Title: Baby Skyrmion Superconductivity in a doped Antiferromagnet K2Fe4S5

Date: Aug 29, 2011 12:05 PM

URL: http://pirsa.org/11080144

Abstract: Strongly correlated electron systems are play grounds for exotic quantum states such as high Tc superconductivity, quantum spin liquids, non-fermi liquids and so on. Recently high Tc superconductivity has been observed in an iron based compound K2Fe4Se5. I will present a model and outline an effective theory [1] that describes physics of this complex system - a non linear O(3) sigma model in 2 + 1 dimensions coupled to Dirac fermions. Topological solitons and induced quantum numbers are well known in Skyrme model for protons and neutrons. In our context, we get topological baby Skyrmions with an induced charge 2e. Baby Skyrmions conduct themselves `super'.

Baby Skyrmion Superconductivity in doped Mott Insulator $K_2Fe_4Se_5$

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Introduction

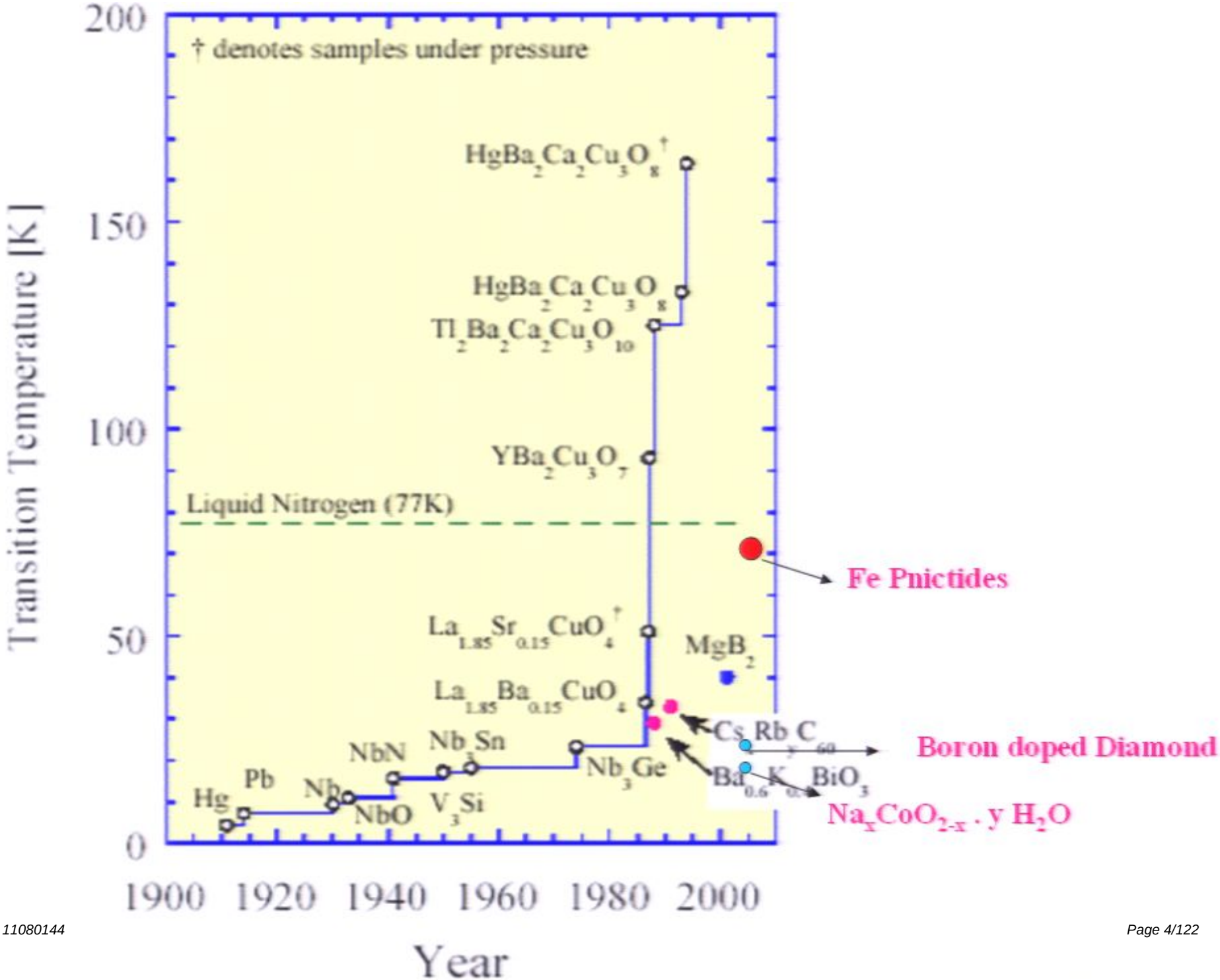
Phenomenology

Model Building for $K_2Fe_4Se_5$

Induced 2e Charge in Skyrmions

Spin gap, spin-8 Quantum Liquid & Superconductivity

Predictions and ways of increasing Tc


† denotes samples under pressure
Transition Temperature [K]
Year
200
150
100
50
0
1900
1920
1940
1960
1980
2000
HgBa2Ca2Cu3O8†
HgBa2Ca2Cu3O8
Tl2Ba2Ca2Cu3O10
YBa2Cu3O7
Liquid Nitrogen (77K)
La1.85Sr0.15CuO4†
La1.85Ba0.15CuO4
MgB2
Nb3Sn
NbN
Nb3Ge
Pb
Hg
Nb
NbO
V3Si
Fe Pnictides
Boron doped Diamond
NaxCoO2-x . y H2O

Routes to High Tc Superconductivity

Theoretical

Little's mechanism

Ginzburg's mechanism

Hydrogen under pressure

Doped Mott insulators & RVB mechanism

Experimental

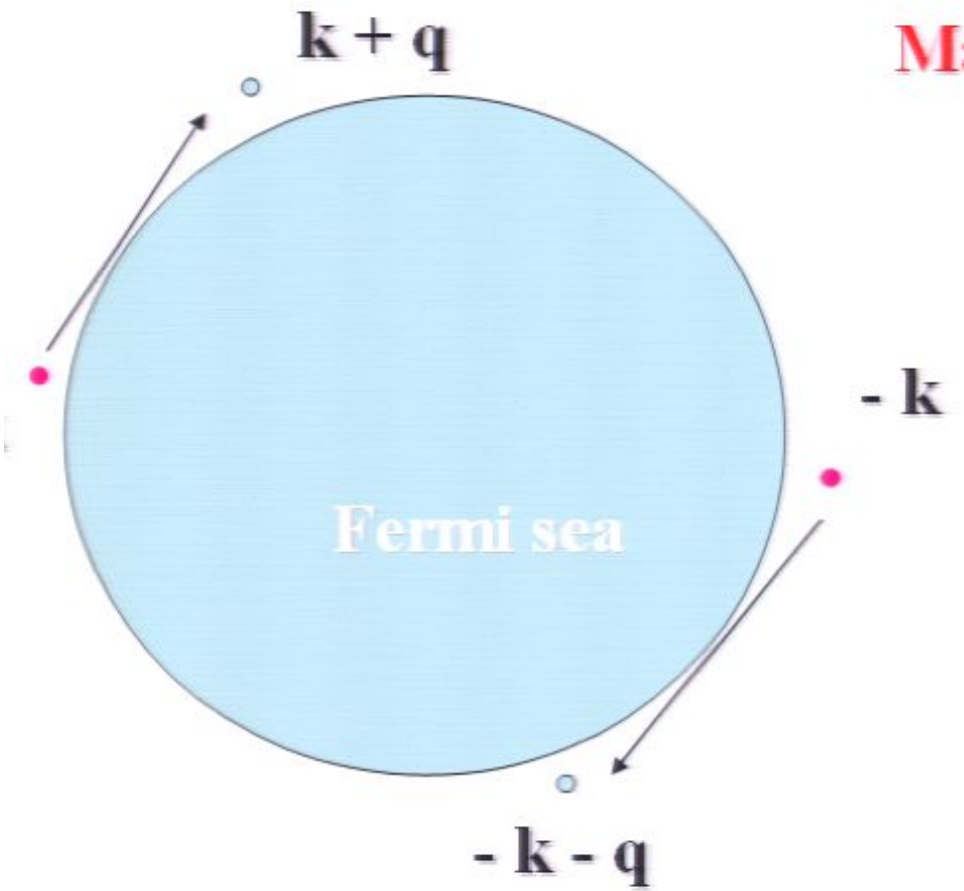
Cuprates - 32 K to 163 K

A15	23 K,
Chevrel Phase	15 K
$(SN)_x$, Organics - 1 K to	13 K
Oxides, .. $Ba_{1-x}Na_x BiO_3$	40 K
Nickel borocarbides	24 K
Fullerits 40 K, Graphite	50 K (?)
Boride MgB_2	40 K
Li Intercalated HfNCl	27 K
Fe Arsenide Family	56 K

CS theory

Fermi liquid reference state

m^*, fermi liquid parameters, ..



Matrix elemenet for phonon mediated scattering is negative

Cooper instability

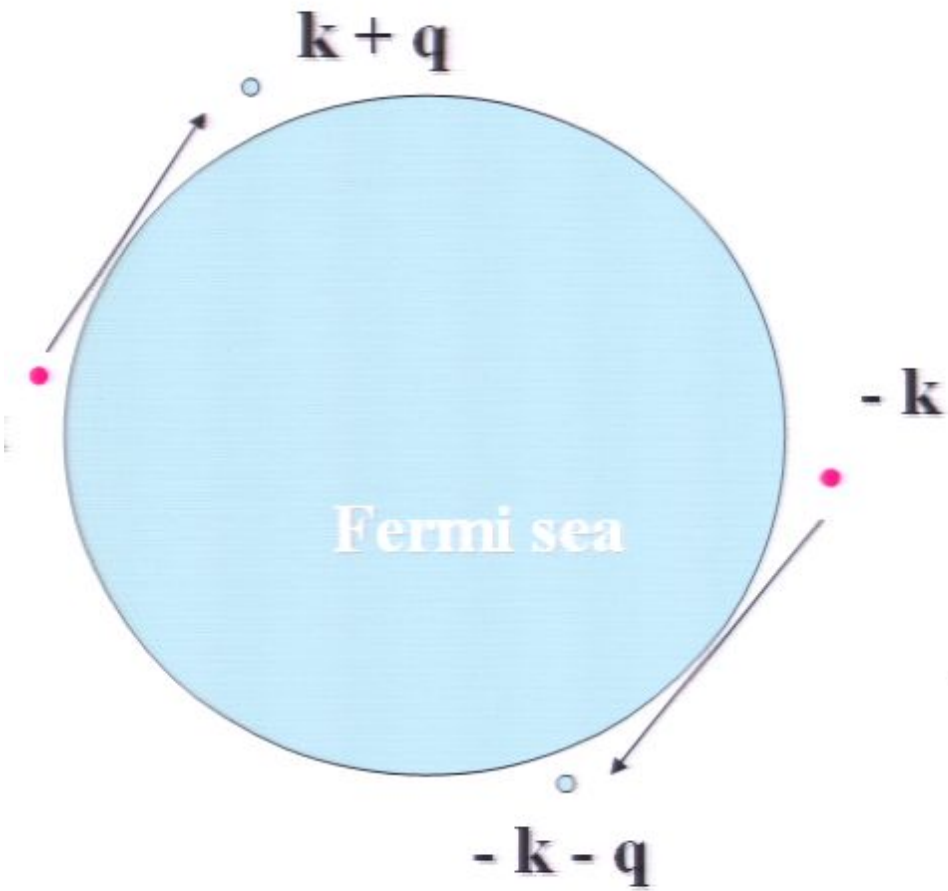
BCS superconducting state

CS theory

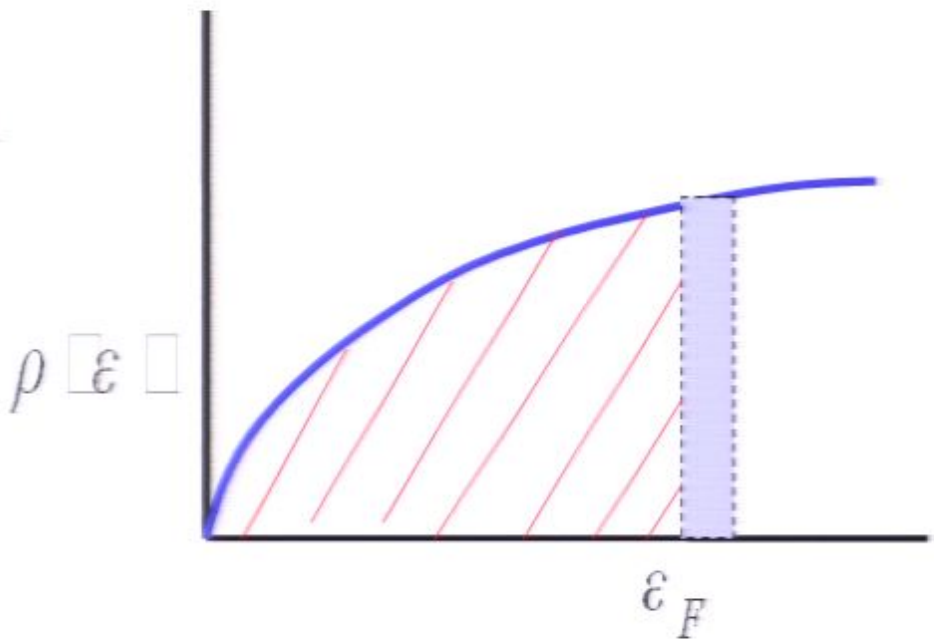
Fermi liquid reference state

m^*, fermi liquid parameters, ..

Fraction of participating electrons $\frac{\hbar\omega_D}{\varepsilon_F} << 1$



Severe Pauli Blocking



BCS theory inspired
traditional route
to new superconductors

$$k_B T_c = \hbar\omega_D e^{\frac{-1}{\rho \cdot g}}$$

Look for

Large Debye frequency
Large density of states
Large electron phonon coupling constant

$$k_B T_c = \hbar \omega_D e^{\frac{-1}{\rho \cdot g}}$$

Serious constraints from stability point of view
-McMillan, Anderson, Cohen

Phonon mediated maximum Tc ~ 30 K

raction of electrons
articipating in
uperconductivity is

$$\frac{\hbar\omega_D}{\varepsilon_F} << 1$$

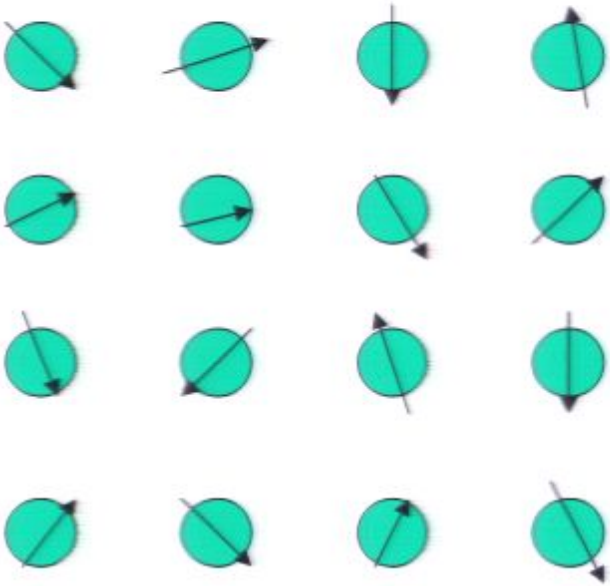
his roughly defines low temperature superconductors

ow do we make more electron participate in superconductivity ?

'uprates showed a new way: Doped Mott insulators

(RVB theory: absence of fermi surface, Mott localization, superexchange, preformed Cooper pairs …)

Mott Insulator

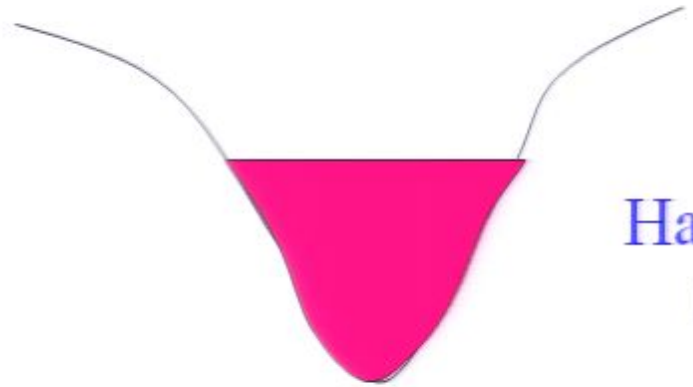


$a >> a_B$

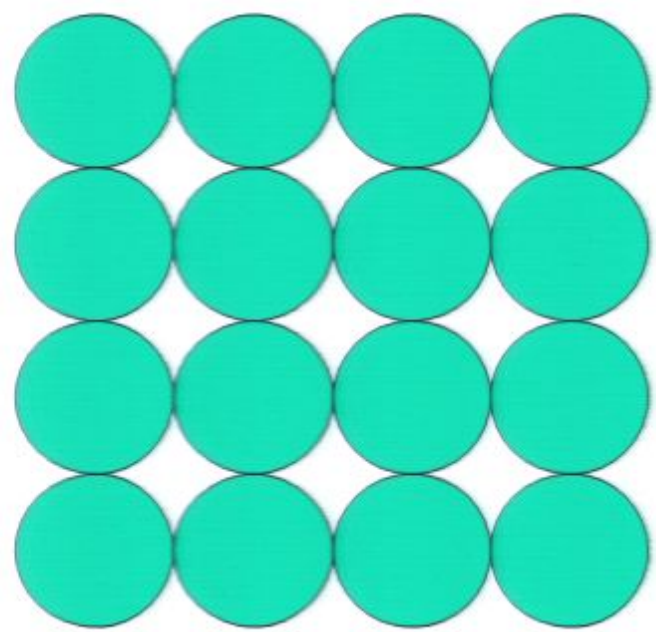
upper Hubbard band

lower Hubbard band

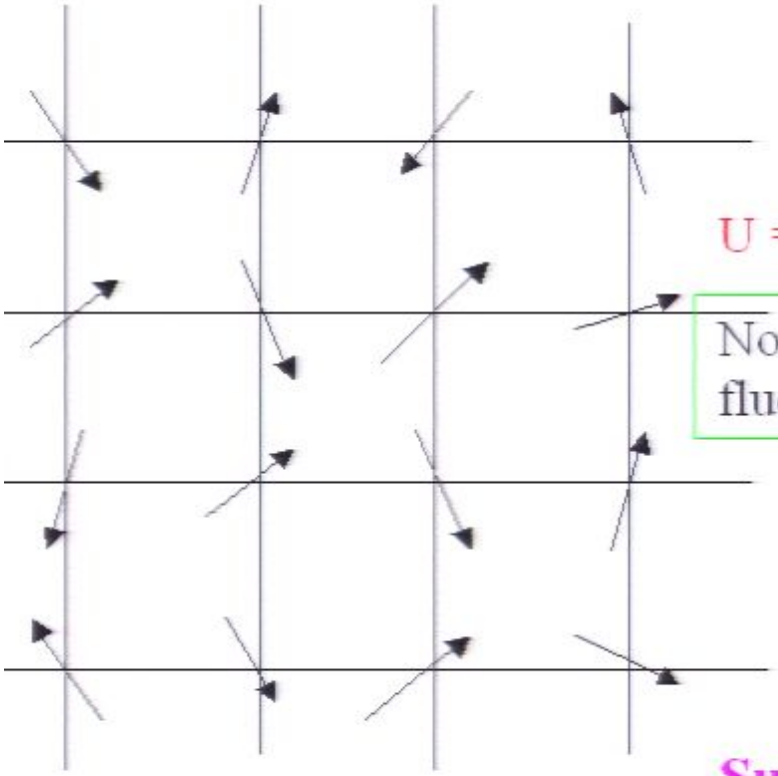
Metal



Half filled band



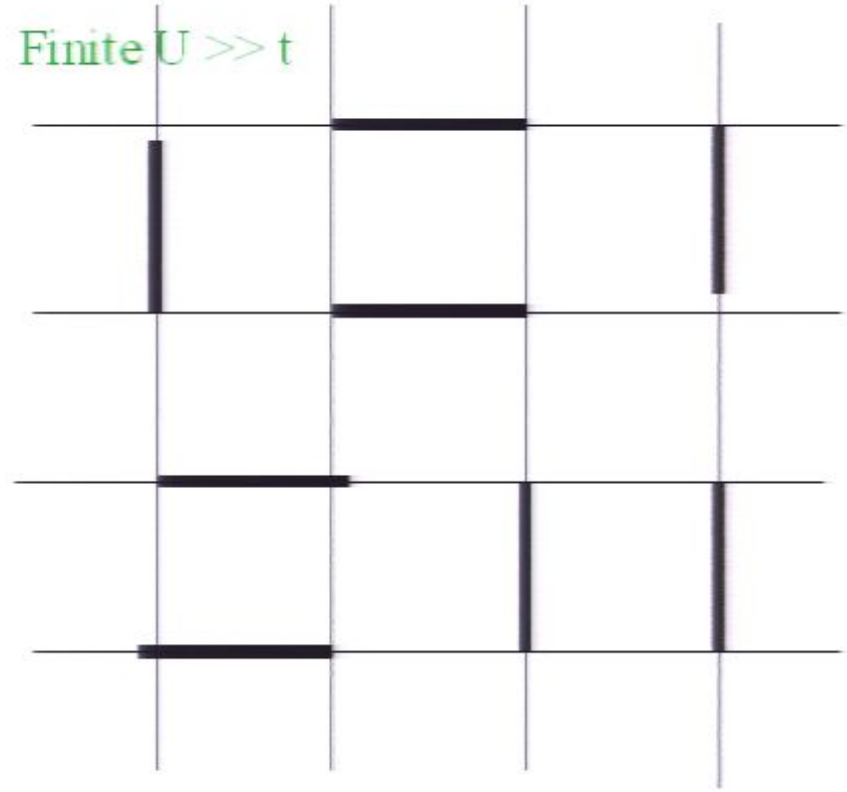
$a \sim a_B$



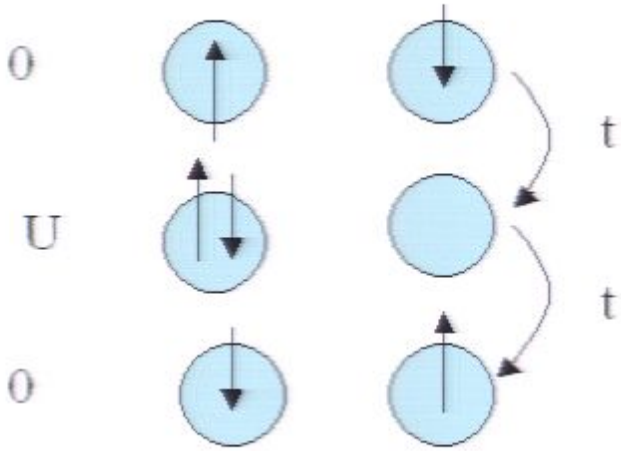
U = infinity

No quantum fluctuations

Finite U >> t



Superexchange or Kinetic exchange process

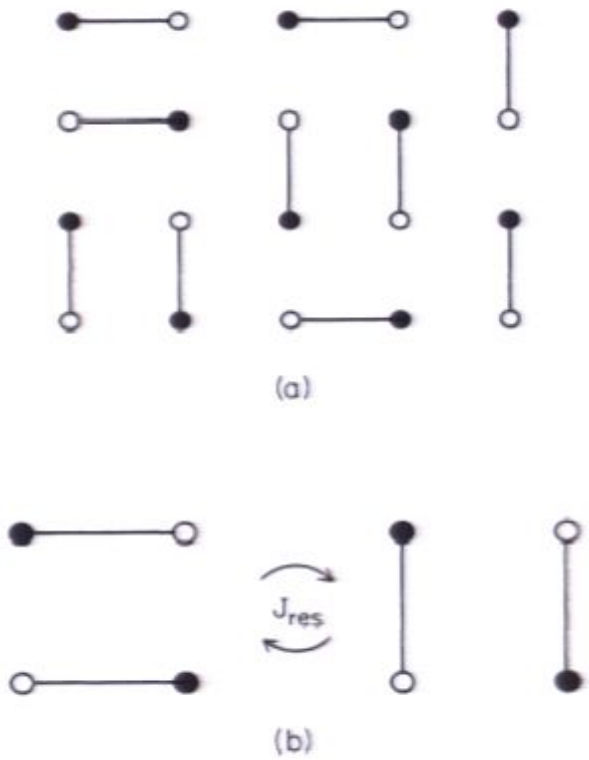


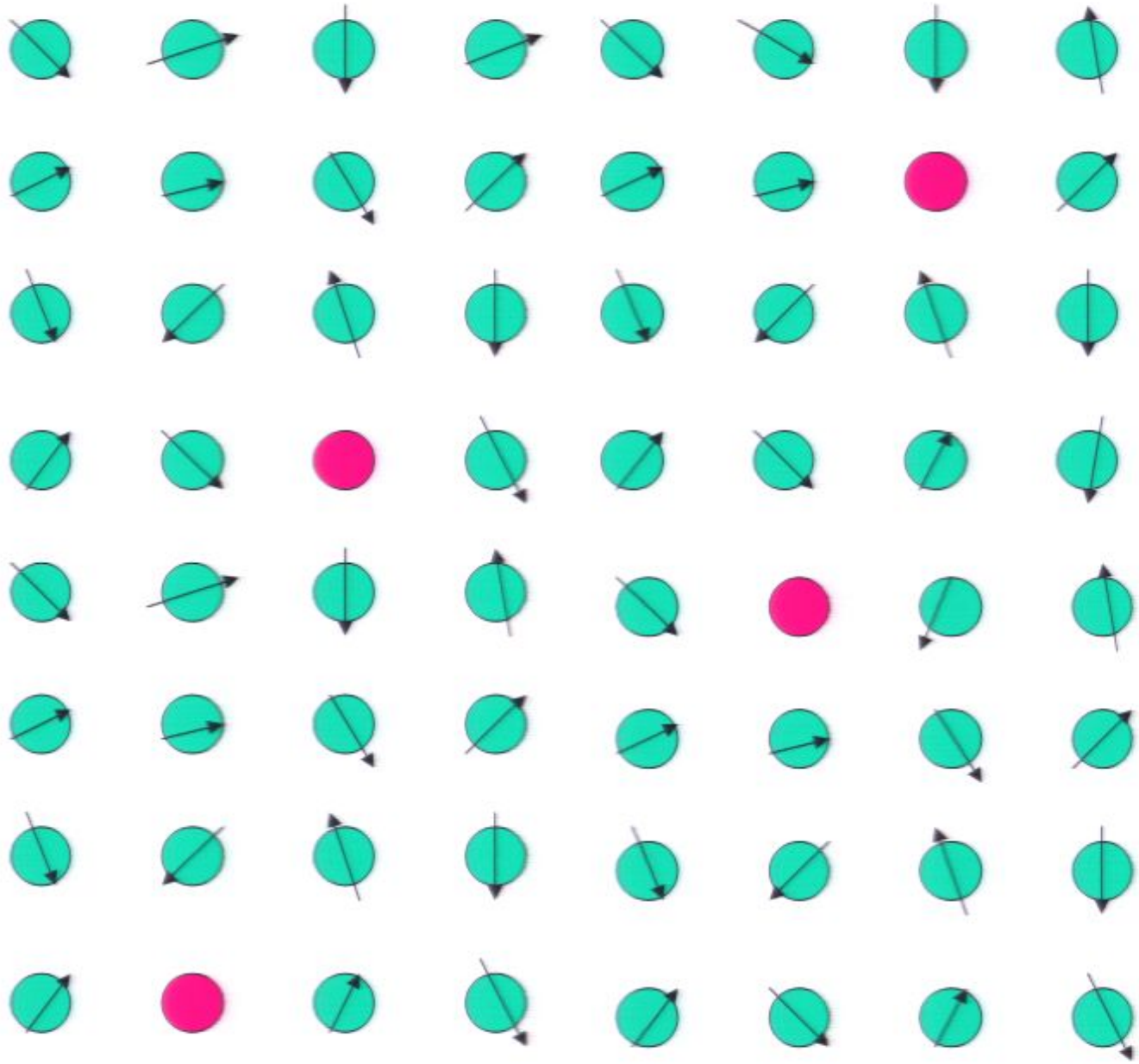
$$\text{Energy gain} = J = \frac{-4t^2}{U}$$

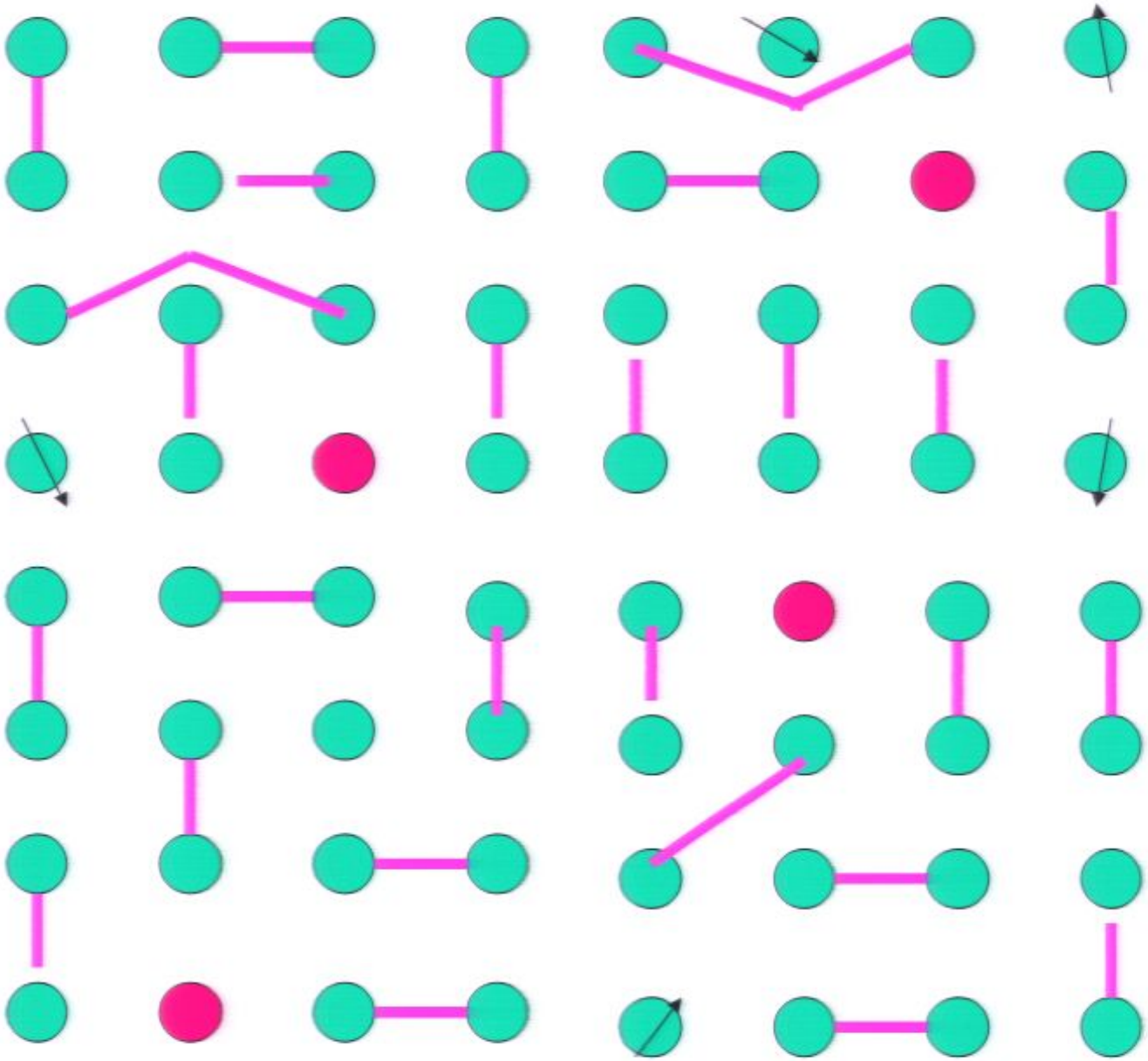
$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

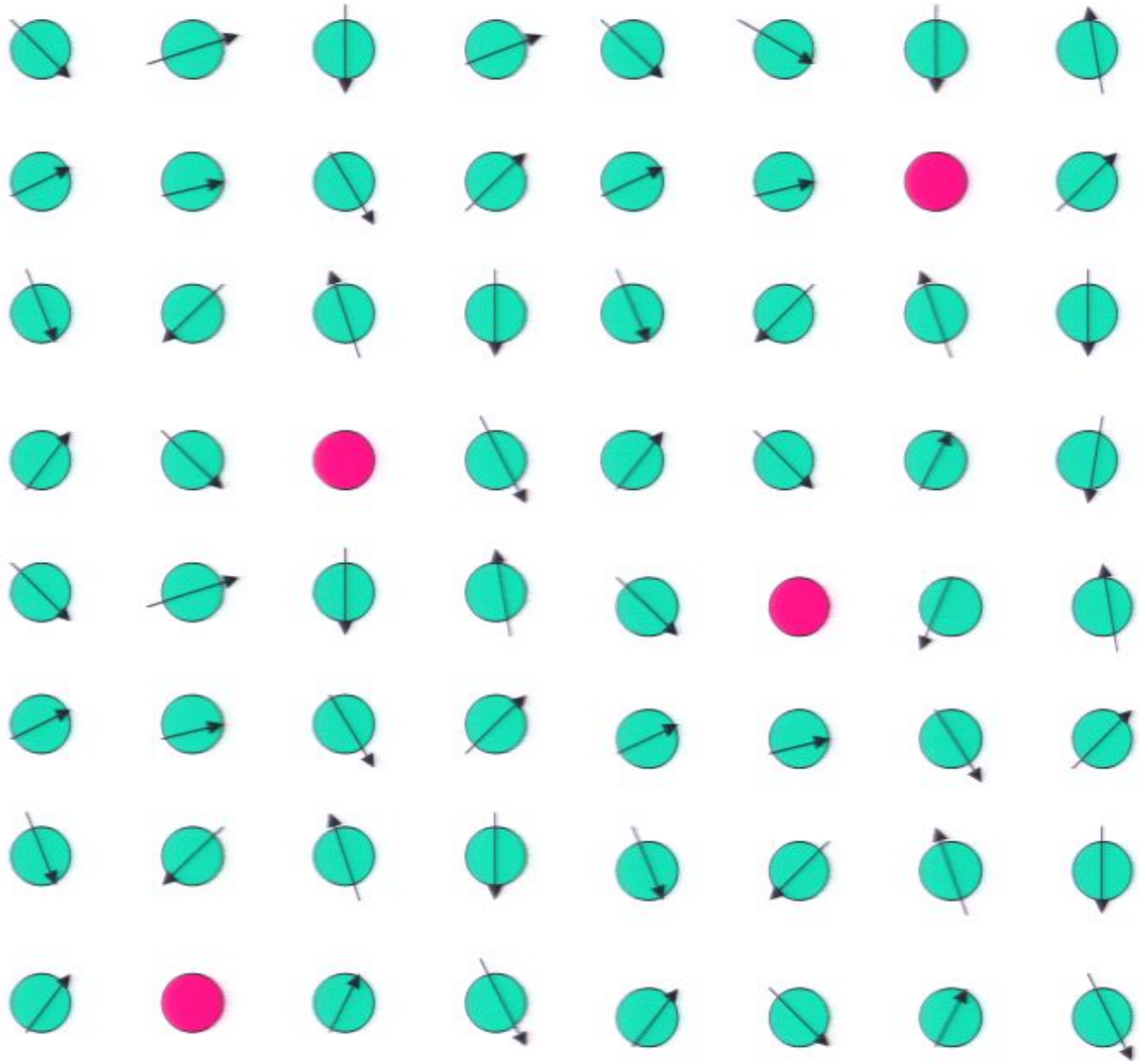
$$H = J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4}\right)$$

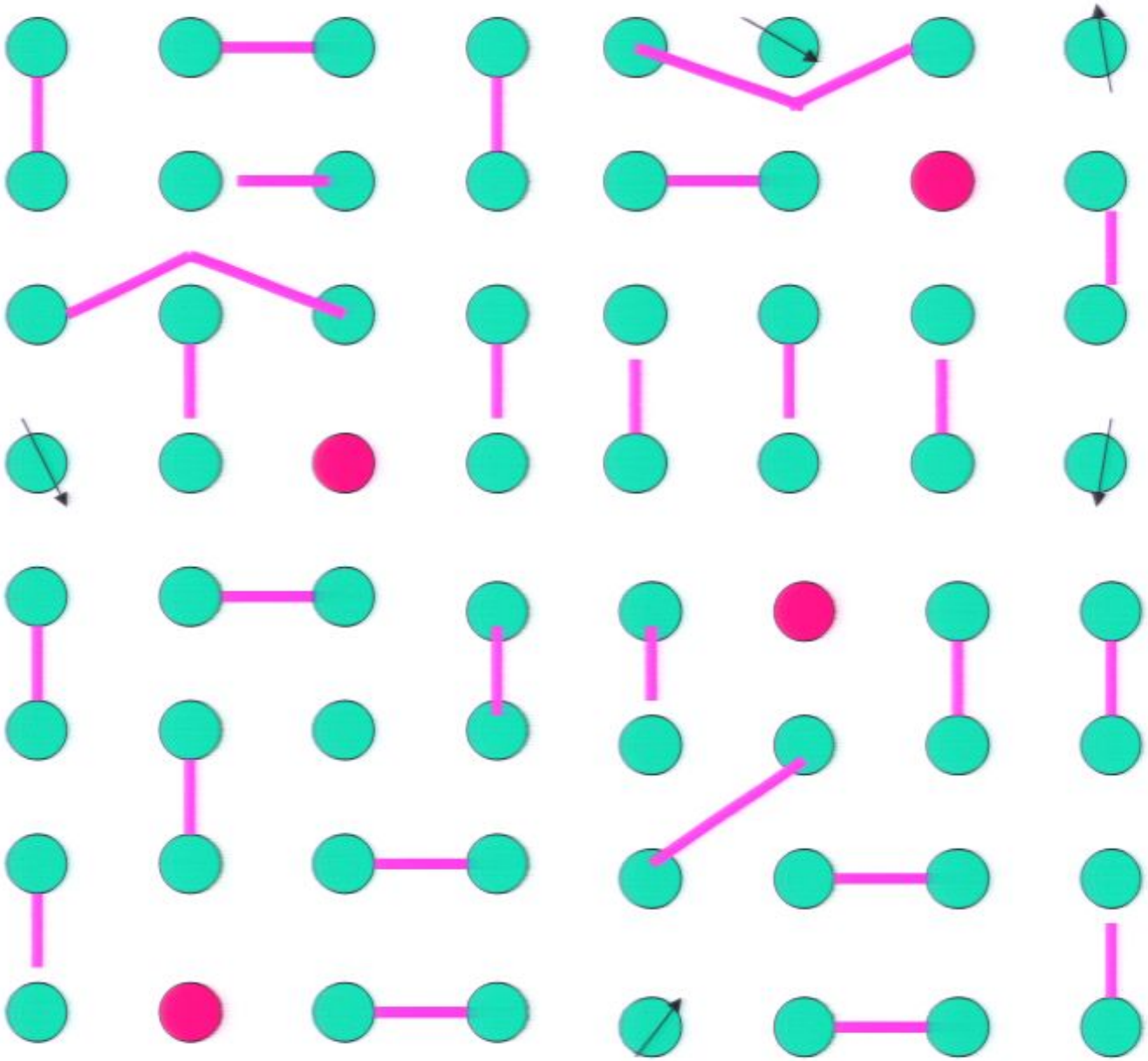
Energy gain = 0


(a)
J_{res}
(b)







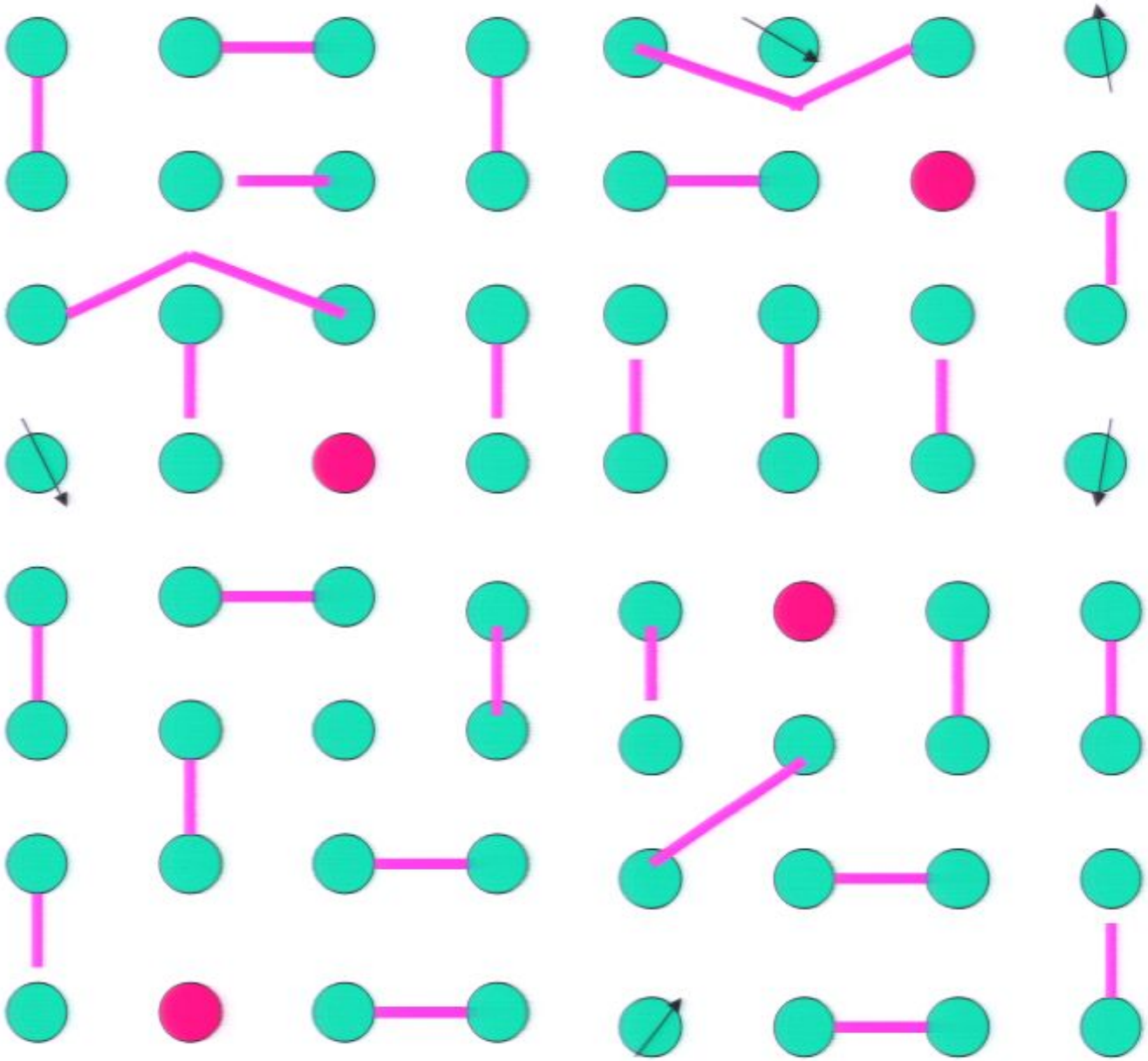


inglet correlations (arising from antiferromagnetic couplin
a Mott insulator are pre-existing neutral cooper pairs
hey carry spin current and no charge current)

Doping charges the neutral singlets

Resonating charge singlets form a superconducting state
rovided they do it in a phase coherent manner)

1987 P W Anderson
GB, Zou and Anderson



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Message from
Resonating Valence Bond (RVB) theory

Mott insulators are seats of high Tc Superconductivity

Superexchange is the GLUE

Fraction of electrons participating in superconductivity

is not $\frac{\hbar\omega_D}{\varepsilon_F}$ **but x**

Therefore $k_B T_c \sim xt$ **(here t is the hopping parameter)**

nother Message from RVB Theory (1987-88)

nportance of Topological Excitations of an
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tatistics Transmutation, induced charge,
lidgap states, two spinon states,
ooper pair as a topological excitation …

olyakov, Wiegmann, Dzhyaloshinski (1988)
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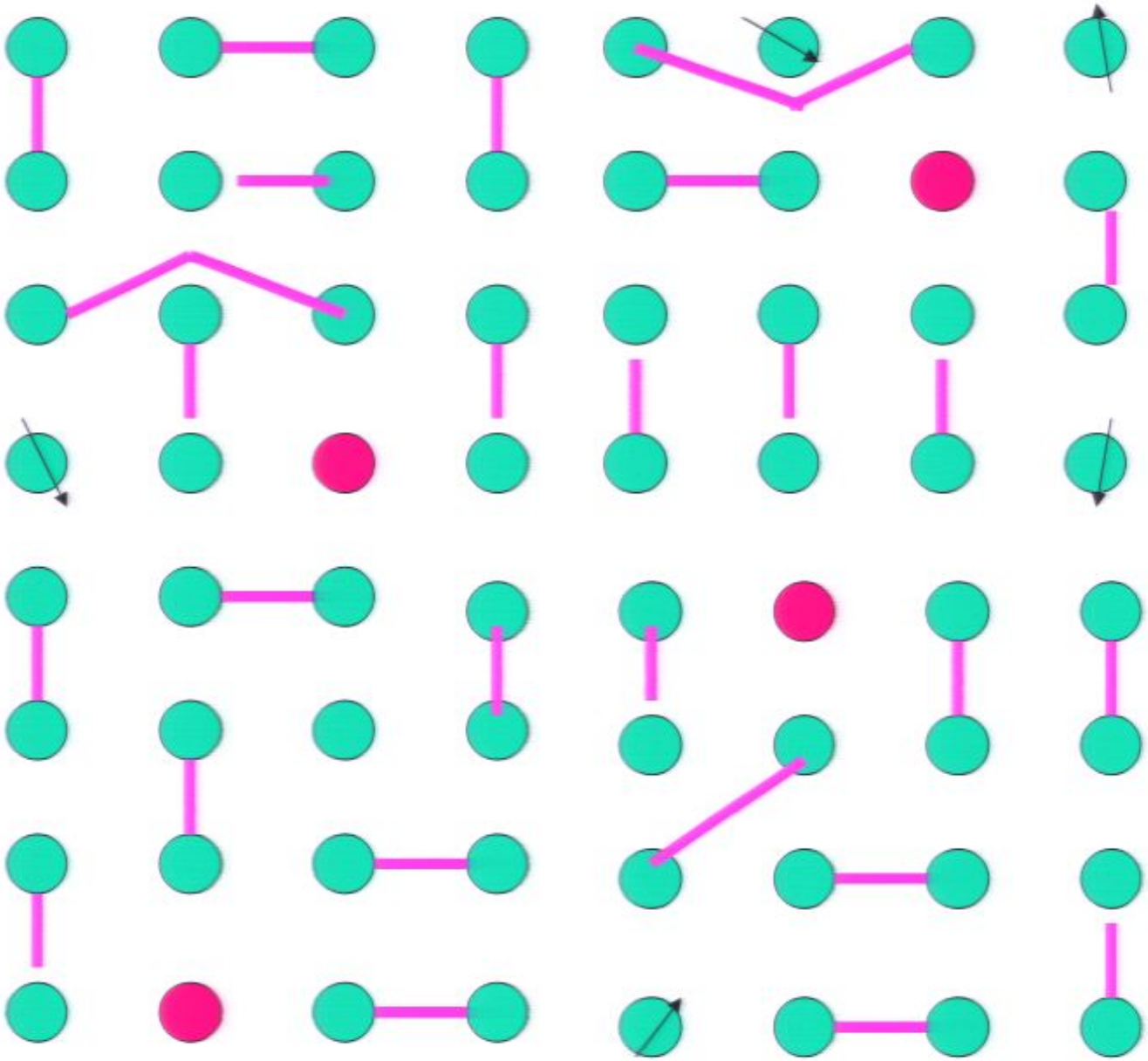
ohn, Golubentsev, Berciu
Viegmann, Abanov …



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J|A|C|S
COMMUNICATIONS

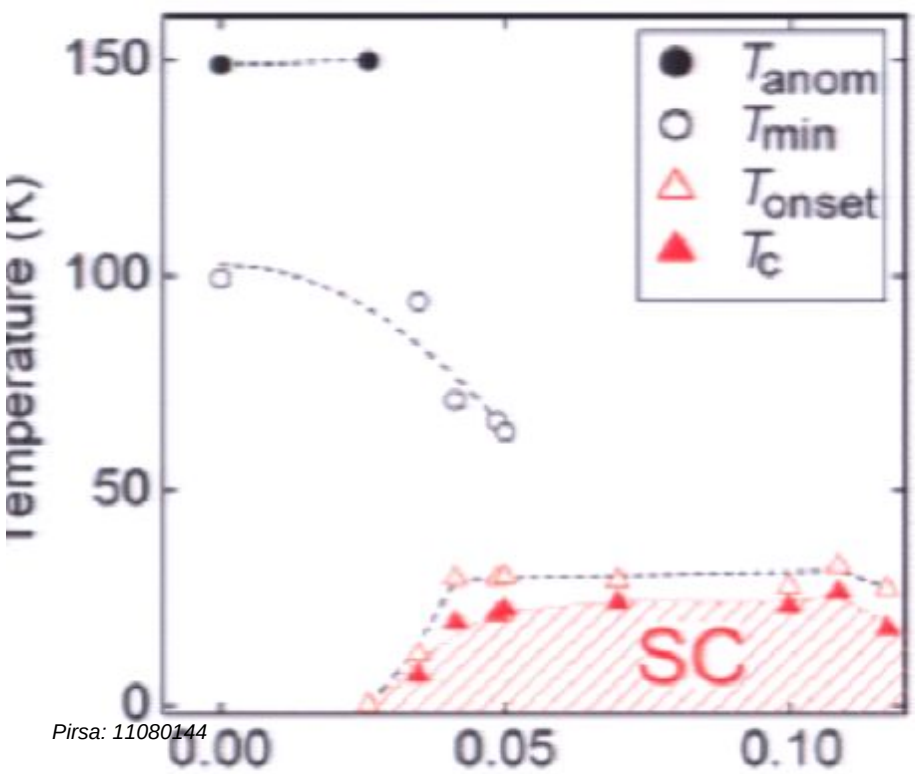
Published on Web 02/23/2008

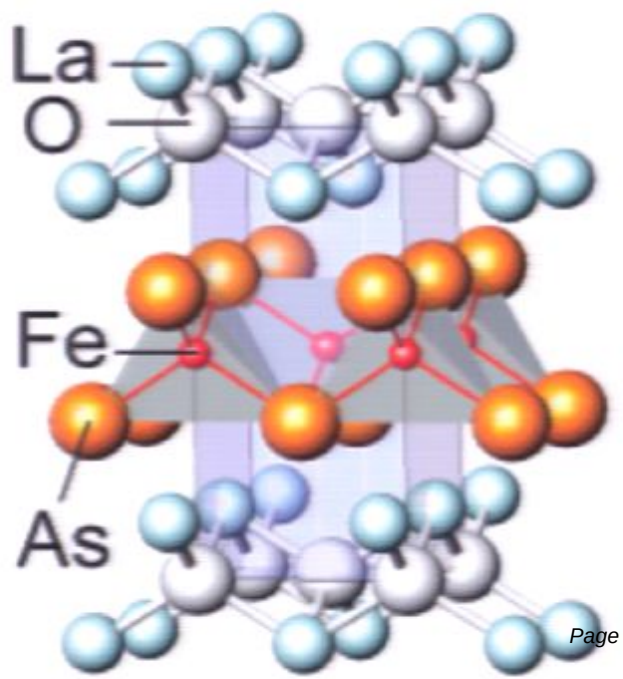
Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05-0.12$) with $T_c = 26$ K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

E-mail: hosono@msl.titech.ac.jp



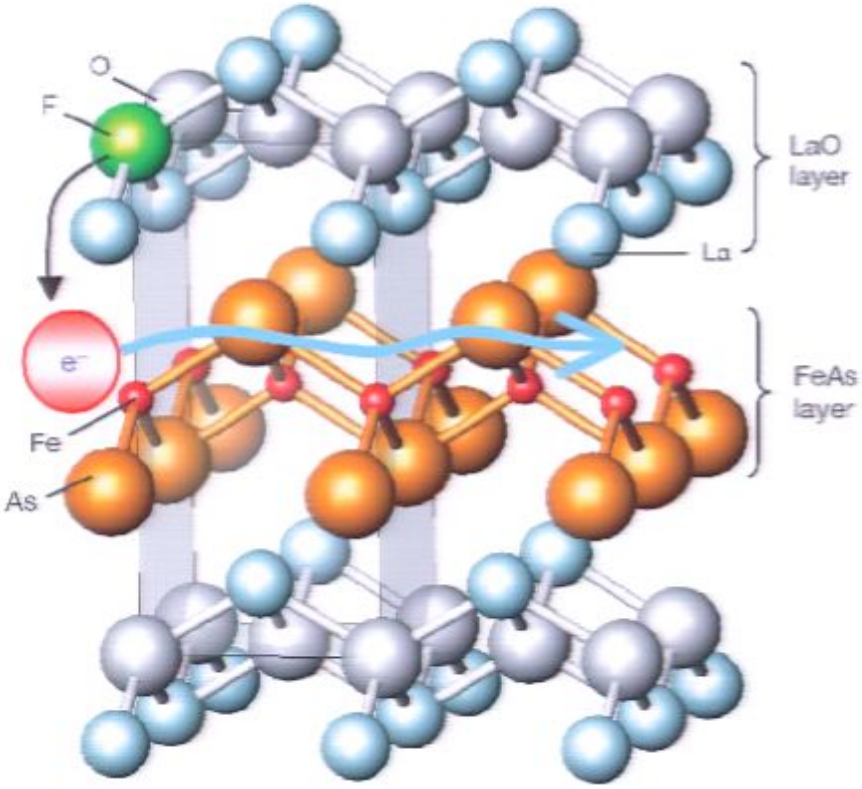


$Re[O_{1-x}F_x]FeAs$

Re=La, Ce, Pr, Nd, Sm, Gd, Tb

space group : tetragonal (P4/nmm)

lattice constant : a =4.02Å, c =8.71Å



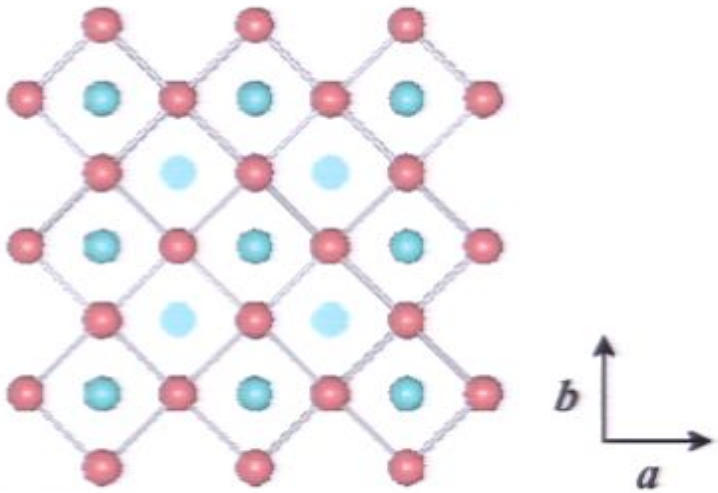
H. Takahashi *et al.*,Nature **453**, 376 (2008)

From *c*-axis

Fe : 2D-square lattice

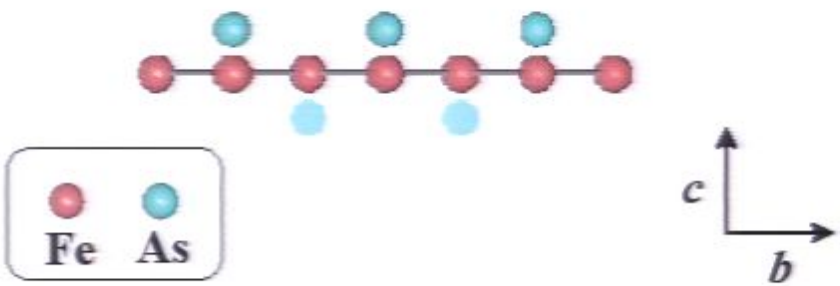
Fe-As distance : 2.327Å

Fe-Fe distance : 2.854Å



From *a*-axis

As : above and below Fe-plane

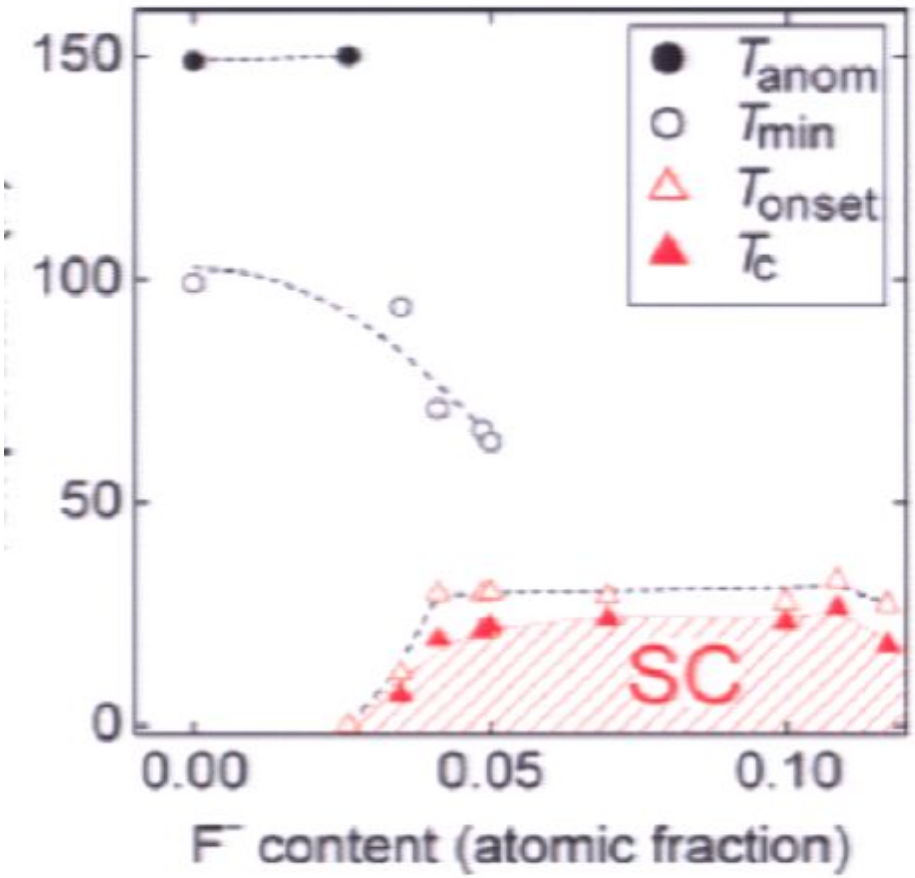


slide: Hosono

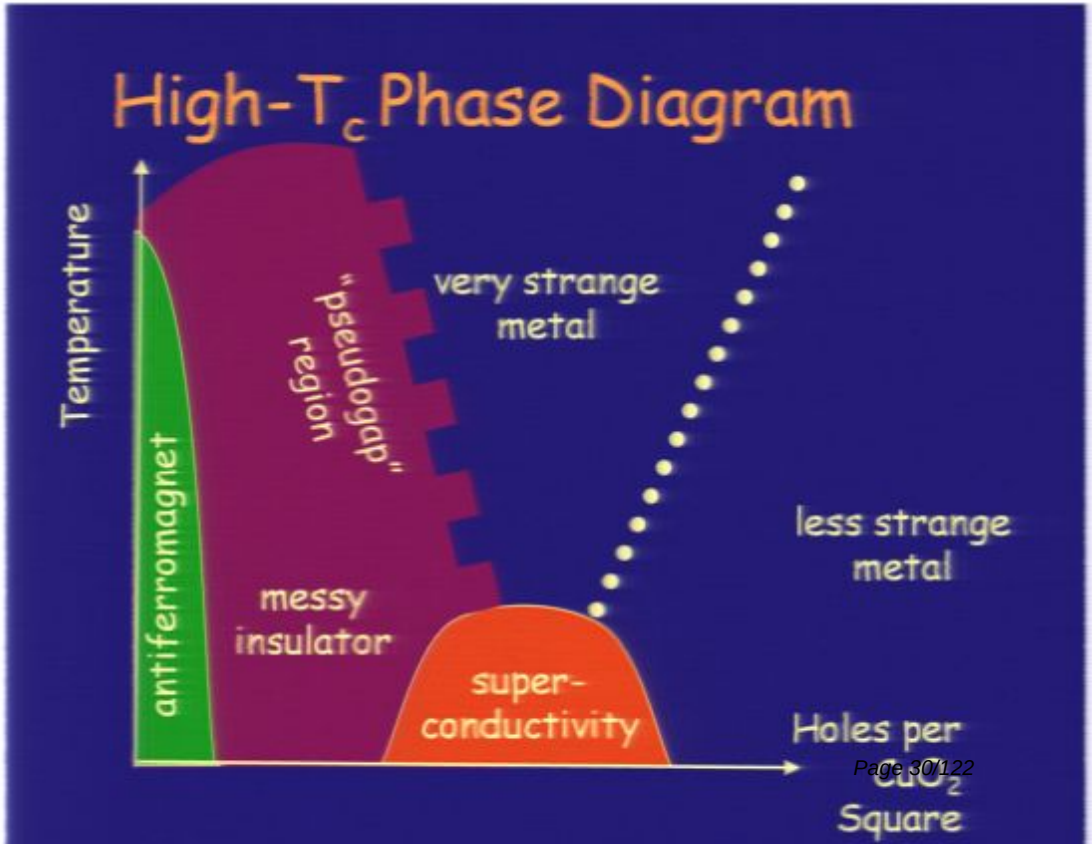
LaO FeAs
Nominal Valence: $La^{3+}\ O^{2-}\ Fe^{2+}\ As^{3-}$

Fe^{2+} : $3d^6$

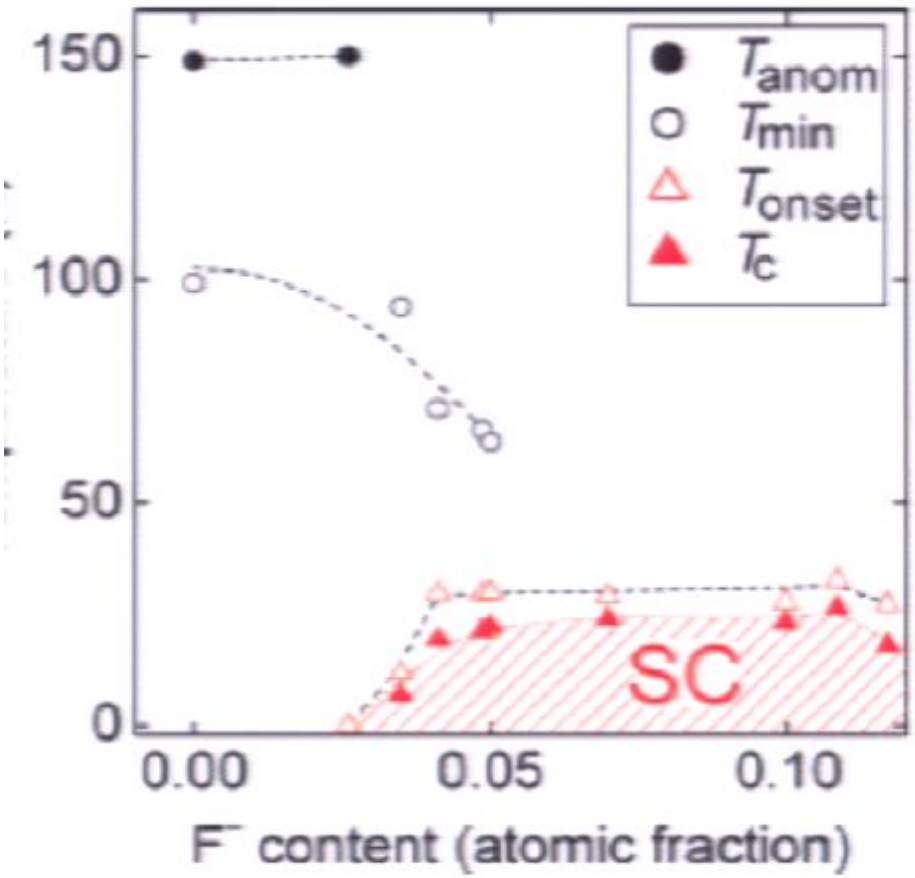
LaO1-xFxFeAs



Similarity to cuprate phase diagram



LaO1-xFxFeAs



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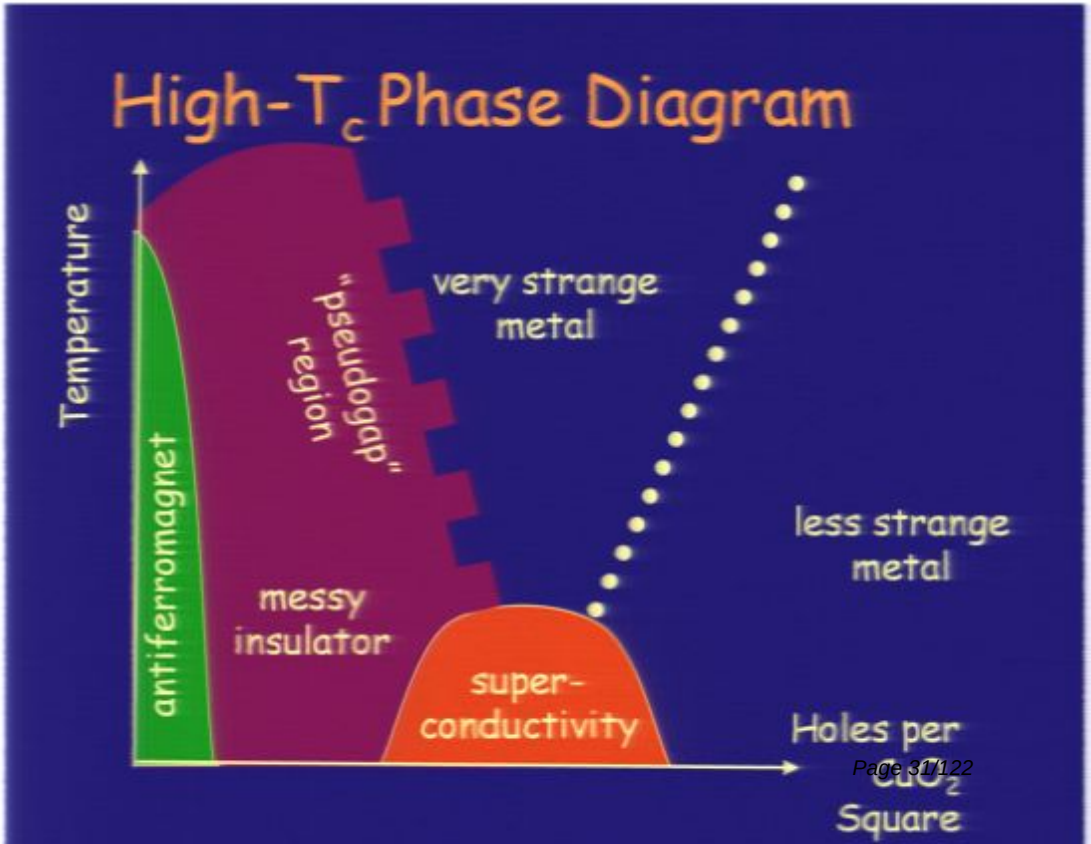

LaO FeAs
Nominal Valence: $La^{3+}\ O^{2-}\ Fe^{2+}\ As^{3-}$

Fe^{2+} : $3d^6$

Odd electrons

La_2CuO_4	$3d^9$
CuO	$3d^9$
VO_2	$3d^1$
K_3C_{60}	

Even electrons

NiO	$3d^8$
$LaMnO_3$	$3d^4$
V_2O_3	$3d^2$
$LaCoO_3$	$3d^6$
$LaOFeAs$	$3d^6$
$FeSe$	$3d^6$
$K_2Fe_4Se_5$	$3d^6$

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Fe^{2+} : $3d^6$

Fe^{2+} : $\boxed{3d^6}$

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— $S = 2$ ✓

— $S = 1$

— $S = 0$

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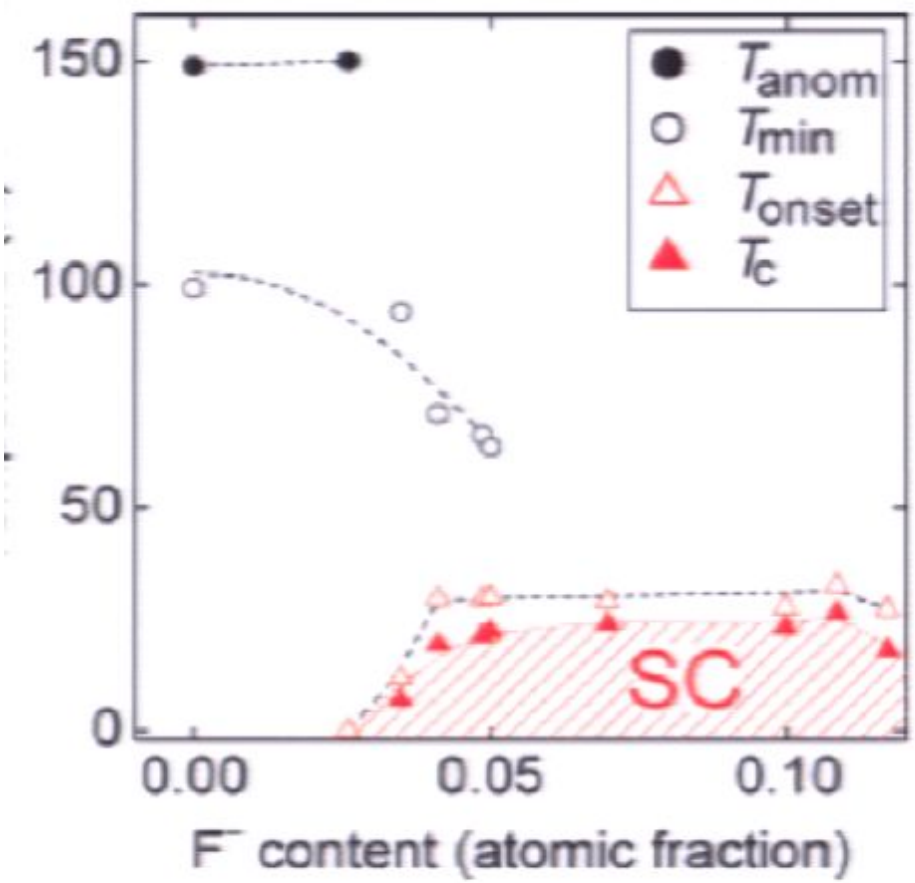
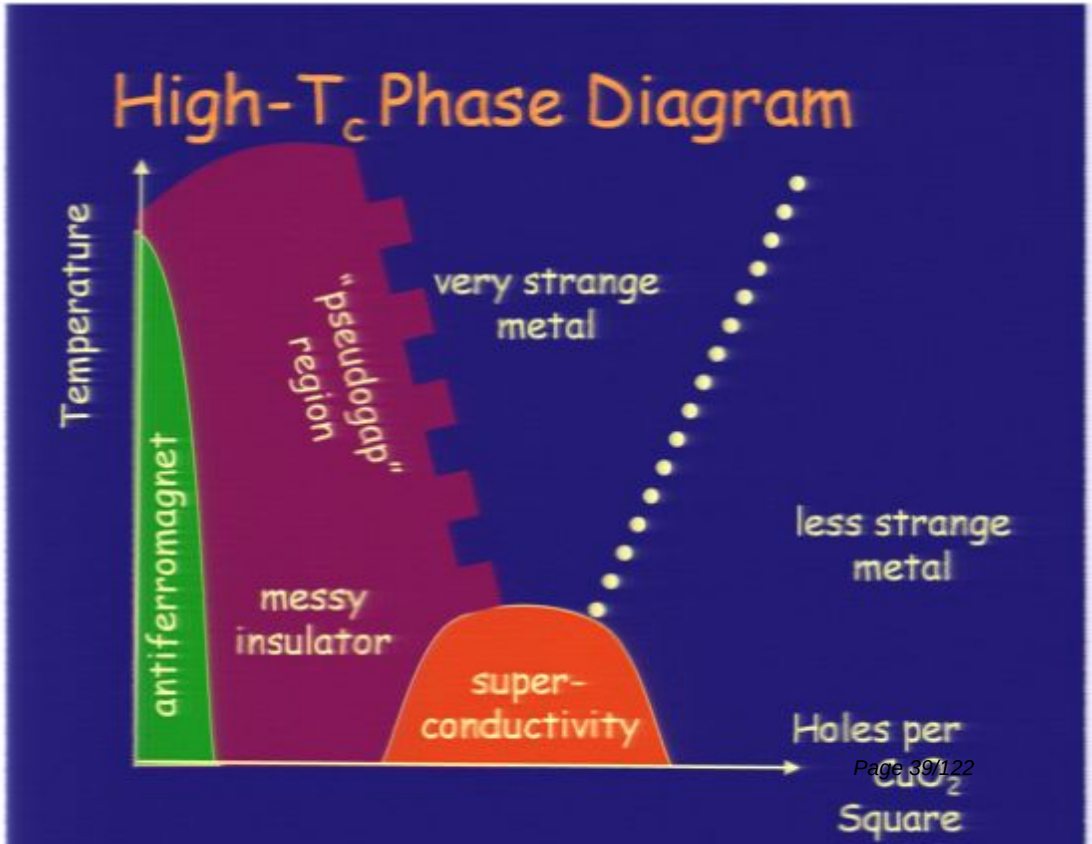
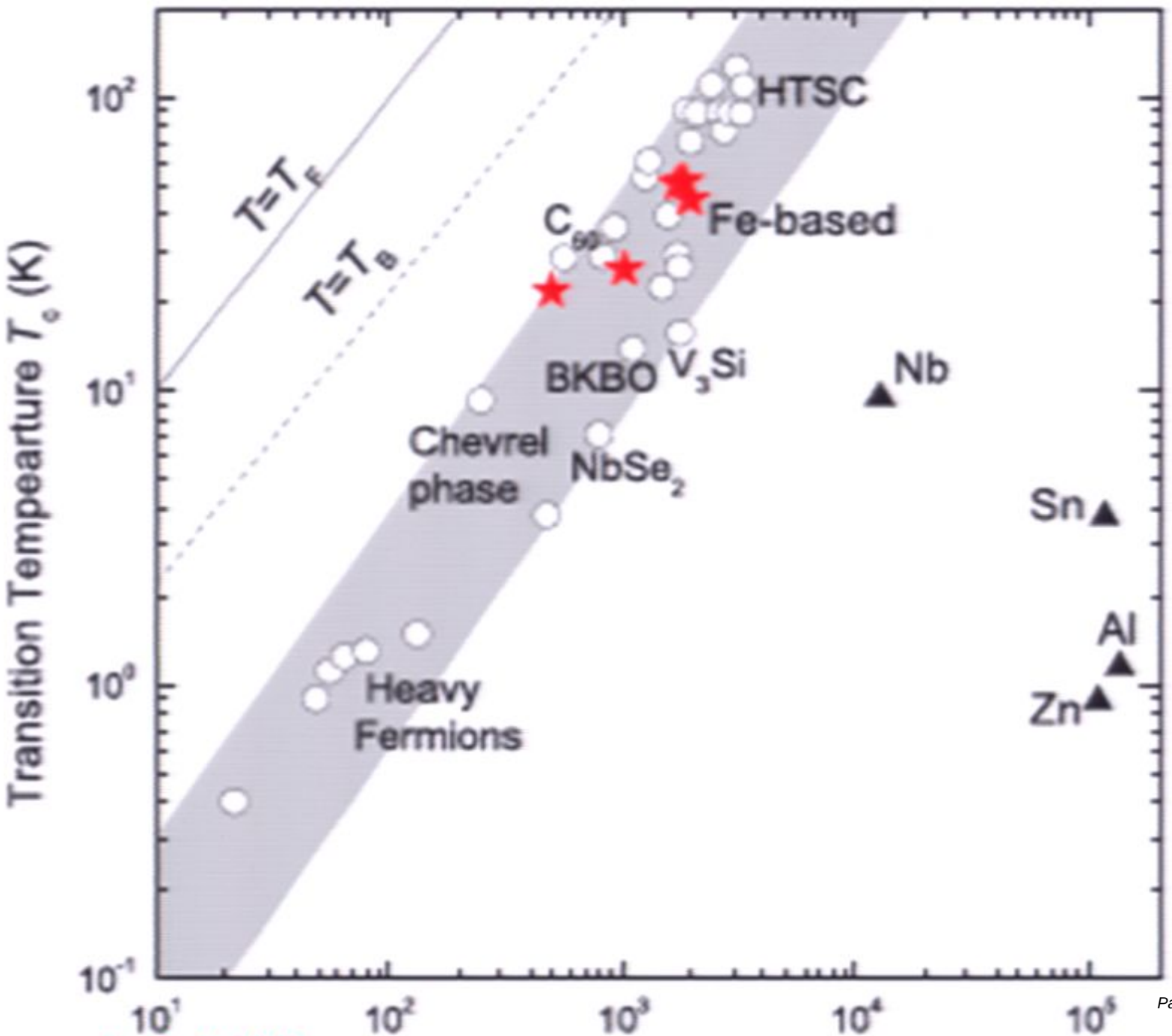
LaO1-xFxFeAs



Similarity to cuprate phase diagram





Khasanov et al. 2008

New Fe based systems

Superconducting Tc increases from 27 K to 55 K

REOFeAs - RE: rare earth Sm, Nd, Pr …

$SrFe_2As_2$, $BaFe_2As_2$, …..

α- FeSe, FeTe

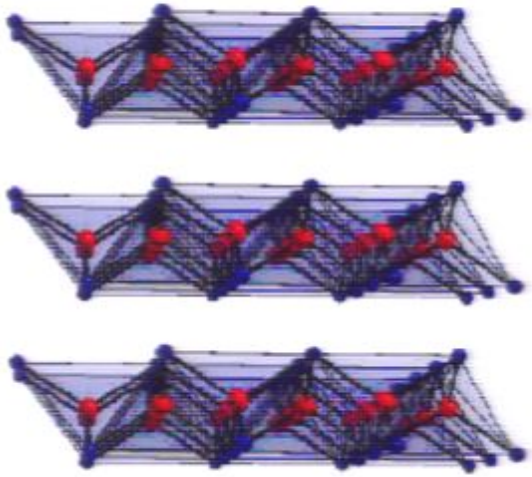
intercalated $K_2Fe_4Se_5$ family, ..

Strong Coupling Theory of Superconductivity In Fe pnictide systems:

G Baskaran, J. Phys. Soc. Jap., Nov. 2008 (arXiv:0804.1341)

Q Si and E Abrahams, PRL 2008 (arXiv: 0804.2480)

Property	Cuprate	Fe pnictide/chalcogenide
ott Insulator rentage	yes (spin-half)	? (spin-1, GB)
oping	external	internal and external
in gap (NMR, Susceptibility)	yes	yes
perconducting Dome	yes	yes
ectrical transport	anomalous/bad metal	anomalous/bad metal
H	T dependent	T dependent
RPES	anomalous QP	anomalous QP
ttinger theorem	violated in low doping	violated
in-1 resonance in eutron scattering (pi,pi)	yes	yes
arge variation of FM Moment and T_c	yes	yes

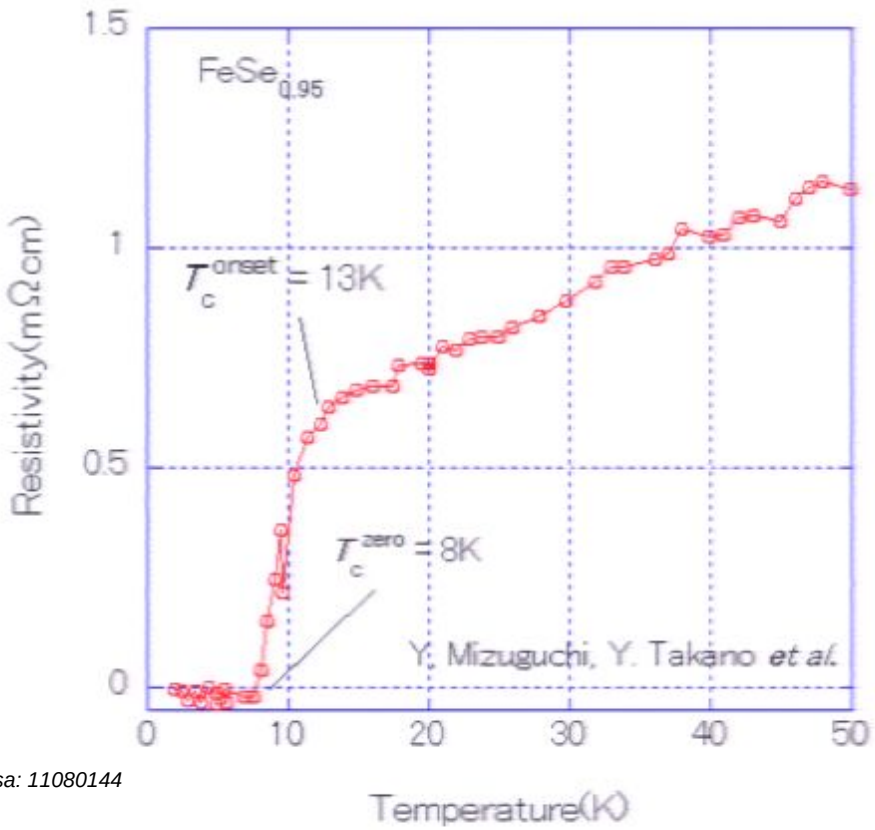


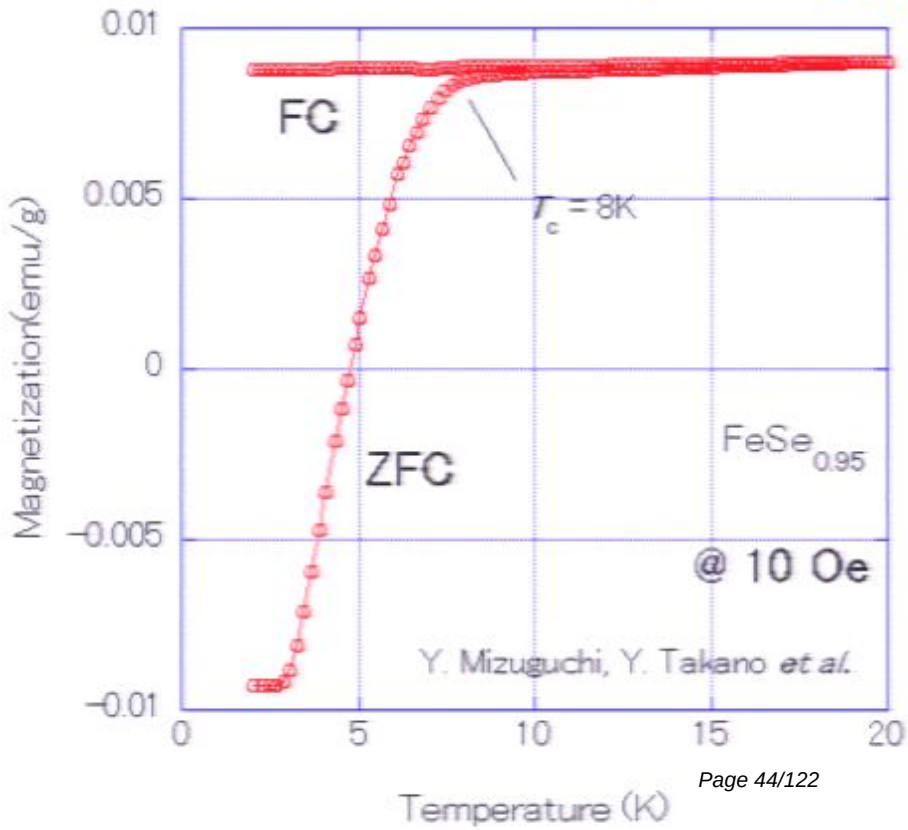
α-FeSe

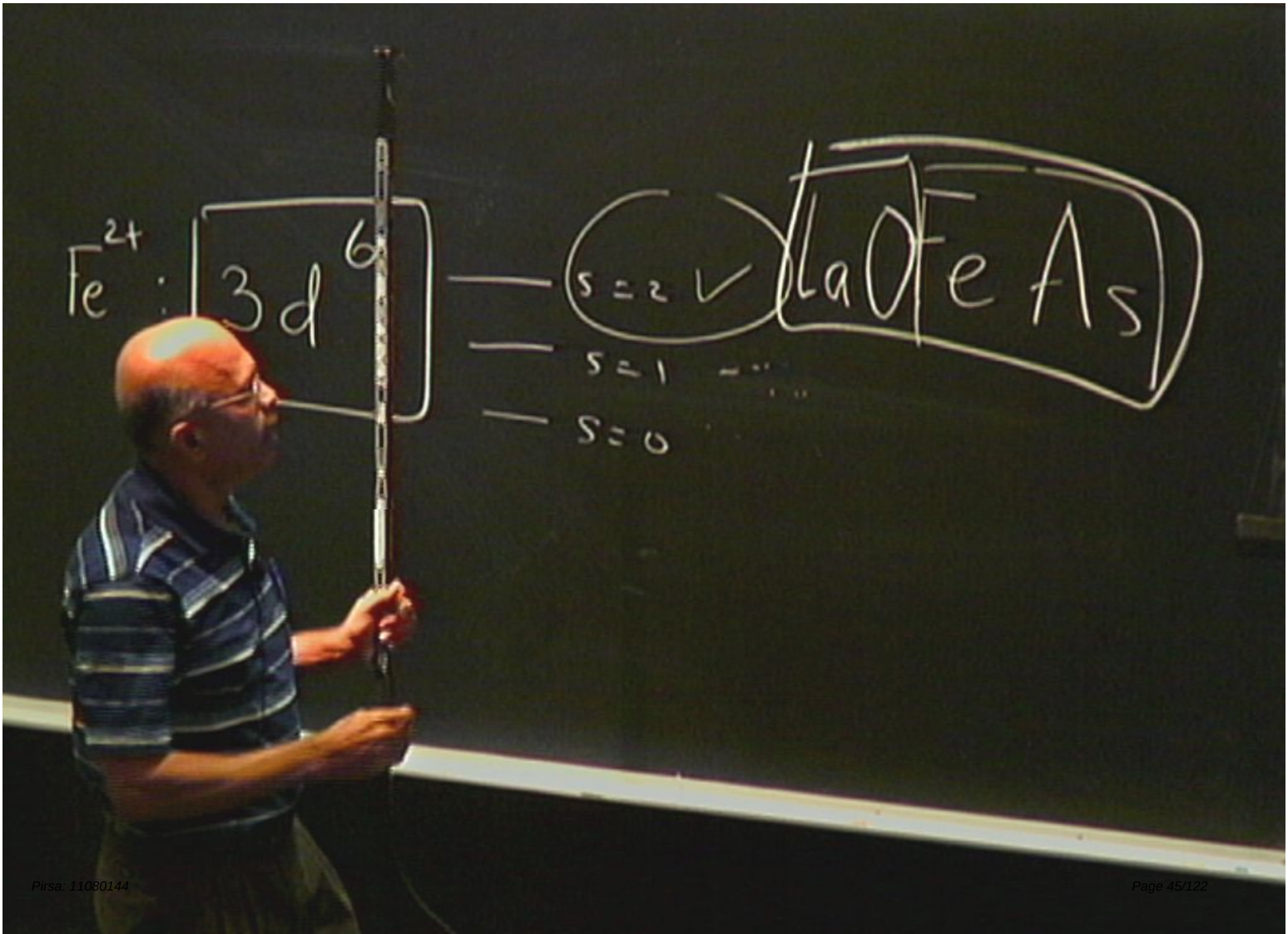
M. K. Wu (Taiwan)

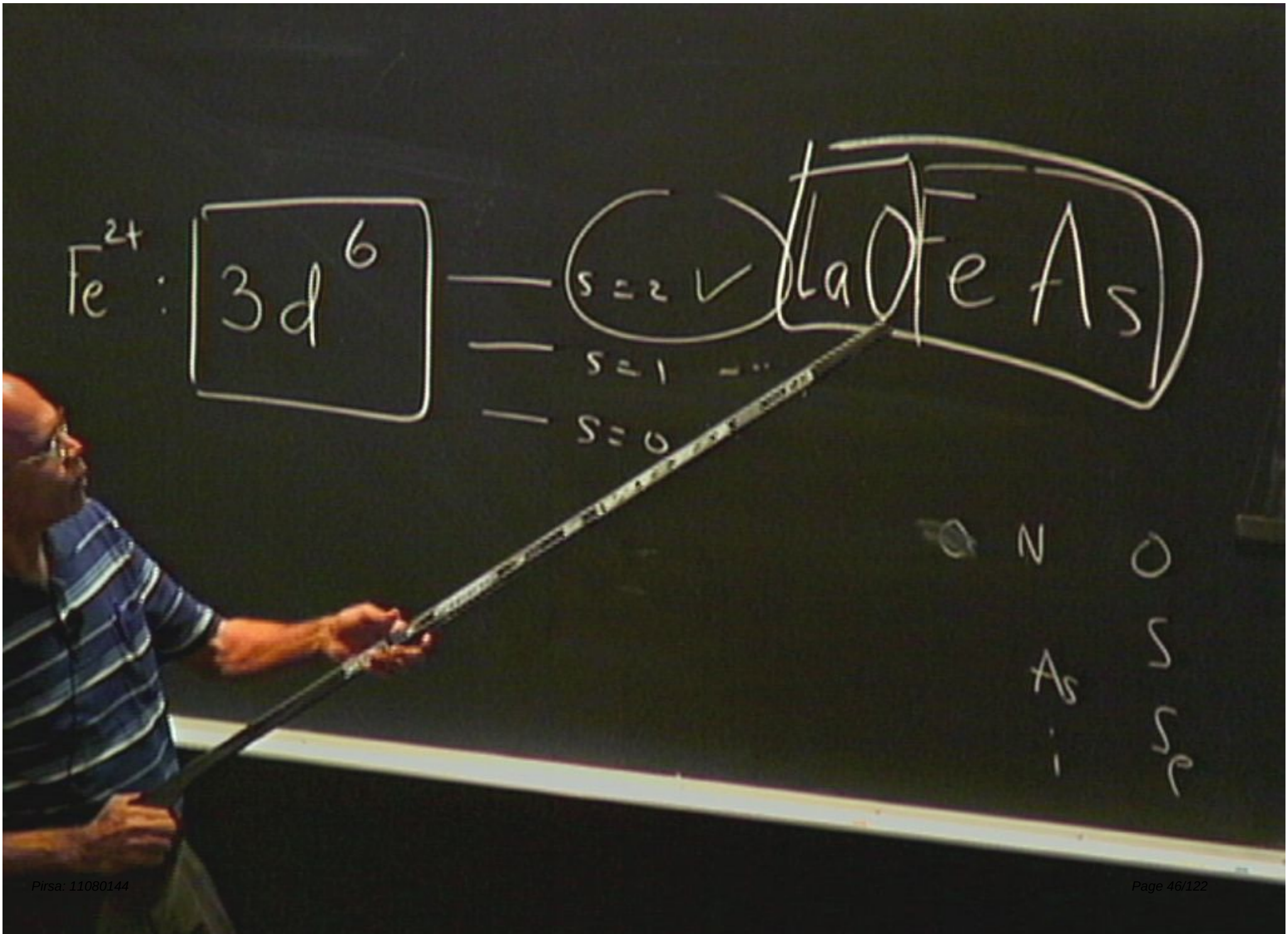
Y. Mizuguchi (NIMS)

Y. Takano et al. POSTER





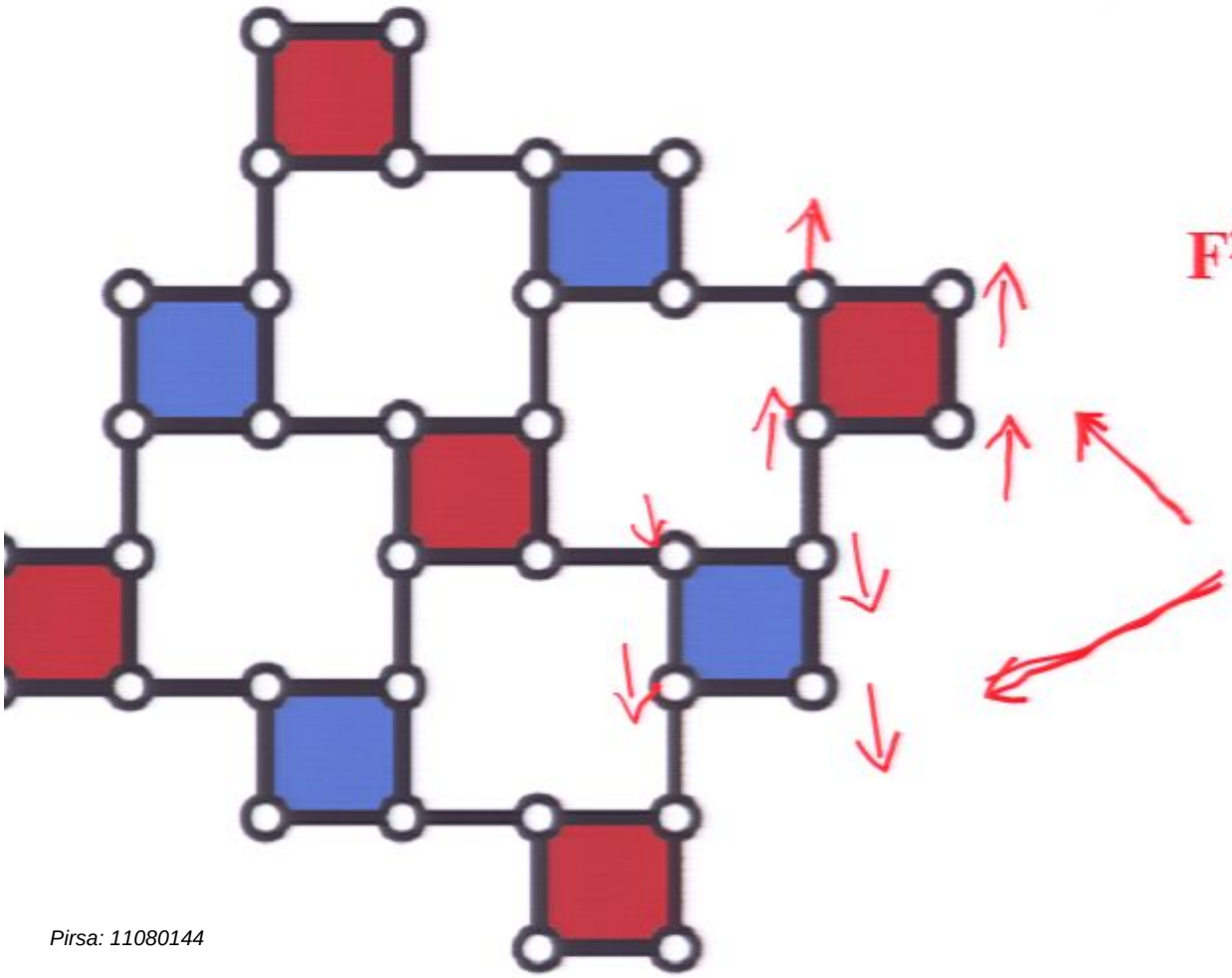

Fe 2+ : 3d 6
S = 2 ✓
S = 1
S = 0
LaOFeAs


Fe 2+ : 3d 6
S=2 ✓
S=1
S=0
LaOFeAs
N O
As S
Se

Intercalated $K_2Fe_4Se_5$ Mott insulator Family

J. Guo et al., Phys. Rev. B 82, 180520(R) (2010).

$\sqrt{5} \times \sqrt{5}$ Ordered Vacancies



F^{2+} carries S = 2 moment

S = 8

F_4 Ferromagnetic plaquette

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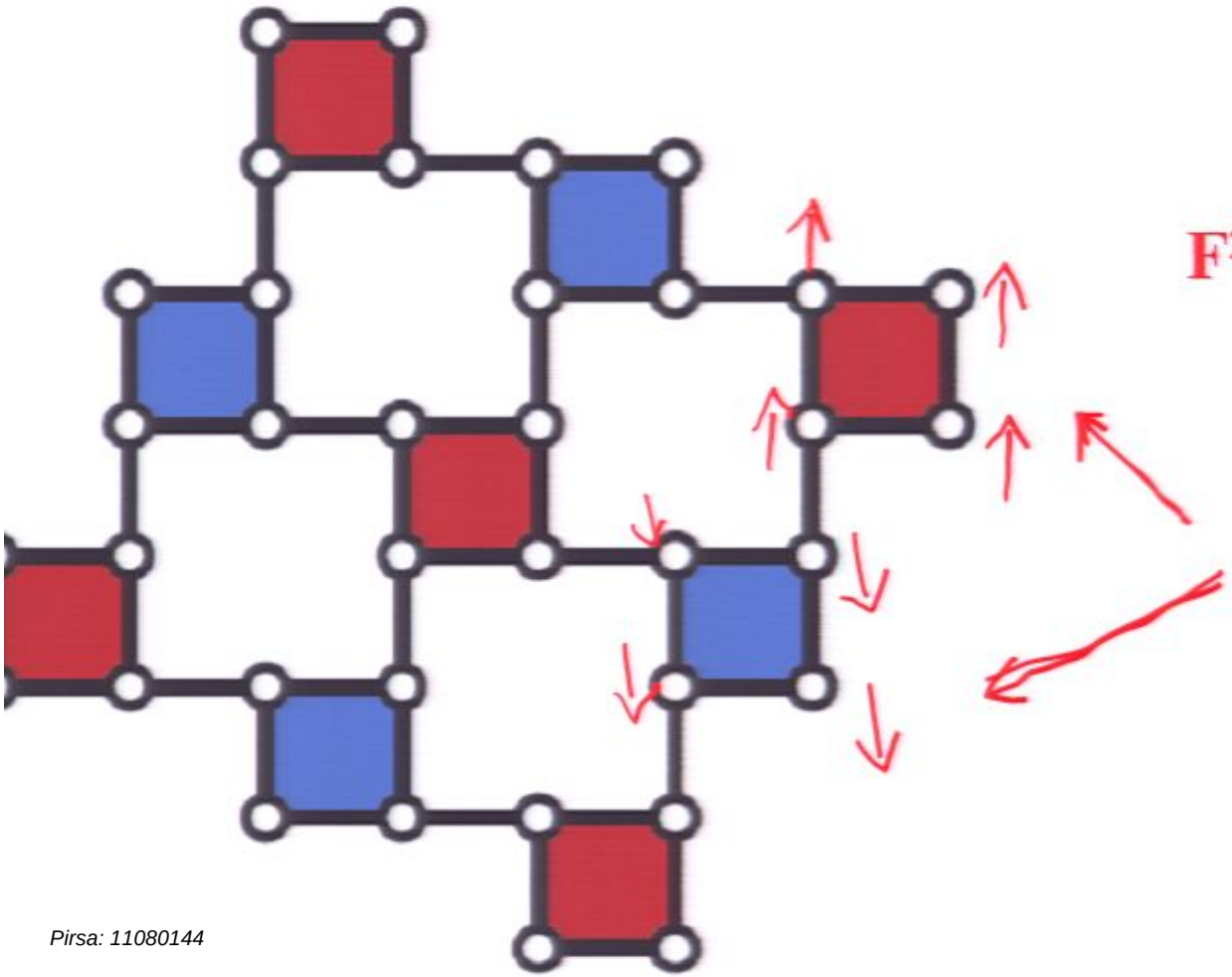

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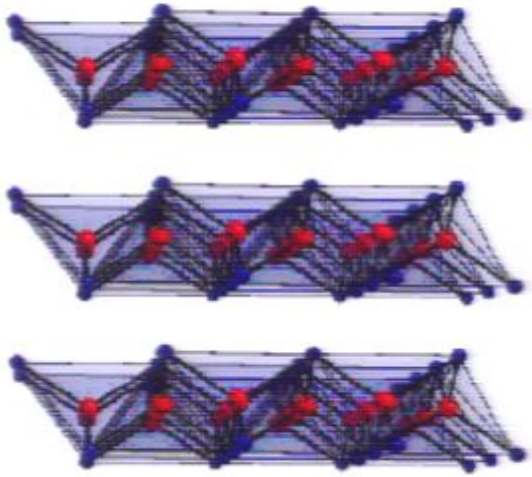
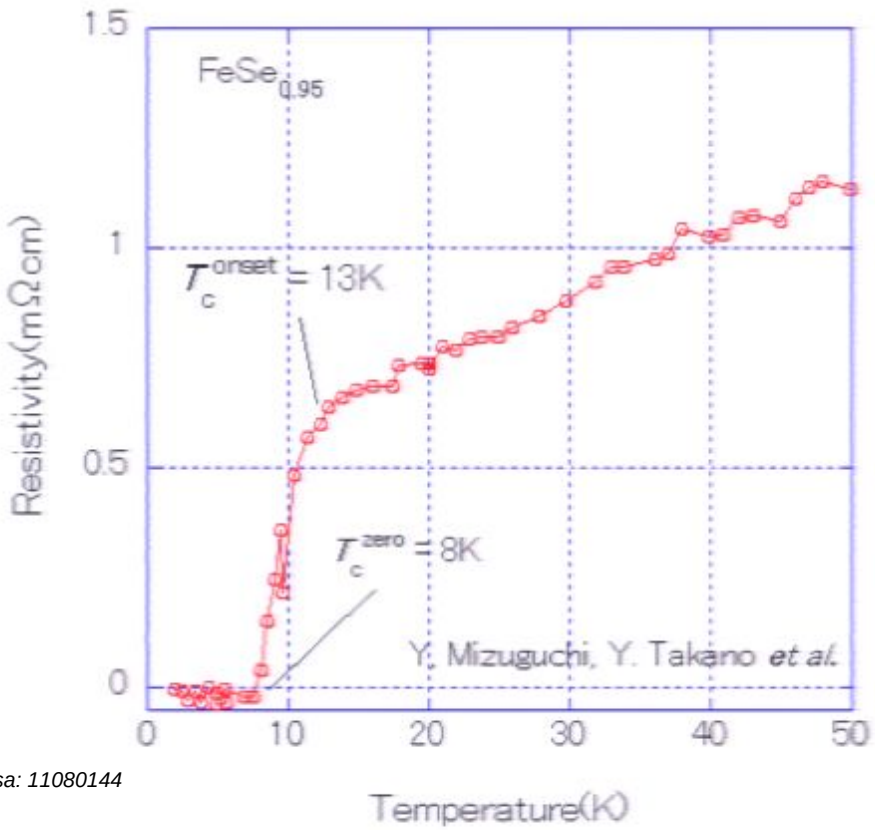


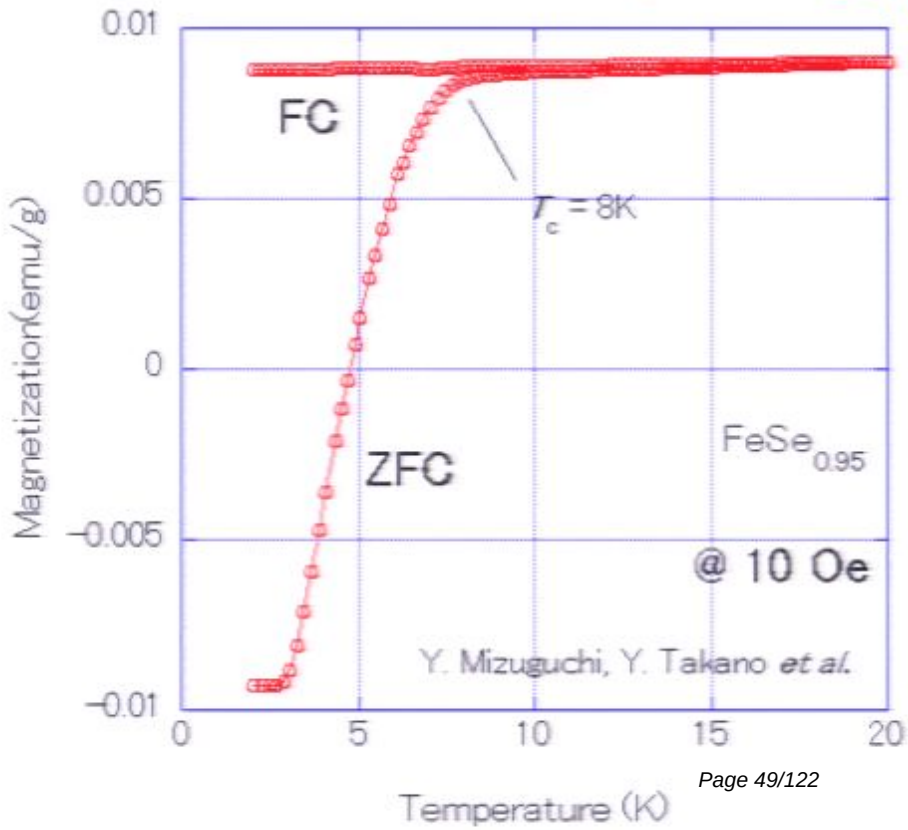
α-FeSe

M. K. Wu (Taiwan)

Y. Mizuguchi (NIMS)

Y. Takano et al. POSTER





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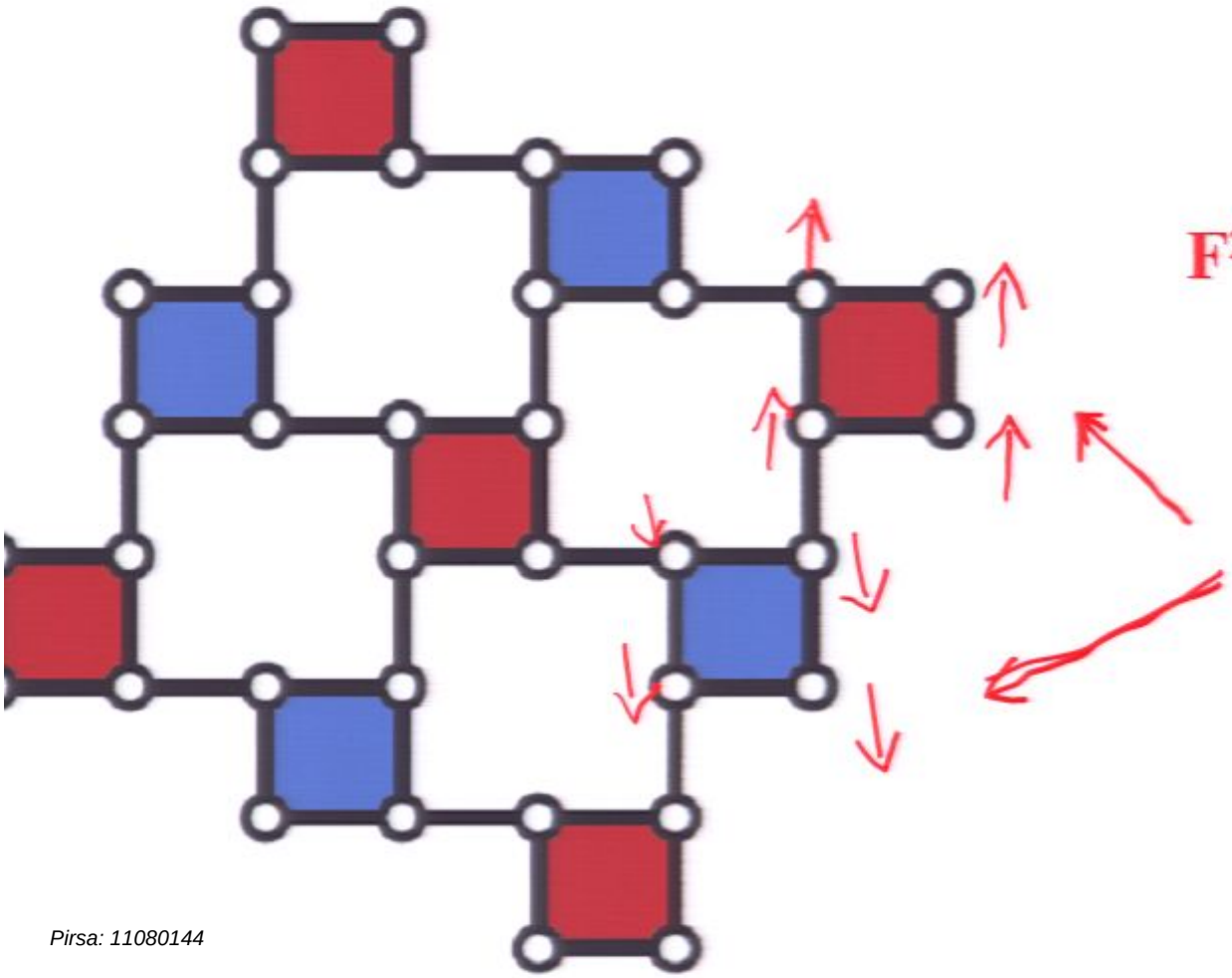

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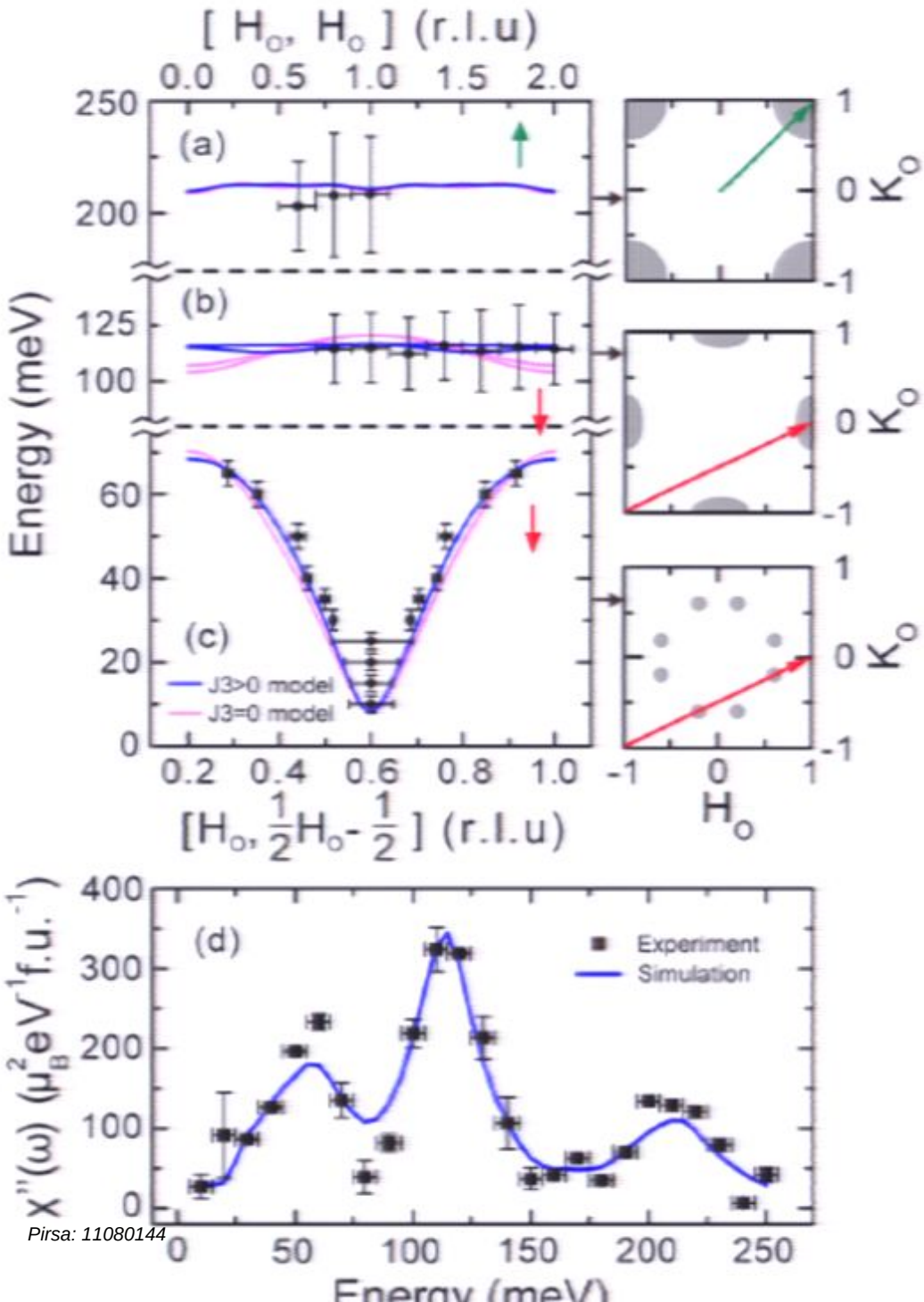


Wang et al. arXiv:1105.4675

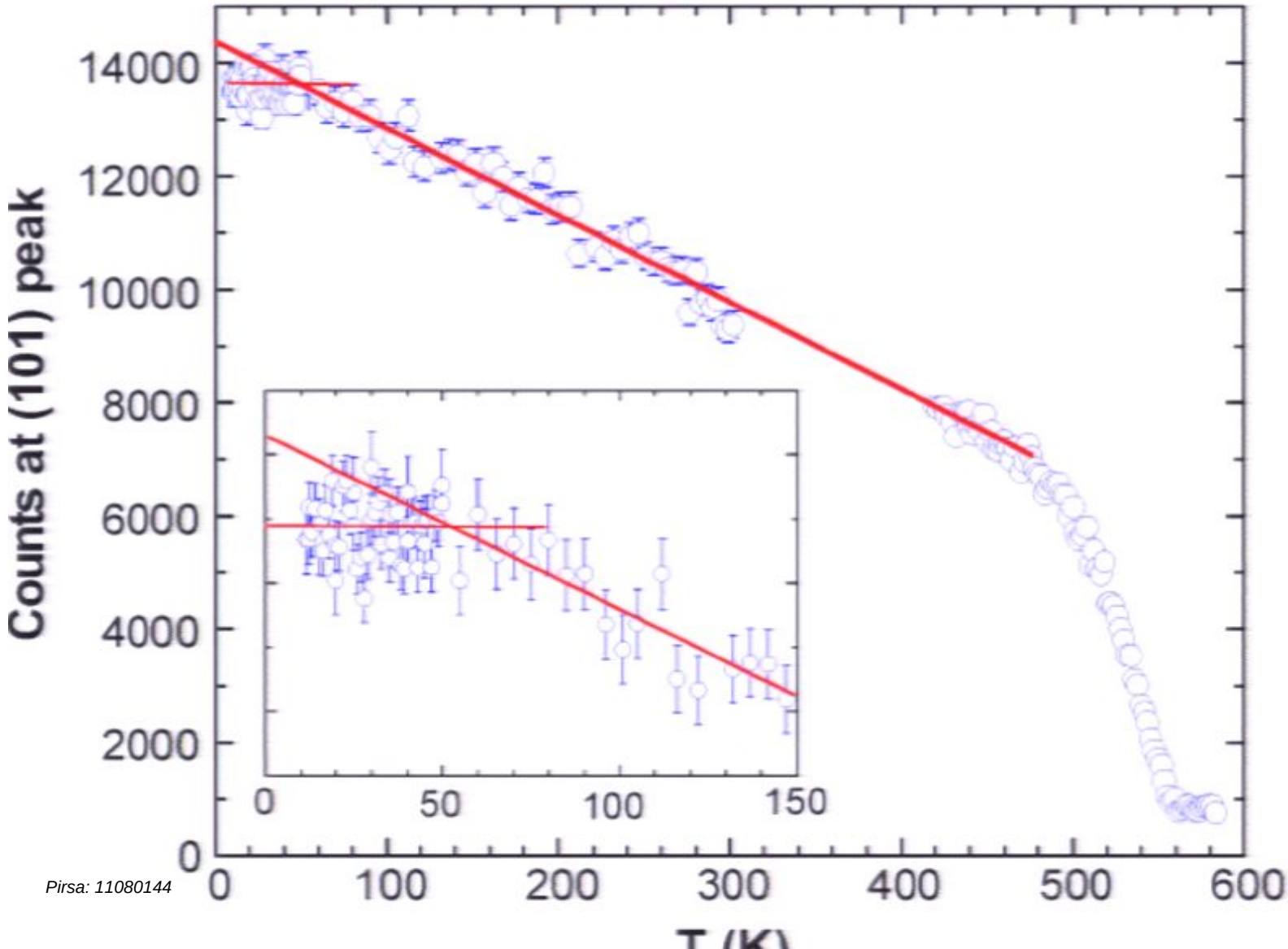
Neutron scattering

Spin wave dispersion

W Biao et al. arXiv:1102.0830 (superconducting sample)

Order parameter square

$T_N \sim 560$ K



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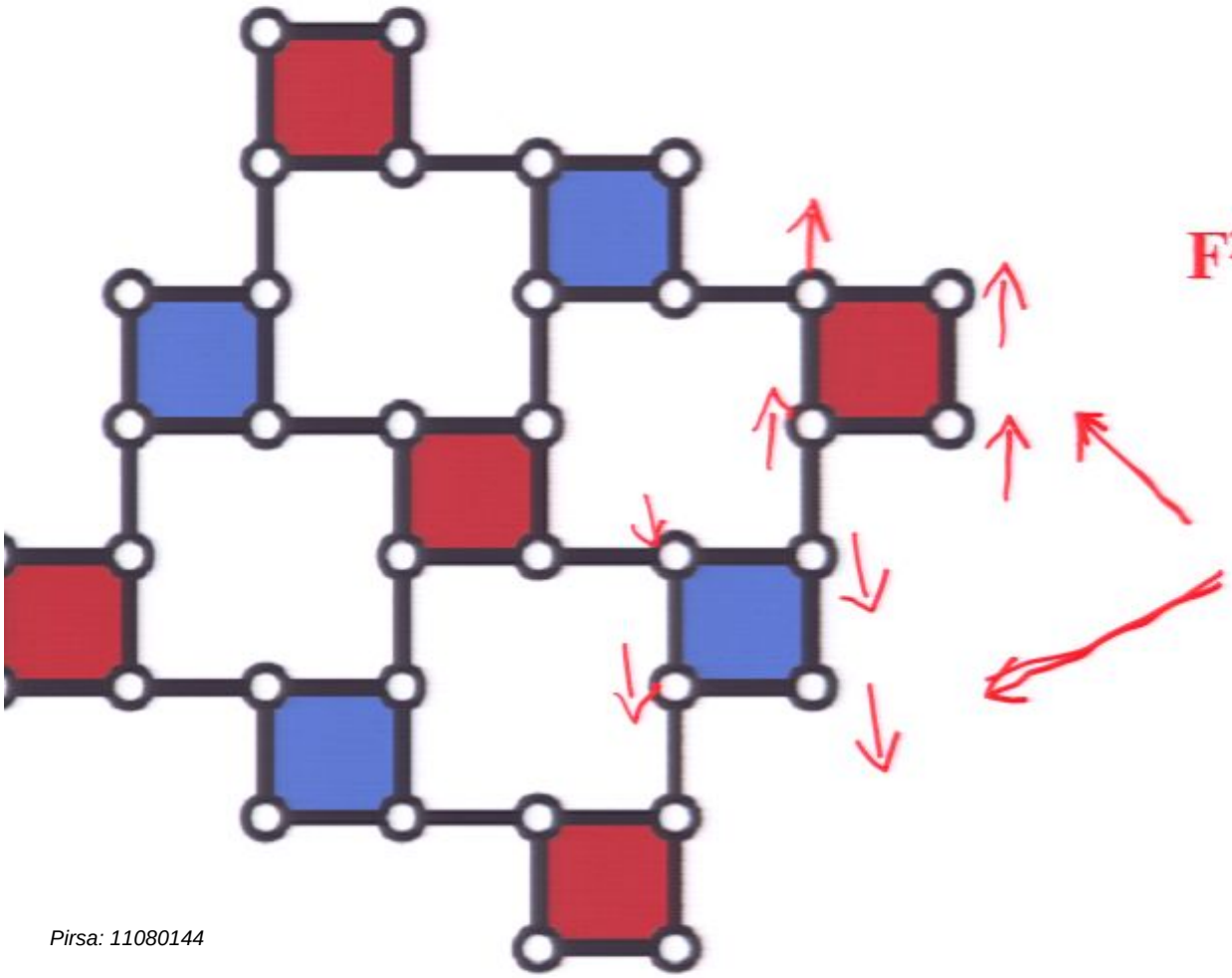

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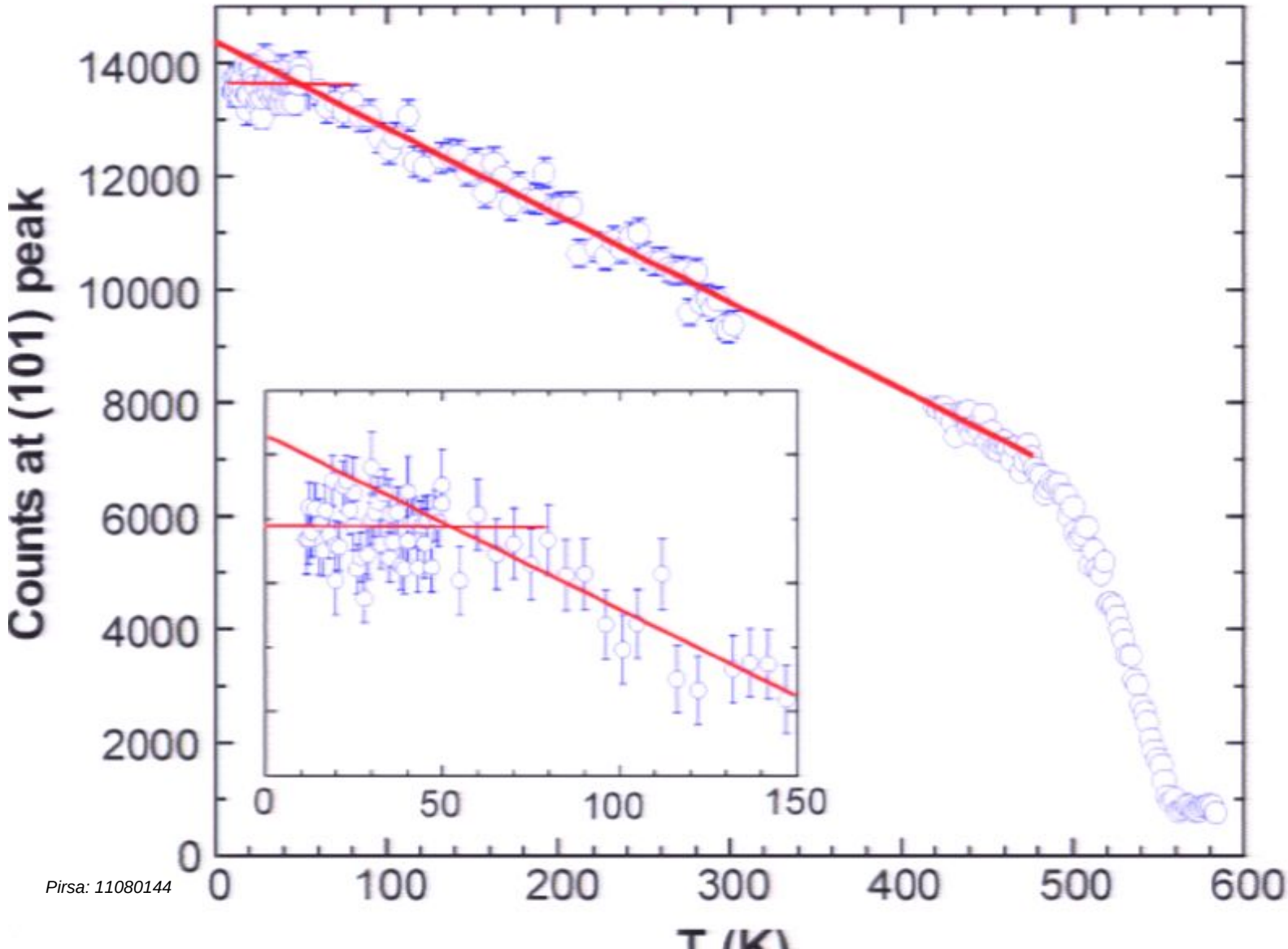
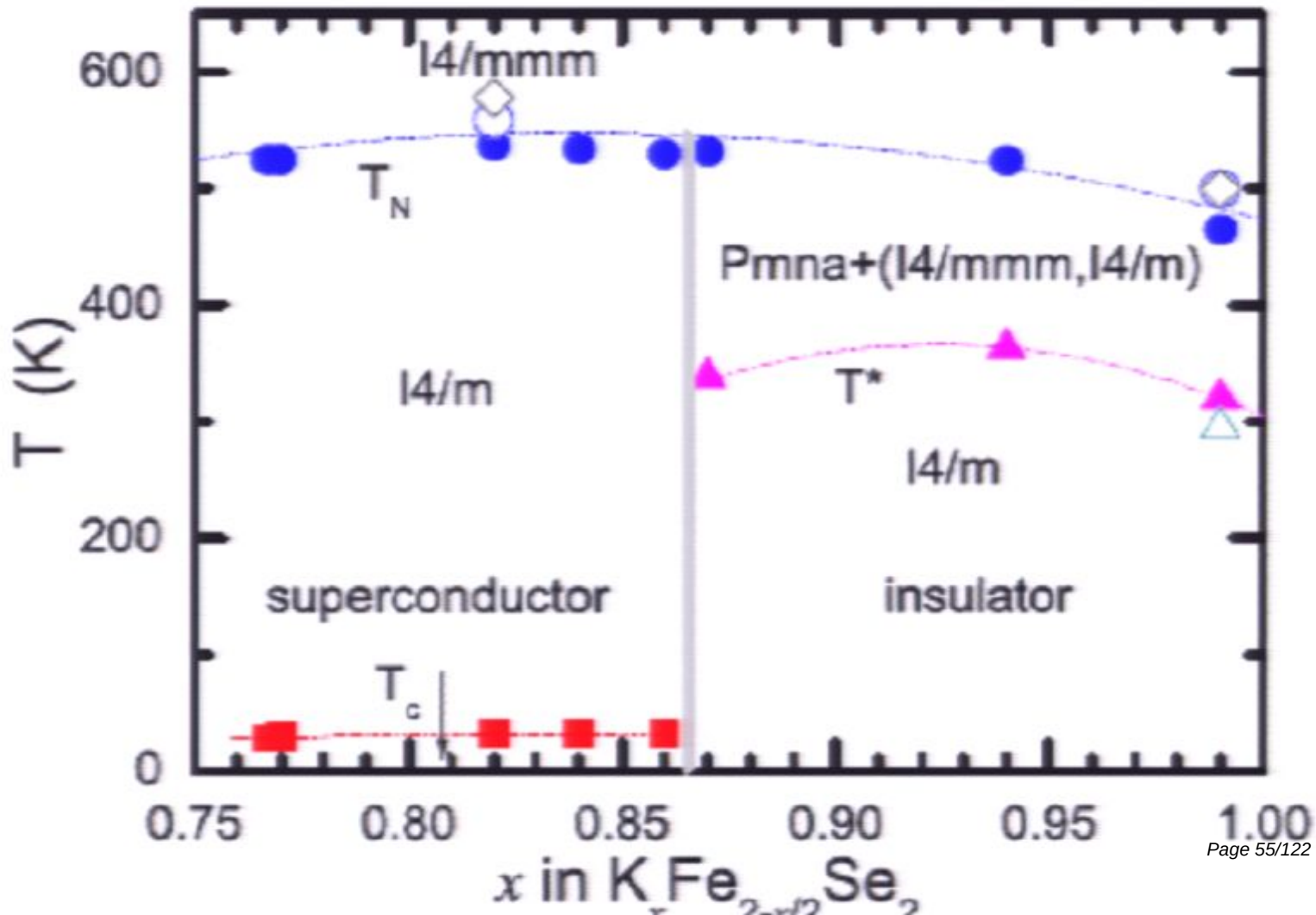
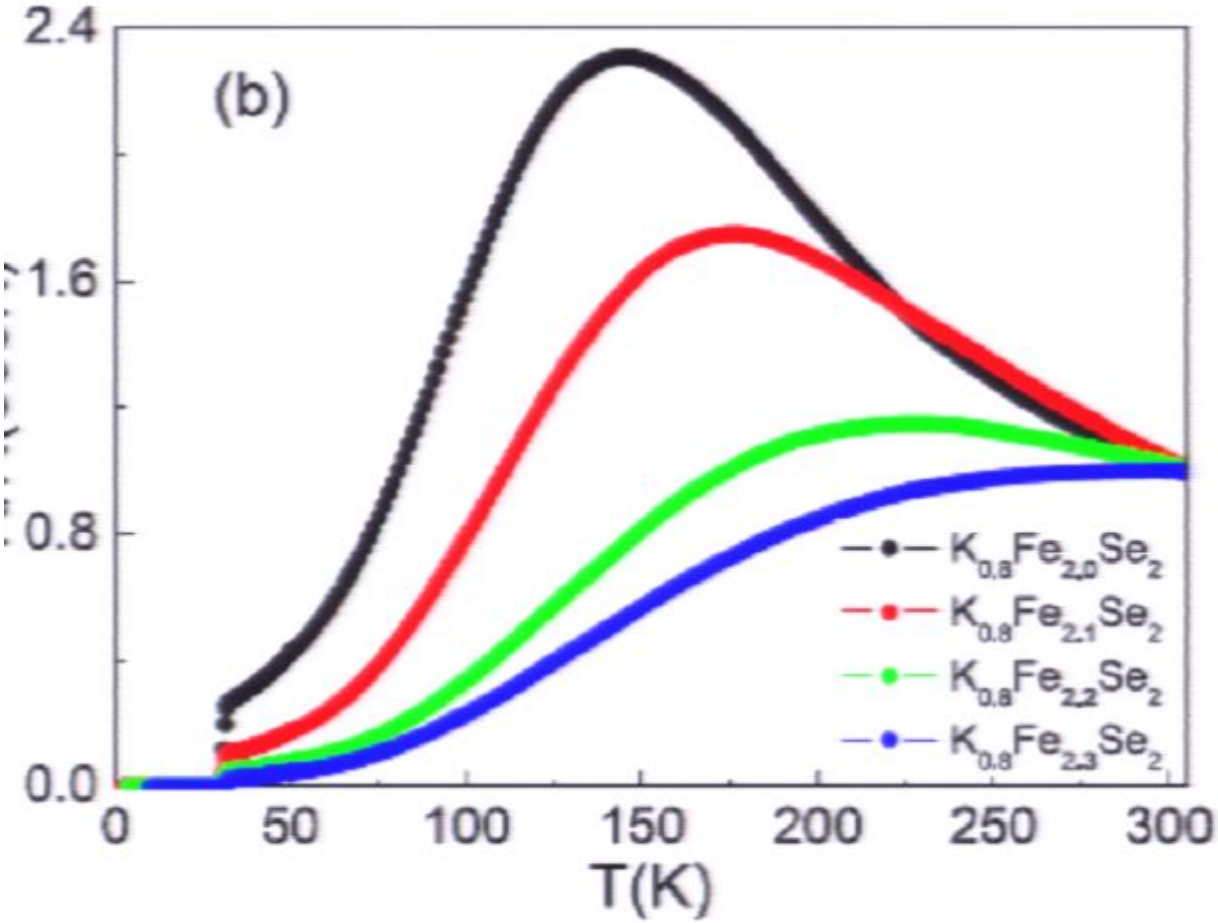


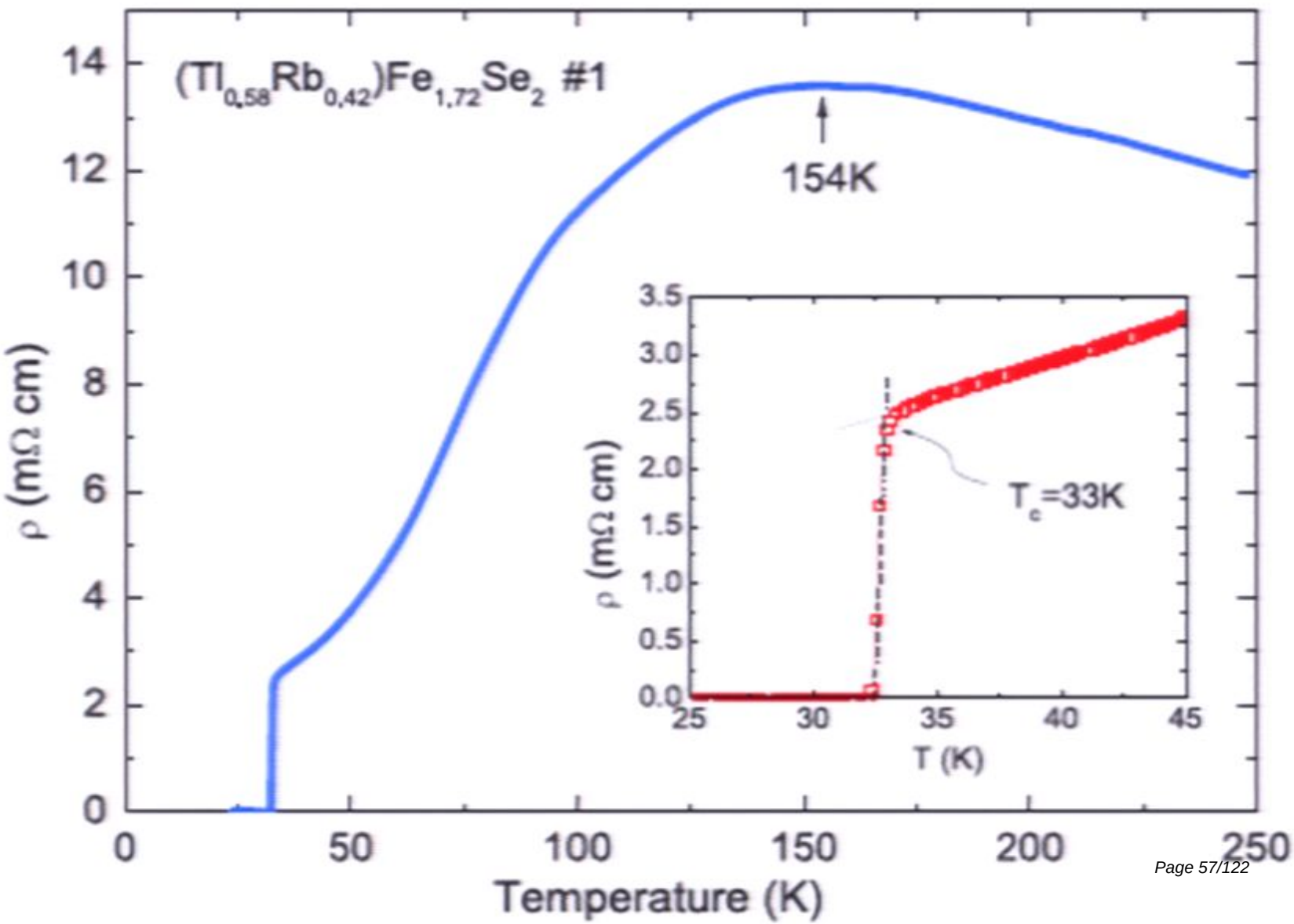
Wei Bao et. al., arXiv:1102.3674



Wang et al. arXiv:1101.0789



. Jiao et al.,
rXiv:1106.2283v1



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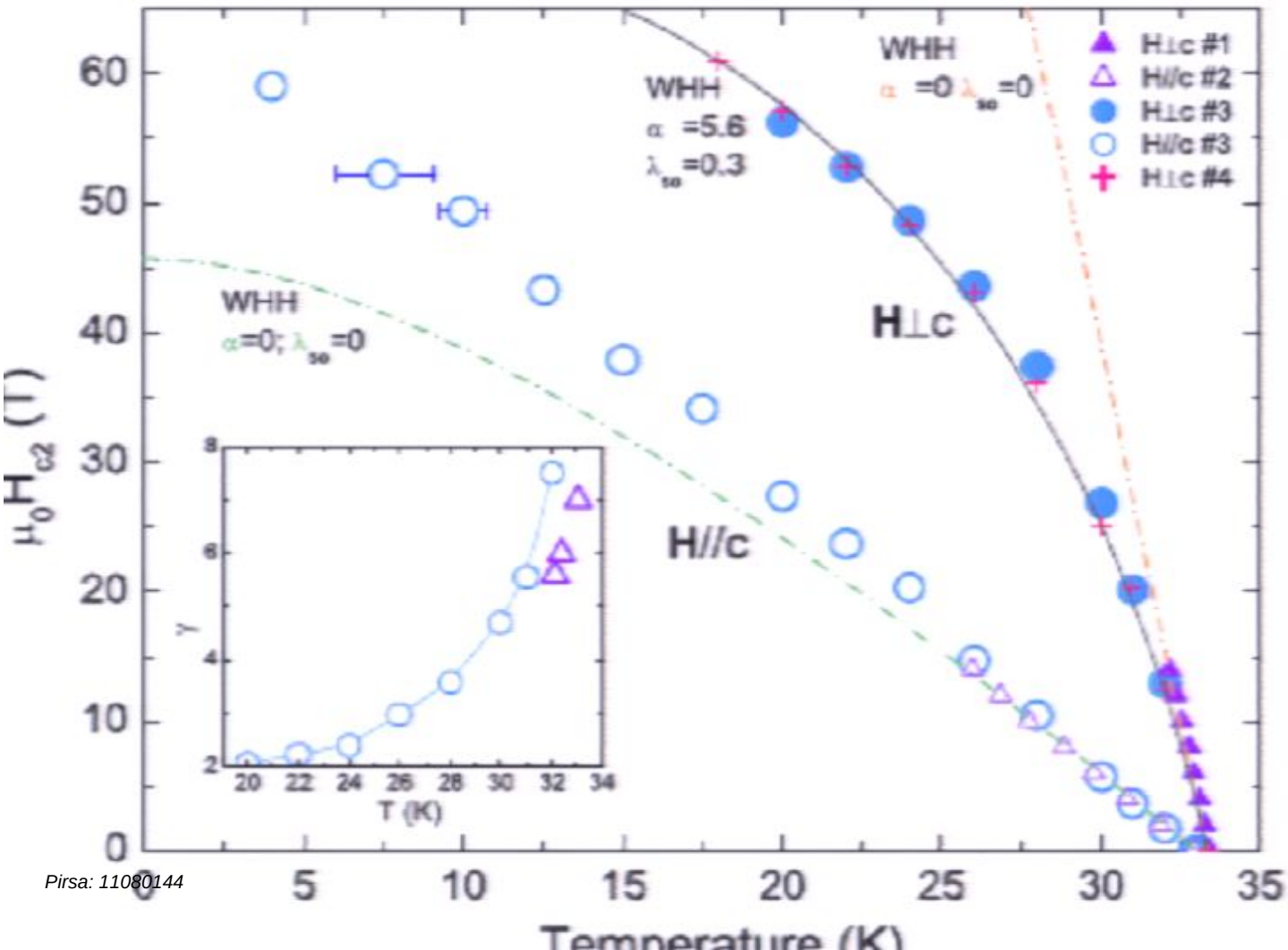
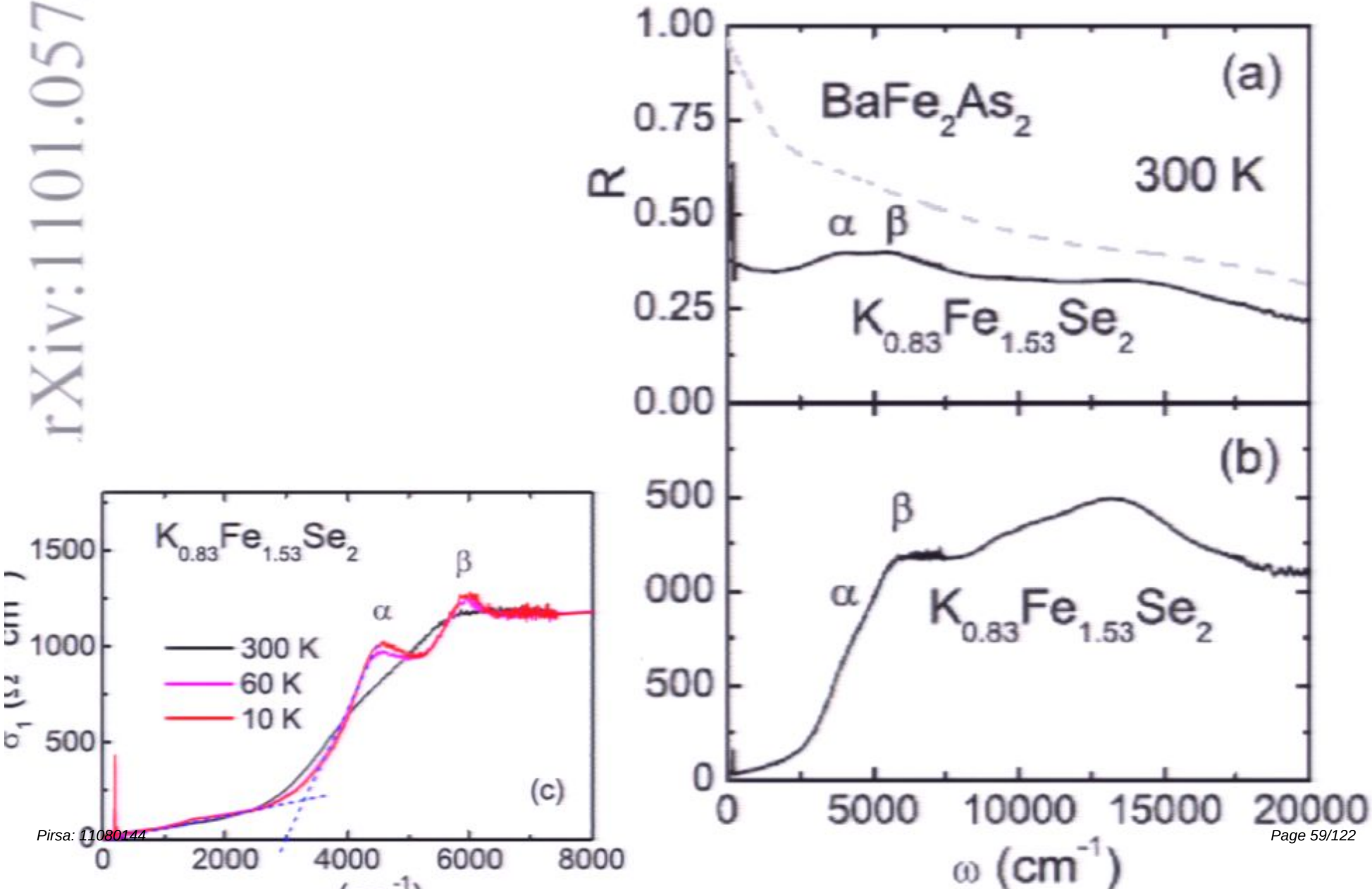
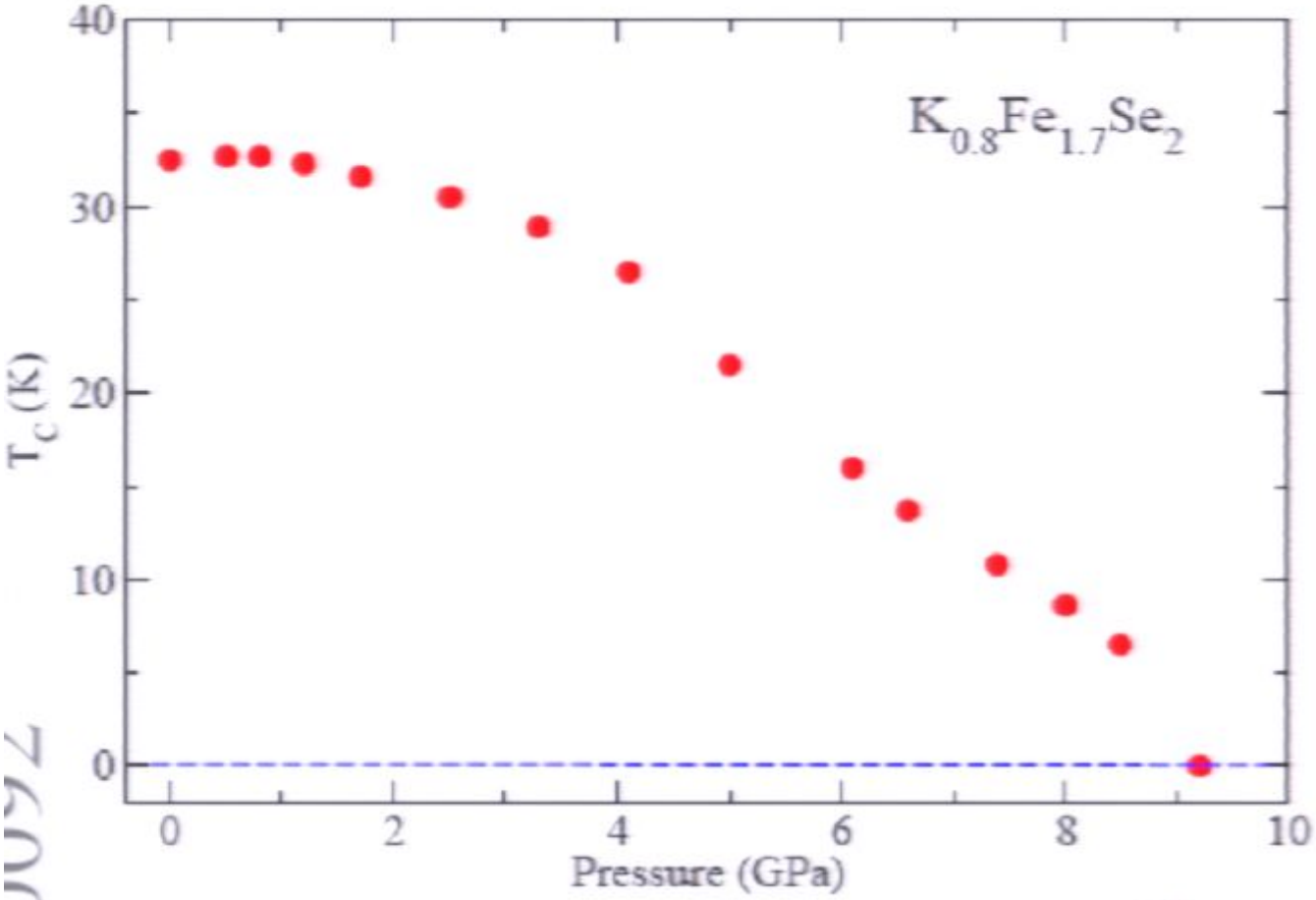


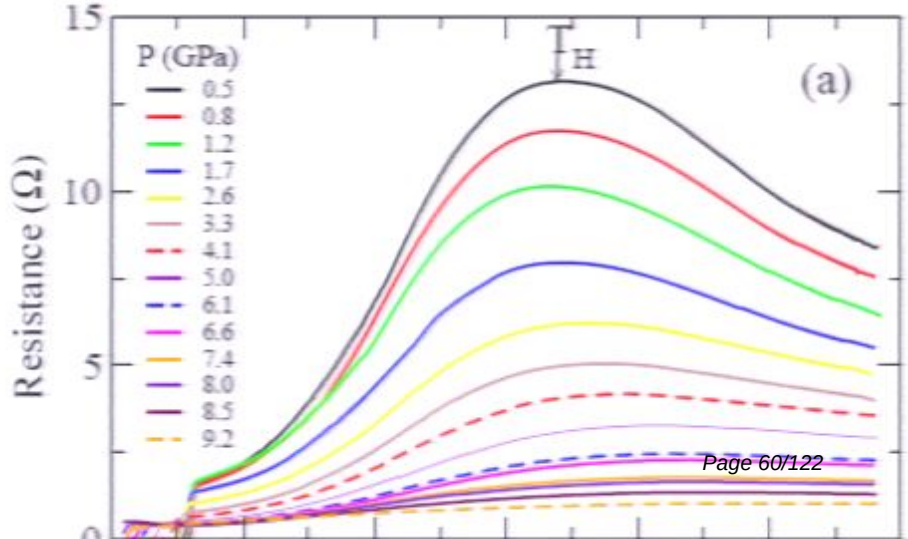
rXiv:1101.0572v3

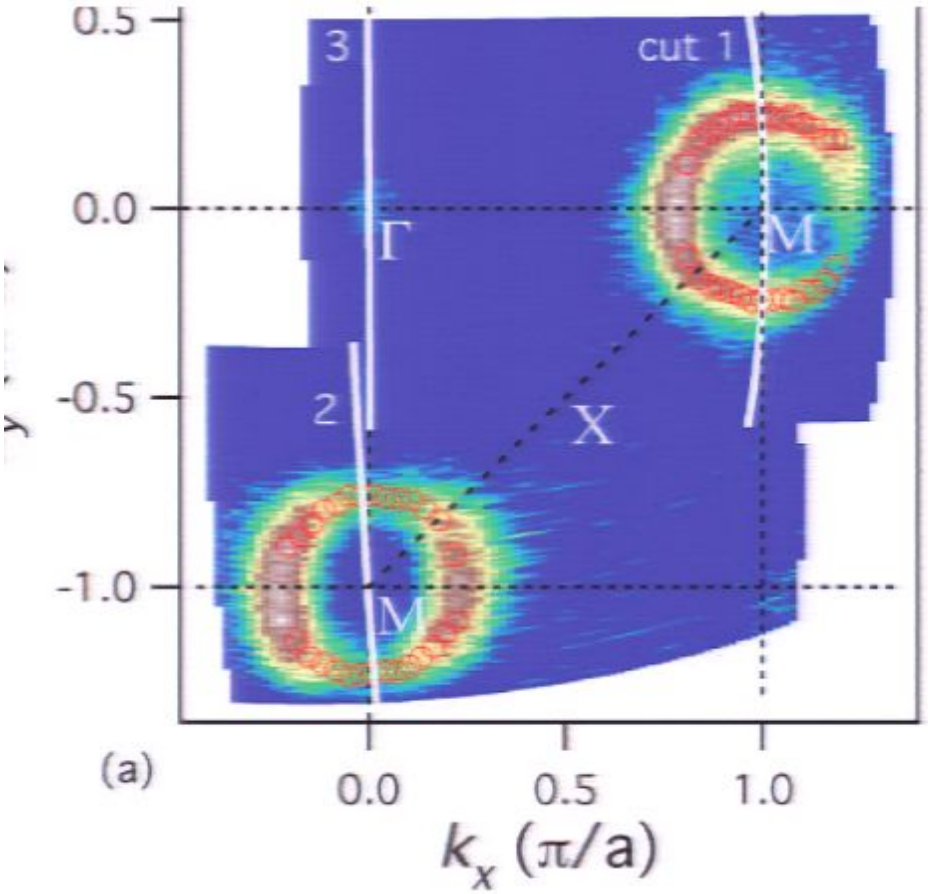
Z.G. Chen et al.



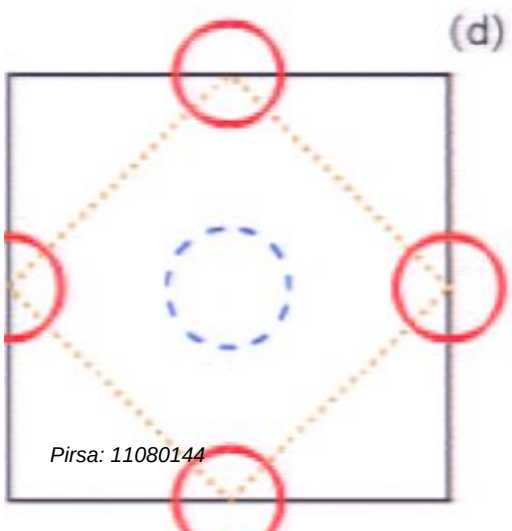


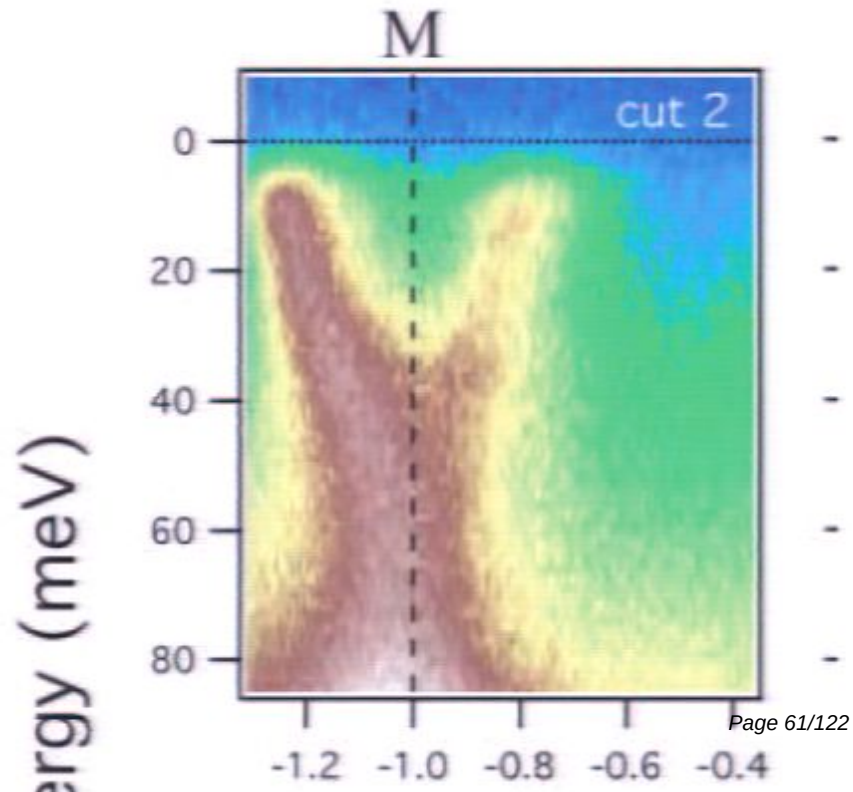
Jing Guo et al.,

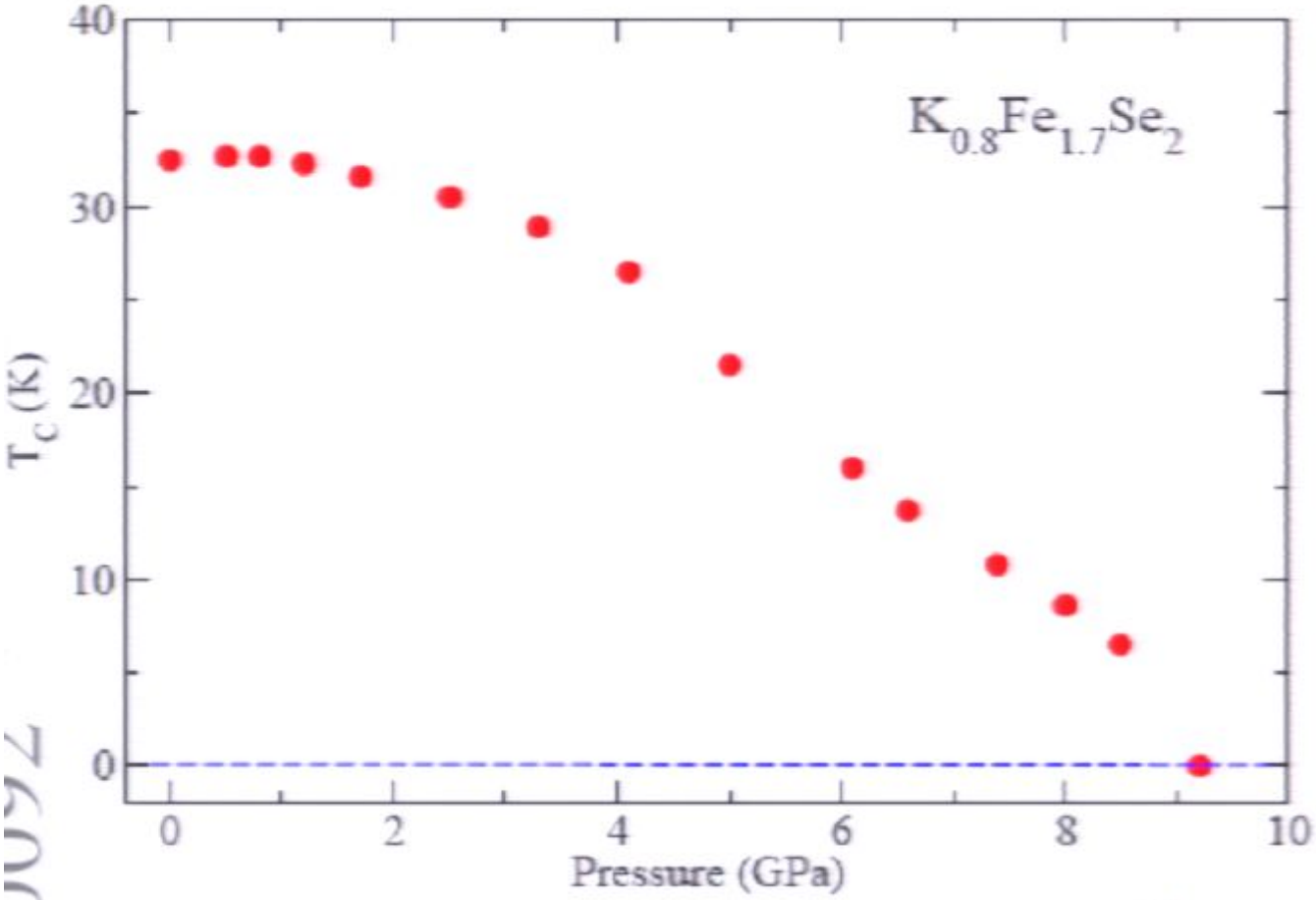




X.-P. Wang et al.
arXiv:1101.4923







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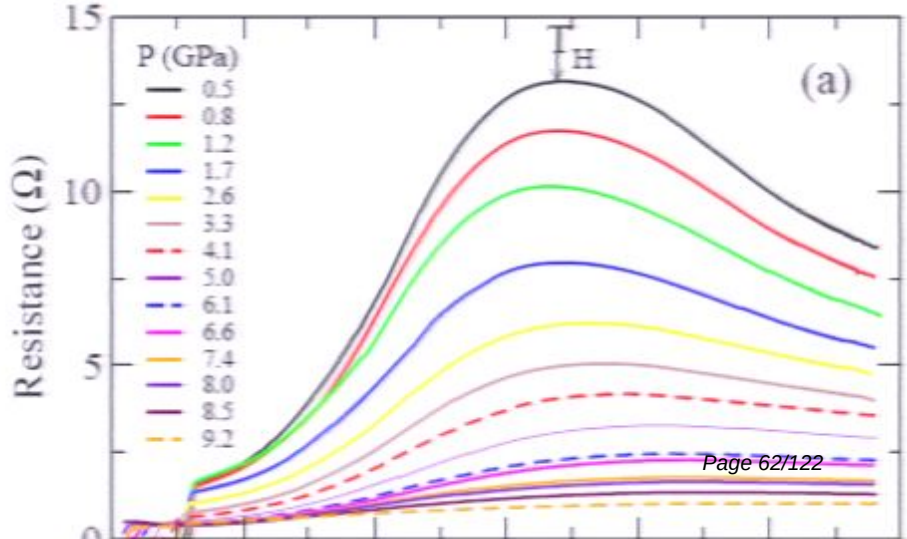

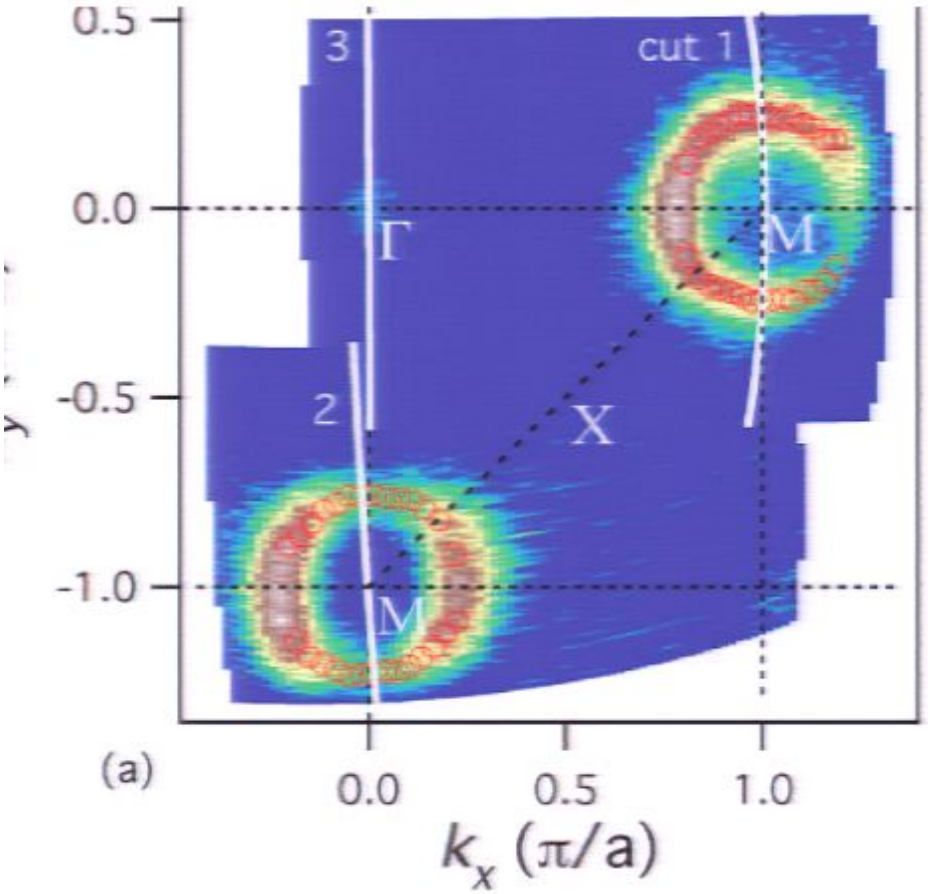

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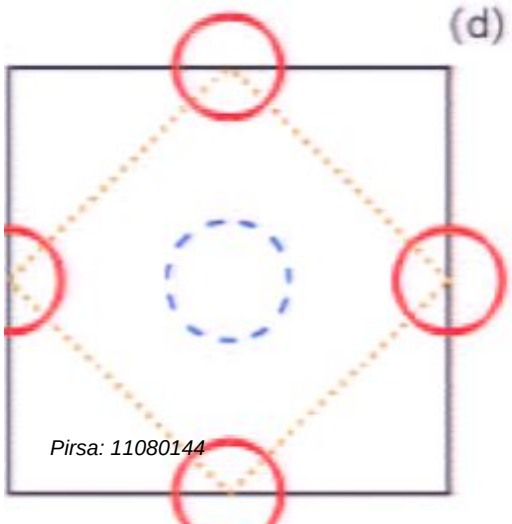
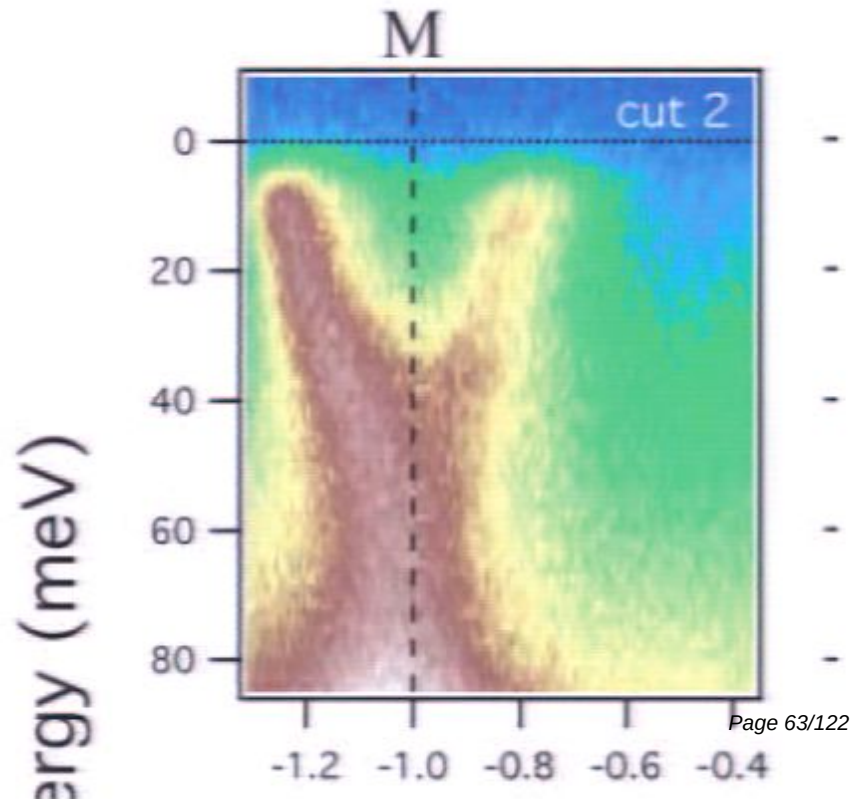
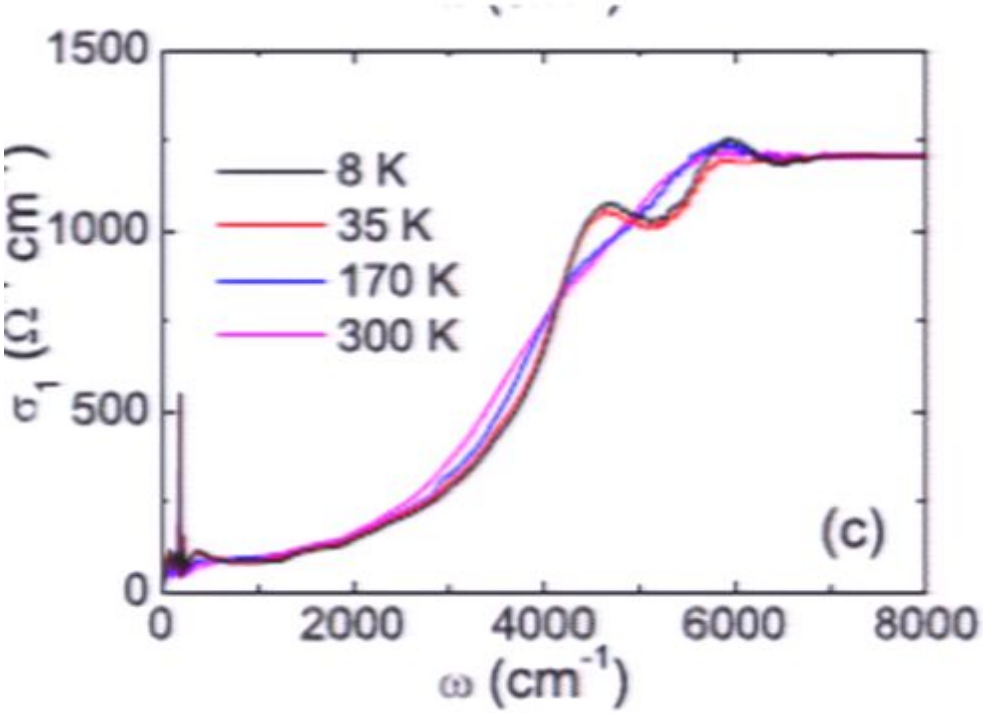
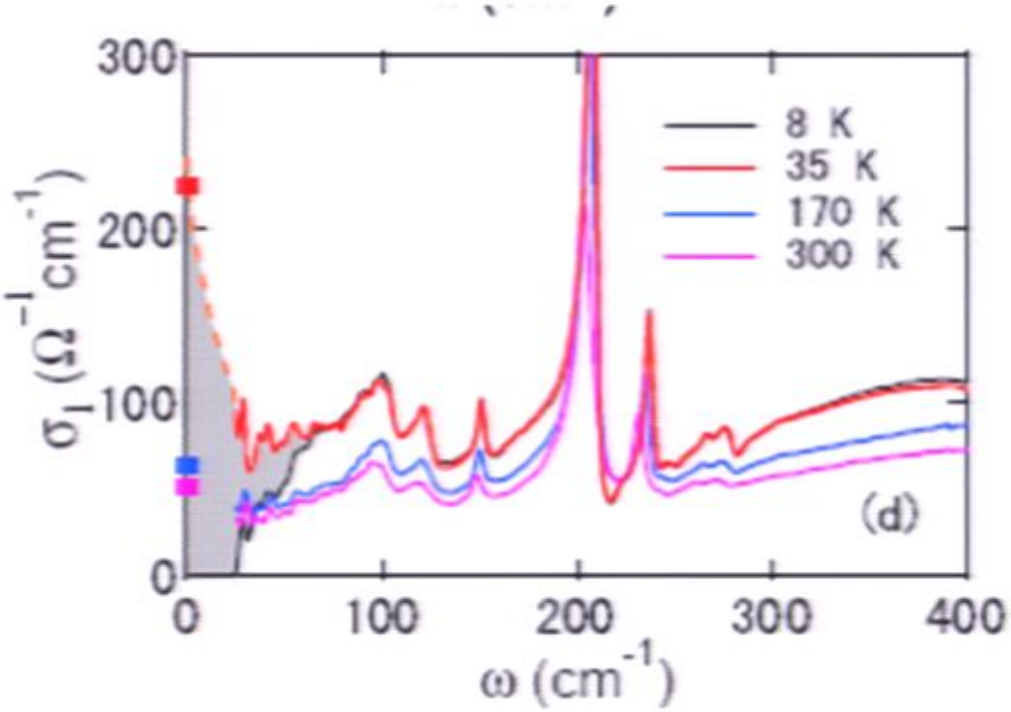




R.H. Yuan et al. arXiv:1102.1381

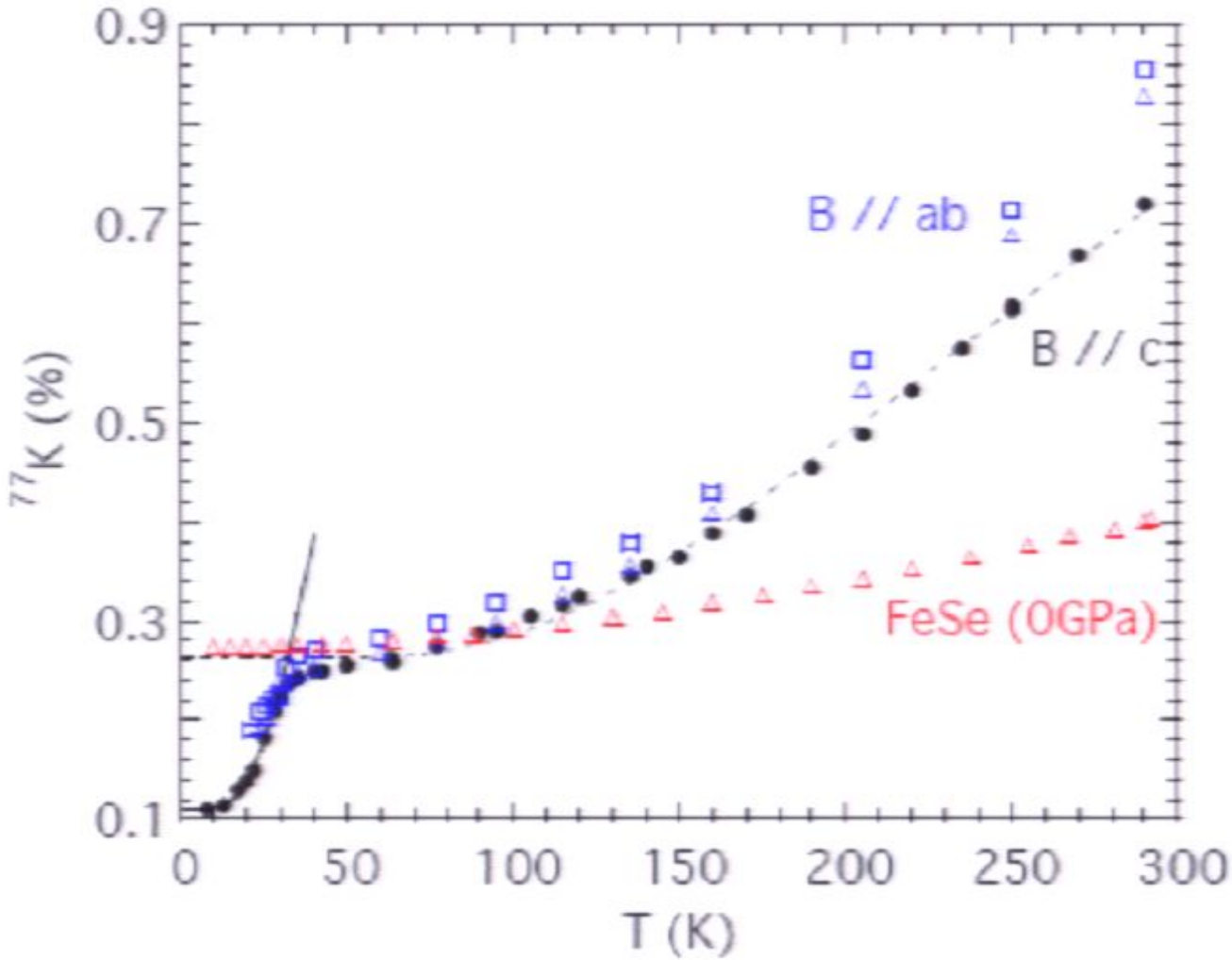




^{77}Se NMR

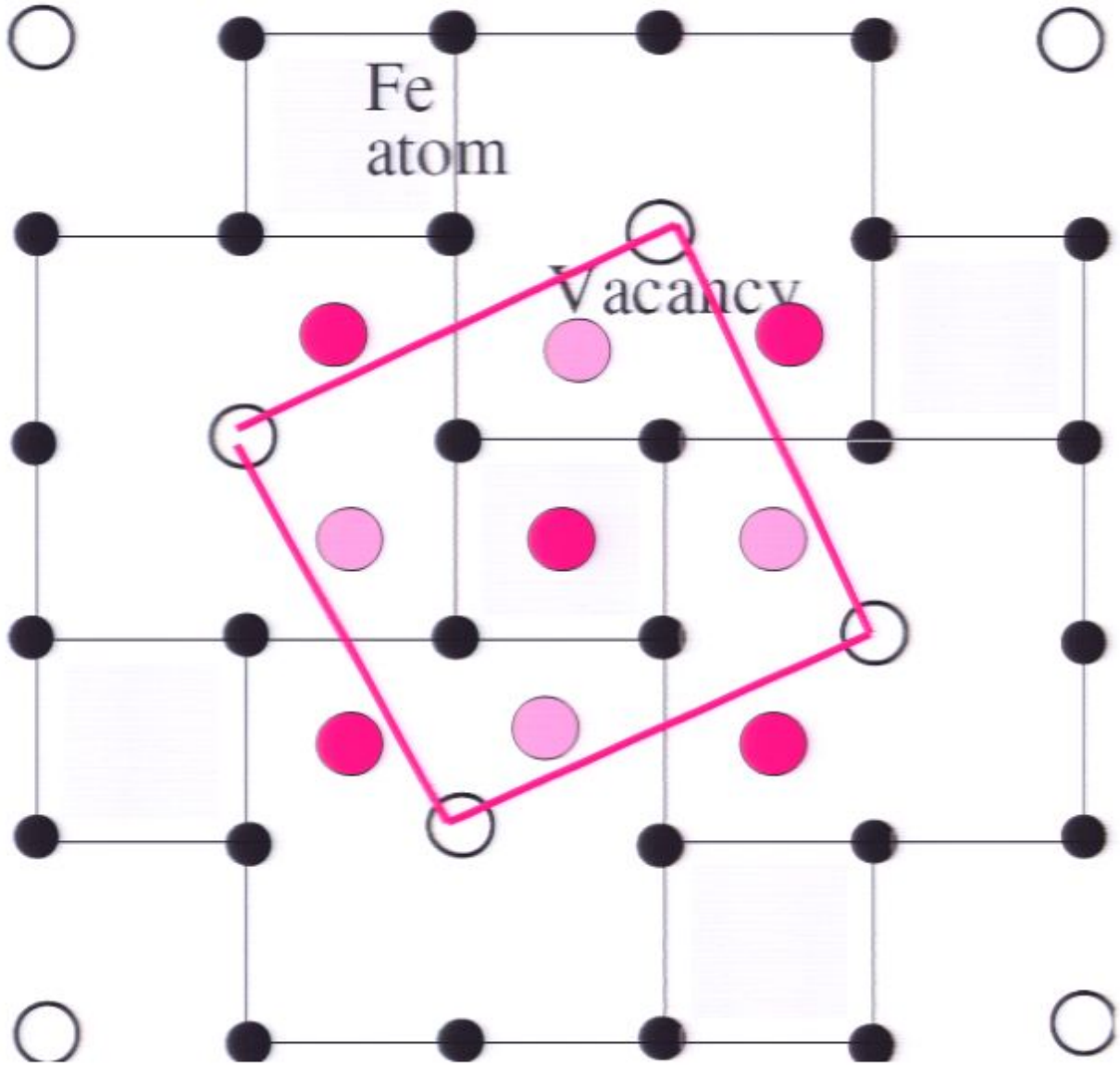
Knight shift

$K_xFe_{2-y}Se_2$



Torchetti et al. PRL 2011 (Imai group)

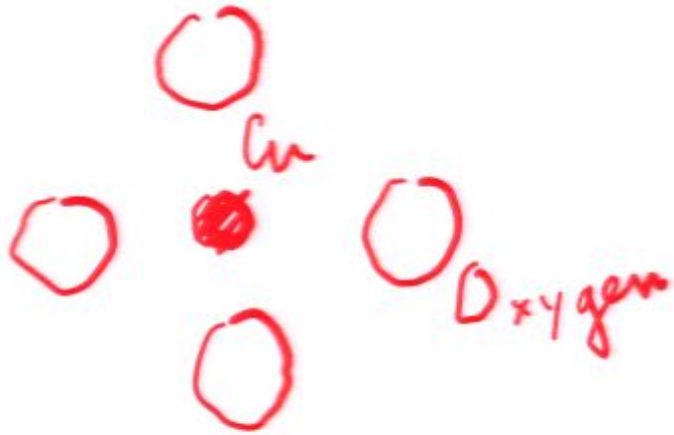
$\sqrt{5} \times \sqrt{5}$ Ordered Vacancies



Theory

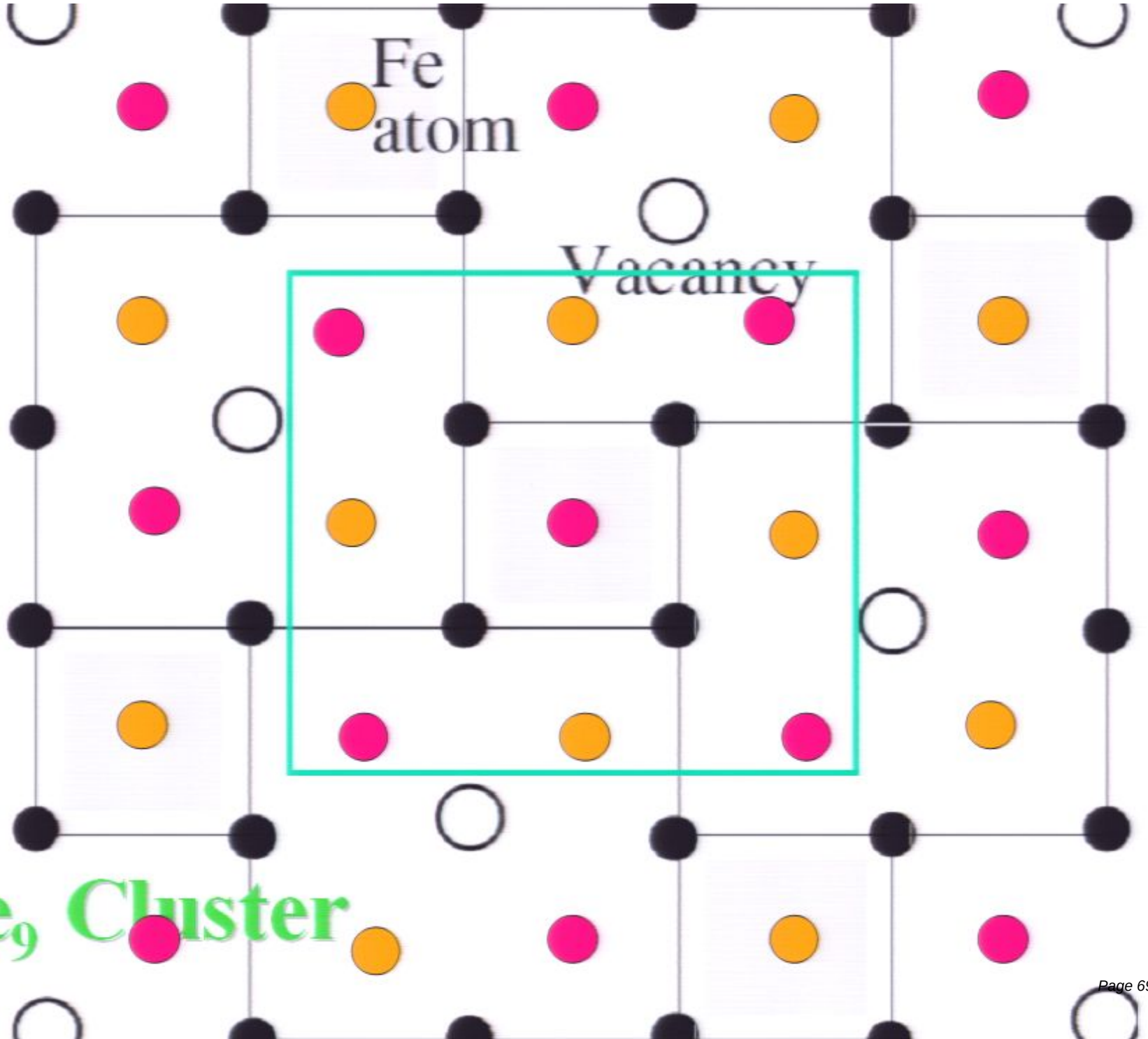
GB, arXiv:1108.3562

C. Platt et al., arXiv:1106.5964
T. A. Maier et al. PRB 2011
Yi Zhou et al., arXiv:1101.4462
Fa Wang, EPL 2011
T Das & Balatsky, arXiv:1106.3289
R Yu et al., PRL 2011



Analogue of CuO_4 plaquett is

F_4Se_9 plaqutte where each Fe is Tetrahedrally coordinated by 4 Se atoms



F_4Se_9 Cluster

GB arXiv:1108.3562

Minimal Model

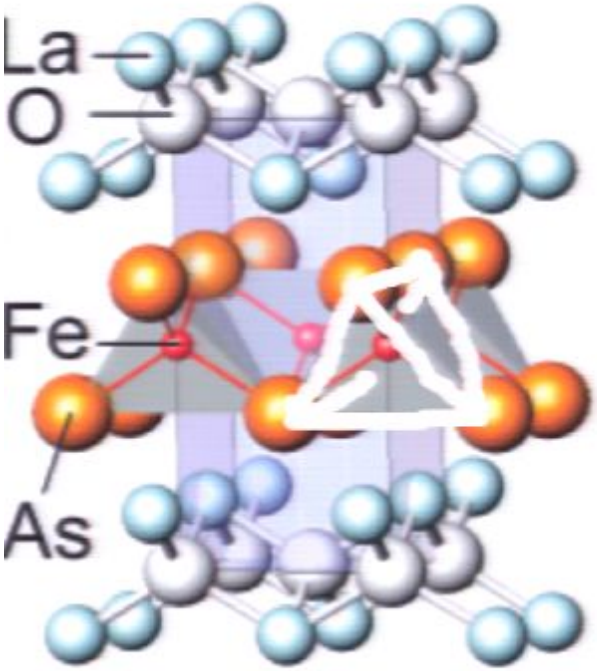
for Low Energy Electronic properties

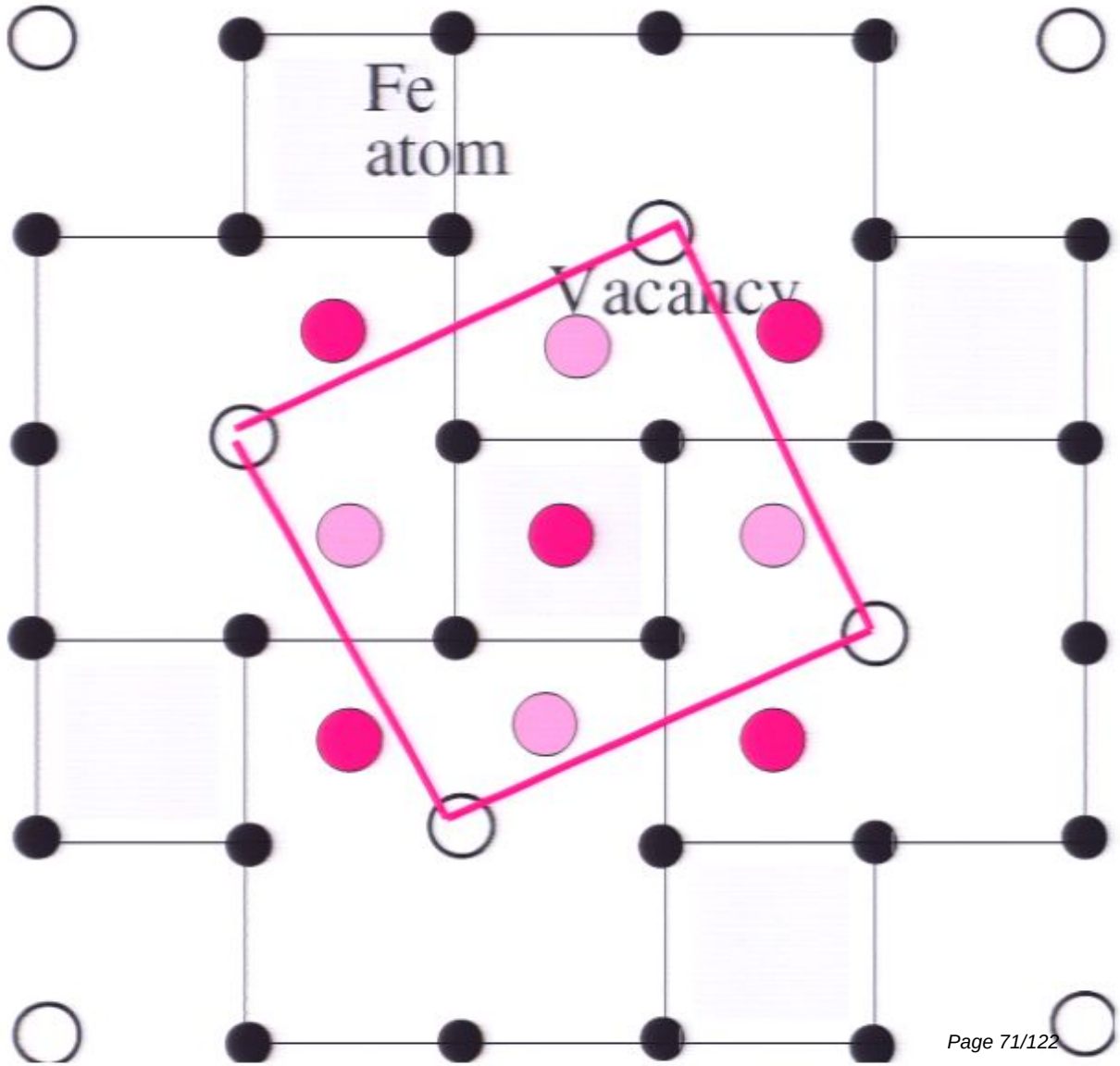
F_4 plaquette is the basic building block

It has an electronic integrity
As seen from its large and robust **S = 8** magetic moment

Where do the moments come from ?

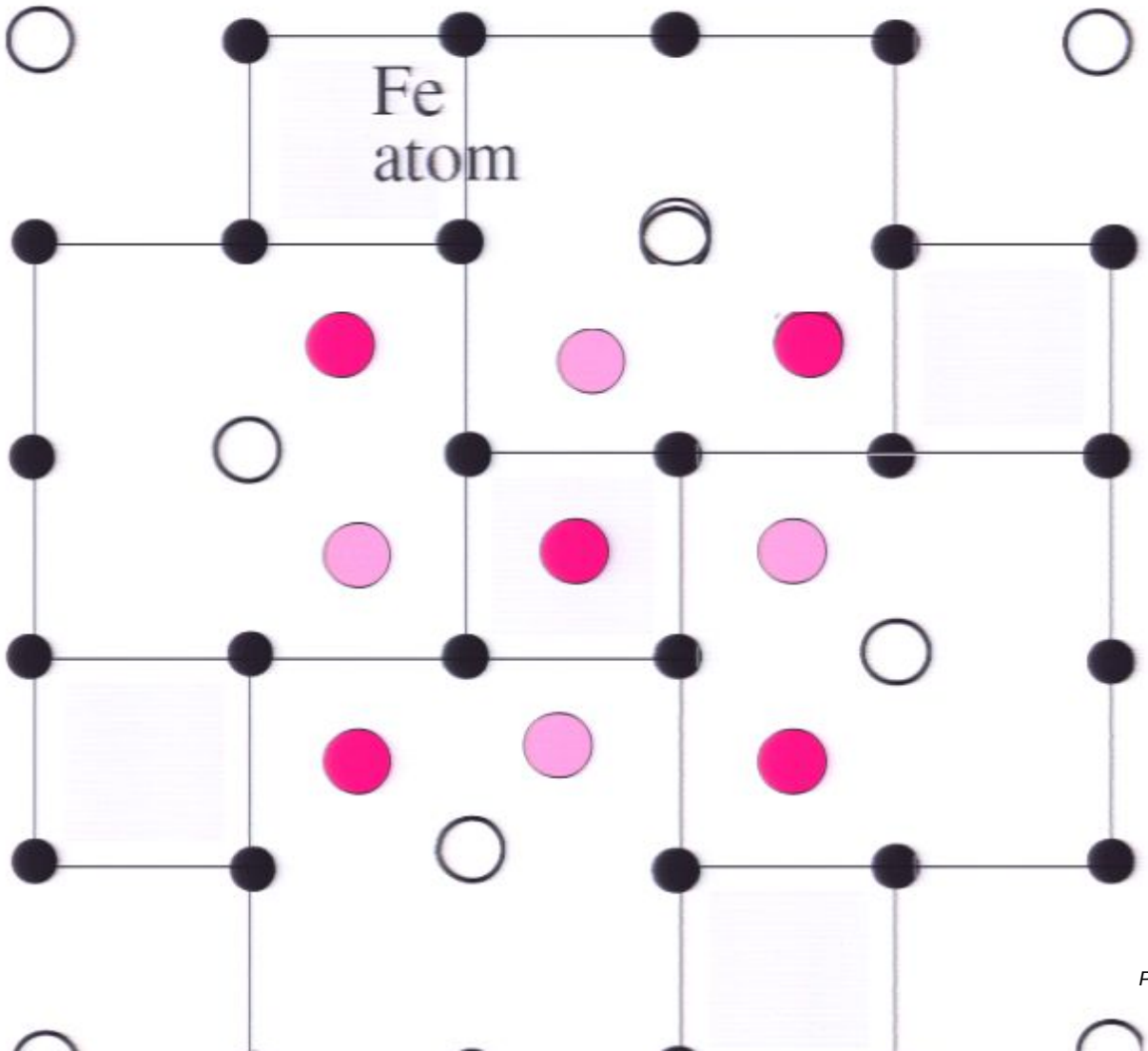
F_4Se_9 Cluster





F_4Se_5 Se_4 Cluster

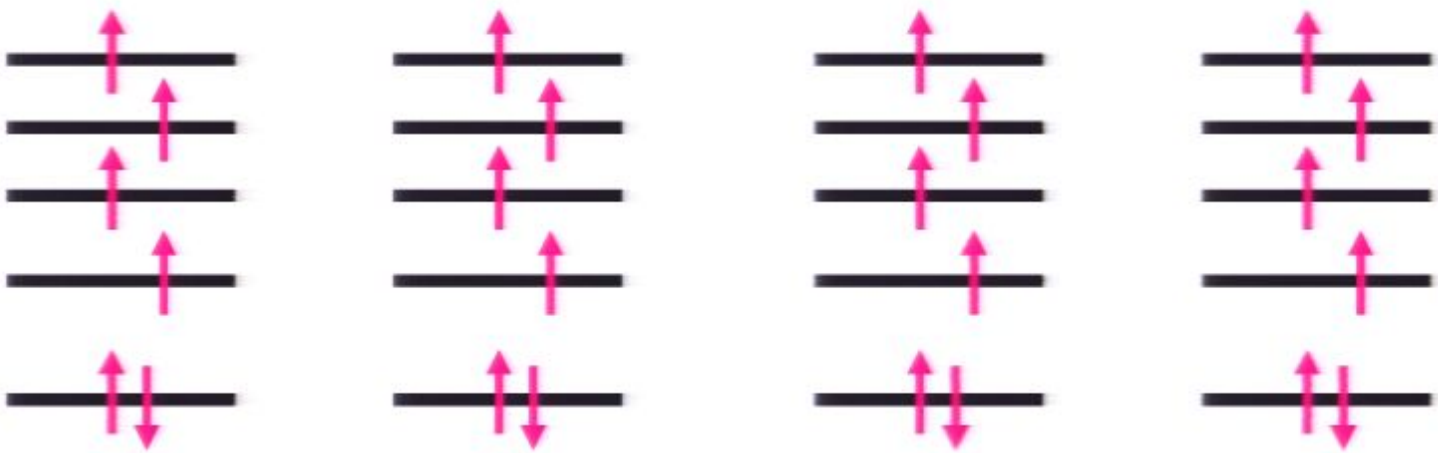
= 4 edge sharing $FeSe_2Se_2$ tetrahedra



F_4Se_9 Cluster Ferromgnetism

Spin state of F^{2+} is S = 2

'e atoms are ferromagnetically coupled - we get S = 8 state

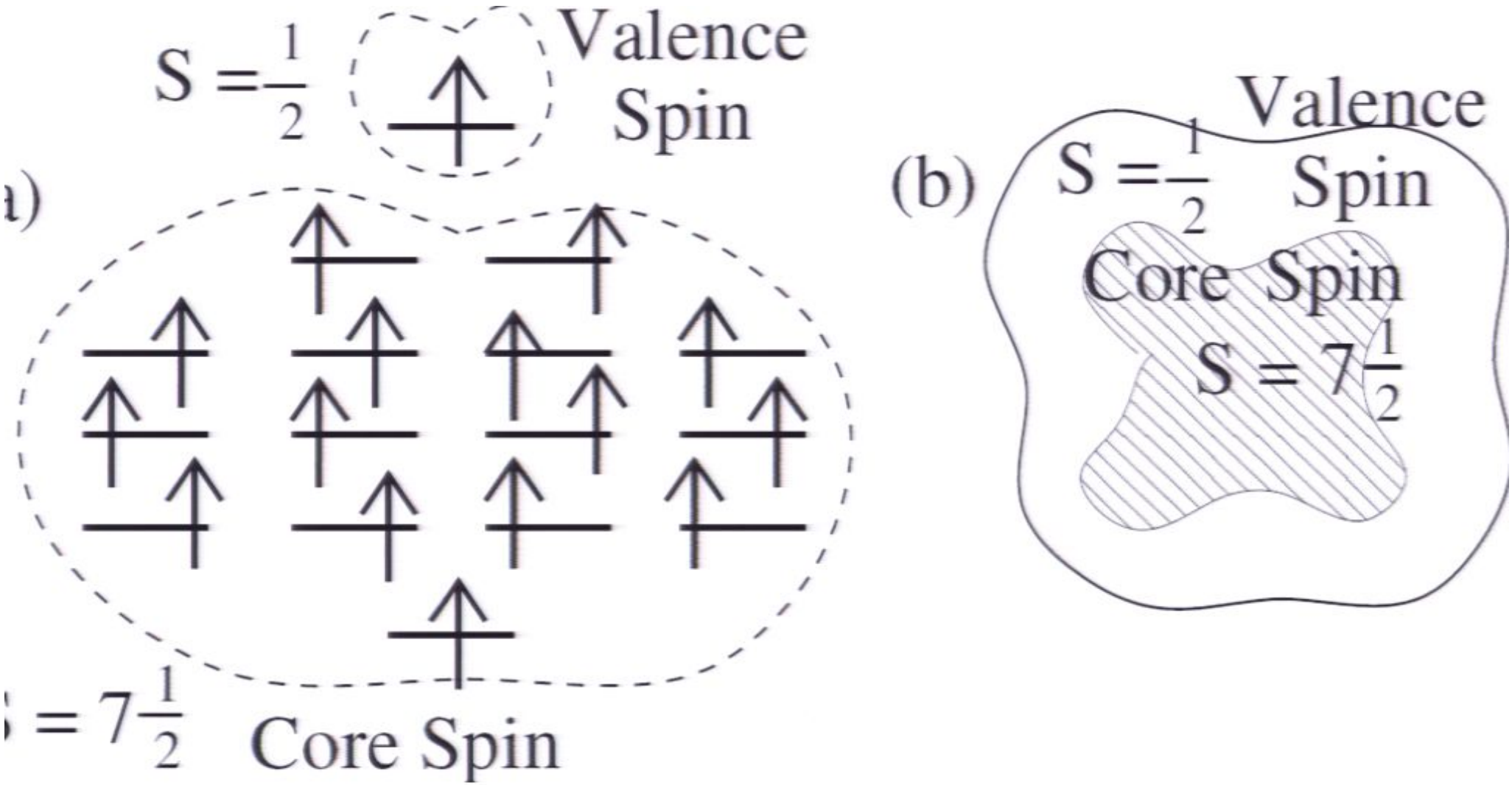


4s and 4p orbitals of Se
strongly hybridize with 3d orbitals of Fe

Fe-Fe distance is comparable to that in metal iron

3d orbitals of 4 Fe atoms have strong direct overlap

(part of the reason for F_4 cluster ferromagnetism)



16 Spin polarized level of F_4Se_9 Cluster

A hybrid of 3d levels of Fe and 4s and 4p levels of Se

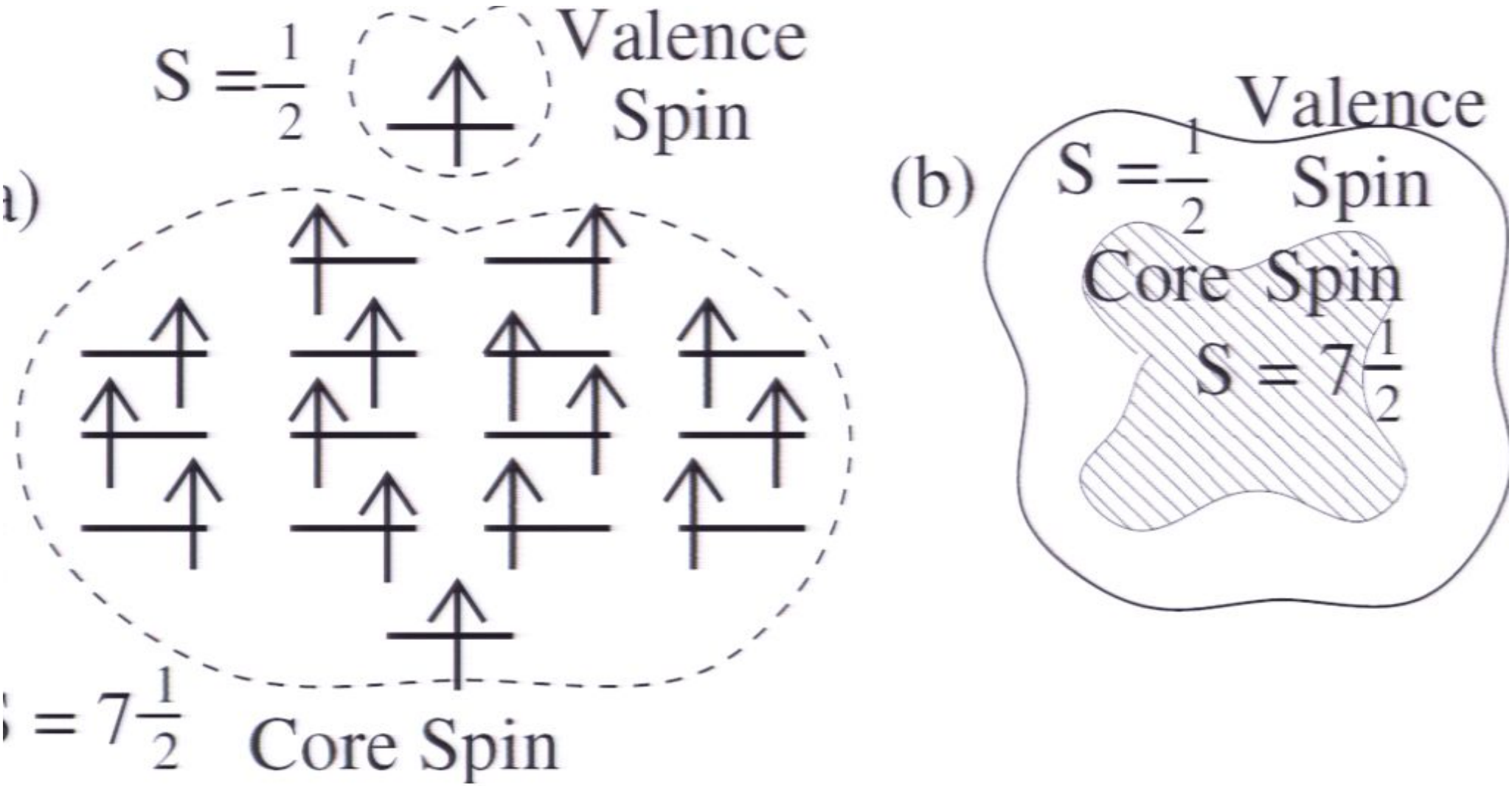
S = 7 ½ core moment **S = ½ valence moment**

$$H_{\mathrm{AFM}} = -J_{\mathrm{H}} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i + J \sum_{\langle ij \rangle} (\mathbf{S}_i + \mathbf{s}_i) \cdot (\mathbf{S}_j + \mathbf{s}_j)$$

J_H ~ 100 meV is Ferromagnetic Hund like coupling within F_4 plaquette

J ~ 20 meV is interplaquette effective AFM coupling

$J_H >> J$ we get S = 8 Heisenberg Antiferromgnet



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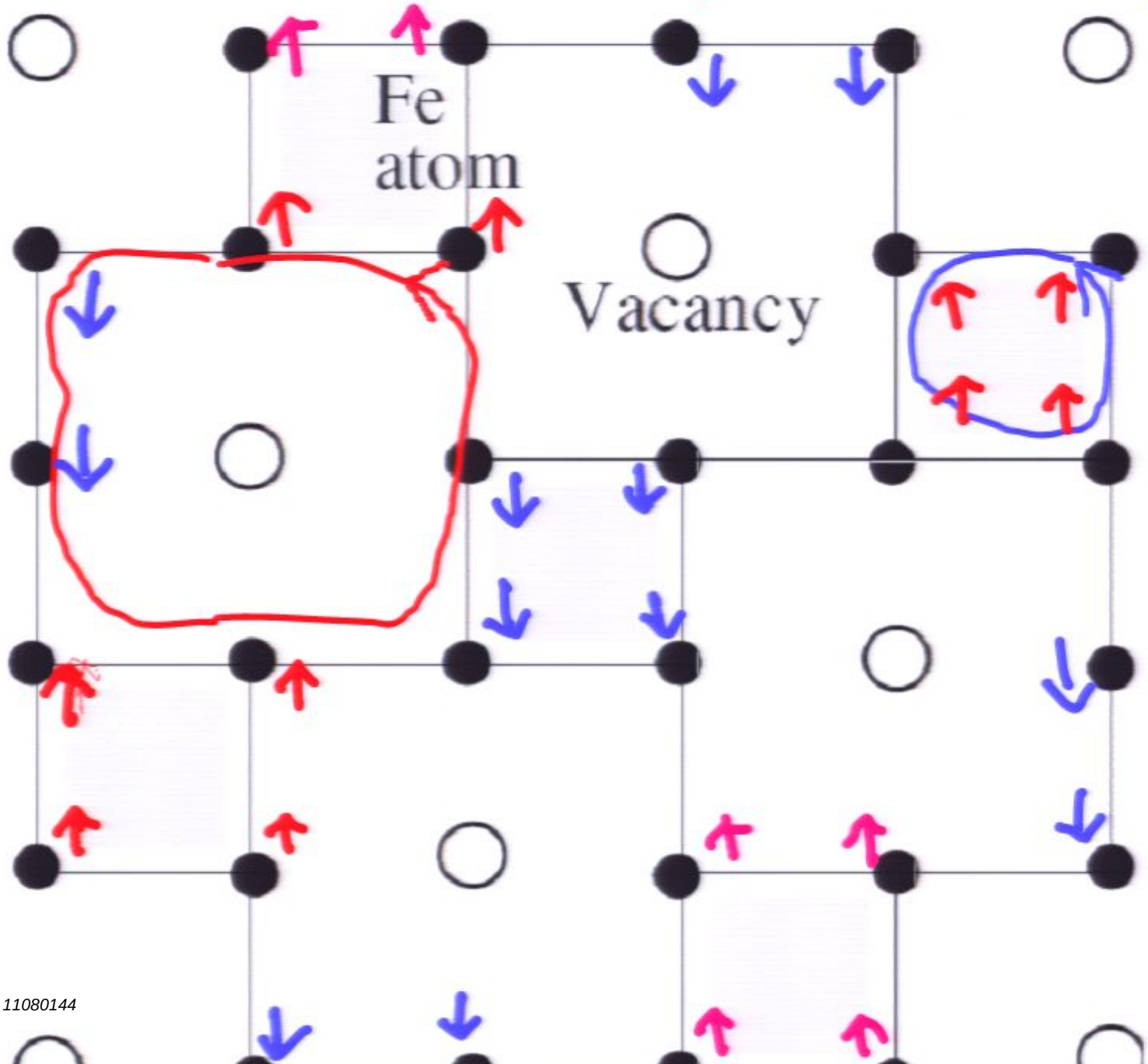
Where does a doped electron go ?



Where does a doped hole go ?

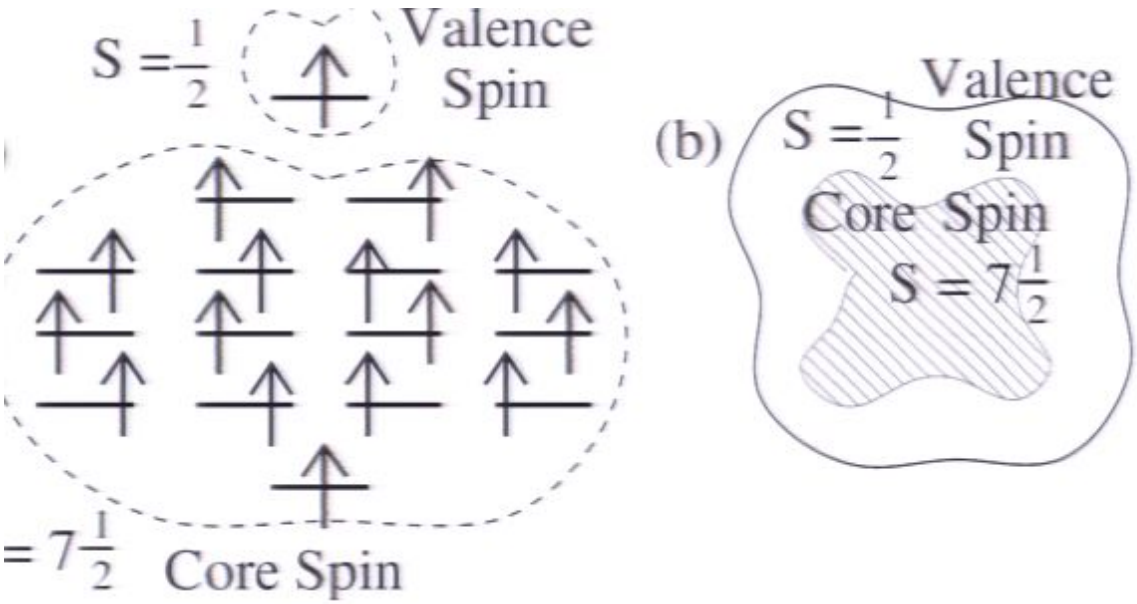
Hypothesis

a doped hole enters a
non degenerate singly occupied valence orbital

Any orbital degeneracy will lead to lifting of degeneracy
by plaquette distortion (not seen in experiments)

This state is similar to Zhang-Rice Singlet in cuprates

In the present case a doped hole creates a S = 7 ½
Hexadecatric State



Model Hamiltonian for the doped S=8 Mott Insulator

$$H_{tJ} = -\sum_{ij} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c} + J \sum_{\langle ij \rangle} (\mathbf{S}_i + \mathbf{s}_i) \cdot (\mathbf{S}_j + \mathbf{s}_j)$$

$$- J_{\text{H}} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i$$

and width 4t ~ 200 meV

$$\sum_\sigma c^{\dagger}_{i\sigma} c_{i\sigma} \neq 2$$

charging energy **500 meV**

$(U_{eff}) \approx \frac{e}{\epsilon_0 R}$ of the $(Fe_2Se_5)^{2+}$ plaquette.

AFM order blocks hole delocalization
(strings of flipped bonds)

Spins cant/twist and allow delocalzation and
gain kinetic Energy

Double exchange theory
Zener, Anderson, Hasegawa, de Gennes
in 3D ferromagnetis (manganites)

In 2D there is an alternate way
(Create Skyrmions and gain delocalization energy)

In 2D there is an alternate way

Skyrmions Can help

Skyrme Model (1962)

Model for neutron, proton
(A low energy field theory for Standard model)

Non-linear sigma model of Pion field

Topological excitations (solitons)

Collective quantization of zero modes
topological terms, induced charges …

$$\pi_3(SU(N)) = \mathbb{Z}$$

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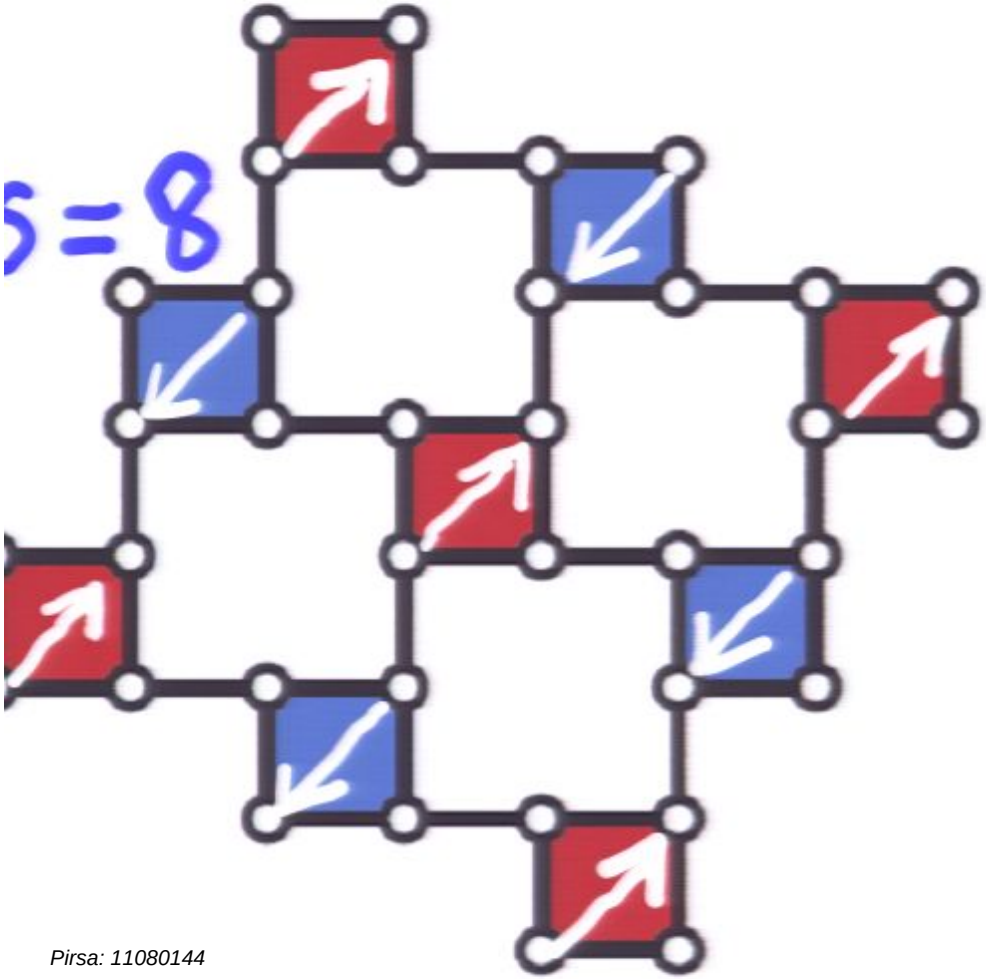
We have a 2-dimensional Heisenberg antiferromagnet



Sublattice magnetization is the order parameter

$$\vec{n}_i \rightarrow \vec{n}(\vec{r})$$

$$\vec{n}\cdot\vec{n}=1$$

2-dimensional Heisenberg antiferromagnet

Its low energy physics is described by a

O(3) Non linear σ-model

$$S \sim \int dx\ dy\ d\tau [\frac{1}{v_s^2}(\partial_\tau \mathbf{n}(\mathbf{r}))^2 + (\partial_x \mathbf{n}(\mathbf{r}))^2 + (\partial_y \mathbf{n}(\mathbf{r}))^2]$$

Collective excitations: **spin waves (Goldstone modes) (non-topological)**

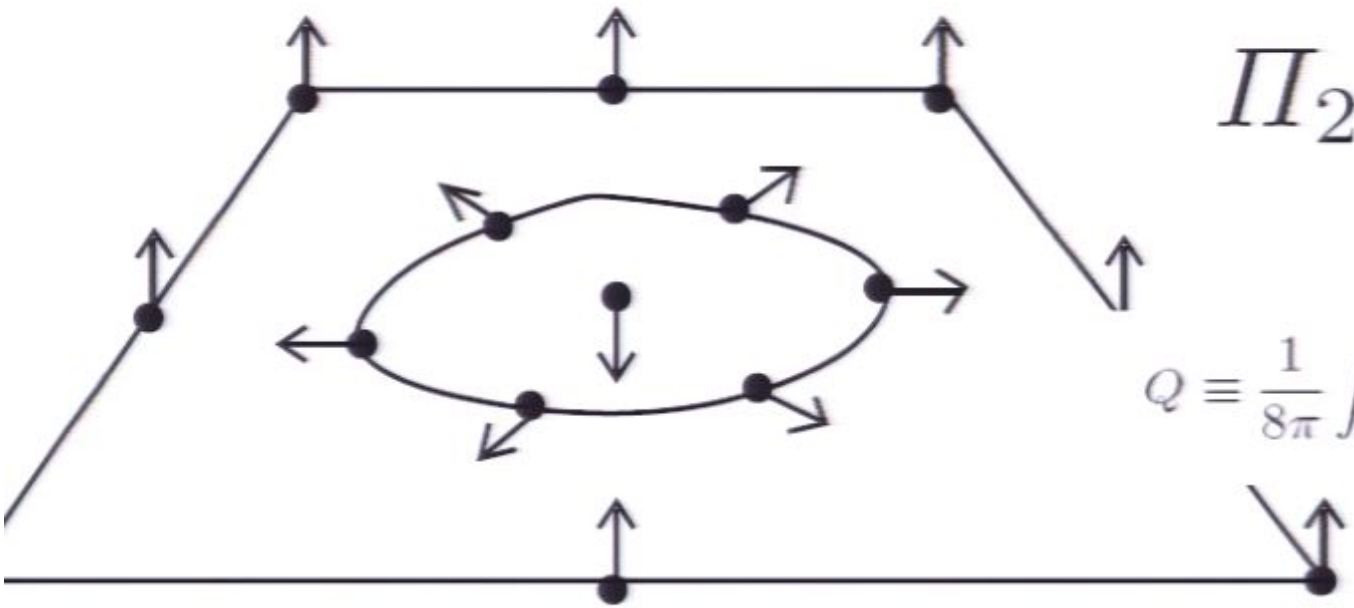
Baby Skyrmions (topological)

Topological index

Pontryagin index

$$Q \equiv \frac{1}{8\pi} \int dx\ dy\ \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_y \mathbf{n})$$

Sublattice spin pattern in 2D plane



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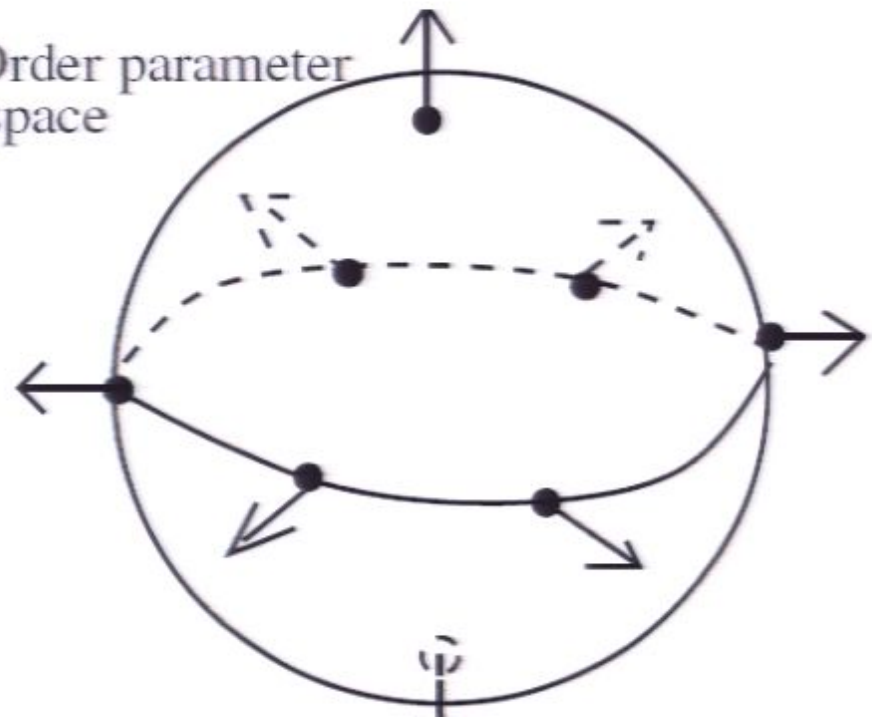
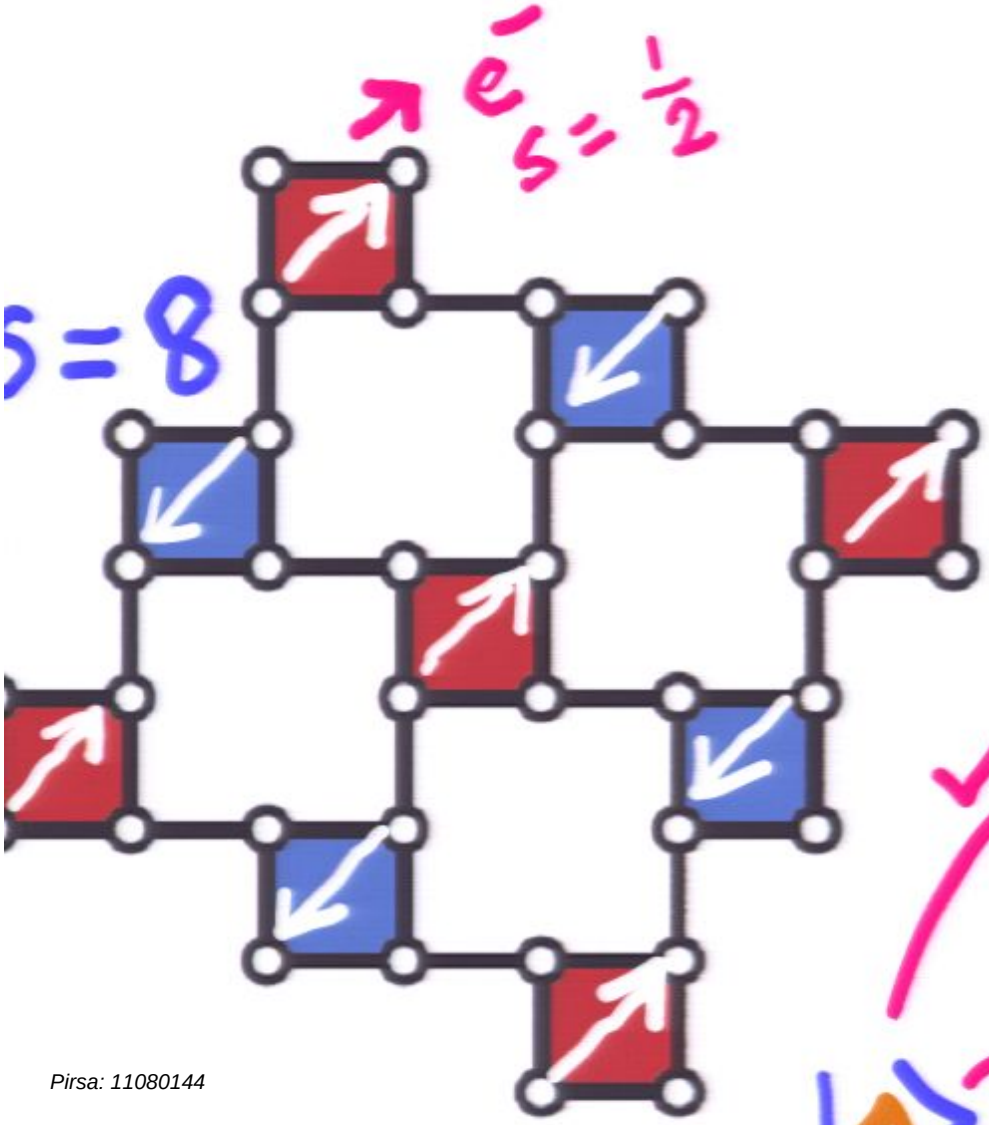
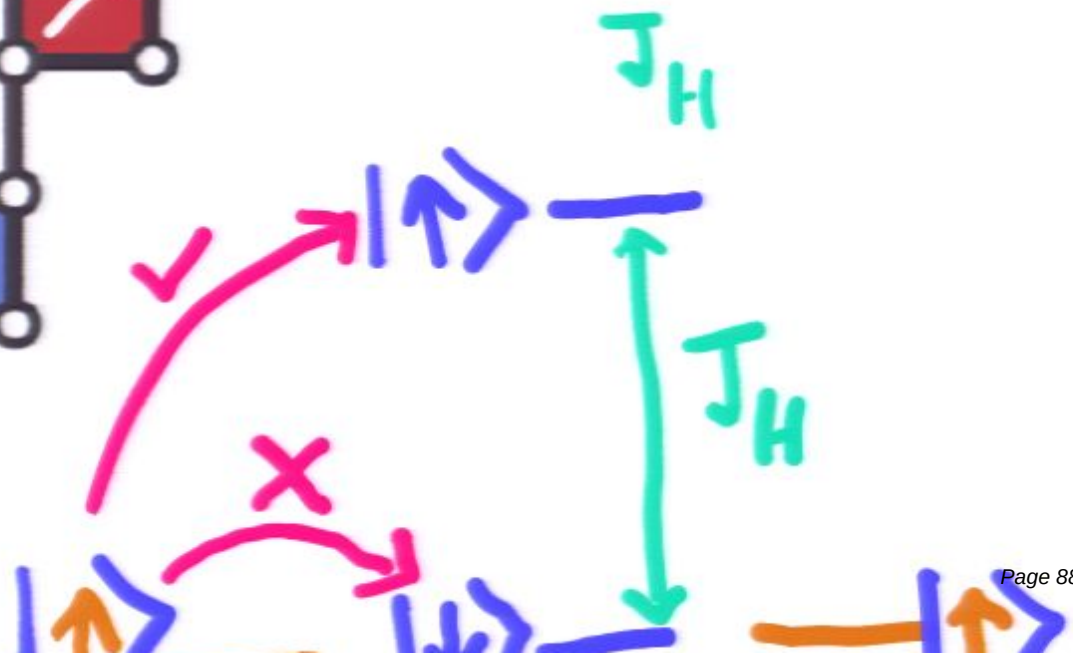


How do Slyrmions Help ?

A rigid AFM background prevents hopping and delocalization through a high exchange barrier





Double exchange theory

Zener, Anderson, Hasegawa

$$H = -t \sum_{\tau} (c^{\dagger}_{1\tau} c_{2\tau} + h.c.) - J_H \sum_{i=1}^{2} \vec{S}_i . \vec{\sigma}_i + J \vec{S}_1 . \vec{S}_2$$

hopping $\to 0$

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$$H_{\text{eff}} = \sum_i \epsilon_i n_i - t \sum_{<ij>} \cos(\theta_{ij}/2)(c^{\dagger}_i c_j + H.C.)$$

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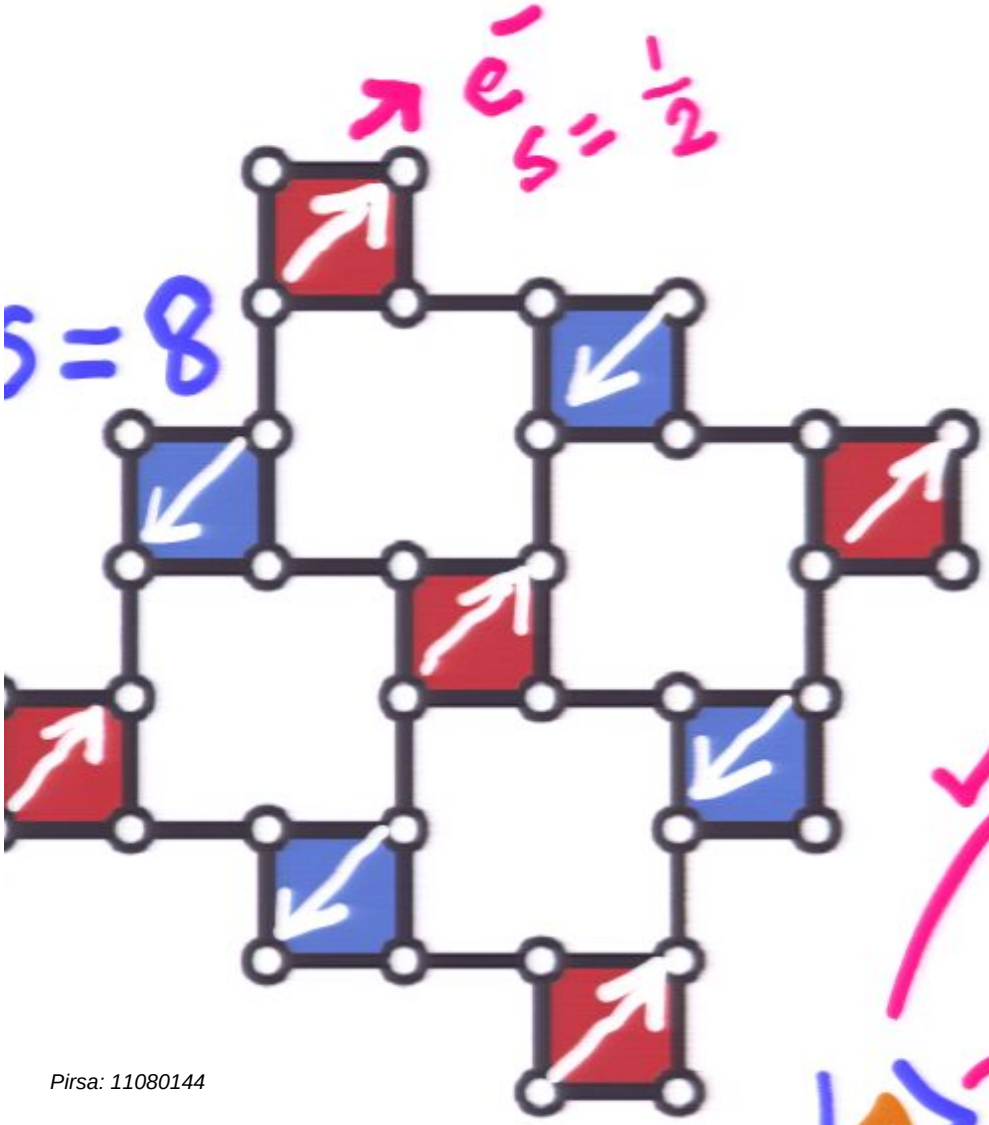
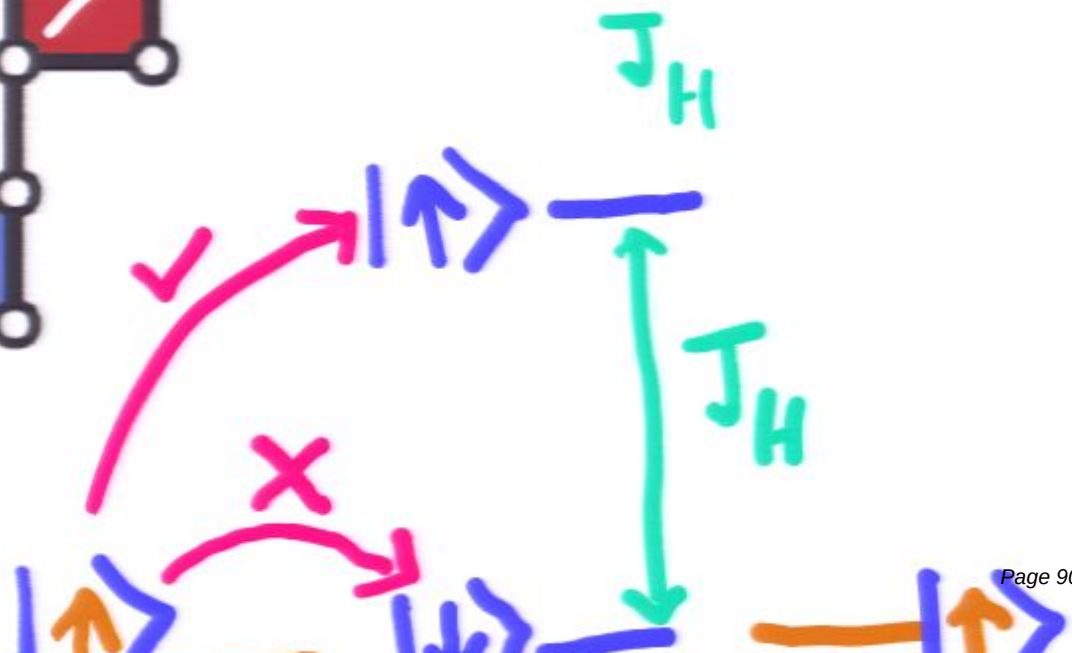
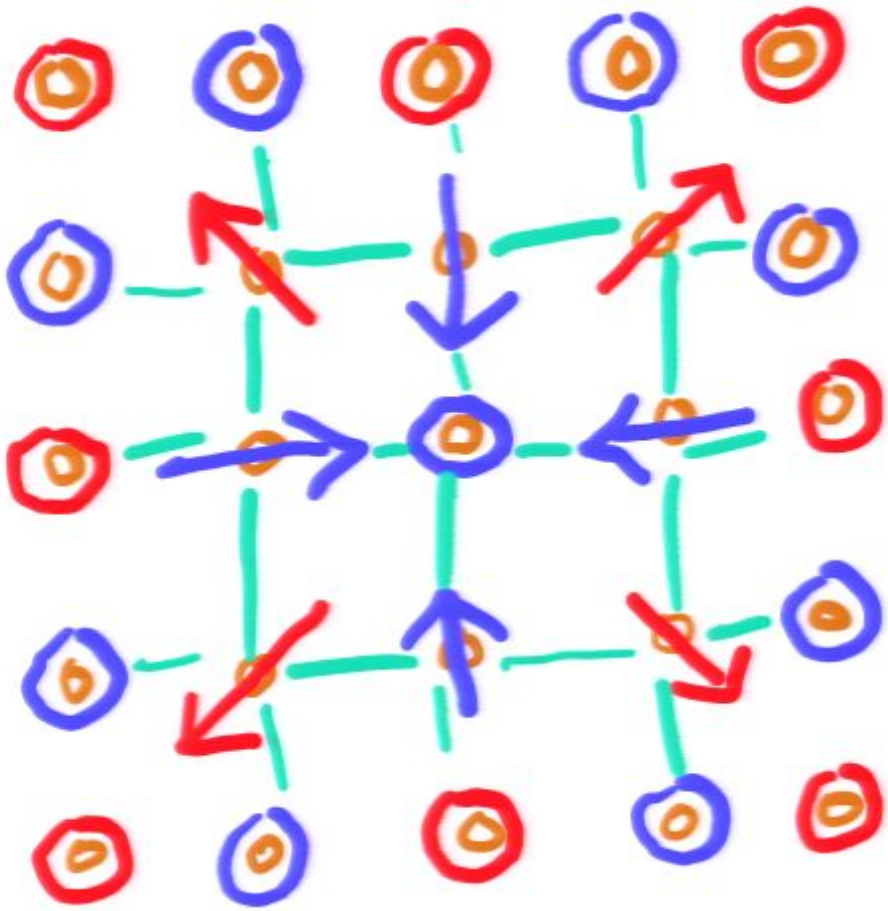




Lattice AFM
skyrmion



Spin density wave picture

1D Domain wall (pi-twist) in an AFM
Traps a mid gap state
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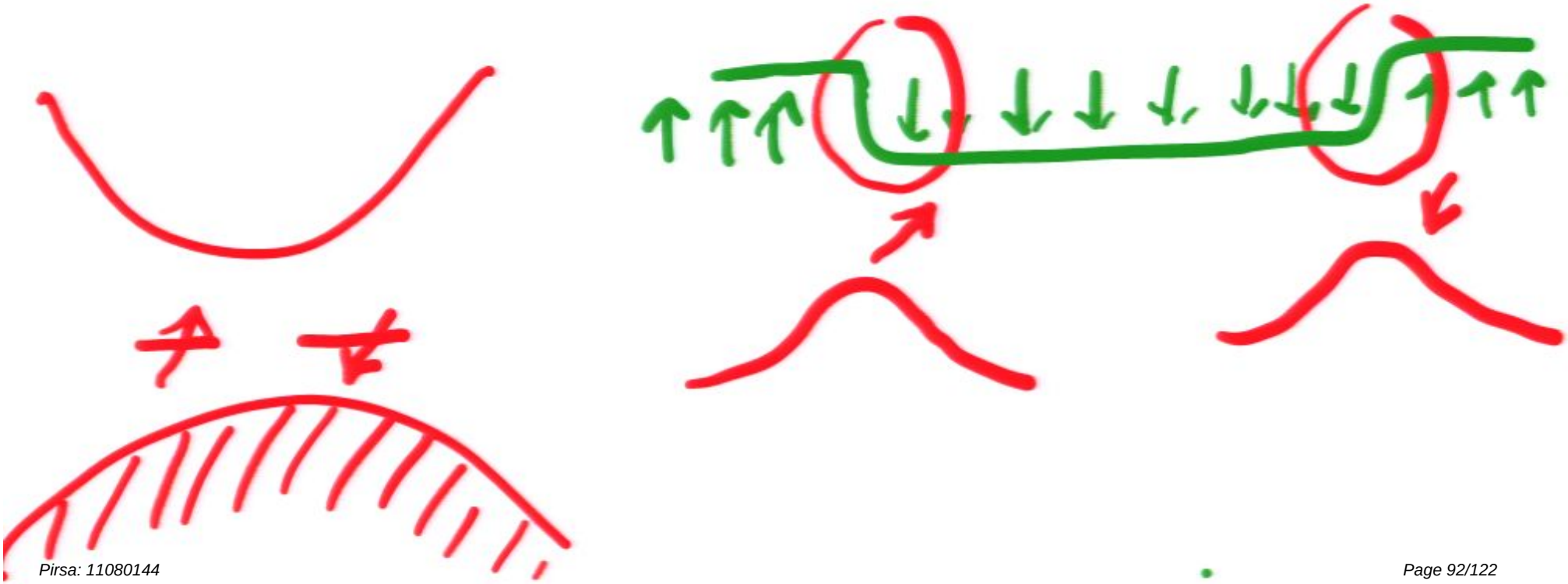

A skyrmion traps 2 spins in 2 midgap states

Sajeev John
Bernie
(1999)

G.B (2002)

$$H_{\mathrm{mF}} \approx \sum_{ij} \tilde{t}_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{h.c} - J_{\mathrm{H}} S \sum_{i} \mathbf{n}_i \cdot c^{\dagger}_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta}$$

$$S \sim \int d^3x \; \bar{\psi} \left[-i\gamma_\mu (\partial_\mu + A^c_\mu) + im \; \vec{\sigma} \cdot \mathbf{n}(\mathbf{r}) \right] \psi$$

$$\bar{\psi} = i\psi^\dagger \gamma^0, \text{ and } \gamma^0, \gamma^x, \gamma^y \equiv \sigma^z, \sigma^y, -\sigma^x$$

$$S = S_{\mathrm{R}} + 2iA^c_\mu J_\mu$$

Wiegmann 1999
Wiegmann, Abanin

$$J^T_\mu = \frac{1}{8\pi}\epsilon^{\mu\nu\lambda}\mathbf{n}\cdot\partial_\nu\mathbf{n}\times\partial_\lambda\mathbf{n}$$

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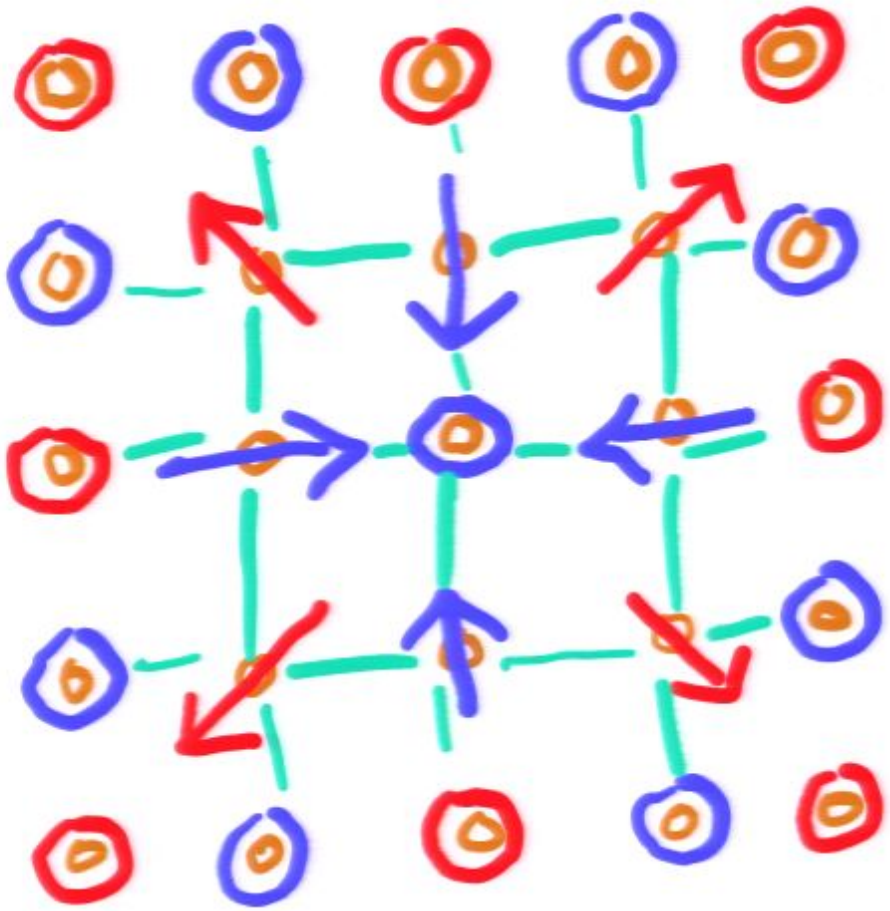

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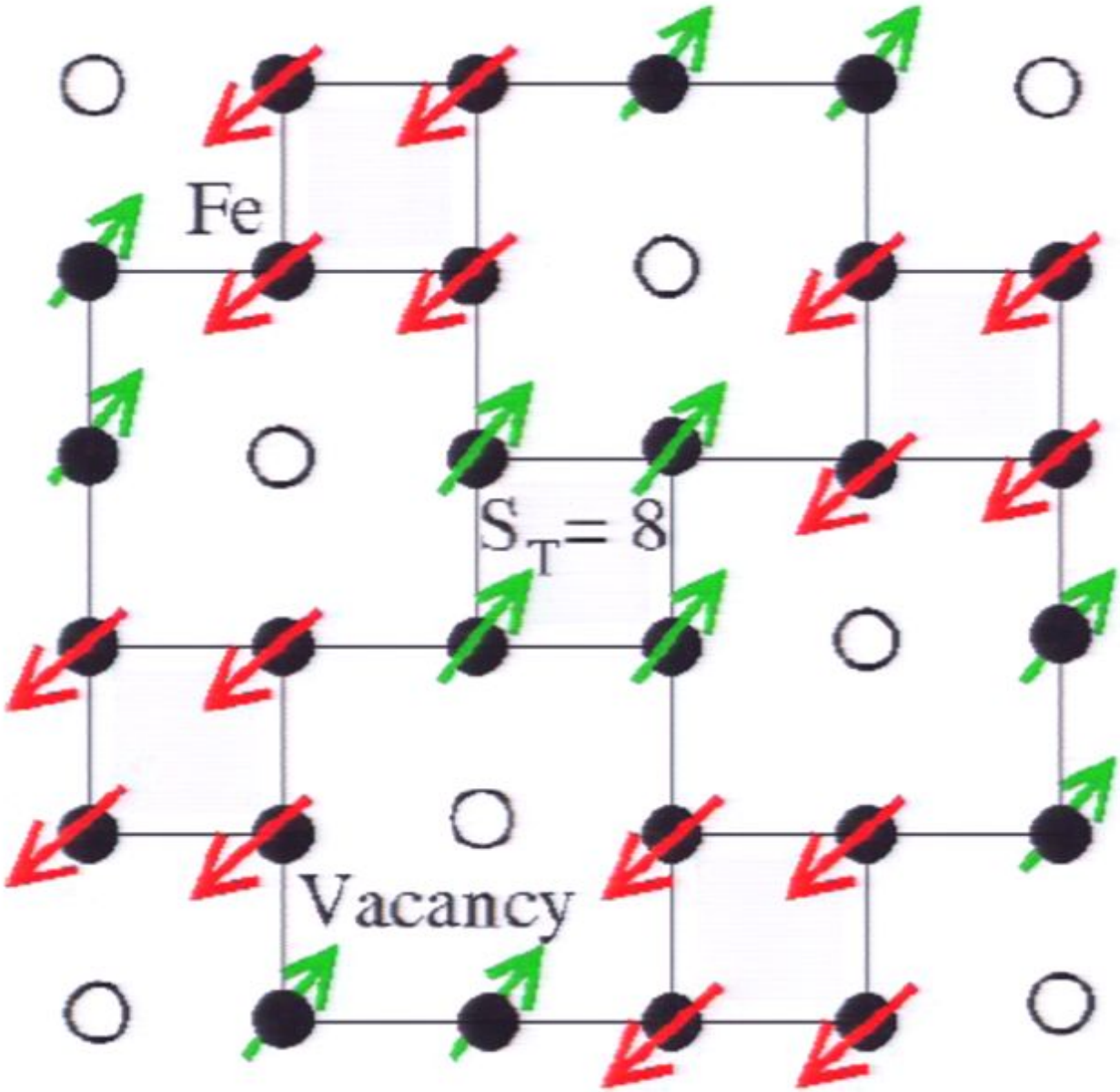
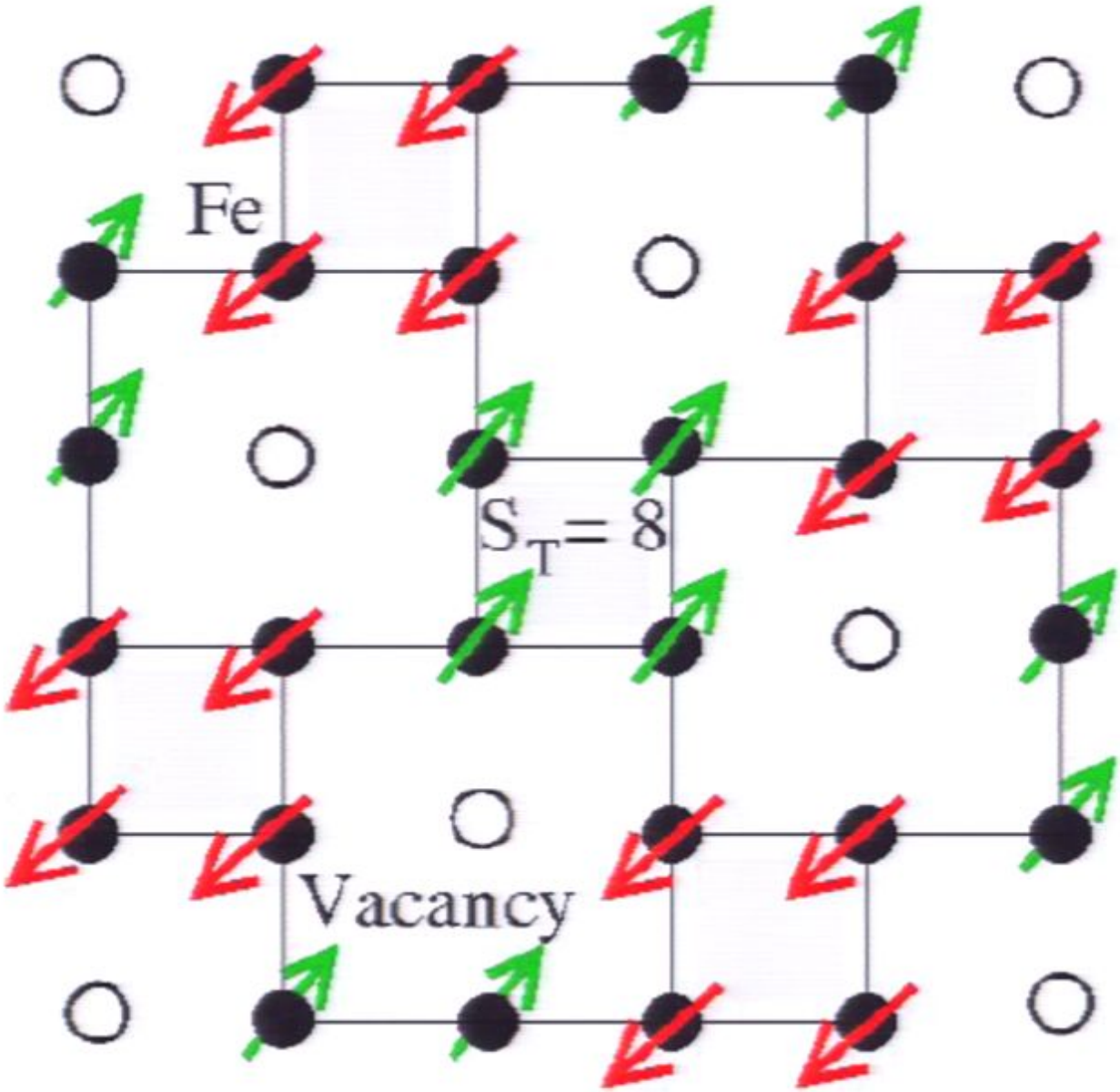

Fe
$S_T = 8$
Vacancy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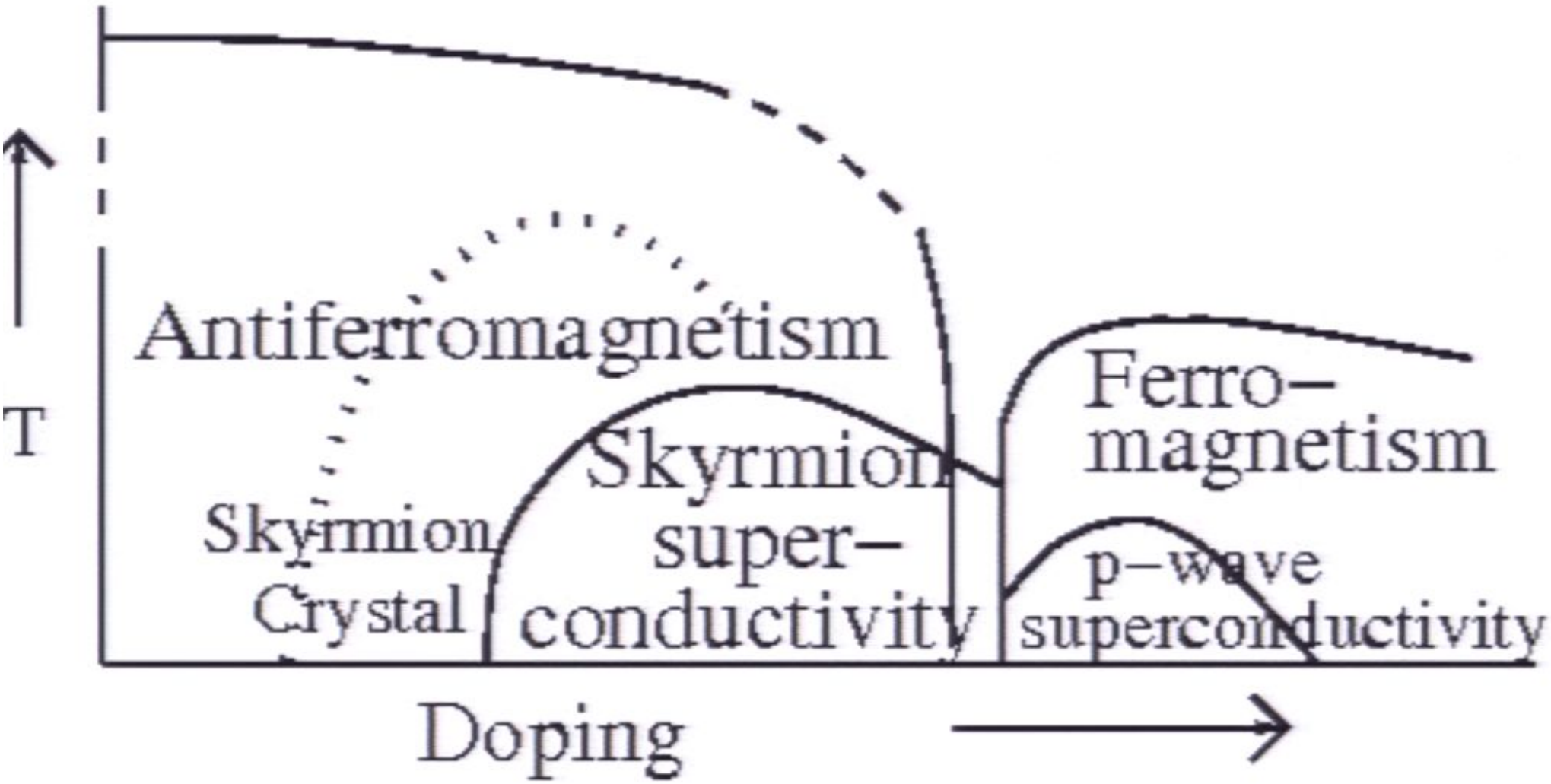
T
Antiferromagnetism
Skyrmion
Crystal
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super–
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Doping

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2-dimensional Heisenberg antiferromagnet

Its low energy physics is described by a

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Baby Skyrmions (topological)

Topological index

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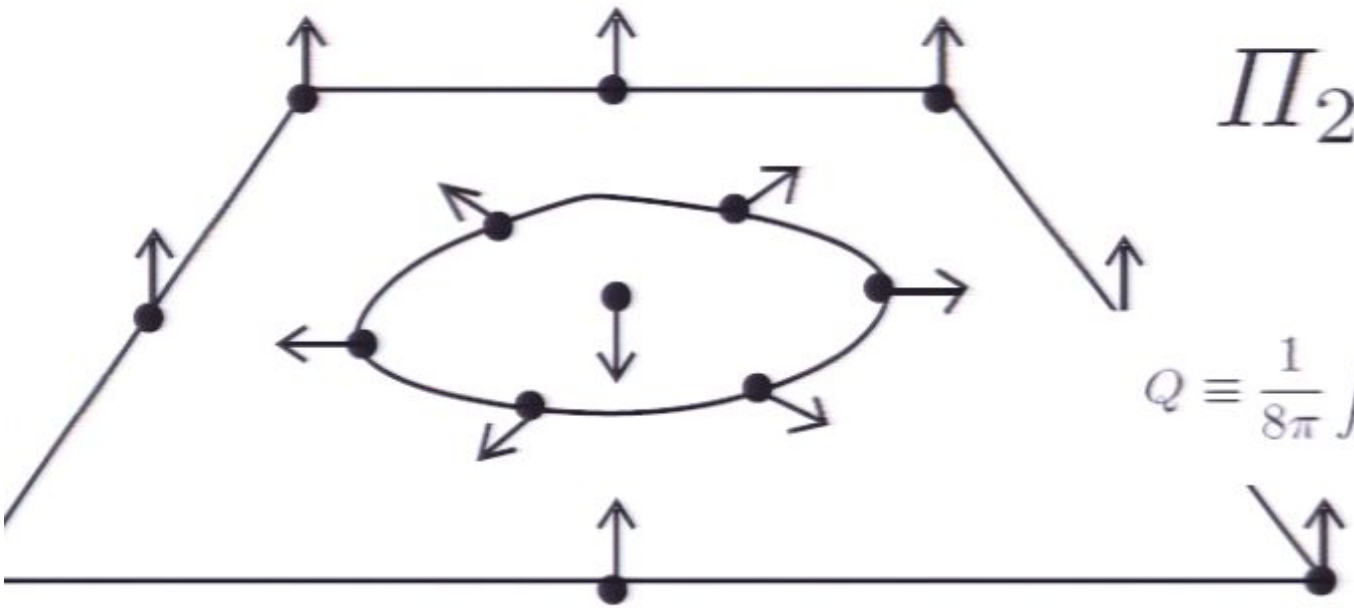

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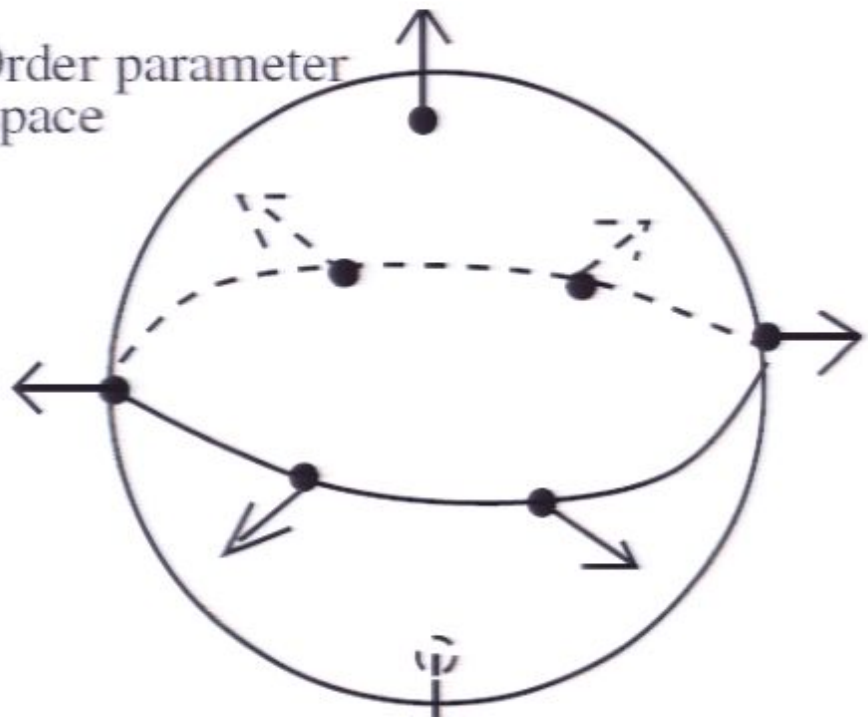

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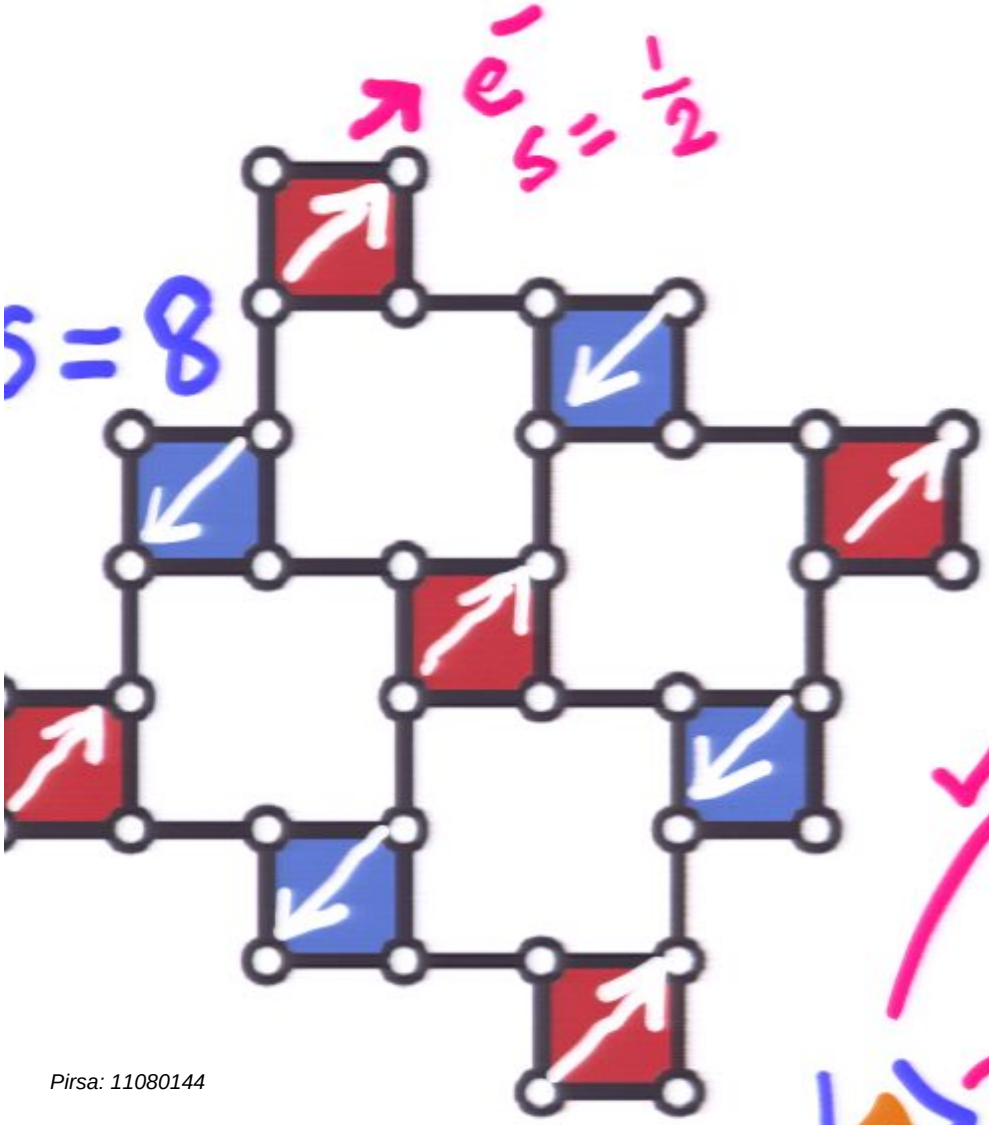

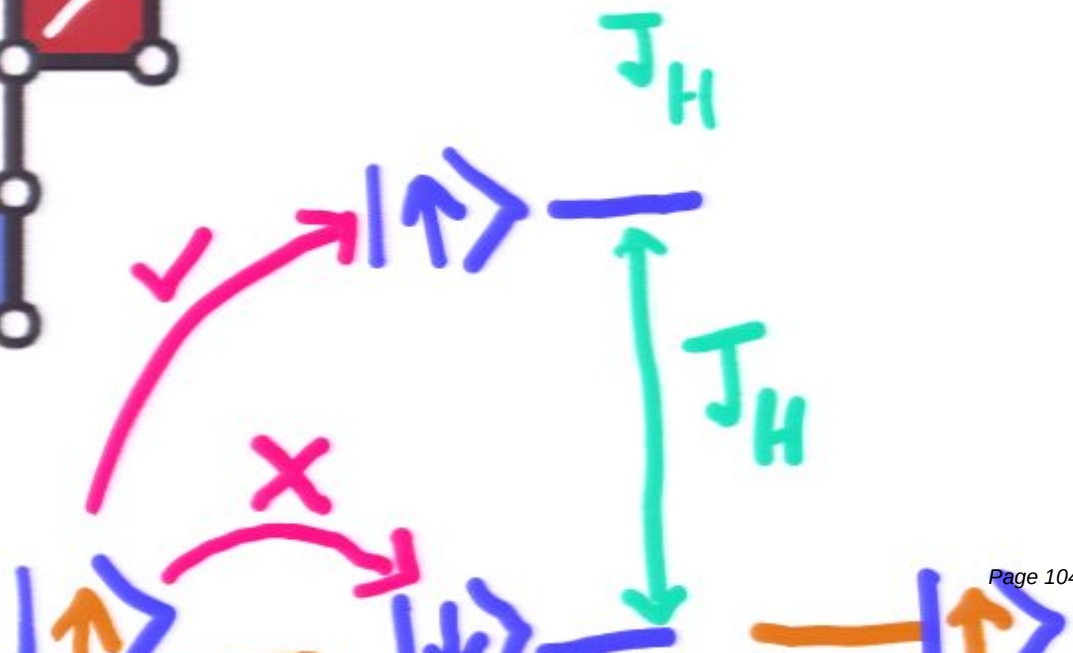

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Robuts antiferromagnetic background

2e Charged Skyrmions as cooper pairs

Singlet or triplet pairing ?

Tl-2201 92K

Hg-2201 92K

ALIKE !

Explanations and Predictions

50 K Structural Transition:

Self Doping and Ordering of Singlet Chains

30 K SDW order: SDW within Singlet Chain

cale of Tc – SCOPE FOR HIGHER T_c

rediction: Mutully Perpendicular SDW and CDW order

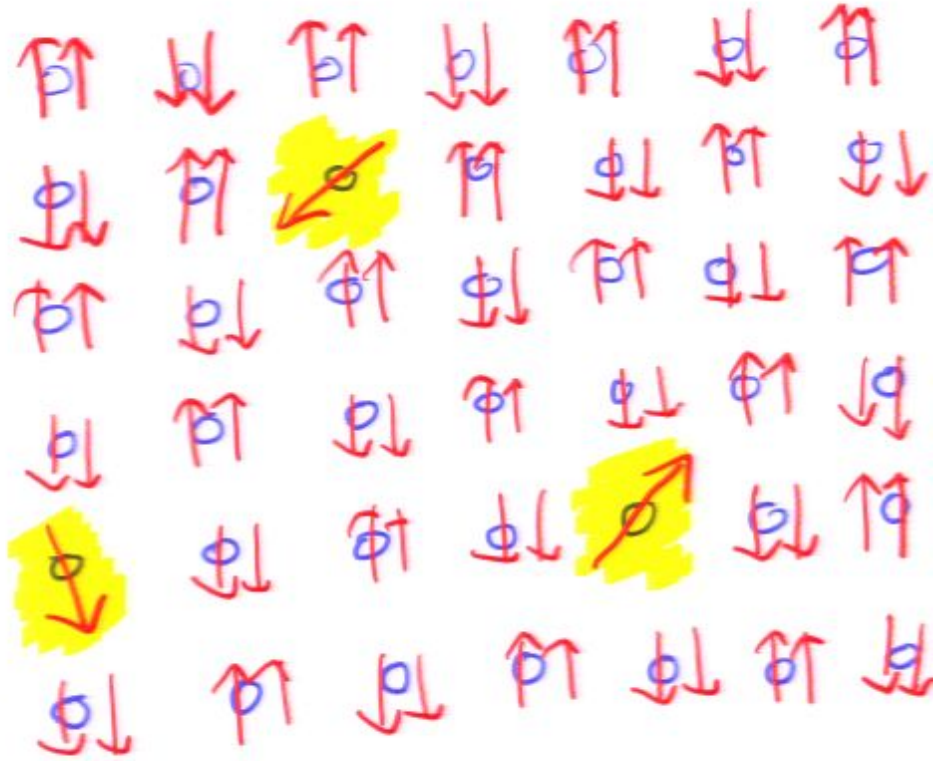
lew Systems ? Doped LaOFeP

Band Picture

No. of Charges N_x

No of Spins N_x

Doped Mott Insulator Picture



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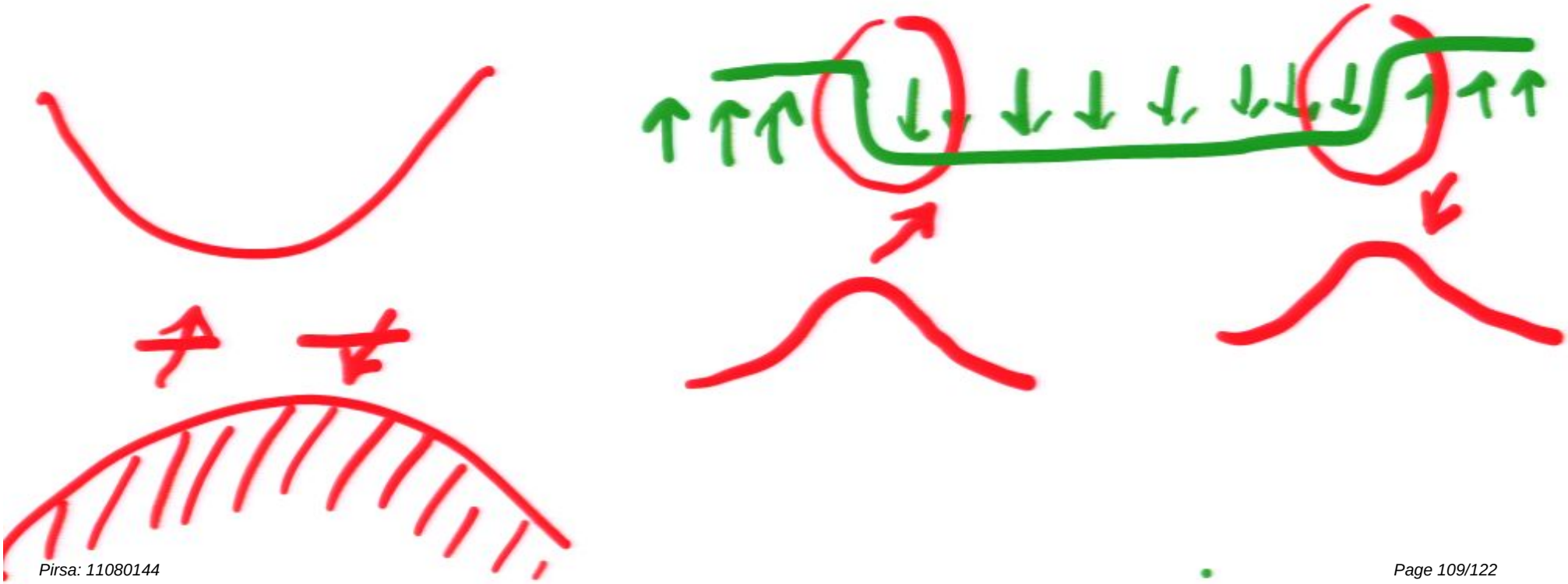

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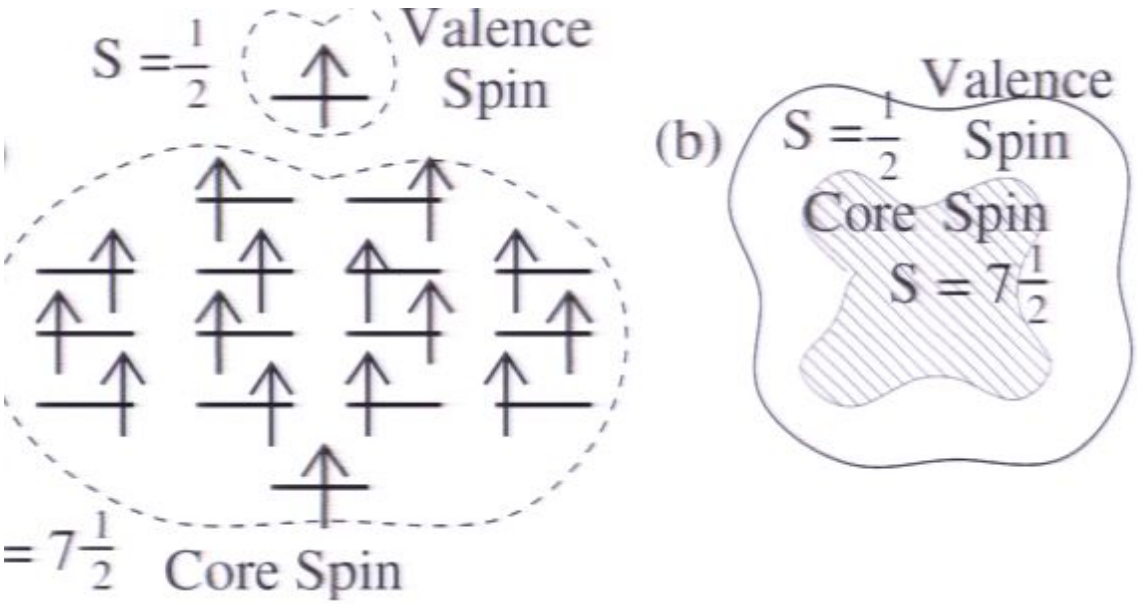


Model Hamiltonian for the doped S=8 Mott Insulator

$$H_{tJ} = -\sum_{ij} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c} + J \sum_{\langle ij \rangle} (\mathbf{S}_i + \mathbf{s}_i) \cdot (\mathbf{S}_j + \mathbf{s}_j)$$

$$- J_{\text{H}} \sum_i \mathbf{S}_i \cdot \mathbf{s}_i$$

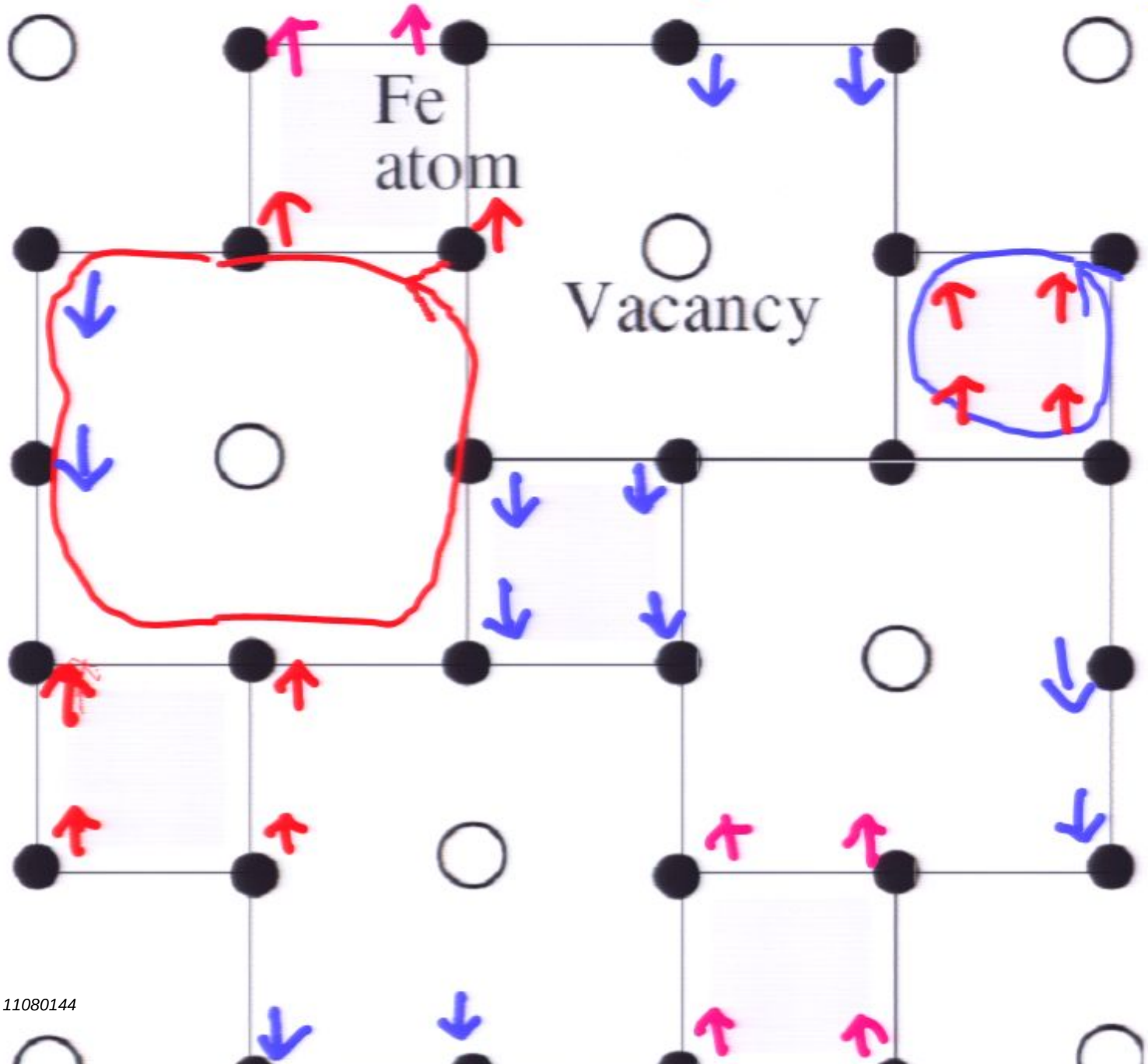
and width 4t ~ 200 meV

$$\sum_\sigma c^{\dagger}_{i\sigma} c_{i\sigma} \neq 2$$

charging energy **500 meV**

$(U_{eff}) \approx \frac{e}{\epsilon_0 R}$ of the $(Fe_2Se_5)^{2+}$ plaquette.

Where does a doped electron go ?



GB arXiv:1108.3562

Minimal Model

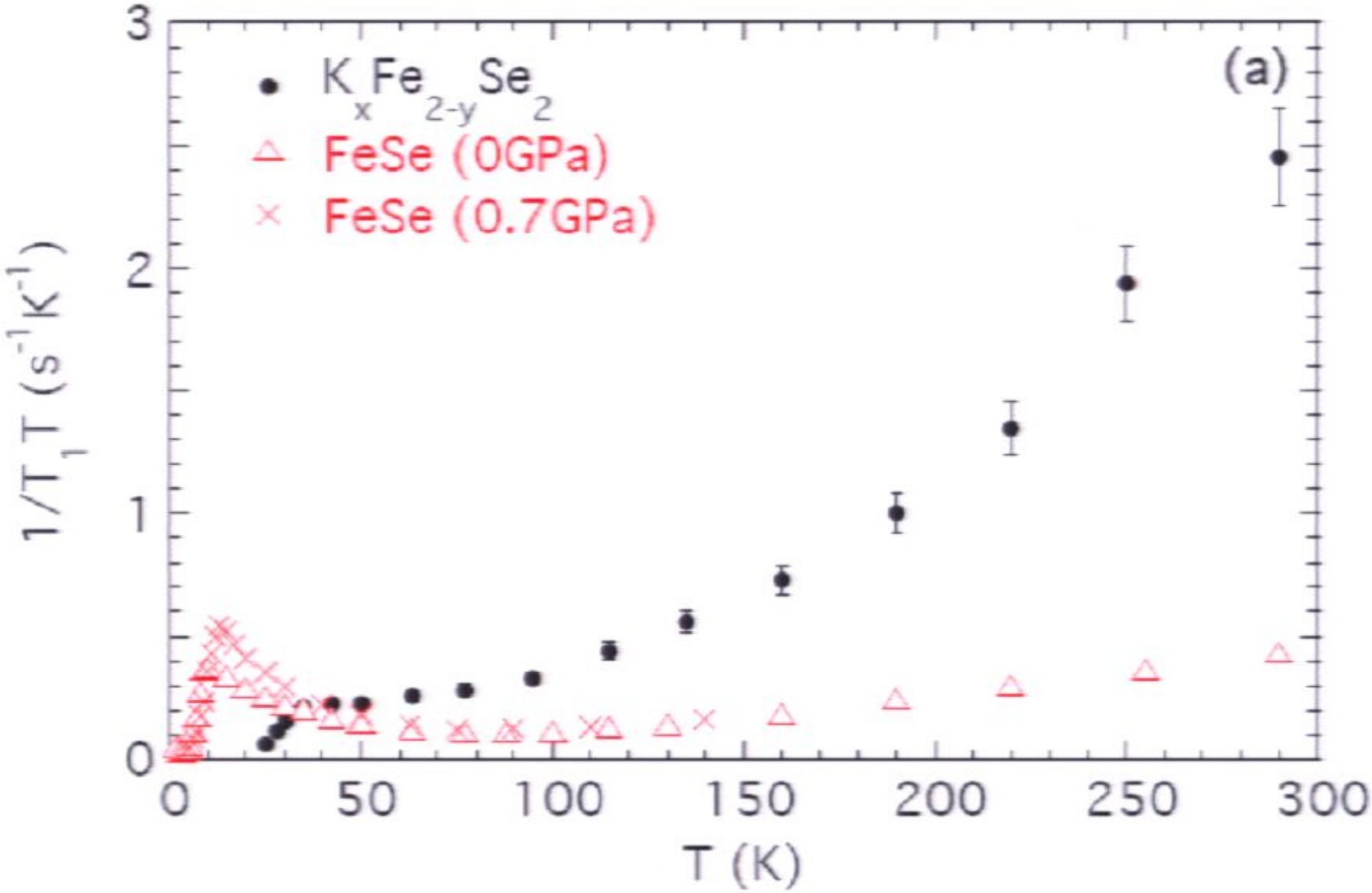
for Low Energy Electronic properties

F_4 plaquette is the basic building block

It has an electronic integrity
As seen from its large and robust **S = 8** magetic moment

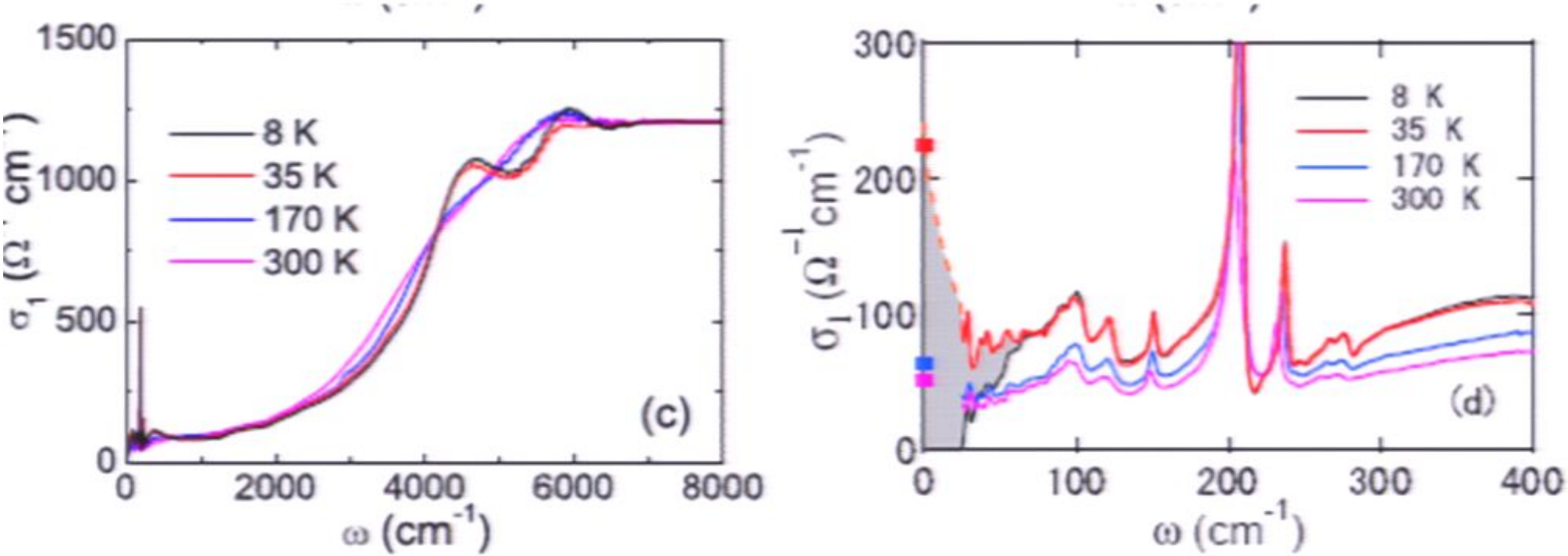
Where do the moments come from ?

^{7}Se NMR $K_xFe_{2-y}Se_2$

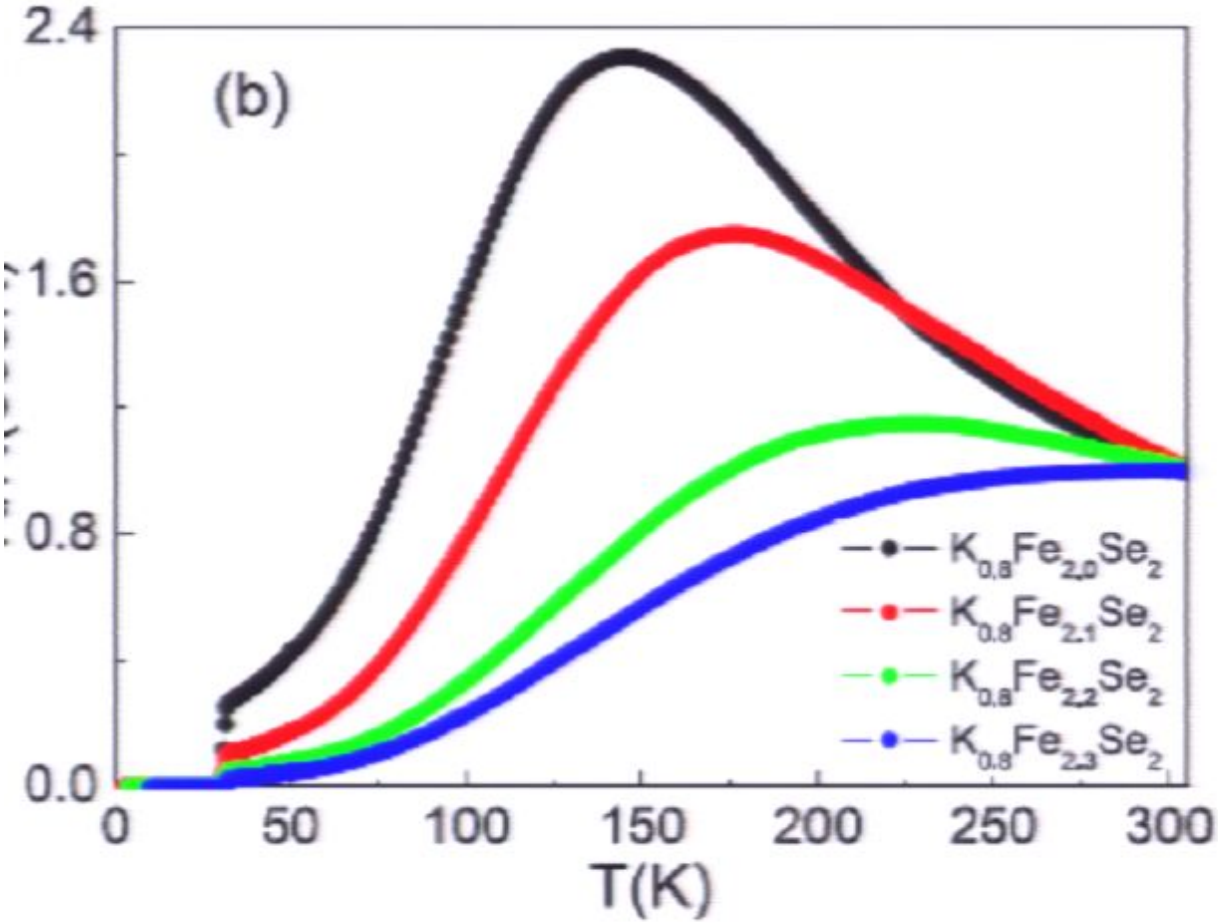


Torchetti et al. PRL 2011

R.H. Yuan et al. arXiv:1102.1381



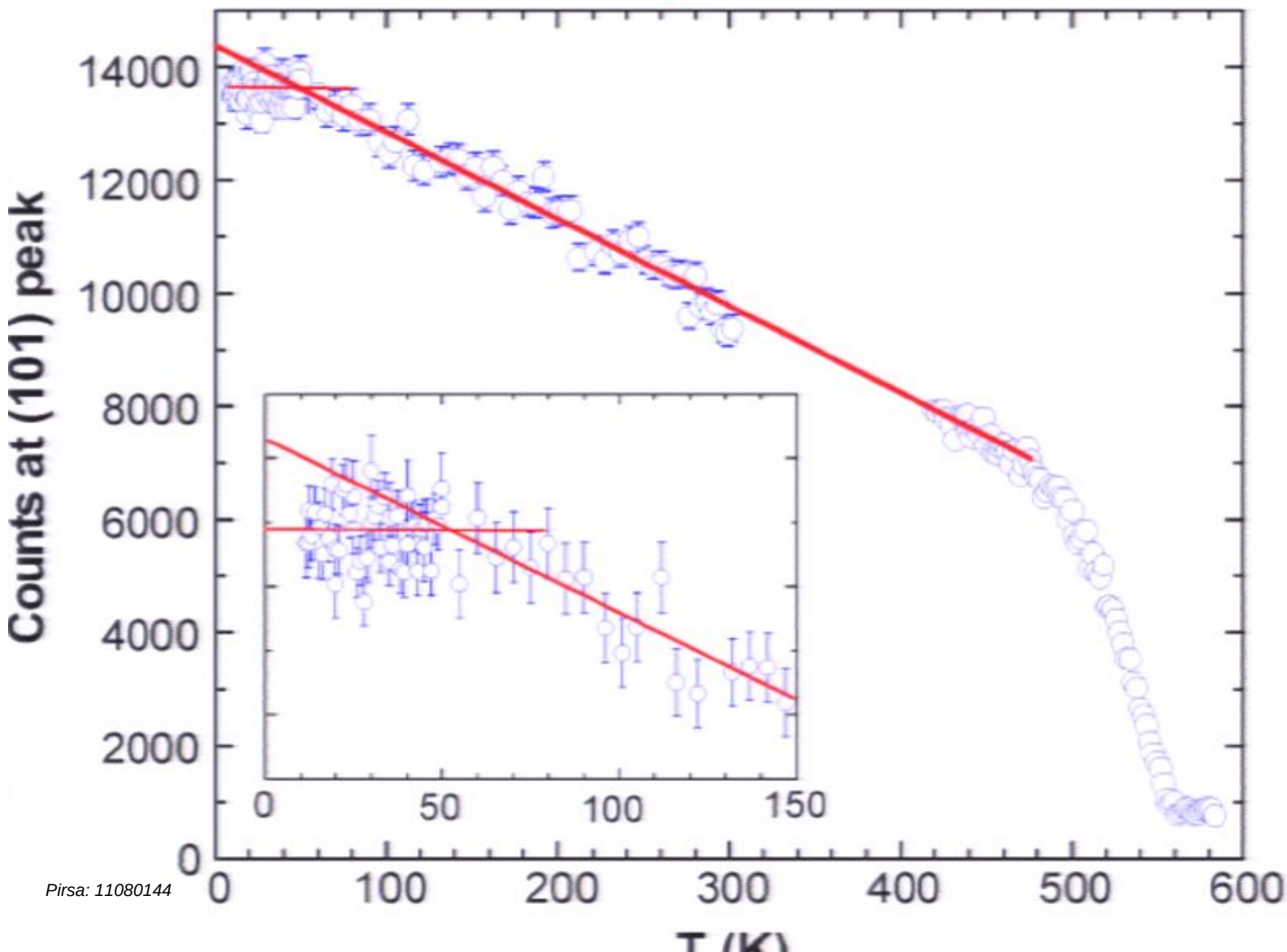
Wang et al. arXiv:1101.0789

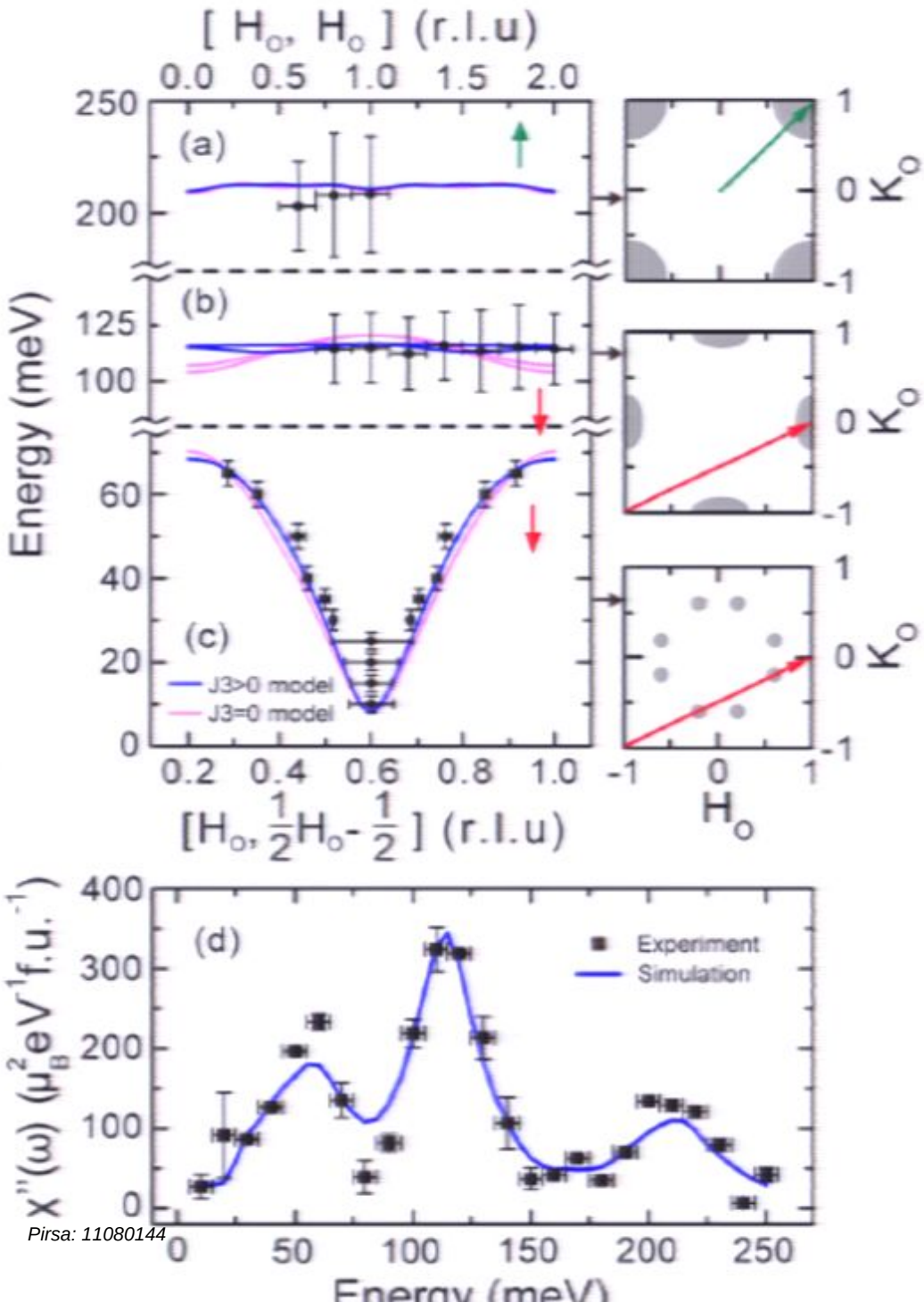


W Biao et al. arXiv:1102.0830 (superconducting sample)

Order parameter square

$T_N \sim 560$ K





Wang et al. arXiv:1105.4675

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Spin wave dispersion

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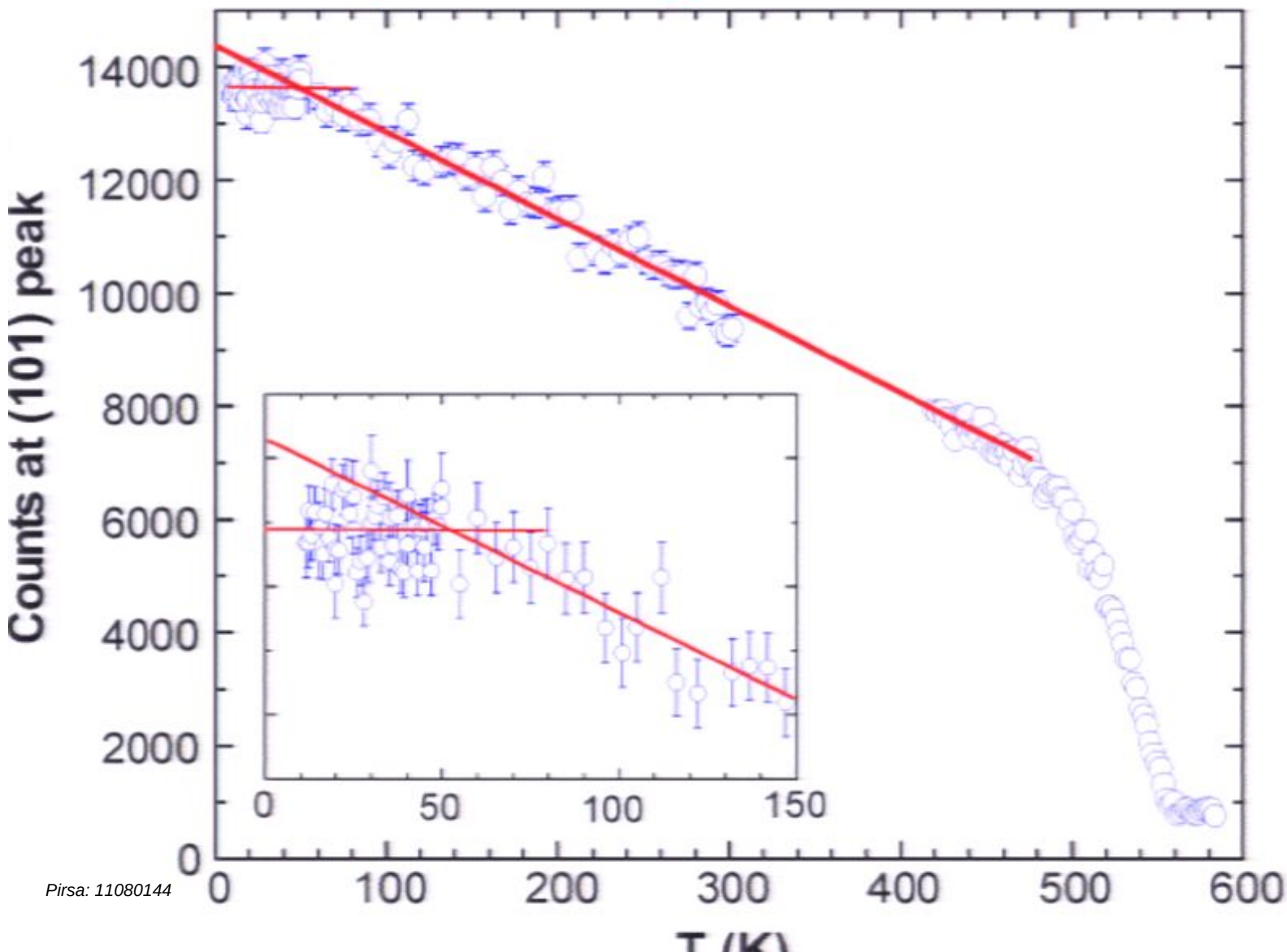

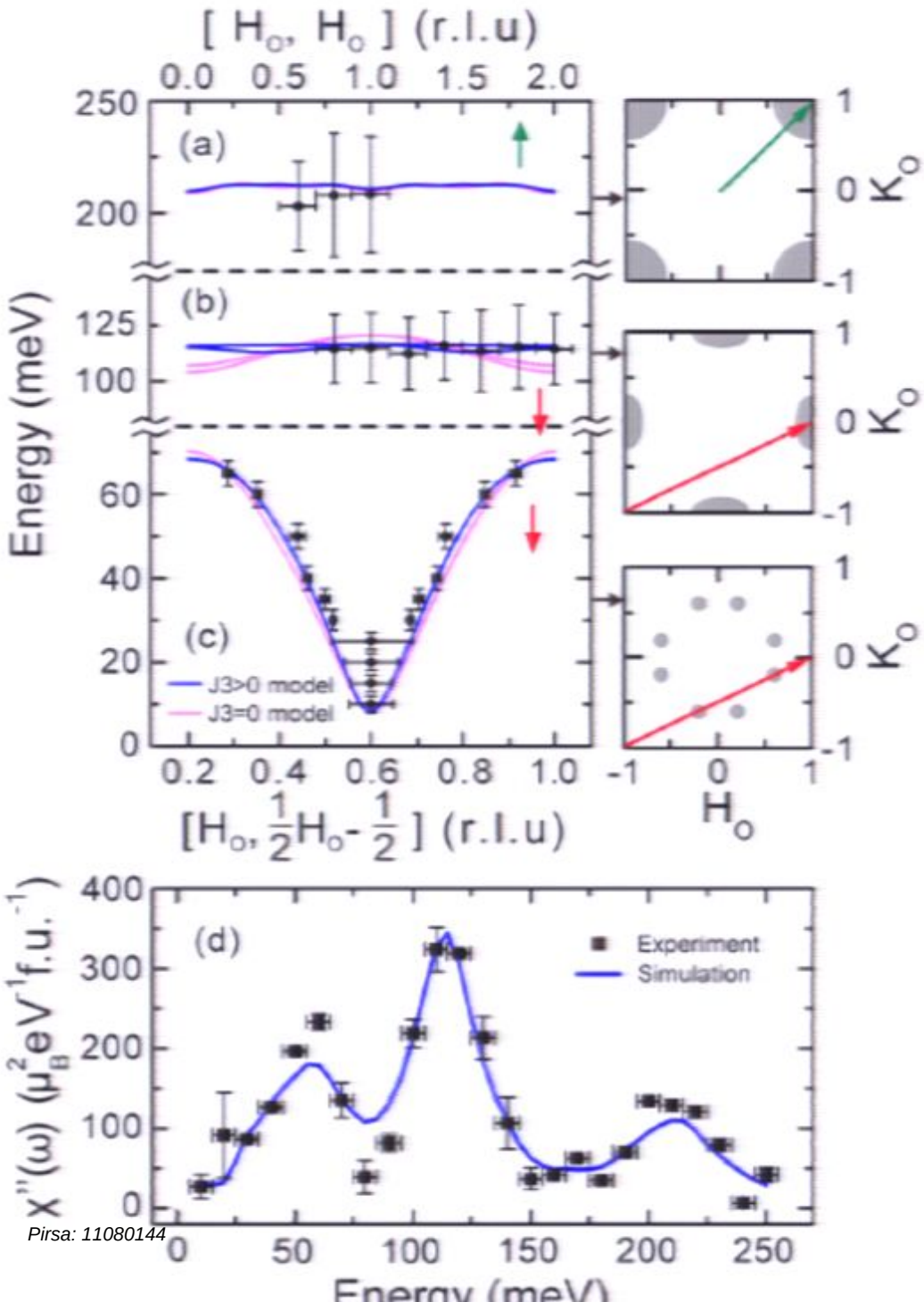

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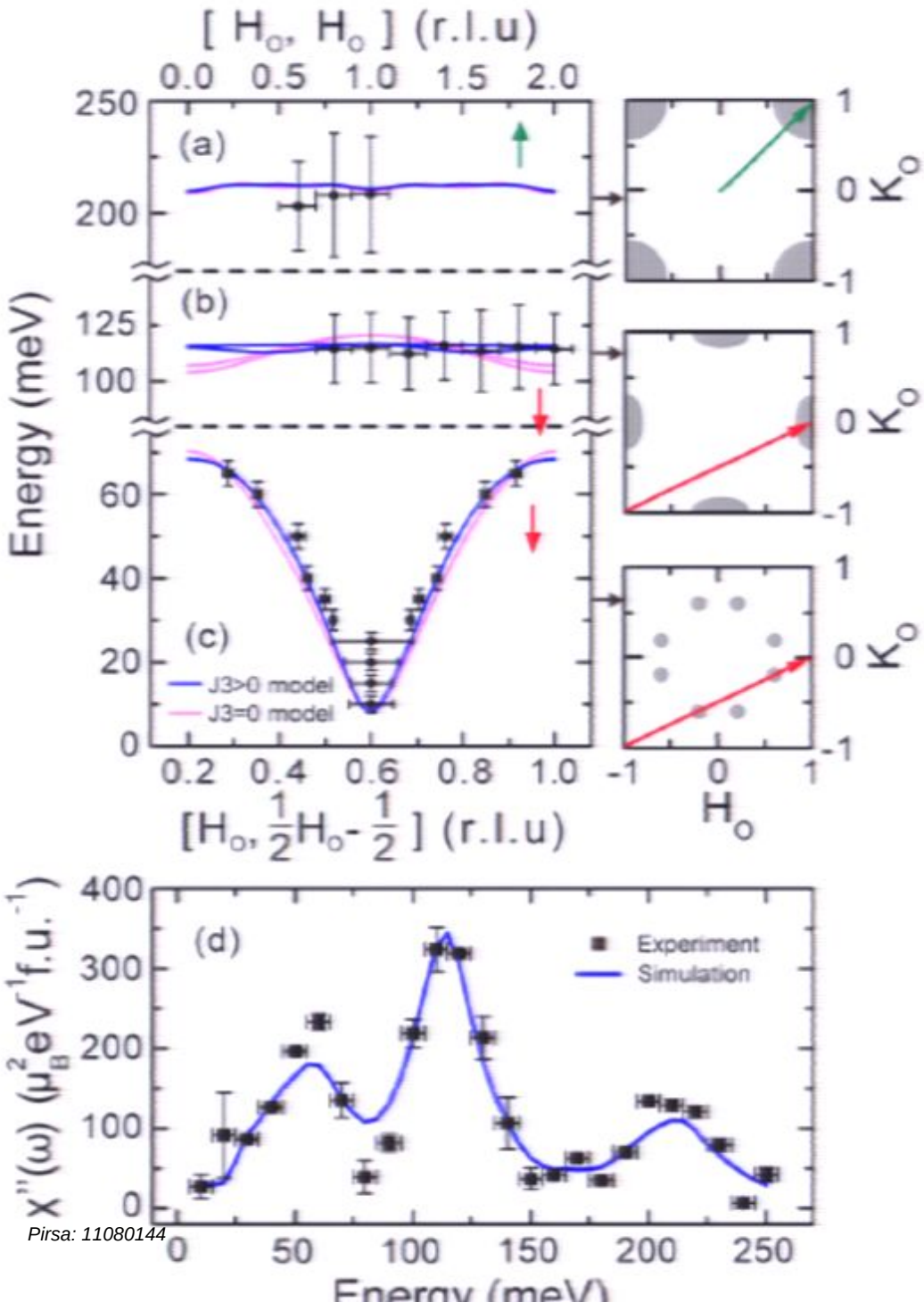

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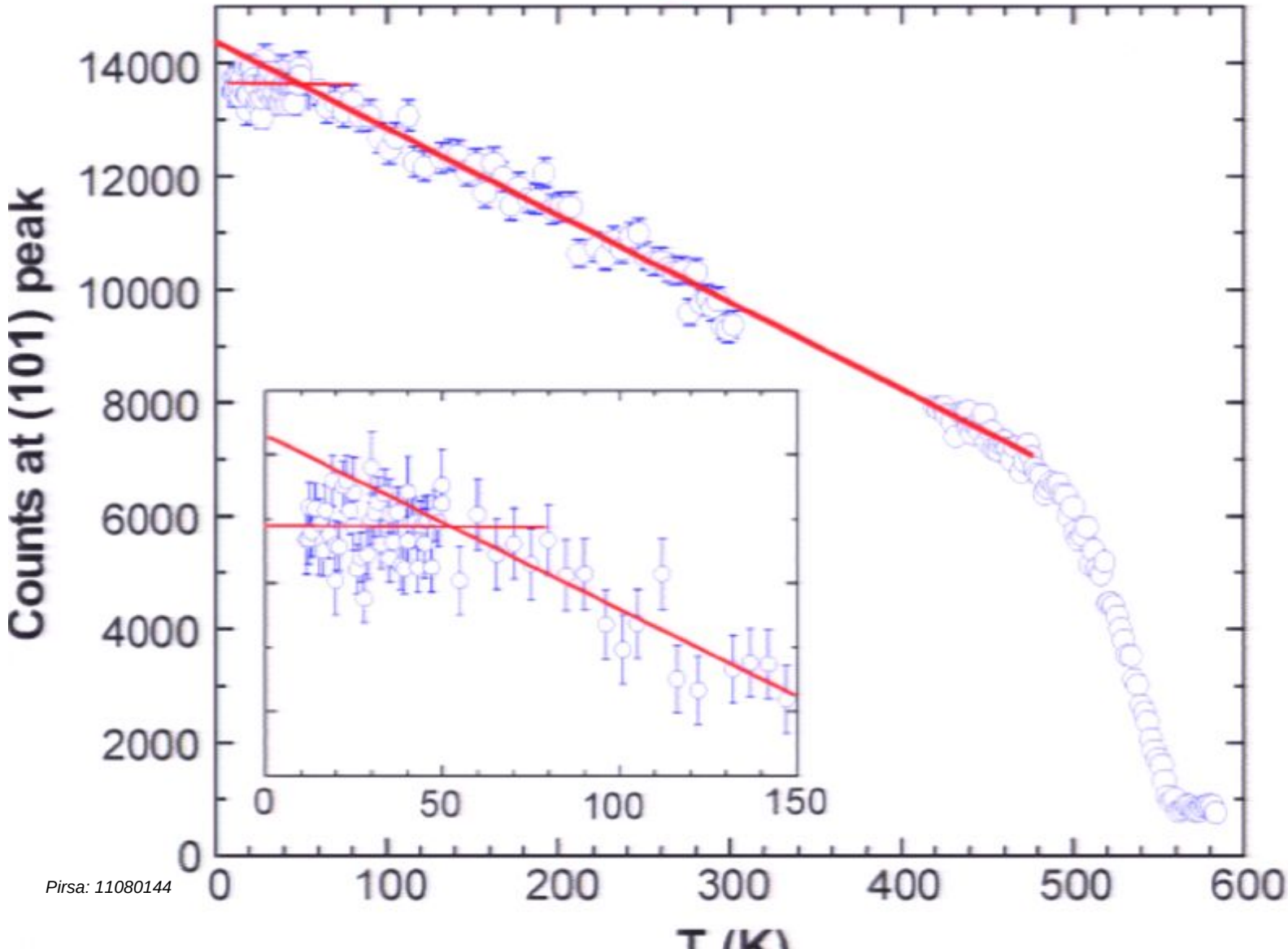
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