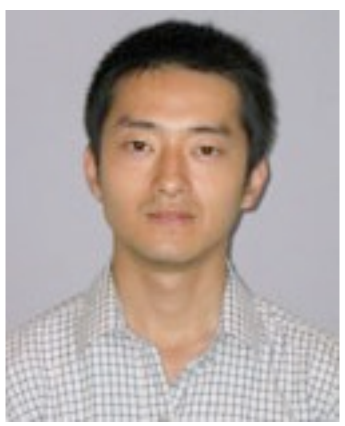
Twisted Hubbard model for Sr2IrO4: Magnetism and possible high temperature superconductivity



T. Senthil (MIT)

Collaboration with Fa Wang (MIT, now at Beijing Univ)

Iridium oxide materials: various kinds of exotic physics

$Na_4Ir_3O_8$: insulating quantum spin liquid (Okamoto, Takagi et al, 2007)

Sr_2IrO_4: $J_{eff} = 1/2$ spin-orbit entangled Mott insulator (B.J. Kim et al, 2008)

Other interesting proposals:

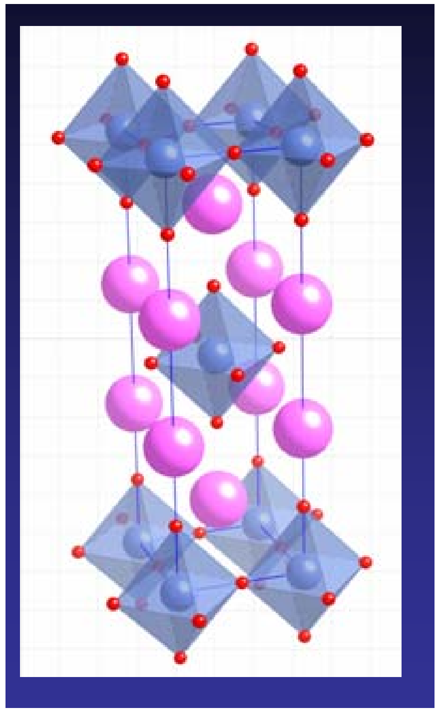
A_2IrO_3: quantum spin Hall effect? (Shitade, Nagaosa et al, PRL 2009), realization of Kitaev spin liquid? (Jackeli, Khaliullin, PRL 2009)

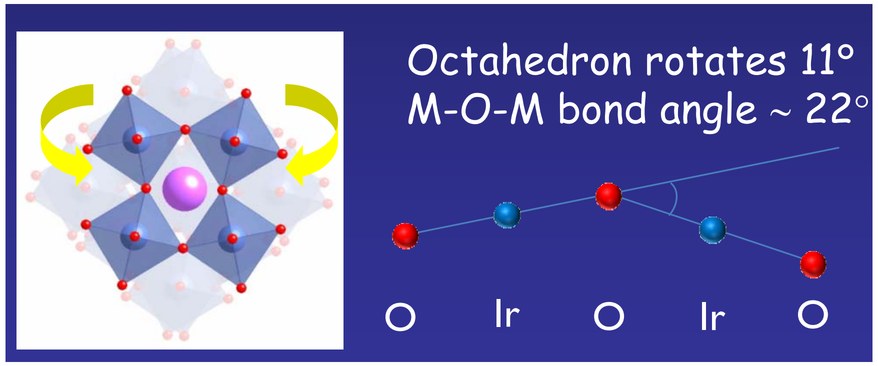
$Ln_2Ir_2O_7$ pyrochlore iridates:
(i) spontaneous anomalous Hall effect (Nakatsuji et al, 2010) for Ln = Pr;
(ii) other Ln: 3d correlated topological insulator? (Pesin, Balents, Nat Phys 2010, Kim et al, 2010), Weyl semi-metals? (Wan, Turner, Vishwanath, Savrasov 2011).

(More iridates: Invited Session F2 Tuesday 8 am)

Sr_2IrO_4: preliminaries

K_2NiF_4 structure similar to La_2CuO_4

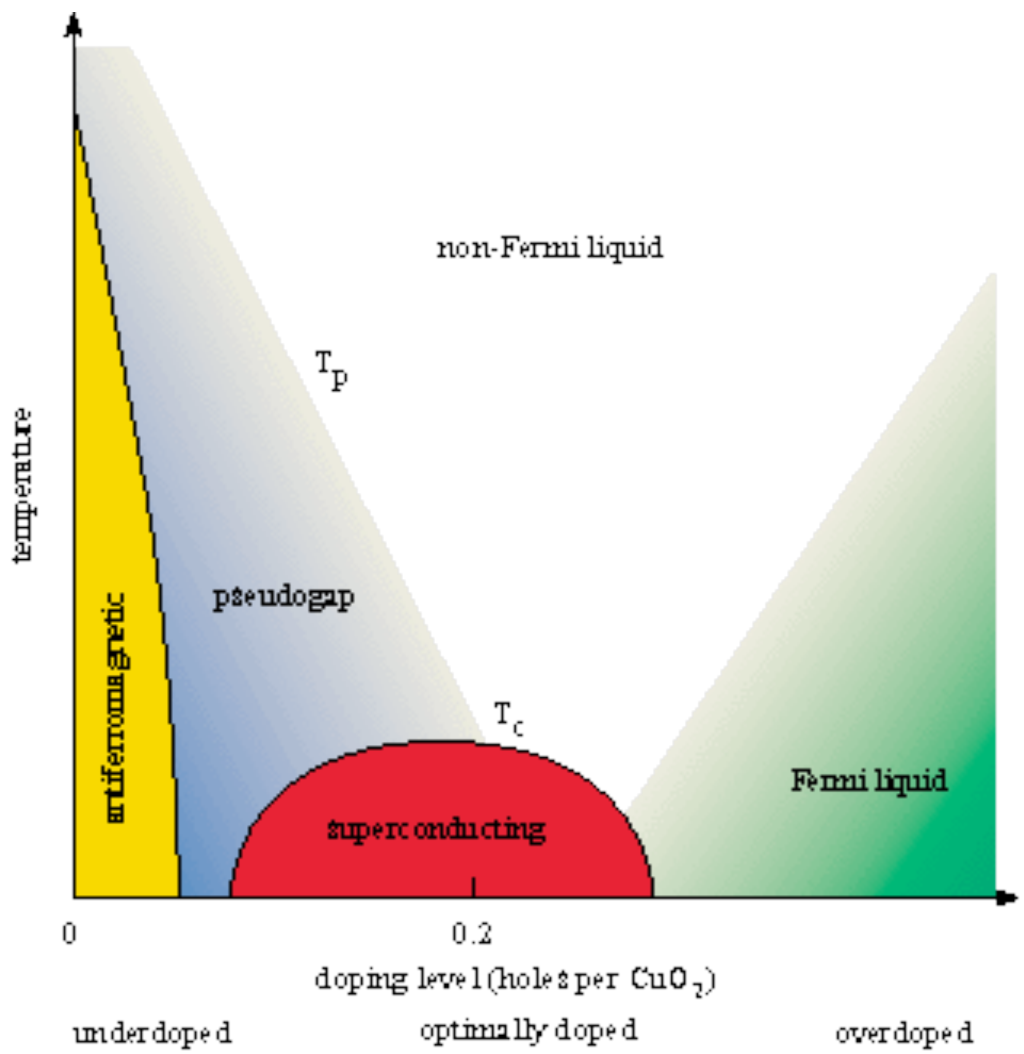




Layers of IrO2 ;
Ir4+ ions on a 2d square lattice.
Each Ir surrounded by O octahedra.

Similarity to cuprates noticed in 1990s: M.A.Subramanian, Gang Cao, ...

Cuprates are interesting

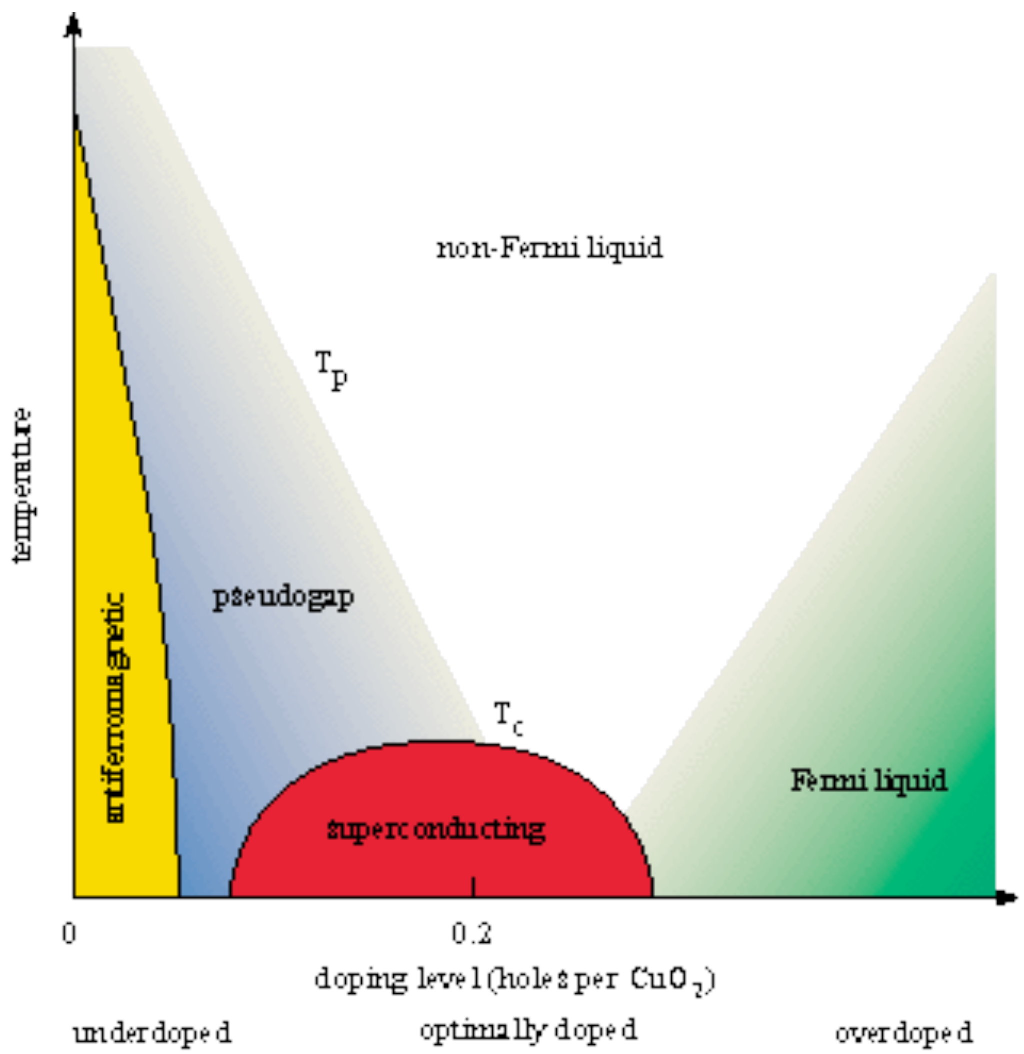


Still the best high temperature superconductors!

Many other novel broken symmetries found in recent years in underdoped side.

1. Antiferromagnetism
2. Broken translation (stripes)
3. Nematic
4. Broken T-reversal
5. Loop currents (break T-reversal, rotation but preserve combination, translation invariant)

Cuprates are interesting (cont'd)



Apart from high Tc superconductivity/other broken symmetries, cuprates show a number of fascinating and mysterious phenomena.

Eg: pseudogap, strange non-Fermi liquid metal,.....

For some of these the superconductivity is a nuisance that people work hard to get rid of so they can be studied at low-T.

Cuprates are challenging for theory

1. Some understanding of origin and properties of superconductivity, stripes, and some of the other broken symmetries.

2. Very little understanding of how these different orders compete/ cooperate.

3. Almost no understanding of essence of pseudogap phenomenon

3. No understanding of strange metal

Do parts of the cuprate story play out elsewhere?

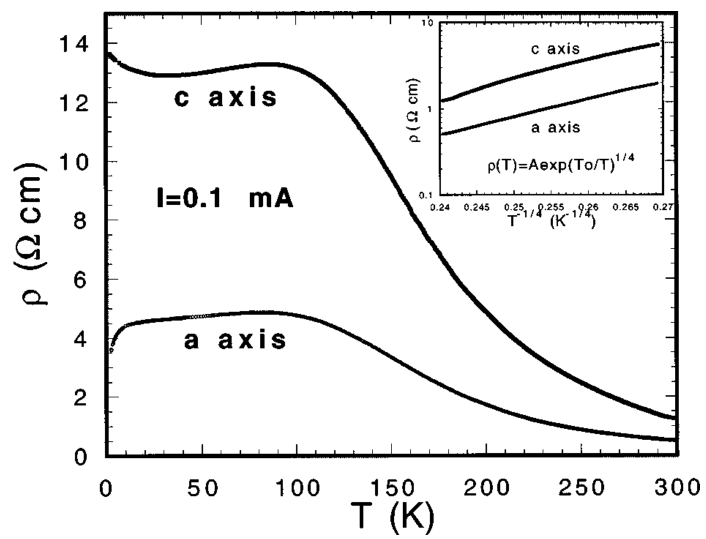
1. Organics: SC proximate to AF Mott insulator, pseudogap in some cases.

2. Pnictides: SC proximate to magnetism in quasi-2d layered square lattice systems, evidence for nematic order but very different microscopically.

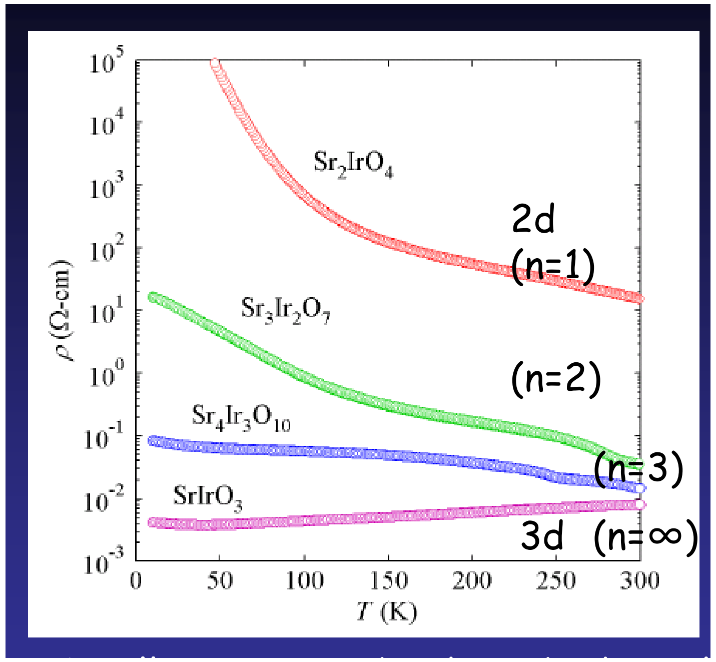
No serious sign of pseudogap, strange metal or (in most cases) Mott insulation

3. Iridates ????

Sr2IrO4: Mott insulator*



Cao et al, PR B 1998

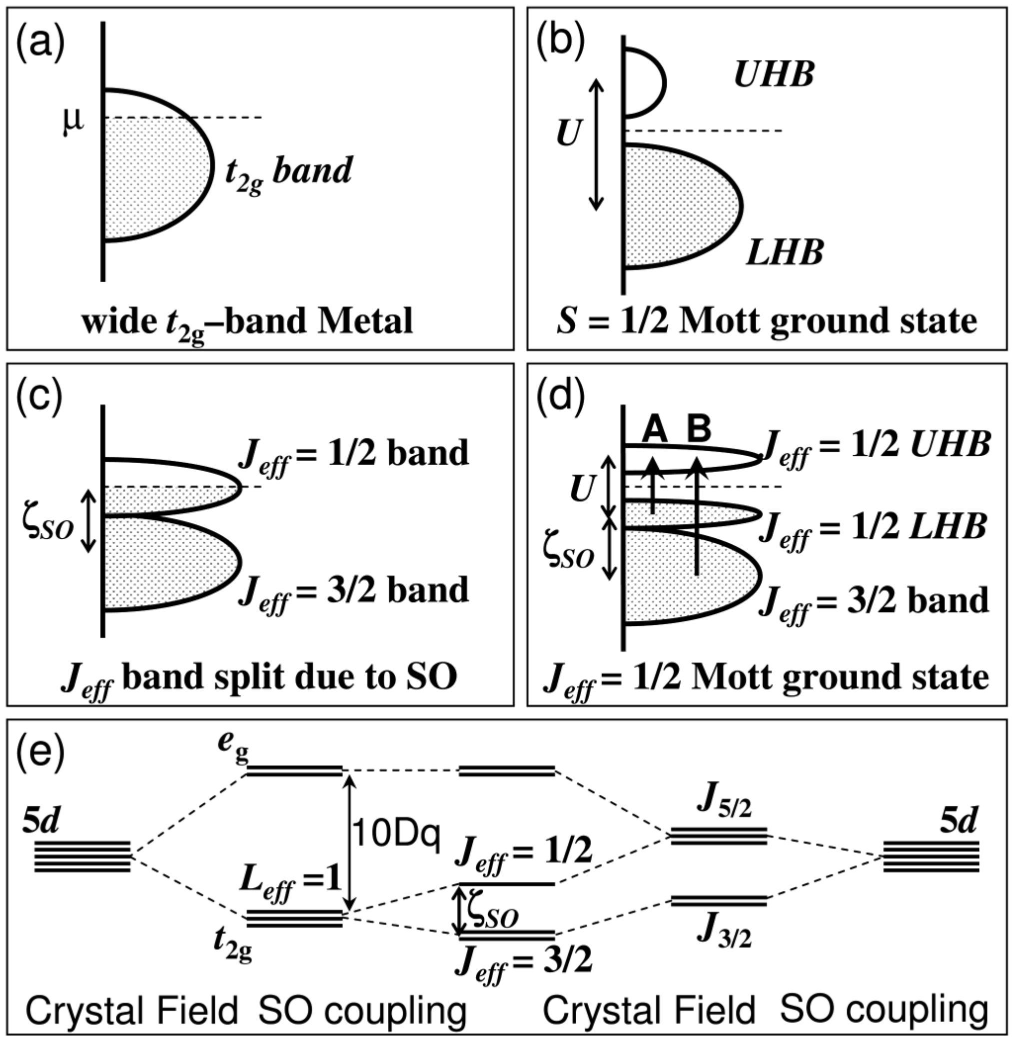


H. Takagi et al, 2008

*Later..how much Mott?

Why a Mott insulator?

Ir 4+ is in a $5d^5$ configuration.



B. J. Kim et al, PRL 08

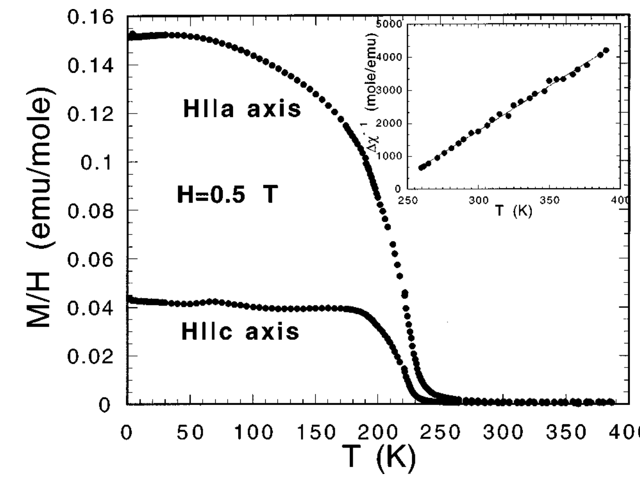
Cubic environment: big t2g - eg splitting.

SO coupling splits t_{2g} level into J_{eff} = 1/2 and J_{eff} = 3/2 bands.

J_{eff} = 1/2 band is half-filled and narrow
=> moderate U can drive it into a Mott insulator

Spin-orbit entangled Mott insulating magnet

$$J_{eff,+1/2} = \frac{1}{\sqrt{3}} \left(|xy, +1/2\rangle + |yz, -1/2\rangle + i|zx, -1/2\rangle \right)$$
$$J_{eff,-1/2} = \frac{1}{\sqrt{3}} \left(|xy, -1/2\rangle - |yz, +1/2\rangle + i|zx, -1/2\rangle \right)$$



G. Cao et al, 1998

J_{eff} moments order into a magnetic state below 240 K.
Weak ferromagnetism (from canting of AF moments): 0.7 - 0.14 μ_B

Spin-orbital content confirmed by resonant magnetic X-ray diffraction
(B.J. Kim, Takagi et al, Science 2009)

How similar to cuprates??

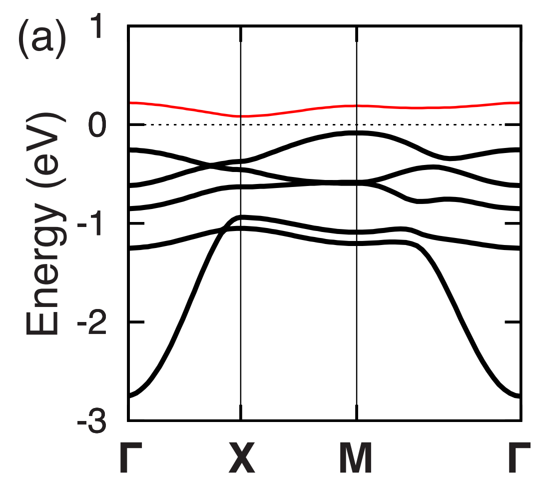
Despite obvious similarities, some worries

1. Different active orbitals
2. Spin anisotropy and related strong spin orbit coupling

Is there a useful effective model which can be compared with, eg, Hubbard model popular for cuprates?

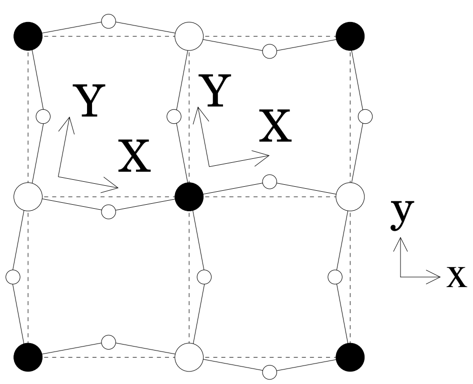
LDA + Spin-Orbit + U bandstructure

Jin, Jaejun Yu, et al, PR B 2009



Fit to obtain tightbinding model (+ U) in t2g subspace: real orbital diagonal hoppings (i.e only xy -> xy, yz->yz, xz->xz) + on-site spin-orbit term

Similar result: H. Watanabe et al, PRL 2010



Interpretation of tightbinding model

Wang and TS, 2011

Rotation of oxygen octahedra => must carefully distinguish between local X,Y, Z basis and global x,y, z basis.

Note
1. Crystal field splitting between t_{2g} and e_g is diagonal in local X,Y,Z basis => define t_{2g} orbitals in local orbital basis.

2. If Ir - Ir hopping is mediated by O p-orbitals, symmetry => Ir-Ir hopping diagonal in local orbital basis

3. Global basis for spin S = 1/2 => Ir-Ir hopping real.

Conclusion: LDA+SO+U tight-binding fit involves Wannier states with t_{2g} orbitals in local X,Y,Z basis but spin in global basis.

Effective model for J_{eff} = 1/2 states: strategy

Wang and TS, 2011

What are correct J_{eff} = 1/2 states?

Must define both t2g orbitals and spin in local X,Y, Z basis.

$$|J^z_{\rm eff} = +1/2\rangle = \frac{1}{\sqrt{3}}\left(+\mathbb{i}|XY,\uparrow\rangle - |XZ,\downarrow\rangle + \mathbb{i}|YZ,\downarrow\rangle\right),$$
$$|J^z_{\rm eff} = -1/2\rangle = \frac{1}{\sqrt{3}}\left(-\mathbb{i}|XY,\downarrow\rangle + |XZ,\uparrow\rangle + \mathbb{i}|YZ,\uparrow\rangle\right).$$

Effective model in J_{eff} = 1/2 subspace:

Start with full tightbinding t2g tightbinding model.

Rotate spin from global to local basis, then project onto J_{eff} = 1/2 states.

Effective model for Jeff = 1/2 states: result

$$H = -\sum_{<jk>,\alpha} (t + \mathbb{i}\epsilon_\alpha \epsilon_j \bar{t})\, d^\dagger_{j,\alpha} d_{k,\alpha} - \sum_{<<jk>>,\alpha} t'\, d^\dagger_{j,\alpha} d_{k,\alpha} - \sum_{<<<jk>>>,\alpha} t''\, d^\dagger_{j,\alpha} d_{k,\alpha} + U \sum_j d^\dagger_{j,\uparrow} d_{j,\uparrow} d^\dagger_{j,\downarrow} d_{j,\downarrow}$$

Effective tight-binding parameters $t \approx 0.26eV$, $t' \approx t/4$, $t" \approx t/10$.

Imaginary spin-dependent hopping $\bar{t} \approx -t/60$: ignore.

Hubbard $U \approx 2eV$.

Effective t-t'-t''-U Hubbard model for Jeff = 1/2 band.

Consequence: pseudospin isotropy

At half-filling, expect can describe Mott insulator by
usual isotropic pseudospin Jeff = 1/2 model

$$H_{AFM} = I \sum_{<ij>} \vec{J}_i.\vec{J}_j + ... \qquad (1)$$

Exchange $I \sim 4t^2/U$.

"....." further neighbor, ring exchange

Similar prior conclusion in spin model limit: Jackeli, Khaliullin 2009

Coupling to external Zeeman field is `twisted'

Wang, TS, 2011

$$H_B = -\mu_B \sum_i \vec{B}.(\vec{L} + 2\vec{S}) \tag{1}$$

Project to Jeff $= 1/2$ states

$$H_B = 2\mu_B (B_X J_X + B_Y J_Y + B_Z J_Z) \tag{2}$$

Subscripts X, Y, Z: components in local basis.

Rotate back to global basis: staggered anisotropic g-tensor.

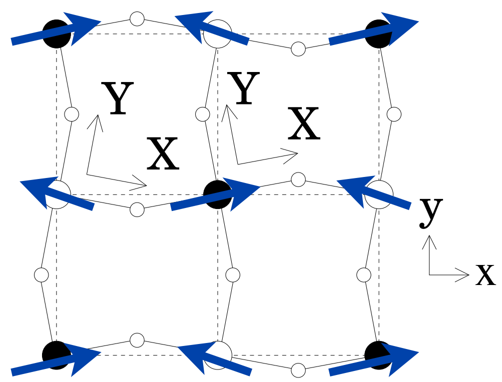
Observable moment M related to J through

$$\begin{pmatrix} M_{j,x} \\ M_{j,y} \\ M_{j,z} \end{pmatrix} = -2\mu_B \begin{pmatrix} \cos\theta & -\epsilon_j \sin\theta & 0 \\ \epsilon_j \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} J_{j,1} \\ J_{j,2} \\ J_{j,3} \end{pmatrix}$$

Twisted magnetic field coupling => anisotropic magnetization even though intrinsic physics is isotropic.

Consequences for magnetism in Sr2IrO4

Isotropic pseudospin ordering => observed moment rotates with octahedra rotation.
=> weak ferromagnetism.



$$\text{FM moment} = (\text{AF moment})\sin\theta$$
$\theta =$ octahedron tilt angle

Known AF moment of $J = 1/2$ Heisenberg model => FM moment $\approx 0.14\mu_B$ similar to experiment.

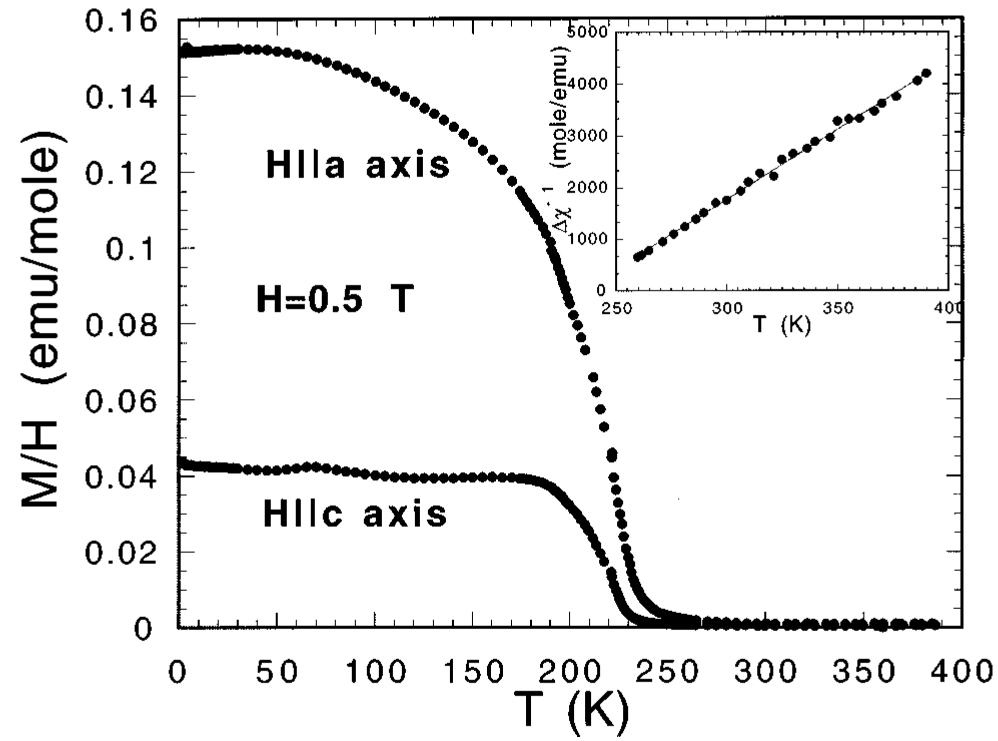
Consequences for magnetism (cont'd)

1. Measured susceptibility near q = 0 is mixture of uniform and staggered susceptibilities

2. Anisotropy between susceptibility to field along ab-plane versus along c axis.

3. Despite apparent spin anisotropy, spin correlation length above T_N should behave like that of isotropic magnet.

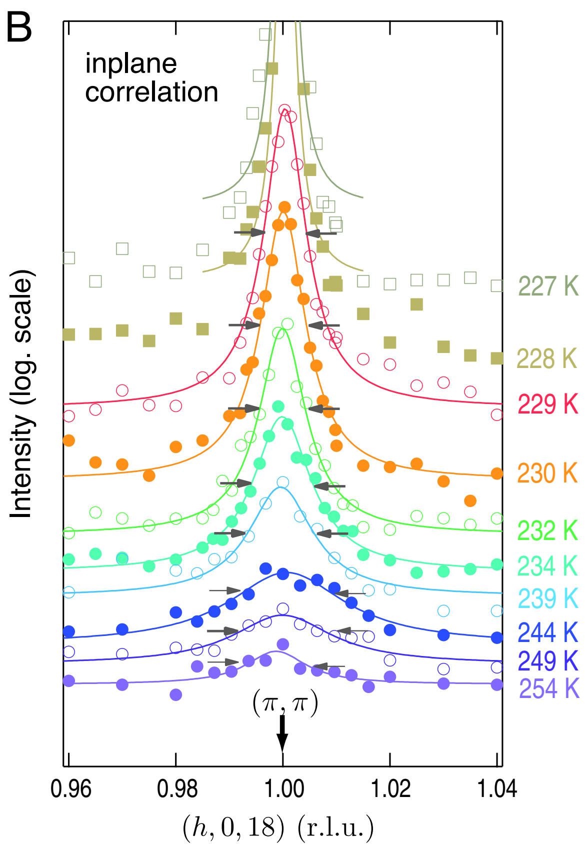
All of these agree with experiment.



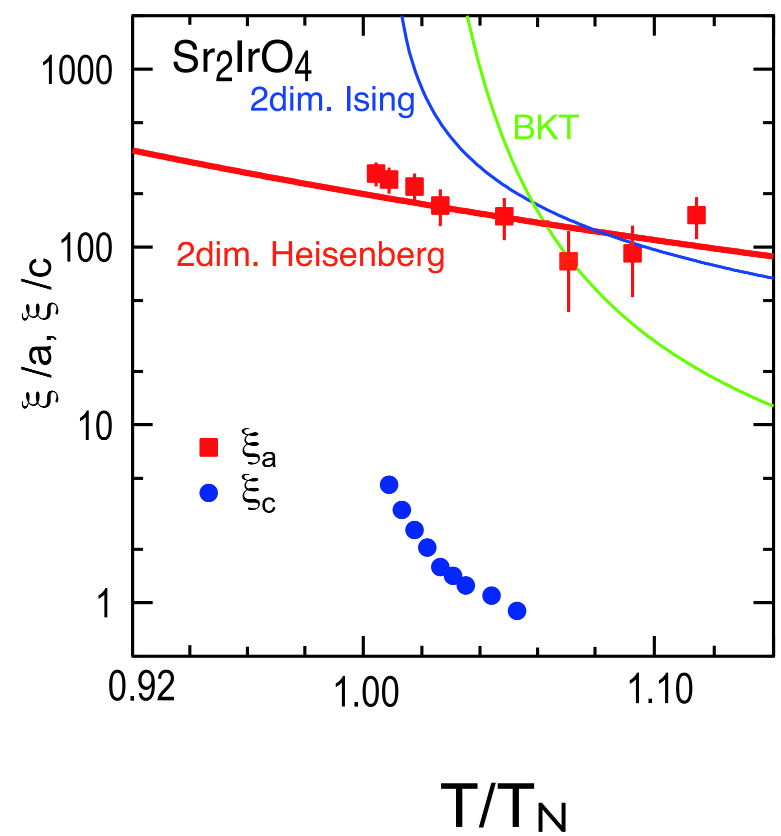
G. Cao et al, 1998

Spin correlation length above T_N

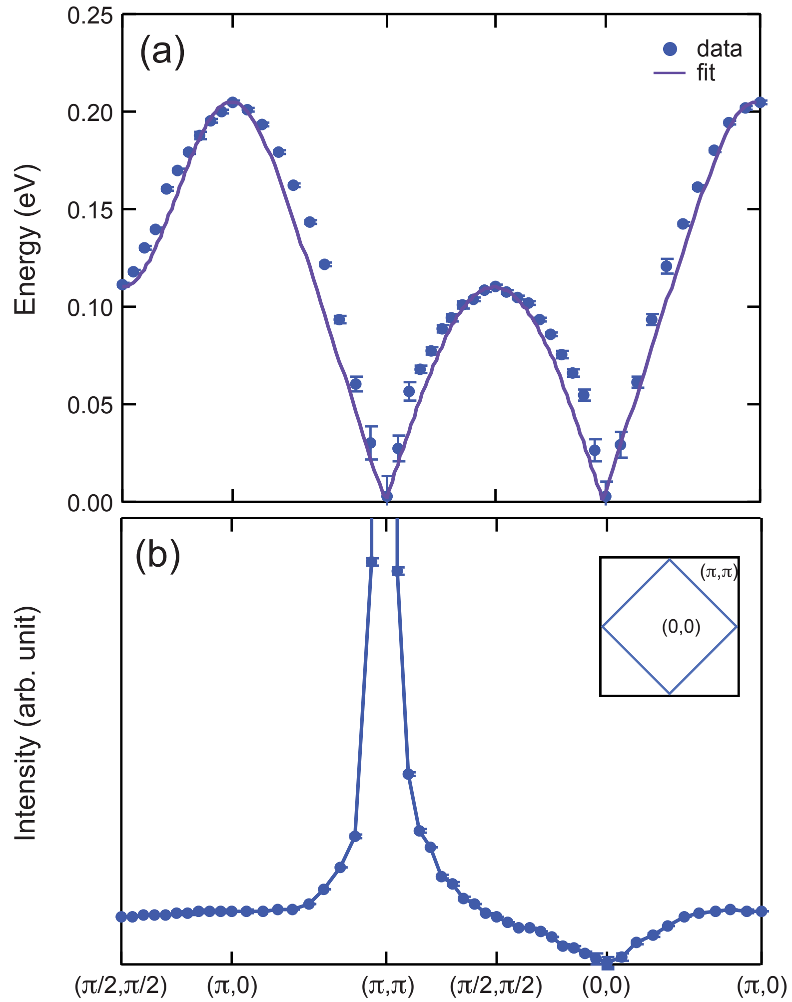
Shigeki Fujiyama, H. Takagi et al, 2012



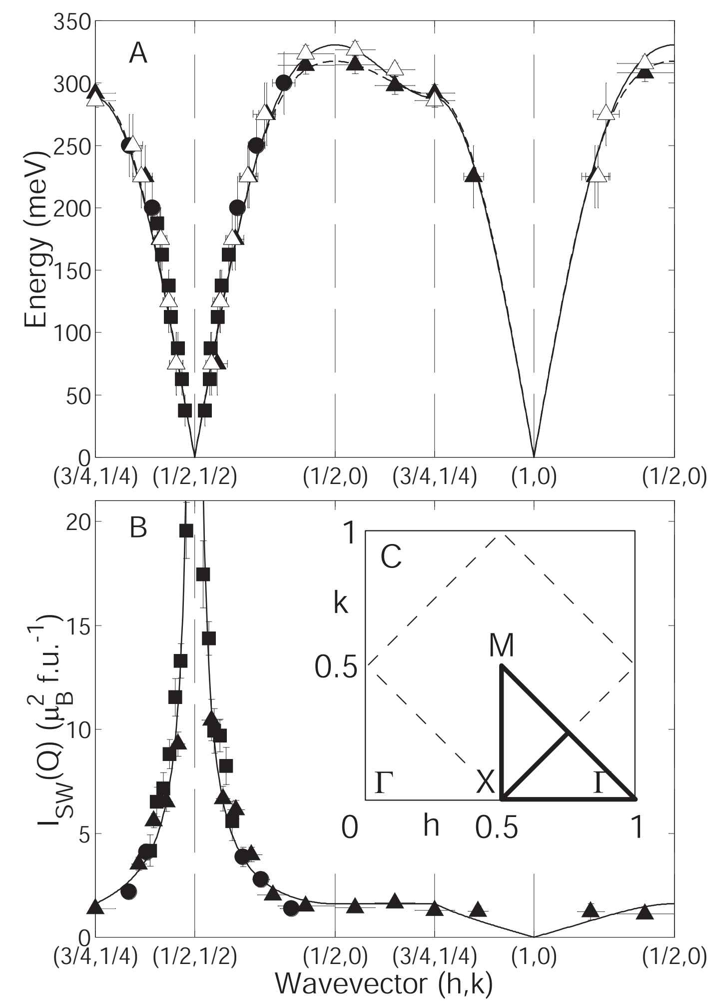
Diffuse magnetic X-ray scattering



Spin wave dispersion (B.J. Kim) through RIXS



Contrast with cuprate



Sr2IrO4, Jungho Kim et al, 2011

LSCO, Coldea et al, 2001

B.J. Kim talk, Session F2 Tuesday

Compare model to cuprate

Effective isotropic Hubbard model parameters:
$t \approx 0.2eV$, $t' \approx \frac{t}{4}$, $t" \approx -\frac{t}{10}$, $U \approx 10t$.

Similar to cuprate?
1. Roughly same parameter range as cuprate Hubbard model except overall energy scale smaller by ≈ 2.
2. t'/t positive for iridate - opposite to cuprate

Doped system - superconductivity?

If the doped square lattice 2d Hubbard model is superconducting, can we expect doping the iridate will give a `high temperature' superconductor?

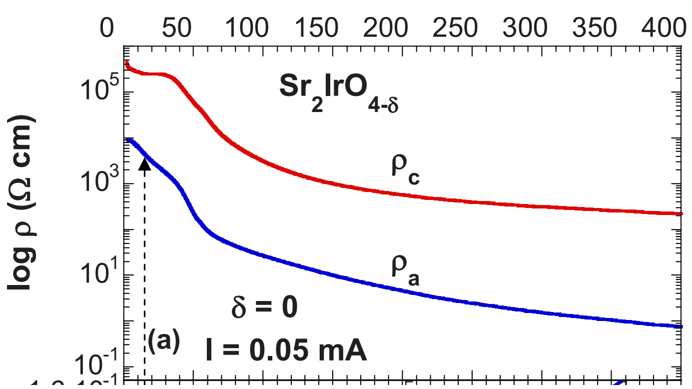
From comparison to cuprate
(i) $t'/t > 0$ => Electron doping better than hole doping for iridate
(Example: Replace Sr by La)

(ii) Overall energy scale smaller by 2 => Tc in range of 50 K???

Differences with cuprates: more coherent c-axis transport?

Interlayer tunneling matrix element in cuprate:
$(cosk_x - cosk_y)^2$ factor which blocks c-axis transport of nodal states.

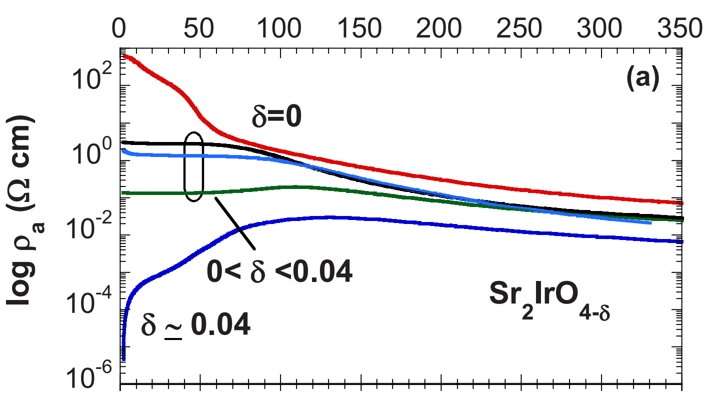
Iridate: different orbital content implies no suppression of nodal c-axis hopping.
Better c-axis coherence?

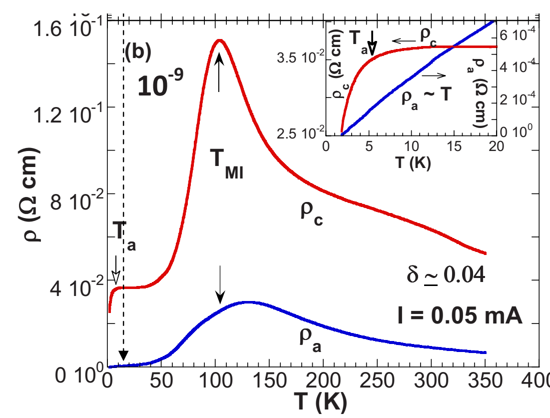


Overall resistivity anisotropy of about 100 in undoped insulator

Experimental prospects?

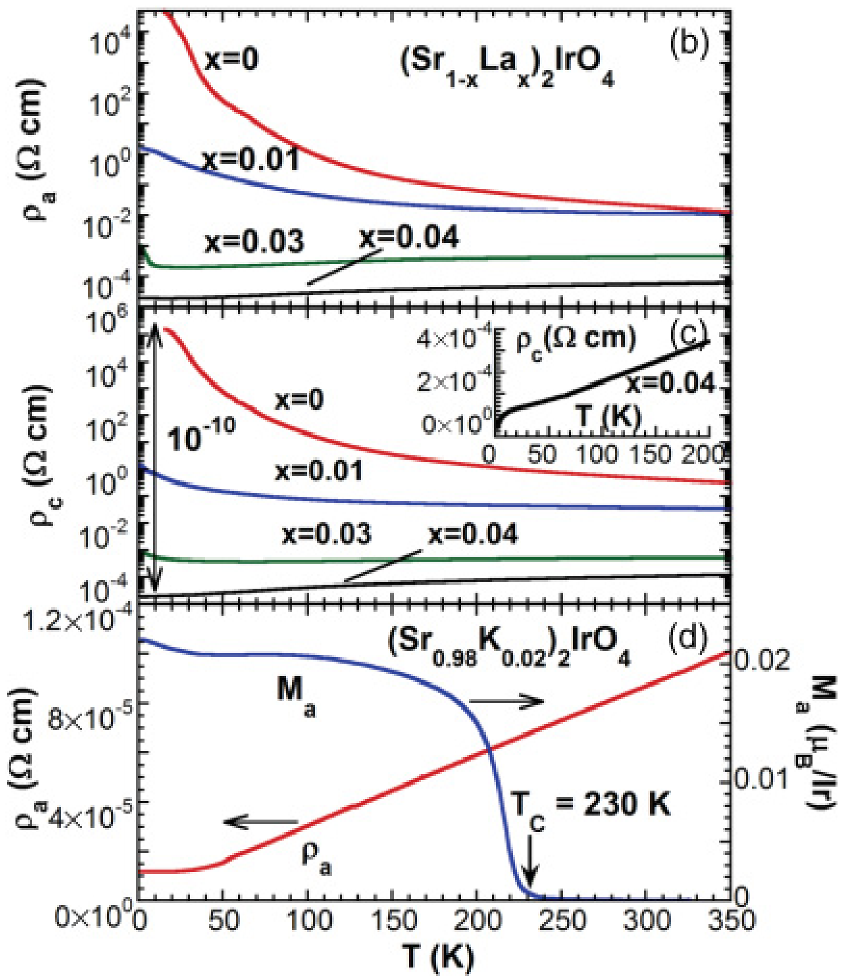
Metal-insulator transition with Oxygen doping





Cornetta, Cao et al, PR B 2010

MIT with La (electron) or K (hole) doping



Ge, Cao et al, 2011

Will it be possible to dope Sr2IrO4
to higher doping levels?

May be try field-effect doping or making
oxide interface? ???

Some important basic issues to settle

1. Sr2IrO4: Mott or Slater insulator?

Issue raised in recent theory and expt papers. (Arita, Imada et al PRL, 2012; Hsieh et al, 2012, Carter, Kee 2012)

Naive Slater picture cleary not legtimate:

Insulator above T_N, no Fermi surface nesting.

Almost certainly intermediate U.

Similar issue still being debated in cuprates (eg Millis 2010).

2. Legitimacy of one-band Hubbard description

More serious is whether a one-band description is legitimate at all.

1. Do J = 3/2 states start playing a role in doped system?

May be not for electron doped.....

2. Complications due to enlarged unit cell from octahedra rotation (eg: suggested semimetal in $SrIrO_3$ (Takagi APS 2012 talk).

If one-band description breaks down similarity with cuprates can also be expected to break down.......

3. Magnetism in doped Sr-214

Fate of magnetic ordering across metal-insulator transition ?

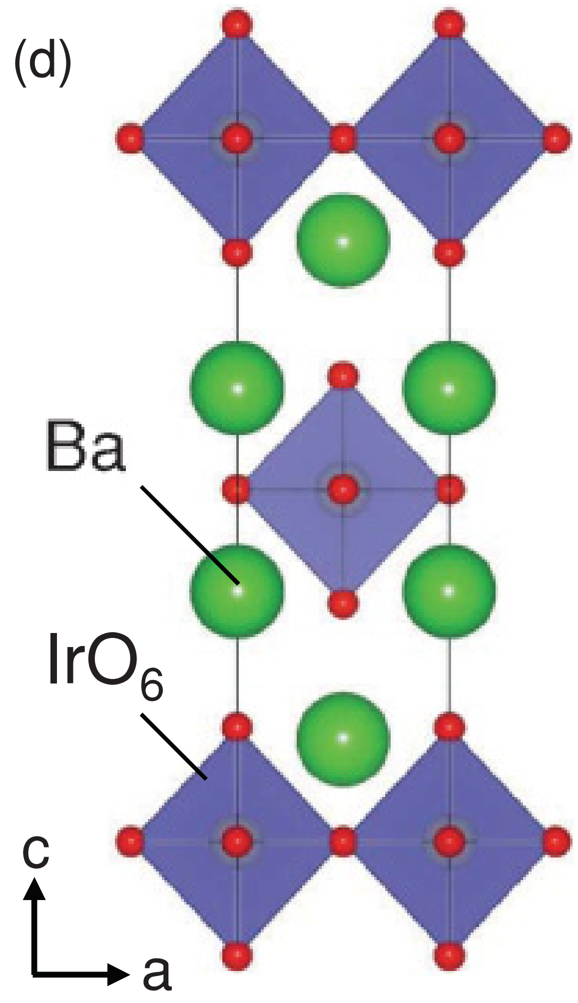
Do long range or at least short range (possibly incommensurate) magnetic correlations persist across MIT?

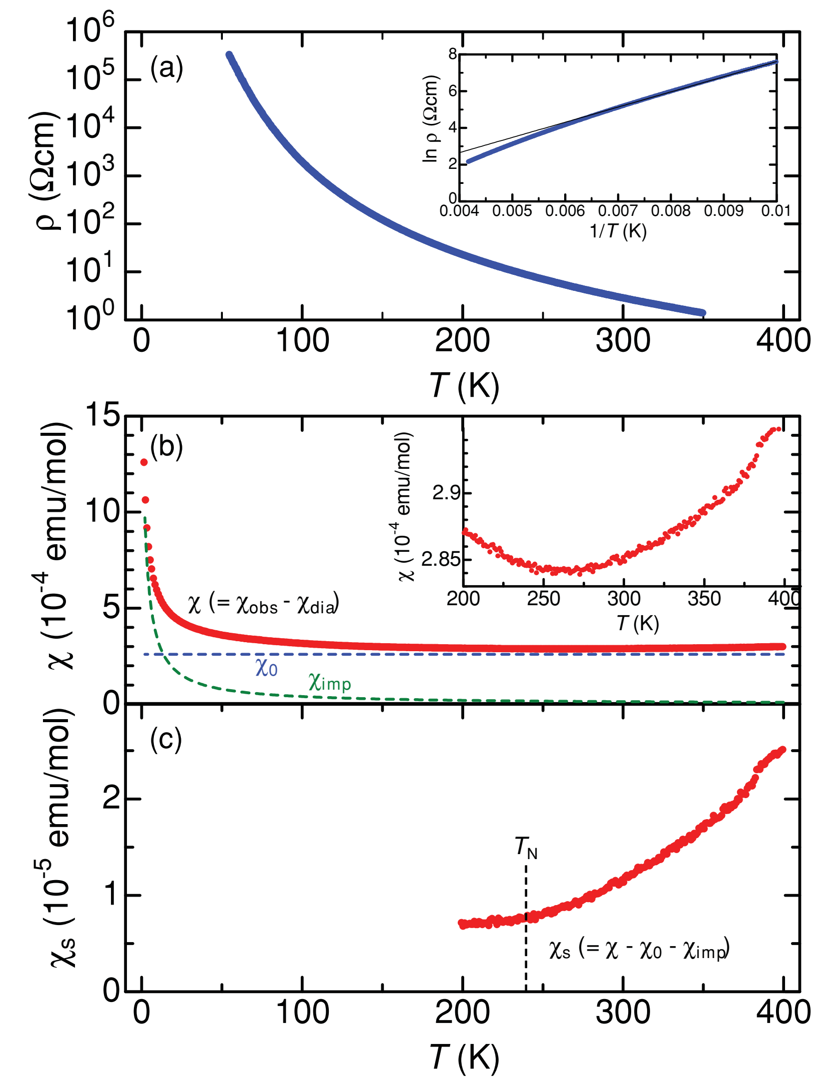
Resonant X-ray studies of magnetism in doped systems?

New 214 iridate: Ba2IrO4

Okabe,..Akimitsu et al, 2011

Same structure as Sr-214 but no rotation of Ir-O octahedra.

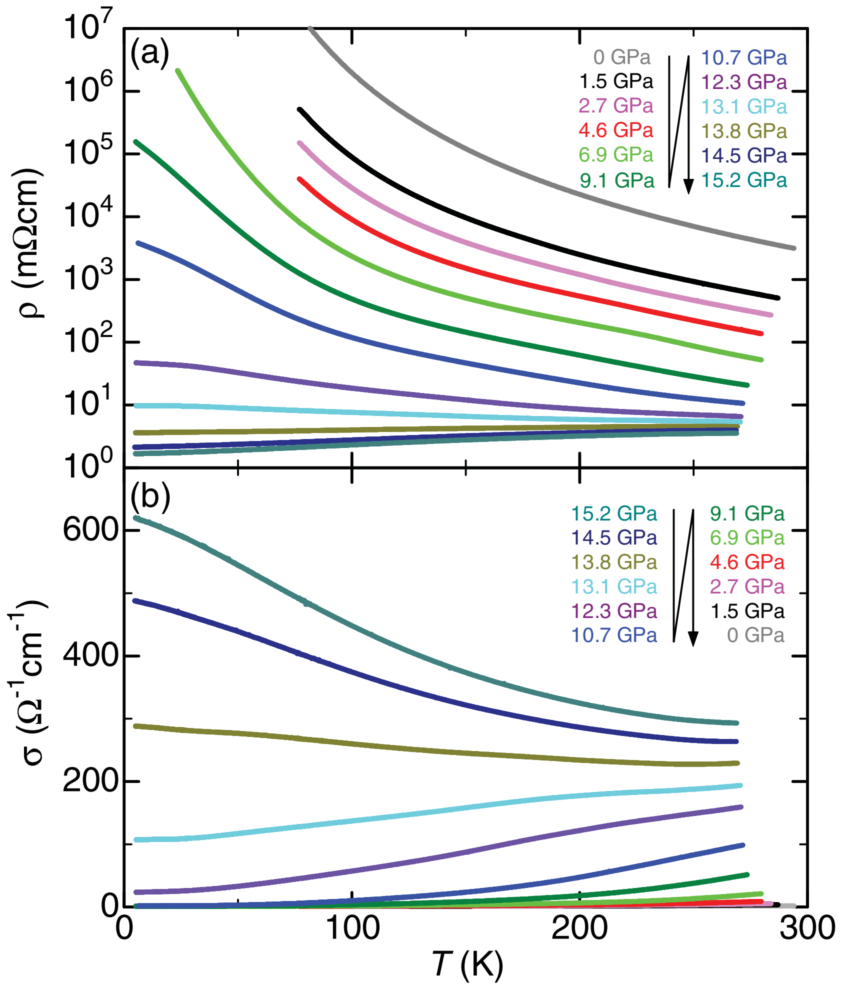




AF seen by muSR

Ba2IrO4: Metal-insulator transition under pressure

Okabe,..Akimitsu et al, 2011

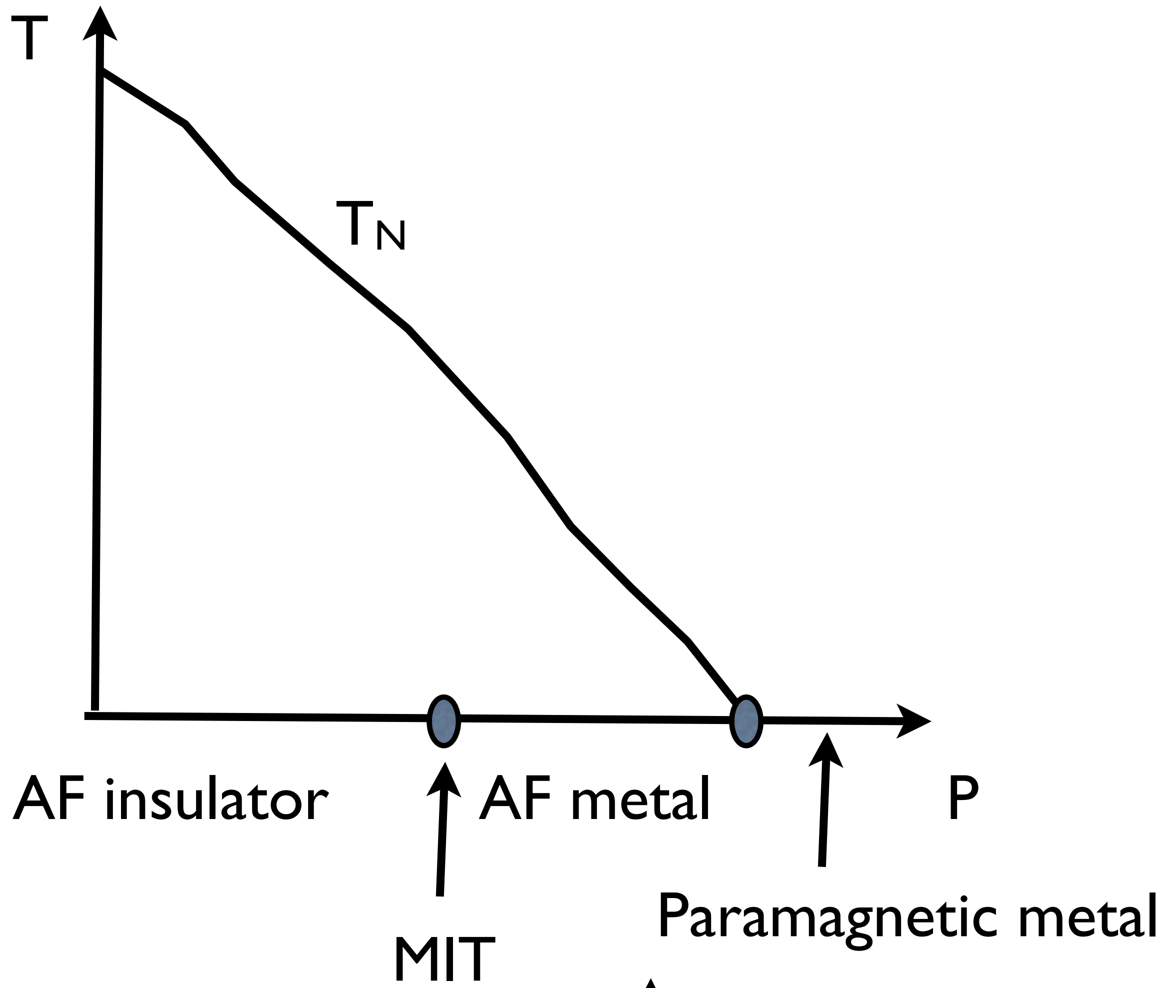


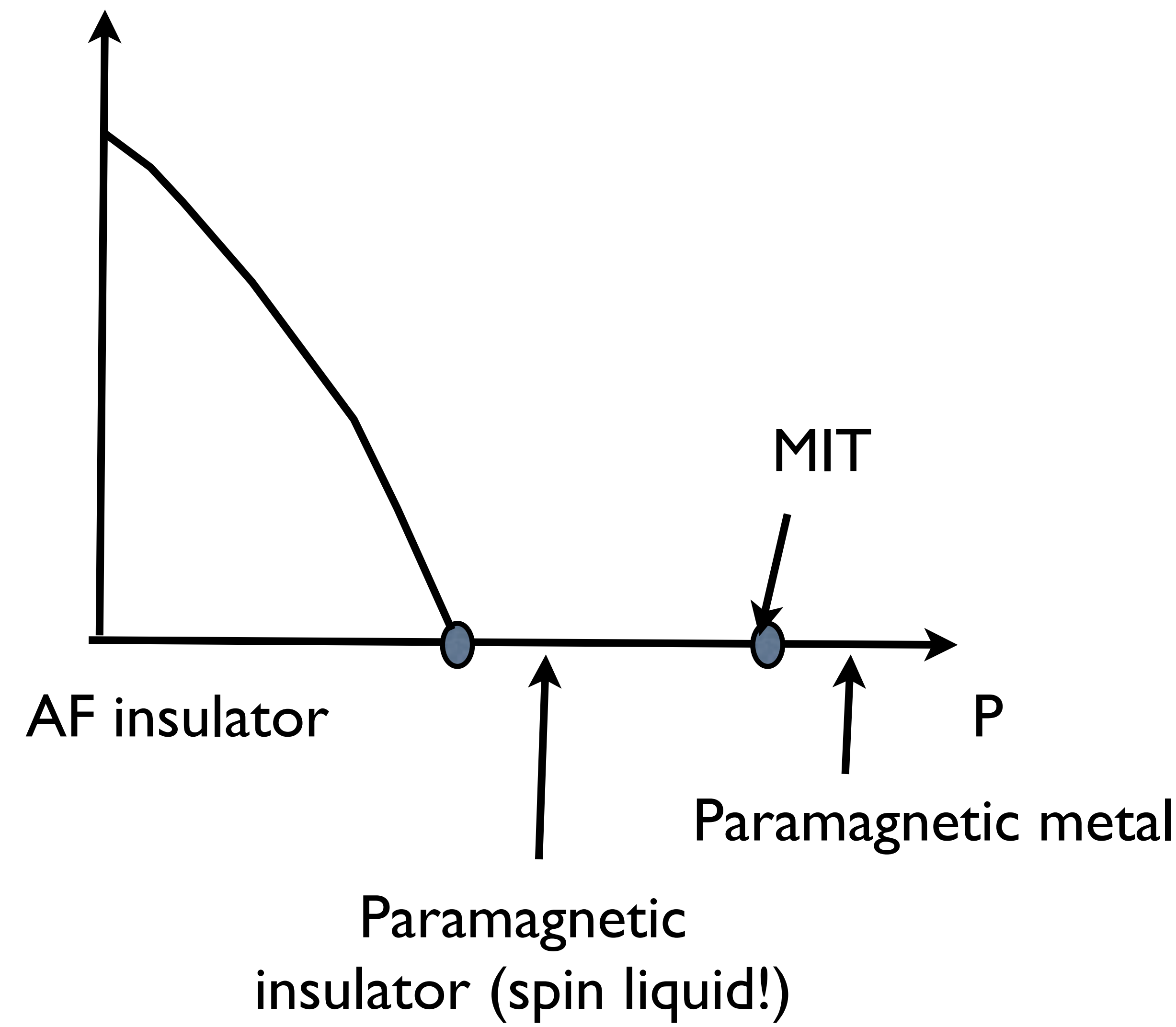
Apparently continuous T = 0 metal-insulator transition!

Nice opportunity to study interplay of magnetism and metal-insulator transition.

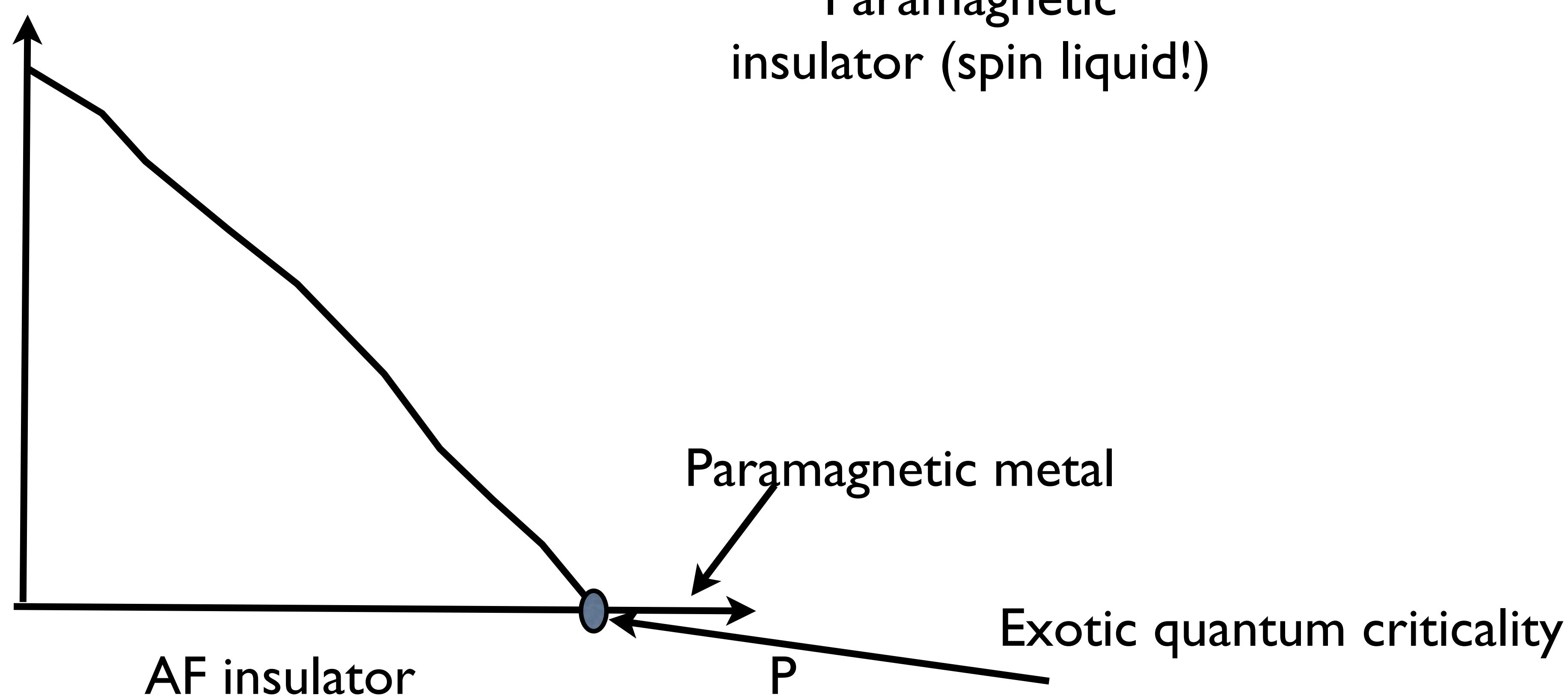
17O NMR under pressure?

Possibilities





Even more exotic



Summary

Sr2IrO4: spin-orbit entangled moments in a Mott insulator
Hubbard model similar to cuprates but smaller overall energy scale.

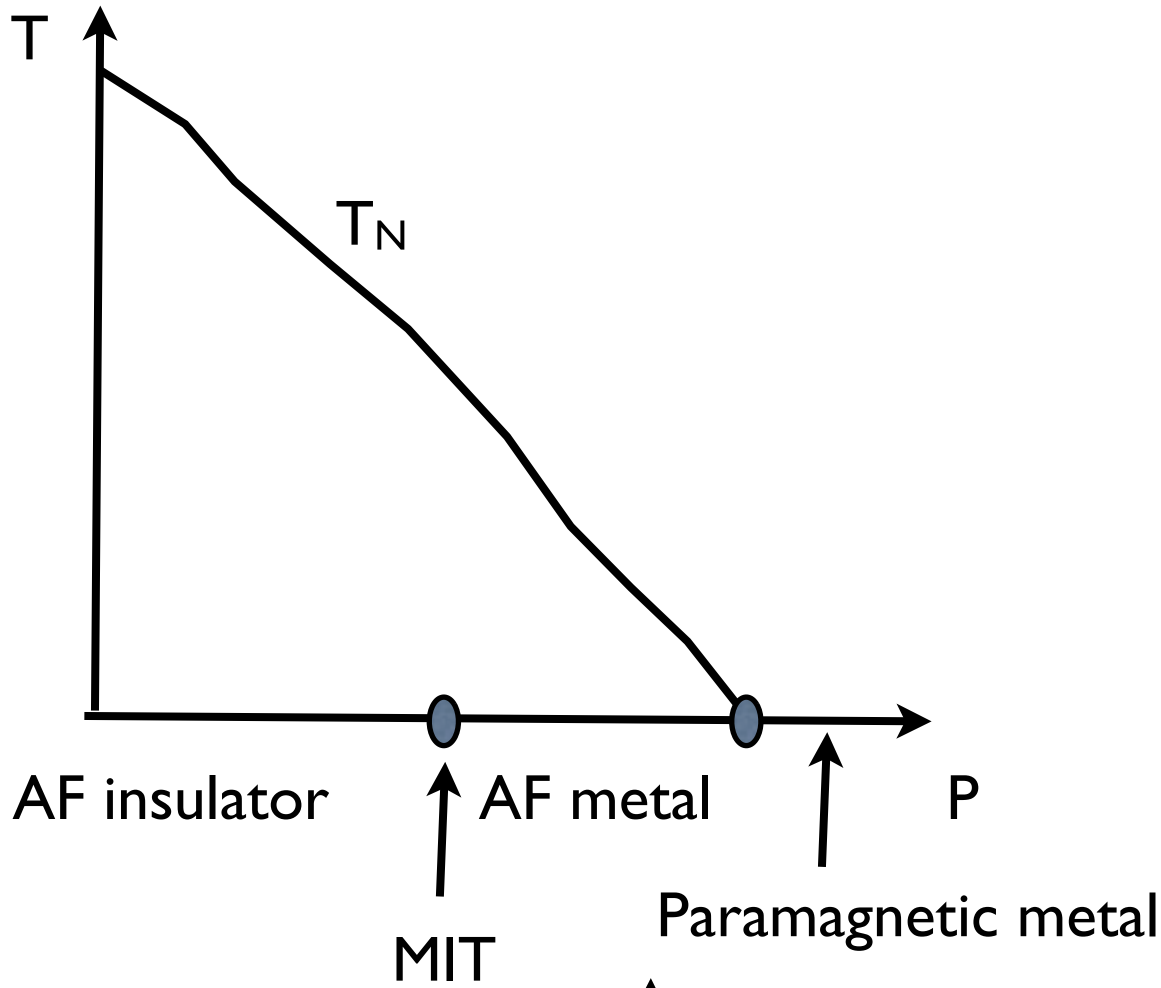
Electron doping may be analagous to hope doping of cuprates.

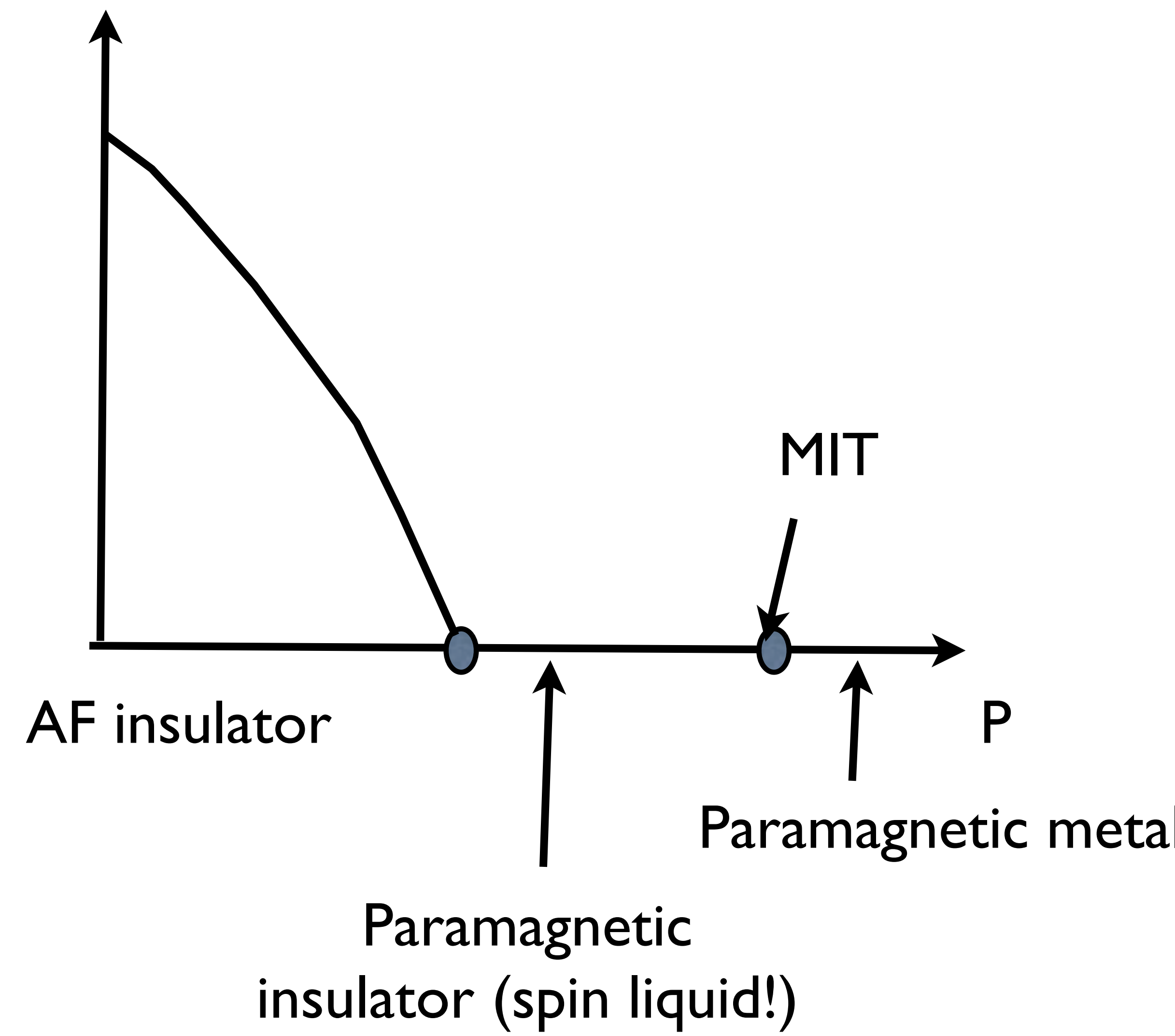
Doping: Finding superconductivity will obviously be exciting

BUT

Not finding superconductivity may also be equally or more exciting if the doped metal is strange or is pseudogapped.

Possibilities





Even more exotic