Magnetic response of the J_1-J_2 Spin Hamiltonian and its Implication for FeAs

arXiv:0904.3809

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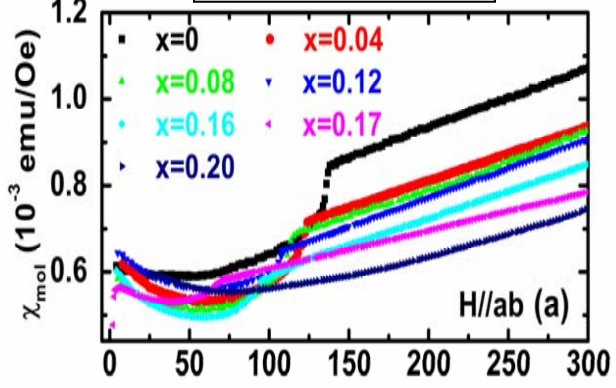
Magnetic properties of parent FeAs compounds

- Uniform magnetic susceptibility above SDW ordering(<200K)

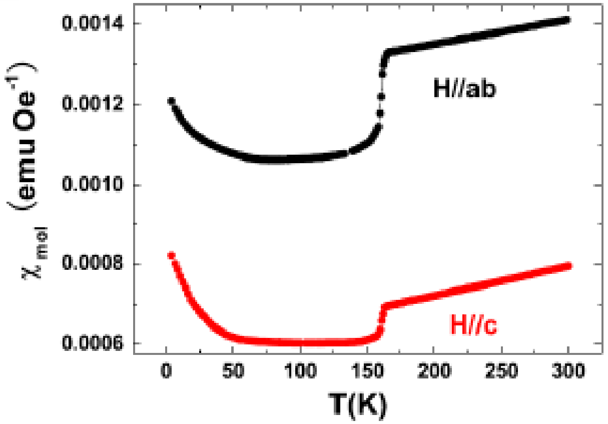
  - **Experiments:** T-linear over, *ie*., 150~500-700K!

$BaFe_{2-x}Co_xAs_2$



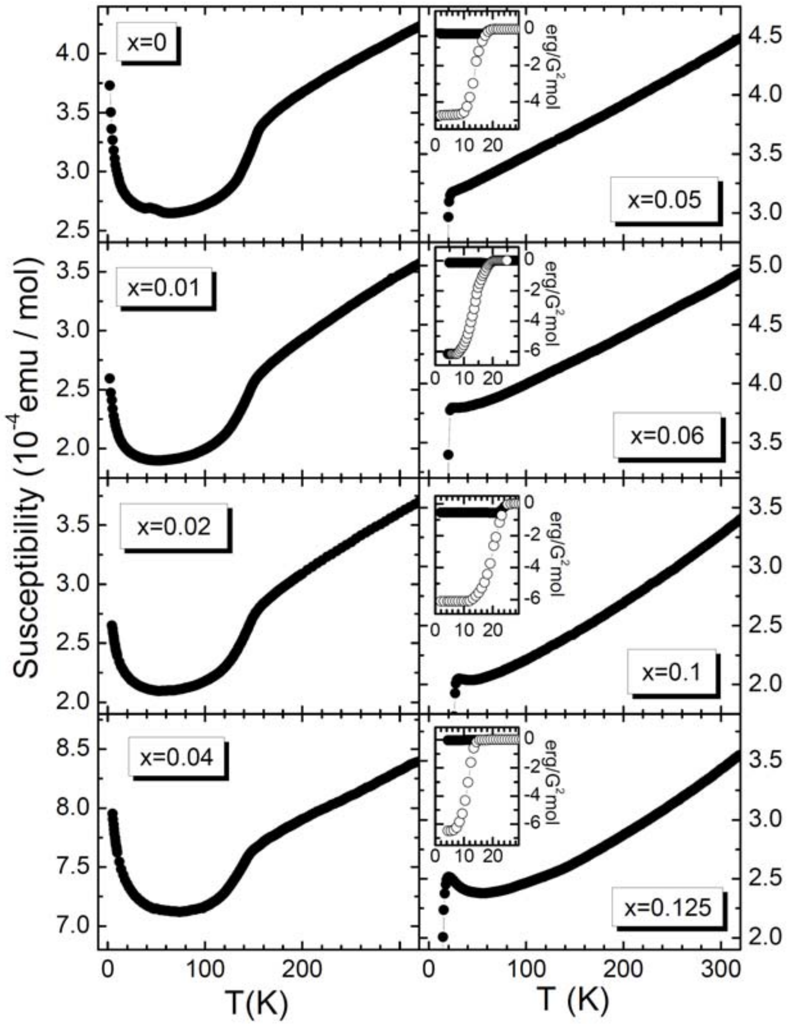
X.F.Wang, *et al*. NJP. 11, 0405(09)

$Ca_{1-x}Na_xFe_2As_2$



G. Wu, *et al*. JPhysC.20, 422201 (09)

$LaFeAsO_{1-x}F_x$



R.Klingeler,et al., arXiv:0808.0708v1

- In **disagreement with**

  Pauli-like (itinerant) or Curie-Weiss-like (local)

- T<T_{SDW} , AF SDW magnetic order: $(\pi, 0)$

  C.de la Cruz, *et al*., Nature(08)

- T>T_{SDW} , no global AF, ***a form of "correlated paramagnet"?***

Motivation

- **J_1-J_2 Spin Hamiltonian**

$$H \sim \sum_{ij} J_{ij}^{\alpha\beta} S_{i\alpha} \cdot S_{j\beta}$$

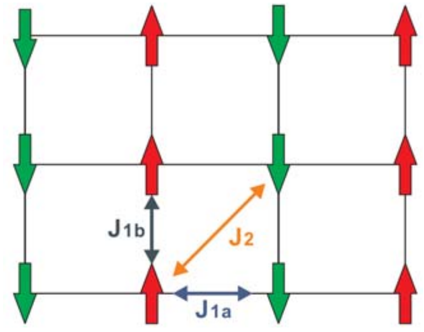
(Si & Abrahams, PRL(08))

Disregarding multi-orbital nature →

$$H = J_1 \sum_{<ij>} S_i \cdot S_j + J_2 \sum_{<<ij>>} S_i \cdot S_j$$

(Ma, Lu & Xiang, PRB (08))

- **Physical $2J_2/J_1$ parameters:** first-principles calculation by Han,Yin,Pickett & Savrasov, PRL (09))



Fe moments (in B),
in-plane exchange interactions (in meV)
using experimental z(As).

$2J_2/J_{1a}$:0.64~1.05

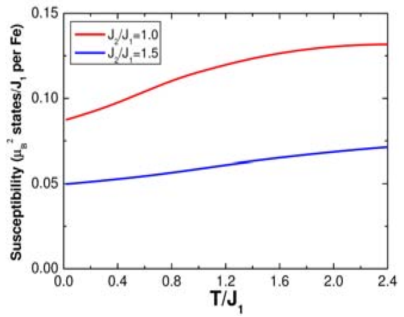
System	Moment	J_{1a}	J_2	J_{1b}	$J_{1a}/2J_2$	$J_{1a}+2J_2$
LaFeAsO	1.69	47.4	22.4	−6.9	1.06	92.2
CeFeAsO	1.79	31.6	15.4	2.0	1.03	62.4
PrFeAsO	1.76	57.2	18.2	3.4	1.57	93.6
NdFeAsO	1.49	42.1	15.2	−1.7	1.38	72.5
$CaFe_2As_2$	1.51	36.6	19.4	−2.8	0.95	75.4
$SrFe_2As_2$	1.69	42.0	16.0	2.6	1.31	74.0
$BaFe_2As_2$	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

- **Spin Hamiltonian for $T>T_{SDW}$, preformed moments exist (** G.M.Zhang, *et al*. EPL(09) **)**

- Linear-T uniform susceptibility

ie. Zhang *et al.(EPL,09)* $\chi_u = \chi_0 (1 + a(\frac{T}{J_1}))$ for J_2/J_1=1, 1.5

Kou *et al.(arXiv:0811.0411v3)* $\chi_u = \chi_{lo} + \chi_{it}$



How about the uniform and staggered susceptibilities in the whole range $2J_2/J_1$?

Abstract

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Classical Monte Carlo method   Schwinger boson mean field theory

↓

Antiferromagnetic J_1-J_2 Spin Hamiltonian

↓

$$\chi_k^\alpha = \frac{\left\langle S_{-k}^\alpha S_k^\alpha \right\rangle - \left\langle S_{-k}^\alpha \right\rangle \left\langle S_k^\alpha \right\rangle}{TN}$$

$S_k^\alpha = \sum_i S_i^\alpha e^{-ik\cdot r_i}$

$\alpha = x, y, z$

$N = L \times L$ is lattice size

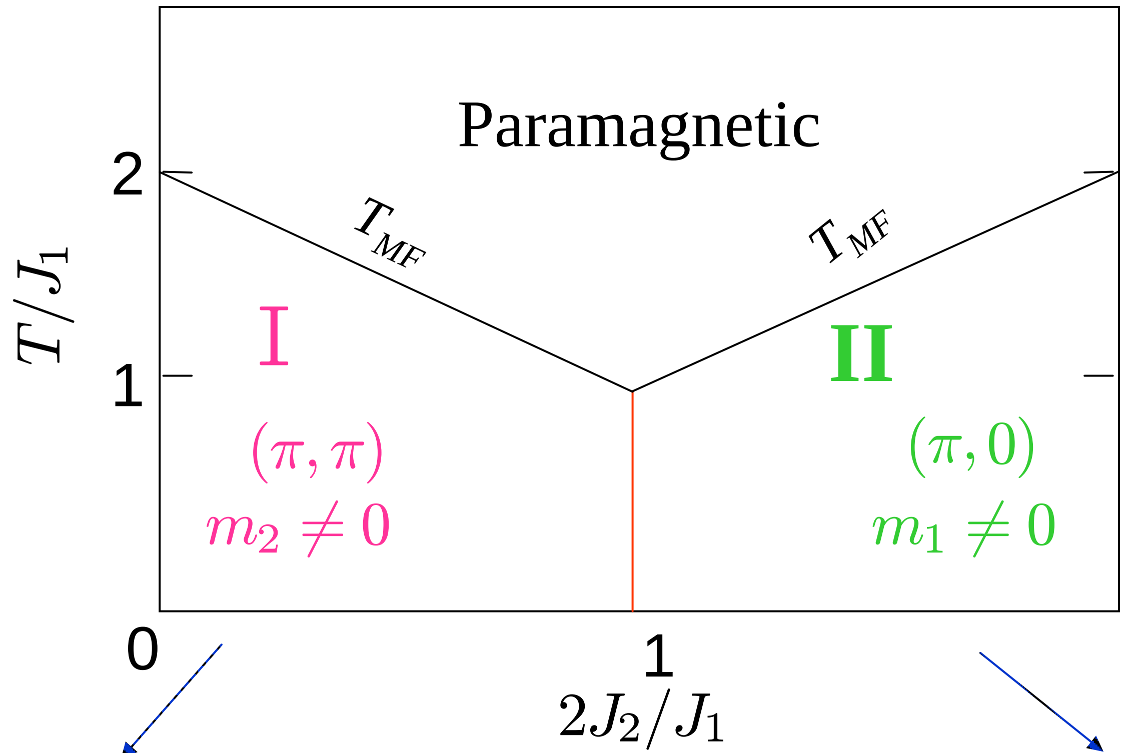
k =any vector !!

Magnetic susceptibilities at wave vecters : $k = (0,0),\ (\pi,0),\ (0,\pi), (\pi,\pi)$

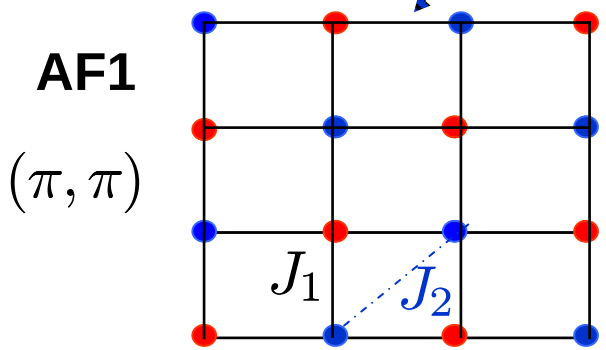
- A nearly linear-T behavior for the uniform susceptibility
- Implication for parent FeAs compounds

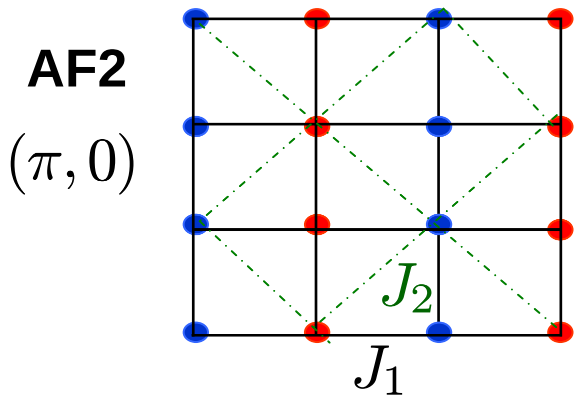
Review of Classical Mean Field Phase Diagram

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

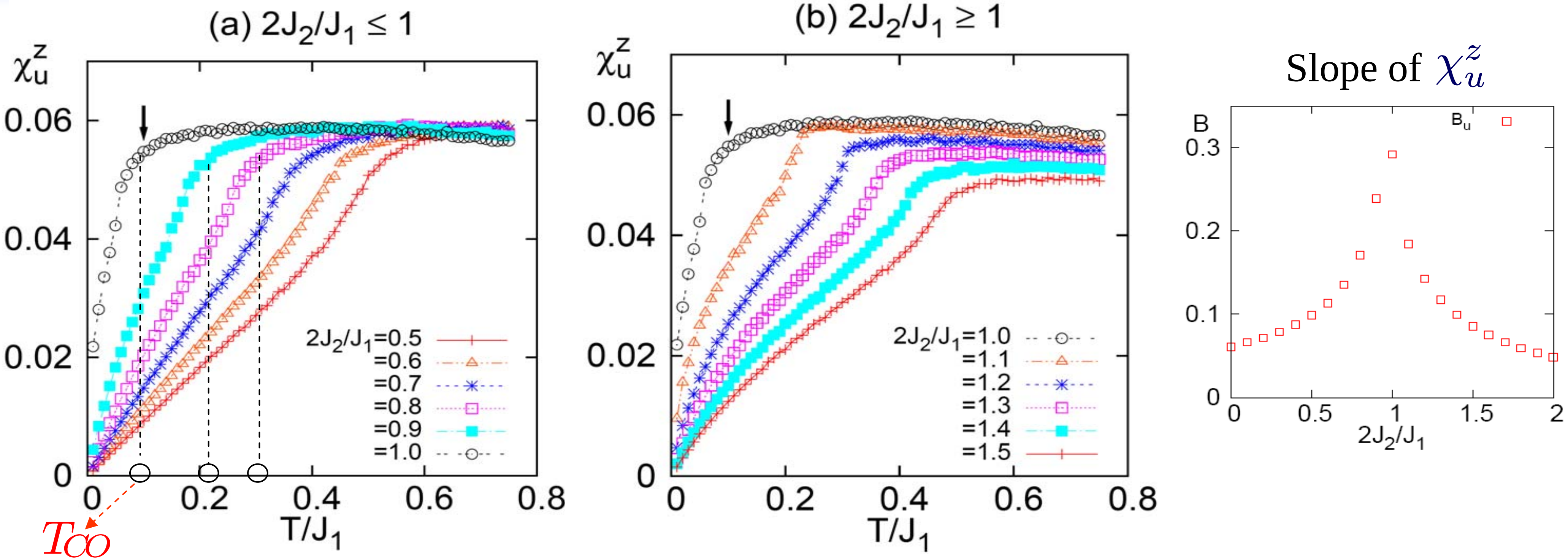


$(2J_2/J_1)_c$=1





Uniform susceptibility (classical Monte Carlo(CMC))



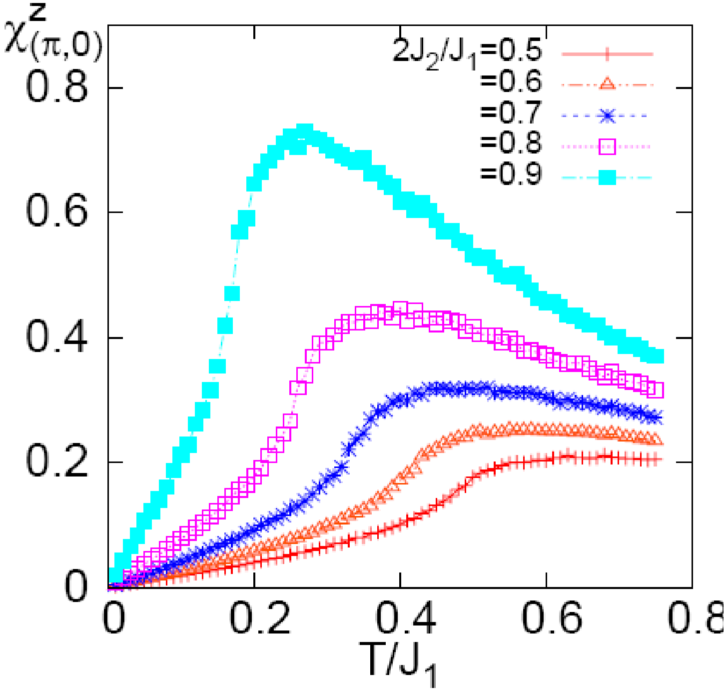
- The linear-T behavior of χ_u^z is a natural aspect of the J_1-J_2 spin model ;

- The crossover temperature T_{CO}~$0.8J_1$~400K ;

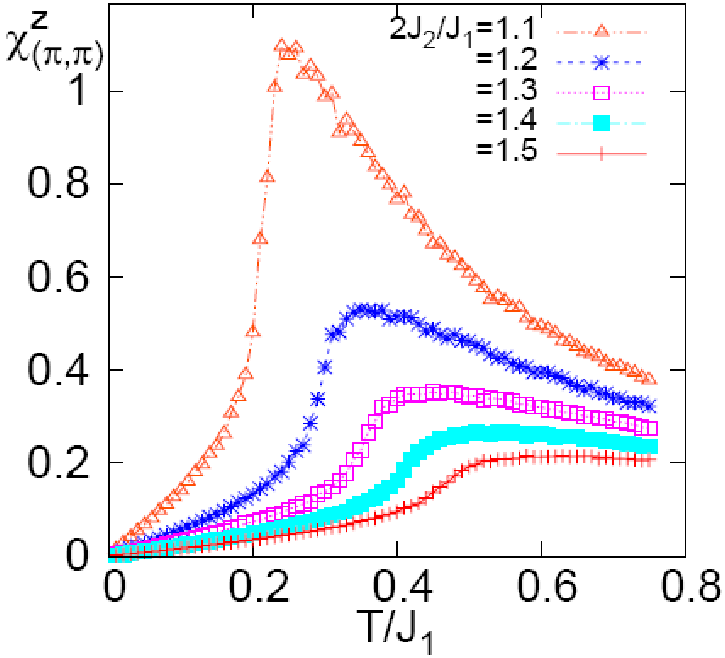
- The linearity of χ_u^z persists over a wider temperature range when the system is away from the critical value.

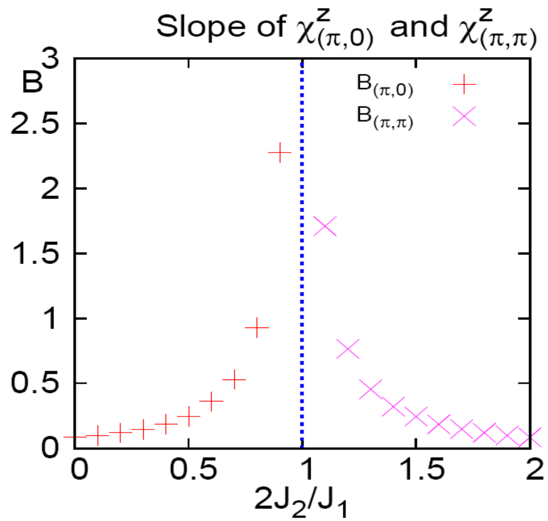
Staggered susceptibility (CMC)

In (π,π) order



In $(\pi,0)$ order





- Non-dominant, non-divergent susceptibilities , roughly linear
- A linear-T behavior with slope B

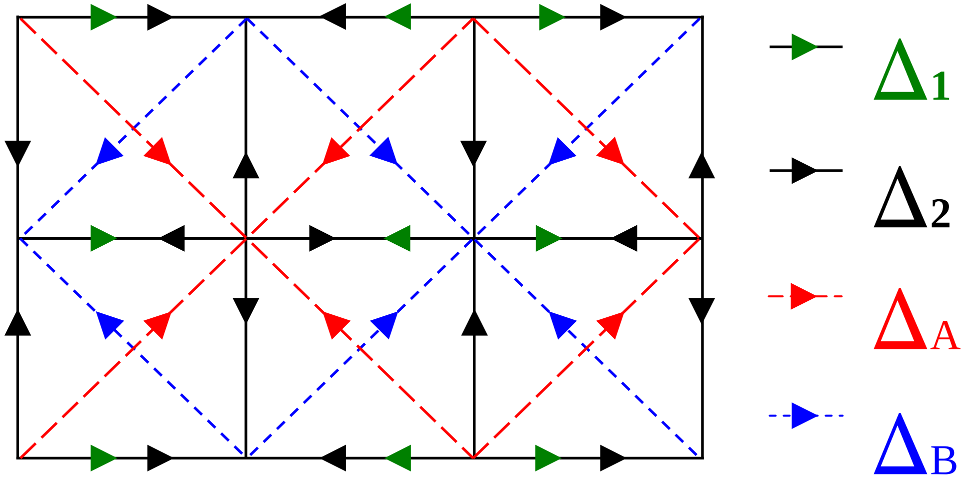
Schwinger Boson mean field theory(SBMFT)

- **J_1-J_2 Hamiltonian in mean field form**

$$\vec{S} = \frac{1}{2} b^\dagger_\alpha \vec{\sigma}_{\alpha\beta} b_\beta$$

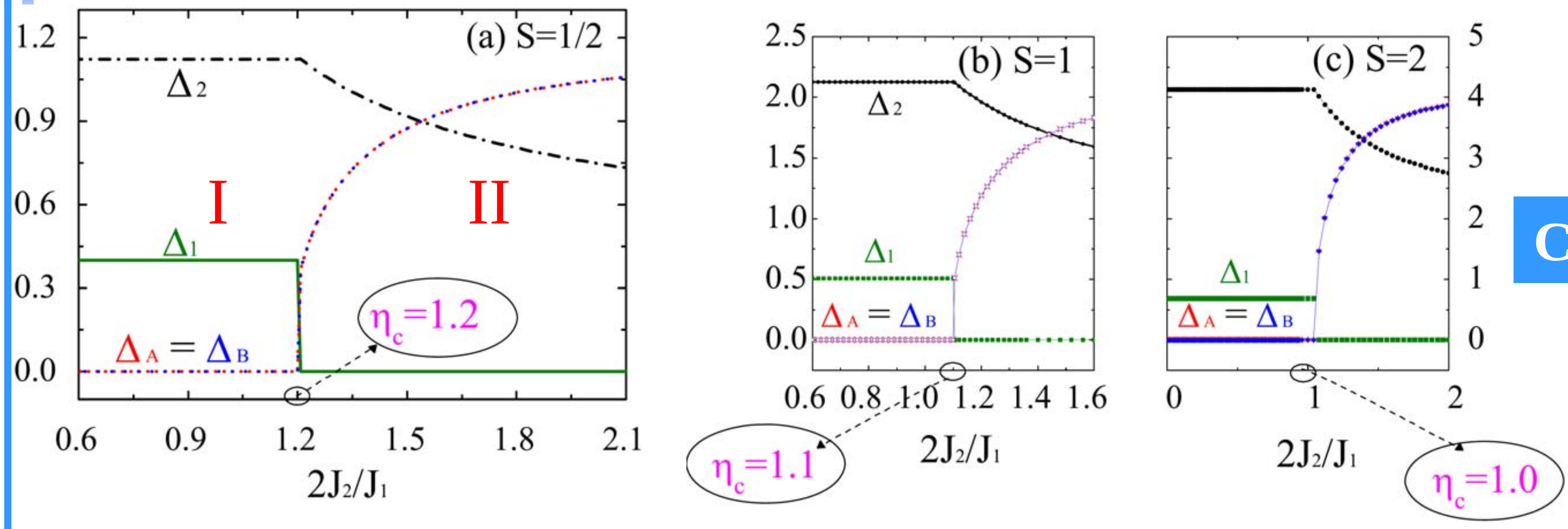
$$H_{MF} = -\frac{J_1}{2}\sum_{\langle ij\rangle}\Delta^*_{ij}A_{ij} - \frac{J_2}{2}\sum_{\langle\langle ij\rangle\rangle}\Delta^*_{ij}A_{ij} + h.c. + \sum_i \lambda_i\left(b^\dagger_{i1}b_{i1} + b^\dagger_{i2}b_{i2} - 2S\right)$$

where the operators are $A_{ij} = b_{i1}b_{j2} - b_{i2}b_{j1} = -A_{ji}$, $\Delta_{ij} = \langle A_{ij}\rangle$.



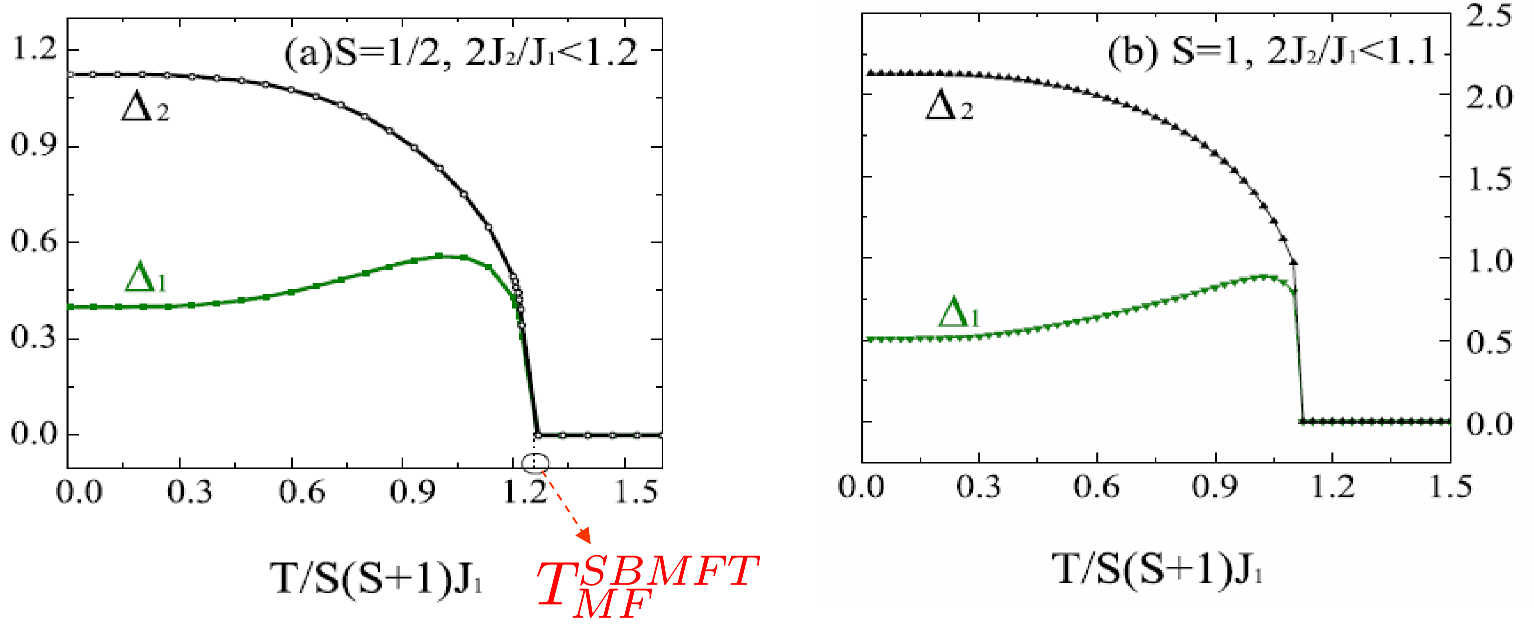
k	Gap parameters
(π,π)	Δ_2
$(\pi,0)$	$\Delta_{1,A,B}$

Gap parameters(SBMFT)



Critical point η_c

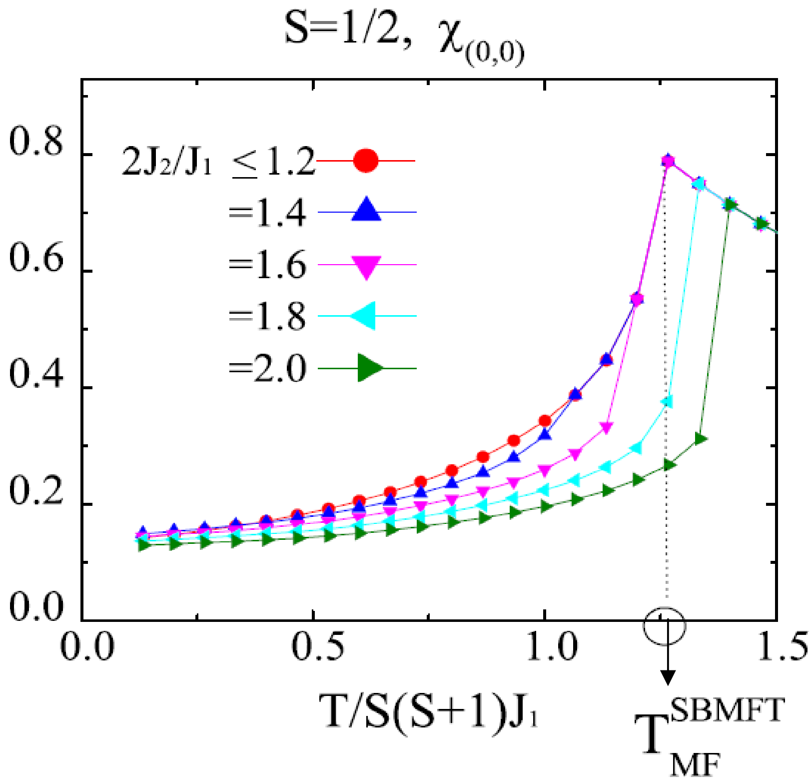
consistent with Capriotti,PRL (04)

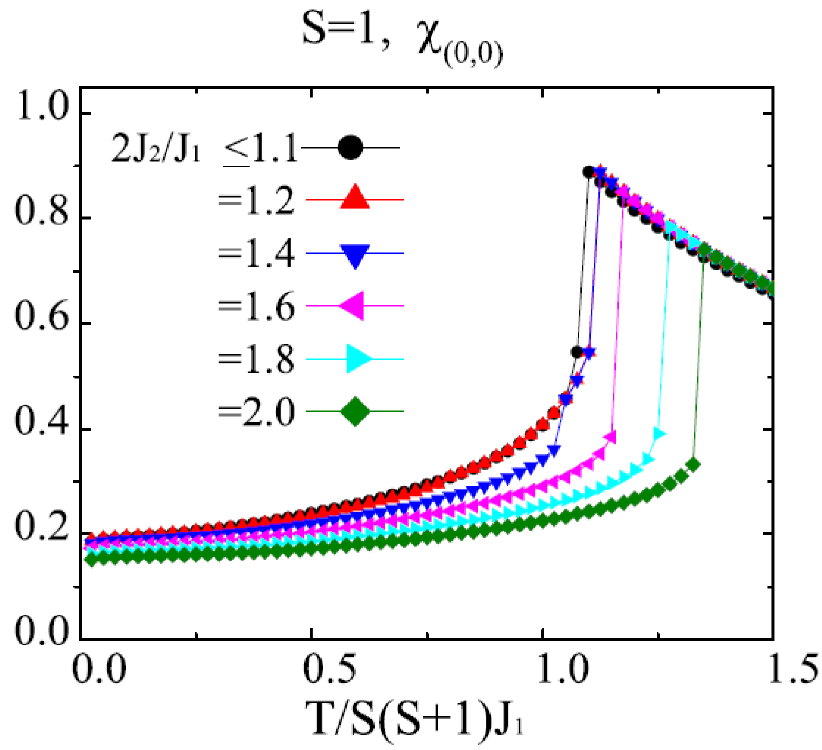


$T > T_{CO}^{SBMFT}$

Gap parameters=0

Uniform susceptibility(SBMFT)





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

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

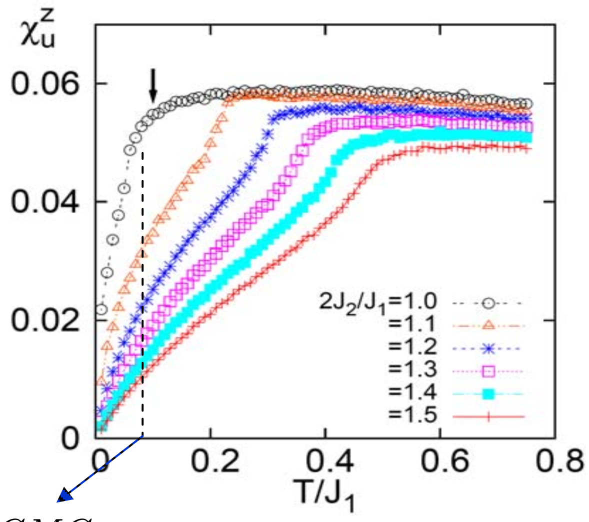
$$\text{T} \in [0 \rightarrow (0.4J_1 \sim 1.0J_1)]\ (S = 1)$$

- **In the J_1 only limit**

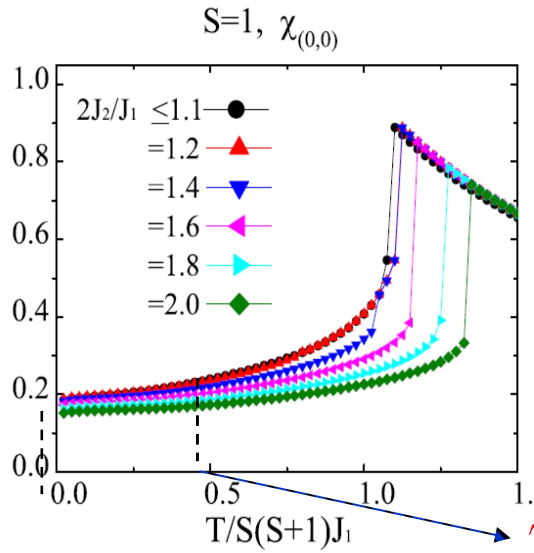
$$A = \frac{2}{C^2},\ C \sim 3.2,\ A \sim 0.19;. \quad B = \frac{ln(L/a)}{\pi \Delta_2^2}$$

CMC vs. SBMFT: uniform susceptibility &phase diagram

CMC

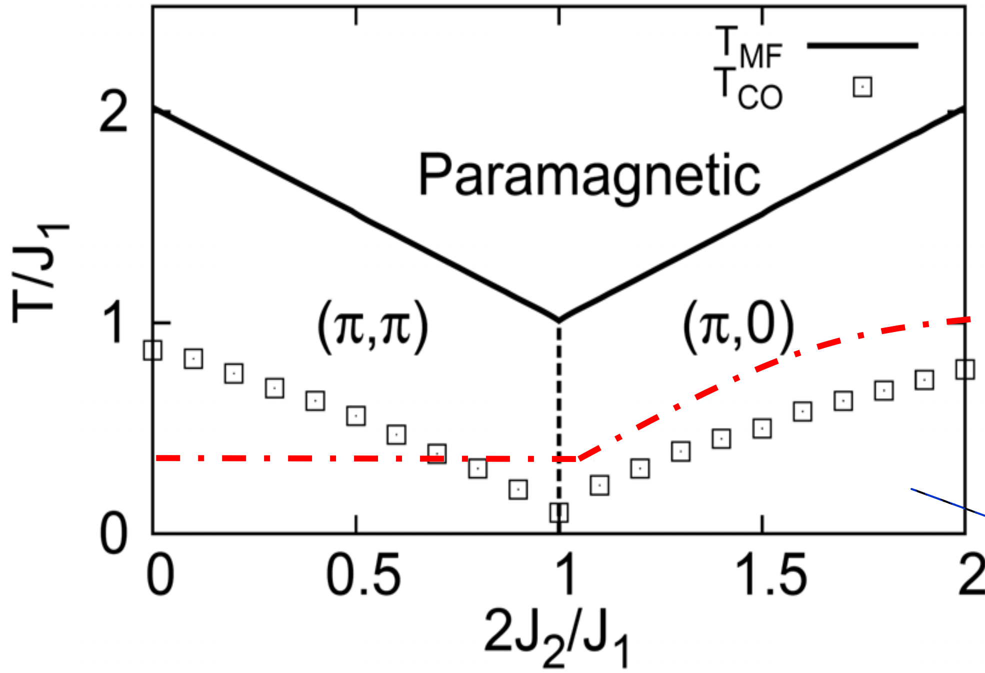


T_{CO}^{CMC}



SBMFT

T_{CO}^{SBMFT}

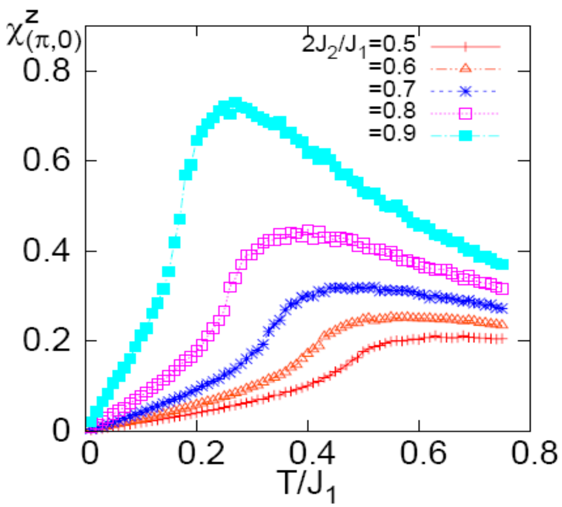
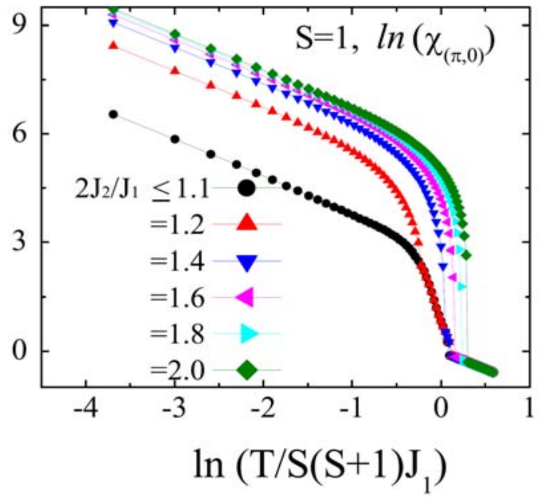
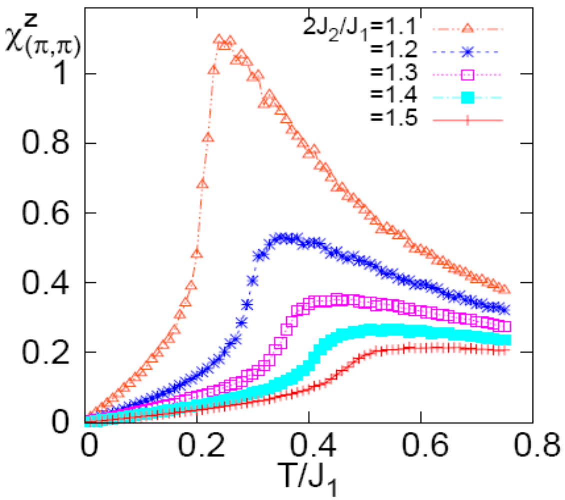
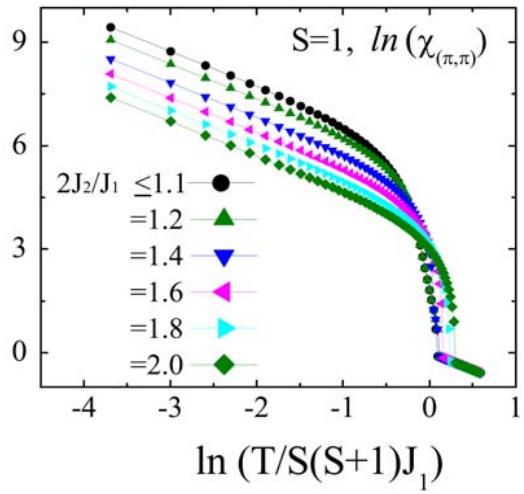


T_{CO}^{SBMFT}

T_{CO}^{CMC}

Linear-T region

CMC vs. SBMFT: staggered susceptibility

	CMC	SBMFT
in (π, π) order $\chi_{(\pi,0)}$		
in $(\pi, 0)$ order $\chi_{(\pi,\pi)}$		

Summary

- **We calculated the susceptibilities of J_1-J_2 model in $0<2J_2/J_1<2$**

  classical Monte Carlo(CMC) + Schwinger Boson mean field theroy(SBMFT)

- **The uniform susceptibilities by the two methods are consistent**

- $0< 2J_2/J_1<2$, uniform susceptibility--linear T dependence

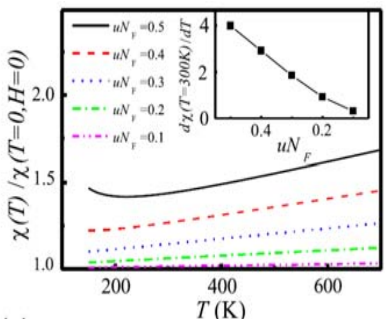
- largely independent of the degree of frustration in the spin model

- a wider linear temperature range when $2J_2/J_1$ is further removed from the critical point ,i.e. away from the critical point, $T\sim0.8J_1$-J_1→400K~500K

- in agreement with the persistence of linear susceptibility in FeAs compounds.

- **Future:local moments &itinerant electrons**

Itinerate electron model



Korshunov,et al., arXiv:0901.0238v1