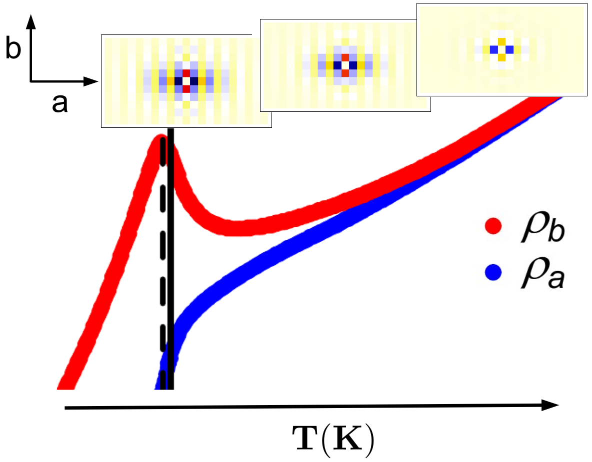
Emergent impurity effects and their observable consequences in Fe-based superconductors

Brian Møller Andersen

Niels Bohr Institute, University of Copenhagen



LUNDBECKFONDEN

Collaborators

Peter J. Hirschfeld

Maria Navarro
Gastiasoro

Talk outline

1) Emergent defect states

- experimental overview (transport, STM).
- model and results; origin and consequences of nematogens.
- new scenario for understanding the resistivity of pnictides.

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- induced magnetic phases and extreme T_c suppression.

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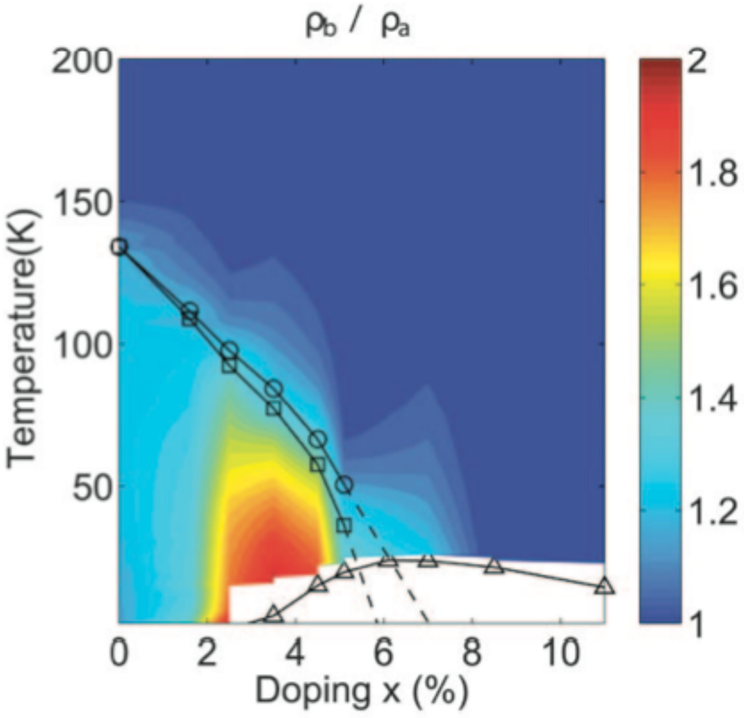
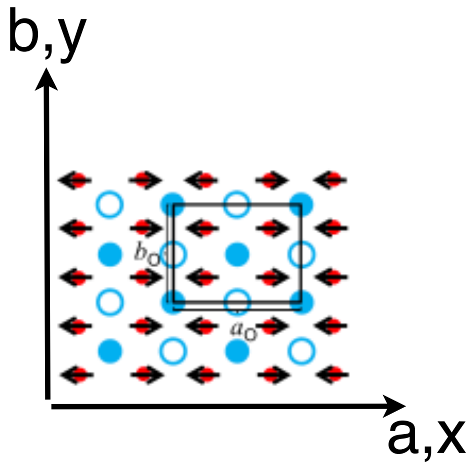
Resistivity anisotropy

Crystal detwinning
allowing transport
anisotropy
measurements





J. Chu et al
Science 2011

NB: Diminishing AF & Orthorhombicity

PRL **110,** 207001 (2013) PHYSICAL REVIEW LETTERS week ending 17 MAY 2013

Anisotropy of the In-Plane Resistivity of Underdoped Ba$(Fe_{1-x}Co_x)_2As_2$ Superconductors Induced by Impurity Scattering in the Antiferromagnetic Orthorhombic Phase

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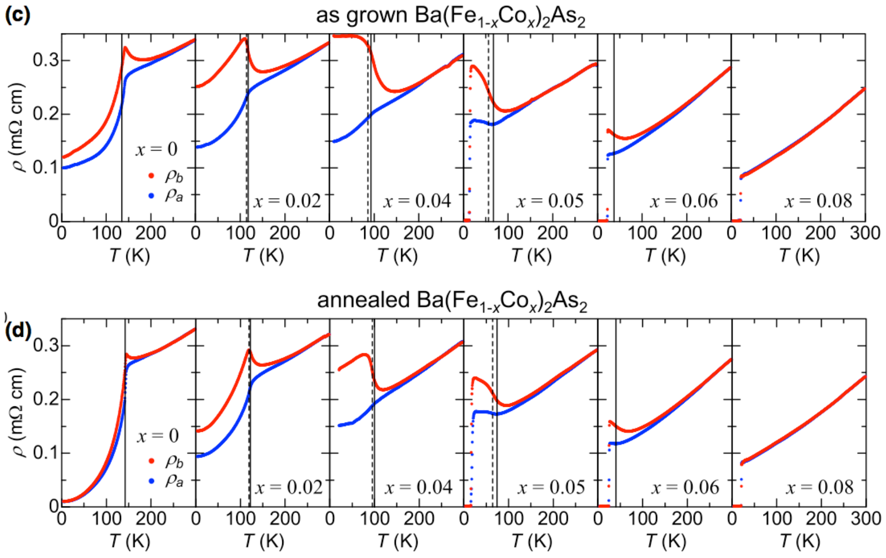

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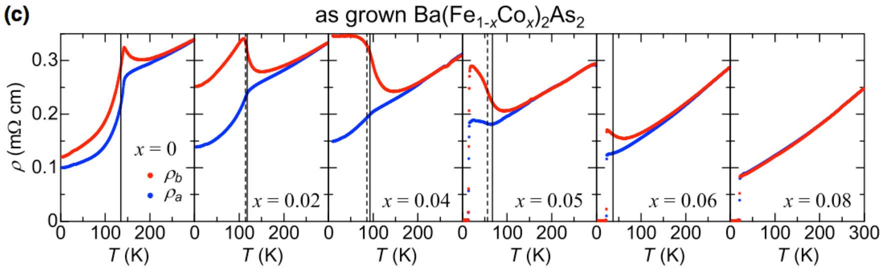

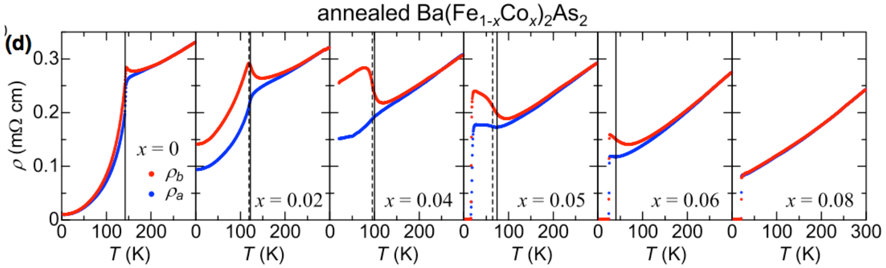

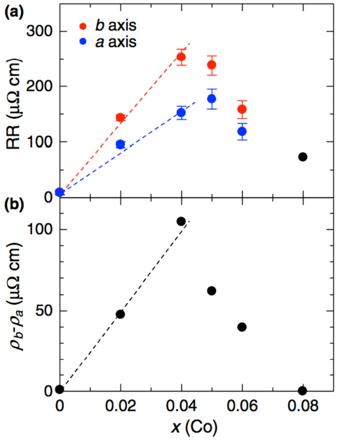

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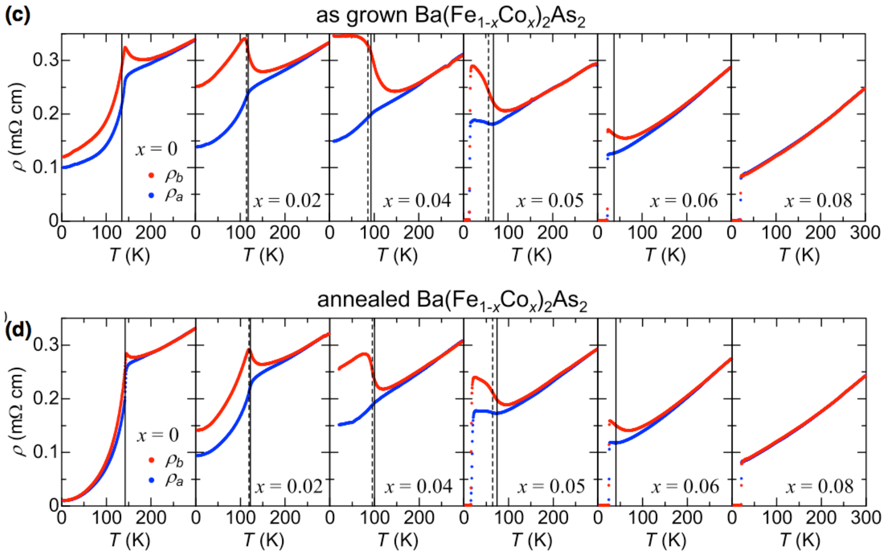
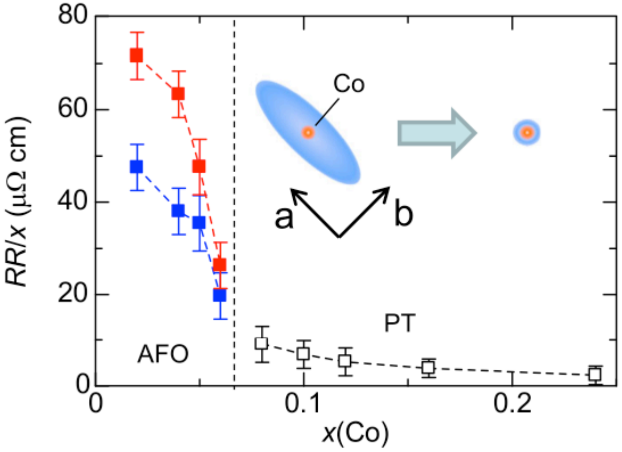


Impurity-induced resistivity anisotropy



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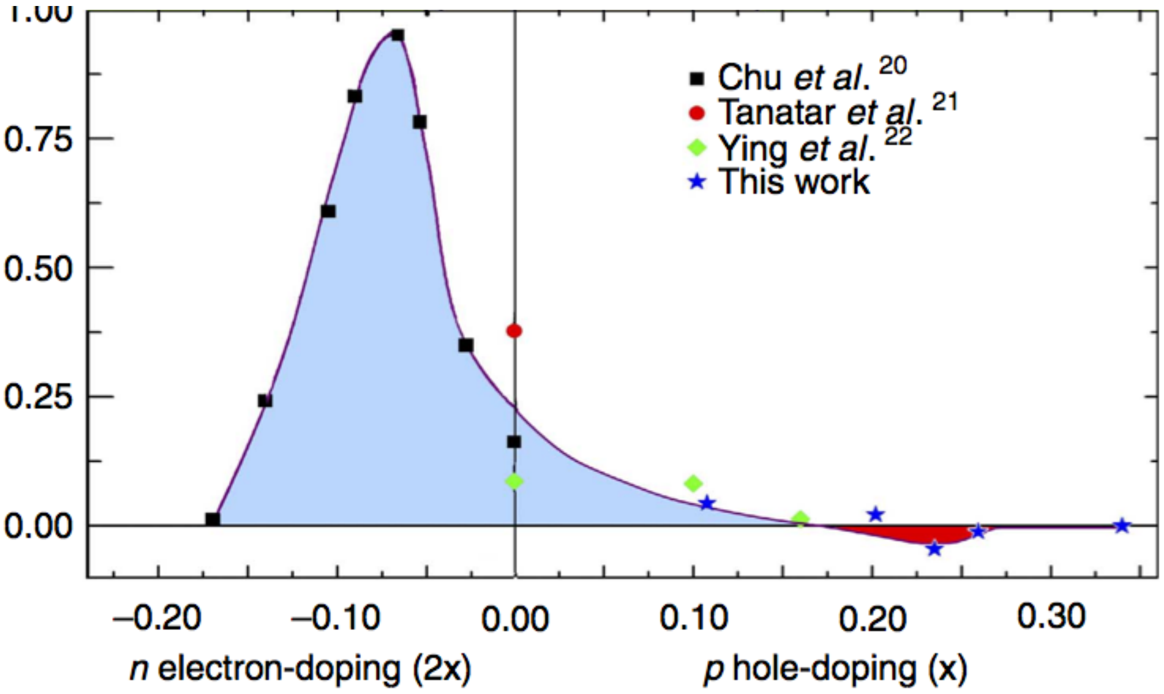
Sign-reversal of the in-plane resistivity anisotropy in hole-doped iron pnictides

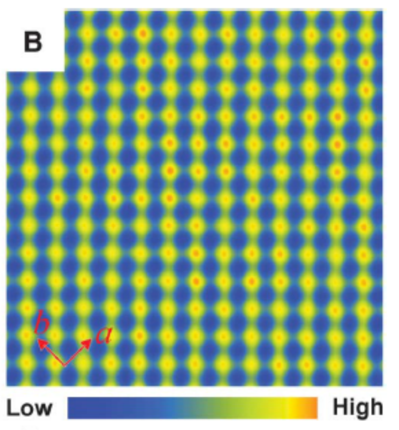
E.C. Blomberg[1,2], M.A. Tanatar[1,2], R.M. Fernandes[3], I.I. Mazin[4], Bing Shen[5,6], Hai-Hu Wen[5,6], M.D. Johannes[4], J. Schmalian[7] & R. Prozorov[1,2]



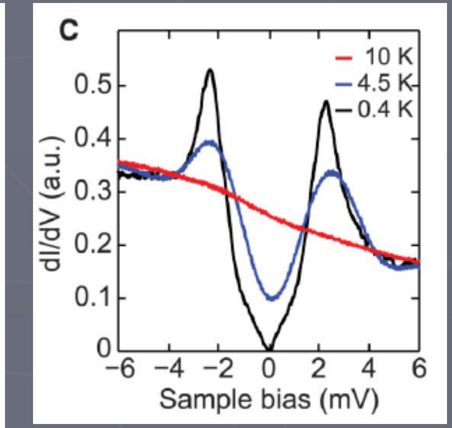
What does the disorder “look like”?

Signatures of electronic nematicity in FeSC
II. STM in SC state

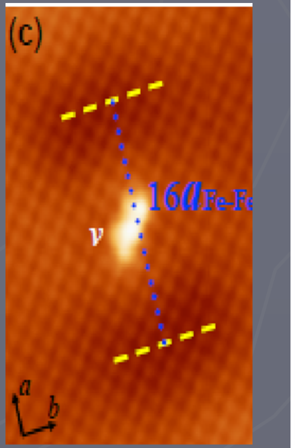
FeSe: CL Song et al, Science 2011, PRL 2012



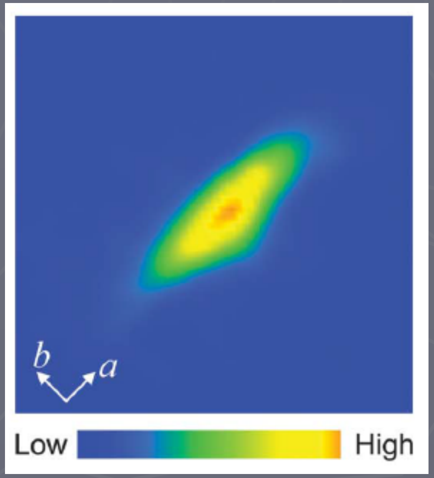
topography



spectrum



defect



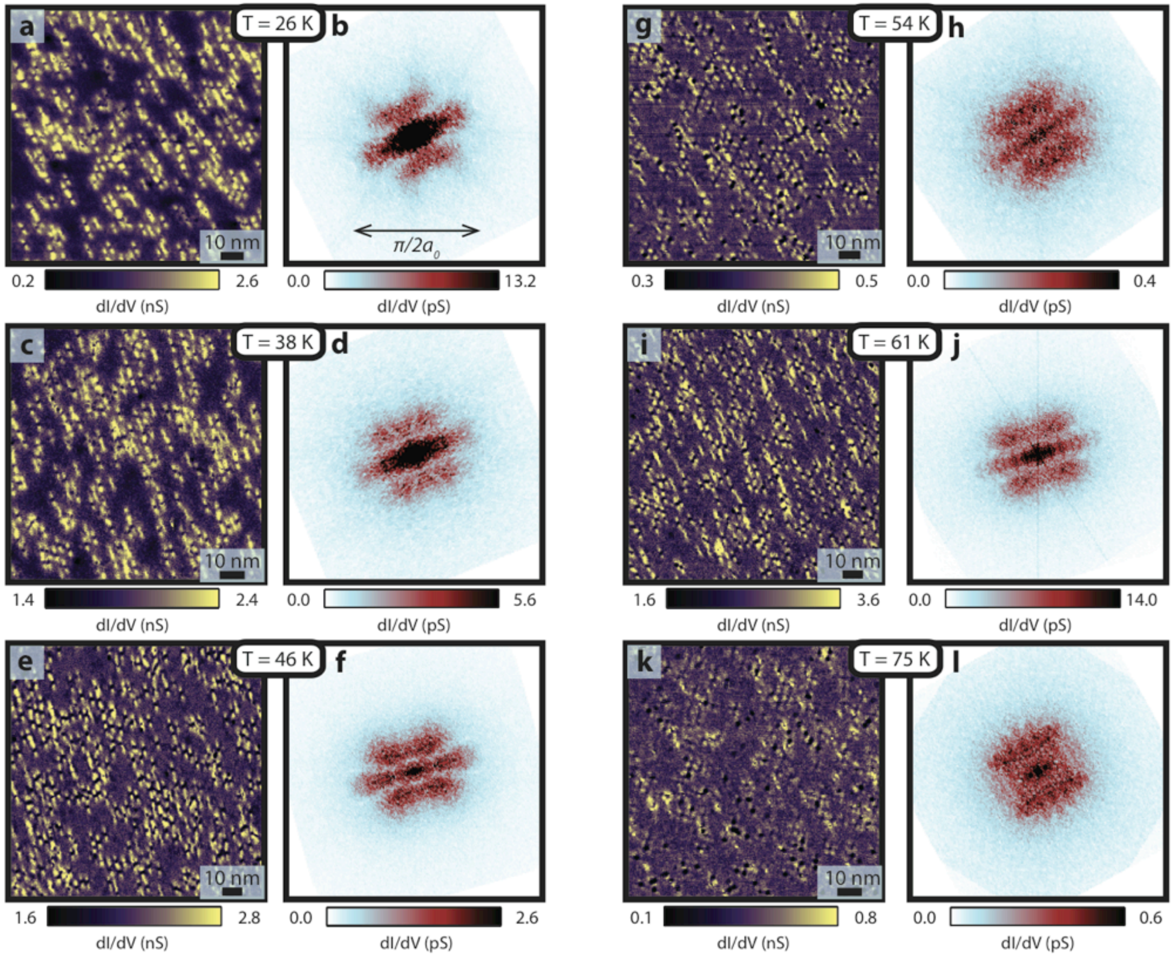
vortex

a and b are only ~0.1% different!   But strong C_4 symmetry breaking in SC state.

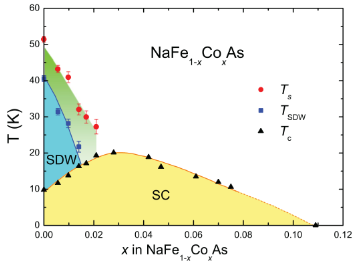
Origin of electronic dimers in the SDW phase

T_N=39K

T_S=54K



E. Rosenthal *et al*, Nat. Phys 2014



Summary of main exp. facts

Challenges for theory:

1) The emergence of strongly C2 symmetric impurity states

2) The counterintuitive sign of the resistivity anisotropy on the electron-doped side, where $\rho_b > \rho_a$ although $b < a$.

3) The decrease of the anisotropy upon annealing.

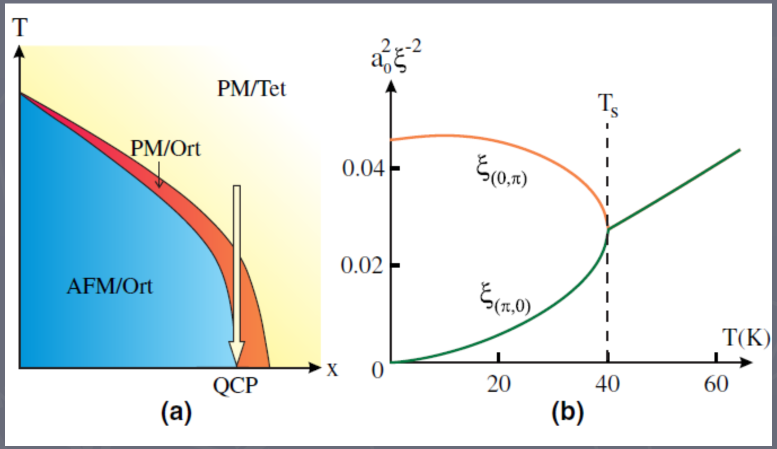
4) The pronounced increase in ρ_b as T_N is approached, with ρ_a remaining metallic like

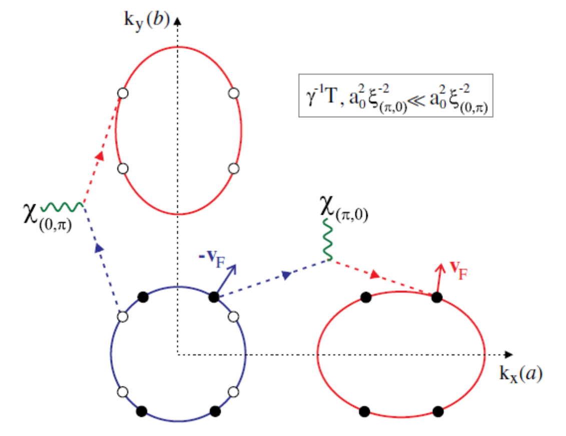
5) The possible sign change but also significant decrease of the anisotropy on the hole-doped side.

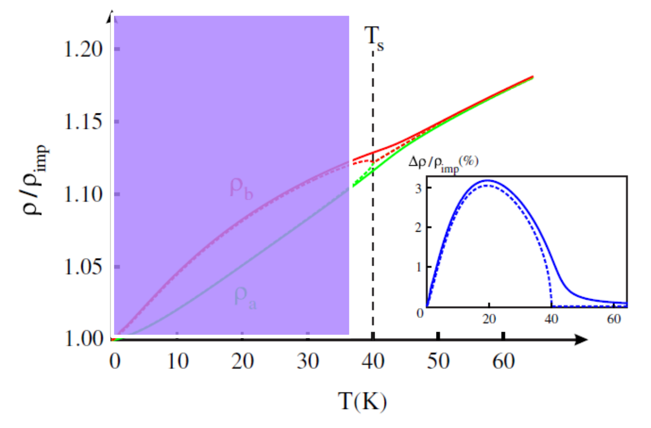
6) The decrease in anisotropy both with increasing T and electron overdoping.

Spin-nematic theory of resistivity anisotropy in nematic phase

Fernandes, Abrahams and Schmalian PRL 2011







Fluctuations in $(\pi,0)$ direction soften at T_s

No description of magnetically ordered phase

Anisotropic AF spin fluctuations

↓

Resistivity anisotropy

Anisotropic AF spin fluctuations

↓

Emergent anisotropic impurity states

↓

Resistivity anisotropy

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Model

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{oo} + \mathcal{H}_{int} + \mathcal{H}_{imp}$$

$$\mathcal{H}_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t_{\mathbf{ij}}^{\mu\nu} c_{\mathbf{i}\mu\sigma}^{\dagger} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu\sigma}$$

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$$\mathcal{H}_{oo} = \frac{\delta}{2} \sum_{\mathbf{i}} \left(n_{\mathbf{i}yz} - n_{\mathbf{i}xz} \right)$$

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$$\mathcal{H}_{oo} = \frac{\delta}{2} \sum\nolimits_{\mathbf{i}} \left(n_{\mathbf{i}yz} - n_{\mathbf{i}xz} \right)$$

$$H_{int} = U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'}$$

$$- 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c^{\dagger}_{\mathbf{i}\mu\sigma} c^{\dagger}_{\mathbf{i}\mu\bar{\sigma}} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma},$$

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$$H_{imp} = \sum_{\mathbf{i}^*\mu\sigma} V_{imp}^{\mu\sigma} c_{\mathbf{i}^*\mu\sigma}^{\dagger} c_{\mathbf{i}^*\mu\sigma},$$

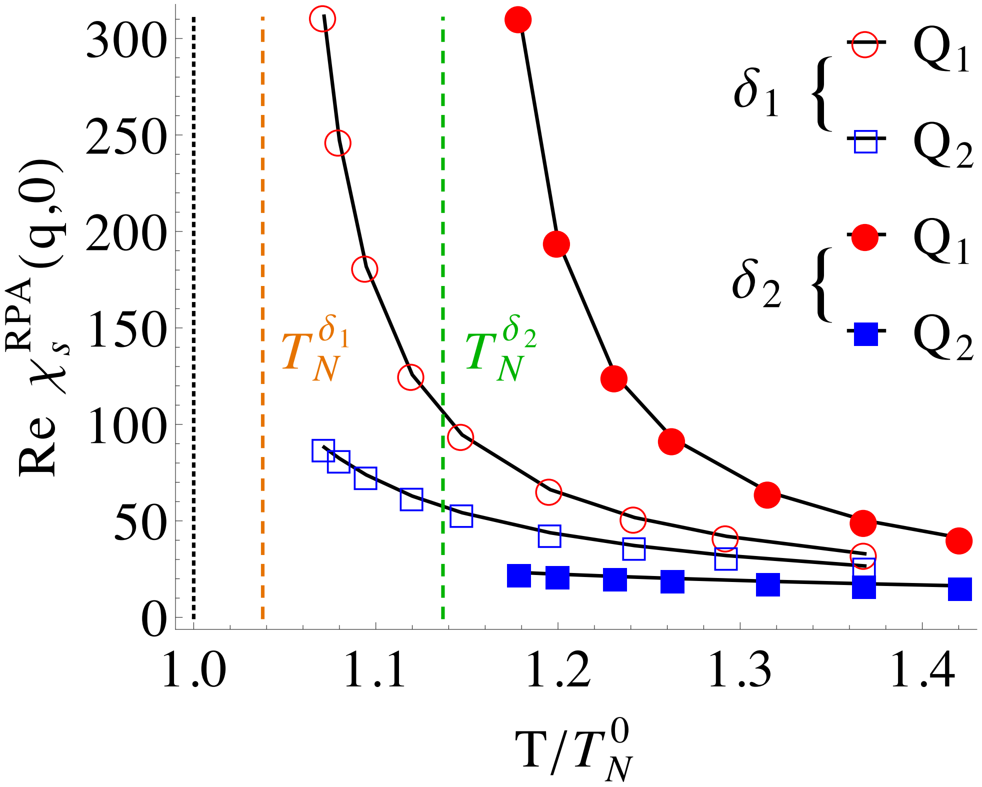
Model

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{oo} + \mathcal{H}_{int} + \mathcal{H}_{imp}$$

$$\Big\downarrow$$

$$\begin{aligned} H^{\mu\nu}_{\mathbf{ij}\sigma} &= t^{\mu\nu}_{\mathbf{ij}} + \delta_{\mathbf{ij}}\delta_{\mu\nu}[-\mu_0 + \delta(\delta_{\mu yz} - \delta_{\mu xz}) + \delta_{\mathbf{ii}^*}V_{imp} \\ &+ U\langle n_{\mathbf{i}\mu\bar{\sigma}}\rangle + \sum_{\mu'\neq\mu}(U'\langle n_{\mathbf{i}\mu'\bar{\sigma}}\rangle + (U'-J)\langle n_{\mathbf{i}\mu'\sigma}\rangle)], \end{aligned}$$

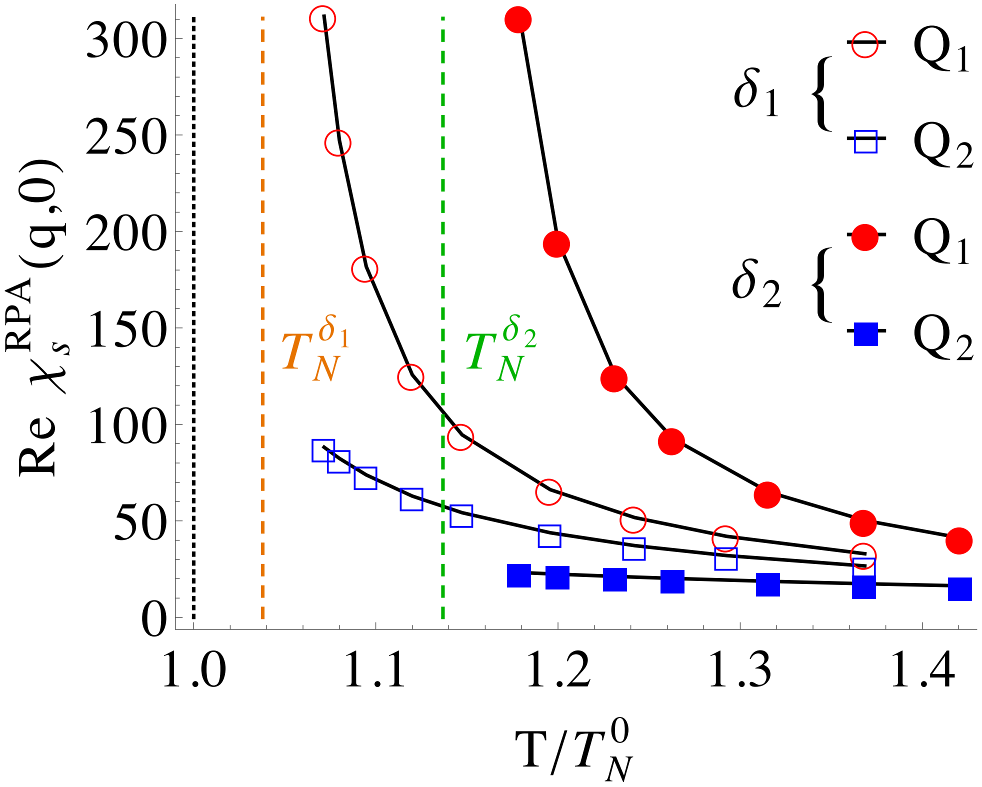
Results

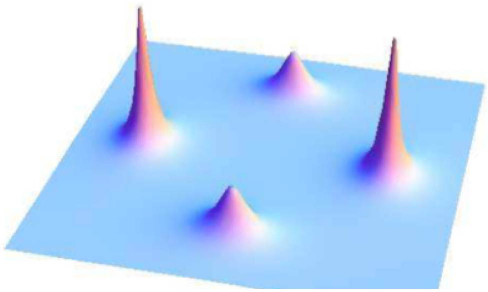


$$\mathcal{H}_{oo} = \frac{\delta}{2} \sum_{\mathbf{i}} \left(n_{\mathbf{i}yz} - n_{\mathbf{i}xz} \right)$$

$$\delta_1 = 16 \text{ meV } (T_N^{\delta_1}) \text{ and } \delta_2 = 80 \text{ meV } (T_N^{\delta_2})$$

Results





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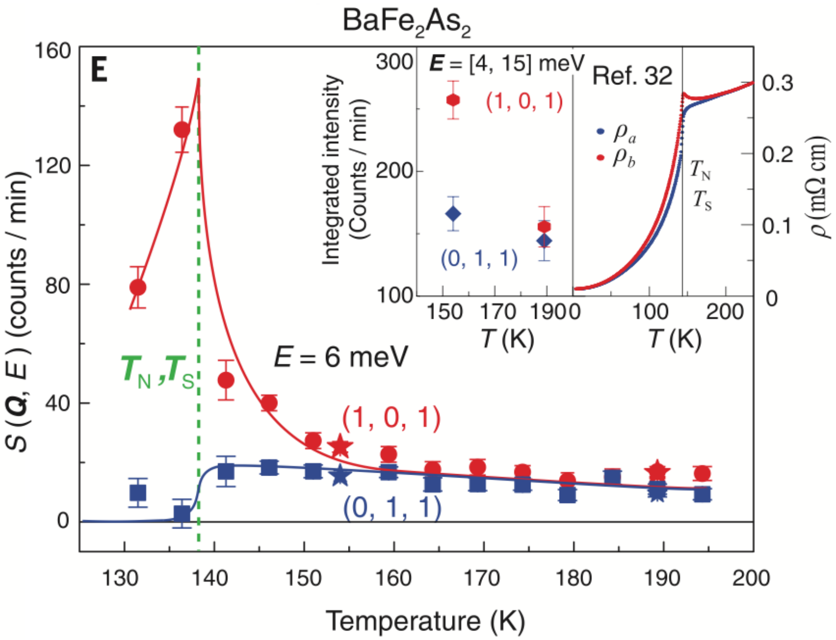
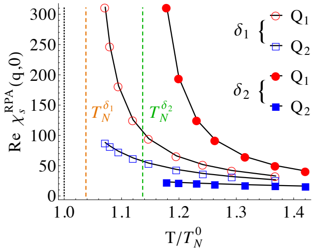
Nematic spin correlations in the tetragonal state of uniaxial-strained $BaFe_{2-x}Ni_xAs_2$

Xingye Lu,[1] J. T. Park,[2] Rui Zhang,[1] Huiqian Luo,[1] Andriy H. Nevidomskyy,[3] Qimiao Si,[3] Pengcheng Dai[3,1*]



X. Lu *et al*
Science 2014

Results: Impurity response

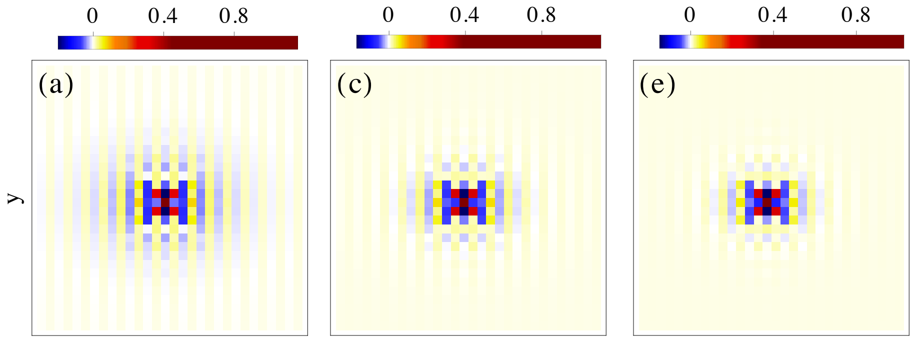


+

$$H_{imp} = \sum_{\mathbf{i}^* \mu\sigma} V_{imp}^{\mu\sigma} c^{\dagger}_{\mathbf{i}^* \mu\sigma} c_{\mathbf{i}^* \mu\sigma},$$

||

$T/T_N^{\delta_2}$ =1.06 (a), 1.14 (c), and 1.23(e).



$\delta_2 = 80$ meV

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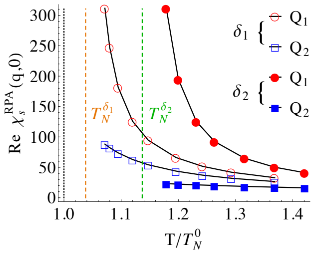

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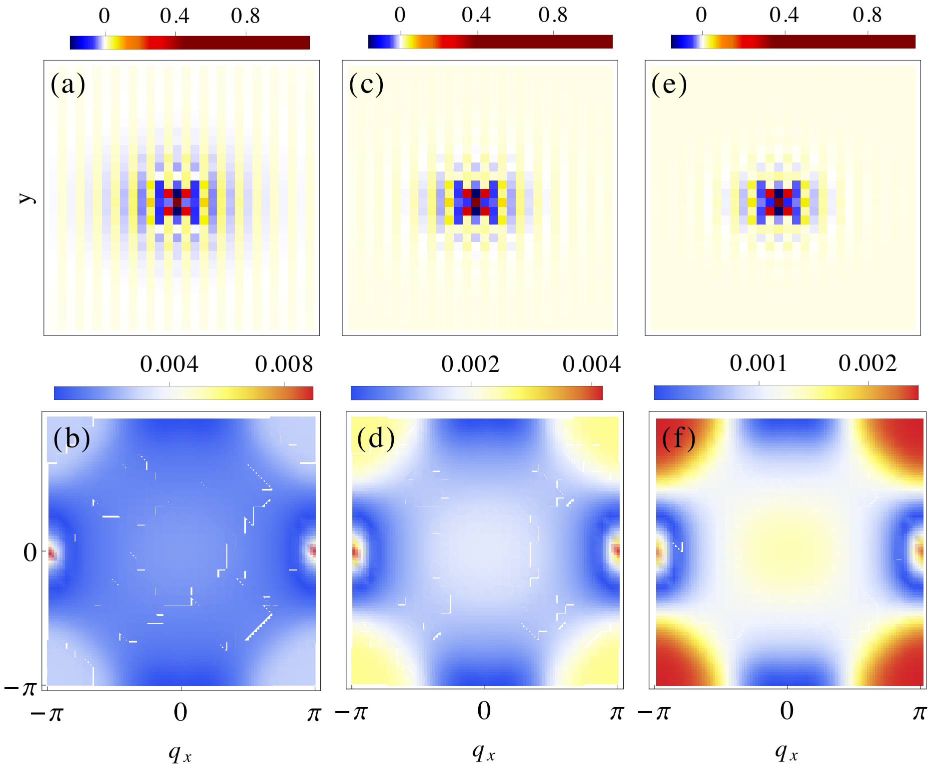

$\delta_2 = 80$ meV

Results: Scattering rate

$$\frac{1}{\tau^{l}_{\mathbf{k}\alpha}} = n_{imp}\frac{2\pi}{\hbar}\frac{1}{V}\sum_{\mathbf{k}'\beta}\left|\mathrm{tr}\left(\hat{\sigma}_l\hat{\mathcal{V}}^{imp}_{\sigma\sigma'}(\mathbf{k}\alpha,\mathbf{k}'\beta)\right)\right|^2\times$$

$$\delta(\epsilon_{\mathbf{k}\alpha}-\epsilon_{\mathbf{k}'\beta})\left(1-\frac{\mathbf{v}^{\alpha}_{F}(\mathbf{k})\cdot\mathbf{v}^{\beta}_{F}(\mathbf{k}')}{|\mathbf{v}^{\alpha}_{F}(\mathbf{k})||\mathbf{v}^{\beta}_{F}(\mathbf{k}')|}\right),$$

where $l=0$ ($l=3$) corresponds to the charge (magnetic) scattering rate and $1/\tau_{\mathbf{k}\alpha}\equiv 1/\tau^{0}_{\mathbf{k}\alpha}+1/\tau^{3}_{\mathbf{k}\alpha}$ is the total scattering rate on band α. The term $\hat{\mathcal{V}}^{imp}_{\sigma\sigma'}(\mathbf{k}\alpha,\mathbf{k}'\beta)\equiv$ $\langle\mathbf{k}'\beta\sigma'|\mathcal{V}^{imp}|\mathbf{k}\alpha\sigma\rangle \equiv \langle\mathbf{k}'\beta\sigma'|\mathcal{H}-\mathcal{H}_{(V_{imp}=0)}|\mathbf{k}\alpha\sigma\rangle$

$$\hat{\mathcal{V}}^{imp}_{\sigma\sigma'}(\mathbf{k}\alpha,\mathbf{k}'\beta)=\sum_{\mu\nu}a^{\alpha *}_{\mathbf{k}\mu}\omega^{\mu\nu}_{\mathbf{k}\sigma\mathbf{k}'\sigma'}a^{\beta}_{\mathbf{k}'\nu}-\epsilon_{\mathbf{k}\alpha}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\alpha\beta}$$

$$\omega^{\mu\nu}_{\mathbf{k}\sigma\mathbf{k}'\sigma'} = \tfrac{1}{N}\textstyle\sum_n\sum_{\mathbf{ij}}u^{n*}_{\mathbf{j}\nu\sigma'}u^{n}_{\mathbf{i}\mu\sigma}E_{n\sigma}e^{-i\mathbf{k}'\mathbf{r_j}}e^{i\mathbf{k}\mathbf{r_i}}$$

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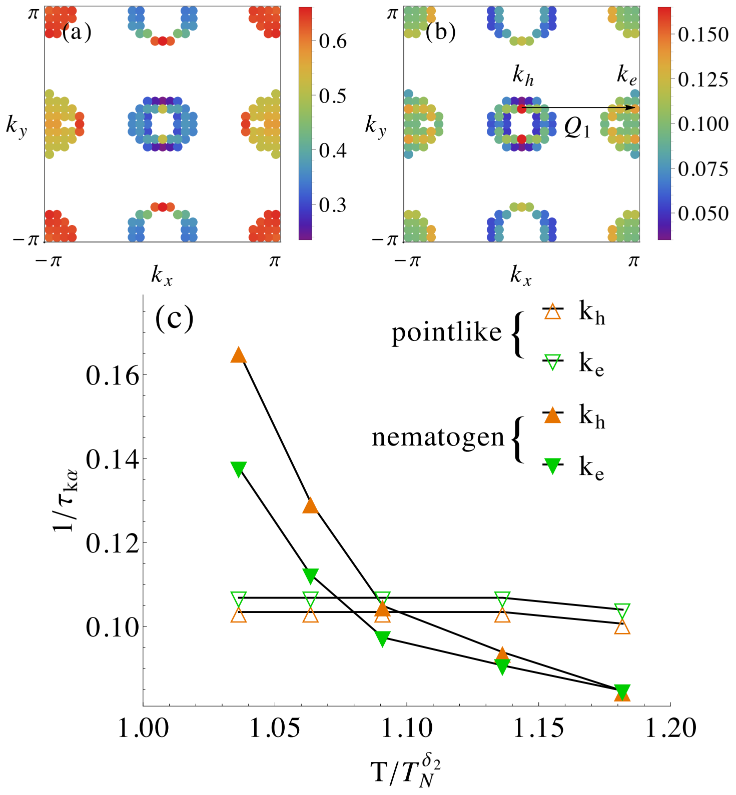

$$T/T_N^{\delta_2} = 1.036.$$

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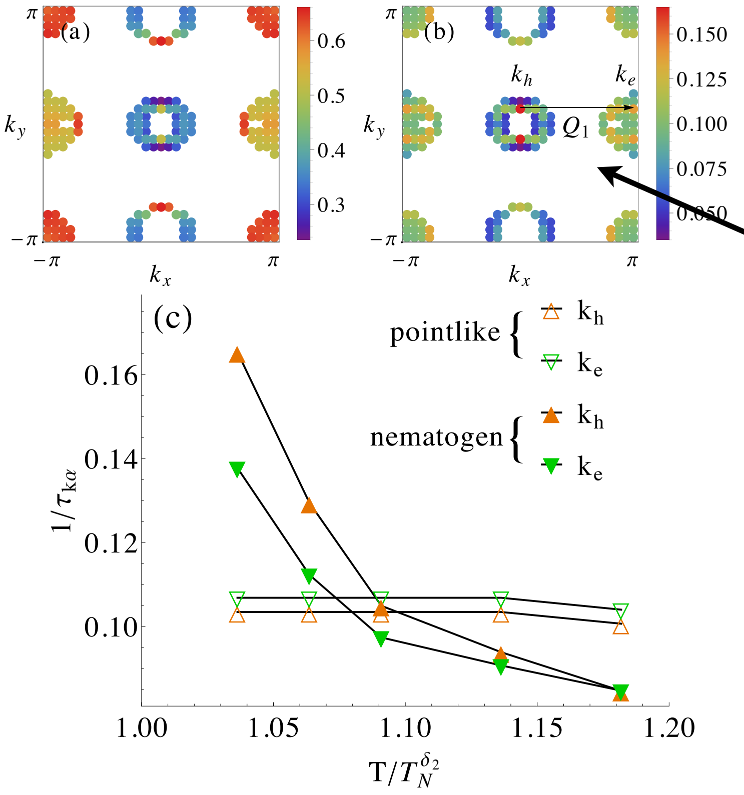
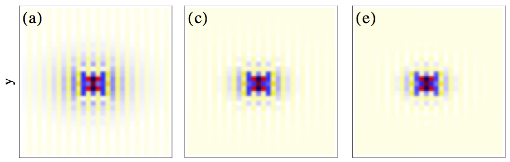
$$\delta(\epsilon_{\mathbf{k}\alpha}-\epsilon_{\mathbf{k}'\beta})\left(1-\frac{\mathbf{v}^{\alpha}_{F}(\mathbf{k})\cdot\mathbf{v}^{\beta}_{F}(\mathbf{k}')}{|\mathbf{v}^{\alpha}_{F}(\mathbf{k})||\mathbf{v}^{\beta}_{F}(\mathbf{k}')|}\right),$$



$$T/T_N^{\delta_2} = 1.036.$$

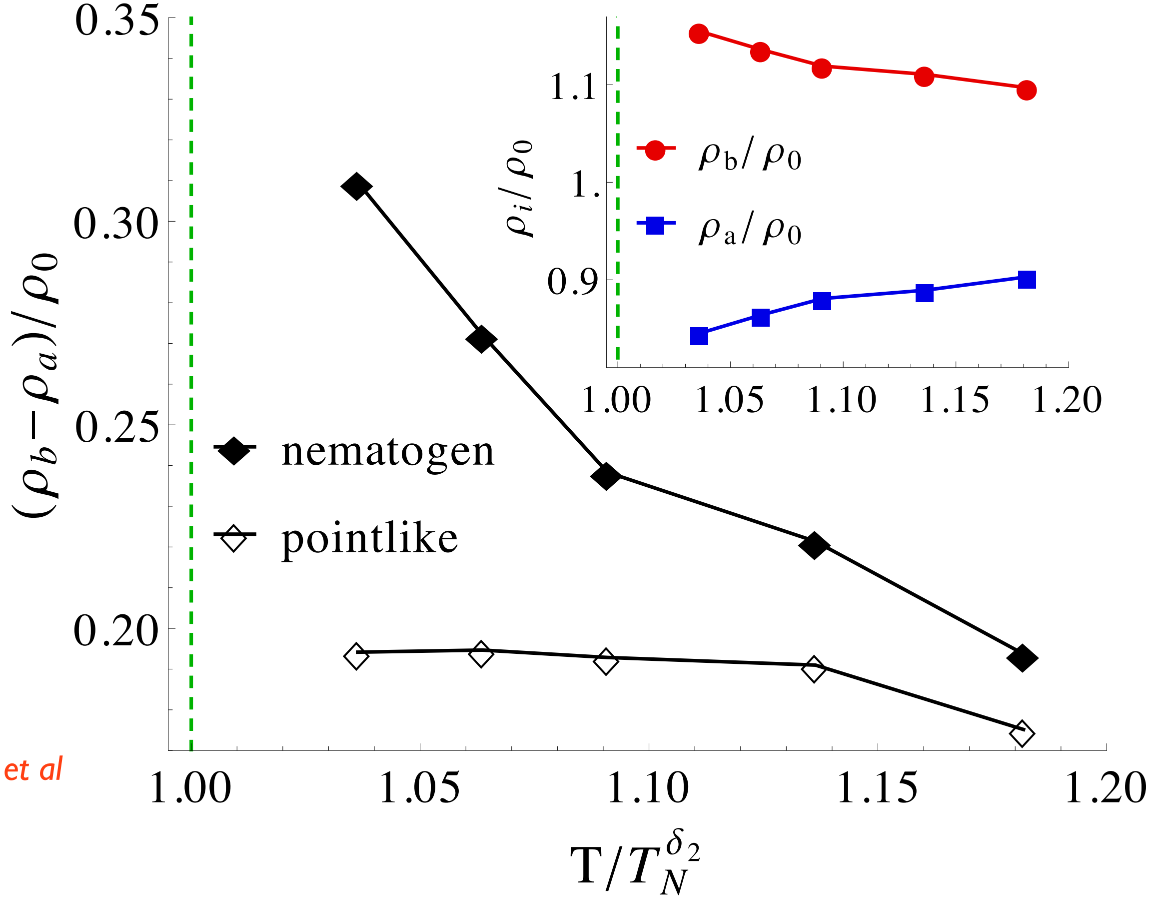
$\hat{\mathcal{V}}^{imp}_{\sigma\sigma'}(\mathbf{k}\alpha,\mathbf{k}'\beta) = \hat{\sigma}_0 V_{imp}\sum_{\mu} a^{\alpha *}_{\mathbf{k}\mu}a^{\beta}_{\mathbf{k}'\mu}$



M. N. Gastiasoro *et al*
PRL 2014

Results: Transport

$$\sigma_{ij} = e^2 \frac{1}{V} \sum_{\mathbf{k}\alpha} \mathbf{v}_i^\alpha(\mathbf{k}) \mathbf{v}_j^\alpha(\mathbf{k}) \tau(\epsilon_{\mathbf{k}\alpha}) \left(-\frac{\partial f}{\partial \epsilon_{\mathbf{k}\alpha}} \right)$$



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PRL **110,** 207001 (2013) PHYSICAL REVIEW LETTERS week ending 17 MAY 2013

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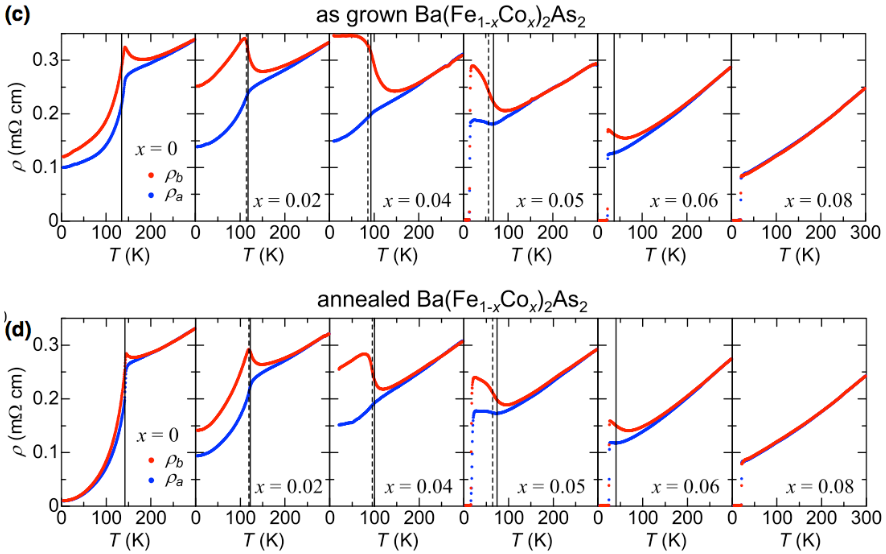
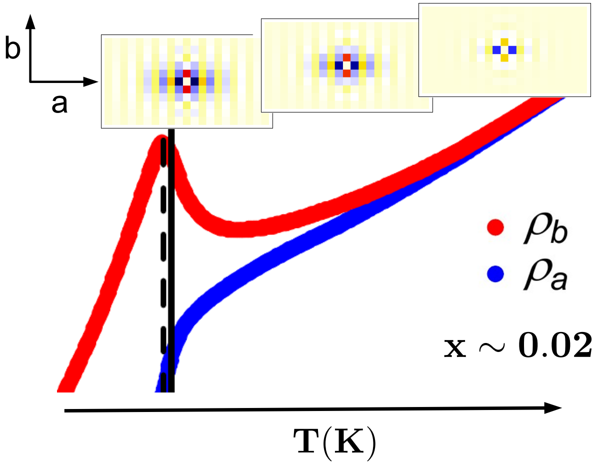
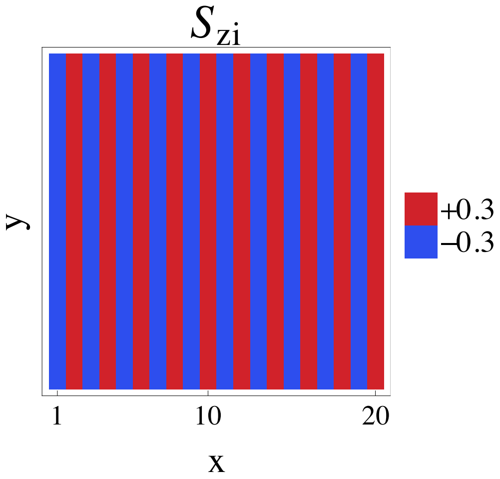




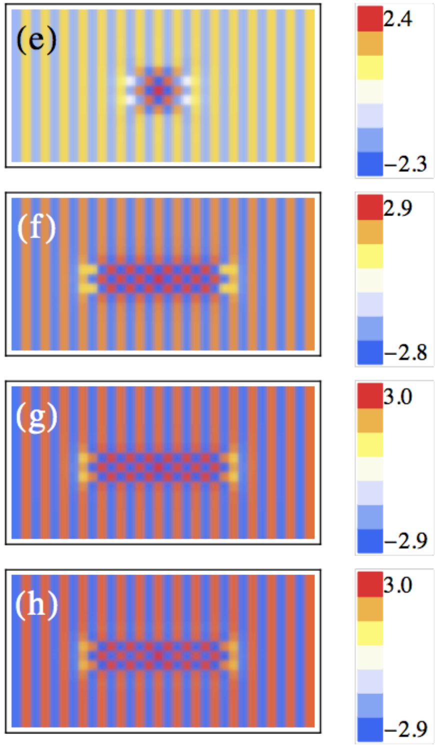
What happens to nematogens at $T<T_N$?

What do point-like impurities actually do in the SDW phase?



Origin of electronic dimers in the SDW phase

Cooling down



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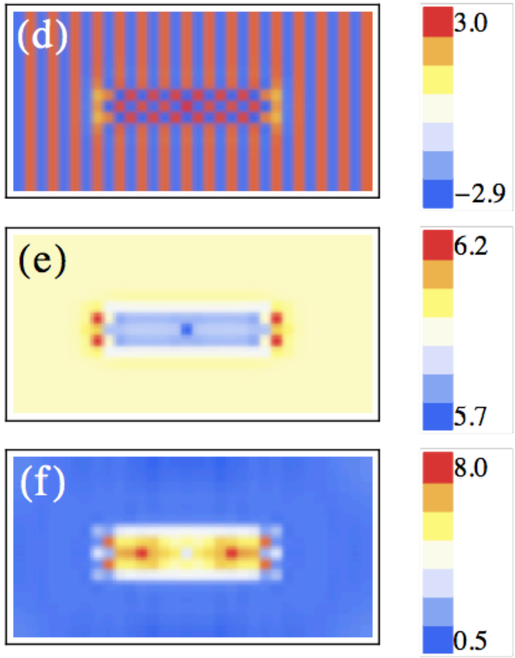


magnetization

(pi,pi) order
below T_N
(neutrons)

density

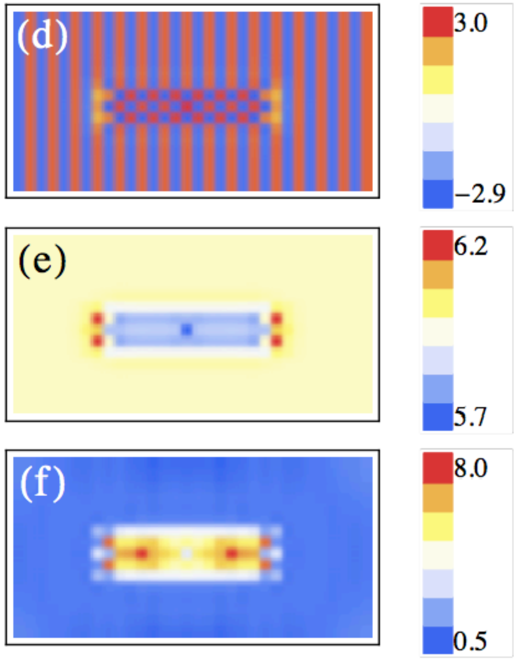
strong, anisotropic
charge potential
(transport)

LDOS

Electronic dimer
(STM)

$$I(\mathbf{r}, -37\ \text{meV}) = \int_0^{E\approx -37\ \text{meV}} g(\mathbf{r},\omega)\, d\omega$$

Origin of electronic dimers in the SDW phase



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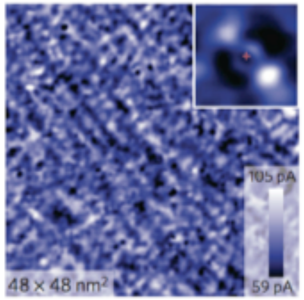


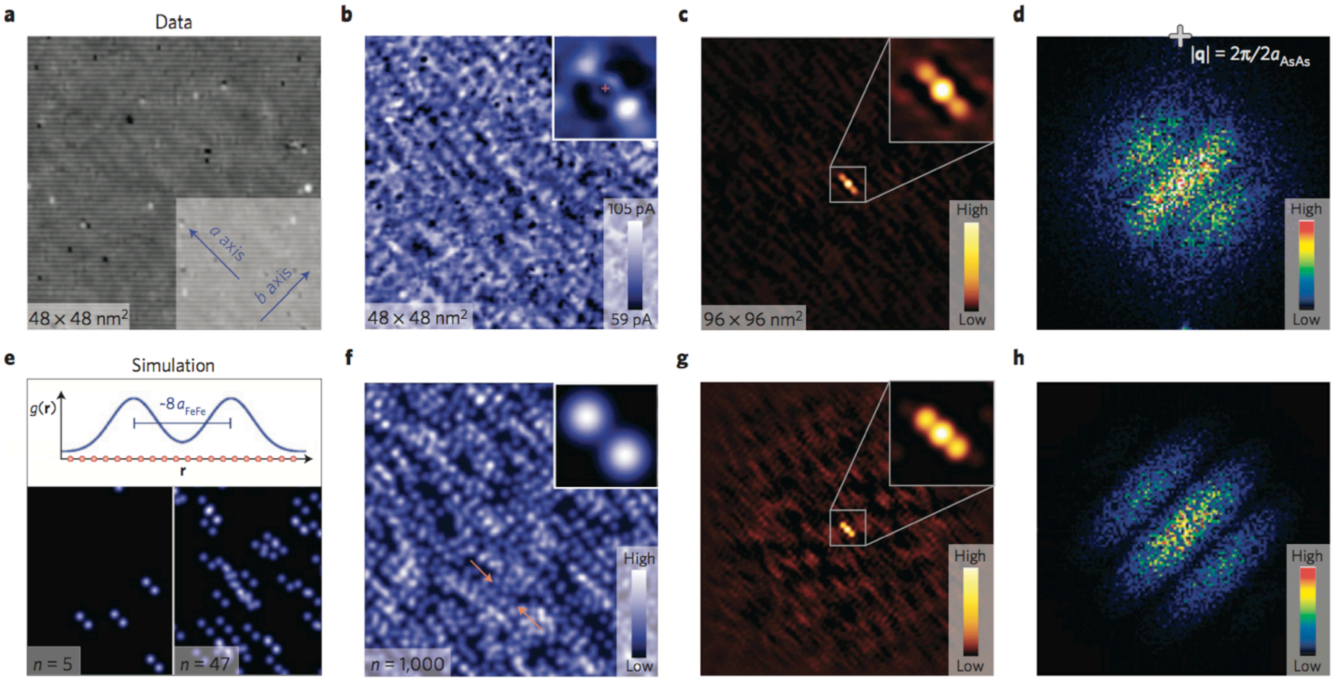
Electronic dimer
(STM)

M. Gastiasoro, P. J. Hirschfeld, BMA,
Phys. Rev. B(R) 89, 100502 (2014)

LETTERS
PUBLISHED ONLINE: 17 FEBRUARY 2013 | DOI: 10.1038/NPHYS2544
nature physics

Anisotropic impurity states, quasiparticle scattering and nematic transport in underdoped $Ca(Fe_{1-x}Co_x)_2As_2$

M. P. Allan[1,2,3], T-M. Chuang[2,3,4,5], F. Massee[2,3,6], Yang Xie[2], Ni Ni[7,8], S. L. Bud'ko[7,8], G. S. Boebinger[5], Q. Wang[9], D. S. Dessau[9], P. C. Canfield[7,8], M. S. Golden[6] and J. C. Davis[2,3,10,11]*



$$I(\mathbf{r}, -37\ \text{meV}) = \int_0^{E\approx -37\ \text{meV}} g(\mathbf{r}, \omega)\, d\omega$$

Talk outline

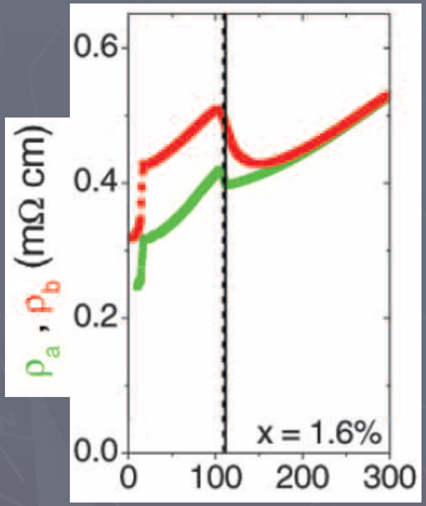
1) Emergent defect states

- experimental overview (transport, STM).
- model and results; origin and consequences of nematogens.
- ➡ scenario for understanding the resistivity of pnictides.

2) Impurity-induced long-range ordered phases

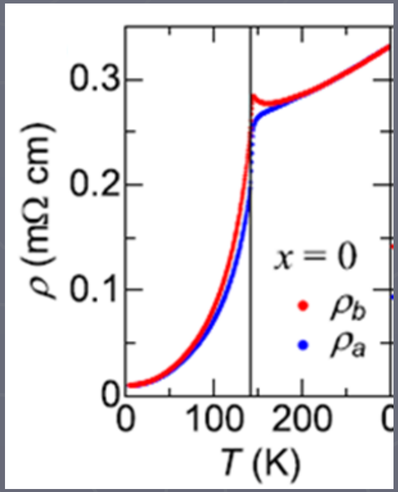
- experimental overview (X-rays, neutron, muSR).
- model and results; origin and consequences of unusual “RKKY” exchange couplings.
- induced magnetic phases and extreme T_c suppression.

Nematogens automatically give correct sign, annealing dependence of transport anisotropy

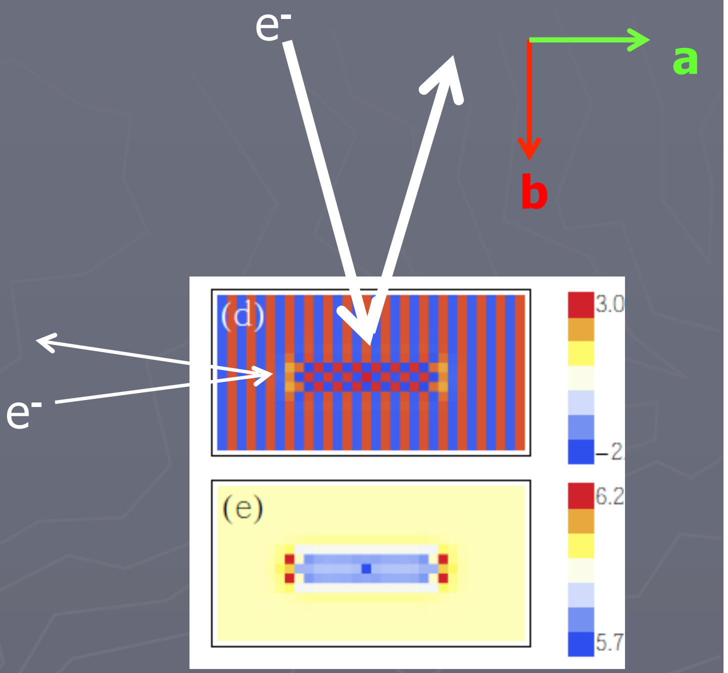


Chu et al, Science (2010)
Tanatar et al, PRB (2010)

annealed!



Ishida et al 2013



- Maximum resistivity in ferromagnetic direction
- Disappearance of anisotropy when parent compound is annealed

Anomalous effect of Lifshitz transitions on DC transport in magnetic phases of Fe-based superconductors

Y. Wang,[1] Maria N. Gastiasoro,[2] Brian M. Andersen,[2] Indranil Paul,[3] and P. J. Hirschfeld[1]
[1] *Department of Physics, University of Florida, Gainesville, Florida 32611, USA*
[2] *Niels Bohr Institute, University of Copenhagen,*
Universitetsparken 5, DK-2100 Copenhagen, Denmark
[3] *Laboratoire Matériaux et Phénomènes Quantiques,*
Université Paris Diderot-Paris VII & CNRS, UMR 7162, 75205 Paris, France

ArXiv:1408.1933

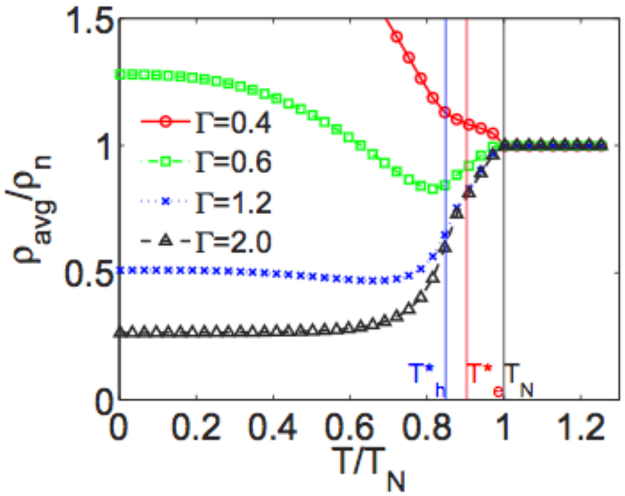
$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_f + \mathcal{H}_{\rm SDW} + \mathcal{H}_{imp}.$$

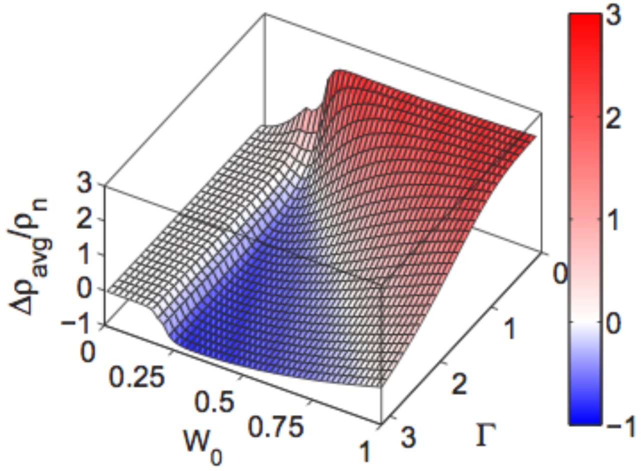
$$\mathcal{H}_{\rm SDW} = \sum_{\mathbf{k},\sigma} \sigma W c^{\dagger}_{\mathbf{k},\sigma} f_{\mathbf{k}+\mathbf{Q},\sigma}$$

$$\mathcal{H}_{imp} = \sum_{\mathbf{k},\mathbf{q},\sigma} V_{\mathbf{q}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} + (c \to f),$$

$$W = W_0 \tanh(2\sqrt{T_N/T - 1}) \text{ for } T \leq T_N,$$

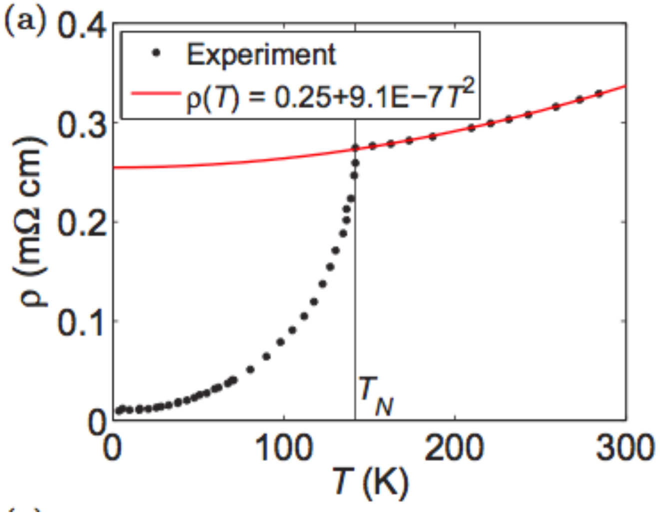
$$V_{\mathbf{q}} = V_0 + V_1(1 + 2\cos q_x),$$





$$\Delta\rho_{avg} \equiv \rho_{avg}(T = 0) - \rho_{avg}(T = T_N)$$

Impurity scattering dominates



$$\rho_{avg} = A + BT^2$$

$$A \gg BT_N^2$$

Anomalous effect of Lifshitz transitions on DC transport in magnetic phases of Fe-based superconductors

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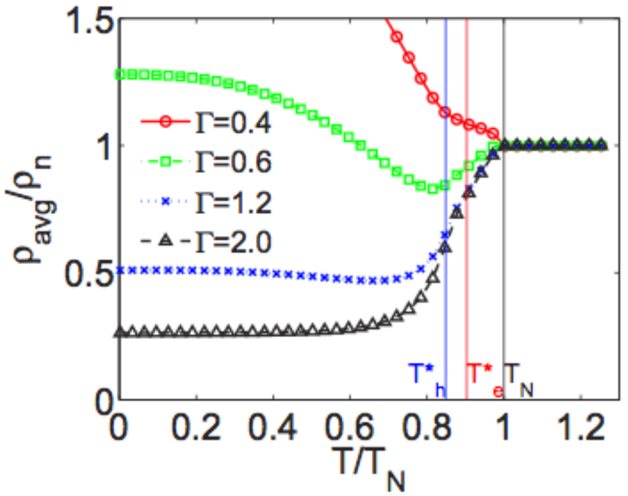

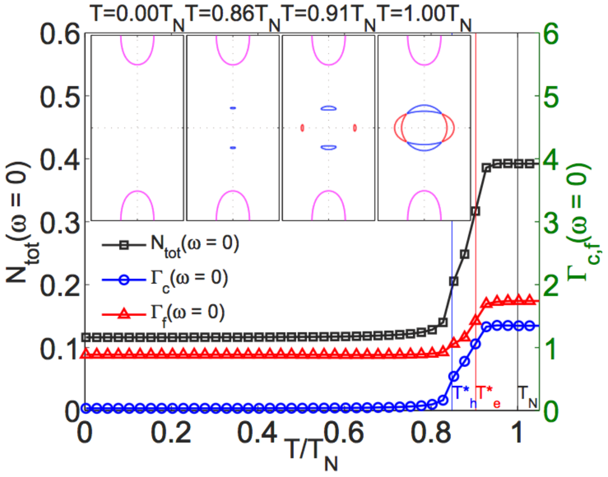

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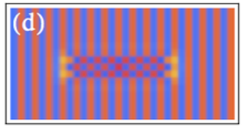
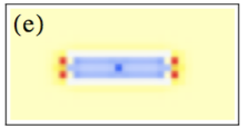
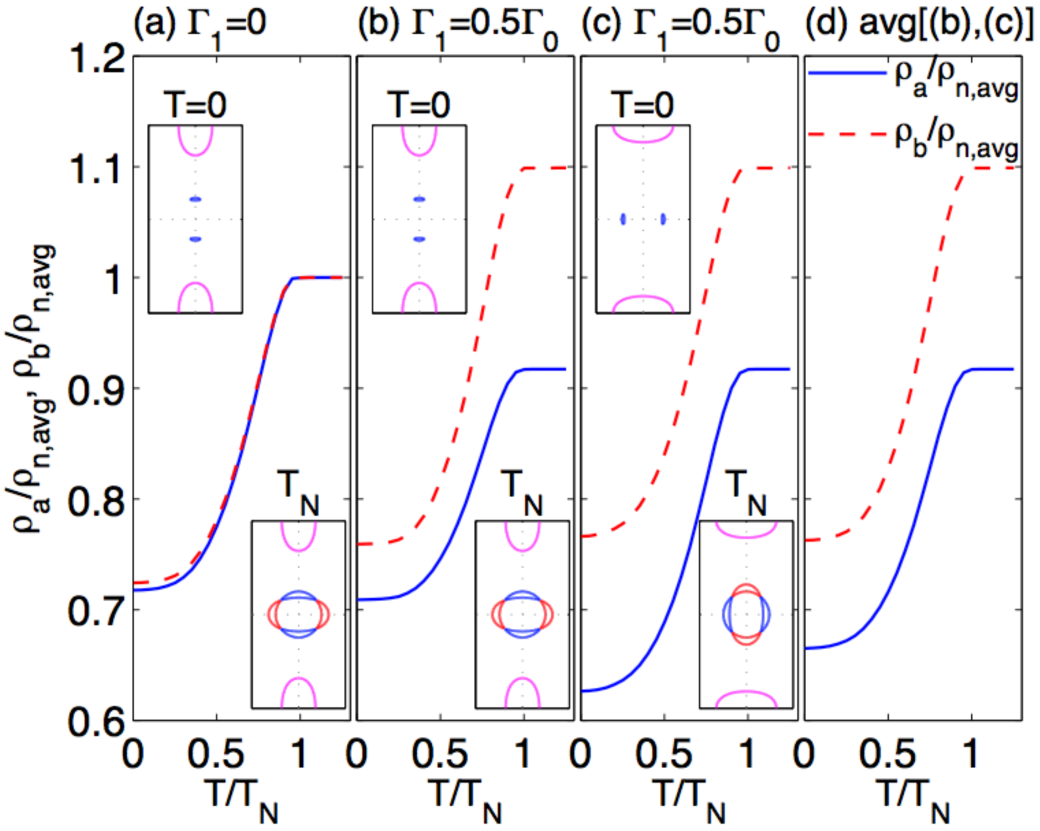
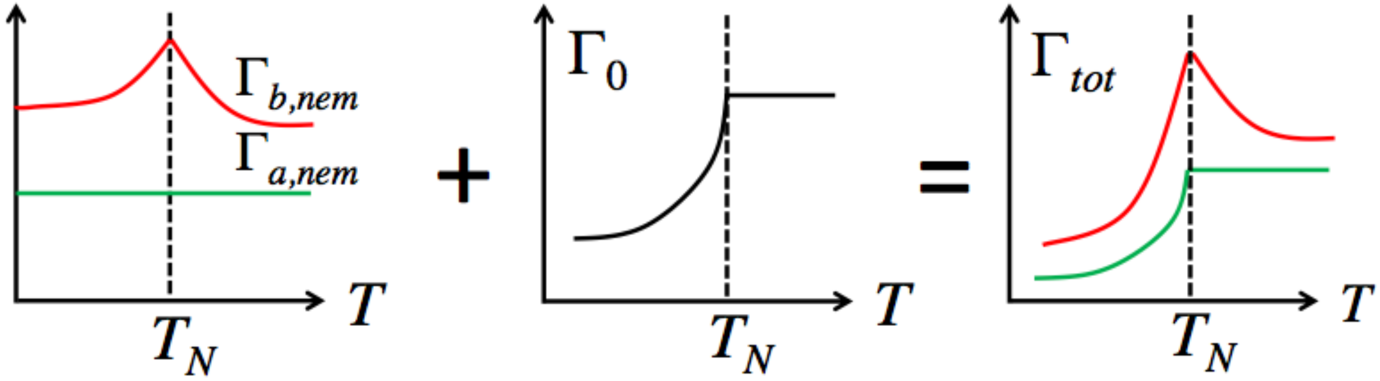






Summary T-dependence



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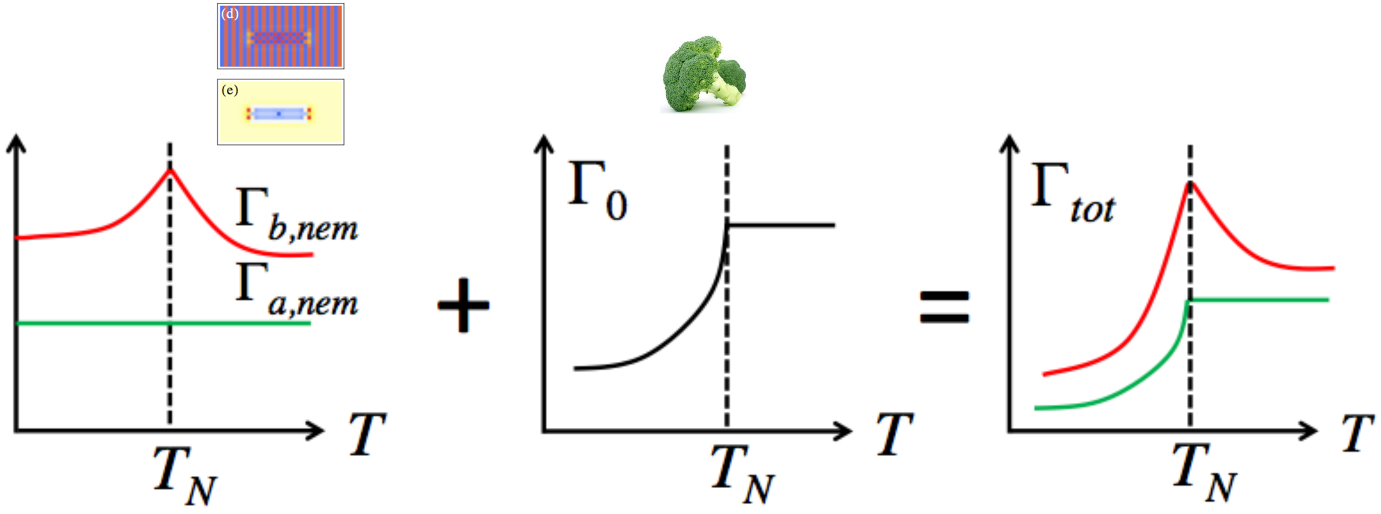

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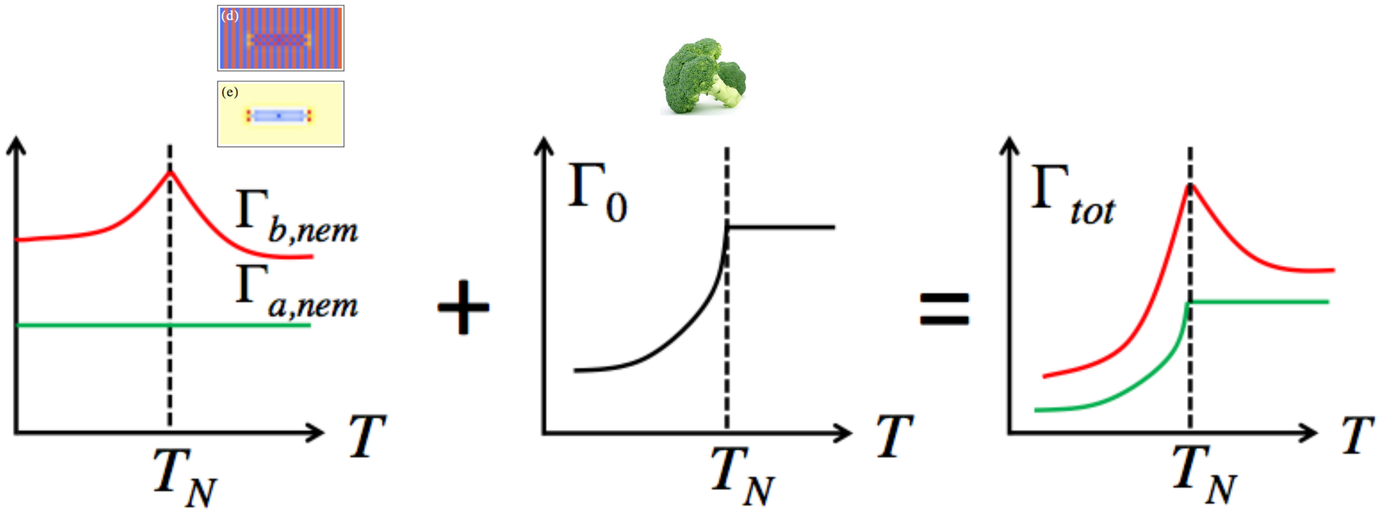
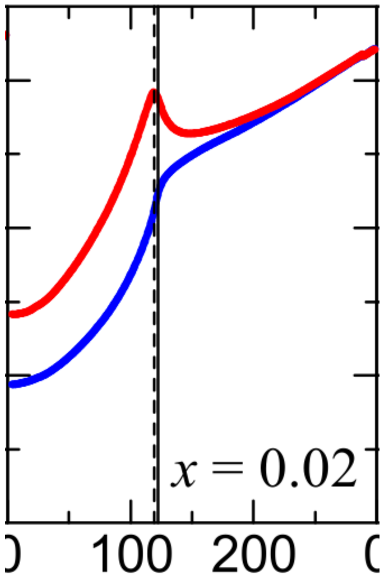
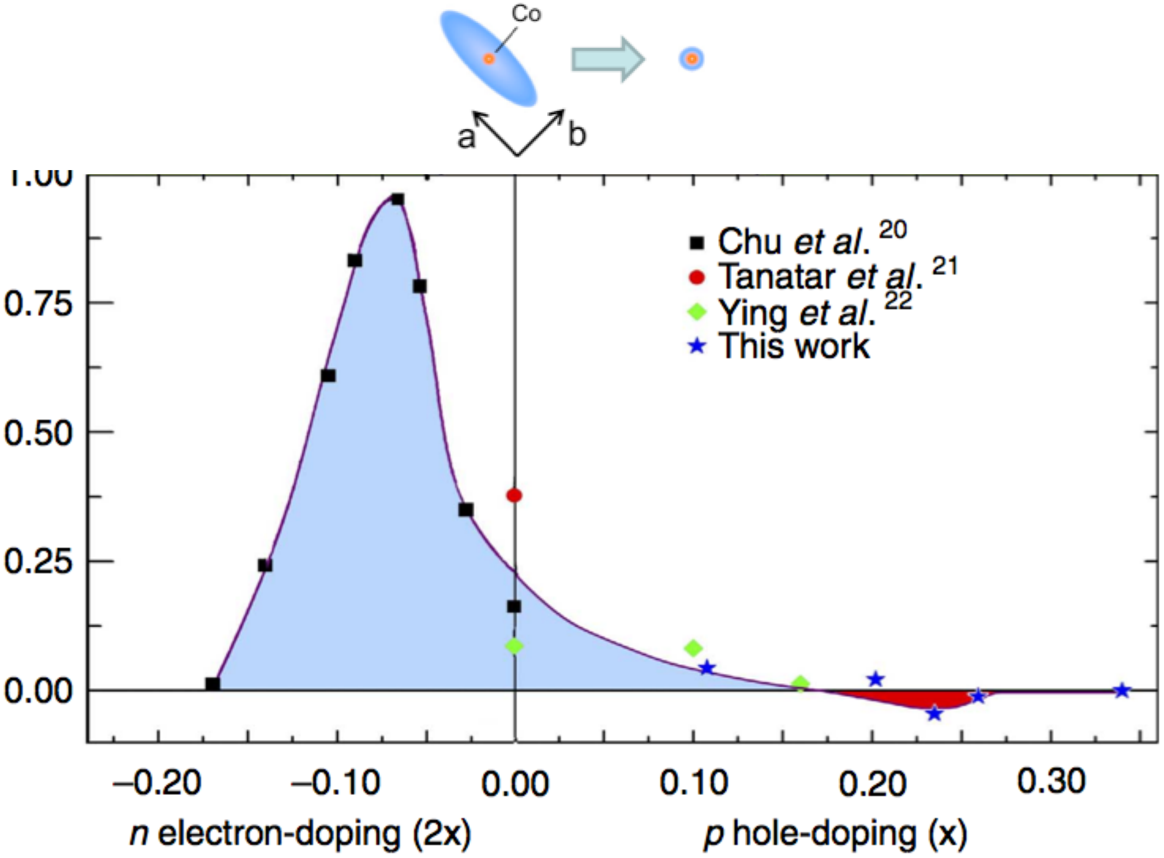




Ishida *et al*, PRL 2013

Summary doping-dependence



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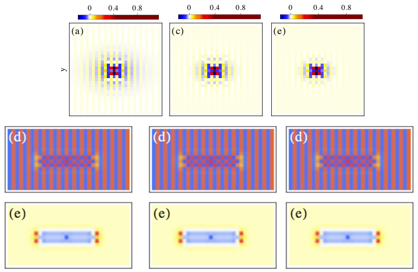

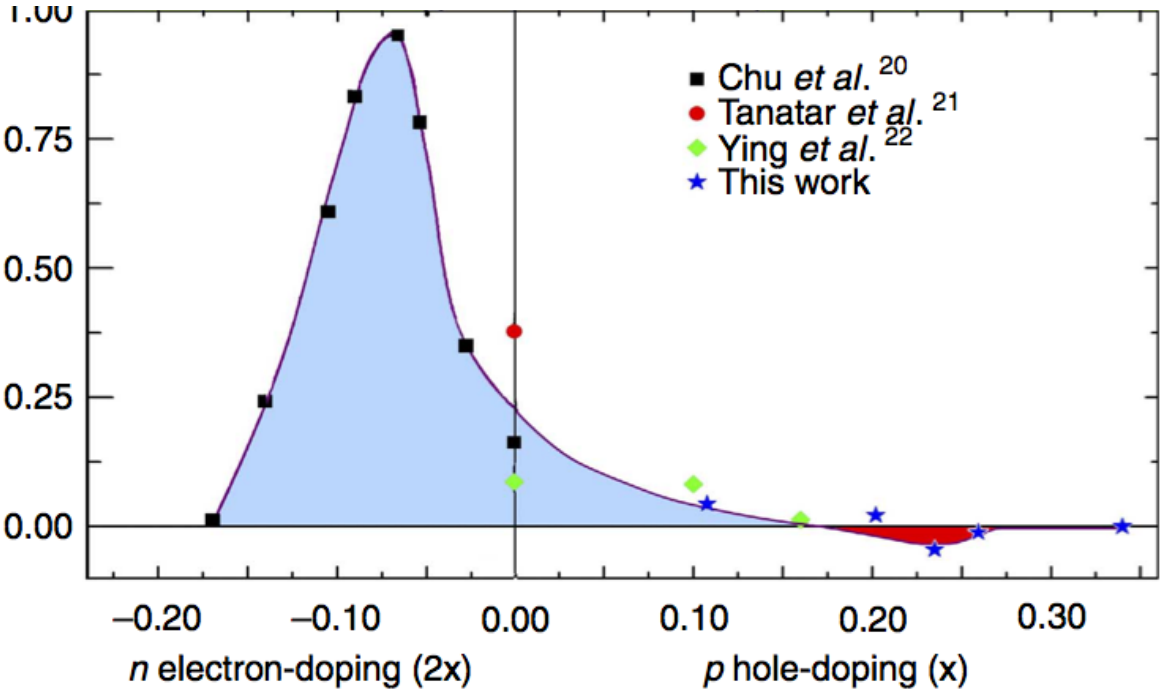

Summary of main exp. facts

Challenges for theory:

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2) The decrease of the anisotropy upon annealing.

3) The pronounced increase in ρ_b as T_N is approached, with little or no increase in ρ_a.

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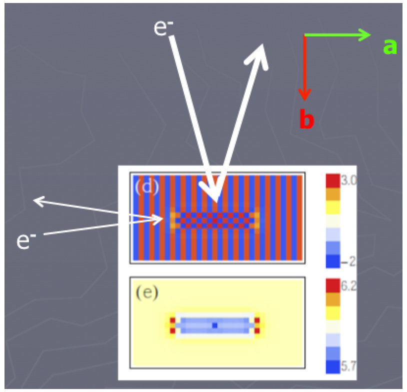

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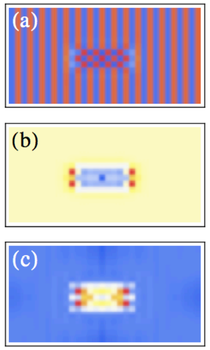

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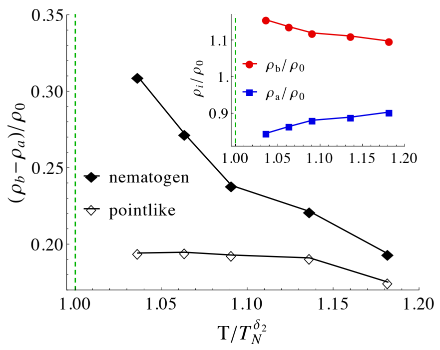

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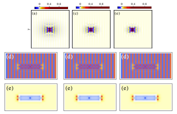

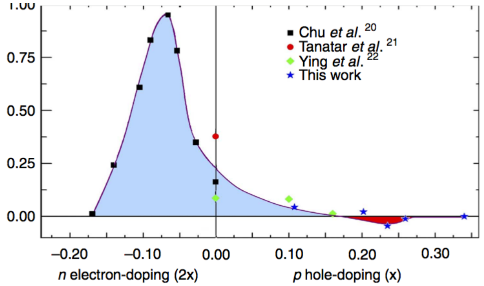

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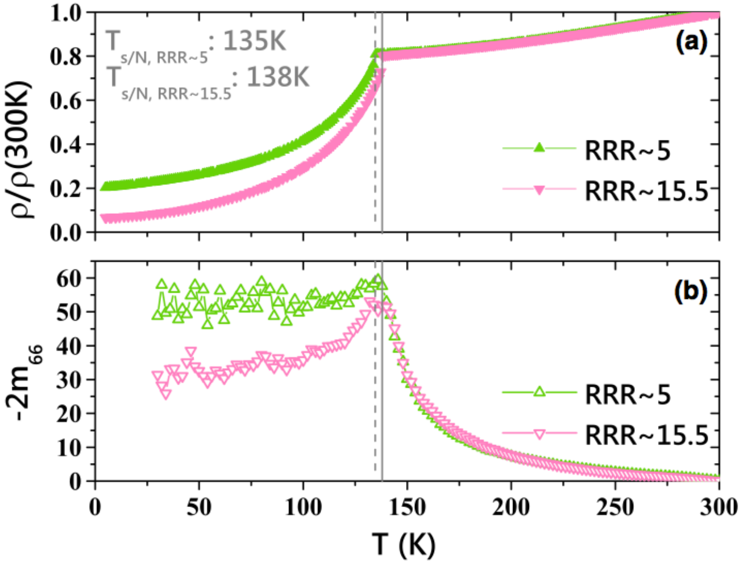
PRL **112,** 227001 (2014) PHYSICAL REVIEW LETTERS week ending 6 JUNE 2014

Effect of Disorder on the Resistivity Anisotropy Near the Electronic Nematic Phase Transition in Pure and Electron-Doped $BaFe_2As_2$

Hsueh-Hui Kuo[1,3] and Ian R. Fisher[2,3]



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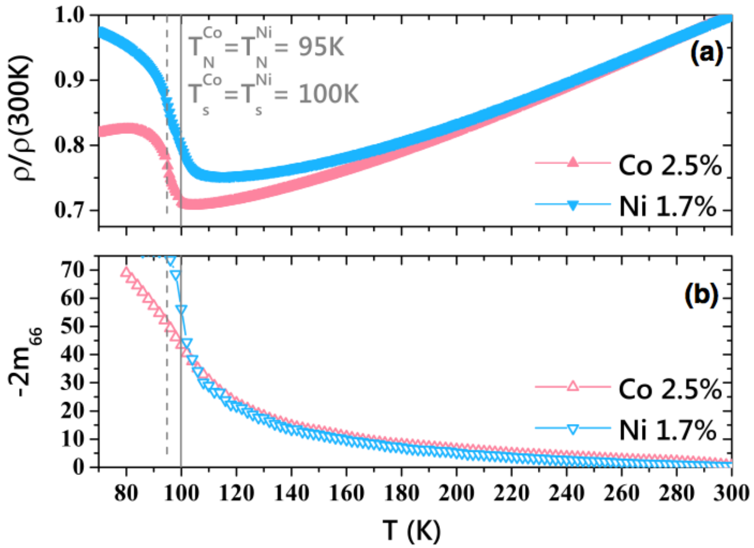

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A magnetic tetragonal phase

PHYSICAL REVIEW B **82**, 220503(R) (2010)

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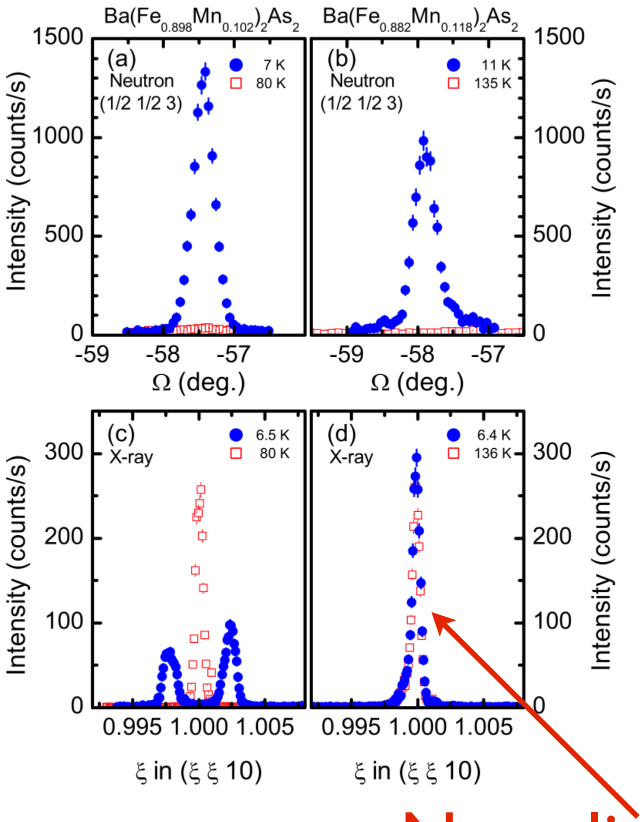

No splitting!

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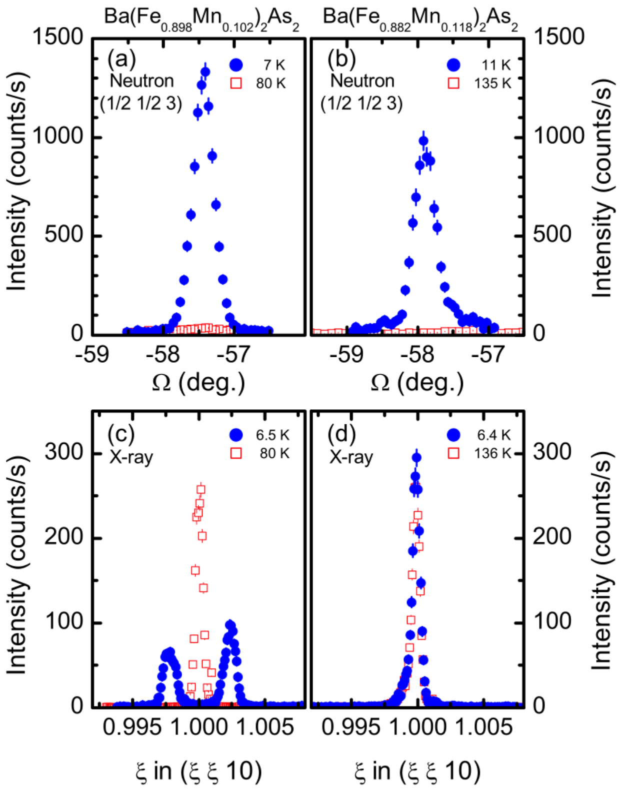

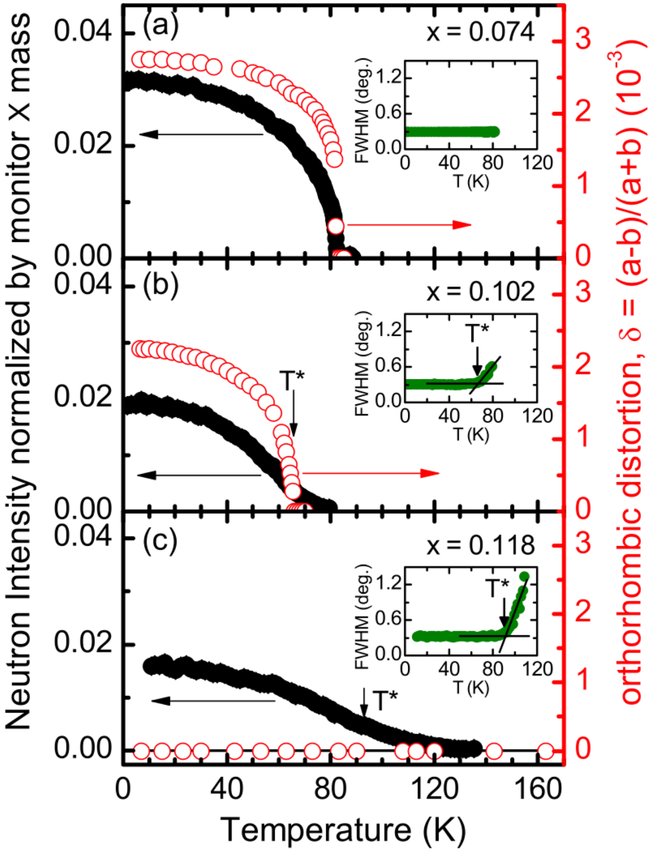

A possibility of unusual magnetic order

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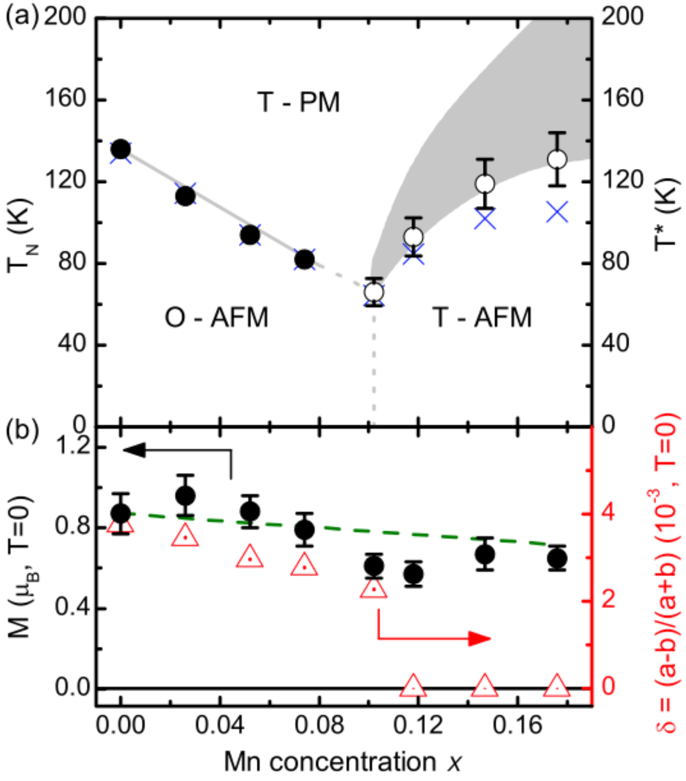

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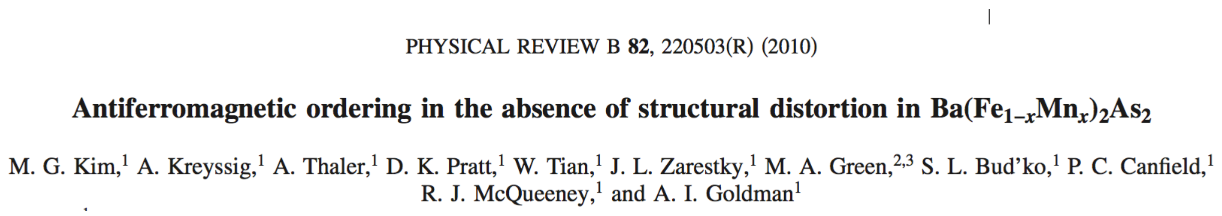

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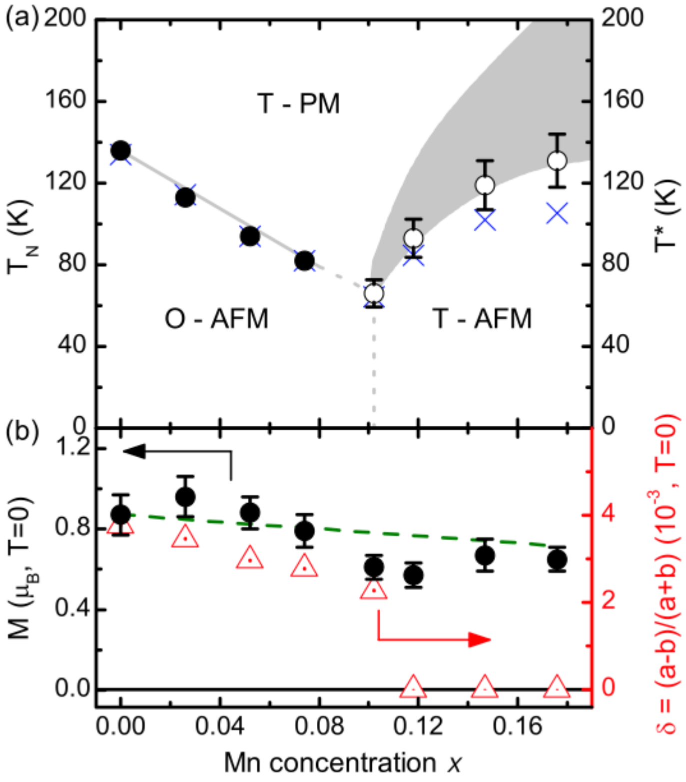
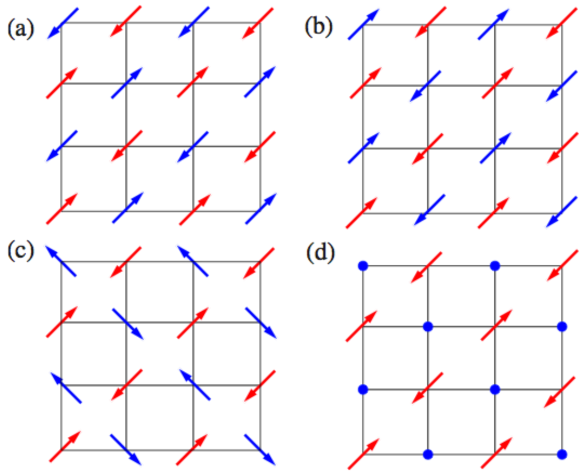


Is this proof that orbital ordering is not driving orthorhombicity and concomitant SDW?

$$\Delta_1 e^{iQ_1 R} + \Delta_2 e^{iQ_2 R}$$



I. Eremin & A. Chubukov
PRB 2009

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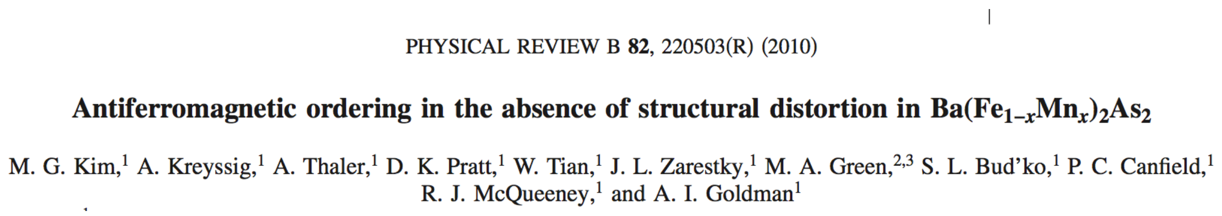

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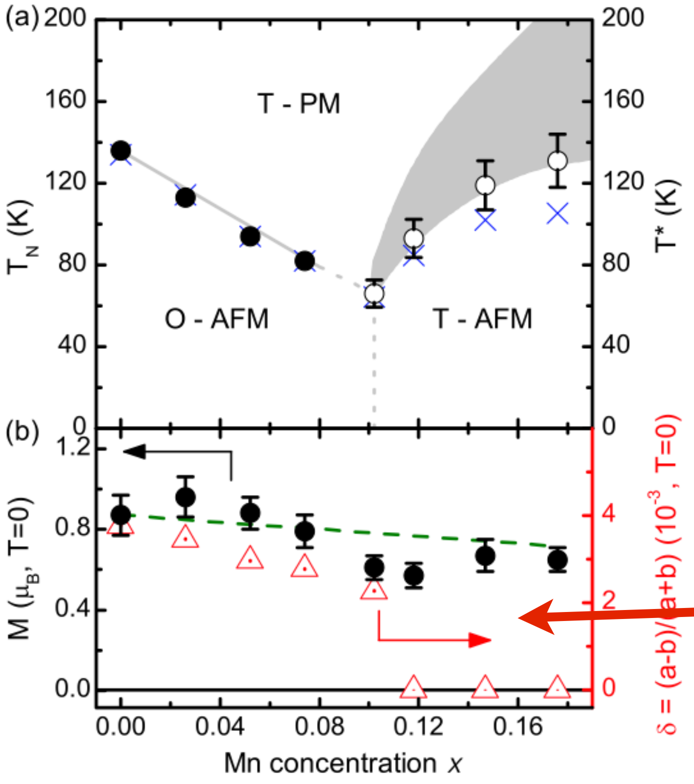

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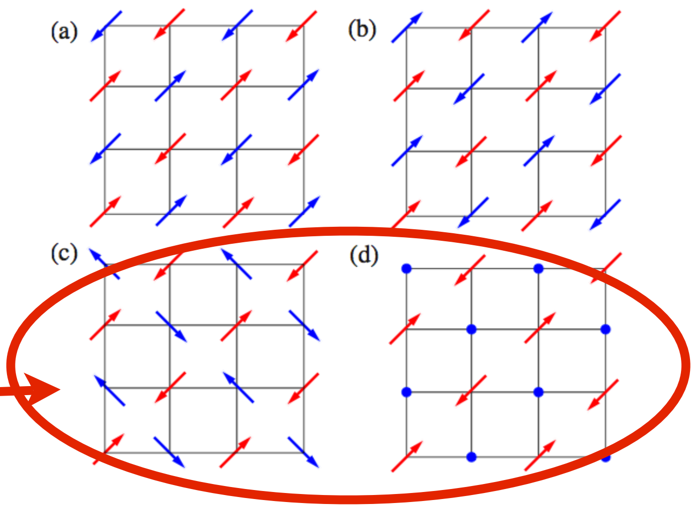
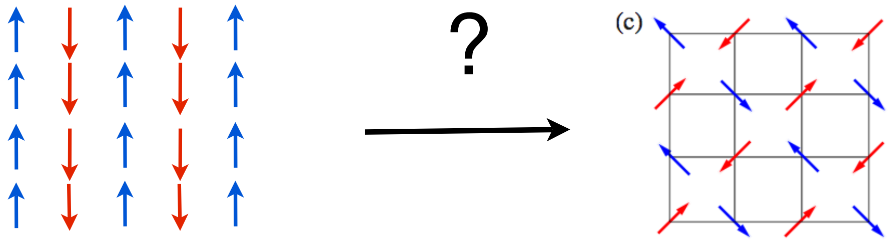


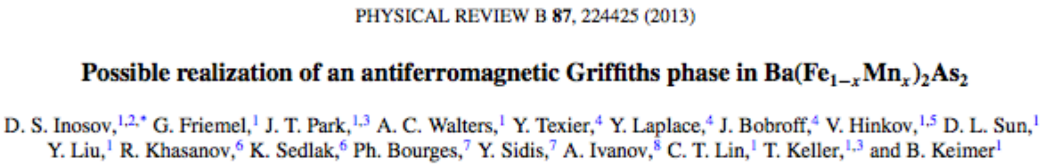
I. Eremin & A. Chubukov
PRB 2009

Puzzling

How can magnetic (non-doping) random disorder tune



Phase coexistence



PHYSICAL REVIEW B **87**, 224425 (2013)

Possible realization of an antiferromagnetic Griffiths phase in $\mathrm{Ba(Fe_{1-x}Mn_x)_2As_2}$

D. S. Inosov,[1,2,*] G. Friemel,[1] J. T. Park,[1,3] A. C. Walters,[1] Y. Texier,[4] Y. Laplace,[4] J. Bobroff,[4] V. Hinkov,[1,5] D. L. Sun,[1]
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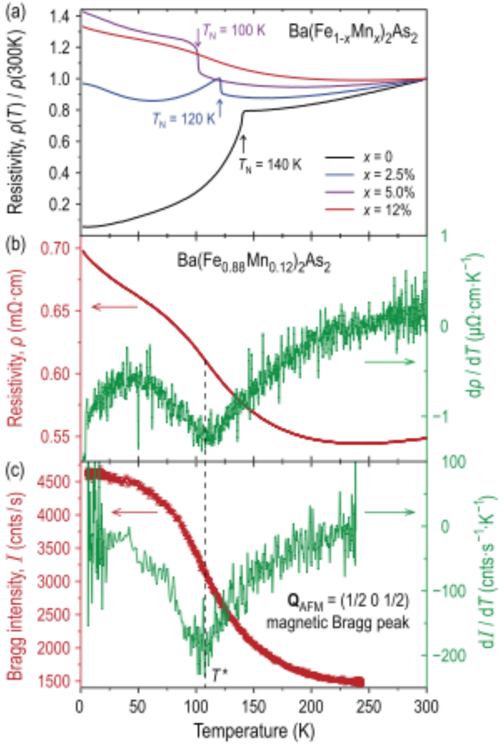
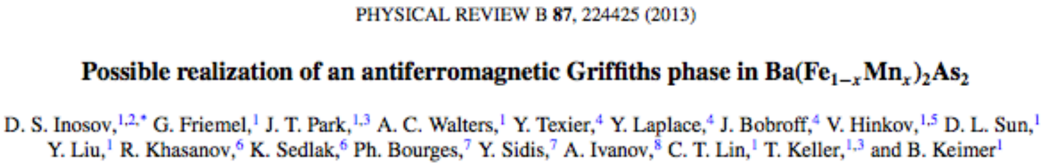


Initial suppression of T_N followed by a cooperative impurity effect stabilizing (pi,0) order at high T.

Phase coexistence



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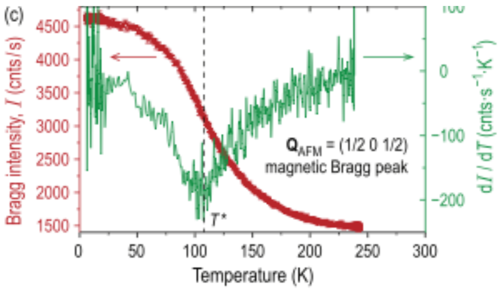
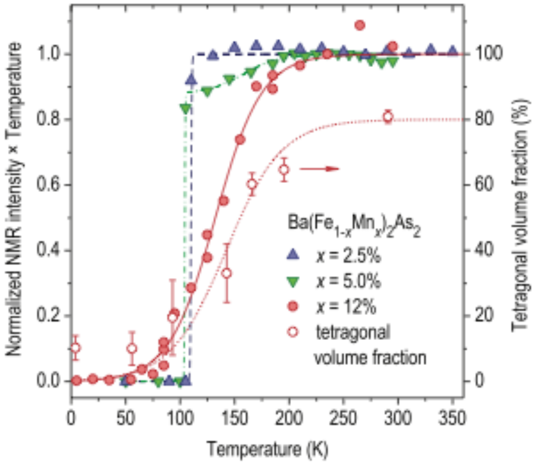
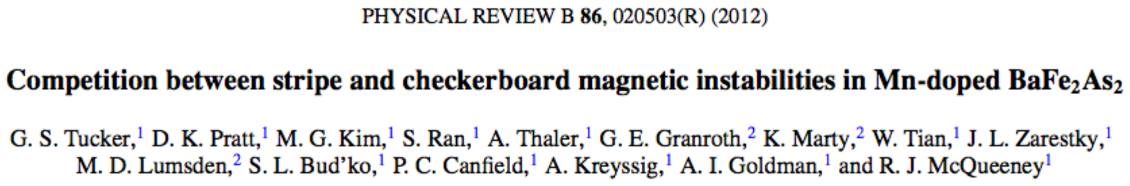




12% Mn sample exhibits *coexistence* of tetragonal and orthorhombic phases

Induced magnetic (pi,pi) scattering

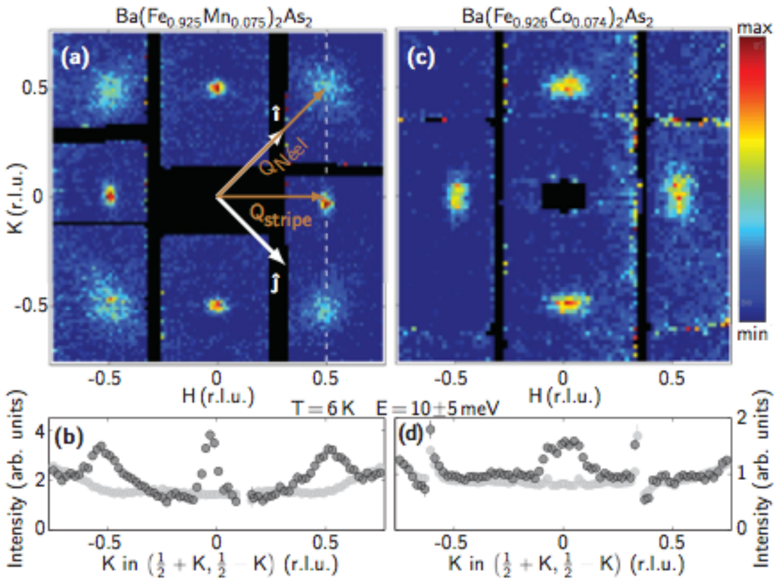


PHYSICAL REVIEW B **86**, 020503(R) (2012)

Competition between stripe and checkerboard magnetic instabilities in Mn-doped $BaFe_2As_2$

G. S. Tucker,[1] D. K. Pratt,[1] M. G. Kim,[1] S. Ran,[1] A. Thaler,[1] G. E. Granroth,[2] K. Marty,[2] W. Tian,[1] J. L. Zarestky,[1]
M. D. Lumsden,[2] S. L. Bud'ko,[1] P. C. Canfield,[1] A. Kreyssig,[1] A. I. Goldman,[1] and R. J. McQueeney[1]

6.0K
10meV



Summary of main exp. facts for Mn-122

Challenges for theory:

1) Mn impurities are a source of (non-doping) magnetic impurities.

2) Mn induce local (pi,pi) order in their vicinity both above and below T_N

3) (pi,0) order is induced above T_N but only for enough Mn.

4) Explain apparent absence of orthorhombicity.

Talk outline

1) Emergent defect states

- experimental overview (transport, STM).
- model and results; origin and consequences of nematogens.
- scenario for understanding the resistivity of pnictides.

2) Impurity-induced long-range ordered phases

- experimental overview (X-rays, neutron, muSR).
- model and results; origin and consequences of unusual "RKKY" exchange couplings.
- induced magnetic phases and extreme T_c suppression.

The 5-band model + magnetic impurity

$$H = H_0 + H_{int} + H_{imp};$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t_{\mathbf{ij}}^{\mu\nu} c_{\mathbf{i}\mu\sigma}^{\dagger} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}$$

$$\begin{aligned} H_{int} = {} & U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'} \\ & - 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c_{\mathbf{i}\mu\sigma}^{\dagger} c_{\mathbf{i}\mu\bar{\sigma}}^{\dagger} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma}, \end{aligned} \quad (3)$$

$$\mathcal{H}_{imp} = \sum_{\{\mathbf{i}^*\}\mu\sigma\sigma'} \mathbf{S}_{\mathbf{i}^*} \cdot (c_{\mathbf{i}^*\mu\sigma}^{\dagger} \sigma_{\sigma\sigma'} c_{\mathbf{i}^*\mu\sigma'}),$$

M. N. Gastiasoro *et al*
PRL 2014

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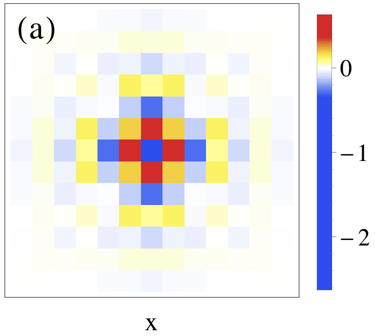
Mean-field decoupling and self-consistent solution for all densities at all orbitals and sites.

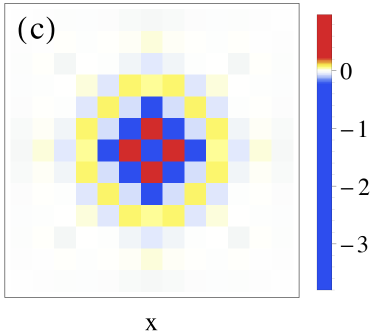
Single magnetic impurity

$T>T_N$

m(r)



$V_{imp}=0.3eV$



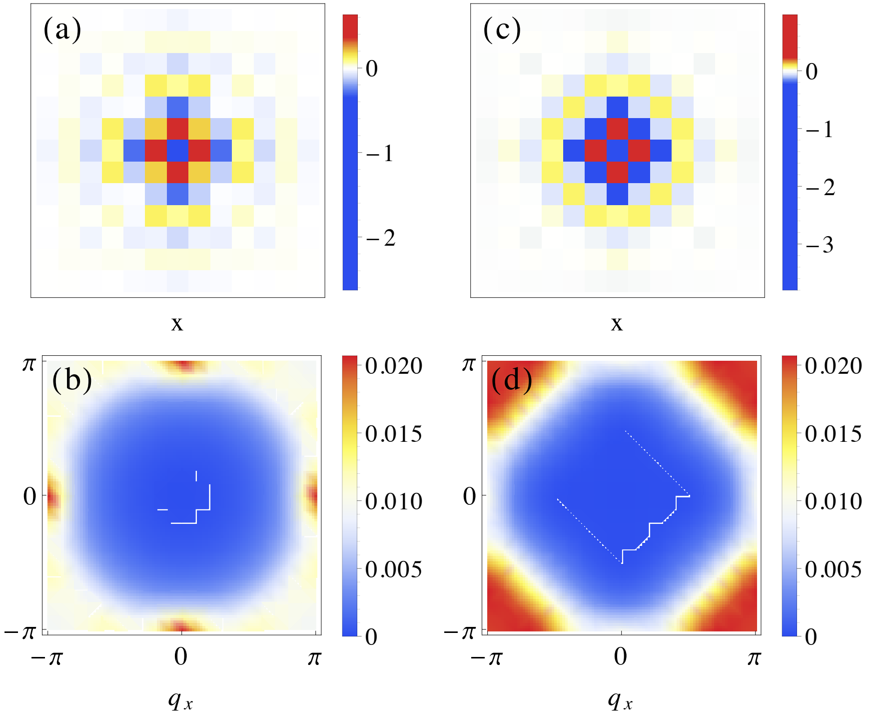
$V_{imp}=0.8eV$

Single magnetic impurity

$T>T_N$

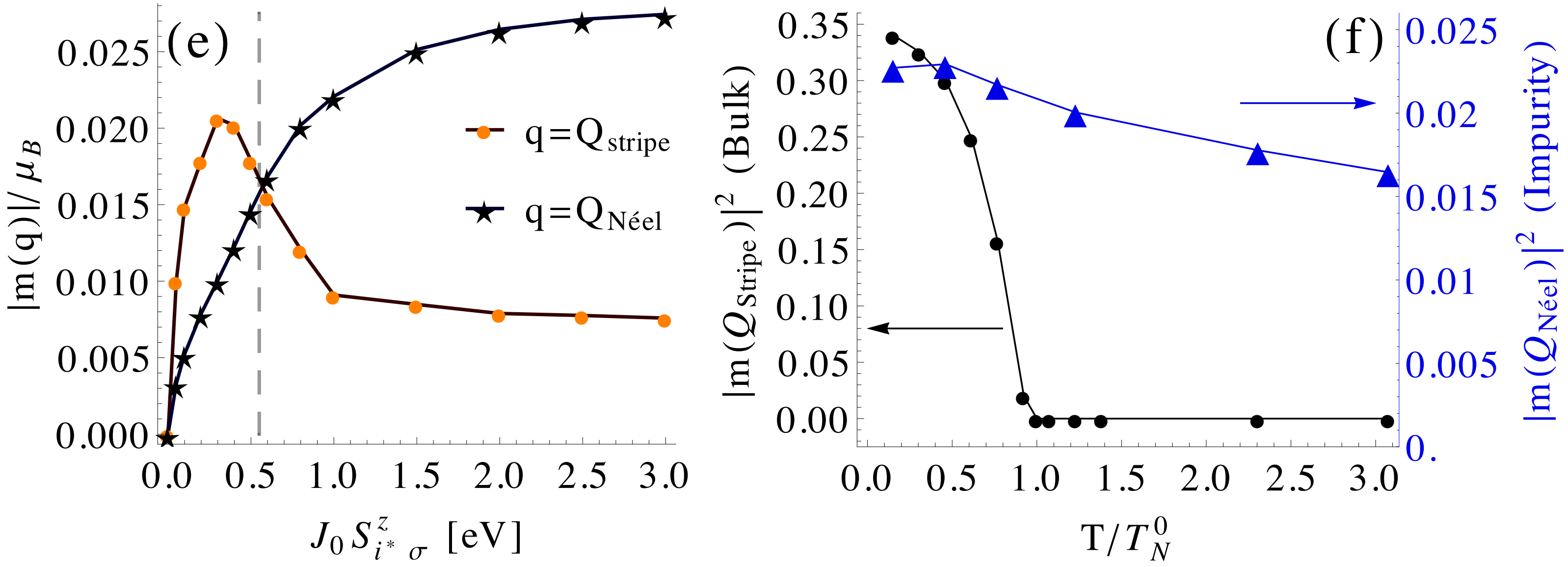
m(r)

|m(q)|



$V_{imp}=0.3eV$ $V_{imp}=0.8eV$

Two different kinds of magnetic impurities



M. N. Gastiasoro *et al*
PRL 2014

Multiple magnetic impurities

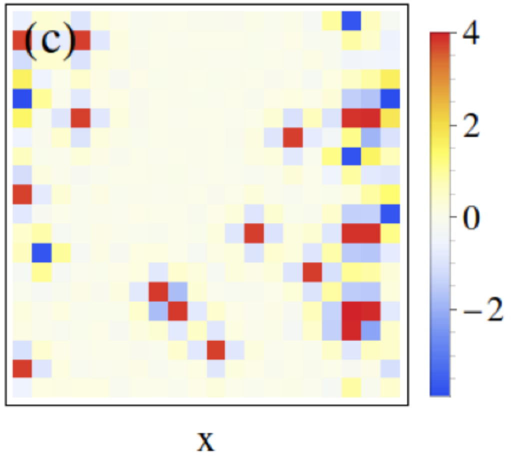
Energy calculation : “Monte Carlo”

$$F = U - TS$$

$$U = \langle H \rangle$$

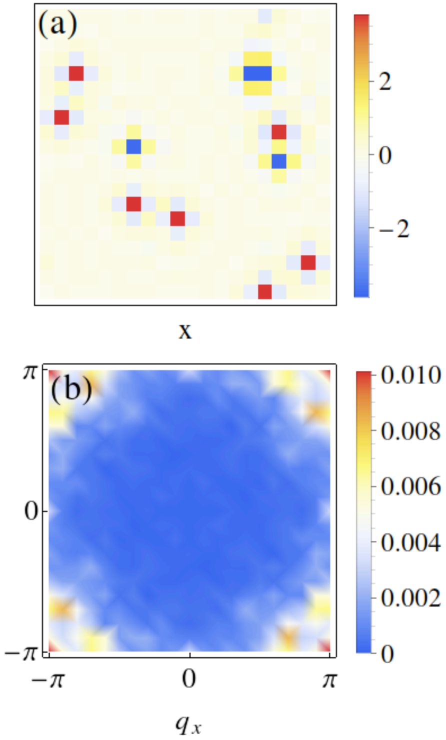
$$S = -k_B \sum_n (f(E_n) Lnf(E_n) + f(-E_n) Lnf(-E_n))$$

Find the configuration that minimizes F



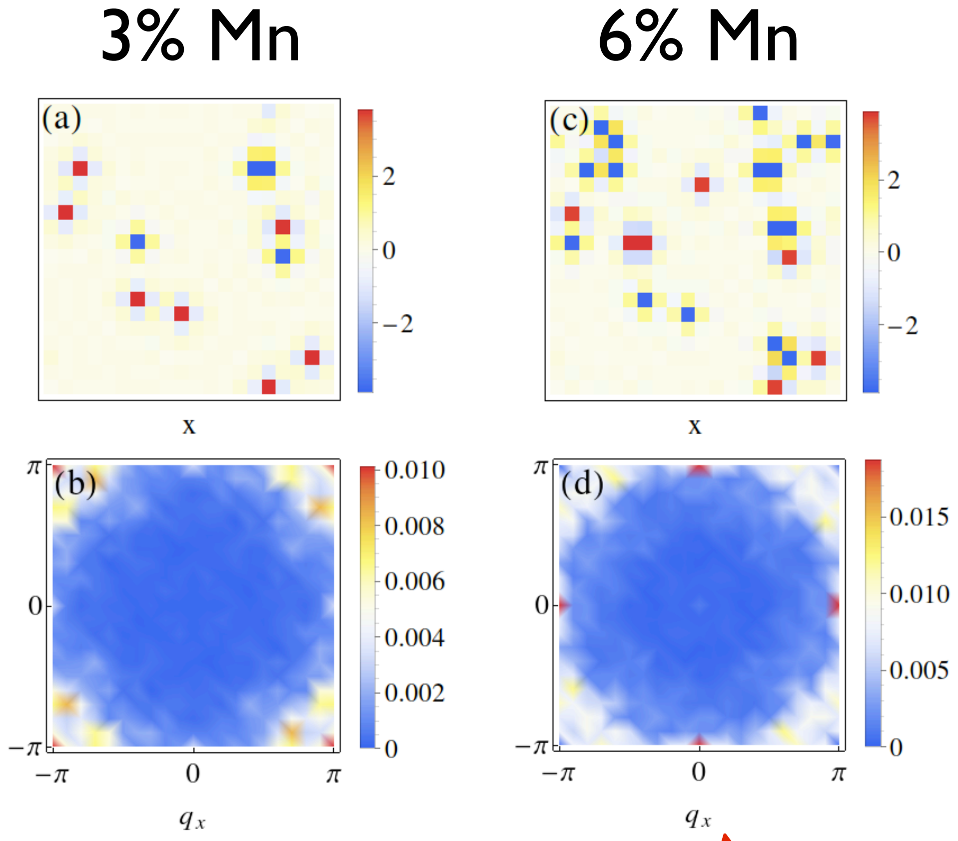
Generation of (0,pi) order-from-disorder

3% Mn



Only (pi,pi) at low Mn
concentrations

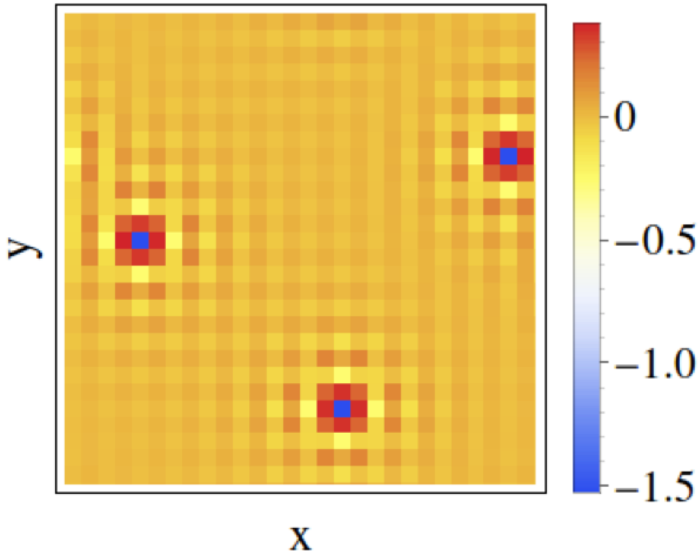
Generation of (0,pi) order-from-disorder

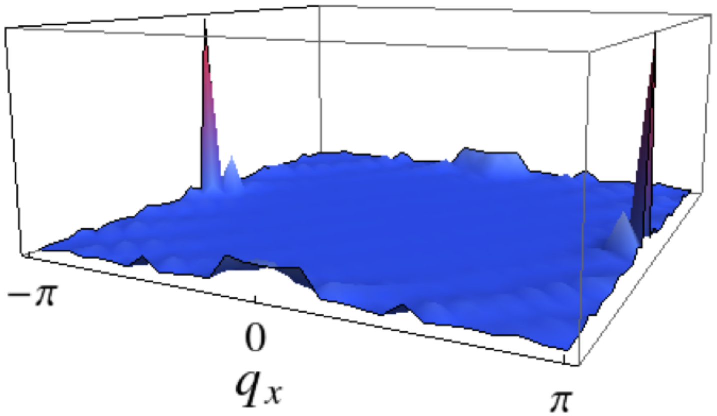


(pi,pi) at low Mn concentrations

(pi,0) at high enough Mn concentrations

Generation of (0,pi) order-from-disorder
- in a nutshell





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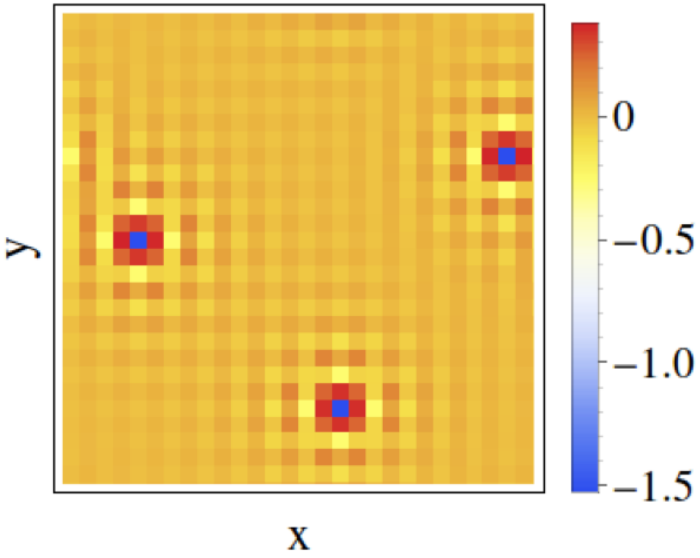

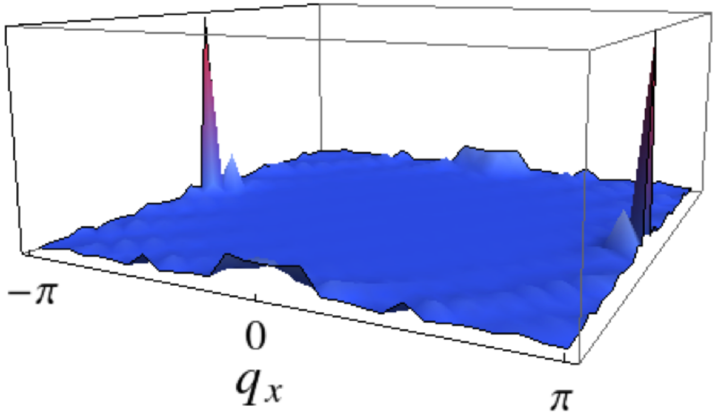

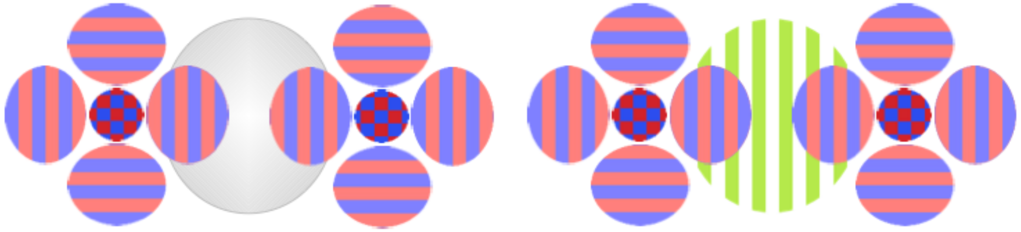

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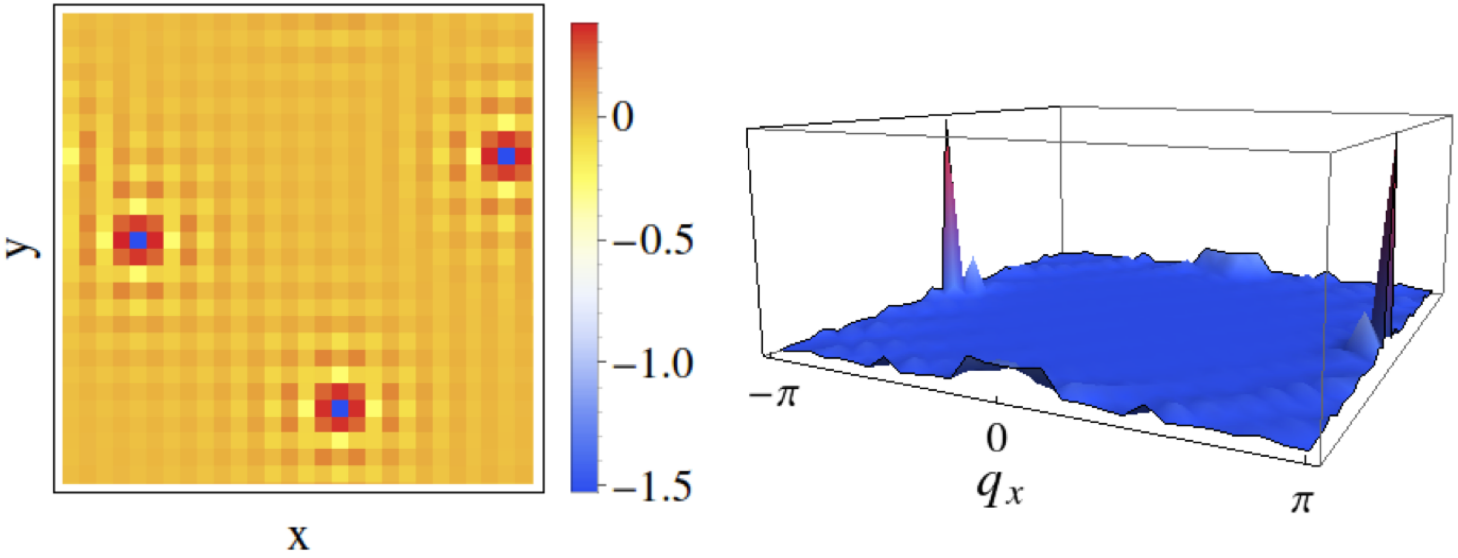
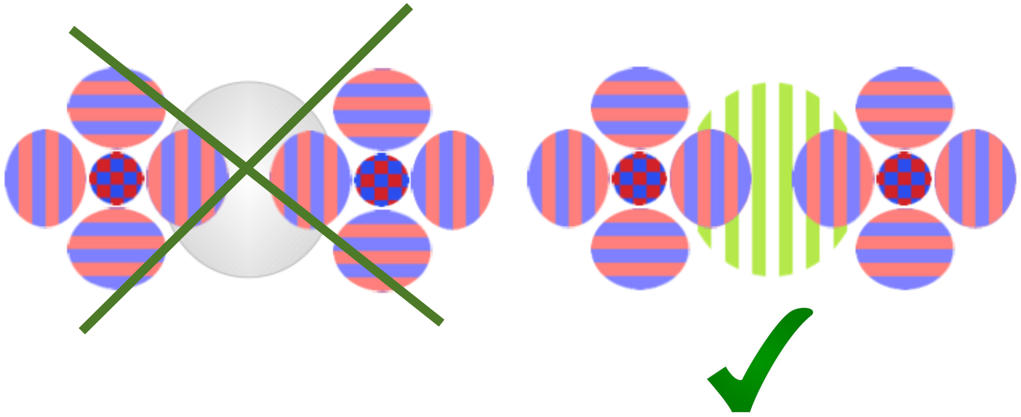
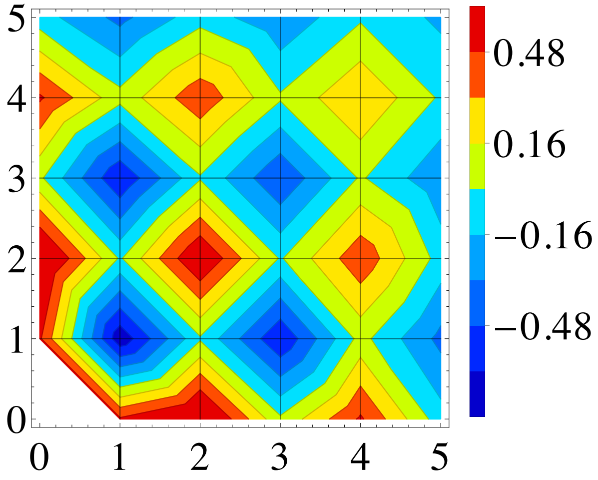
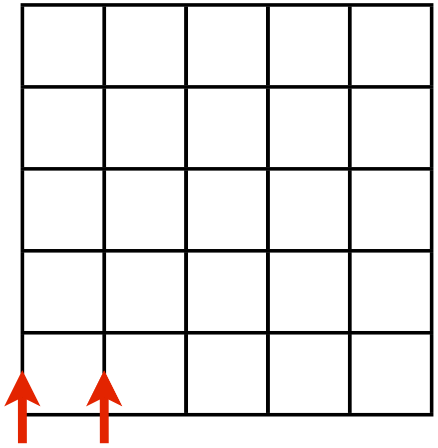




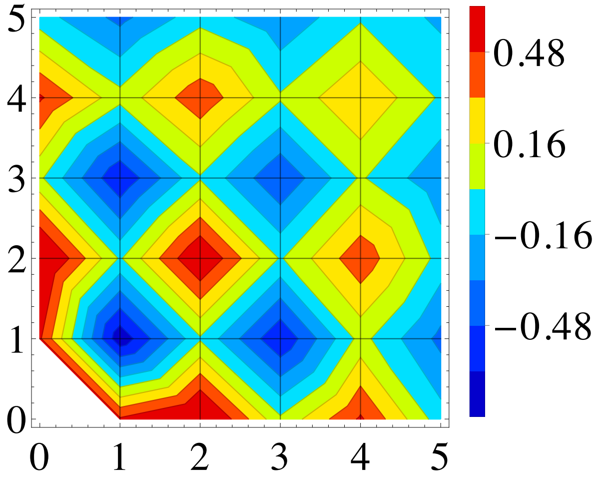
Exchange map

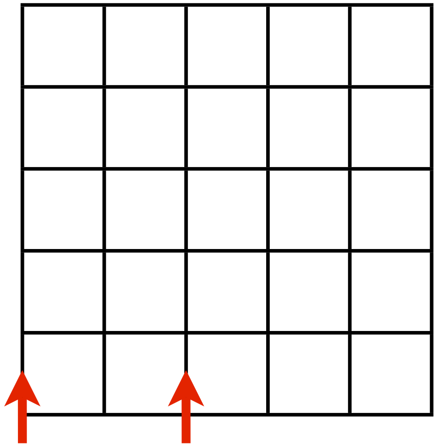




$$E_{\sigma\sigma'} - E_{\sigma\sigma}$$

Exchange map





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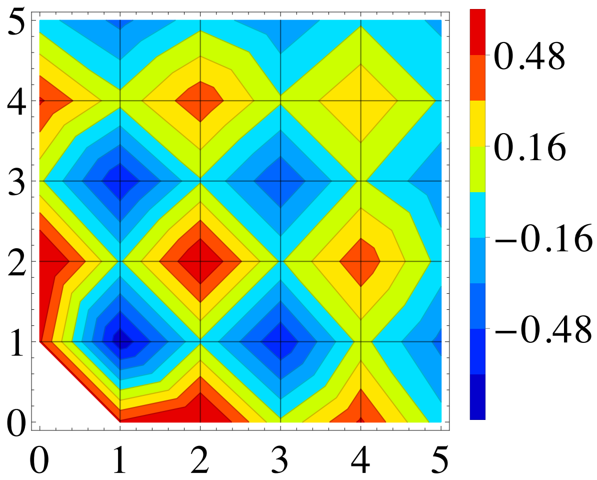

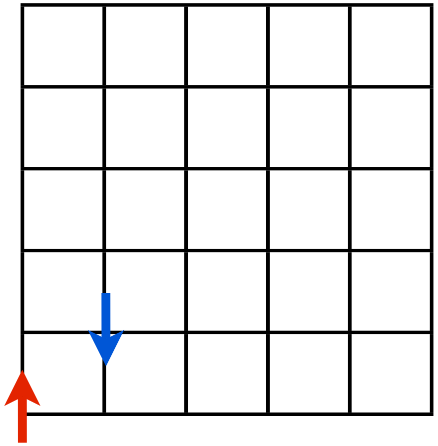

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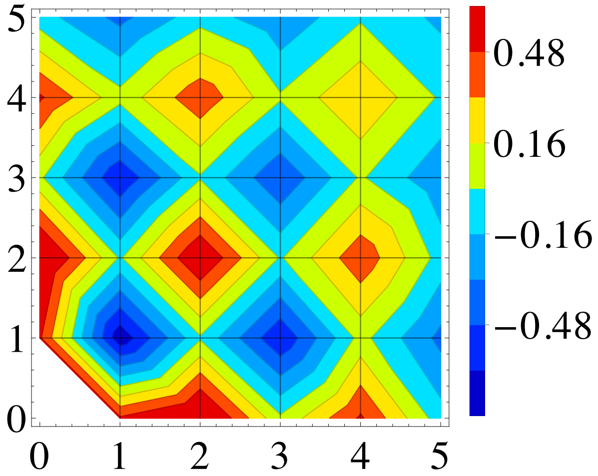

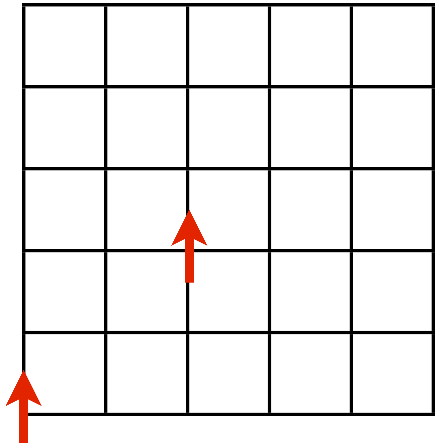

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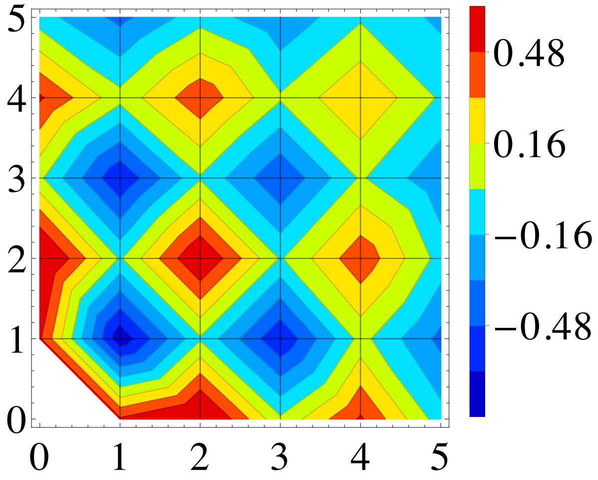

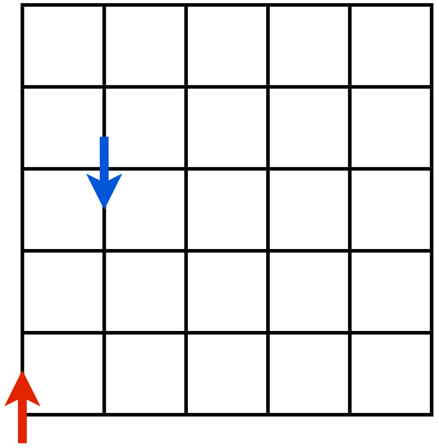

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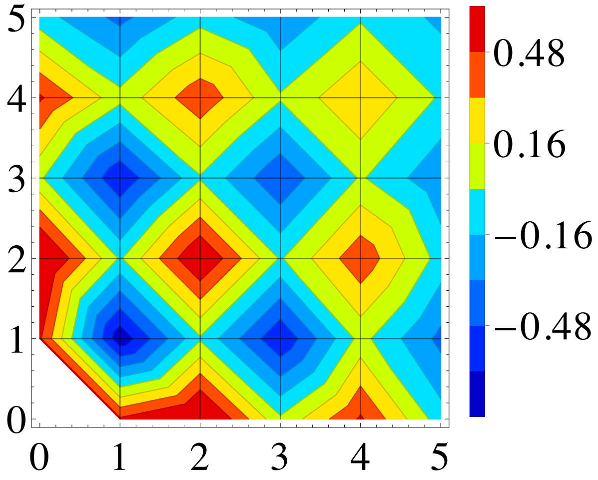
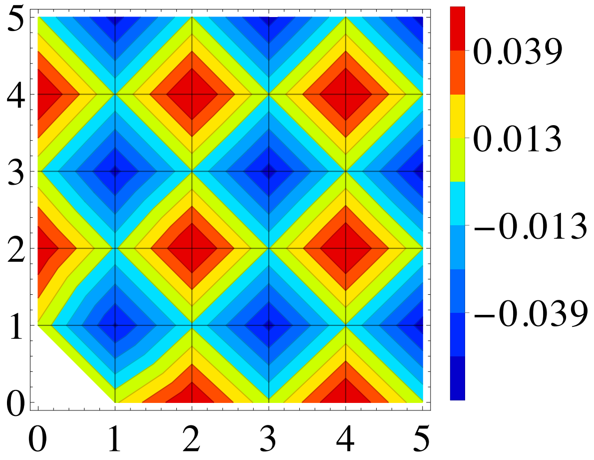
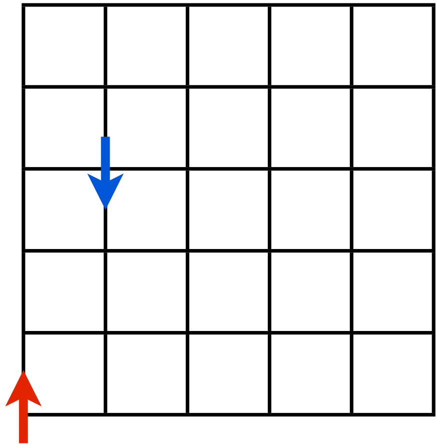


Max Stripe order map





$$E_{\sigma\sigma'} - E_{\sigma\sigma}$$

$$I = M_s(\sigma\sigma) - M_s(\sigma\sigma')$$

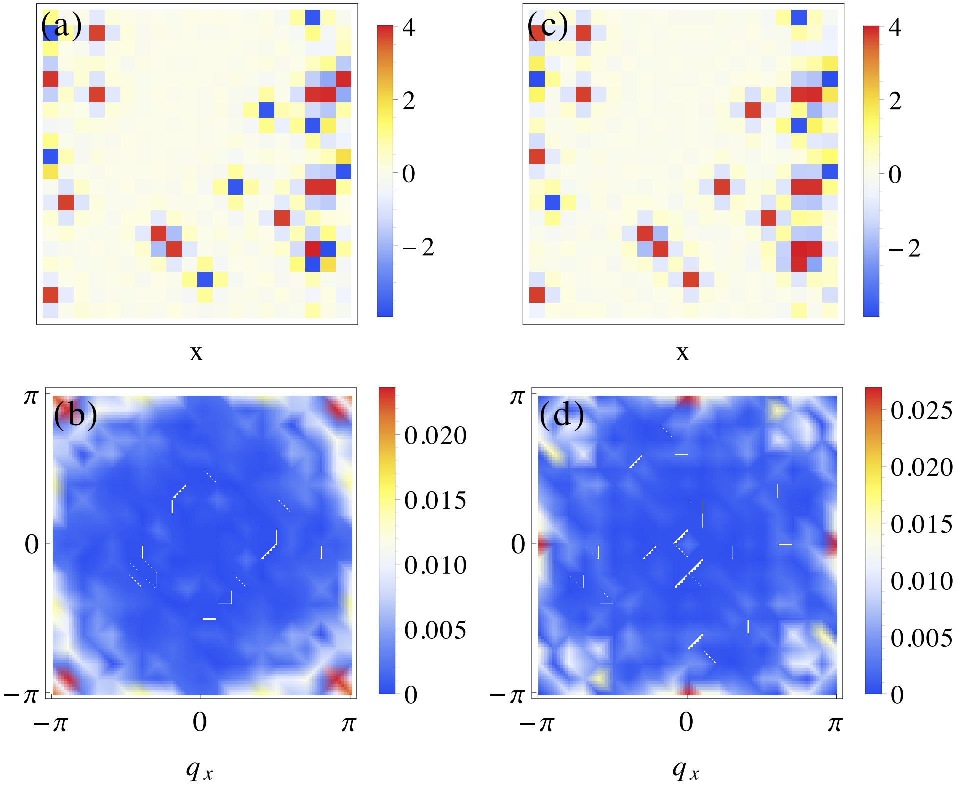
$$M_s = m(Q_1) + m(Q_2)$$

Generation of (0,pi) order-from-disorder

“Quenched” F minimized

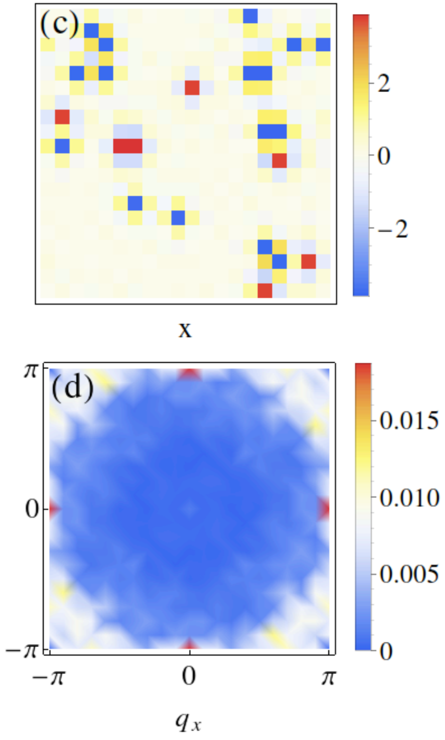
Real-space

$|m(q)|^2$

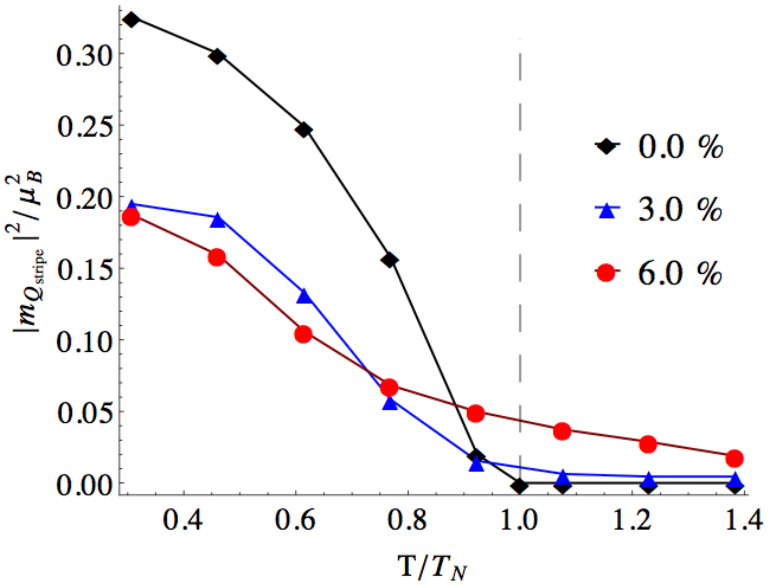


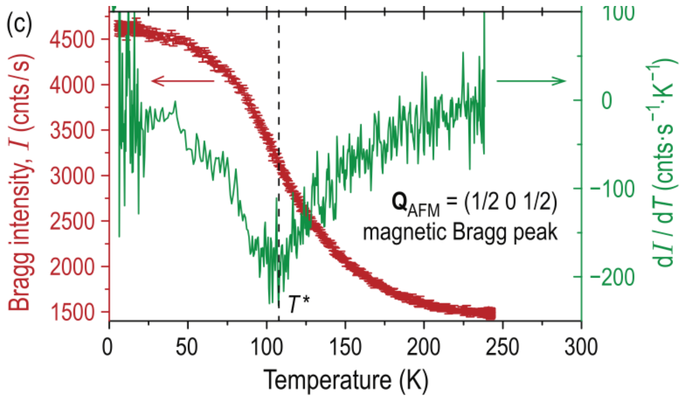
Cooperative spin alignment cause
(pi,0) Bragg peak above T_N

T-dependence of Mn-induced (0,pi) order



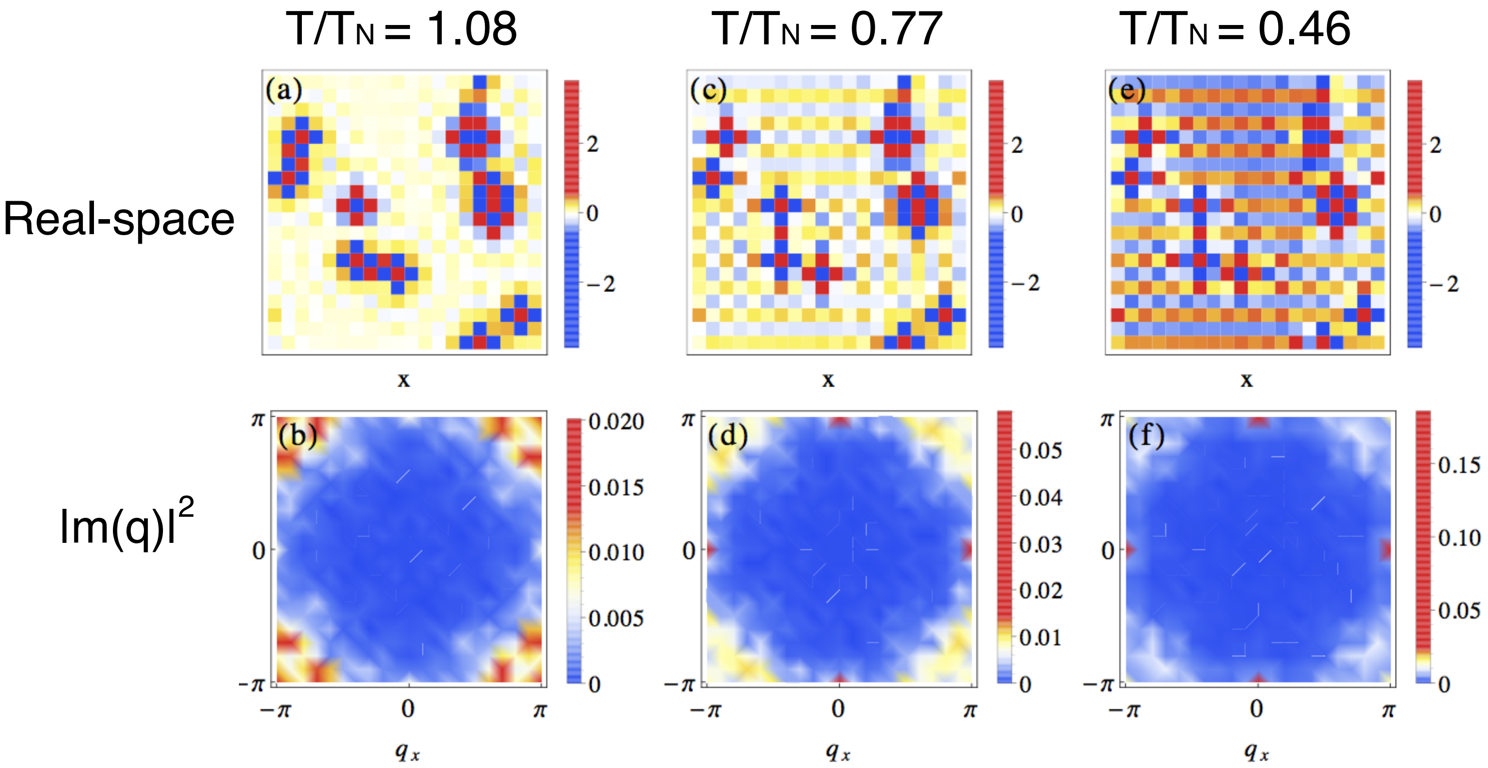
(pi,0) at high enough Mn concentrations





T-dependence in real space for dilute concentrations

3% Mn



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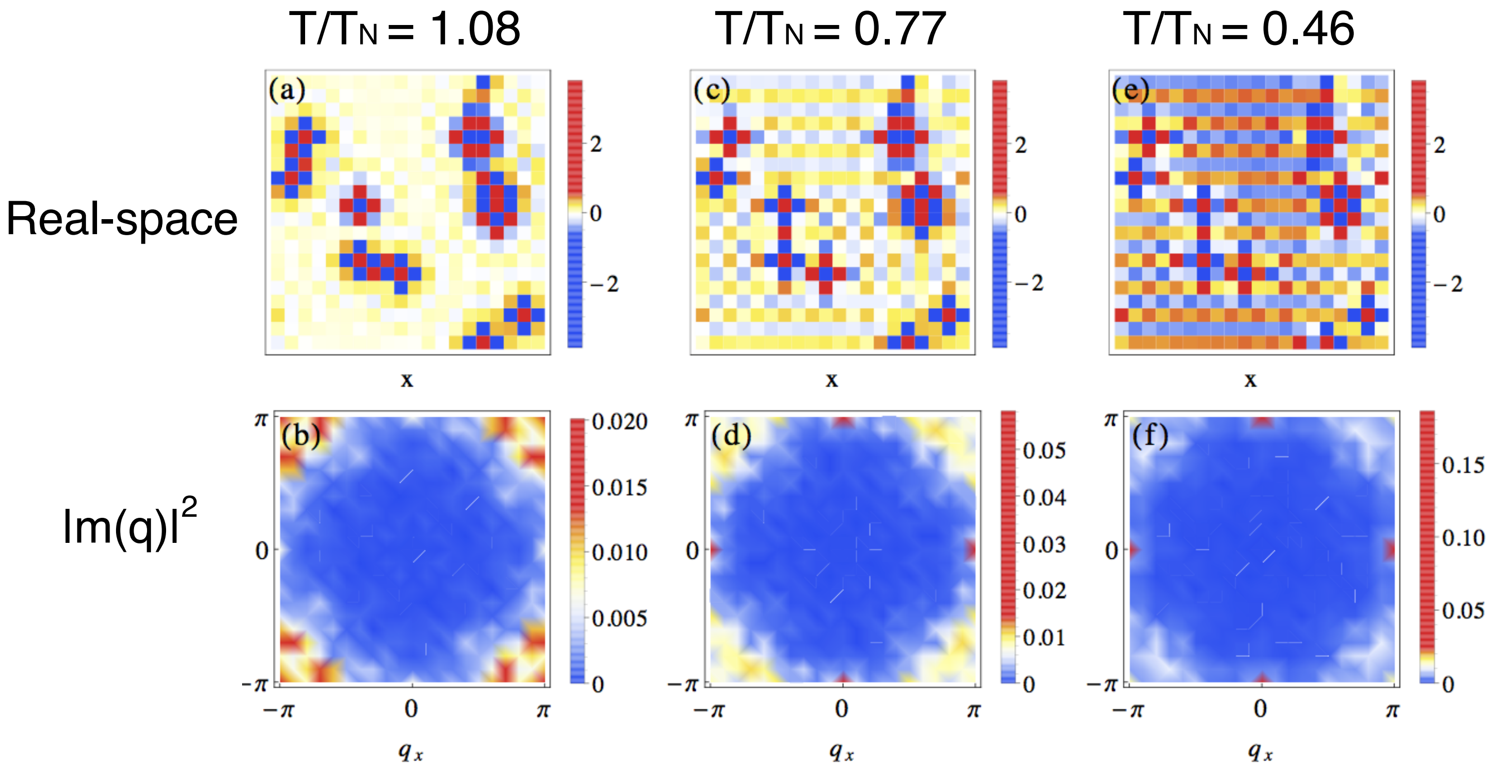

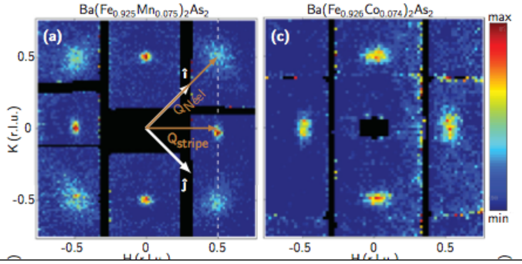

PHYSICAL REVIEW B **86**, 020503(R) (2012)

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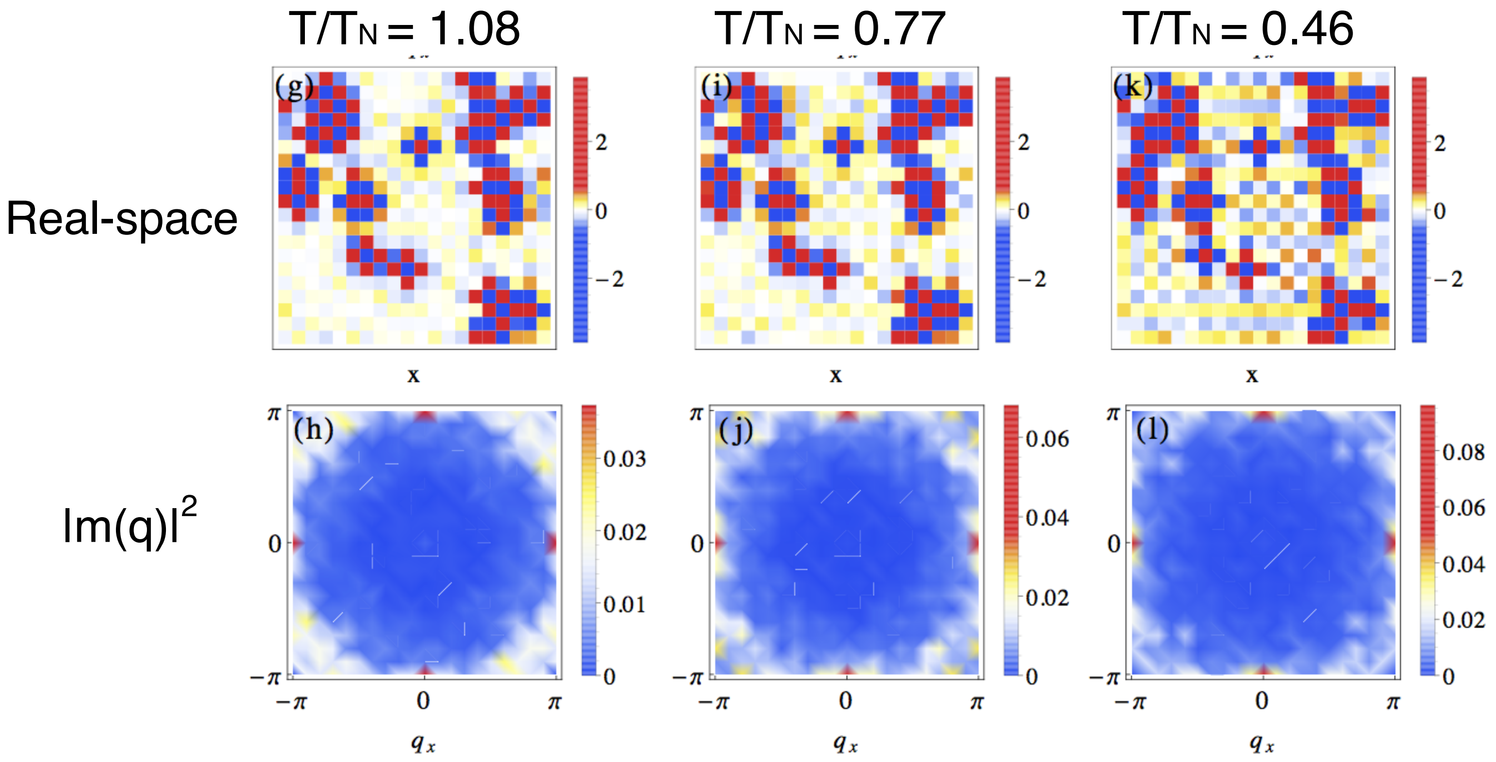
T-dependence in real space for dilute concentrations

6% Mn



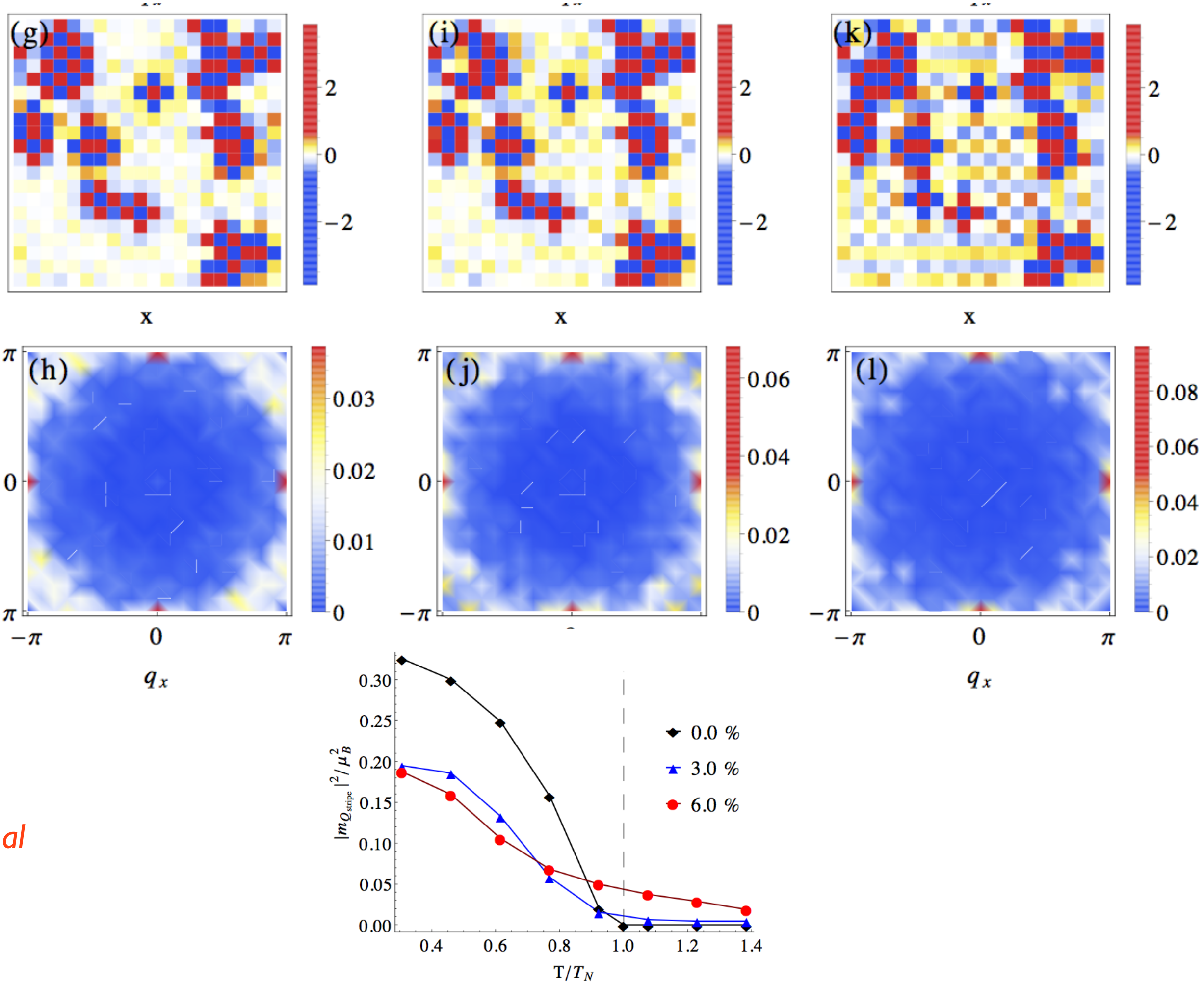
T-dependence in real space for dilute concentrations

6% Mn

$T/T_N = 1.08$ $T/T_N = 0.77$ $T/T_N = 0.46$

Real-space

$|m(q)|^2$



M. N. Gastiasoro *et al*
PRL 2014

Conclusions

Challenges for theory:

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- experimental overview (X-rays, neutron, muSR).
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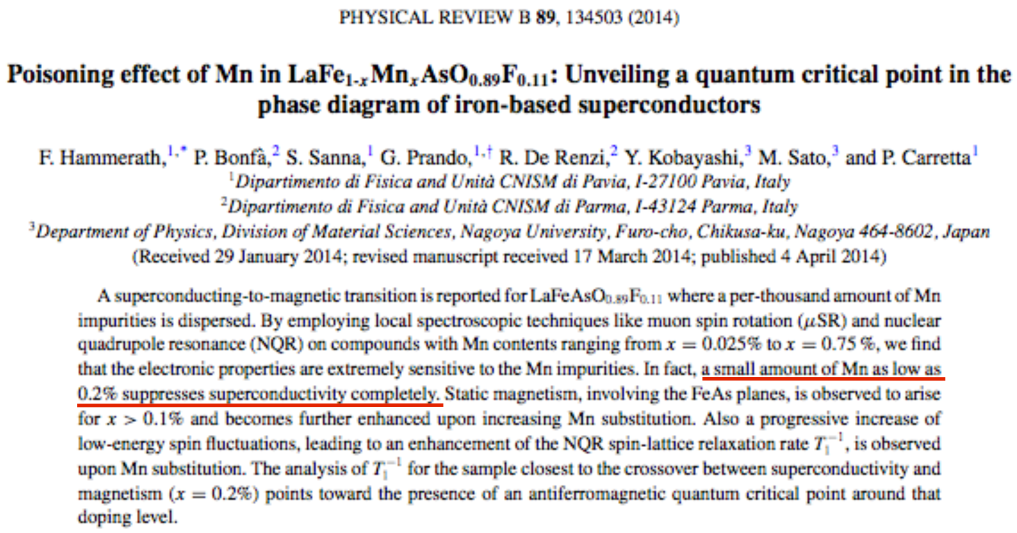
Poisoning effects



PHYSICAL REVIEW B **89**, 134503 (2014)

Poisoning effect of Mn in LaFe$_{1-x}$Mn$_x$AsO$_{0.89}$F$_{0.11}$: Unveiling a quantum critical point in the phase diagram of iron-based superconductors

F. Hammerath,[1,*] P. Bonfà,[2] S. Sanna,[1] G. Prando,[1,†] R. De Renzi,[2] Y. Kobayashi,[3] M. Sato,[3] and P. Carretta[1]
[1]*Dipartimento di Fisica and Unità CNISM di Pavia, I-27100 Pavia, Italy*
[2]*Dipartimento di Fisica and Unità CNISM di Parma, I-43124 Parma, Italy*
[3]*Department of Physics, Division of Material Sciences, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan*
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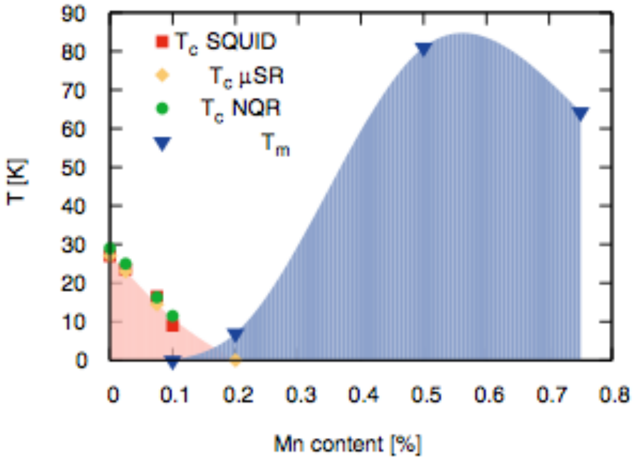
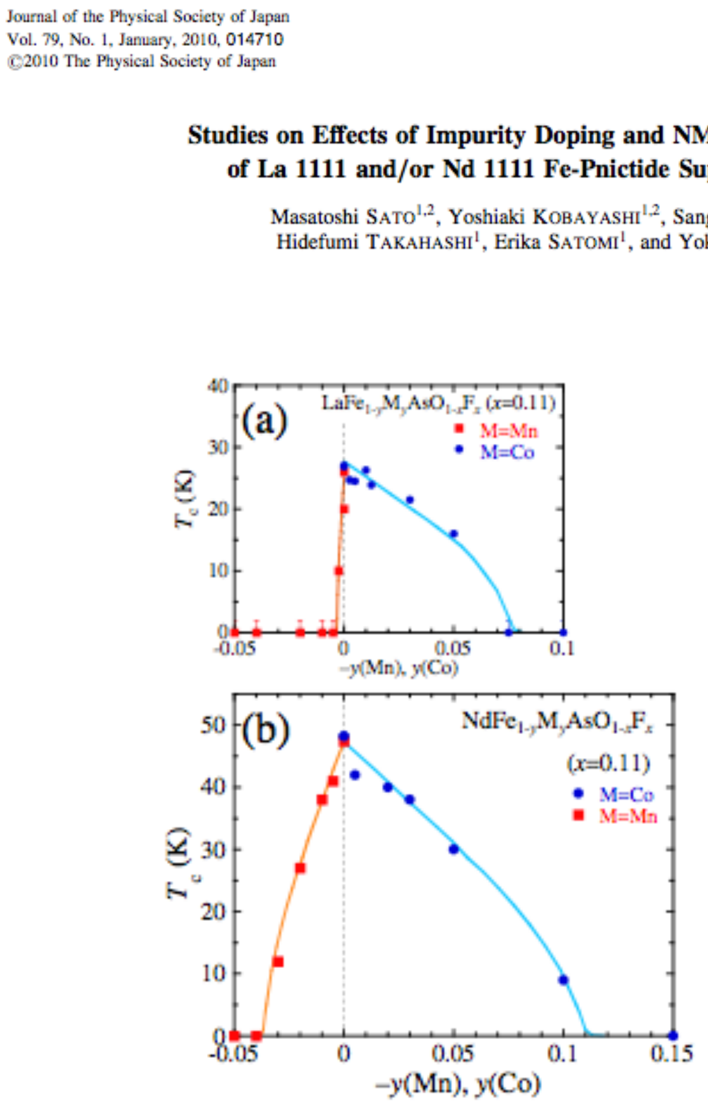
A superconducting-to-magnetic transition is reported for LaFeAsO$_{0.89}$F$_{0.11}$ where a per-thousand amount of Mn impurities is dispersed. By employing local spectroscopic techniques like muon spin rotation (μSR) and nuclear quadrupole resonance (NQR) on compounds with Mn contents ranging from $x = 0.025\%$ to $x = 0.75\,\%$, we find that the electronic properties are extremely sensitive to the Mn impurities. In fact, a small amount of Mn as low as 0.2% suppresses superconductivity completely. Static magnetism, involving the FeAs planes, is observed to arise for $x > 0.1\%$ and becomes further enhanced upon increasing Mn substitution. Also a progressive increase of low-energy spin fluctuations, leading to an enhancement of the NQR spin-lattice relaxation rate T_1^{-1}, is observed upon Mn substitution. The analysis of T_1^{-1} for the sample closest to the crossover between superconductivity and magnetism ($x = 0.2\%$) points toward the presence of an antiferromagnetic quantum critical point around that doping level.





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Studies on Effects of Impurity Doping and NMR Measurements of La 1111 and/or Nd 1111 Fe-Pnictide Superconductors

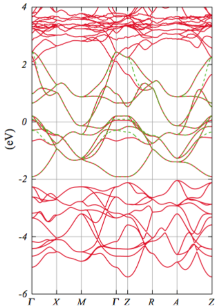
Masatoshi SATO[1,2], Yoshiaki KOBAYASHI[1,2], Sang Chul LEE[1],
Hidefumi TAKAHASHI[1], Erika SATOMI[1], and Yoko MIURA[1,2]

Extreme Tc
suppression

Five band model

$$H = H_0 + H_{int} + H_{BCS} + H_{imp},$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t_{\mathbf{ij}}^{\mu\nu} c^{\dagger}_{\mathbf{i}\mu\sigma} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}.$$



LaFeAsO 1111

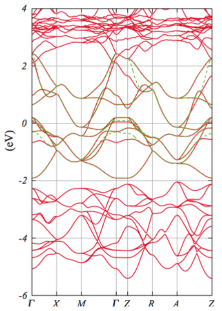
Five band model

$$H = H_0 + H_{int} + H_{BCS} + H_{imp},$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t^{\mu\nu}_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\mu\sigma} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}.$$

$$H_{int} = U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'}$$

$$- 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c^{\dagger}_{\mathbf{i}\mu\sigma} c^{\dagger}_{\mathbf{i}\mu\bar{\sigma}} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma},$$

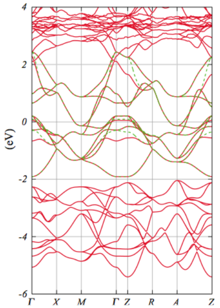


LaFeAsO 1111

Five band model

$$H = H_0 + H_{int} + H_{BCS} + H_{imp},$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t_{\mathbf{ij}}^{\mu\nu} c^{\dagger}_{\mathbf{i}\mu\sigma} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}.$$



$$H_{int} = U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'}$$

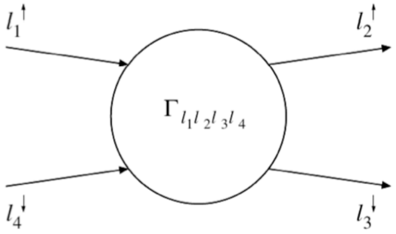
LaFeAsO 1111

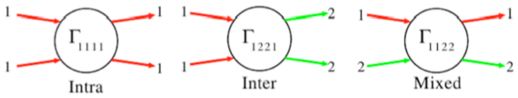
$$- 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c^{\dagger}_{\mathbf{i}\mu\sigma} c^{\dagger}_{\mathbf{i}\mu\bar{\sigma}} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma},$$

$$H_{BCS} = - \sum_{\mathbf{i}\neq\mathbf{j},\mu\nu} [\Delta_{\mathbf{ij}}^{\mu\nu} c^{\dagger}_{\mathbf{i}\mu\uparrow} c^{\dagger}_{\mathbf{j}\nu\downarrow} + H.c.],$$

Pairing

$$H_{BCS} = -\sum_{\mathbf{i}\neq\mathbf{j},\mu\nu}[\Delta^{\mu\nu}_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\mu\uparrow} c^{\dagger}_{\mathbf{j}\nu\downarrow} + H.c.],$$



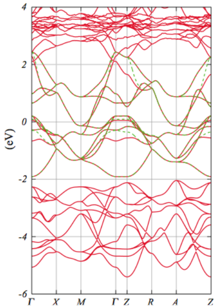


The pairing vertex in the singlet channel:

$$\Gamma_{pqst}(k-k',0) = \left[\frac{3}{2}U^s\chi_s^{RPA}(k-k',0)U^s + \frac{1}{2}U^s - \frac{1}{2}U^c\chi_c^{RPA}(k-k',0)U^c + \frac{1}{2}U^c\right]_{pq}^{st}$$

Five band model

$$H = H_0 + H_{int} + H_{BCS} + H_{imp},$$



LaFeAsO 1111

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t^{\mu\nu}_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\mu\sigma} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}.$$

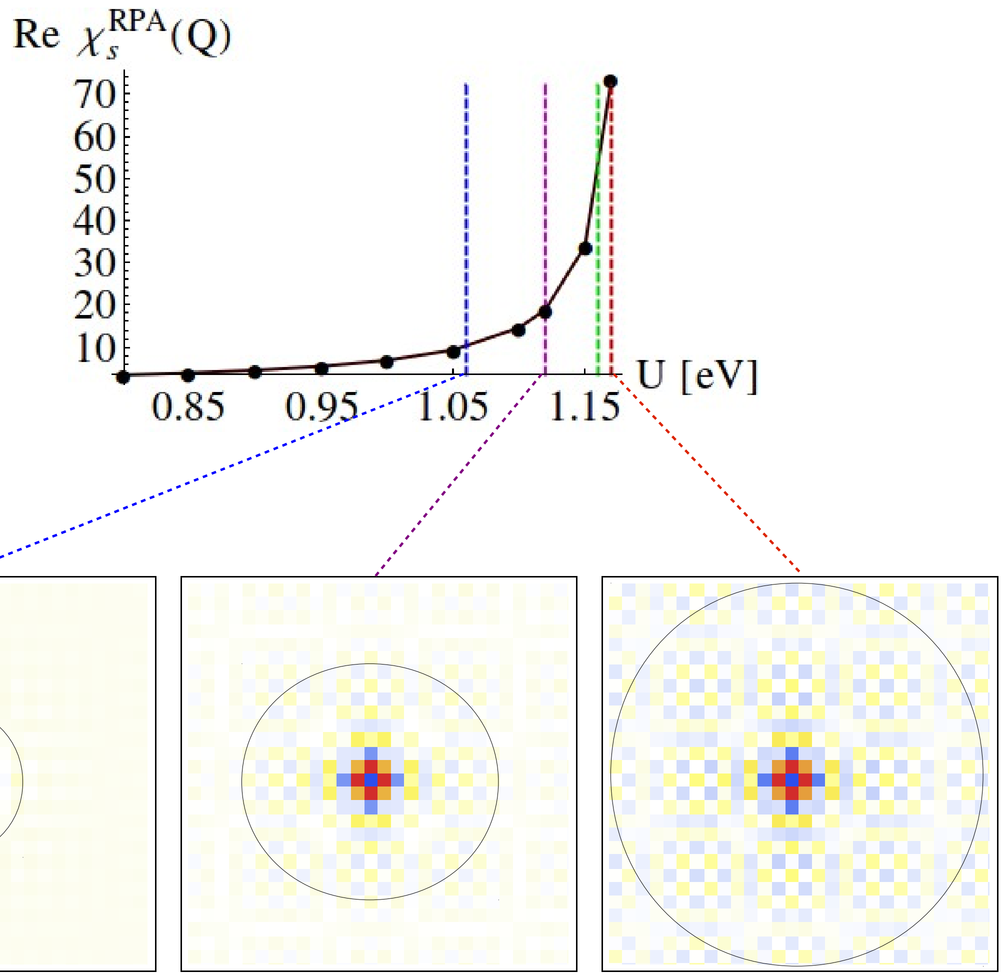
$$H_{int} = U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'}$$

$$- 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c^{\dagger}_{\mathbf{i}\mu\sigma} c^{\dagger}_{\mathbf{i}\mu\bar{\sigma}} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma},$$

$$H_{BCS} = - \sum_{\mathbf{i}\neq\mathbf{j},\mu\nu} [\Delta^{\mu\nu}_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\mu\uparrow} c^{\dagger}_{\mathbf{j}\nu\downarrow} + H.c.],$$

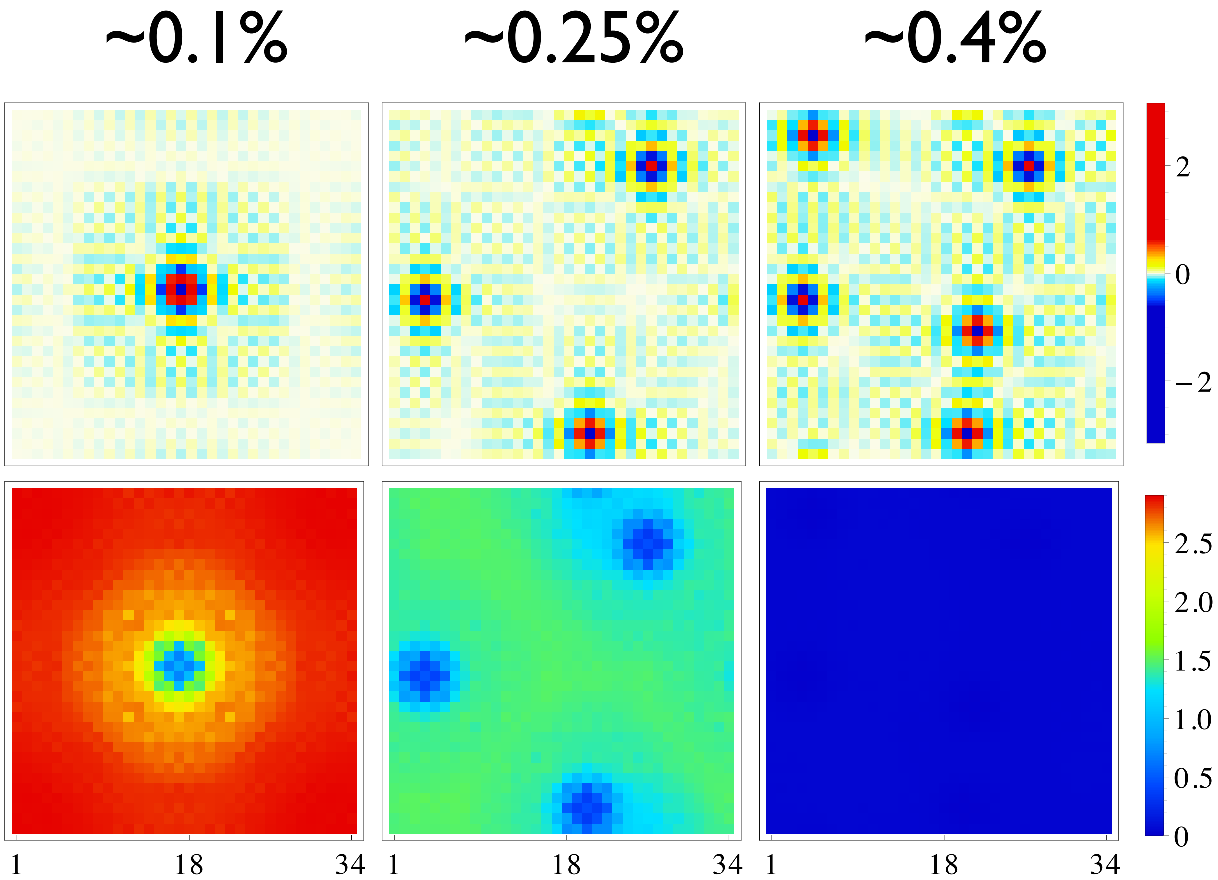
$$\mathcal{H}_{imp} = \sum_{\{\mathbf{i}^*\}\mu\sigma\sigma'} \mathbf{S}_{\mathbf{i}^*} \cdot (c^{\dagger}_{\mathbf{i}^*\mu\sigma} \sigma_{\sigma\sigma'} c_{\mathbf{i}^*\mu\sigma'}),$$

Study of magnetic disorder in the superconducting phase



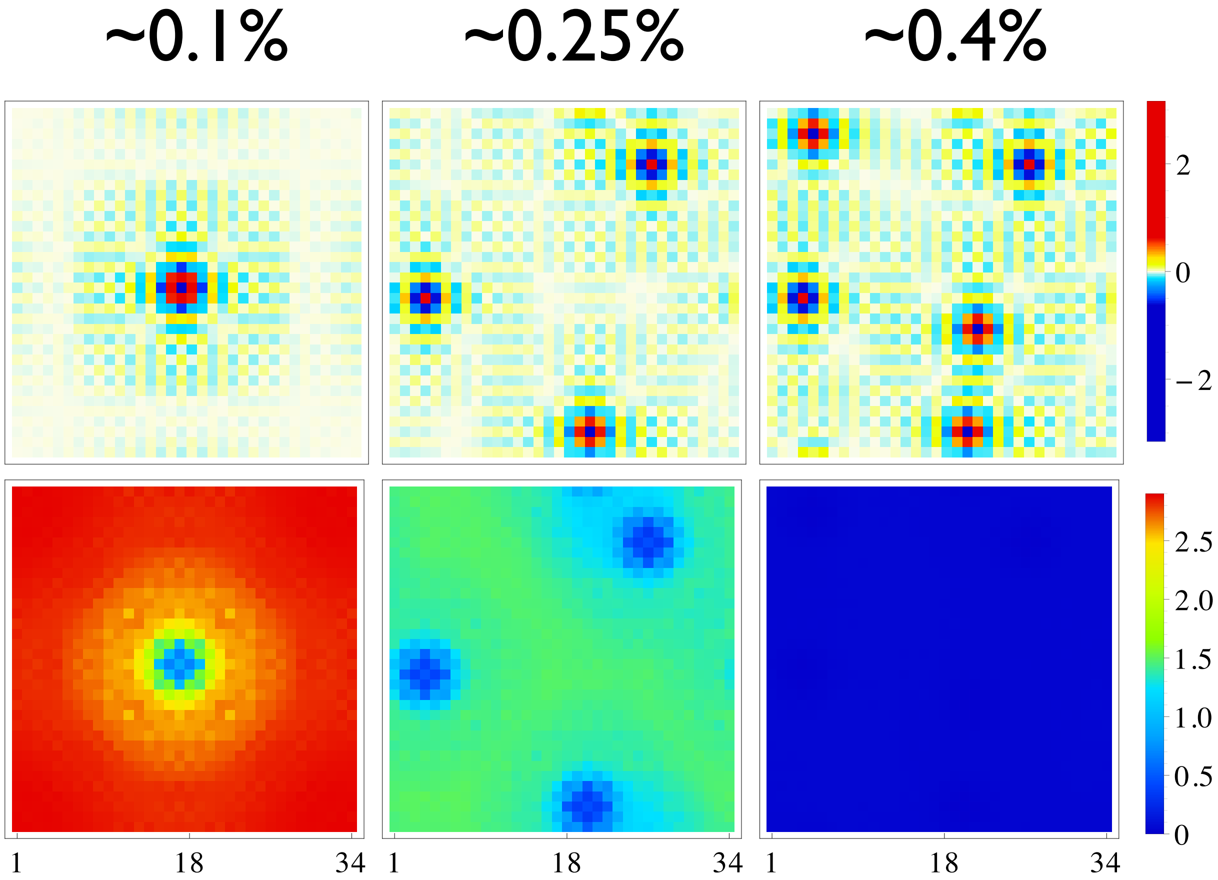
Growing magnetization bubble upon approaching the QCP

Study of magnetic disorder in the superconducting phase



Quasi-long-range magnetic order induced by very dilute disorder concentrations

Study of magnetic disorder in the superconducting phase



Quasi-long-range magnetic order induced by very dilute disorder concentrations

Thank you for your attention