Magnetism in Low-Dimensional Systems
From Frustration to Complex Order

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April 18, 2009
Outline

1. Cool-down

2. Full-Potential ASW Method

3. A Short Walk Through Dimensions
   - Where are the Moments?
   - How to Build a Spin-Ladder
   - Greetings from High-$T_c$
   - A Recipe Against Frustration
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Delafossites $\text{ABO}_2$

**Delafossite Structure**

**Building Blocks**

- rhombohedral lattice
- triangular A-atom layers
- $\text{BO}_2$ sandwich layers
- B-atoms octahedrally coordinated
- linear $\text{O}–\text{A}–\text{O}$ bonds
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**Issues**
- dimensionality
- frustration effects
- play chemistry
Delafossites $\text{ABO}_2$

### Delafossite Structure

### Prototype Materials
- $\text{CuFeO}_2$, $\text{CuCrO}_2$
- $\text{CuCoO}_2$, $\text{CuRhO}_2$
- $\text{CuAlO}_2$, $\text{CuGaO}_2$, $\text{CuInO}_2$, …
- $\text{PdCrO}_2$, $\text{PdCoO}_2$, $\text{PdRhO}_2$, $\text{PtCoO}_2$

### Properties
- Semiconductors, AF interactions, (distorted) triangular
- Non-magnetic semiconductors, high TEP
- Wide-gap semiconductors, p-type TCO
- Very good metals, highly anisotropic
Delafossites $\text{ABO}_2$

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Delafossites ABO$_2$

### Delafossite Structure

![Delafossite Structure Diagram]

### Prototype Materials

- CuFeO$_2$, CuCrO$_2$
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![Delafossite Structure Diagram]

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Magnetism in Low-Dimensional Systems
PdCoO$_2$ and PtCoO$_2$

**Delafossite Structure**

**Facts**
- very low resistivity
- anisotropy factor $\approx 200$
- PES: only Pd 4$d$ states at $E_F$
- PES/IPES: $E_F$ in shallow DOS minimum
**PdCoO$_2$ and PtCoO$_2$**

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**Open Issues**
- role of Pd 4$d$ orbitals?
- role of Co 3$d$ and O 2$p$ orbitals?
Electronics Properties of PdCoO$_2$

**Results**
- Co 3$d$-O 2$p$ hybridization
- CoO$_6$ octahedra: Co 3$d$ $\Rightarrow$ $t_{2g}$ and $e_g$
- Co 3$d^6$ (Co$^{3+}$) LS
- Co 3$d$, O 2$p$: very small DOS at $E_F$
- Pd 4$d^9$ (Pd$^{1+}$)

Electronic Properties of PdCoO$_2$

**Partial Densities of States**

- **Pd 4d**
  - $x^2-y^2$
  - $x^2_y^2$
  - $3z^2-r^2$
- **O 2p**
  - $z$

**Results**

- Pd 4d-O 2p hybridization
- Broad Pd $d_{xy}, x^2-y^2$ bands
- States at $E_F$: Pd $d_{xy}, x^2-y^2$, $d_{3z^2-r^2}$

Electronic Properties of PdCoO$_2$

**Band Structure**

\[ (E - E_F) \ (eV) \]

\[ \Gamma M K \Gamma A L H A \]

**Results**
- quasi-2D
- single band crossing $E_F$

**Brillouin Zone**

Electronic Properties of PdCoO$_2$

**Results**
- strong anisotropy
- but: bands below $E_F$ disperse along $\Gamma$-$A$

**VE, R. Frésard, A. Maignan, Chem. Mat. 20, 2370 (2008)**
The Fingerprint of Dimensionality

Band Dispersions

Pd $4d_{xy,x^2-y^2}$

Pd $4d_{3z^2-r^2}$
The Fingerprint of Dimensionality

Free Electron Density of States

\[ \rho(E) \sim \int_{\Omega_{BZ}} d^d k \, \delta \left( E - \frac{\hbar^2 |k|^2}{2m} \right) \]

\[ \sim \int_{\Omega_{BZ}} d|k||k|^{d-1} \, \delta \left( |k| - \sqrt{\frac{2mE}{\hbar^2}} \right) \]

\[ \sim \frac{m}{\hbar^2} \sqrt{\frac{2mE}{\hbar^2}}^{d-2} \]
The Fingerprint of Dimensionality

Free Electron Density of States

- Bulk (3D)
- Quantum Well (2D)
- Quantum Wire (1D)
- Quantum Dot (0D)

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Magnetism in Low-Dimensional Systems
The Fingerprint of Dimensionality

Tight-Binding Bands

\[ \varepsilon_k = E_0 + E_1 \sum_{\{\Delta\}} e^{ik\Delta} \]

\( d = 1 \)
\( d = 2 \)
\( d = 3 \)

(from: G. Czycholl, Theoretische Festkörperphysik, Springer)
The Fingerprint of Dimensionality

Single-layer $SrTiO_3$

$\text{DOS (1/eV)}$ vs $(E - E_V)$ (eV)

- $\text{Ti 3d}_{xy}$
- $\text{Ti 3d}_{xz,yz}$
- $\text{Ti 3d}_{3z^2-r^2}$
- $\text{Ti1 3d}_{x^2-y^2}$

$d_{3z^2-r^2} : d = 0$

$d_{xz,yz} : d = 1$

$d_{xy} : d = 2$
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Augmented Spherical Wave (ASW) Method

Characteristics

- a “dialect” of Andersen’s LMTO method
  - different linearization schemes
  - different interstitial energies
  - different implementations
Augmented Spherical Wave (ASW) Method

**Characteristics**
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- different interstitial energies
- different implementations

**0th Generation (Williams, Kübler, Gelatt, 1970s)**

PRB 19, 6094 (1979)
Augmented Spherical Wave (ASW) Method

1st Generation (VE, 1990s)  IJQC 77, 1007 (2000)

- monolithic implementation from scratch
- new algorithms $\rightarrow$ improved accuracy, numerical stability
- much improved functionality, usability, and portability
- xAnderson convergence acceleration scheme
- all LDA-parametrizations, most GGA-schemes
- still based on atomic-sphere approximation
Wave Function Expanded in Basis Functions

\[ \psi_\sigma (\mathbf{r}) = \sum_{L_\kappa i} c_{L_\kappa i\sigma} H_{L_\kappa \sigma} (\mathbf{r}_i) \]

\[ \longrightarrow c_{L_\kappa i\sigma} \text{ determined variationally} \]
ASW Method: Basic Formalism

Wave Function Expanded in Basis Functions

$$\psi_\sigma(r) = \sum_{L\kappa i} c_{L\kappa i\sigma} H_{L\kappa\sigma}^\infty(r_i)$$

$$\longrightarrow c_{L\kappa i\sigma} \text{ determined variationally}$$

Basis Functions: Augmented Spherical Waves

$$H_{L\kappa\sigma}^\infty(r_i) = \begin{cases} H_{L\kappa}^I(r_i) & \text{interstitial region} \\ \tilde{H}_{L\kappa\sigma}(r_i) & \text{on-centre sphere } i \\ \sum'_{L'j} \tilde{J}_{L'\kappa\sigma}(r_j) B_{L'L\kappa} & \text{off-centre spheres } j \end{cases}$$

$$B_{L'L\kappa}(R_j - R_i): \text{ structure constants}$$

ASW classified by atomic site $R_i$, $L = (l, m)$, decay $\kappa$, spin $\sigma$
Envelope Functions

\[ H^l_{\kappa l}(\mathbf{r}_i) := i \kappa^{l+1} h^{(1)}_l(\kappa r_i) Y_L(\hat{r}_i) \]

\( h^{(1)}_l(\kappa r_i) \): spherical Hankel function
ASW Method: Basic Formalism

Envelope Functions

\[ H_{L\kappa}^l(r_i) := i^{l+1} h_l^{(1)}(\kappa r_i) Y_L(\hat{r}_i) \]

\( h_l^{(1)}(\kappa r_i) \): spherical Hankel function

Augmented Functions

\[ \tilde{H}_{L\kappa\sigma}(r_i) := \tilde{h}_{l\kappa\sigma}(r_i) Y_L(\hat{r}_i) \]
\[ \tilde{J}_{L'\kappa\sigma}(r_j) := \tilde{j}_{l'\kappa\sigma}(r_j) Y_{L'}(\hat{r}_j) \]

\( \tilde{h}, \tilde{j} \): numerical solutions of radial Kohn-Sham equation boundary conditions from envelope functions correspond to \( \varphi \) and \( \dot{\varphi} \) of LMTO
ASW Method: Basic Formalism

Augmented Spherical Waves

envelope functions
augmented spherical waves

A B

A B

r
ASW Method: Further Reading

Eyer
The Augmented Spherical Wave Method

The Augmented Spherical Wave (ASW) method is one of the most powerful approaches for handling the requirements of limited basis sets in DFT calculations. It is particularly suited for the calculation of the electronic, magnetic, and optical properties of solid-state materials. Recent developments allow application to the elastic properties and phonon spectra. The book addresses all those who want to learn about methods for electronic structure calculations, especially the ASW method in particular.
Towards a Full-Potential Spherical-Wave Method

Status

- ASA (space-filling atomic spheres)
  - $O(ASA)$ speed
  - systematic error in total energy
- non-overlapping muffin-tin spheres
  - prerequisite for accurate total energies
  - larger basis set $\rightarrow$ inefficient
**Towards a Full-Potential Spherical-Wave Method**

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### Requirements

- restore interstitial region
  - go to non-overlapping muffin-tin spheres
  - go beyond constant-potential approximation
- inside muffin-tin spheres
  - non-spherical contributions
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Guidelines

- interstitial quantities expanded in plane waves
  - straightforward to implement
  - inefficient

- interstitial quantities expanded in spherical waves
  - elegant, no periodicity required
  - efficient
  - difficult to implement
Towards a Full-Potential Spherical-Wave Method

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Steps to be Taken

- **remove total energy error** due to overlap of atomic spheres
  - reintroduce non-overlapping muffin-tin spheres
  - restore interstitial region
Cool-down
Full-Potential ASW Method
A Short Walk Through Dimensions

Basic Principles

Steps to be Taken

- remove total energy error due to overlap of atomic spheres
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  - restore interstitial region

- find representation of electron density and full potential

  - inside muffin-tin spheres
  - in the interstitial region
Basic Principles

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    - use spherical-harmonics expansions
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- find representation of products of the basis functions
  - inside muffin-tin spheres
    - use spherical-harmonics expansions
  - in the interstitial region
  - no exact spherical-wave representation available!
From Wave Functions to Electron Density

Density inside MT-Spheres

$\rho_v / \text{a.u.}$
Products of Basis Functions in Interstitial Region

\[ p^I(r) = \sum_n d_n F_n(r) \]

\[ \int d^3r \ F^*_n(r) p^I(r) = \sum_n d_n \int d^3r \ F^*_n(r) F_n(r) \]
From Wave Functions to Electron Density

Products of Basis Functions in Interstitial Region

\[ p^I(r) = \sum_n d_n F_n(r) \]

\[ \int d^3r \ F^*_{n'}(r) p^I(r) = \sum_n d_n \int d^3r \ F^*_{n'}(r) F_n(r) \]

- \( F_n(r) \): plane waves
  - integrals exact
  - inefficient
From Wave Functions to Electron Density

Products of Basis Functions in Interstitial Region

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- \( F_n(r) \): spherical waves
  - would be efficient
  - integrals not known analytically
From Wave Functions to Electron Density

**Products of Basis Functions in Interstitial Region**

\[ p^I(r) = \sum_n d_n F_n(r) \]

\[ \int d^3 r F_{n'}^*(r)p^I(r) = \sum_n d_n \int d^3 r F_{n'}^*(r)F_n(r) \]

- \( F_n(r) \): spherical waves
  - would be efficient
  - integrals not known analytically
  - Methfessel 1988: match values and slopes at MT-sphere surfaces
From Wave Functions to Electron Density

Density from Value/Slope Matching at MT-Radii (Al)

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From Electron Density to Full Potential

Inside Muffin-Tin Spheres
- density, Hartree-potential and xc-potential numerically

Interstitial Region
- density from value/slope matching
- Hartree-potential analytically
- xc-potential from value/slope matching
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From Full Potential to Basis Functions

Previous Approaches
- project full potential to muffin-tin potential
- construct basis functions from muffin-tin potential
- no minimal basis set! (large basis set!)

Present Approach
- project full potential to ASA potential
- construct basis functions from ASA potential
- minimal basis set!
From Full Potential to Basis Functions

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- project full potential to ASA potential
- construct basis functions from ASA potential
- minimal basis set!
Comparison of Approaches

Ole K. Andersen

- ASA geometry used for basis functions → minimal basis set good!
- ASA geometry used for density and potential → error in total energy bad!
### Comparison of Approaches

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Full-Potential ASW Method

2nd Generation ASW (VE, 2000s)

- based on 1st generation code
- full-potential ASW method
  - electron densities, spin densities
  - electric field gradients
  - elastic properties, phonon spectra
- optical properties
  - based on linear-response theory
  - direct calculation of $\Re \sigma$ and $\Im \sigma$
  - no Kramers-Kronig relations needed
- transport properties, thermoelectrics
- LDA+U method
  - all „flavours“ for double-counting terms (AMF, FLL, DFT)

at $O(\text{ASA})$ speed!
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LTO(Γ)-Phonon in Silicon

ASA⁺ Code

Bad
- no stable Si position # nature
LTO(\Gamma)-Phonon in Silicon

**ASA\(^+\) Code**

\[
E_{\text{Si}}(\text{Ryd}) = -1156.0698
\]

**Full-Potential Code**

\[
E_{\text{Si}}(\text{Ryd}) = -1156.1070
\]

New!

- phonon frequency: \( f_{\text{calc}} = 15.34 \text{ THz} \) \( (f_{\text{exp}} = 15.53 \text{ THz}) \)

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La$_2$BaCuO$_5$: A 0D(?) Ferromagnetic Semiconductor

**Crystal Structure**

**Building Blocks**

- $P4/mbm$ ($D^5_{4h}$)
- $a = 6.8447$ Å, $c = 5.8637$ Å
- Ba-Cu and La-O1 layers
- O2 interlayers
- LaO$_8$ and BaO$_{10}$ polyhedra
- CuO$_4$ plaquettes
  - Cu-Cu distance 4.84 Å
  - chains $\parallel c$
  - $\perp$ in (a,b) planes
  - coupled by La atoms
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**Magnetic Properties**
- $T_C = 5.2$ K
- $m = 0.95 \mu_B / Cu \parallel c$
- $T > 80$ K: Curie-Weiss
  - $\mu_{\text{eff}} = 1.54 \mu_B$
  - $\Theta < 0$ K
- $T < 80$ K: Curie-Weiss
  - $\Theta = 5$ K
- 3D Spin-$\frac{1}{2}$ Heisenberg Model
- + Ising-like anisotropy

**Electronic Properties**
- Cu$^{2+} \rightarrow d^9$
- Cu $d$ hole $\hat{d} = d_{x^2-y^2}$ plaquette orbital

**Cluster Model**
- ferromagnetic order
- interference of different exchange paths

---

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Open Issues

- Role of Cu $3d$, O $2p$, La $5d$ Orbitals?
- Dimensionality?
- Effective Magnetic Sites?
- Exchange Paths?
- Heisenberg model?
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TODOs
- Spin-Degenerate Calculations
  - Role of Orbitals
  - Chemical Bonding
- Spin-Polarized Calculations
  - Magnetic Instability
  - Exchange Paths
Spin-Degenerate Calculations for La$_2$BaCuO$_5$

**Band Structure**

- Graph showing the band structure with labels $\Gamma$, M, X, $\Gamma$, Z, A, R, Z.
- Axes: $(E - E_F)$ (eV) vs. Energy level.

**Partial DOS**

- Graph showing the partial density of states (DOS) with labels Cu 3d, O1 2p, O2 2p, La 5d.
- Axes: $(E - E_F)$ (eV) vs. DOS (1/eV).

**References**


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Spin-Degenerate Calculations for La$_2$BaCuO$_5$

**Cu 3d Partial DOS**

**O 2p Partial DOS**

**Bonding/Antibonding Splitting from $p$-$d$ Overlap**

$\approx 2.5 - 3.0$ eV for $t_{2g}$-like states ($\pi$-type)

$\approx 5.5$ eV for $d_{x^2-y^2}/p_{\parallel}$ states ($\sigma$-type)

$= 0$ eV for $d_{3z^2-r^2}$ states (apex $\rightarrow \infty$)
Spin-Polarized Calculations for $\text{La}_2\text{BaCuO}_5$

### Magnetic Moments ($\mu_B$)

<table>
<thead>
<tr>
<th></th>
<th>$\uparrow\uparrow$</th>
<th>$\uparrow\downarrow$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>0.51</td>
<td>0.53</td>
</tr>
<tr>
<td>O2</td>
<td>0.12</td>
<td>0.07</td>
</tr>
<tr>
<td>La</td>
<td>0.02</td>
<td>0.03</td>
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<tr>
<td>Ba</td>
<td>-0.01</td>
<td>0.00</td>
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<tr>
<td>O1</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>f.u.</td>
<td>1.00</td>
<td>0.87</td>
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### Total Energies (mRyd/f.u.)

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<th>spin-deg.</th>
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<tbody>
<tr>
<td>$\text{La}_2\text{BaCuO}_5$</td>
<td>0.0</td>
<td>-9.35</td>
<td>-3.30</td>
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### Band Gap (eV)

<table>
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<th>spin-deg.</th>
<th>$\uparrow\uparrow$</th>
<th>$\uparrow\downarrow$</th>
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</thead>
<tbody>
<tr>
<td>$\text{La}_2\text{BaCuO}_5$</td>
<td>0.0</td>
<td>0.66</td>
<td>0.38</td>
</tr>
</tbody>
</table>

Spin-Polarized Calculations for La$_2$BaCuO$_5$

Results

- extended localized moments on plaquettes
- carried by Cu $3d_{x^2-y^2}$ and O2 $2p_{||}$ states
Spin-Polarized Calculations for La$_2$BaCuO$_5$
Results

- extended localized moments on plaquettes
  - carried by Cu 3d_{x^2-y^2} and O2 2p_|| states
Spin-Polarized Calculations for $\text{La}_2\text{BaCuO}_5$

**Results**
- extended localized moments on plaquettes
  - carried by Cu $3d_{x^2−y^2}$ and O2 $2p_{||}$ states
  - coupled via La $5d_{x^2−y^2}$ states

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Magnetism in Low-Dimensional Systems
Outline

1. Cool-down

2. Full-Potential ASW Method

3. A Short Walk Through Dimensions
   - Where are the Moments?
   - How to Build a Spin-Ladder
   - Greetings from High-$T_c$
   - A Recipe Against Frustration
Orbital Ordering Transition in La$_2$RuO$_5$

Semiconductor-Semiconductor Transition at 160 K

Orbital Ordering Transition in La$_2$RuO$_5$

**Basics**
- Ru$^{4+} \rightarrow 4d^4$
- low-spin ($S = 1$)
- above 160 K: CW
- below 160 K:
  - $\chi \neq \chi(H), H < 9$ T
  - no supercell reflects.
  - no AF order (?)
  - local moments?
  - $S = 1, S = 0$?

**Magnetism, Crystal Structure**

Orbital Ordering Transition in $\text{La}_2\text{RuO}_5$

**HT-Structure**

**Building Blocks**
- $\text{RuO}_6$ octahedra
  - corner-sharing
  - chains $\parallel c$
  - zigzag pattern $\parallel b$
  - double layers $\parallel b, c$
- $\text{LaO}_9$ tricapped trigonal prisms
- $\text{La}_4\text{O}$ tetrahedra
Orbital Ordering Transition in $\text{La}_2\text{RuO}_5$

HT-Structure

LT-Structure
Orbital Ordering Transition in La$_2$RuO$_5$

**HT-Structure**
- monoclinic, $P2_1/c$
- $d_{\text{Ru-Ru}} = 3.975\,\text{Å}$
- $d_{\text{O-Ru-O-Ru-O}} = 7.772\,\text{Å}$

**LT-Structure**
- triclinic, $P\overline{1}$
- $d_{\text{Ru(1)-Ru(2)}} = 3.868, 4.045\,\text{Å}$
- $d_{\text{O-Ru(1)-O-Ru(2)-O}} = 7.579, 7.977\,\text{Å}$

Orbital Ordering Transition in La$_2$RuO$_5$

Where are the Electrons?

Spin-Degenerate Calculations for La$_2$RuO$_5$

**Results**

- quasi-1D dispersion $\parallel c$
- CEF $\rightarrow$ Ru 4$d$ $t_{2g}/e_g$
- strong Ru 4$d$-O 2$p$ overlap
Spin-Degenerate Calculations for La$_2$RuO$_5$

**Results**
- $d_{xy} \approx d_{xz} \approx d_{yz}$
- Hund’s rule: $S = 1$
Spin-Degenerate Calculations for La$_2$RuO$_5$

**Results**

- $d_{xy} \approx d_{xz} \approx d_{yz}$
- Hund’s rule: $S = 1$

**Results**

- $d_{xy} \approx d_{yz}$
- $d_{xy}^1 d_{xz}^2 d_{yz}^1$: $S = 1$
Spin-Polarized Calculations for La$_2$RuO$_5$

<table>
<thead>
<tr>
<th>structure</th>
<th>funct.</th>
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<th>$m_{\text{RuO}_6}$</th>
<th>$E_g$</th>
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<td>-70.1</td>
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</table>


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Magnetism in Low-Dimensional Systems
Spin-Polarized Calculations for La$_2$RuO$_5$

**Results**

- $\text{Ru}(1) \approx \text{Ru}(2)$
- $d_{xy} \approx d_{yz}$
- $\text{m}(\text{Ru})$: $d_{xy}$ and $d_{yz}$ ($d_{xy}^1 d_{xz}^2 d_{yz}^1$)
- $\text{m}(\text{Ru}(1)) \neq -\text{m}(\text{Ru}(2))$

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Magnetism in Low-Dimensional Systems
Scenario for La₂RuO₅

HT-Structure

LT-Structure

Spin-Ladders

- AF coupling on rungs
- $m(\text{Ru}(1)\text{O}_6) = -m(\text{Ru}(2)\text{O}_6)$

Outline

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3. A Short Walk Through Dimensions
   - Where are the Moments?
   - How to Build a Spin-Ladder
   - Greetings from High-$T_c$
   - A Recipe Against Frustration
Magnetic Order in $K_2\text{NiF}_4$ and $K_2\text{CuF}_4$

- “classical” two-dimensional systems
- based on $K_2\text{NiF}_4$ structure
- parent compounds of $\text{La}_2\text{CuO}_4$
- magnetic semiconductors
- role of TM 3$d$ and F 2$p$ orbitals?
- intralayer/interlayer magnetic coupling?
- antiferromagnetism vs. ferromagnetism
- symmetry breaking by magnetic order vs. symmetry breaking by orbital order
Magnetic Order in $\text{K}_2\text{NiF}_4$ and $\text{K}_2\text{CuF}_4$

**K$_2$NiF$_4$ Structure**

**Basics**
- I4/mmm (centered tetragonal)
- NiF$_2$ planes ($\cong$ CuO$_2$ planes)
- K and F interlayers
- corner sharing NiF$_6$ octahedra
- $d(\text{Ni} - \text{F}_{\text{apex}}) < d(\text{Ni} - \text{F}_{\text{plane}})$
- AF order
  - Cmca (side-centered orthorh.)
  - $a \rightarrow \sqrt{2}a$
K₂NiF₄

- Magnetic Properties
  - \( T_N = 97.23 \text{ K} \)
  - \( m = 2.22 \mu_B \)
  - magnetic moments \( \parallel c \)
  - \( J/k_B \approx -100 \text{ K} \)
  - 2D spin-wave dispersion
    - \( J'/J < 0.0037 \)
  - 2D (\( S = 1 \)) Heisenberg Model
  - + Ising-like anisotropy

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K$_2$NiF$_4$: Spin-Degenerate Calculations

Band Structure

Partial DOS

Results

- $E < -4$ eV: $d$-$p$ bonding
- $E > -2$ eV: $d$-$p$ antib.
- 2D dispersion
- at $E_F$: Ni 3$d$ $e_g$
K$_2$NiF$_4$: Weighted Bands

**Partial DOS**

**Results**
- CEF ($t_{2g}/e_g$) $\approx$ 0.9 eV
- $W(d_{x^2-y^2}) \approx 2 W(d_{3z^2-r^2})$
- perfect FS nesting
K₂NiF₄: Doubling the Unit Cell

centered tetragonal

side-centered orthorh.
K$_2$NiF$_4$: Spin-Polarized Calculations

### Band Structure

![Band Structure Graph](image)

### Partial DOS

![Partial DOS Graph](image)

### Moments ($\mu_B$)

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<th>Moment</th>
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<tr>
<td>F2</td>
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</tr>
<tr>
<td>sublattice</td>
<td>1.38</td>
</tr>
</tbody>
</table>

### Results

- Moment: $d_{3z^2-r^2}$, $d_{x^2-y^2}$
- $\Delta E_{\text{tot}} = -30.5$ mRyd
K$_2$CuF$_4$

**Magnetic Properties**

- $T_C = 6.26$ K
- $m = 1.00 \mu_B$
- Magnetic moments $\perp c$
- 2D spin-wave dispersion
  - $J'/J < 0.00066$
- 3D ($S = \frac{1}{2}$) Heisenberg Model
- + 1% XY-like anisotropy
- $J/k_B = 11.2$ K
**K₂CuF₄**

**Magnetic Properties**
- \( T_C = 6.26 \text{ K} \)
- \( m = 1.00 \mu_B \)
- magnetic moments \( \perp c \)
- 2D spin-wave dispersion
  - \( J'/J < 0.00066 \)
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- + 1\% XY-like anisotropy
- \( J/k_B = 11.2 \text{ K} \)

**Early XRD (Knox)**
- “K₂NiF₄” structure
- \( d_{\text{Cu–F}_\text{apex}} < d_{\text{Cu–F}_\text{plane}} \)
- # related Cu-compounds
K₂CuF₄

Khomskii and Kugel Model
- Heisenberg Hamiltonian
- + Pseudospin Hamiltonian
  - orbital ordering
- compressed octahedra
  - # ferromagnetic order
- antiferrodistortive structure proposed
  - side-centered orthorh.

Early XRD (Knox)
- “K₂NiF₄” structure
- \( d_{\text{Cu–F}_{\text{apex}}} < d_{\text{Cu–F}_{\text{plane}}} \)
  - # related Cu-compounds
K$_2$CuF$_4$

**Khomskii and Kugel Model**

- Heisenberg Hamiltonian
- + Pseudospin Hamiltonian
- orbital ordering
- compressed octahedra
- ♯ ferromagnetic order
- antiferrodistortive structure proposed
- side-centered orthorh.

**In-Plane Structure**

Cu

F

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Magnetism in Low-Dimensional Systems
K$_2$CuF$_4$

**In-Plane Structure**

- **Cu**
- **F**

**NMR (Le Dang Khoi, Veillet)**

- octahedra elongated, long axis $\perp$ c
$K_2CuF_4$

### In-Plane Structure

- **Cu**
- **F**

### NMR (Le Dang Khoi, Veillet)
- Octahedra elongated, long axis $\perp$ c

### XRD (Hidaka et al.)
- Cmca (side-centered orthorh.)
- F at $\left(\frac{1}{4} - \delta, \frac{1}{4} - \delta, 0\right)$
  - $\delta = 0.0176$

---

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Magnetism in Low-Dimensional Systems
K$_2$CuF$_4$: Spin-Degenerate Calculations

**Band Structure**

**Partial DOS**

**Results**

- similar to K$_2$NiF$_4$
- $d$-$p$ splitting smaller
- electron count!
**K₂CuF₄: Weighted Bands**

**Cu 3d₃z²−r²**

**Cu 3dₓ²−yü²**

**Cu 3dt₂g**

**Partial DOS**

**Results**
- CEF \((t₂g/e₉) \approx 1.0 \text{ eV}\)
- \(W(dₓ²−yü²) \approx 2 \times W(d₃z²−r²)\)
- \(FS(dₓ²−yü²) \approx FS(d₃z²−r²)\)
- no FS nesting

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**K₂CuF₄: Doubling the Unit Cell**

### Bands: centered tetragonal

![Graph of centered tetragonal bands](image1)

### Bands: side-centered orthorh.

![Graph of side-centered orthorh bands](image2)
K$_2$CuF$_4$: Spin-Polarized Calculations

**Band Structure**

**Partial DOS**

**Moments ($\mu_B$)**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Cu</td>
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</tr>
<tr>
<td>F1</td>
<td>0.08</td>
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<tr>
<td>F2</td>
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<tr>
<td>sublattice</td>
<td>1.00</td>
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</tbody>
</table>

**Results**

- moment: $d_{3z^2-r^2}$, $d_{x^2-y^2}$
- $\Delta E_{\text{tot}} = -6.5$ mRyd

Volker@Eyert.de Magnetism in Low-Dimensional Systems
K$_2$NiF$_4$: Orbital and Magnetic Order

Conclusion
- FS nesting
- instability
  - $\delta \neq 0$
- or
  - $m \neq 0$
K₂CuF₄: Orbital and Magnetic Order

Conclusion
- no FS nesting
- instability
  - $\delta \neq 0$
  - and
  - $m \neq 0$
**K\textsubscript{2}NiF\textsubscript{4} and K\textsubscript{2}CuF\textsubscript{4}: Energies and Moments**

**Total Energies**

![Graph of total energies showing the difference in energies for K\textsubscript{2}NiF\textsubscript{4} and K\textsubscript{2}CuF\textsubscript{4}](image)

**Magnetic Moments**

![Graph of magnetic moments showing the variation of moments for K\textsubscript{2}NiF\textsubscript{4} and K\textsubscript{2}CuF\textsubscript{4}](image)


Outline

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Cool-down
Full-Potential ASW Method
A Short Walk Through Dimensions

Where are the Moments?
How to Build a Spin-Ladder
Greetings from High-$T_c$
A Recipe Against Frustration

CuFeO$_2$

Delafossite Structure

Basics
- semiconductor
- AF interactions
- triangular lattice
CuFeO$_2$

**Delafossite Structure**

**Basics**
- semiconductor
- AF interactions
- triangular lattice

**Open Issues**
- frustration vs. long-range order
- role of Cu 3$d$ orbitals?
- role of Fe 3$d$ and O 2$p$ orbitals?
CuFeO$_2$

**Previous Neutron Data**

- $T_{N_1} = 16$ K, $T_{N_2} = 11$ K
- $\Theta_{CW} = -90$ K
- magnetic supercells
- no structural distortion
- $m_{Fe^{3+}} = 4.4 \mu_B$
CuFeO$_2$

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Band Calculations
- rhombohedral structure
- $m_{Fe} = 0.9 \mu_B$, $m_{Fe} = 3.8 \mu_B$
- $E_g = 0$ in LDA, GGA
- PES, XES
CuFeO$_2$

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- $T_{N_1} = 16$ K, $T_{N_2} = 11$ K
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- PES, XES

**New Neutron Data**
- magnetic supercells
- monoclinic structure below 4 K
CuFeO$_2$

**Previous Neutron Data**
- $T_{N_1} = 16$ K, $T_{N_2} = 11$ K
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- magnetic supercells
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- $m_{Fe^{3+}} = 4.4 \mu_B$

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- rhombohedral structure
- $m_{Fe} = 0.9 \mu_B$, $m_{Fe} = 3.8 \mu_B$
- $E_g = 0$ in LDA, GGA
- $\#$ PES, XES

**New Neutron Data**
- magnetic supercells
- monoclinic structure below 4 K

**Open Issues**
- spin-state of Fe?
- influence of monoc. structure?
Electronic Properties of CuFeO$_2$

Partial Densities of States

Results

- Fe 3d-O 2p hybridization
- FeO$_6$ octahedra: Fe 3d $\Rightarrow t_{2g}$ and $e_g$
- Cu 4$d^{10}$ ($Cu^{1+}$)
- Fe 3d $t_{2g}$
  - sharp peak at $E_F$

Electronic Properties of CuFeO$_2$

**Band Structure**

Results
- quasi-2D
- single band crossing $E_F$

Electronic Properties of CuFeO$_2$

Fermi Surface

Results
- strongly 3D

FS PdCoO$_2$

### Magnetic Properties of CuFeO$_2$

<table>
<thead>
<tr>
<th>structure</th>
<th>magn. order</th>
<th>$\Delta E$</th>
<th>$m_{Fe}$</th>
<th>$m_{O}$</th>
<th>$E_g$</th>
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<td>$3.73$</td>
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Magnetic Properties of CuFeO$_2$

**Results**

- LS, IS, HS in rhombohedral structure
- HS: O 2$p$ polarization via Fe 3$d$ $e_g$

### Magnetic Properties of CuFeO$_2$

<table>
<thead>
<tr>
<th>structure</th>
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<th>$\Delta E$</th>
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<td>$-32.0$</td>
<td>3.62</td>
<td>0.19</td>
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Magnetic Properties of CuFeO₂

**Antiferromagnet**

![DOS plot](image)

**Results**
- monoc. structure
- Fe³⁺ HS
- O 2p polarization via Fe 3d eg
- $E_g > 0$ in GGA

### Magnetic Properties of CuFeO$_2$

<table>
<thead>
<tr>
<th>structure</th>
<th>magn. order</th>
<th>$\Delta E$</th>
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<th>$m_{O}$</th>
<th>$E_g$</th>
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<td>$-12.0$</td>
<td>2.02</td>
<td>$-0.02$</td>
<td>-</td>
</tr>
<tr>
<td>rhomb.</td>
<td>ferro (HS)</td>
<td>$-19.2$</td>
<td>3.73</td>
<td>0.21</td>
<td>-</td>
</tr>
<tr>
<td>monoc.</td>
<td>spin-deg.</td>
<td>$-6.0$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>monoc.</td>
<td>ferro (LS)</td>
<td>$-21.5$</td>
<td>1.04</td>
<td>$-0.02$</td>
<td>-</td>
</tr>
<tr>
<td>monoc.</td>
<td>ferro (IS)</td>
<td>$-19.0$</td>
<td>2.08</td>
<td>$-0.02$</td>
<td>-</td>
</tr>
<tr>
<td>monoc.</td>
<td>ferro (HS)</td>
<td>$-32.0$</td>
<td>3.62</td>
<td>0.19</td>
<td>-</td>
</tr>
<tr>
<td>monoc.</td>
<td>antiferro</td>
<td>$-46.0$</td>
<td>$\pm3.72$</td>
<td>$\pm0.08$</td>
<td>0.05</td>
</tr>
</tbody>
</table>

A Short Walk: Fundamental Principles
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La$_2$BaCuO$_5$ Moments

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La$_2$BaCuO$_5$ Moments

La$_2$RuO$_5$ Orbitals

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Thank You for Your Attention!