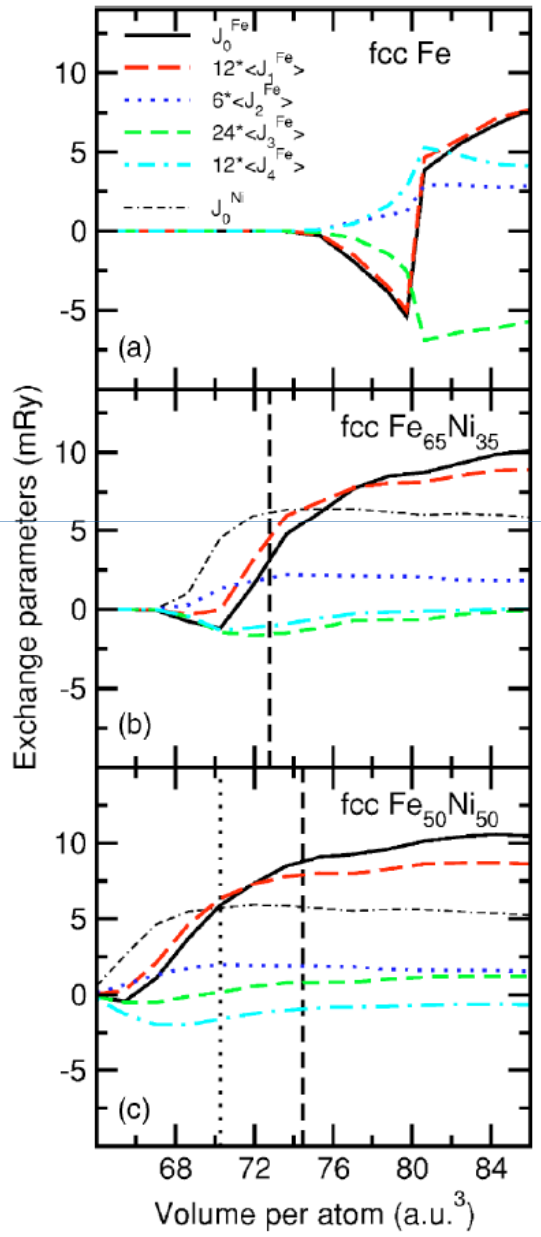
Frustrated magnetism in γ-Fe II

PHYSICAL REVIEW B **71**, 054402 (2005)

Origin of magnetic frustrations in Fe-Ni Invar alloys

A. V. Ruban,[1] M. I. Katsnelson,[2,3] W. Olovsson,[3] S. I. Simak,[3,4] and I. A. Abrikosov[4]

FIG. 1. (Color online) Effective exchange parameters for Fe J_0^{Fe} (thick black solid line) and Ni J_0^{Ni} (thin black dot-double dashed line), as well as average pair exchange parameters $\langle J_p^{\mathrm{Fe}}\rangle = (1/z_p)\Sigma_{j\in p}[cJ_{0j}^{\mathrm{Fe\text{-}Fe}} + (1-c)J_{0j}^{\mathrm{Fe\text{-}Ni}}]$ for the first (red long-dashed line), second (dark blue dotted line), third (green short-dashed line), and fourth (light blue dot-dashed line) shells in (a) fcc Fe, (b) $Fe_{65}Ni_{35}$ alloy, and (c) $Fe_{50}Ni_{50}$ alloy as a function of the volume per atom. z_p is the coordination number of the pth coordination shell, and c is the Fe concentration. In the figure $\langle J_p^{\mathrm{Fe}}\rangle$ are multiplied with z_p in order to show their actual contribution to J_0^{Fe}. Vertical dashed lines in (b) and (c) show calculated equilibrium volume at corresponding concentrations. The vertical dotted line in (c) indicates estimated volume where fcc $Fe_{50}Ni_{50}$ alloy shows Invar behavior under pressure, Ref. 5. Calculations are done within the coherent potential approximation (see text for the discussion).



Total exchange is determined by J_1; long-range oscillating tail favors frustrations. J_1 strongly depend on volume

Frustrated magnetism in γ-Fe III

Okatov, Gornostyrev, Lichtenstein & MIK, PR B 84, 214422 (2011)

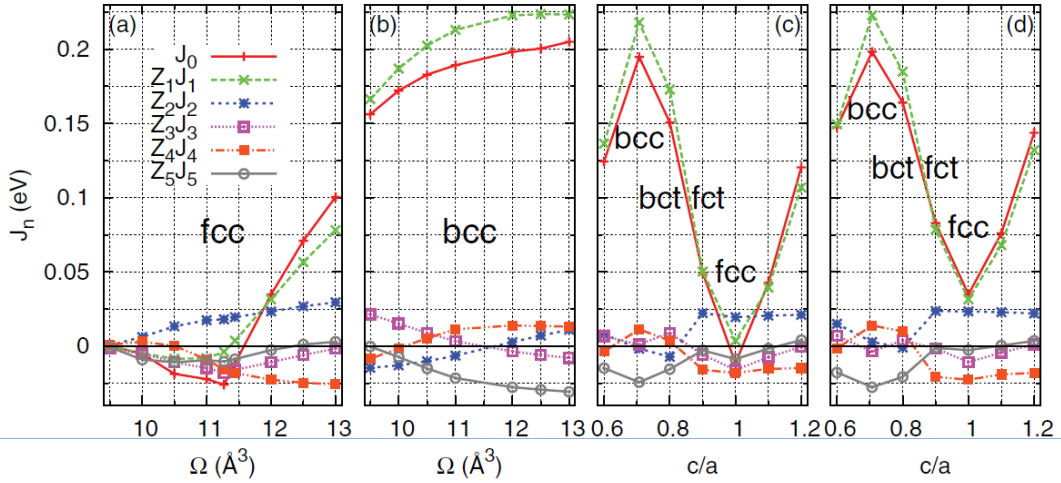


FIG. 3. (Color online) Exchange parameters J_n for $n = 1,2,3,4,5$ for different lattice parameters: dependence J_n on a volume of fcc (a) and bcc (b) Fe; dependence J_n on (c/a) at fixed volumes $\Omega = 11.44$ Å^3 (c) and $\Omega = 12.0$Å^3 (d), respectively.

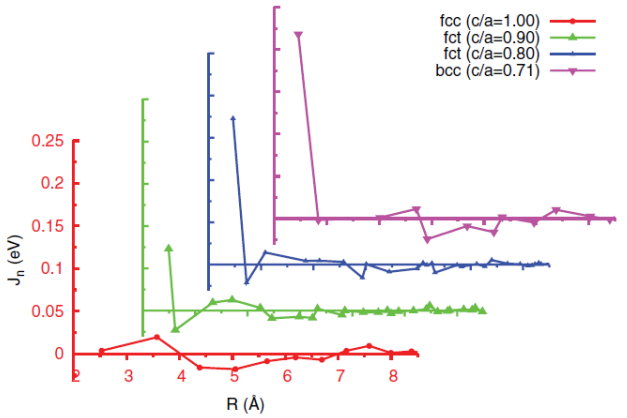


FIG. 5. (Color online) The exchange parameter as a function of interatomic distance to the nth neighbor $J_n(R_n)$ for different c/a ratios.

Exchange parameters are very sensitive not only to volume but also to tetragonal deformations – stabilization of fct phase

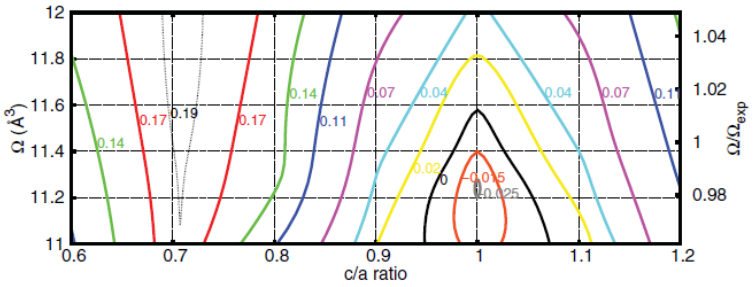
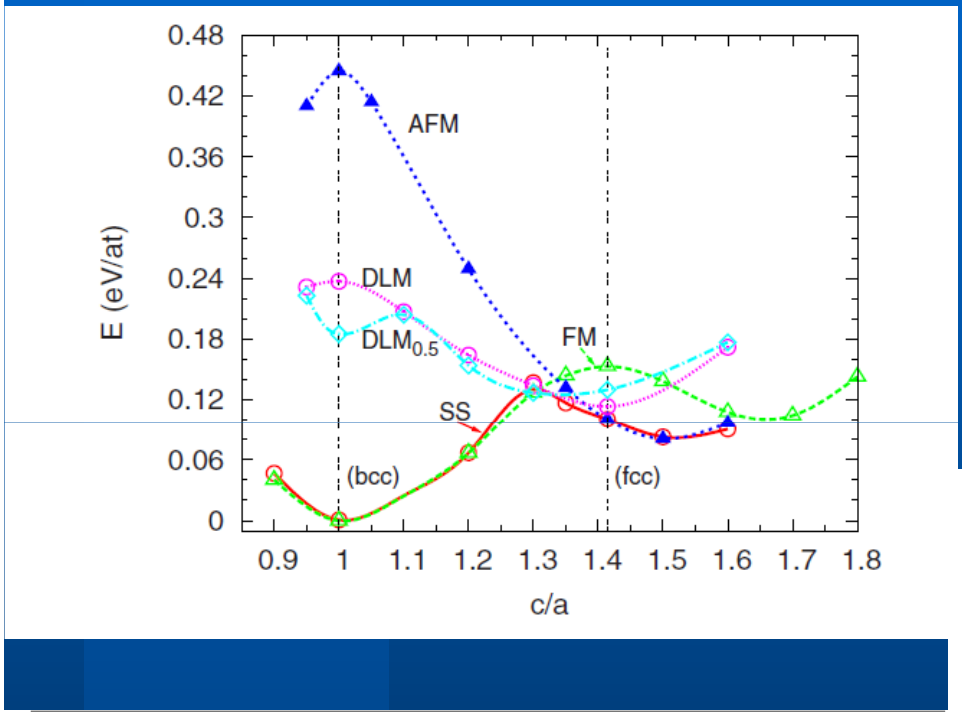


FIG. 4. (Color online) Dependence of the total exchange parameter J_0 on volume Ω and c/a ratio as a contour plot $J_0(\Omega, c/a)$.

Magnetism along the Bain path in Fe

Okatov, Kuznetsov, Gornostyrev, Urtsev & MIK, PR B 79, 094011 (2011)



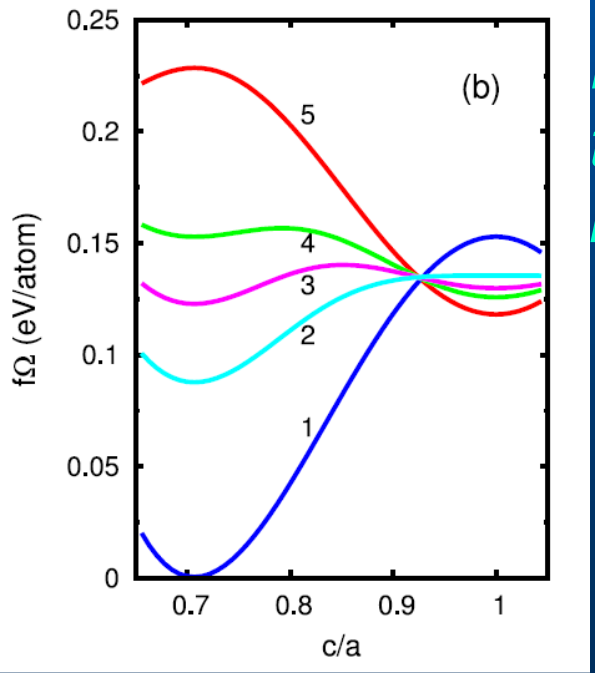
Transition without barrier starting from FM state

A very important consequences for morphology of the transformation

J. Phys.: Condens. Matter **25** (2013) 135401 (9pp) doi:10.1088/0953-8984/25/13/135401

Effect of magnetism on kinetics of $\gamma-\alpha$ transformation and pattern formation in iron

I K Razumov[1,2], Yu N Gornostyrev[1,2] and M I Katsnelson[3]



Free energy to be used in phase field

1-5: T=0K; 700; 1000; 1300; ∞ Magnetic temperature

Carbon impurity in γ-Fe: Role of exchange interactions

PRL 99, 247205 (2007) PHYSICAL REVIEW LETTERS week ending 14 DECEMBER 2007

Magnetism and Local Distortions near Carbon Impurity in γ-Iron

D. W. Boukhvalov
Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 ED Nijmegen, the Netherlands
Institute of Metal Physics, Russian Academy of Sciences, Ural Division, Ekaterinburg 620041, Russia

Yu. N. Gornostyrev
Institute of Metal Physics, Russian Academy of Sciences, Ural Division, Ekaterinburg 620041, Russia
Institute of Quantum Materials Science, Ekaterinburg 620107, Russia

M. I. Katsnelson
Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 ED Nijmegen, the Netherlands

A. I. Lichtenstein
Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany
(Received 25 June 2007; published 13 December 2007)

Long-standing problem: solution enthalpy of C in γ-Fe

Solution: local tetragonal distortions and local FM ordering

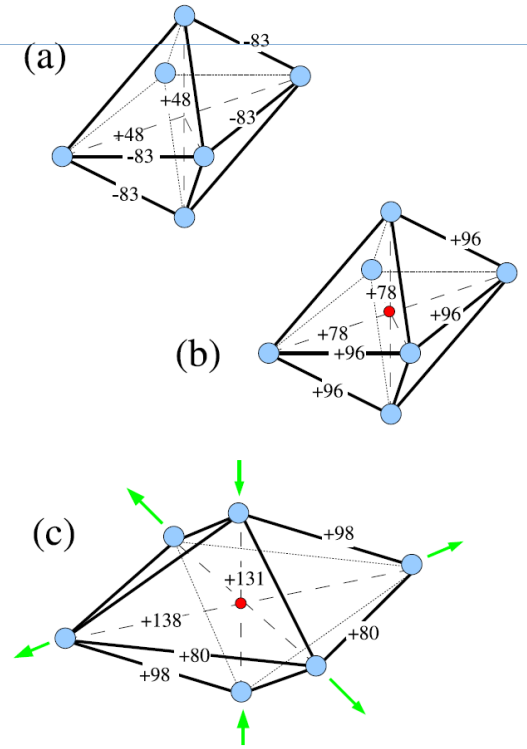


FIG. 2 (color online). Exchange parameters (in K) for different Fe-Fe pairs in original fcc lattice (a); in fcc lattice with carbon interstitial impurity without (b) and with (c) relaxation taken into account. Arrows indicate direction of atomic displacements during the relaxation.

Solution enthalpy 0.55 eV (exp. 0.4 eV)

Deformations make C-C interaction much stronger (not pure dilatation centers)

Beyond the talk

- *Finite-temperature effects*
- *Ab initio spin dynamics for real systems*
- *Intermediate level: TB spin dynamics*
- *And many, many specific applications to real materials*
- *Magnetic interactions out of equilibrium*

Non-equilibrium magnetic interactions in strongly correlated systems

Annals of Physics 333 (2013) 221–271

A. Secchi [a,*], S. Brener [b], A.I. Lichtenstein [b], M.I. Katsnelson [a]

Collaboration

Recent:

A. Lichtenstein and S. Brener (Hamburg)
Yu. Gornostyrev, S. Okatov, A. Kuznetsov (Ekaterinburg)
A. Secchi and A. Rudenko (Nijmegen)
V. Mazurenko (Ekaterinburg)
Ya. Kvashnin and O. Eriksson (Uppsala)
and many other people involved in development of the formalism and calculations for specific materials in 1987-2013, esp. V. Antropov (Ames) and D. Boukhvalov (Seoul)

Thank you for your attention