Gutzwiller wave functions for itinerant ferromagnetism of transition metals

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Collaboration

Theory	J. Bünemann, Marburg; W. Weber, Dortmund
Experiment	R. Claessen, V. Strocov, Würzburg; A. Kakizaki, S. Shin, Tokyo; D. Ehm, G. Nicolay, Saarbrücken; A. Kimura, Hiroshima

Overview

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1. Basic experimental results

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2. Stoner–Slater theory: band magnetism

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6. Results for nickel

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7. Summary

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- g-factor is purely spin, $g \approx 2$;
- magnetic order sets in at the Curie temperature T_C with

$$T_C = \mathcal{O}\left(10^3 \mathrm{K}\right)$$

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2. itinerant $3d$ electrons are responsible for the magnetism (contribution from $4s$ and $4p$ is small);
3. large values for the Curie temperature can only be understood from the competition between
   - the electrons' kinetic energy (bandwidth $W = \mathcal{O}(\text{eV})$)
   - the electrons' potential energy (mutual Coulomb repulsion $U = \mathcal{O}(\text{eV})$).

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2.1 Starting point: non-interacting electrons

$$\hat{H}_0 = \sum_{\vec{l},\vec{m}} \sum_{(b\sigma),(b'\sigma')} t_{\vec{l},\vec{m}}^{b\sigma,b'\sigma'} \hat{c}_{\vec{l},b\sigma}^{+} \hat{c}_{\vec{m},b'\sigma'} = \sum_{\vec{k}} \sum_{b\sigma} \epsilon(\vec{k},b) \hat{d}_{\vec{k},b\sigma}^{+} \hat{d}_{\vec{k},b\sigma}$$

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Density of states per spin direction:

$$D_\sigma(E) = \sum_{\vec{k},b} \delta\left(\epsilon(\vec{k},b) - E\right)$$

In the ground state, all states are filled up to the Fermi energy E_F:

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- metal (OK);
- purely electronic g-factor, $g \approx 2$ (OK);
- paramagnetic (not OK).

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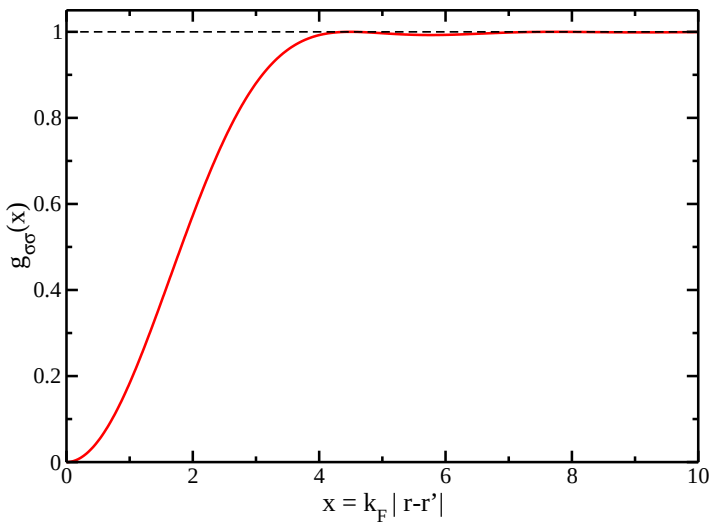

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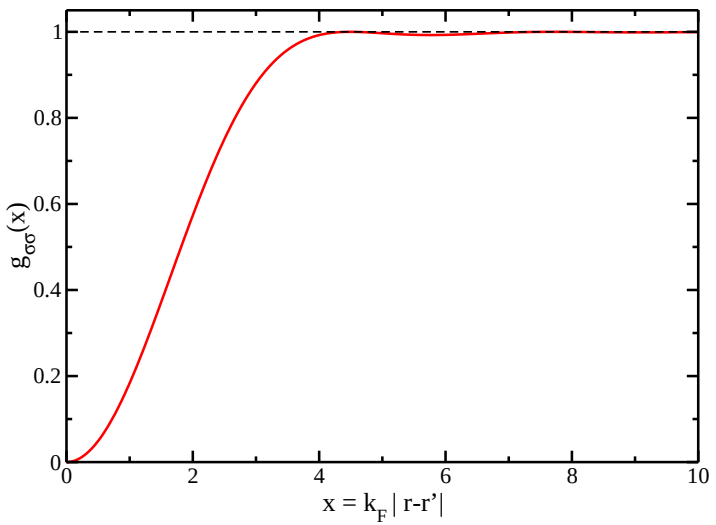

The Coulomb interaction between electrons with like spins is smaller than the Coulomb interaction between electrons with different spins because of the Pauli or exchange hole.

Energy difference: “exchange energy”

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U measures the strength of the Coulomb interaction,
$D_\sigma(E_F) \sim 1/W$ measures the importance of the kinetic energy.

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- Conclusion:
  A large density of states at the Fermi energy promotes ferromagnetism (Stoner criterion).

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For spherical symmetry and d electrons, the Coulomb parameters U may be expressed in terms of 3 Racah parameters A, B, C.
Atomic eigenstates $|\Gamma\rangle$

$$\hat{H}_{\mathrm{at}}|\Gamma\rangle = E_\Gamma|\Gamma\rangle$$

The ground state $|\Gamma\rangle$ has maximum spin: atomic physics naturally provides magnetic moments.

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Effective theory:

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For $J_{\vec{l},\vec{m}} > 0$: anti-ferromagnetism for $T < T_{\text{Néel}}$
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Physical picture:

- Pre-formed moments develop long-range order;
- For $T > T_c = \mathcal{O}(J)$: moments decouple, long-range order is lost but the local moments persist.

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- coupling of moments due to electrons' motion –
  long-range order at low temperatures.

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Combination of both (extreme) viewpoints:

$$\hat{H} = \hat{H}_0 + \sum_{\vec{l}} \hat{H}_{\vec{l},\mathrm{at}}$$

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Electron's local Coulomb interaction (starting point of Hund-Heisenberg theory)

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'Solution': use approximate methods

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$$|\Psi_{\mathrm{G}}\rangle = \hat{P}_{\mathrm{G}} |\Psi_0\rangle$$

- Idea: the correlator $\hat{P}_{\mathrm{G}}$ reduces energetically unfavorable configurations in $|\Psi_0\rangle$ (suppression of charge fluctuations)

4 Gutzwiller variational wave functions

- Choice of the correlator:

$$\hat{P}_{\mathrm{G}} = \prod_{\vec{l}} \prod_{\Gamma} \lambda_{\vec{l},\Gamma}^{\hat{m}_{\vec{l},\Gamma}} = \prod_{\vec{l}} \prod_{\Gamma} \left[1 + (\lambda_{\vec{l},\Gamma} - 1) \hat{m}_{\vec{l},\Gamma} \right] = \prod_{\vec{l}} \sum_{\Gamma} \lambda_{\vec{l},\Gamma} \hat{m}_{\vec{l},\Gamma}$$

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- The operators

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- The quantities $\lambda_{\vec{l},\Gamma}$ are real variational parameters; further parameters may be contained in $|\Psi_0\rangle$, e.g., the magnetization.

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- Task: calculate expectation values with $|\Psi_G\rangle$;
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- This is a

difficult many-body problem!

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- Important steps:
  1. Develop a diagrammatic perturbation theory with 'Vertices' $x_{\vec{l},\Gamma_1,\Gamma_2}$ and 'Lines' $\widetilde{P}^0_{\sigma,\sigma'}(\vec{l},\vec{m})$.
  2. The expansion parameters $x_{\vec{l},\Gamma_1,\Gamma_2}$ can be chosen such that at least four lines meet at every inner vertex, there are no Hartree bubble diagrams, and the single-particle density matrices obey

$$\widetilde{P}^0_{\sigma,\sigma'}(\vec{l},\vec{l}) = 0\,. \qquad (*)$$

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  3. In the limit $Z \to \infty$, all skeleton diagrams collapse in position space, i.e., they have the same lattice site index. As a consequence of Eq. (*), they all vanish and not a single diagram must be calculated.

4 Gutzwiller variational wave functions

- The results remain non-trivial because of the contributions from the external vertices, e.g., the sites $\vec{i}$ and $\vec{j}$ in the one-particle density matrix $P_{\sigma,\sigma'}(\vec{i},\vec{j})$.

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- Effective electron transfer matrix elements (cubic symmetry)

$$\tilde{t}_{\vec{l}\neq\vec{m}}^{\,b\sigma,b'\sigma'} = \sqrt{q_{\vec{l},b\sigma}} \sqrt{q_{\vec{m},b'\sigma'}} \, t_{\vec{l}\neq\vec{m}}^{b\sigma,b'\sigma'}$$

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- Landau's idea of quasi-particles

  Fermi gas + hole excitation $\xrightarrow{\text{interactions}}$ Fermi liquid + quasi-hole excitation

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  - Fermi gas $|\Psi_0\rangle$: Fermi-gas ground state

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    $|\Psi_{\mathrm{G}}(\vec{p},b\sigma)\rangle = \hat{P}_{\mathrm{G}}\hat{c}_{\vec{p},b\sigma}|\Psi_0\rangle$: quasi-hole excitation
- Energy of Landau-Gutzwiller quasi-particles

$$E^{\mathrm{QP}}(\vec{p},b\sigma) := \frac{\langle\Psi_{\mathrm{G}}(\vec{p},b\sigma)|\hat{H}|\Psi_{\mathrm{G}}(\vec{p},b\sigma)\rangle}{\langle\Psi_{\mathrm{G}}(\vec{p},b\sigma)|\Psi_{\mathrm{G}}(\vec{p},b\sigma)\rangle} - E_0^{\mathrm{var}}$$

$$\overset{Z=\infty}{=} \widetilde{\epsilon}(\vec{p},b\sigma) + \mu_{b\sigma} - E_{\mathrm{F}}$$

$\widetilde{\epsilon}(\vec{p},b\sigma)$: dispersion relation of $\hat{H}_0^{\mathrm{eff}}$.

5 Generic two-band model

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$$\begin{aligned}\hat{H}_{\text{at}} &= U \sum_b \hat{n}_{b,\uparrow}\hat{n}_{b,\downarrow} + U' \sum_{\sigma\sigma'} \hat{n}_{1,\sigma}\hat{n}_{2,\sigma'} - J \sum_\sigma \hat{n}_{1,\sigma}\hat{n}_{2,\sigma} \\ &\quad + J \sum_\sigma \hat{c}^+_{1,\sigma}\hat{c}^+_{2,-\sigma}\hat{c}_{1,-\sigma}\hat{c}_{2,\sigma} + J_c \left(\hat{c}^+_{1,\uparrow}\hat{c}^+_{1,\downarrow}\hat{c}_{2,\uparrow}\hat{c}_{2,\downarrow} + \text{h.c.}\right)\end{aligned}$$

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- Properties:
  - 16 states per atom
  - cubic symmetry: $J_c = J$, $U - U' = 2J$
  - two parameters: Hubbard-U as in the one-band case, Hund's rule coupling J

5 Generic two-band model

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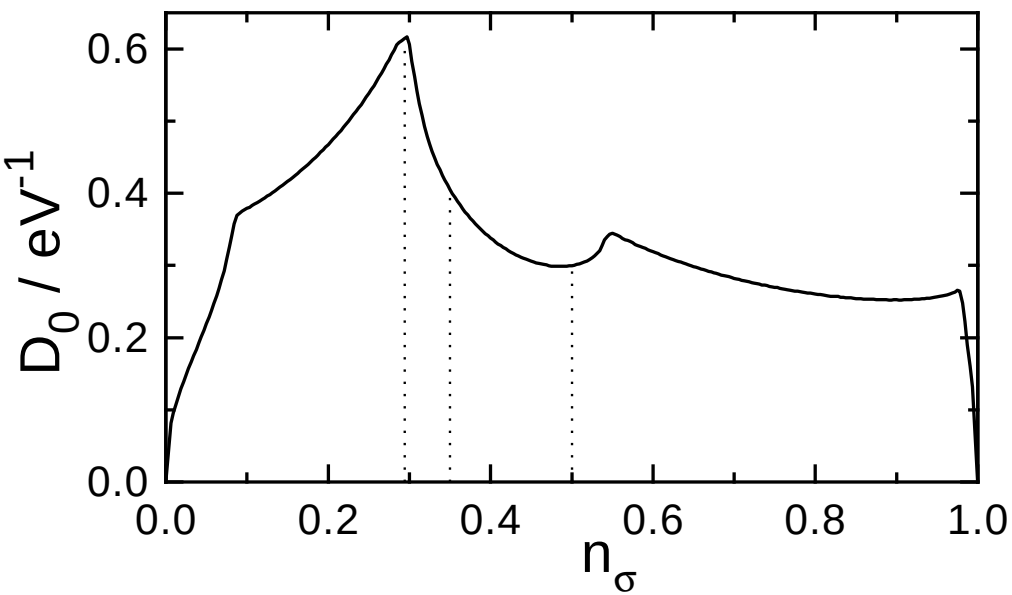
- 'Generic' density of states with no 'perfect nesting' instabilities, no excessive peaks
  Density of states at the Fermi energy (bandwidth $W = 6.6$ eV)



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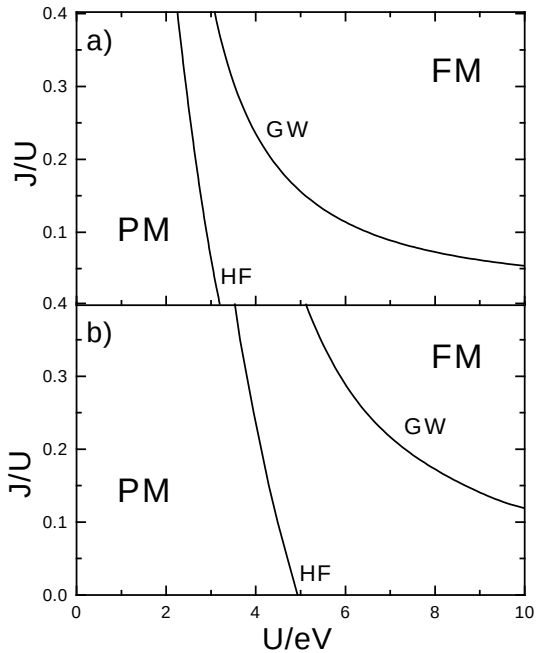

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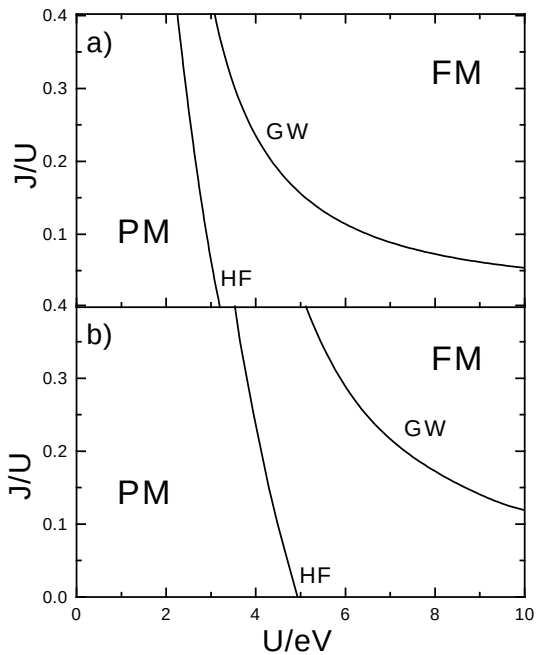
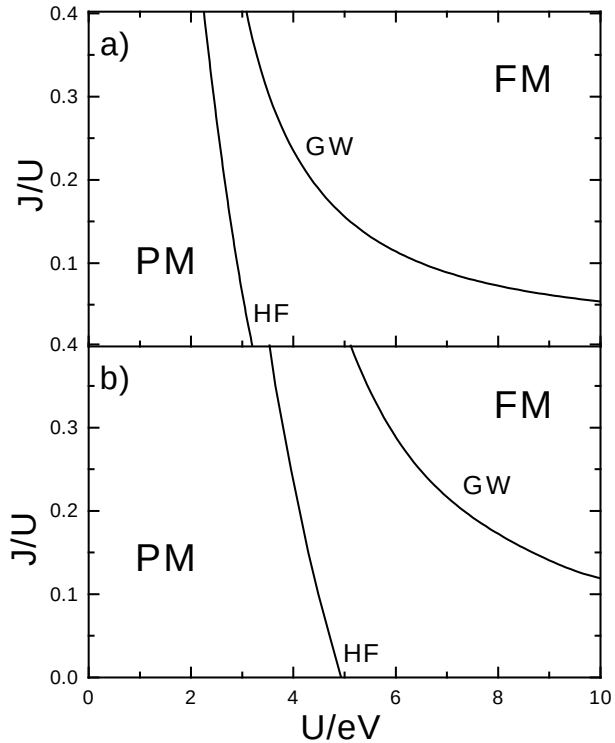


- Stoner theory ≡ Hartree–Fock theory
  - ferromagnetism appears at 'moderate couplings' – **wrong**;
  - Hund's rule coupling is irrelevant – **wrong**;
  - large density of states at the Fermi energy favors ferromagnetism – **correct**.

5 Generic two-band model



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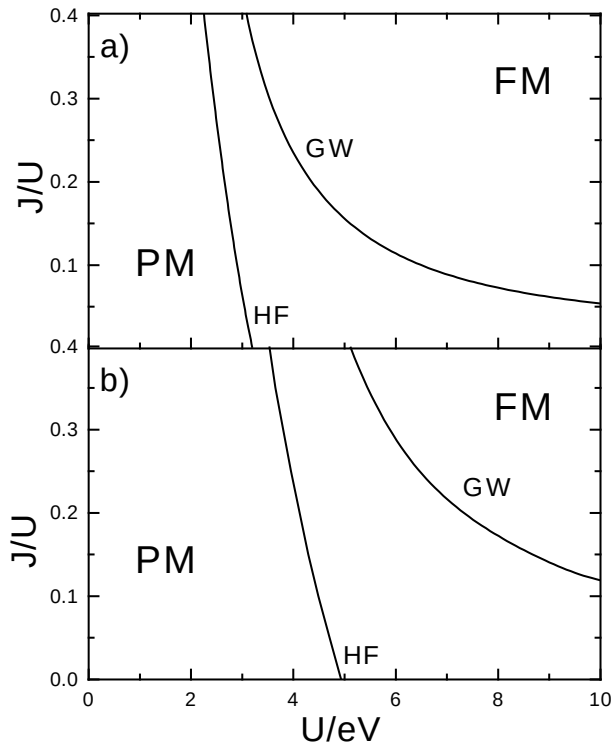
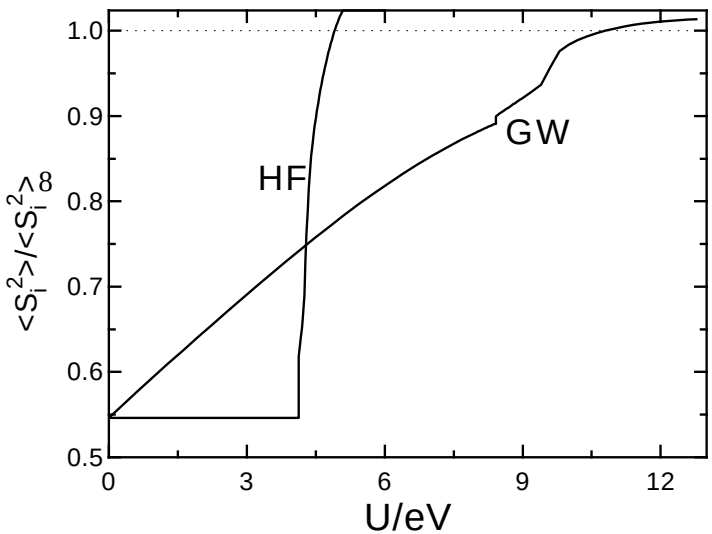


- Gutzwiller correlated electron theory
  - ferromagnetism at $U_c^{\mathrm{GW}} > W$: strong coupling phenomenon;
  - Hund's rule coupling is **decisive** for ferromagnetism;
  - large density of states at the Fermi energy favors ferromagnetism.

5 Generic two-band model

5.3 Local moments

(bandwidth $W = 6.6\,\mathrm{eV}$; $J = 0.2U$, filling $n_\sigma = 0.35$)



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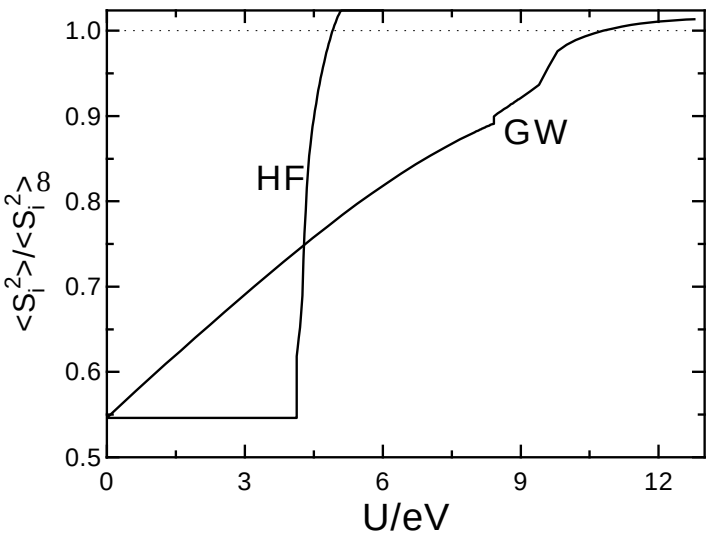

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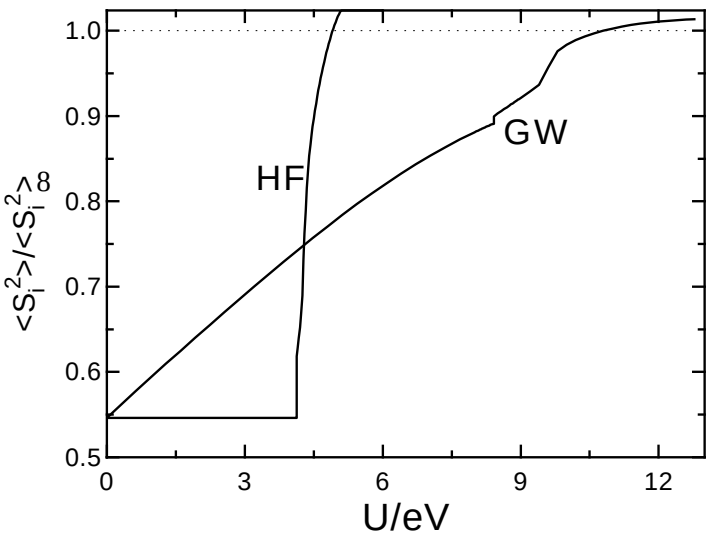

- Hartree–Fock theory:
  moments are formed at the transition
- Gutzwiller correlated electron theory:
  local moments are almost equal at the transition; idea of pre-formed moments applies.

5 Generic two-band model

5.4 Condensation energy (bandwidth $W = 6.6\,\mathrm{eV}$; $J = 0.2U$)

$E_{\mathrm{cond}} := \left| E_0^{\mathrm{para}} - E_0^{\mathrm{ferro}} \right|$; expectation: $E_{\mathrm{cond}} = \mathcal{O}\left(T_{\mathrm{Curie}}\right)$

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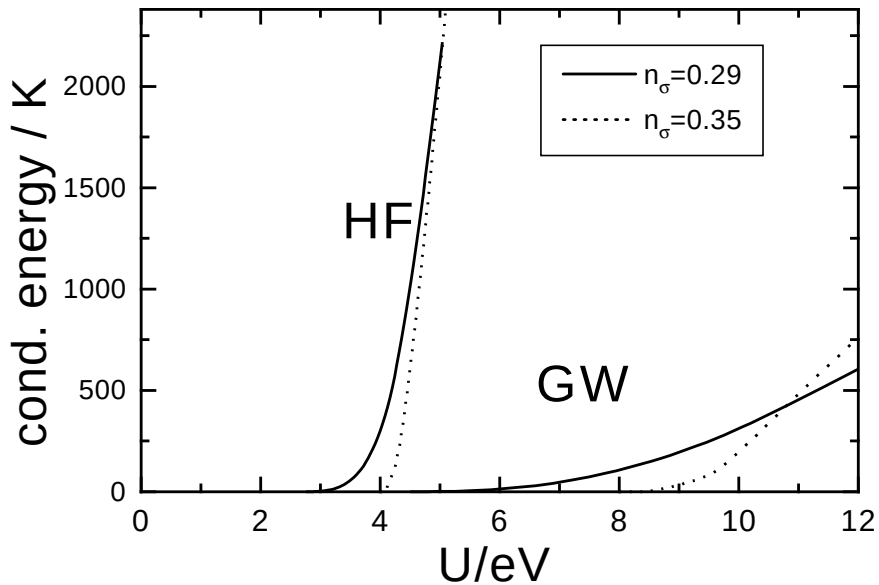

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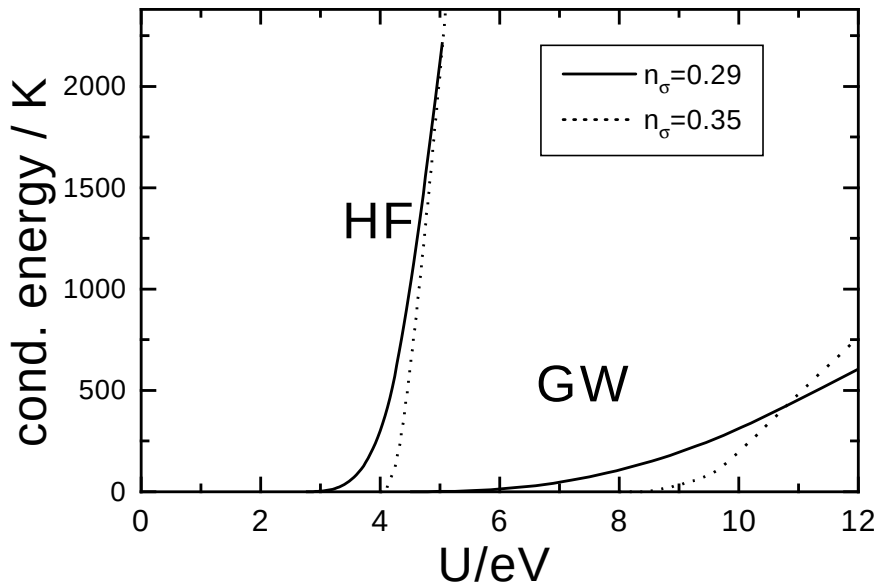

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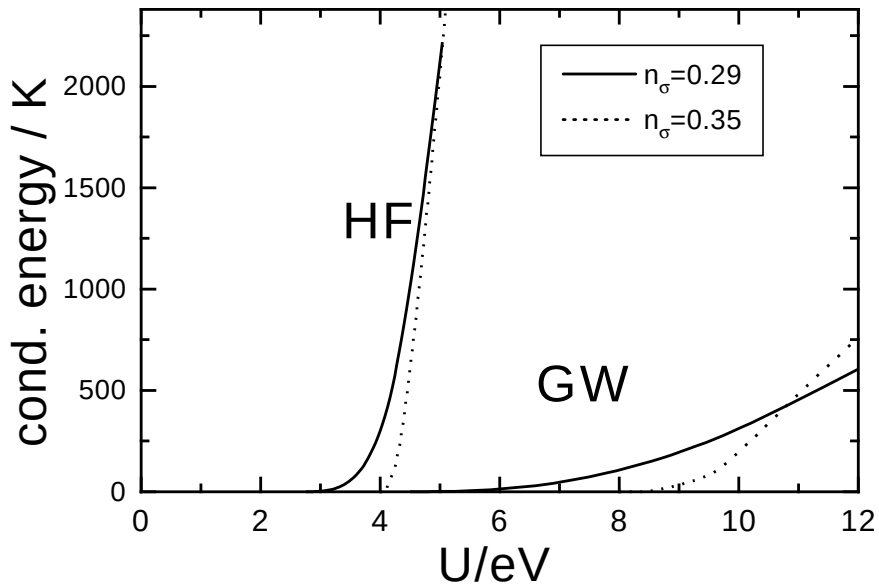

- Hartree–Fock theory: fine tuning of U required!
- Gutzwiller correlated electron theory:
  realistic values for all $U > U_{\mathrm{c}}$;
  not sensitive against variations of U.

6 Results for nickel

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Modern version of Stoner–Slater theory: SDFT

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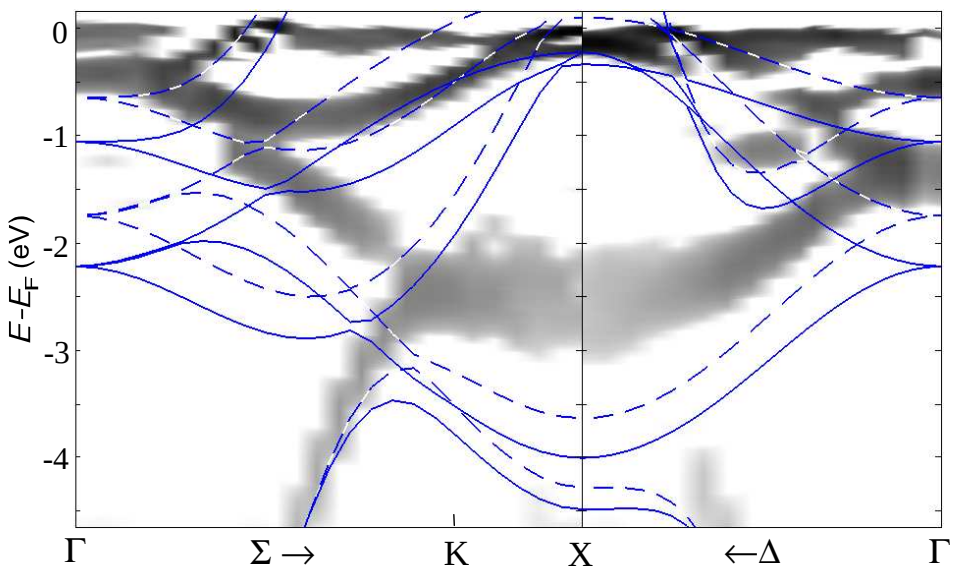

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- A directly controls effective mass, bandwidth, magnetic moment (together with C).

6 Results for nickel

6.3 Results (no spin-orbit coupling, cubic symmetry)

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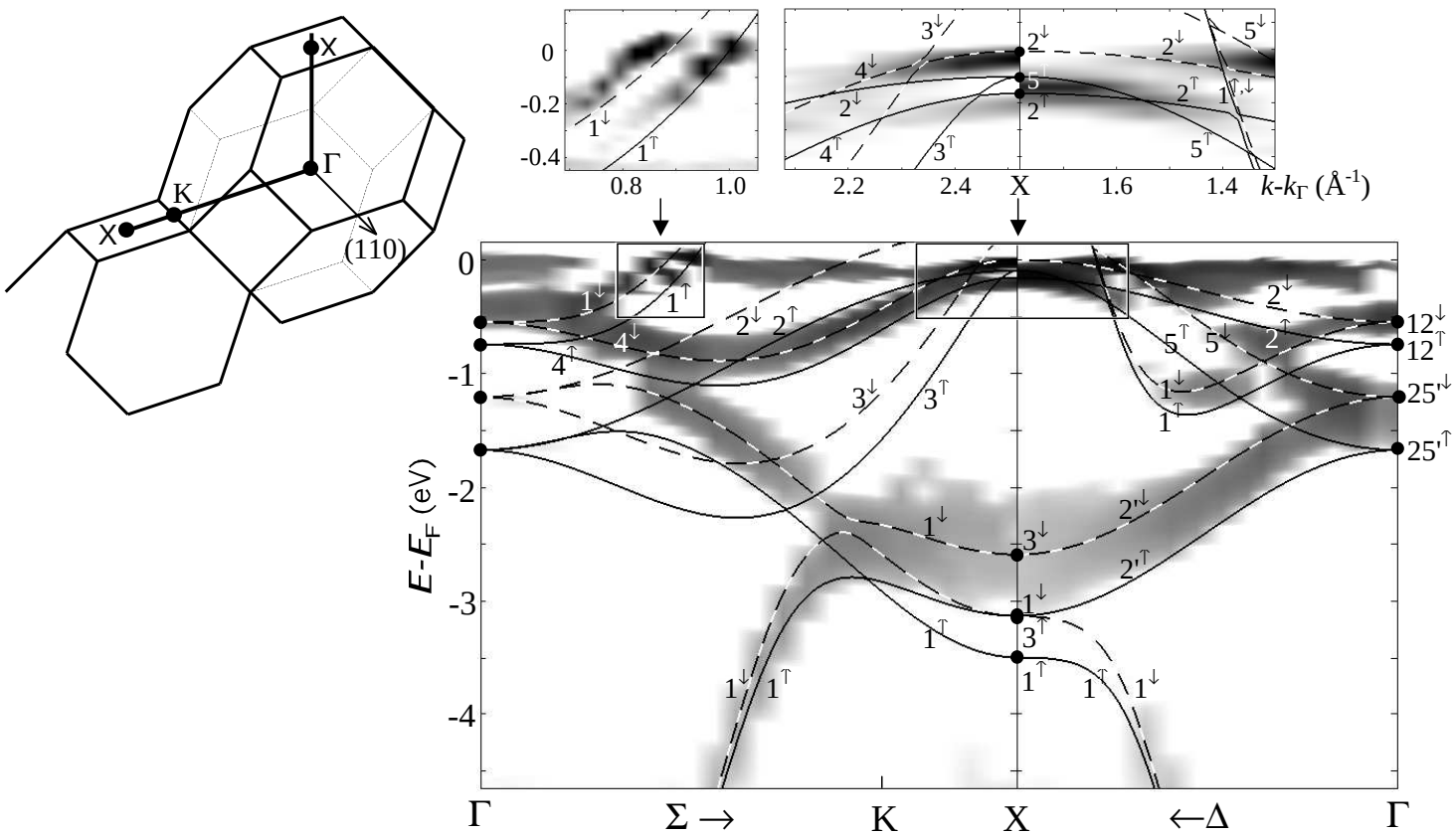
- Band structure



6 Results for nickel

- Data (spin-only moment $\mu_s = 0.55\mu_B$, no spin-orbit coupling)

Symmetry	Experiment	Gutz-DFT	SDFT
$\langle\Gamma_1\rangle$	8.90±0.30	8.86	8.96[−0.11]
$\langle X_1\rangle$	3.30±0.20	3.31[0.36]	4.37[0.20]
$X_{2\downarrow}$	0.04±0.03	0.01	−0.09
$\Delta_{e_g}(X_2)$	0.17±0.05	0.155	0.44
$\Delta_{t_{2g}}(X_5)$	0.33±0.04	0.38	0.56
$\langle L_{2'}\rangle$	1.00±0.20	0.97[0.0]	0.24[−0.12]
$\langle\Lambda_{3;1/3}\rangle$	0.57[0.16±0.02]	0.67[0.22]	0.90[0.42]
$\langle\Lambda_{3;1/2}\rangle$	0.50[0.21±0.02]	0.55[0.26]	0.76[0.44]
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- Important details
  - correct Fermi surface topology: one hole ellipsoid around X
  - correct exchange splitting: small and anisotropic
  - correct $4sp$ level ($L_{2'}$): n_d had to be corrected

6 Results for nickel

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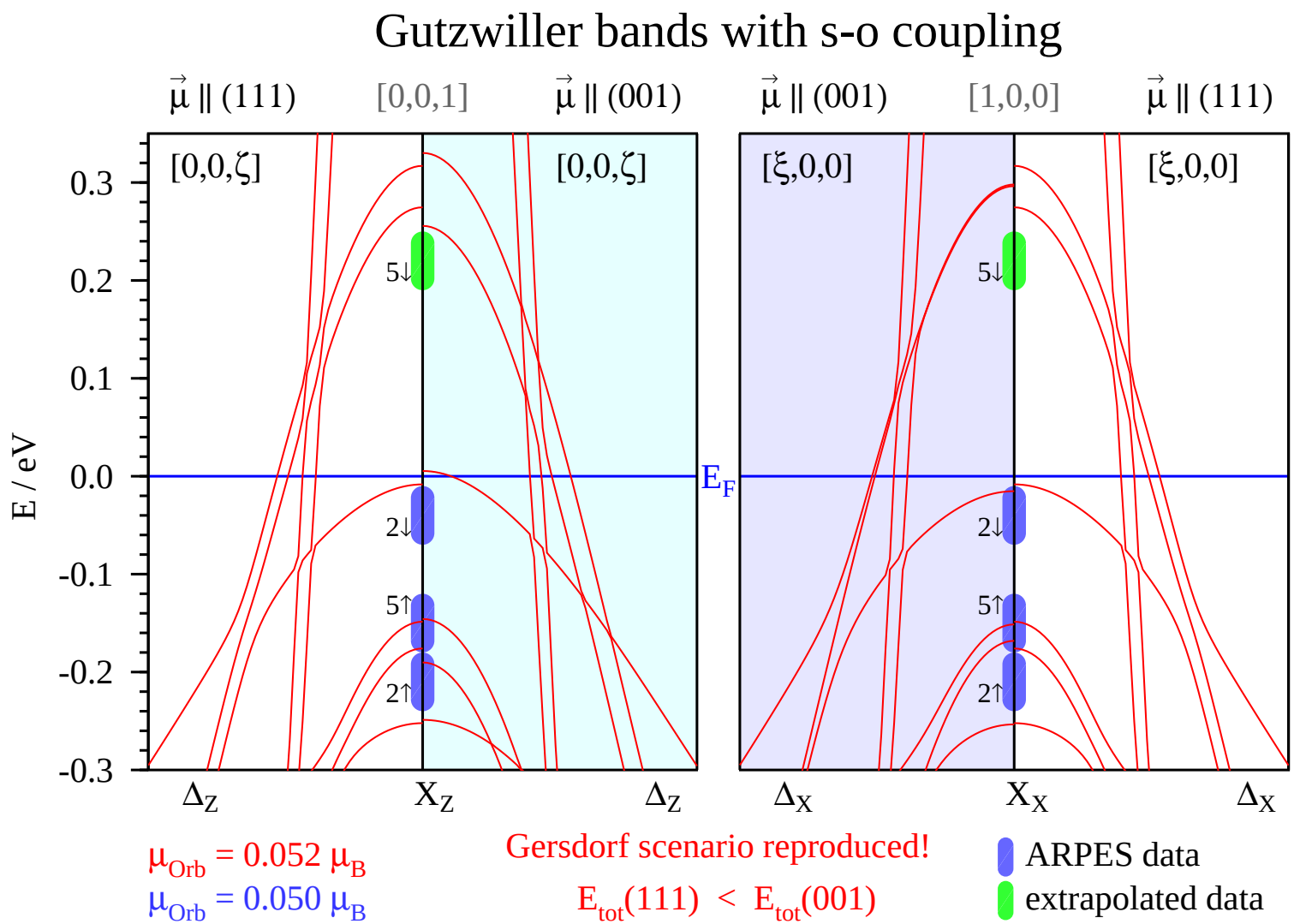

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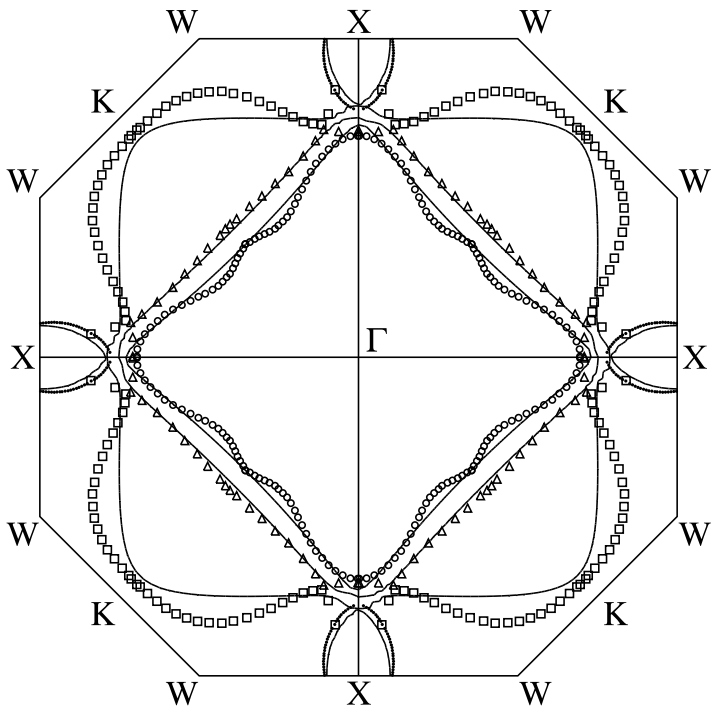

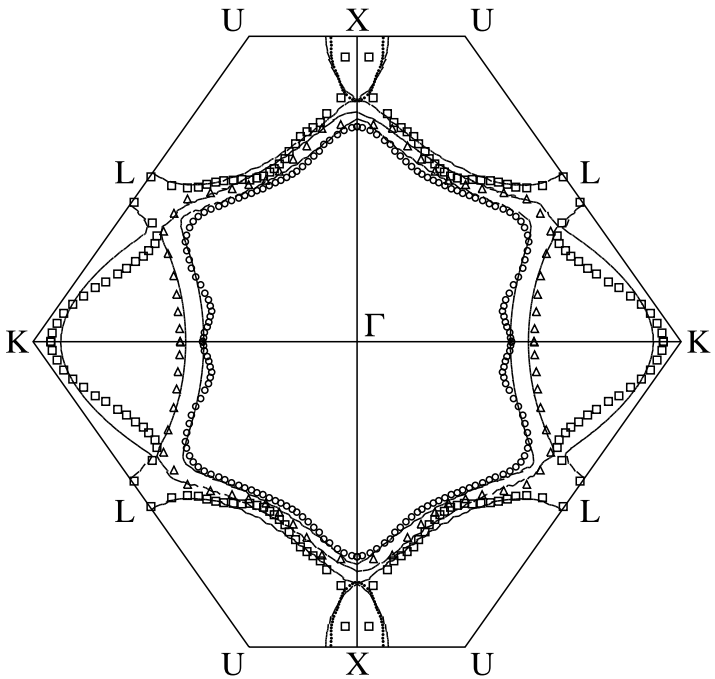

We think that the experimental ‘wiggles’ are not correct.

New ARPES measurements are under way . . .

7 Summary

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