

Nematic Order in $\text{Sr}_3\text{Ru}_2\text{O}_7$

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PRB **79** 214402 (2009)



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I. Overview

Ruthenates: $\text{Sr}_{n+1}\text{Ru}_n\text{O}_{3n+1}$

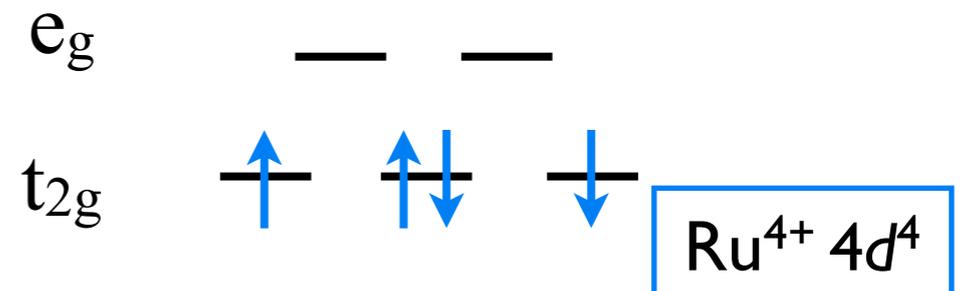
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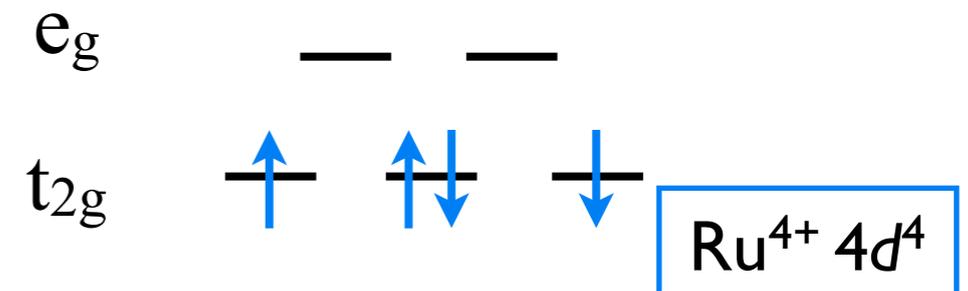
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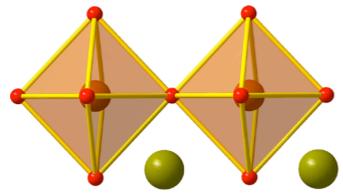


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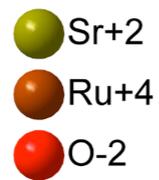
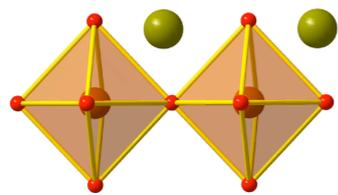
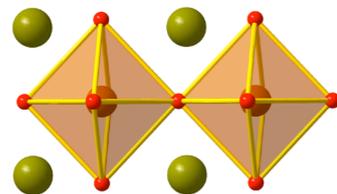
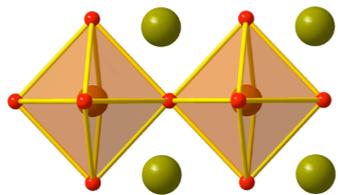
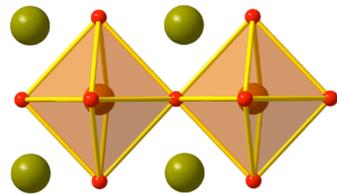
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- 4) Spin-orbit coupling plays an important role (*e.g.* affects Fermi-surface topology).



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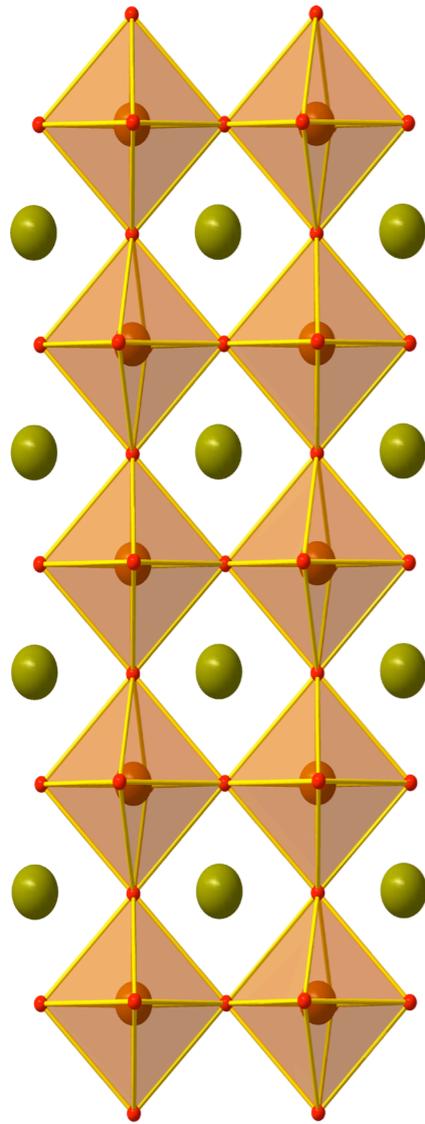


$n = 1$: Sr_2RuO_4 unconventional
superconductivity $T_c=1.5\text{K}$.

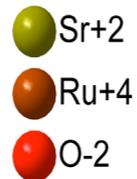


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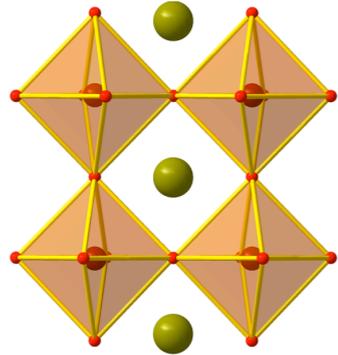
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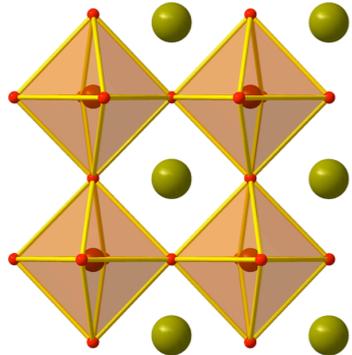
← $n = \infty$: SrRuO_3 Ferromagnetism
 $T_c = 165\text{K}$.



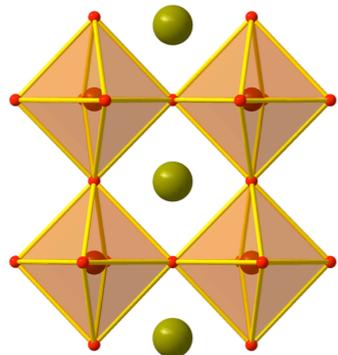
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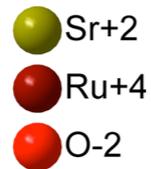
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$n = 2$: $\text{Sr}_3\text{Ru}_2\text{O}_7$ metamagnetism, quantum critical fluctuations.

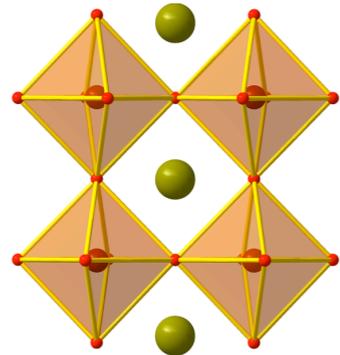


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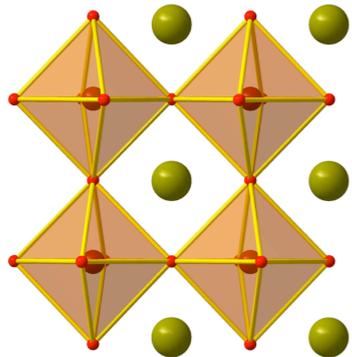


increasing itinerancy with n (FM for $n > 3$).

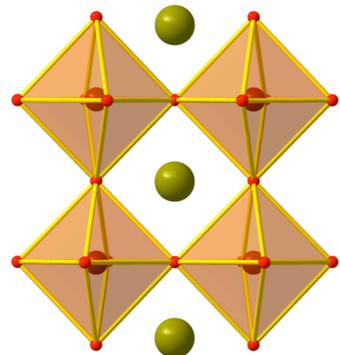
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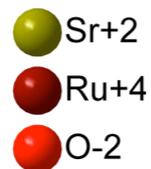
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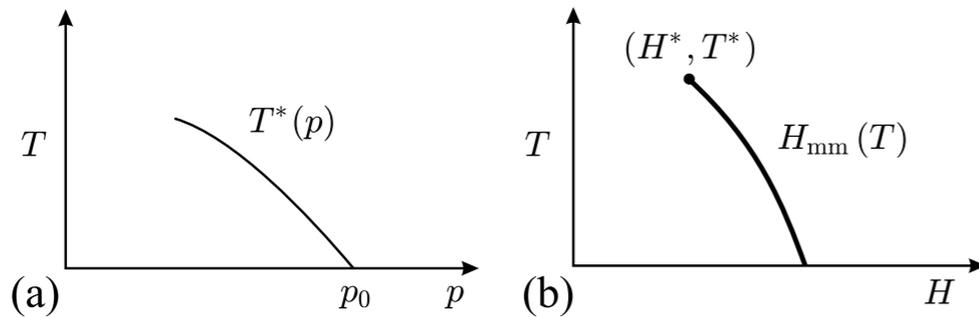
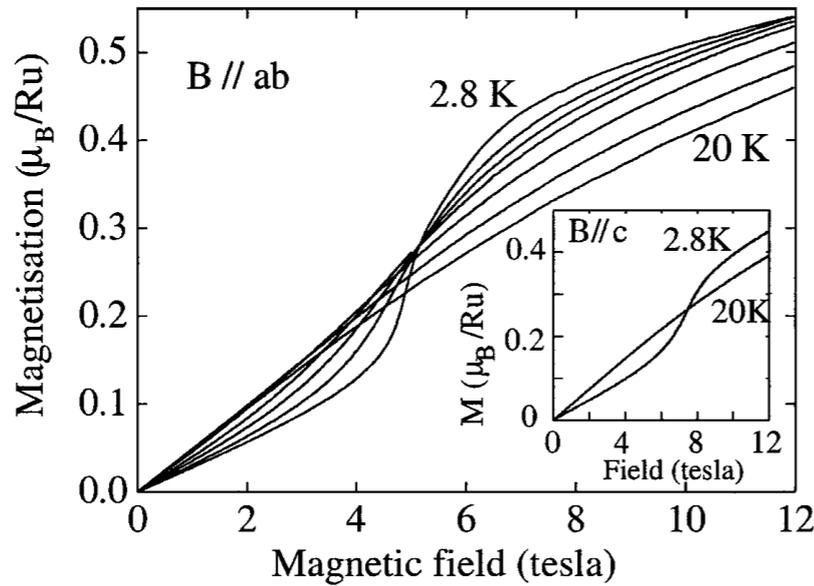
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 $n > 3$).

In this talk: we concentrate on $n=2$: $\text{Sr}_3\text{Ru}_2\text{O}_7$

II. Experimental phase diagram of $\text{Sr}_3\text{Ru}_2\text{O}_7$

Metamagnetism

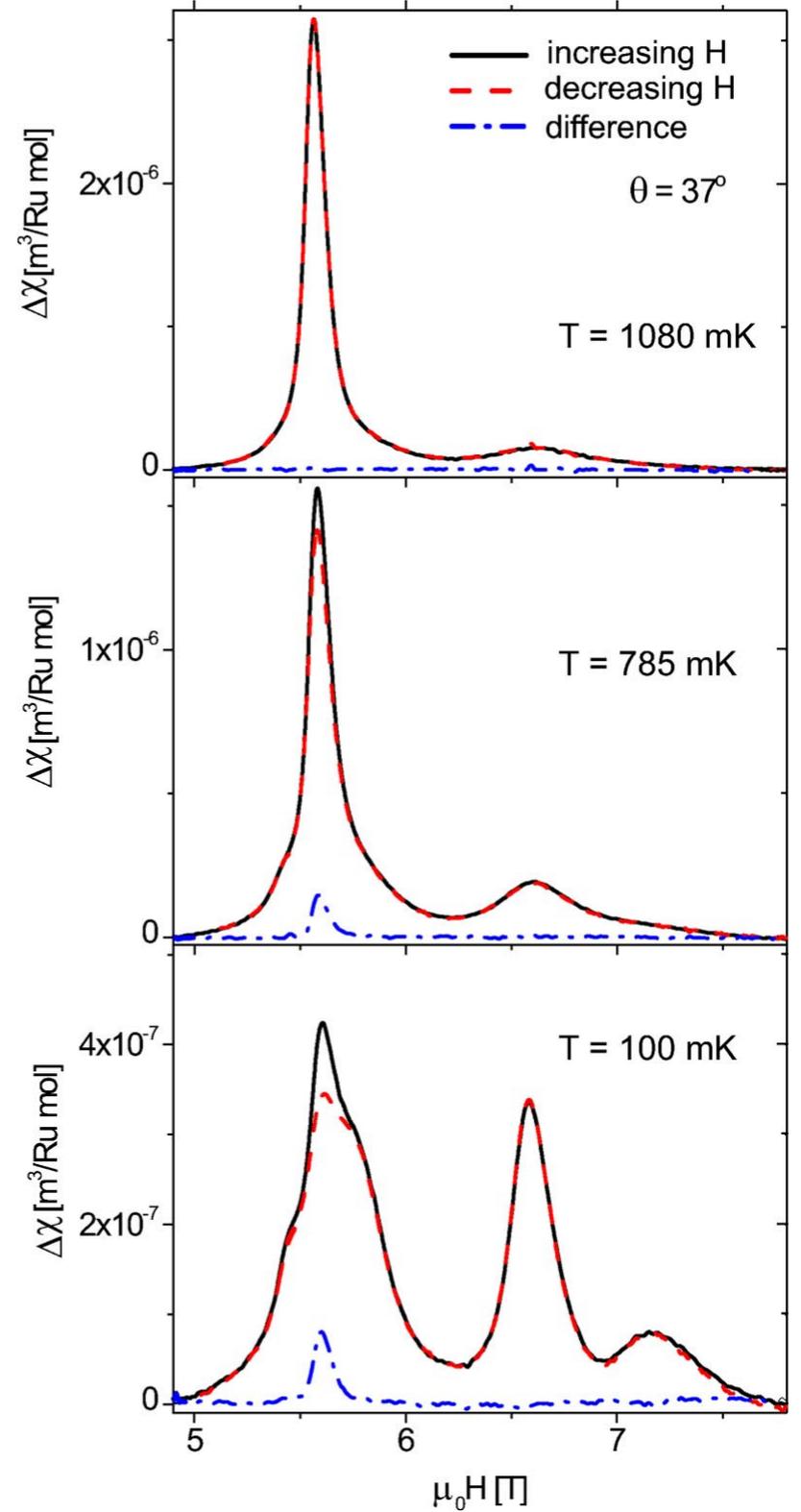
1st order transition
(no symmetry breaking)



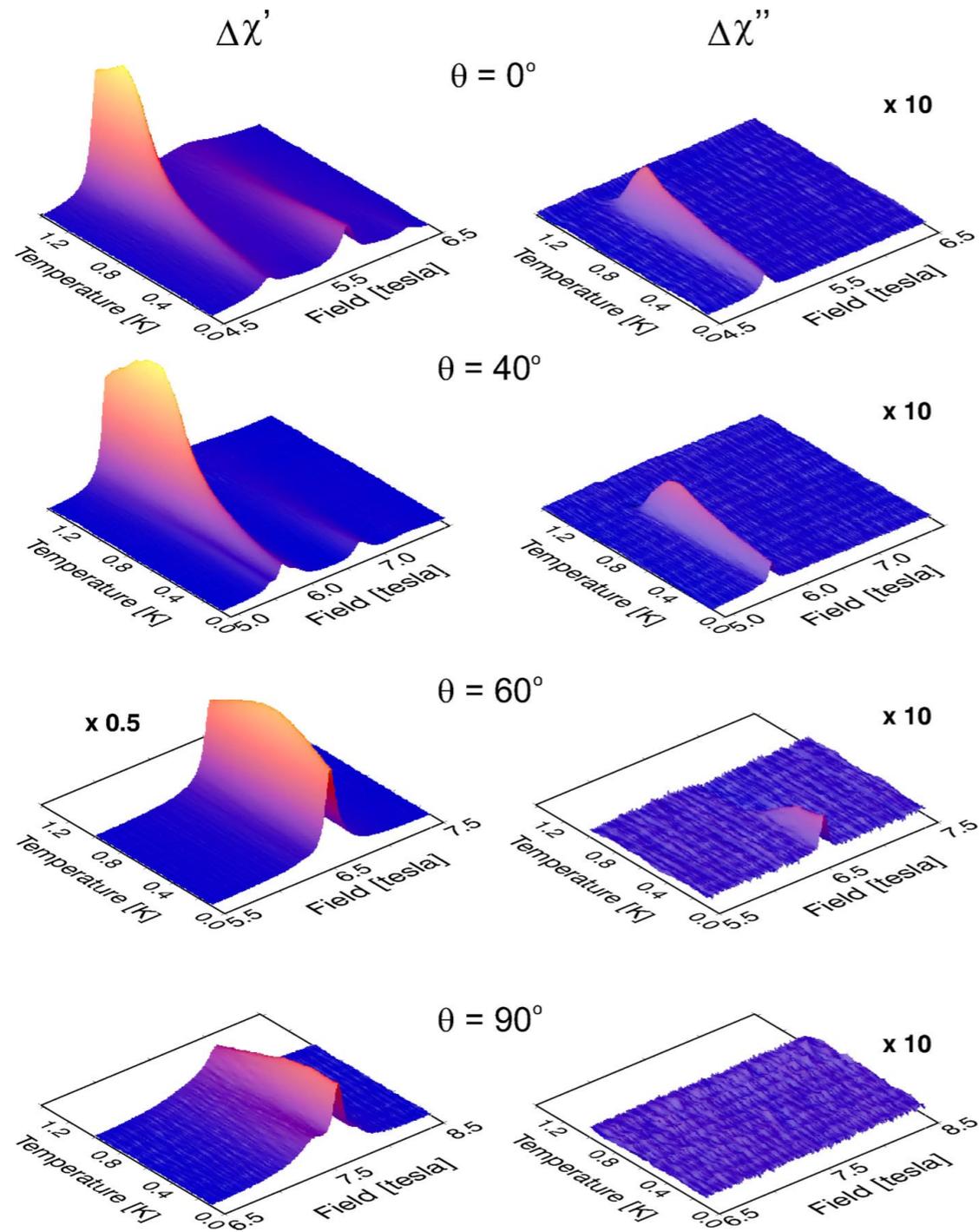
Analogous to Liquid-gas transition:
presence of a critical end point

$T < T^*$: 1st-order transition
 $T > T^*$: crossover

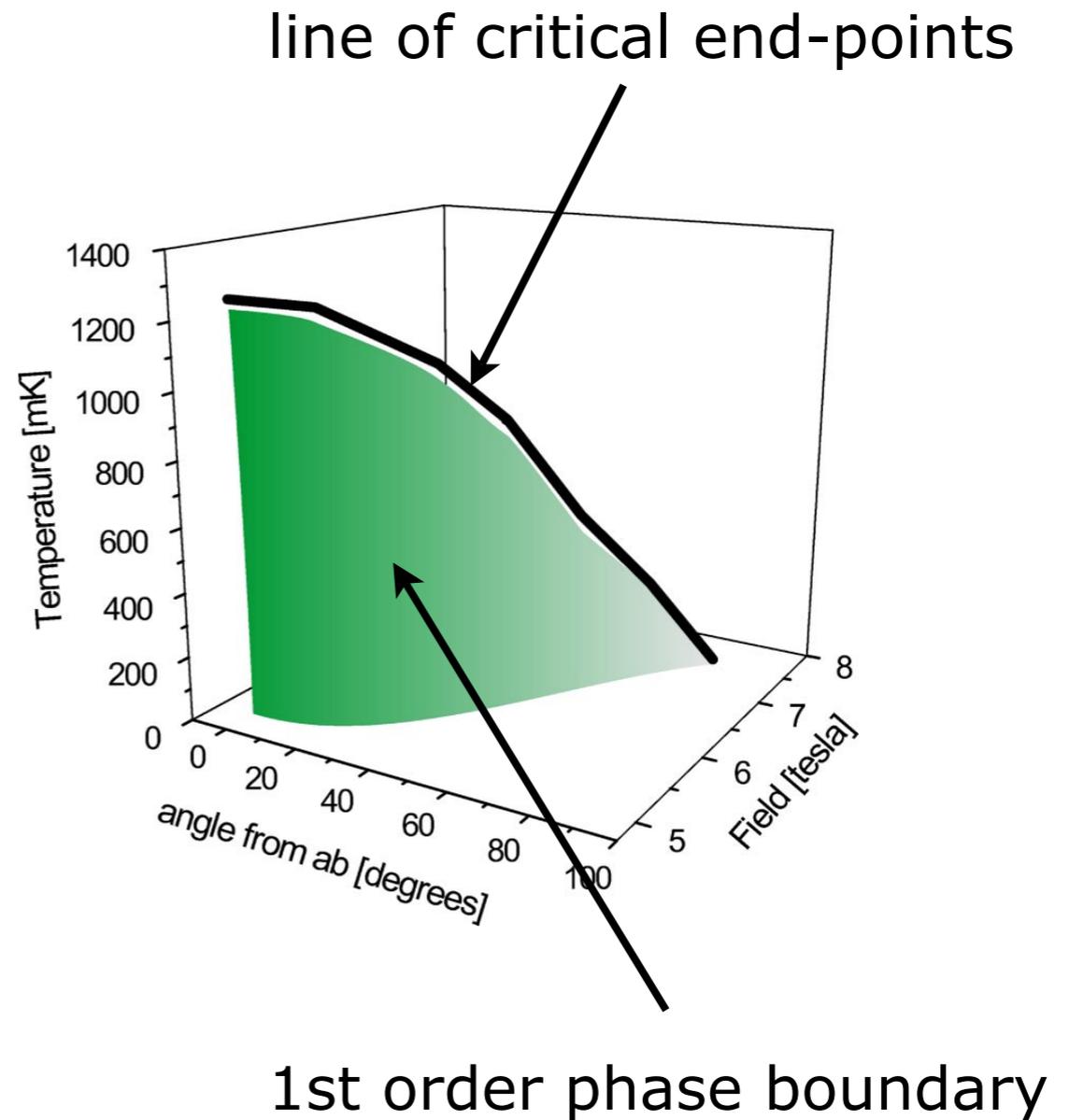
Hysteresis



Dependence on field orientation



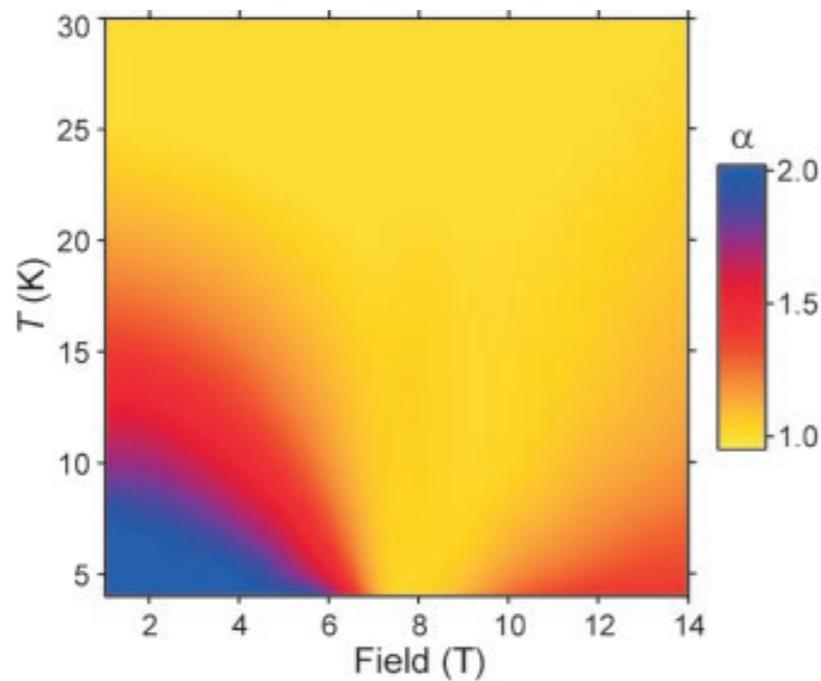
$T^* \rightarrow 0$ for H parallel to c-axis



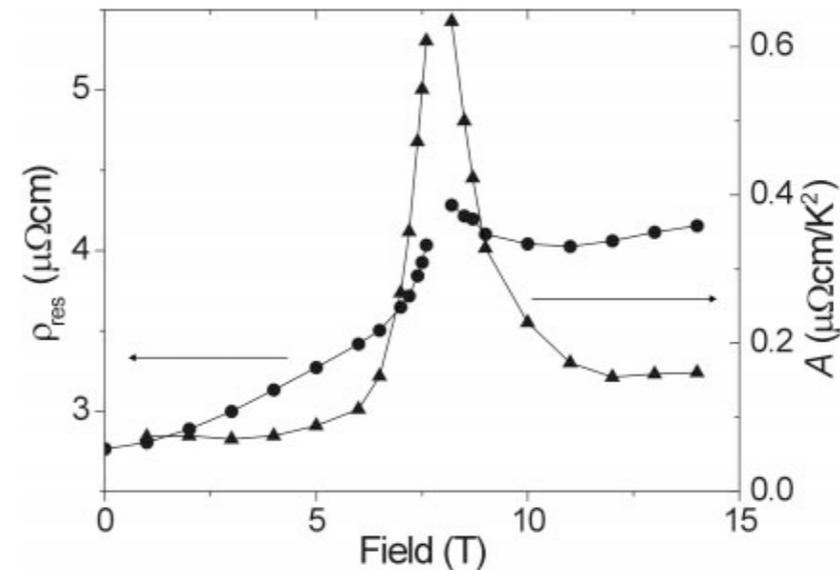
PRB **67**, 214427 (2003)

“Metamagnetic quantum criticality”

$$\rho(T) = \rho_{res} + AT^\alpha$$



non-FL behavior,
quantum critical
fluctuations

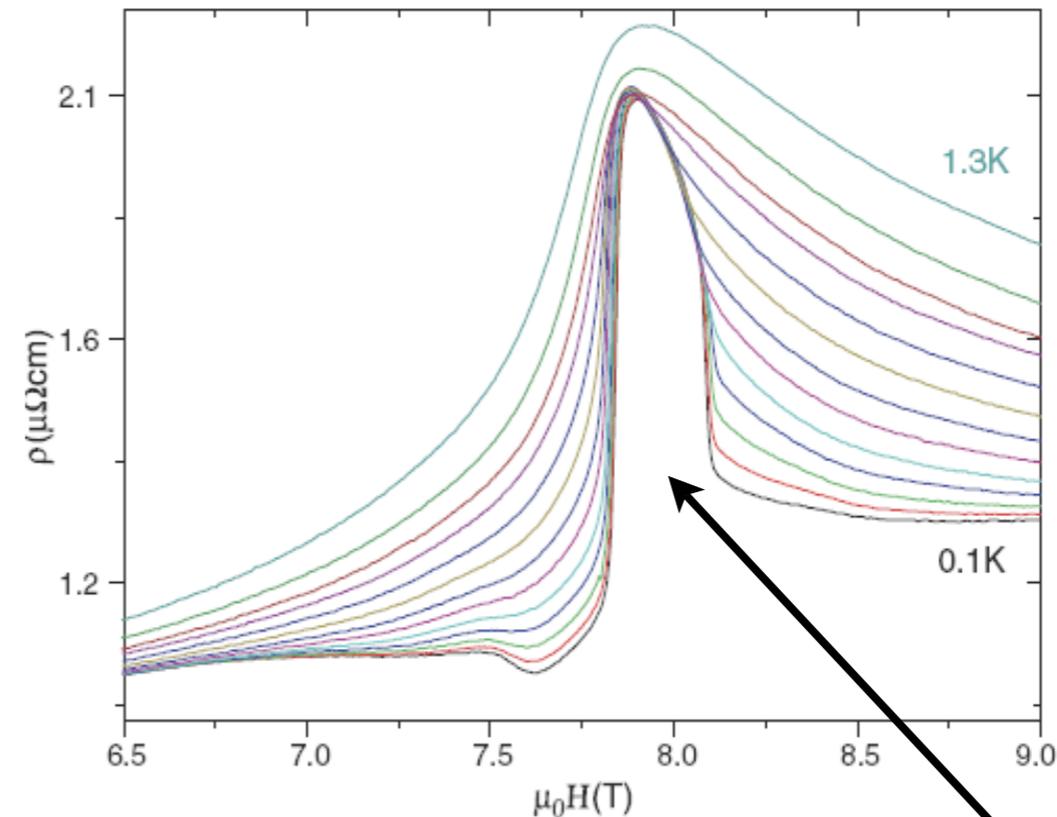
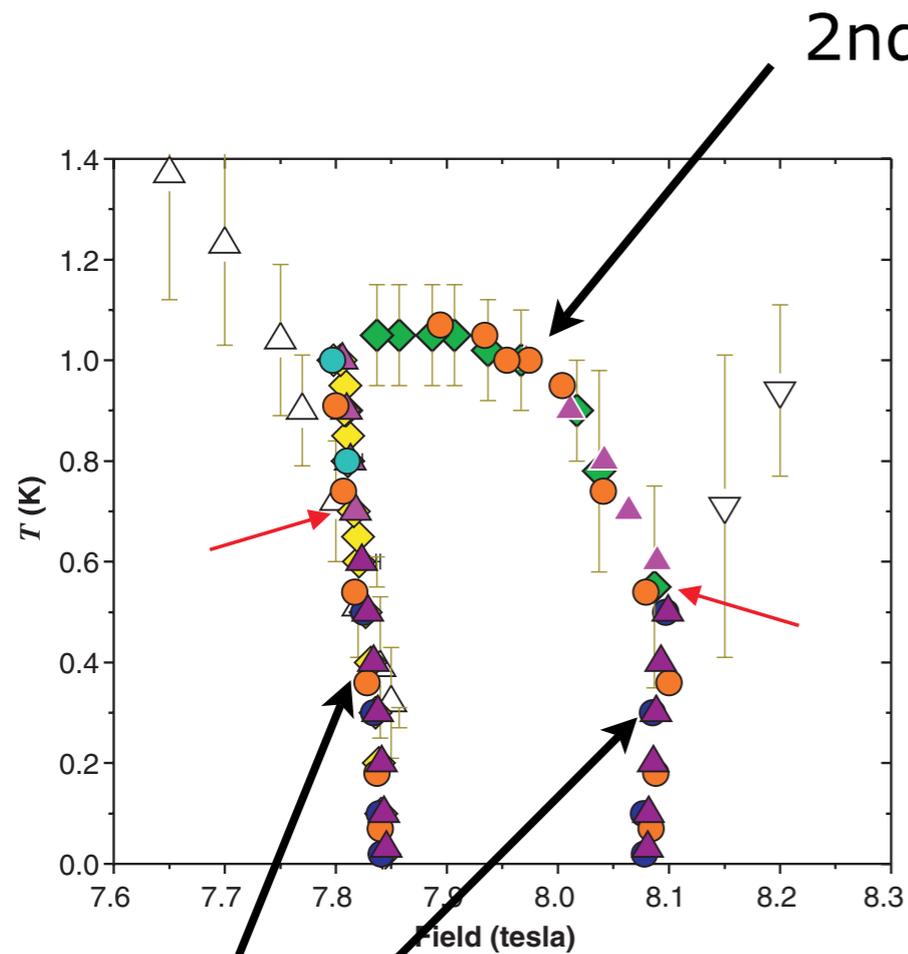


divergence of qp mass
near qcp (also seen in
quantum oscillations).

Science **306**, 1154 (2004)

This is a new type of quantum critical phenomena: associated with a critical end point, and no symmetry breaking. However...

Ultra-pure crystals: new low T phase



Science **306**, 1154 (2004)

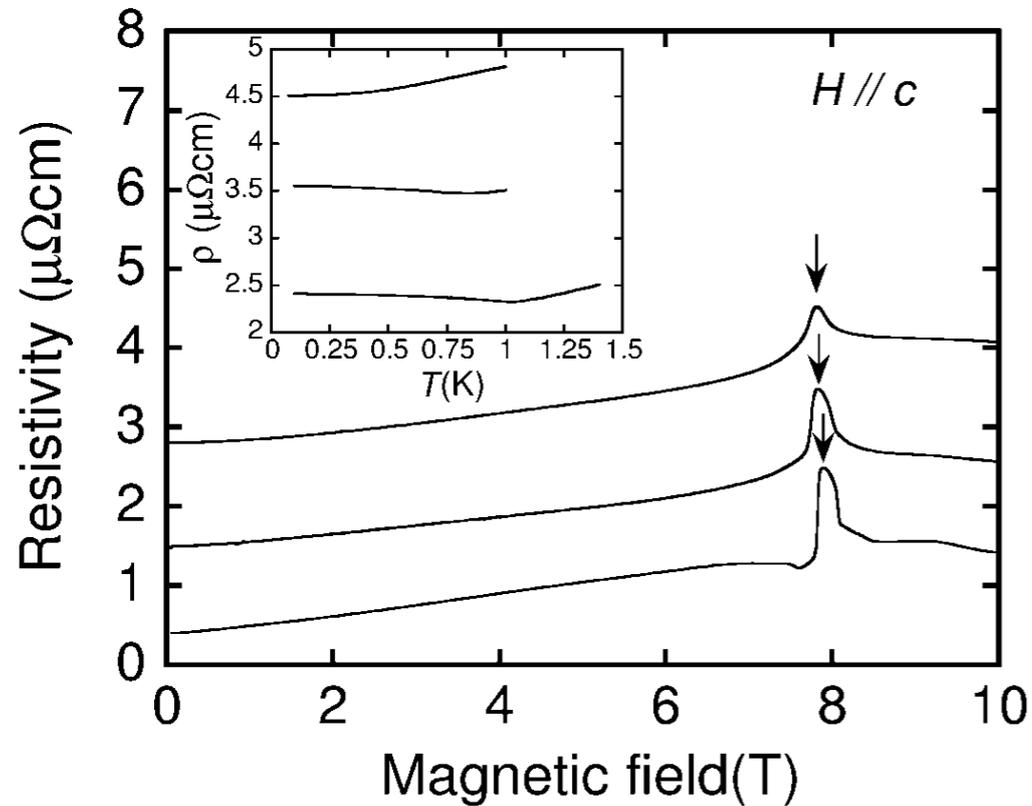
enhanced scattering

1st order boundaries

In the purest crystals, the "metamagnetic qcp" is enveloped by a thermodynamic phase at low T.

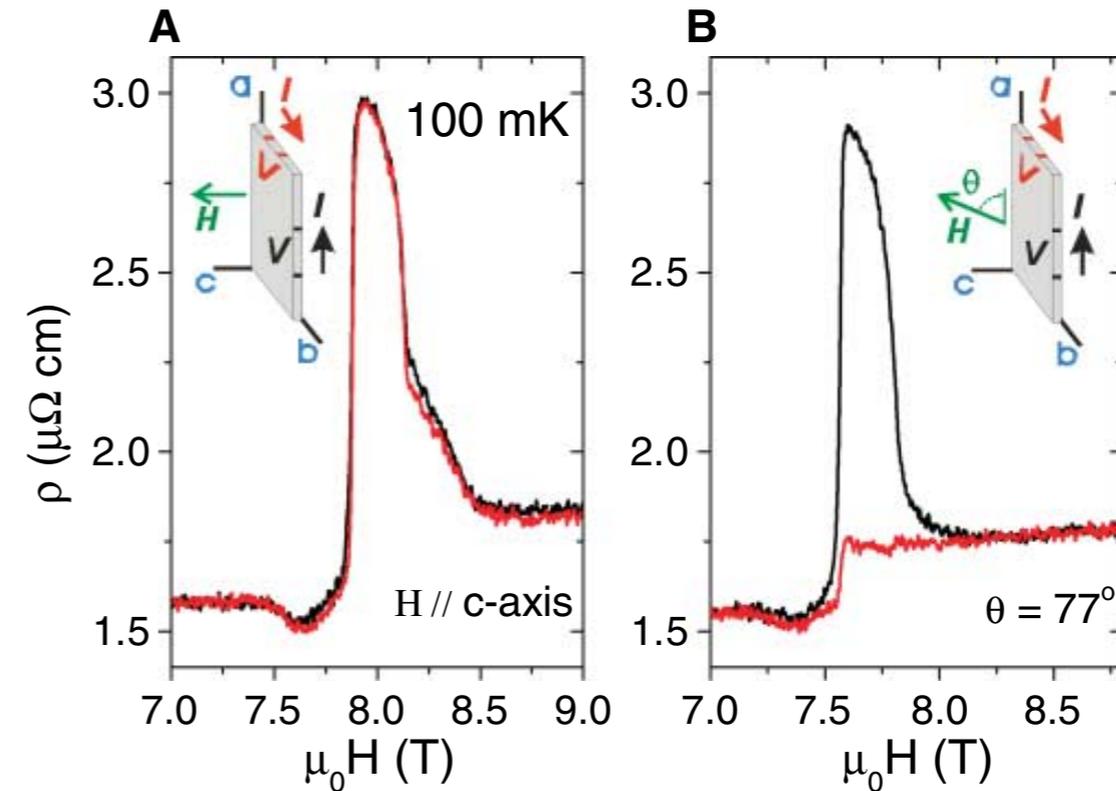
Properties of the low T phase near H_c

PRL **92**, 166602 (2004)



Very sensitive to disorder

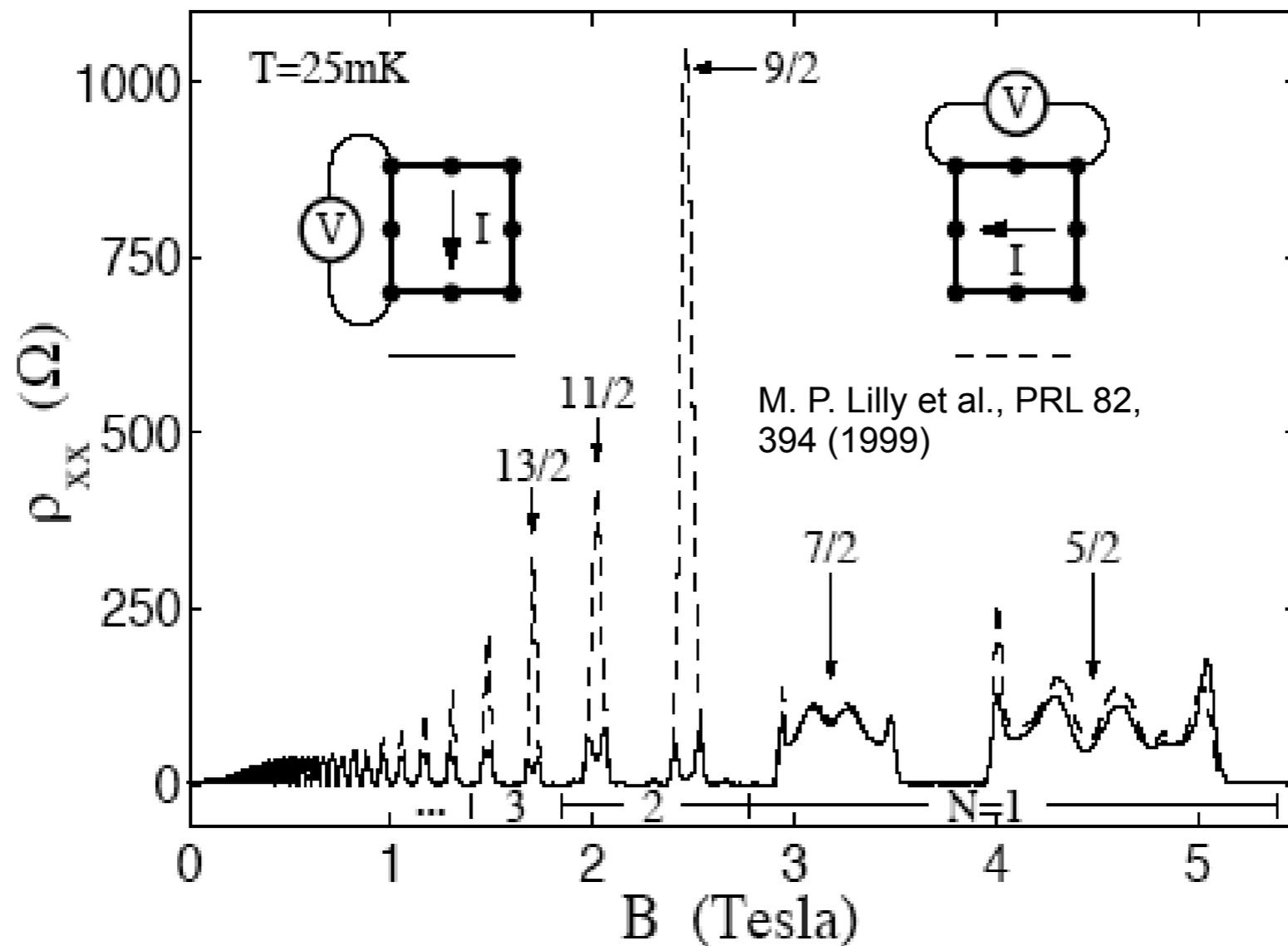
Science **315**, 214 (2007)



Order 1 resistive anisotropy
 C4 symmetry reduced to C2
 (no associated structural transition)

The phase has orientational order, but translational symmetry is preserved
 electronic analog of **nematic** phase.

Similar features observed in 2DEG at high B fields



M. M. Fogler, et al, PRL 76 ,499 (1996), PRB 54, 1853 (1996); E. Fradkin et al, PRB 59, 8065 (1999), PRL 84, 1982 (2000).

III. Microscopic model and theoretical phase diagram

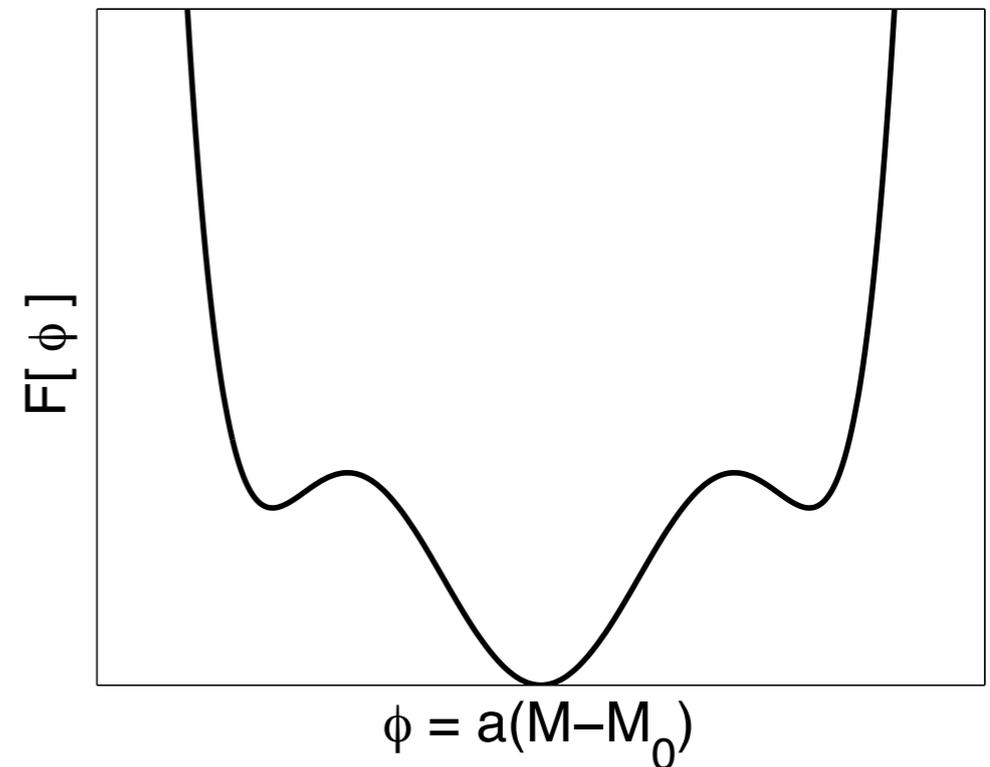
Itinerant electron metamagnetism

First consider effective theory for itinerant electron metamagnetism

$$F = \alpha\phi^2 - \beta\phi^4 + \gamma\phi^6 - H\phi$$

$$1. E = \sum_{\sigma} \int_{-\infty}^{\mu_{\sigma}} d\epsilon \epsilon \nu(\epsilon)$$

$$2. M = \sum_{\sigma} \sigma \int_{-\infty}^{\mu_{\sigma}} d\epsilon \nu(\epsilon)$$



From 1, and 2, we can derive Landau coefficients.

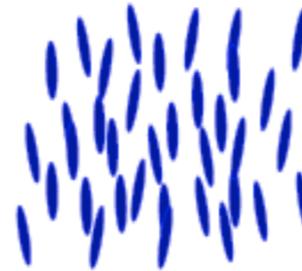
Requirement for weakly first-order metamagnetic transition:
D.O.S at the fermi level must have pronounced positive curvature.

Electronic nematic phases

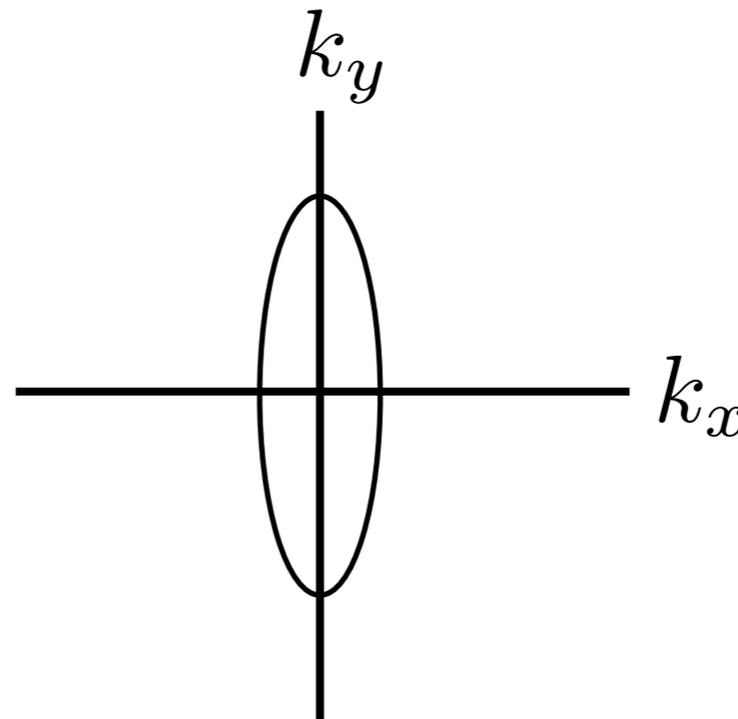
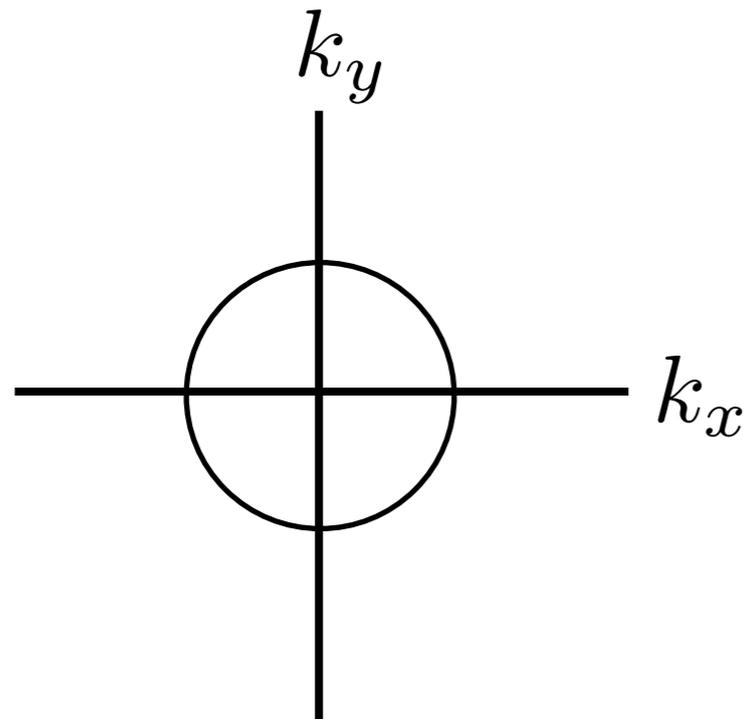
Isotropic



Nematic



Classic nematic liquid crystal:
preserves translation
breaks rotation
symmetry.



Electronic analog:
Fermi surface breaks
underlying rotational
symmetry.

effective theory of the nematic transition: L=2 Fermi-liquid instability.

$$V_{eff} = \sum_{\mathbf{k}, \mathbf{k}'} f_2 P_2(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') \delta n_{\mathbf{k}\sigma} \delta n_{\mathbf{k}'\sigma'}$$

Formulating a microscopic theory

Problems with a microscopic formulation:

- 1) Both metamagnetism and nematic order arise as intermediate to strong-coupling effects: difficult to treat theoretically. Stoner mean-field theory: $N(E_f)U \sim 1$ not a well-controlled method.
- 2) Difficult to imagine why metamagnetism and nematicity should be tied together.

Critical insight into both of these issues: H.-Y. Kee *et al.* PRB (2005). Consider *effective* models close to van Hove singularities.

Proposal of H.-Y. Kee *et al.*

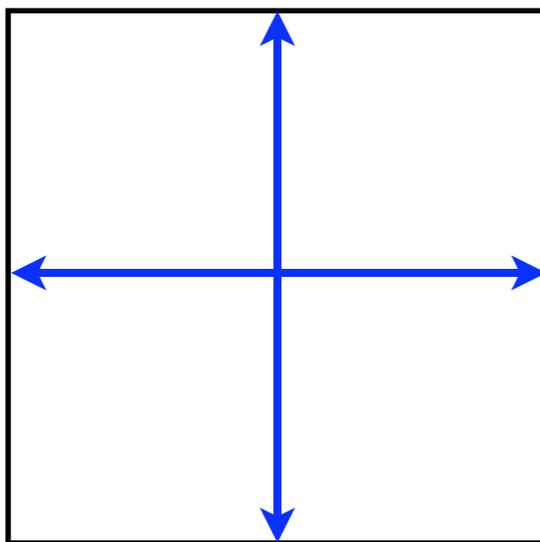
PRB **71**, 184402 (2005)

$$H = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q},\sigma} F_2(\mathbf{q}) \text{Tr}[\hat{Q}_\sigma(\mathbf{q})\hat{Q}_\sigma(-\mathbf{q})] + \text{H.c.}$$

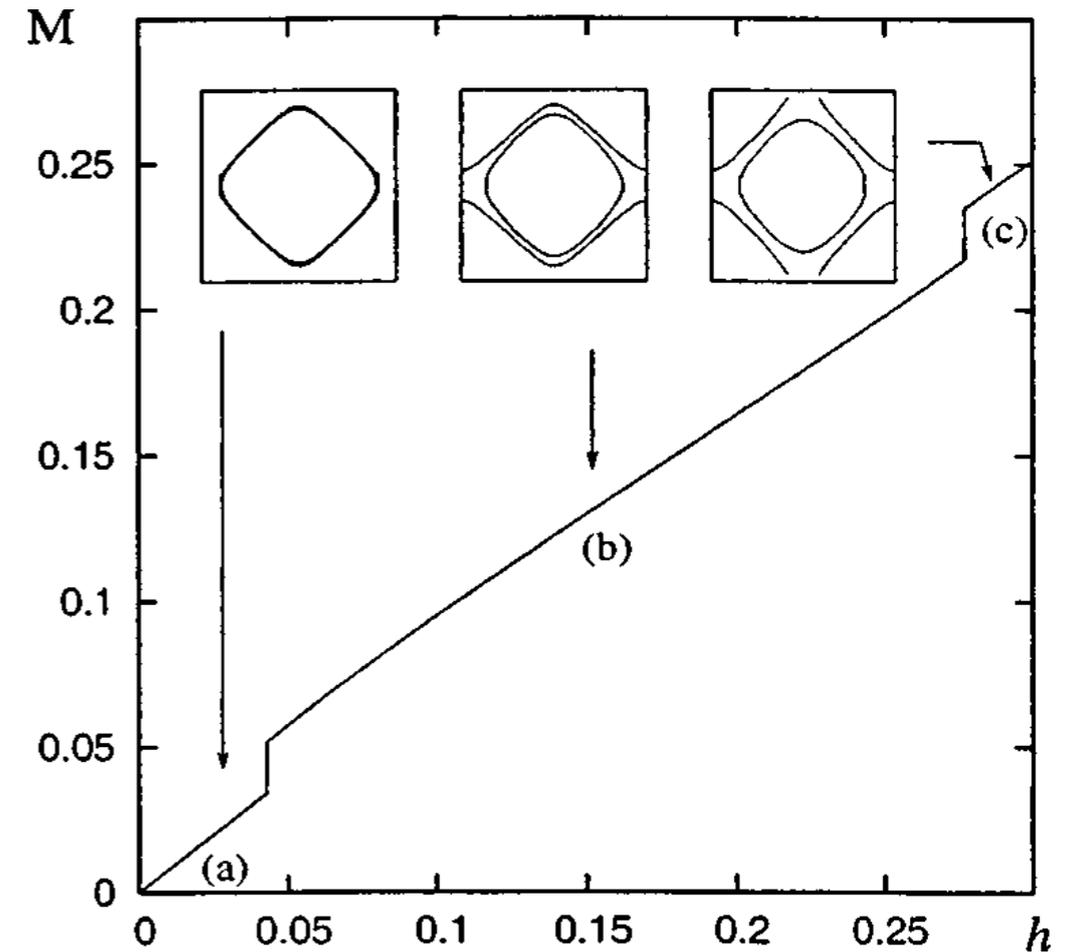
V_{eff} $\hat{Q}_\alpha^{ij}(\mathbf{q}) \sim \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\alpha}^\dagger \left(\hat{k}^i \hat{k}^j - \frac{1}{2} \hat{k}^2 \delta^{ij} \right) c_{\mathbf{k}\alpha}$

effective model of single band near vHS

V_{eff}



Attractive



Proposal of H.-Y. Kee *et al.*

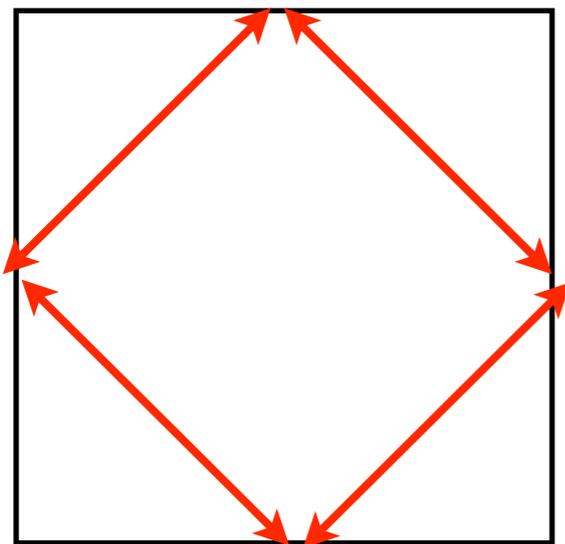
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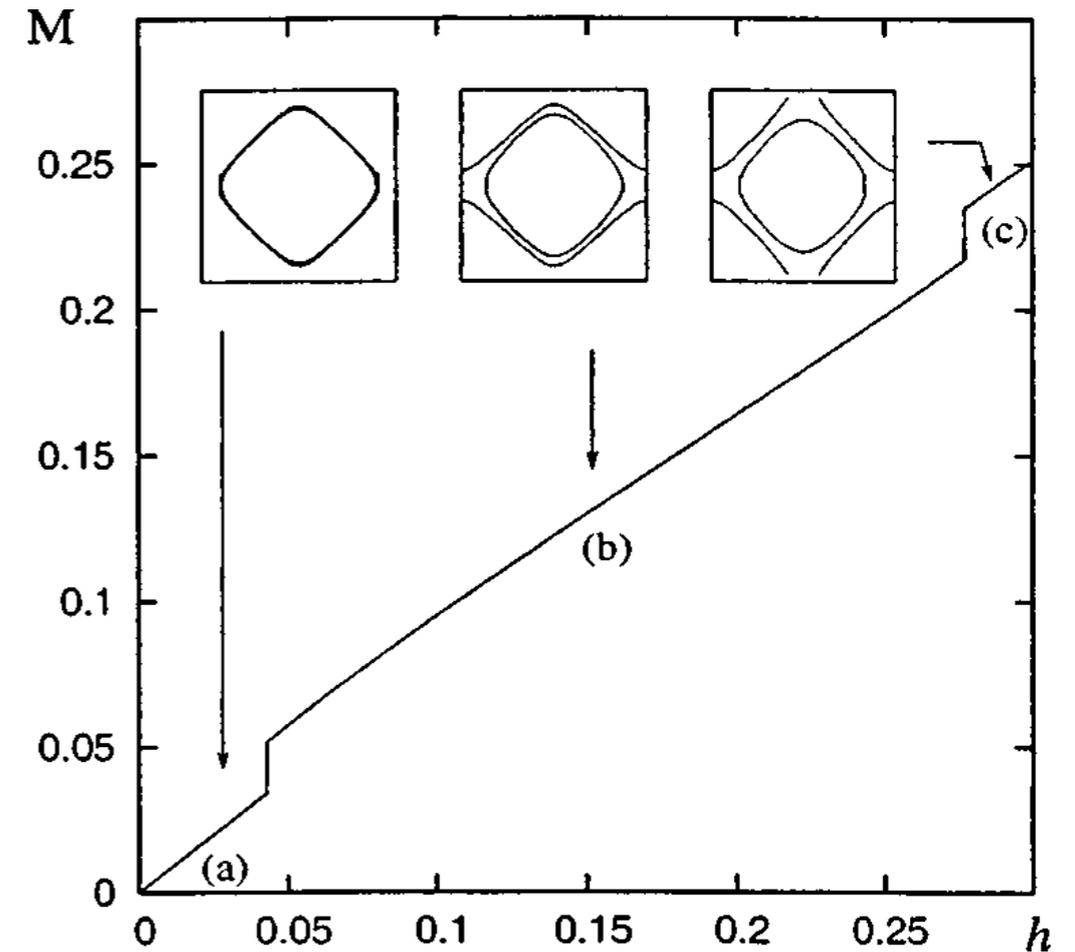
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Repulsive



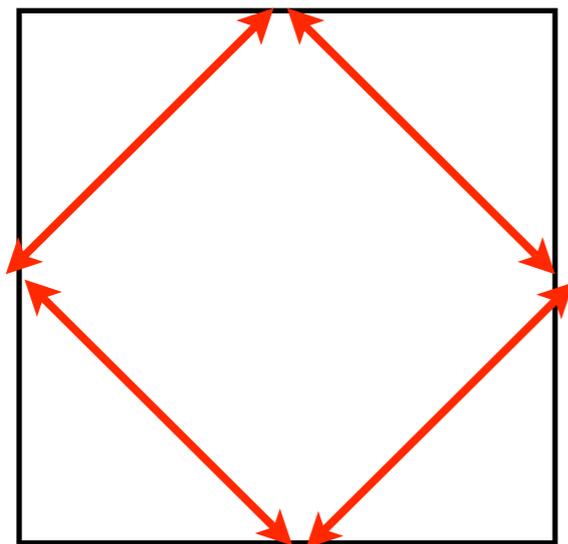
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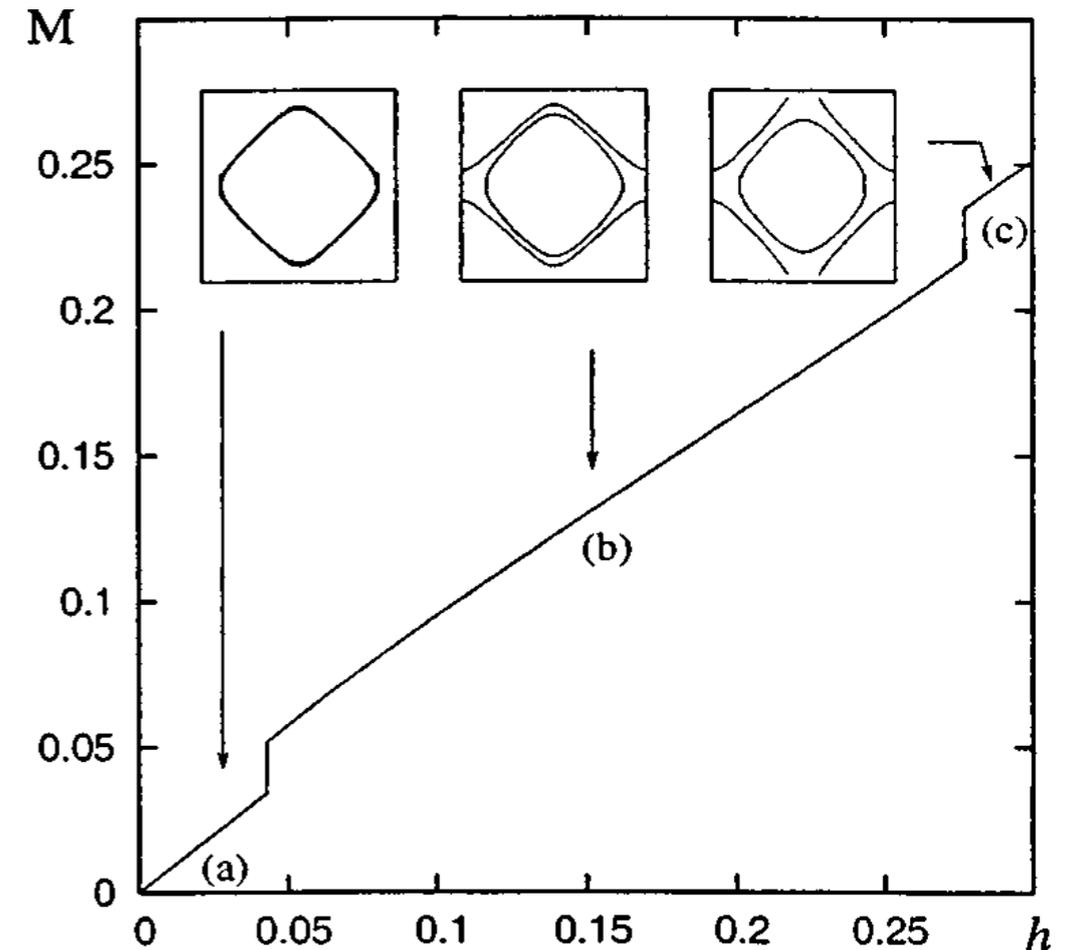
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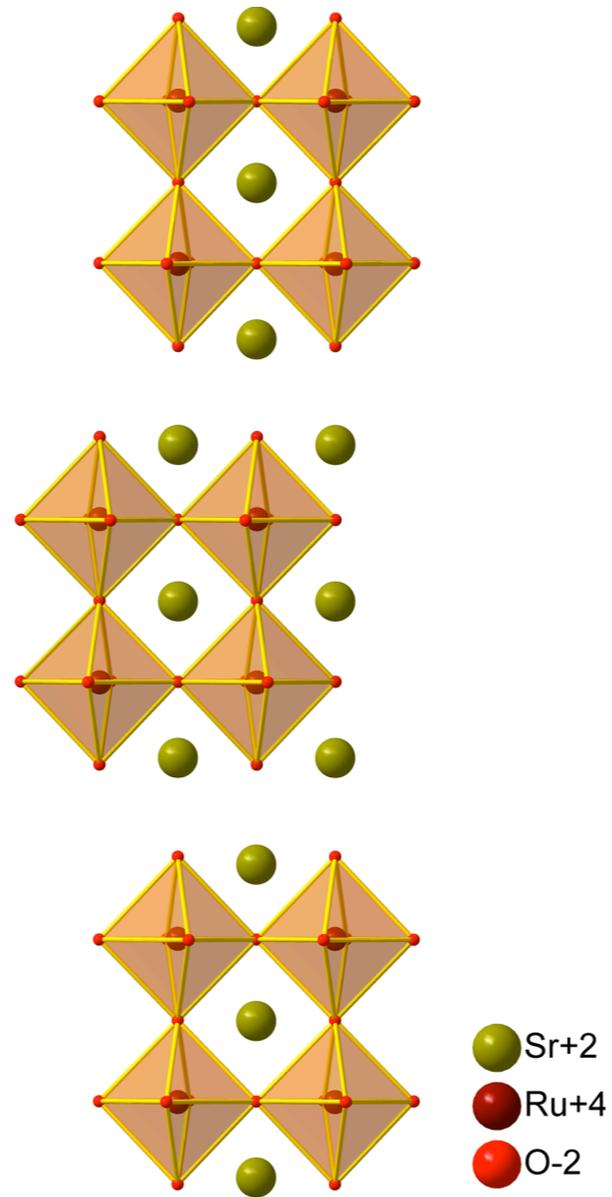
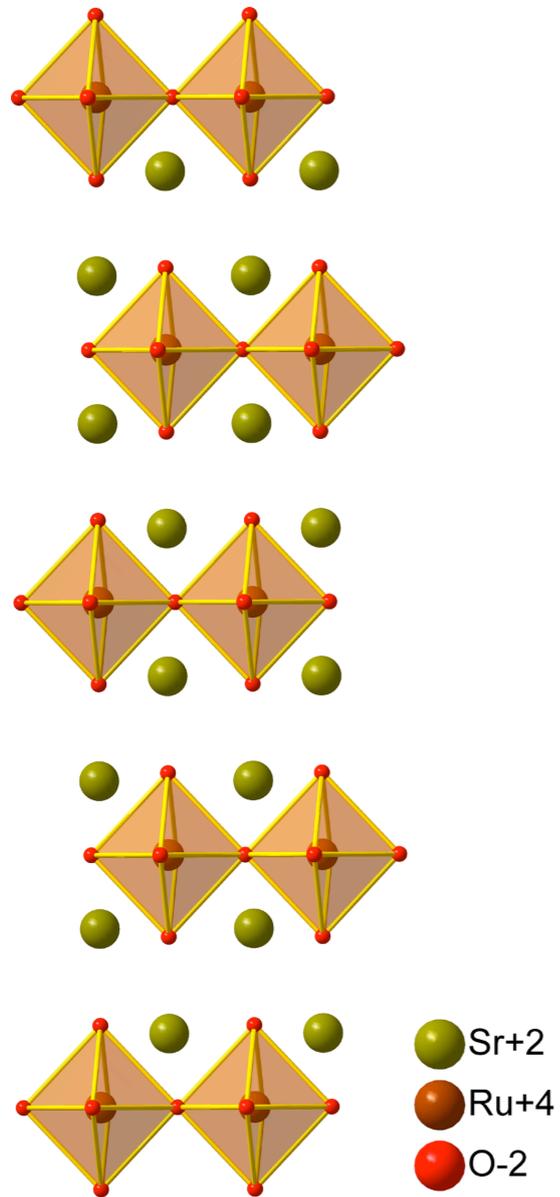


Although the phenomena can be “engineered”,

Microscopic origins of this is still unclear.

Our proposal: metamagnetic and nematic transitions here are both driven by **orbital-ordering** tendency.

Monolayer vs. bilayer ruthenate compounds

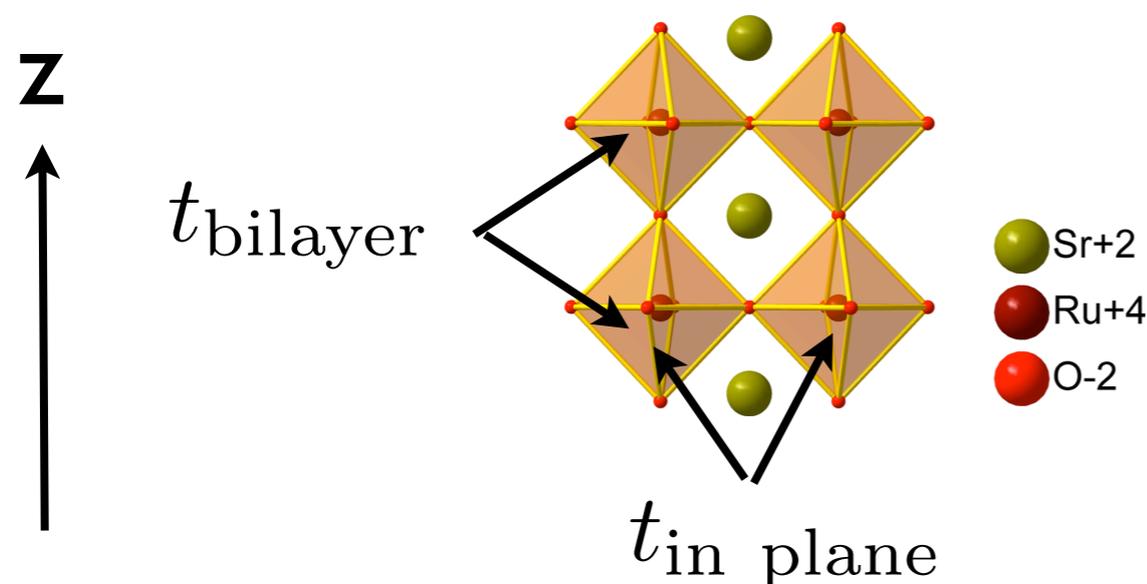
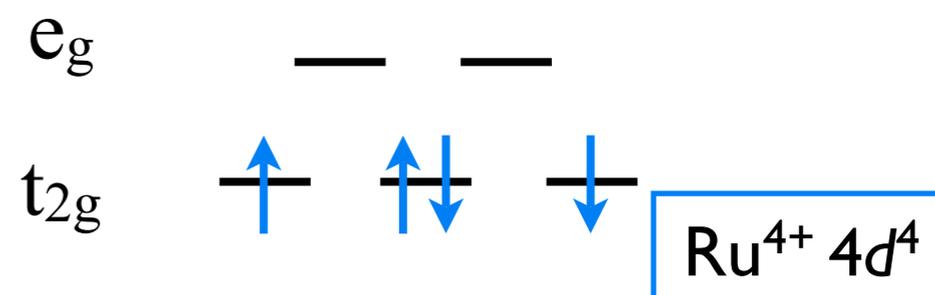


What are the microscopic origins of the low temperature physics of $\text{Sr}_3\text{Ru}_2\text{O}_7$?

i.e. why do Sr_2RuO_4 and $\text{Sr}_3\text{Ru}_2\text{O}_7$ have such different physical properties?

Monolayer vs. bilayer ruthenate compounds

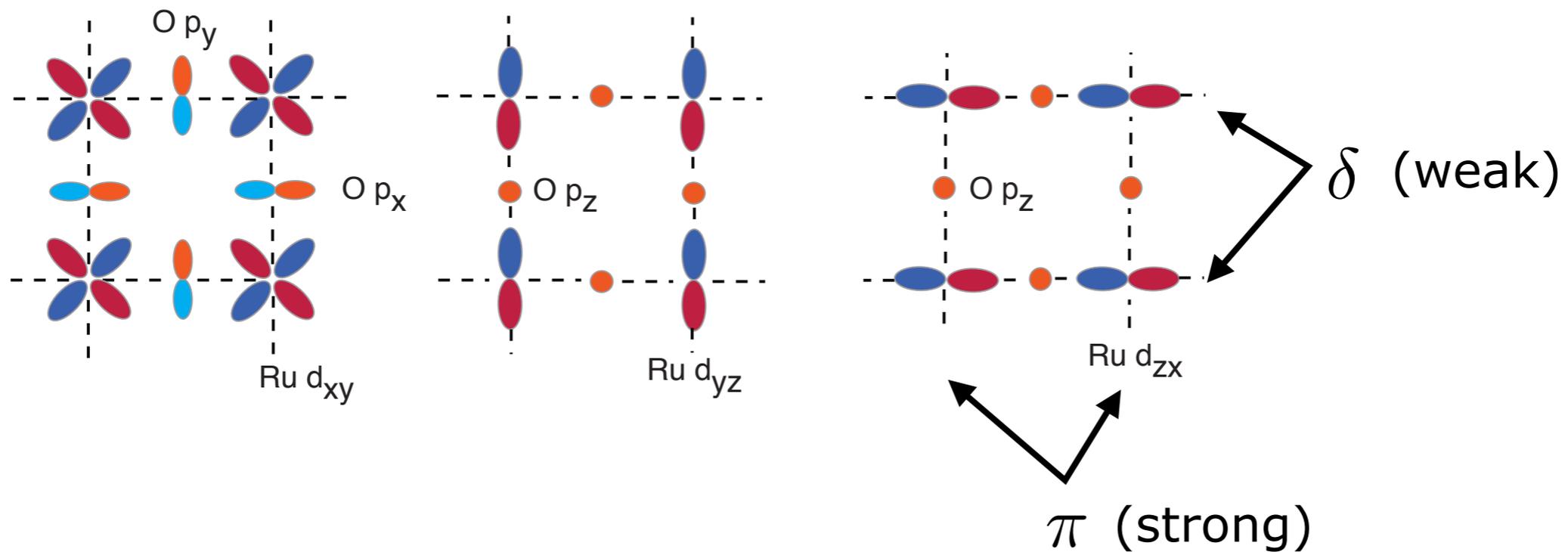
In both of these materials, degeneracy of Ru t_{2g} (d_{xz}, d_{yz}, d_{xy}) orbitals plays a crucial role.



The **strong** bilayer splitting in $Sr_3Ru_2O_7$ is the primary difference between the two materials.

$$t_{in\ plane} \approx t_{bilayer}$$

Which of the t_{2g} orbitals are most affected by the bilayer splitting?



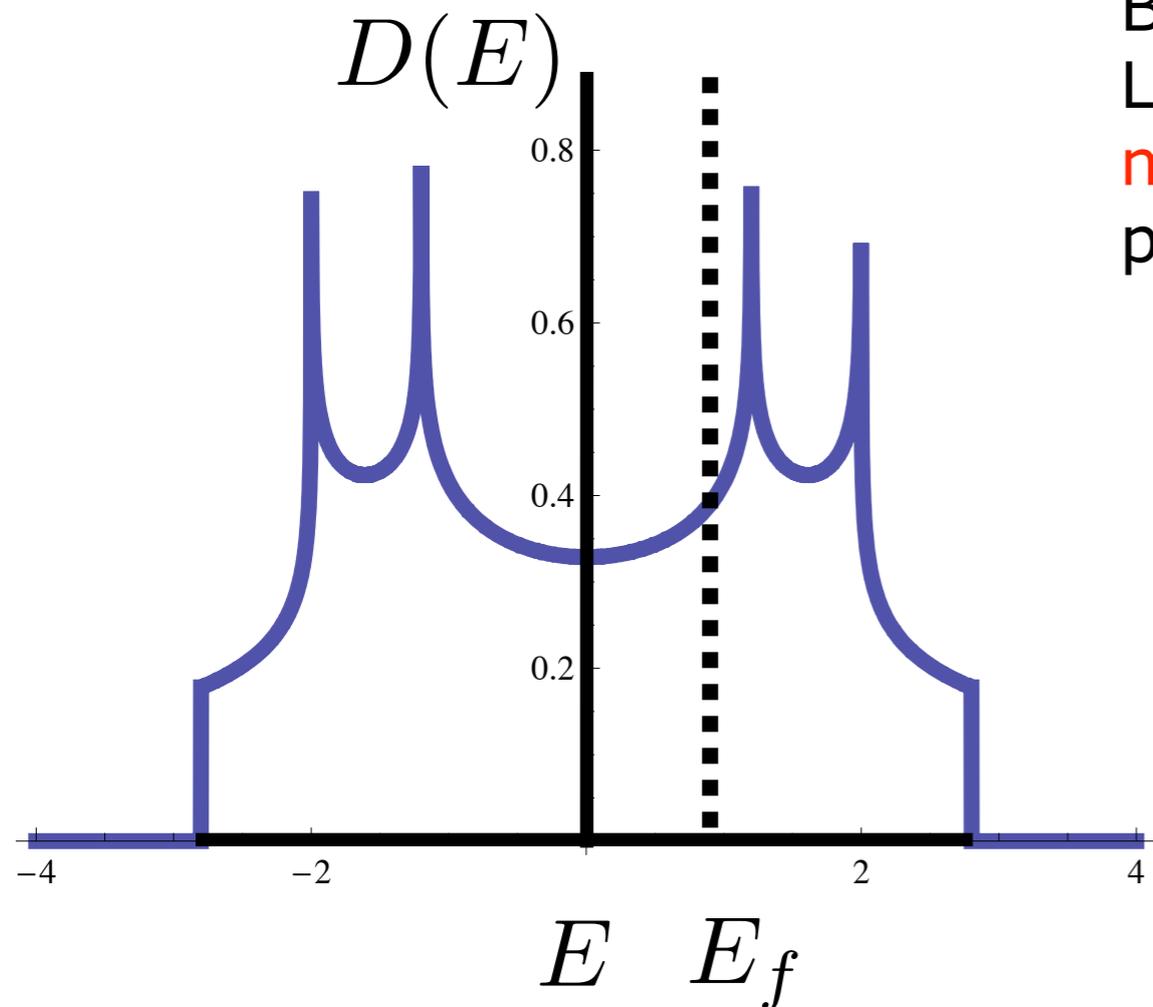
Electrons “hopping” between two adjacent Ru sites make use of intervening oxygen p -orbitals.

xz, yz : quasi-1D bands, *strongly* affected by bilayer splitting.

xy : quasi-2D band, *weakly* affected by bilayer splitting.

Primary difference between Sr_2RuO_4 ($n=1$) and $\text{Sr}_3\text{Ru}_2\text{O}_7$:
bilayer-split quasi-1D bands in $\text{Sr}_3\text{Ru}_2\text{O}_7$.

Metamagnetism and nematicity in quasi-1D bands



Bilayer-split quasi-1D bands satisfy Landau theory of weakly-first order **metamagnetism**: $D(E_f)$ has pronounced positive curvature

xz, yz orbitals also transform as a doublet under C_4 :

$$\begin{pmatrix} xz \\ yz \end{pmatrix} \rightarrow \begin{pmatrix} yz \\ -xz \end{pmatrix}$$

Orbital-ordering among xz, yz : **breaks C_4** , producing **nematic order**. Proximity of Fermi level to a van Hove singularity of the quasi 1D dispersion enables a weak-coupling treatment of this problem.

Metamagnetism and orbital-ordering: weak-coupling

$$H = H_{kin} + U \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \frac{V}{2} \sum_{i\alpha \neq \alpha'} n_{i\alpha} n_{i\alpha'}$$

strongest hybridizations
among t_{2g} orbitals

Intra-orbital
repulsion

Inter-orbital
repulsion

$$\sum_i \langle \vec{M}_{xz,i} + \vec{M}_{yz,i} + \vec{M}_{xy,i} \rangle$$

Total magnetic moment: breaks T.

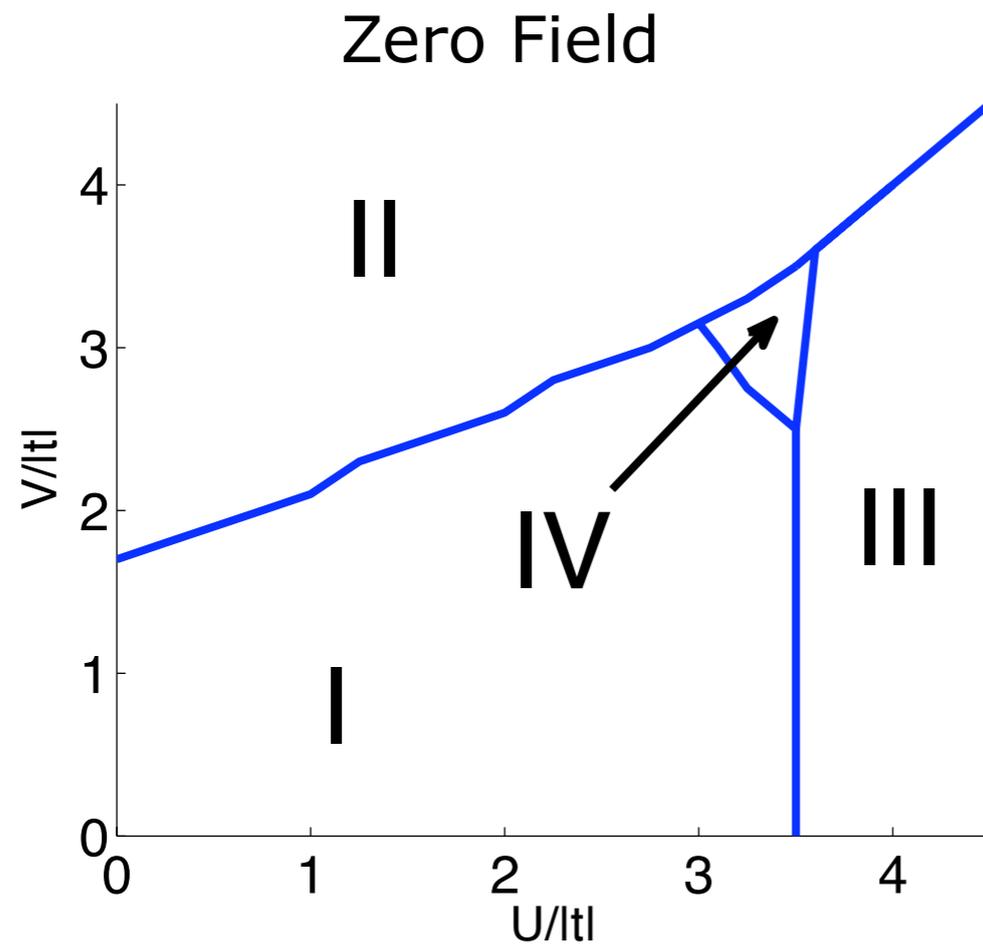
$$\sum_i \langle n_{xz,i} - n_{yz,i} \rangle$$

Nematic: breaks orbital degeneracy, C_4 .

$$\sum_i \langle \vec{S}_{xz,i} - \vec{S}_{yz,i} \rangle$$

Spin nematic: breaks orbital degeneracy,
 C_4 , T, SU(2), but preserves ($C_4 \times T$).

Phase diagram



I: Paramagnet

II: Nematic order

III: Ferromagnet
degenerate with
spin-nematic

IV: Ferromagnet,
nematic and spin-
nematic

Landau theory contains
trilinear coupling:

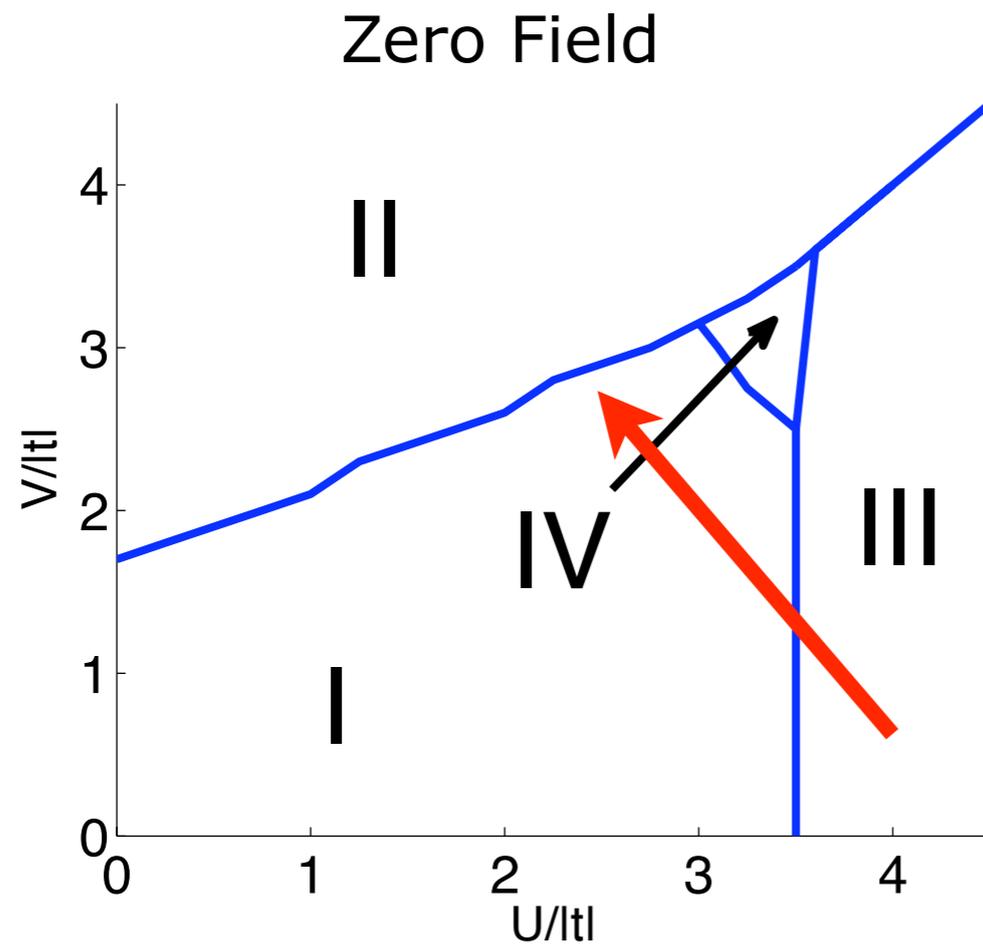
$$c(\rho)N_o\vec{M} \cdot \vec{N}_s$$

relative weight of this term
determines if phase IV wins.

Physical regime: $U \approx V$

All phase boundaries here
mark 1st order transitions.

Phase diagram



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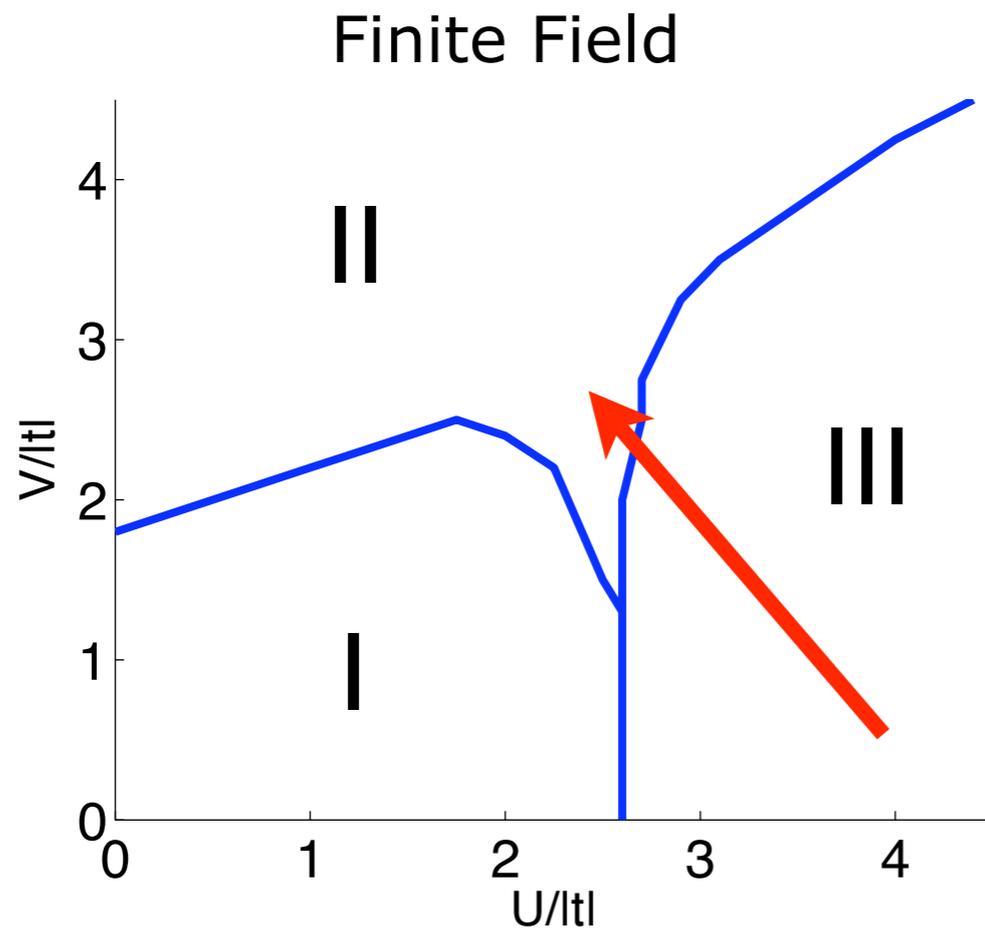
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Phase diagram



I: Small moment

II: Intermediate moment, Nematic

III: Large moment

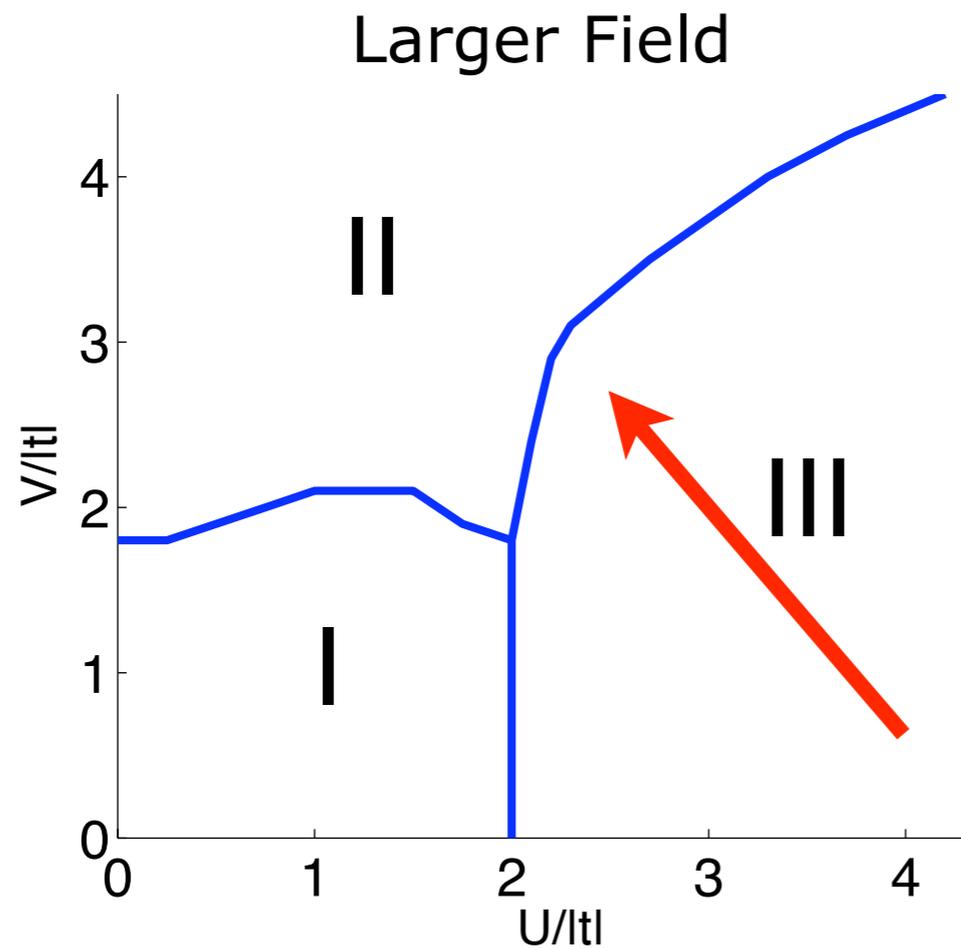
System crosses first metamagnetic boundary into nematic phase.

There is no distinction between nematic and spin-nematic in a finite field.

Physical regime: $U \approx V$

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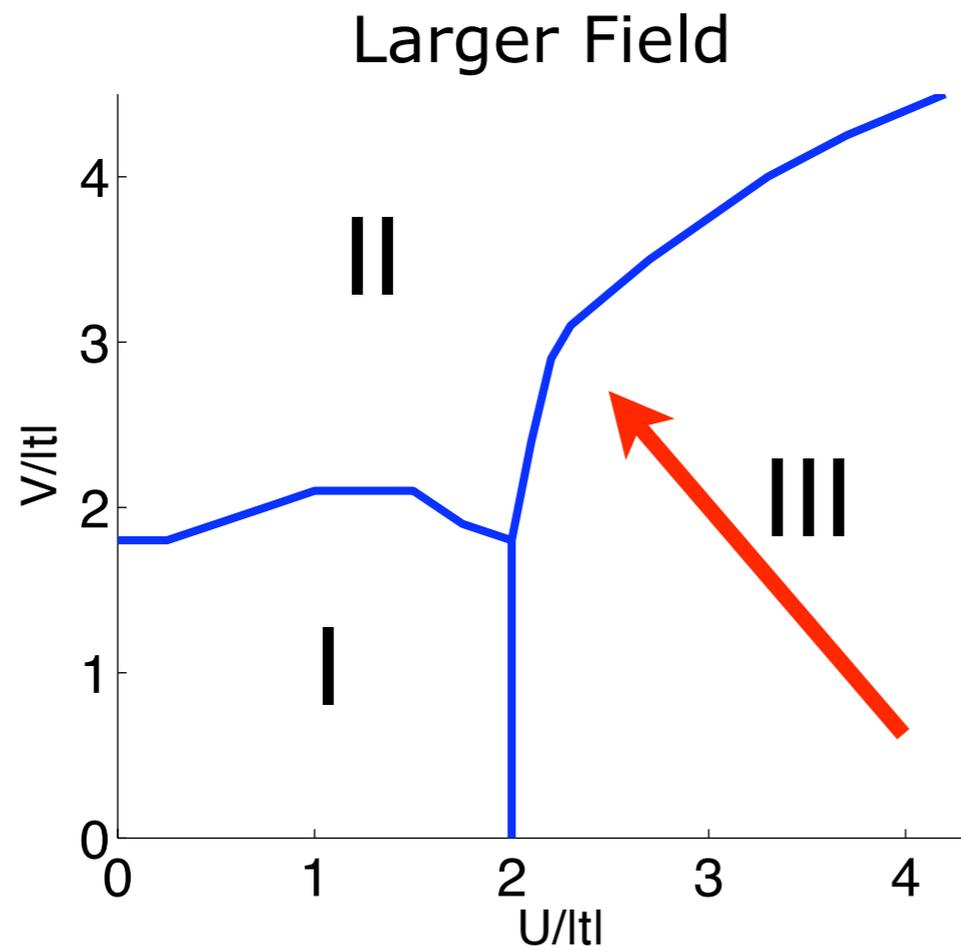
System crosses second metamagnetic boundary into large moment phase.

There is no distinction between nematic and spin-nematic in a finite field.

Physical regime: $U \approx V$

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Phase diagram



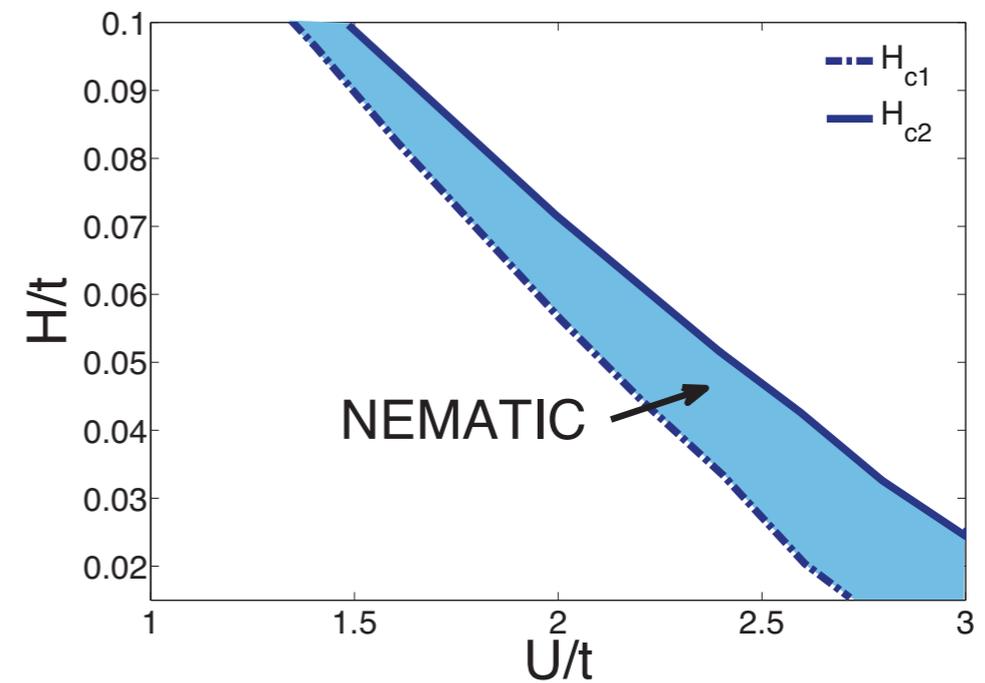
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II: Intermediate moment, Nematic

III: Large moment

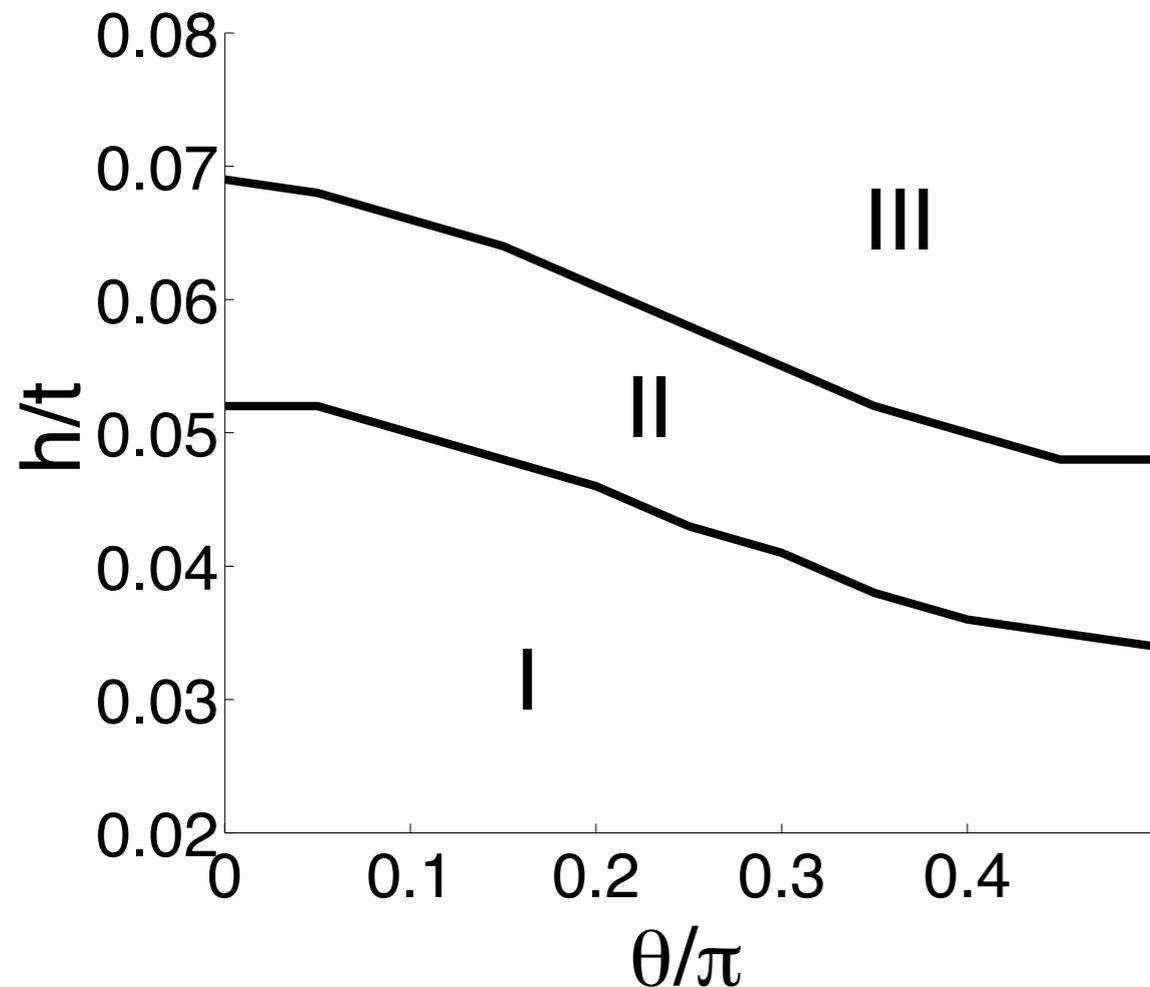
Physical regime: $U \approx V$

All phase boundaries here mark 1st order transitions.



Effect of spin-orbit coupling

SOC changes Fermi surface topology, and therefore plays an important qualitative role.



Phase I: small nematic order, small moment.

Phase II: large nematic order, intermediate moment.

Phase III: small nematic order, large moment.

All phase boundaries mark 1st order transitions.

$$H_{s.o.}(\theta) = \lambda \vec{L} \cdot \vec{S}(\theta)$$

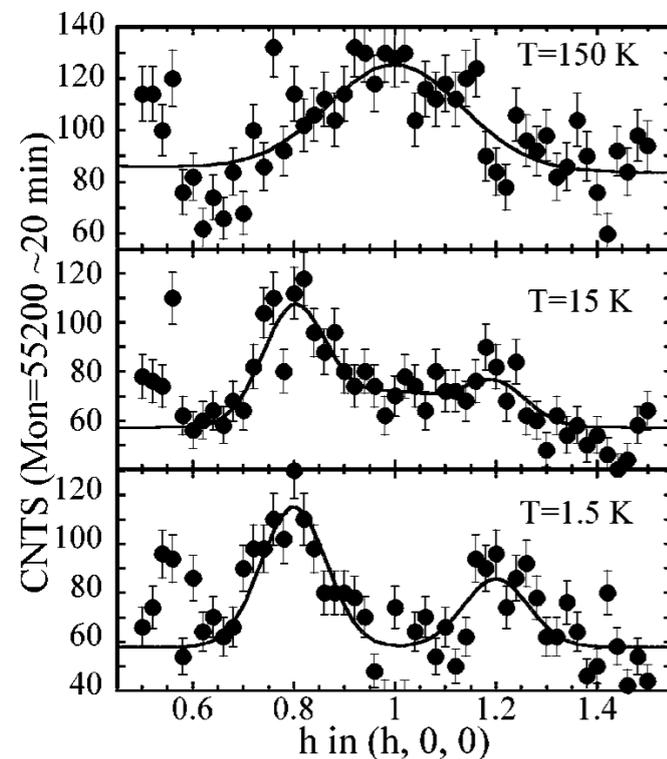
Angle-dependent "metanematic" transitions.

Spin-orbit coupling captures the $O(1)$ anisotropy of critical fields as the field angle is varied.

Comparison to finite-q order

How does the nematic phase here compare with SDW, etc?

PRB **67**, 012504 (2004)



Inelastic neutron scattering: incommensurate fluctuations for $T < 20\text{K}$. Wave-vectors are consistent with FS nesting. However, no static SDW order is present (for $h=0$).

Spin-orbit coupling destroys near-perfect nesting of Fermi surface.

one-loop spin susceptibility

$$[\chi^{ij}(\mathbf{q})]_{ba}^{st} = \int_0^\beta d\tau \sum_{\mathbf{p}\mathbf{p}'} \sum_{\alpha\beta\gamma\delta} \sigma_{\alpha\beta}^i \sigma_{\gamma\delta}^j \times \langle T_\tau d_{s\mathbf{p}\alpha}^\dagger(\tau) d_{t\mathbf{p}+\mathbf{q}\beta}(\tau) d_{a\mathbf{p}'\gamma}^\dagger(0) d_{b\mathbf{p}'-\mathbf{q}\delta}(0) \rangle$$

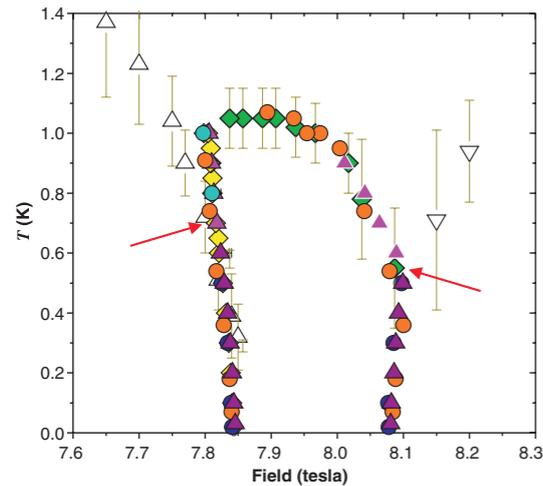
$$\text{RPA: } \frac{U_{c,sdw}}{2} \text{Max}(\text{eig}[\chi]) = 1$$

close to critical coupling for FM. SOC provides a natural explanation for why SDW order is not formed.

Summary

- 1) We have considered the microscopic origins of metamagnetism and nematicity, making use of interplay b/w orbital, spin ordering.
- 2) Relatively small interval over which nematic phase occurs:
- 3) Asymmetry present in the problem (and experimental data). Nematic order decreases monotonically from H_{c1} to H_{c2} .
- 4) Moderate spin-orbit coupling consistent with bandstructure estimates produce an $O(1)$ decrease in critical fields as field angle varies.
- 5) Quasi-1D bands contribute to spin-fluctuations and account for INS peaks. However, spin-orbit coupling efficiently spoils their nesting, plausibly explaining why SDW order does not occur at $h=0$.
- 6) Our model predicts that nematic order should occur for all field orientations (this has not yet been detected experimentally).

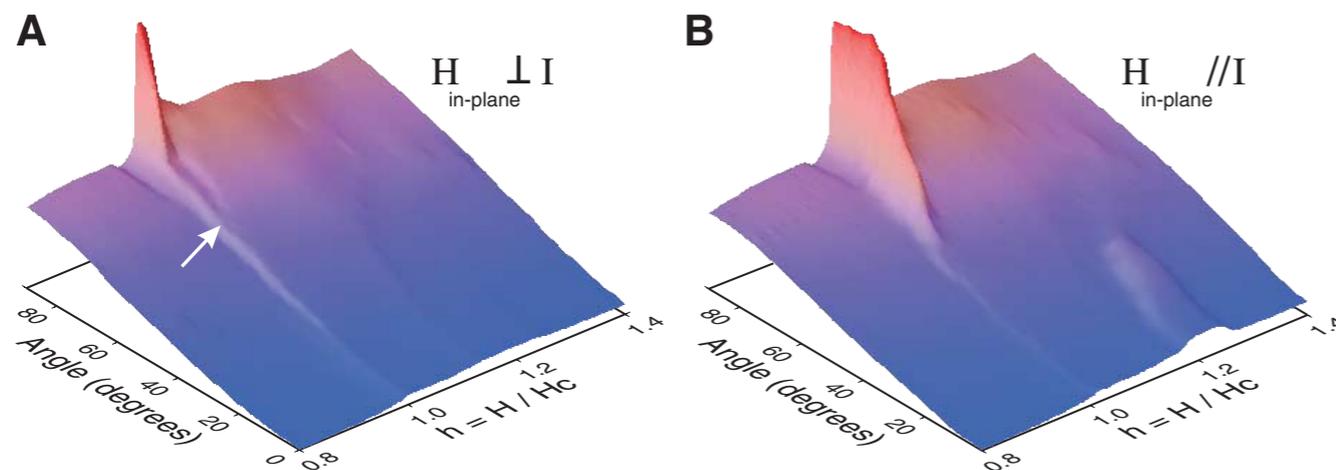
Current and future work



Nematic phase has a *higher* entropy than the surrounding isotropic phases.

Our model does not provide an answer for large resistive anisotropy (just a symmetry argument).

Plausible explanation: scattering off of nematic domains.



average resistivity decreases with angle as domains get aligned.

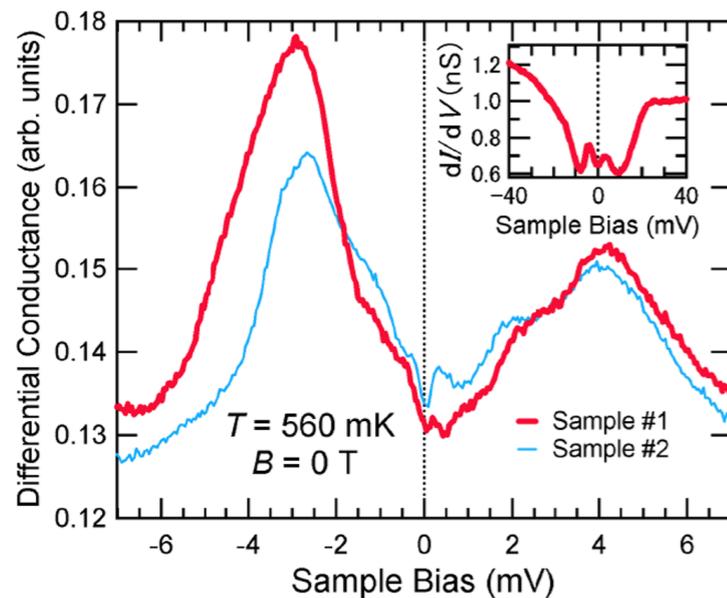
Science **315**, 214 (2007)

Nematic domains could also account for why the phase has higher entropy

Current and future work

Effects of quantum fluctuations

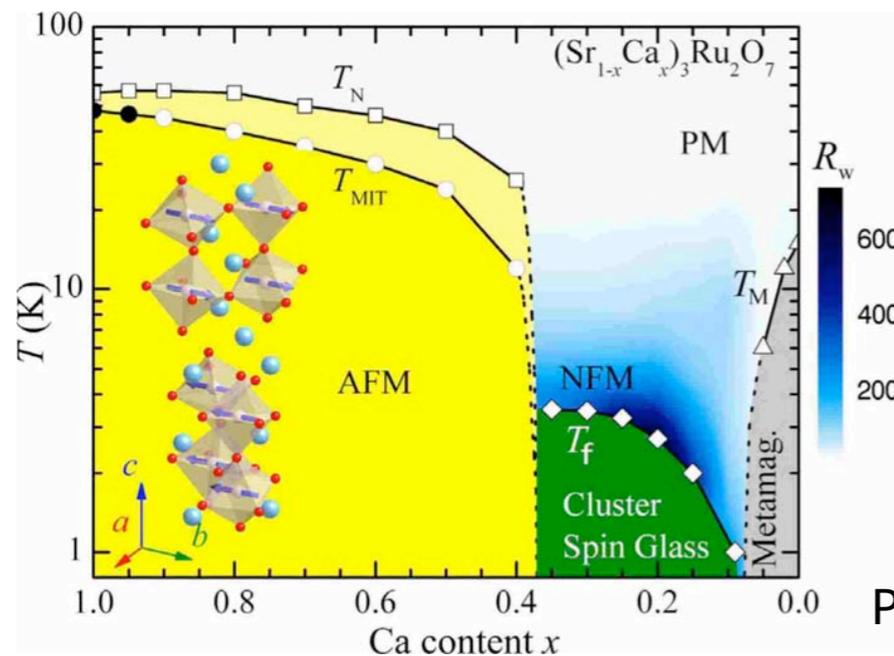
PRL **99**, 057208 (2007)



STM experiments have revealed a “pseudogap” in LDOS which persists at zero field.

Can this feature be explained due to local nematic quantum fluctuations?

This feature could also occur due to incommensurate spin-fluctuations



Calcium doping studies suggest a metamagnetic QCP occurs with doping. Nematic fluctuations might also persist here and could be the basis of a fluctuational theory.

PRB **78**, 180407(R) (2008)