Magnetic Response of the J_1-J_2 spin Hamiltonian and its Implications for FeAs

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arXiv : 0904.3809

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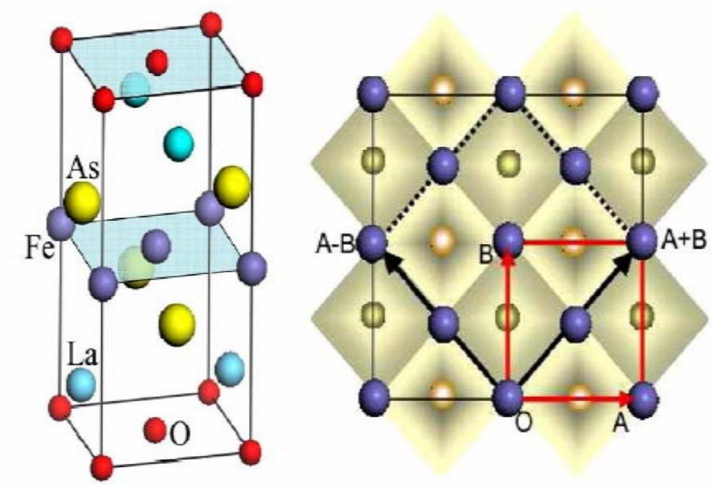
Introduction to FeAs parent compounds

- Consists of multilayered Fe planes
  - Fe^{2+} ions have 6 electrons in 5 *3d*–orbitals
  - Filling these orbitals depends on a delicate balance among a number of factors (*e.g. crystal field splitting, Hund's coupling, etc.)*
  - Electrical resistivity is large : $\rho \sim 5$ mΩcm corresponds to a normalized mean free path of ~ 0.5 Å

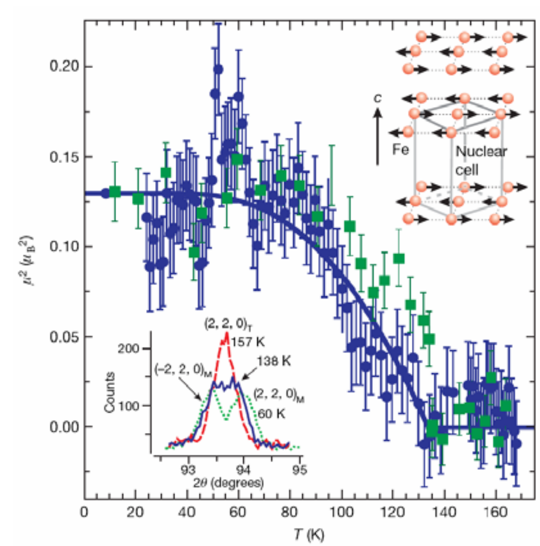
→ Thus it is a multiband bad metal



Yildirim,
PRL 101, 057010 (08)

Magnetic Properties of FeAs parent compounds

- Observed weak magnetic moments $\sim 0.4\ \mu_B$/Fe
  - $\sim$ 7 times smaller than LDA
- SDW order of $(\pi,0)$ sets in at $T_{SDW} \sim 137$ K
  - Preceded by structural phase transition from tetragonal to orthorhomic at ~150K
- <u>Shows linear-T susceptibility above T_{SDW}</u>
  - Since FeAs is a metal, convention dictates that it should follow Pauli (itinerant) or Curie-Weiss (local) susceptibility above T_{SDW}



C. De la Cruz, *et al.*
Nature 453, 899 (08)

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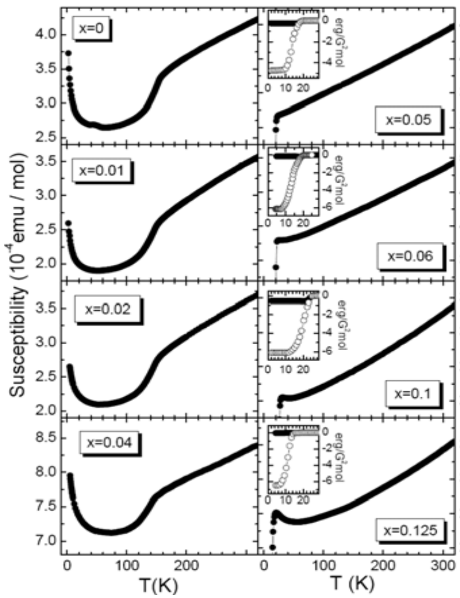
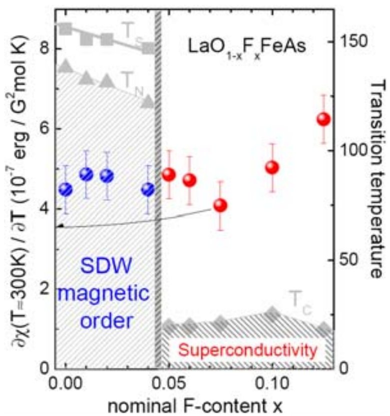
Linear T dependence of the susceptibility

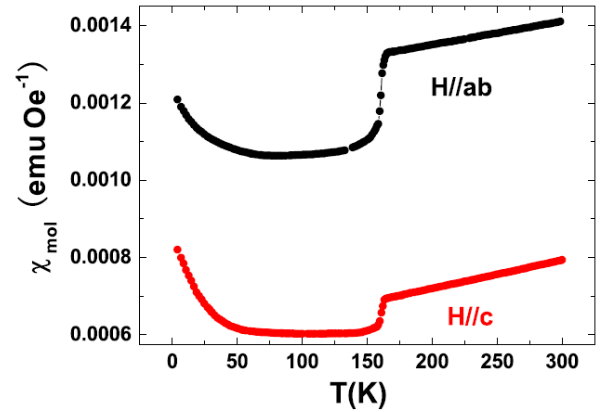
- From Experiments





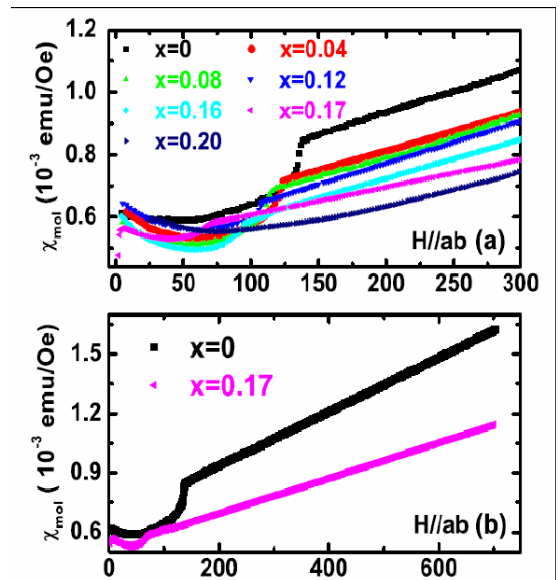
$LaFeAsO_{1-x}F_x$

Klingeler, *et al.*
arXiv:0808.0708v1



$Ca_{1-x}Na_xFe_2As_2$

Wu, *et al.*
JPhysCM 20, 422201 (08)

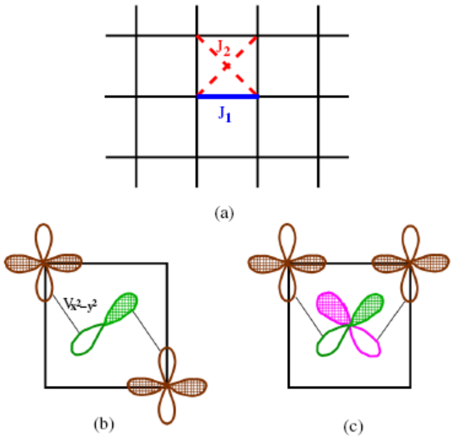


$BaFe_{2-x}Co_xAs_2$

Chen, *et al.*
NJP 11, 045003 (09)

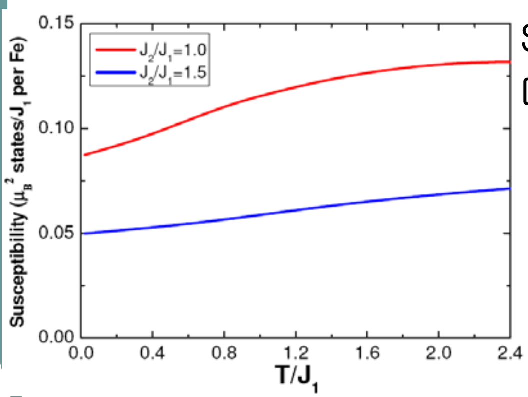
Linear T dependence of the susceptibility

- From Theory
  - Localized picture



J_1-J_2 spin Hamiltonian
Superexchange through As p-orbitals

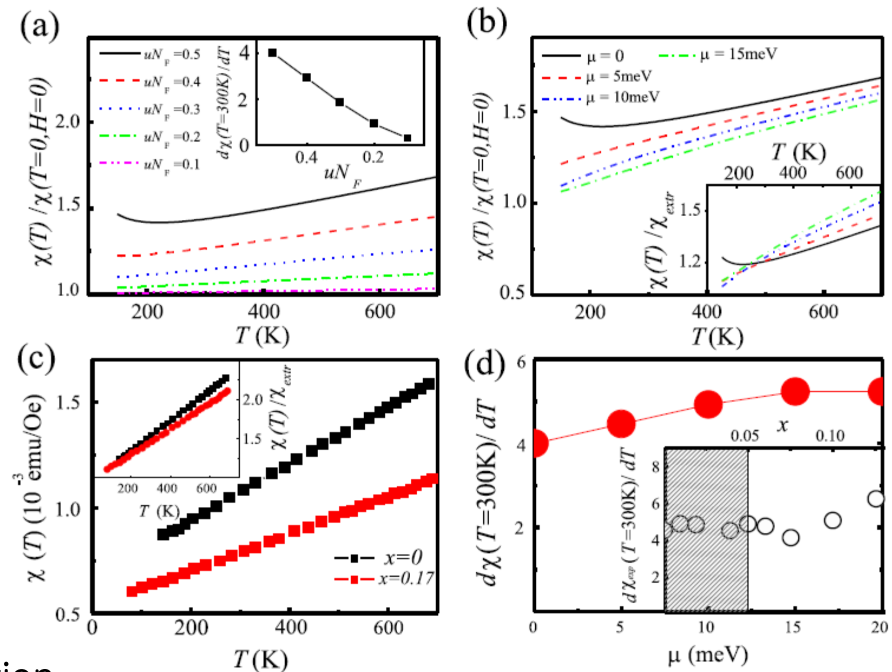
Si & Abrahams
PRL 101, 076401 (08)



SDW moment fluctuations
Dyson–Maleev representation

Zhang *et al.*
EPL 86, 37006 (09)

- Itinerant picture



2-band Hubbard model
Pauli–T^2 + T correction

Korshunov *et al.*
PRL 102, 236403 (09)

Where does FeAs fall?

- From LDA

  - $2J_2/J_1 > 1$

TABLE I: Parameters for AFe_2As_2 (A=Ba, Sr, Ca) in the nonmagnetic state (NM) and the collinear antiferromagnetic state (Col). The units for the carrier density ρ, the electronic specific heat coefficient γ, and the Pauli paramagnetic susceptibility χ are $10^{21}/cm^3$, $mJ/(K^2{*}\text{mol})$, and $10^{-9}m^3/\text{mol}$, respectively. J_1 and J_2 (meV/S^2) are the superexchange antiferromagnetic couplings between the nearest and the next nearest neighbor Fe spins $\vec{S}$, respectively.

AFe_2As_2	State	ρ		γ	χ	Coupling	
		hole	electron			J_1	J_2
$BaFe_2As_2$	NM	2.54	2.54	9.26	1.60	27.2	33.1
	Col	0.69	0.52	5.68			
$SrFe_2As_2$	NM	3.33	3.33	7.71	1.33	18.7	31.4
	Col	0.46	0.27	4.52			
$CaFe_2As_2$	NM	4.21	4.21	9.31	1.60	5.53	23.3
	Col	0.26	0.23	2.87			

Ma *et al.*
arXiv:0806.3526v2

  - $2J_2/J_1 < 1$

TABLE I. Calculated Fe moments (in μ_B) and in-plane exchange interactions (in meV), using experimental z(As).

System	Moment	J_{1a}	J_2	J_{1b}	$J_{1a}/2J_2$	$J_{1a}+2J_2$
LaFeAsO	1.69	47.4	22.4	−6.9	1.06	92.2
CeFeAsO	1.79	31.6	15.4	2.0	1.03	62.4
PrFeAsO	1.76	57.2	18.2	3.4	1.57	93.6
NdFeAsO	1.49	42.1	15.2	−1.7	1.38	72.5
$CaFe_2As_2$	1.51	36.6	19.4	−2.8	0.95	75.4
$SrFe_2As_2$	1.69	42.0	16.0	2.6	1.31	74.0
$BaFe_2As_2$	1.68	43.0	14.3	−3.1	1.51	71.5
KFe_2As_2	1.58	42.5	15.0	−2.9	1.42	72.5
LiFeAs	1.69	43.4	22.9	−2.5	0.95	89.2

Han *et al.*
PRL 102, 107003 (09)

Need to check whole range
$0 \le 2J_2/J_1 \le 2$

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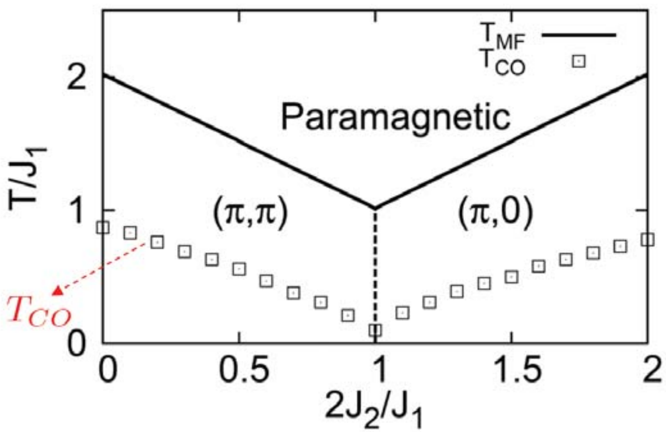
J_1–J_2 spin Hamiltonian (classical)

- Mean-field phase diagram

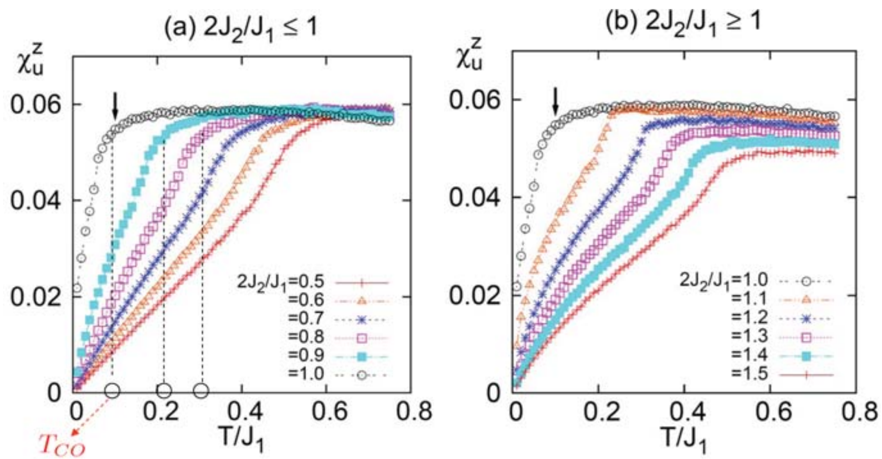


$$\langle S_i \rangle = m_1(-1)^{x_i} + m_2(-1)^{x_i + y_i}$$

(π,π) : $m_1=0$ & $m_2\neq0$

$(\pi,0)$: $m_1\neq0$ & $m_2=0$

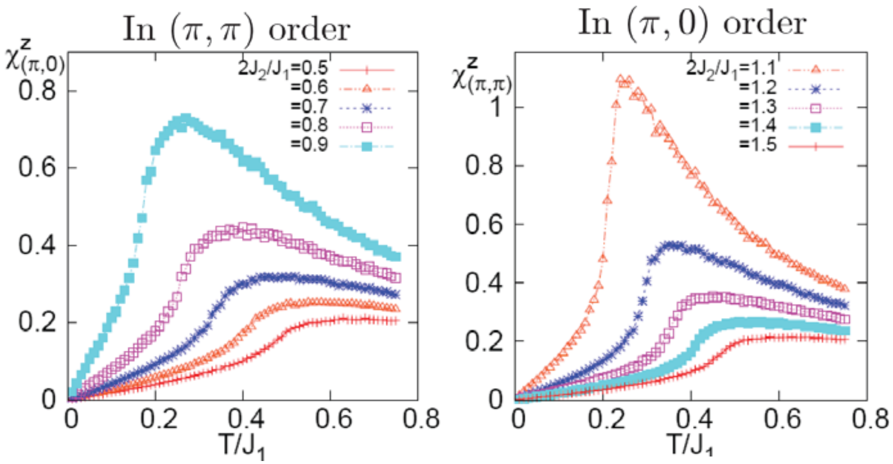
- Monte Carlo
  - Uniform susceptibility



Whole range of $0 \leq 2J_2/J_1 \leq 2$ shows linear T susceptibility

J1–J2 spin Hamiltonian (classical)

- Monte Carlo
  - Staggered susceptibility



- Dominant susceptibility diverges

  In (π,π) order $(2J_2/J_1 \leq 1)$, $\chi^z_{(\pi,\pi)}$

  In $(\pi,0)$ order $(2J_2/J_1 \geq 1)$, $\chi^z_{(\pi,0)}$

- Non-dominant, non-divergent susceptibilities

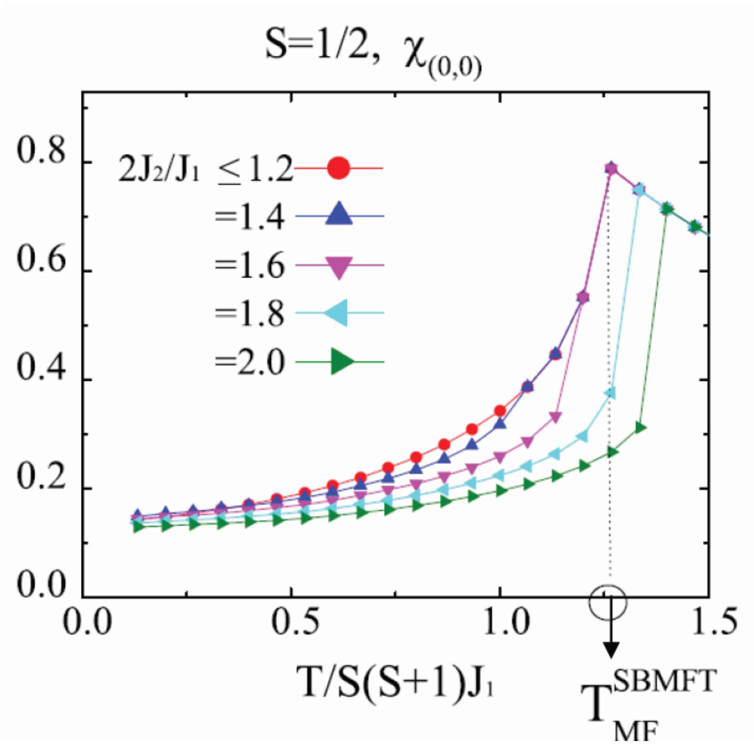
  In (π,π) order $(2J_2/J_1 < 1)$, $\chi^z_{(\pi,0)}$

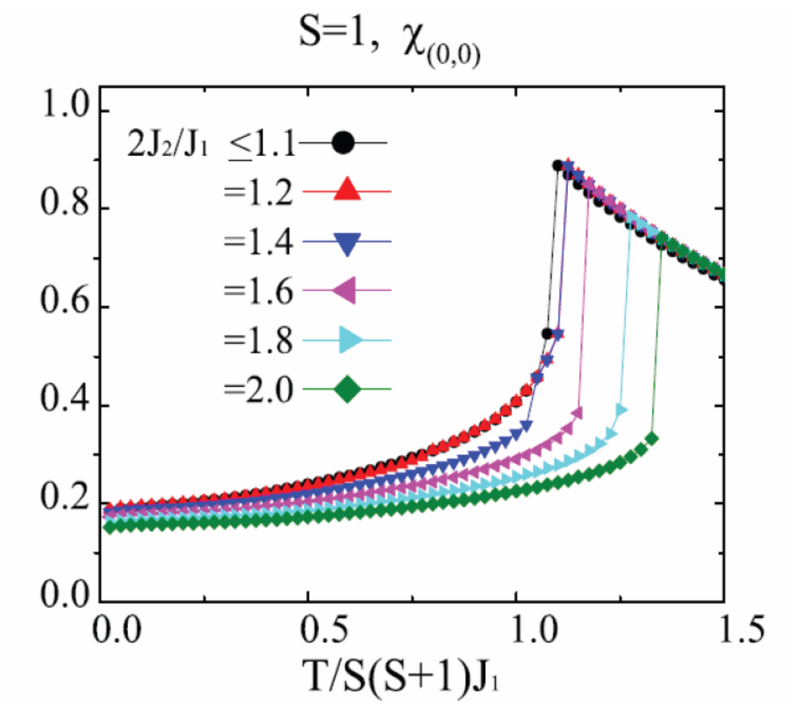
  In $(\pi,0)$ order $(2J_2/J_1 > 1)$, $\chi^z_{(\pi,\pi)}$

- Monte Carlo conclusions
  - Linear T dependence of uniform and staggered susceptibility in $0 \leq 2J_2/J_1 \leq 2$
  - $T_{CO} \sim 0.8J_1 \sim 400K$ which is close to FeAs (500–700K)
  - If localized physics is right, the linear-T susceptibility is well described by the J_1–J_2 classical spin Hamiltonian

J_1–J_2 spin Hamiltonian (quantum)

- Schwinger Boson mean field theory (SBMFT)





- **Linear-T behavior,** $\chi_{(0,0)} \sim A + BT$

  T$\in [0 \rightarrow (0.3J_1 \sim 0.9J_1)]$ $(S = \frac{1}{2})$

  T$\in [0 \rightarrow (0.4J_1 \sim 1.0J_1)]$ $(S = 1)$

- **In the J_1 only limit**

  $A = \frac{2}{C^2},\ C \sim 3.2,\ A \sim 0.19;.\quad B = \frac{ln(L/a)}{\pi \Delta_2^2}$

Conclusions & open questions

- The J_1–J_2 spin Hamiltonian captures the linear T behavior of the susceptibility for the range $0 \leq 2J_2/J_1 \leq 2$.
- The ratio of $2J_2/J_1$ still inconclusive for FeAs (LDA).
- Perhaps dimensionality plays a role (compare with Cr).
- Spin wave excitations well explained by J_1–J_2 spin physics yet other experiments (Haas-van Alphen, ARPES) favor itinerant picture.
- May need to find new scheme where itinerant and local pictures are compromised.