Reconciling spin 1 and orbital degeneracy in $V_2O_3$

Frédéric MILA
Institut de Physique Théorique
Université de Lausanne (Switzerland)

Collaborators: R. Shiina, F.-C. Zhang, A. Joshi, M. Ma, V. A. Anisimov, T. M. Rice

Scope

- Introduction to $V_2O_3$
  - Phase diagram
  - New experiments
- Vertical pair
  - Level crossings
  - Orbital degeneracy
- Pair model
  - In-plane coupling
  - Role of spin-orbit coupling
  - Open issues
- Conclusions
Dr. Frederic Mila, Lausanne (KITP Correlated Electron Materials 10-07-02) Reconciling Spin 1 and Orbital Degeneracy in V203

Structure of V2O3

Vanadium lattice ↔ coupled hexagonal lattices

Corundum structure

Phase diagram of V2O3

\((V_{1-x}Cr_x)O_3\)
New experiments

**Bao et al** (PRB '98) Inelastic neutron scattering

Fluctuations in PI phase **not related** to magnetic order in AFI

\( (1, 0, 1) \) and \( (1, 1, 0) \)

**Park et al** (PRB 2000) Polarized X-ray absorption

Both \( e_g e_g \) and \( a_{1g} e_g \) + Spin 1

**Paolasini et al** (PRL '99) Resonant X-ray scattering

Additional Bragg peaks **not directly related** to magnetic order

**Goulon et al** (PRL 2000) Nonreciprocal X-ray gyrotropy

Magnetic group **non** centrosymmetric

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Single site

Spin 1 but **NO ORBITAL DEGENERACY**!

\[ \Rightarrow \text{consider vertical pairs (Castellani et al., '79)} \]
Theory of V$_2$O$_3$: Basic Ingredients

Relevant states of a vertical pair

$|e_g a_1; e_g e_g\rangle$

or/and

$|e_g e_g; e_g a_1\rangle$

Residual interactions

- Inter-pair couplings
- Spin-orbit coupling
- Coupling to the lattice

Pair model

Effect of interpair coupling on $|e_g a_1; e_g e_g\rangle$ configurations

F. Mila et al. PRL 2000; R. Shina et al. PRB 2001

- Spin 1 on each site + Ferromagnetic coupling $\Rightarrow S = 2$ ($\sigma$)
- Choice for empty $e_g$ orbital $\Rightarrow 2$-fold orbital degeneracy ($\tau$)

$H_{\text{eff}} = (G_1 + \frac{1}{3}G_2 + \frac{1}{2}G_3)\vec{\sigma},\vec{\tau}$

$G = \frac{1}{3}G_1 + \frac{3}{2}G_2 + \frac{1}{2}G_3$

$G_1 = \frac{4\pi^2}{v_F}$

$G_2 = \frac{4\pi^2}{v_F}$

$G_3 = \frac{4\pi^2}{v_F}$

appropriately rotation by $2\pi/3$ for other bonds.
Resonant X-ray scattering (Paulasi et al., PRL 1999)

- Bragg peaks consistent with magnetic structure
- Additional Bragg peaks with orbital ordering?

Pair model

\[
O \left( e_g \right) = \left( \sqrt{2} d_{xy} + d_{xz} \right) / \sqrt{3}
\]

\[
\left( e_g \right) = \left( \sqrt{2} d_{xy} - d_{yz} \right) / \sqrt{3}
\]

Additional Bragg peaks consistent with magnetic scattering

Nonreciprocal X-Ray Gyrotropy (Goulon et al., PRL 2000)

First Proposal (Di Matteo et al., unpublished)

Different \( e_g \) orbitals on different vertical pairs

Inversion center is lost.
**Alternative explanation: Spin canting**

Ferromagnetic bonds **very weak** (Bao et al, unpublished)

Dzyaloshinskii-Moriya interaction $\Rightarrow$ small canting

\[ \text{NB: Exchange constants consistent with pair model if some mixing with } \left| e_g e_g; e_g e_g \right| \text{ is included (Shiina et al, PRB '01).} \]

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**Effect of spin-orbit coupling**

- Magnetic resonant scattering
- Orbital moments $\rightarrow$ Additional Bragg peaks (Lovesey and Knight; Tanaka)
- Tilting of magnetic moments away from z-axis if $\left( e_g e_g; e_g e_g \right)$ not too far (Shiina et al, PRB 2001; see also Tanaka)

More radical point of view

A. Tanaka, cond-mat/0201407

- Degeneracy between $\left| e_g a_1; e_g e_g \right|$ and $\left| e_g a_1; e_g e_g \right|$ lifted

$\rightarrow$ NO ORBITAL DEGENERACY!

- Why 1st order transition? (Pair model OK, see Joshi et al, PRL '00).
- Why $J_{\text{Ferro}}$ and $J_{\text{AF}}$ so different?
- Why treat $t_{\text{in-plane}}$ as second-order effect? ($t_{\text{in-plane}} \gg \Delta_{\text{spin-orbit}}$)
Conclusions

- $\text{V}_2\text{O}_3$ still resists!

- Orbital degeneracy
  - Plays an essential role.
  - No orbital ordering at atomic level.
  - Possible orbital ordering of vertical pairs $\Rightarrow$ \textsc{good case for ferroorbital ordering of vertical pairs}

- Resonant X-Ray scattering
  - Excellent technique to probe orbitals in $\text{V}_2\text{O}_3$ $\Rightarrow$ \textsc{final answer?}