

From 'Why DMFT?' to 'Why not DMFT!'

Swagata Acharya

King's College London

3rd Questaal Workshop, 2019

Daresbury, UK

KING'S
College
LONDON

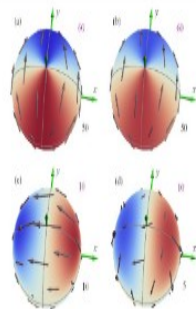
EPSRC, SIMONS FOUNDATION,
ARCHER UK



Quasiparticle Electronic Structure and Augmented LMTOs

MOST RECENT ARTICLE

Spin-orbit Torques in CoPt Multilayers

October 30, 2018 | [PAPERS](#) · [NONEQUILIBRIUM GREEN'S FUNCTIONS](#)

We have demonstrated the feasibility of calculating the spin-orbit torques in layered systems within density-functional theory, augmented by an Anderson model to treat disorder. Terms beyond the usual damping-like and field-like torques were found. While the torques that contribute to damping are almost entirely due to spin-orbit coupling on the Pt atoms, the field-like torque does not require it.

[Read More](#)

MORE ARTICLES

[Metal-insulator transition in copper oxides induced by apex displacements](#) · [EXAMPLES](#)[Many body response functions in the Questaal code](#) · [WORKSHOP](#)[Frolich contribution to energy band shifts in SrTiO3](#) · [NEWS](#)[Ladder Diagrams in QSGW](#) · [NEWS](#)[More Articles](#)

About Questaal

Questaal is a suite of programs for electronic structure simulations.

What are materials made of?

Around 2600 years back: Kanada and Democritus

ATOMS!

Space, time!

From Electrons to Atoms!

Walter Kohn, Landau : electrons!

Mott, Peierls, Van Vleck, Anderson, Hubbard and **Chemists** know it!

When John Hubbard started his career in theoretical physics it was known that a surprisingly good understanding of the electron gas in metals could be obtained by ignoring the Coulomb interaction among the electrons but there was no understanding of how to develop a consistent way to treat these interactions. John Hubbard's doctoral the-

T M Rice, 1980

From Electrons to Atoms: continued

While the importance of correlation in causing the breakdown of band theory and insulating character of magnetic insulators was known from the work of Mott, Peierls, Van Vleck and Anderson, it was John Hubbard who put the problem on a firm foundation. The famous Hubbard Hamiltonian for electron correlation is as crucial and fundamental as the Ising and Heisenberg Hamiltonian for localized spins and by now has spawned almost as much work. However the large literature on the Hubbard Hamiltonian that now exists also serves to emphasize the importance of his original contribution and the depth of his understanding. W.Kohn has described his contribution as "the basis of much of our present thinking about the electronic structure of large classes of metals and insulators". It is also the basis of much of what we are

T M Rice, 1980

Atomic correlations matter! How obvious is it?

From Electrons to Atoms: From Fermi gas to atomic multiplets

For most T and P: quasi-particles (Thanks to Lev Landau) are long lived



Large Fermi energy/quasi-particle coherence scale

From Electrons to Atoms: From Fermi gas to atomic multiplets

Some T, P, dopings: quasi-particles are absent



No Fermi energy/quasi-particle coherence scale -Atomic Multiplets

Most materials are in-between these two-extremes : small enough quasi-particle coherence scale and atomic like excitations

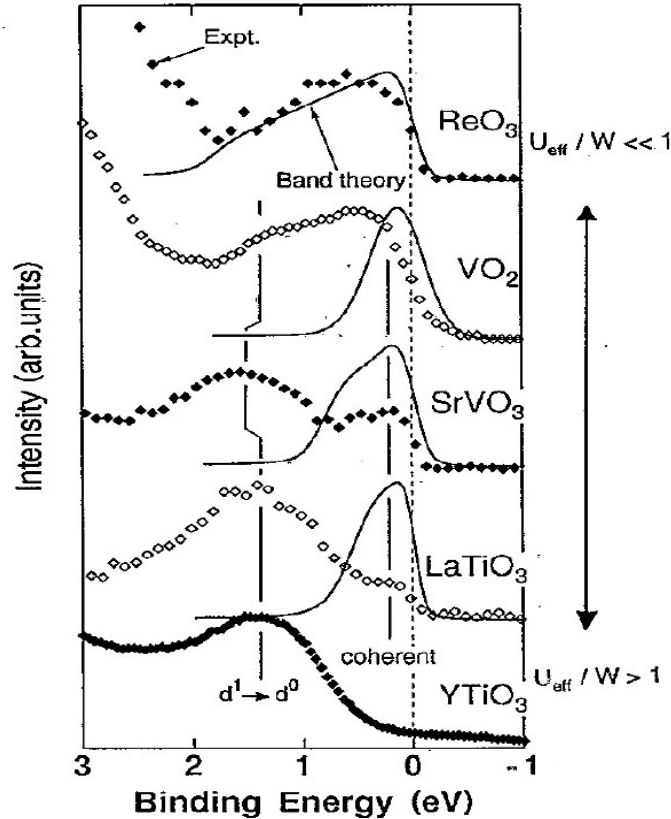
From Fermi gas to atomic multiplets : Do we see them?

Periodic Table of Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
1 H Hydrogen 1.008	2 He Helium 4.003											3 Li Lithium 6.941	4 Be Beryllium 9.012	5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948		
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.883	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80		
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.906	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.905	46 Pd Palladium 106.363	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.757	52 Te Tellurium 127.603	53 I Iodine 126.905	54 Xe Xenon 131.29		
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222		
87 Fr Francium 223	88 Ra Radium 226	89-103 Actinoids	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 263	107 Bh Bohrium 264	108 Hs Hassium 265	109 Mt Meitnerium 266	110 Ds Darmstadtium 267	111 Rg Roentgenium 268	112 Uub Ununbium 269	113 Uut Ununtrium 270	114 Uuq Ununquadium 271	115 Uup Ununpentium 272	116 Uuq Ununhexium 273	117 Uus Ununseptium 274	118 Uuo Ununoctium 276		

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

Design and Interface Copyright © 1997 Michael Dayan (michael@dayan.com), <http://www.ptable.com/>



Fujimori et al, PRL 69, 1796 (1992)

d¹ TM configuration

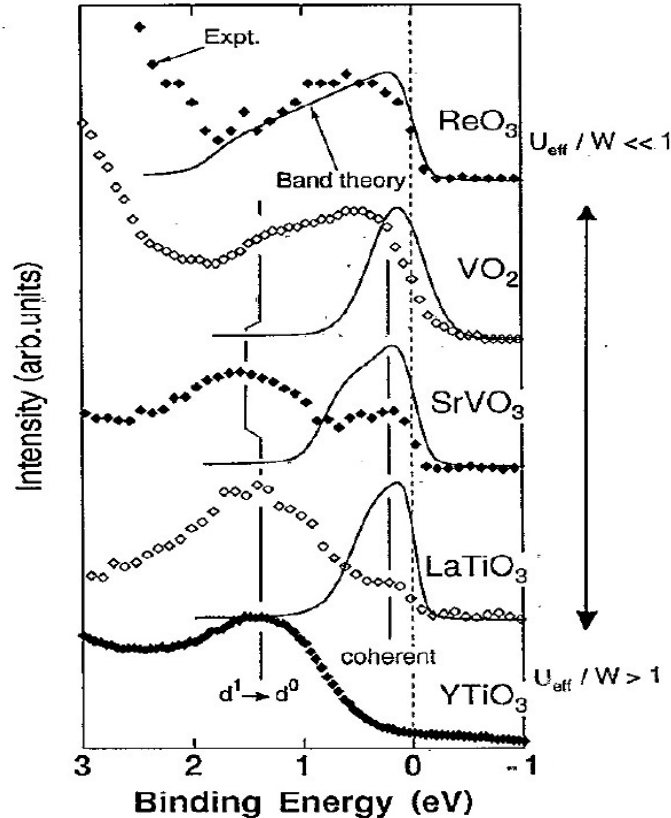
From Fermi gas to atomic multiplets : Do we see them?

Periodic Table of Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
1 H Hydrogen 1.00794	2 He Helium 4.002602											3 Li Lithium 6.941	4 Be Beryllium 9.012182	5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.00643	8 O Oxygen 15.999	9 F Fluorine 18.9984032	10 Ne Neon 20.1797
11 Na Sodium 22.98976928	12 Mg Magnesium 24.304											13 Al Aluminum 26.9815386	14 Si Silicon 28.0855	15 P Phosphorus 30.973762	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.948		
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938044	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.6305	33 As Arsenic 74.9216	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798		
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium 98	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.3631	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.90547	54 Xe Xenon 131.29		
55 Cs Cesium 132.90545196	56 Ba Barium 137.327	57-71 La-Lu Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.9804	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222		
87 Fr Francium 223	88 Ra Radium 226	89-103 Ac-Lr Actinides	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 263	107 Bh Bohrium 264	108 Hs Hassium 265	109 Mt Meitnerium 266	110 Ds Darmstadtium 267	111 Rg Roentgenium 268	112 Uub Ununbium 269	113 Uut Ununtrium 270	114 Uuq Ununquadium 271	115 Uup Ununpentium 272	116 Uuq Ununhexium 273	117 Uuh Ununheptium 274	118 Uuo Ununoctium 276		

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

Design and Interface Copyright © 1997 Michael Dayan (michael@dayan.com), <http://www.ptable.com/>

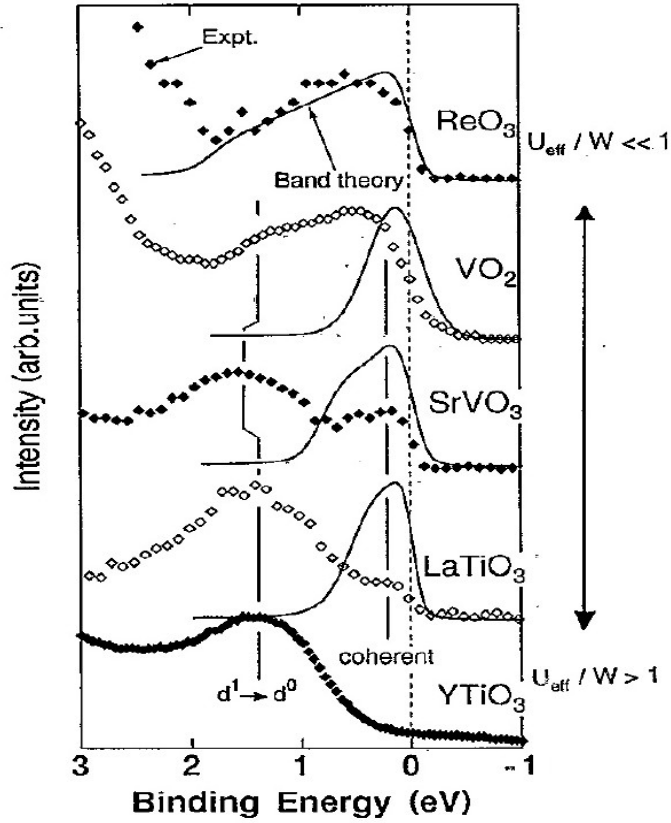
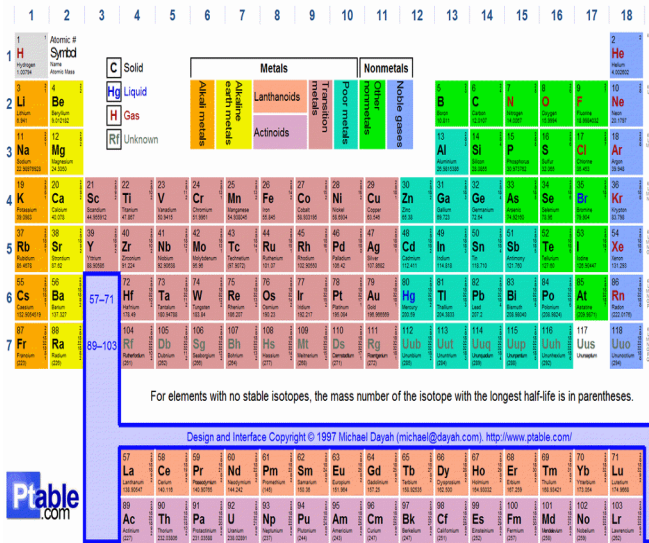


Fujimori et al, PRL 69, 1796 (1992)

d^1-d^0 transition-----LHB--- not a band, rather an atomic transition broadened by solid state env.

From Fermi gas to atomic multiplets : Low energy and high energy !

Periodic Table of Elements

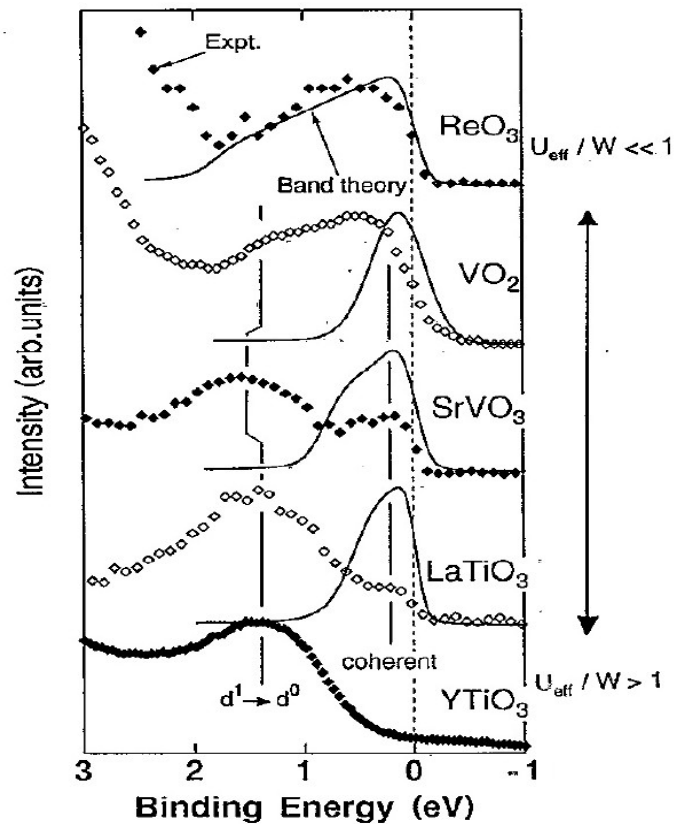


Fujimori et al, PRL 69, 1796 (1992)

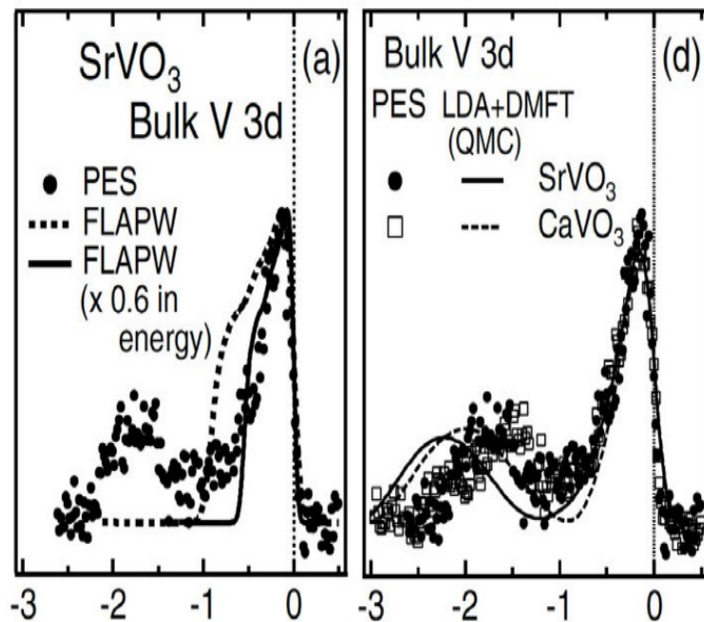
Band theory does not explain the spectral weight at rather high energies---atomic correlations --- the peak at -1.5 eV is there for both metals and Mott insulators: correlation and atomic physics matters in metals too

Band theory—can it explain low energy physics though?

From Fermi gas to atomic multiplets : Low energy and high energy !



Fujimori et al, PRL 69,
1796 (1992)



Low energy quasiparticle coherence scale ($z = m/m^*$) needs to be rescaled by a factor of 2 from band theory calculations ---one would imagine it could driven to 0 by continuously making it narrower

Sekiyama et al.,
PRL 93, 156402
(2004)

Theory for explaining high and low energy physics

The Brinkman-Rice transition

Correlated metallic state. Fermi liquid like approach

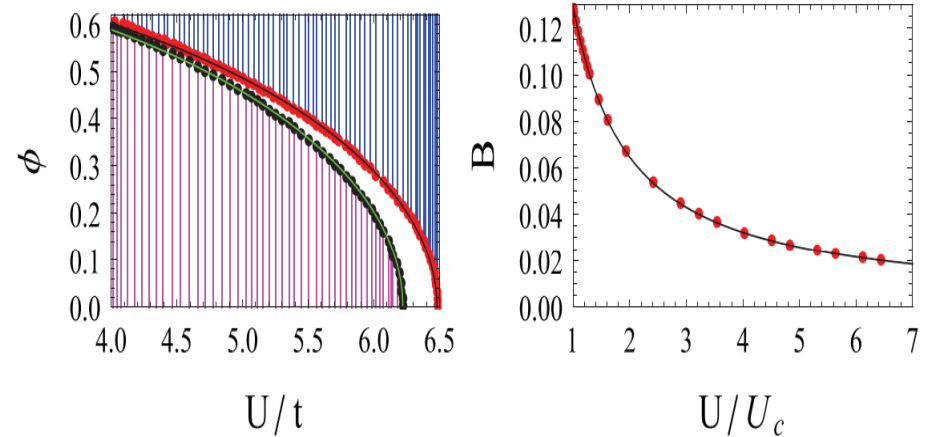
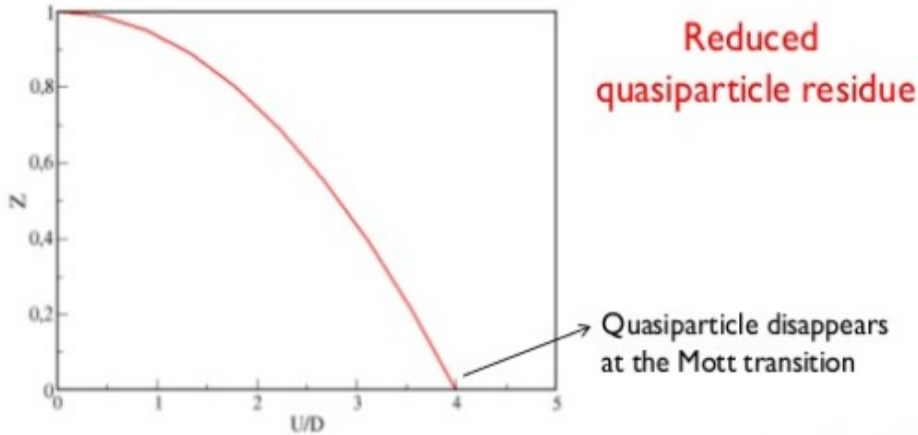
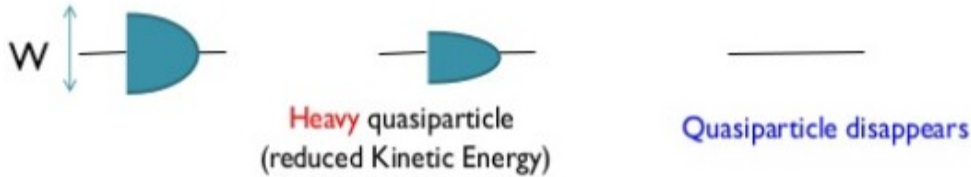


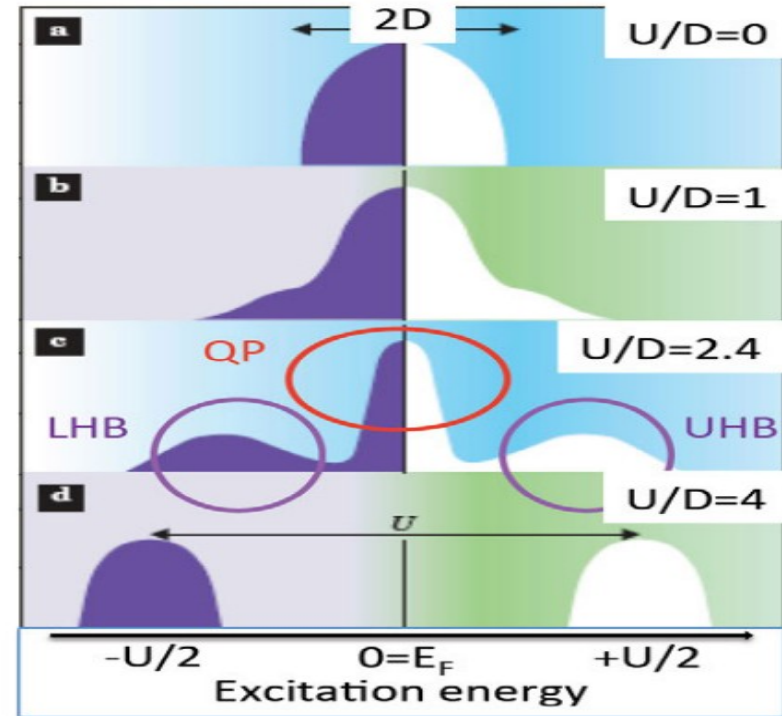
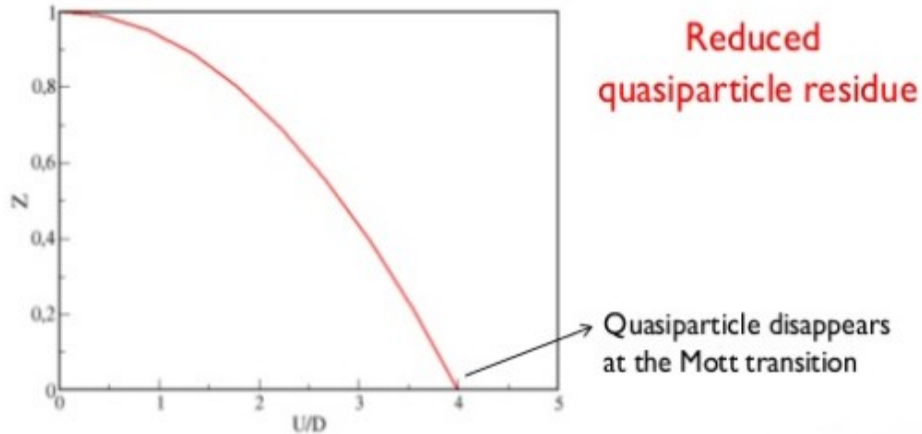
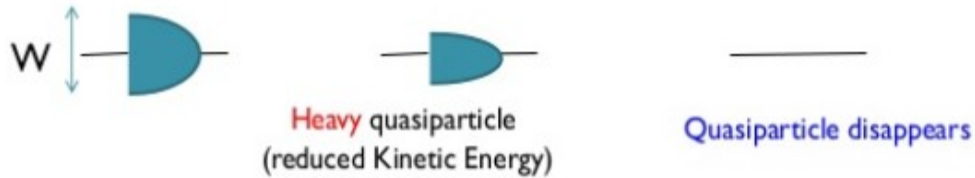
Figure 1. Left: ϕ is plotted against U/t for single-site (red dots are data points and the black continuous curve is a fit to the Brinkman–Rice picture) and cluster approximations (black dots are data points and the continuous green line is the Brinkman–Rice fit). The critical values of U/t for MIT are 6.483 and 6.214 in single-site and cluster analyses, respectively. Right: the inter-site correlation from the cluster analysis in the insulating phase (red dots) and the fit to t^2/U (black curve).

But then what happens to the rest of the spectral weight? Where do they go?

Theory for explaining high and low energy physics

The Brinkman-Rice transition

Correlated metallic state. Fermi liquid like approach



But then what happens to the rest of the spectral weight? Where do they go?

Theory for explaining high and low energy physics

is lowered. This is what Dynamical Mean-Field Theory (DMFT) does. The term *dynamical* is perhaps not ideally chosen, since we are not talking here about the out-of-equilibrium dynamics of the system. Instead, it indicates that the theory handles the different time-scales or energy-scales involved in the excitation spectrum of the system at equilibrium. In order to do so, DMFT introduces a generalization of the classical Weiss mean-field concept to that of a full function of energy (or time scale).

A Georges

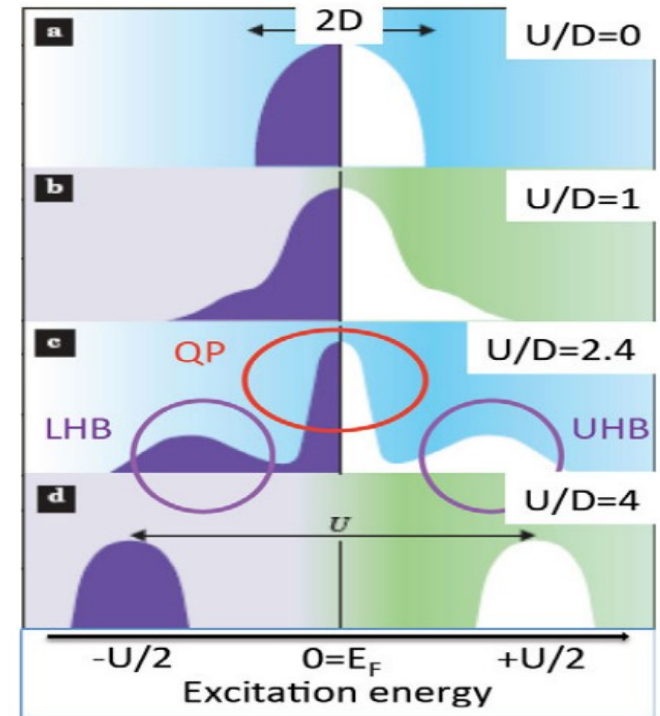
E. Pavarini, E. Koch, D. Vollhardt, and A. Lichtenstein

DMFT at 25: Infinite Dimensions

Modeling and Simulation Vol. 4

Forschungszentrum Jülich, 2014, ISBN 978-3-89336-953-9

<http://www.cond-mat.de/events/correll14>



But then what happens to the rest of the spectral weight? Where do they go?

DMFT: How does it work?

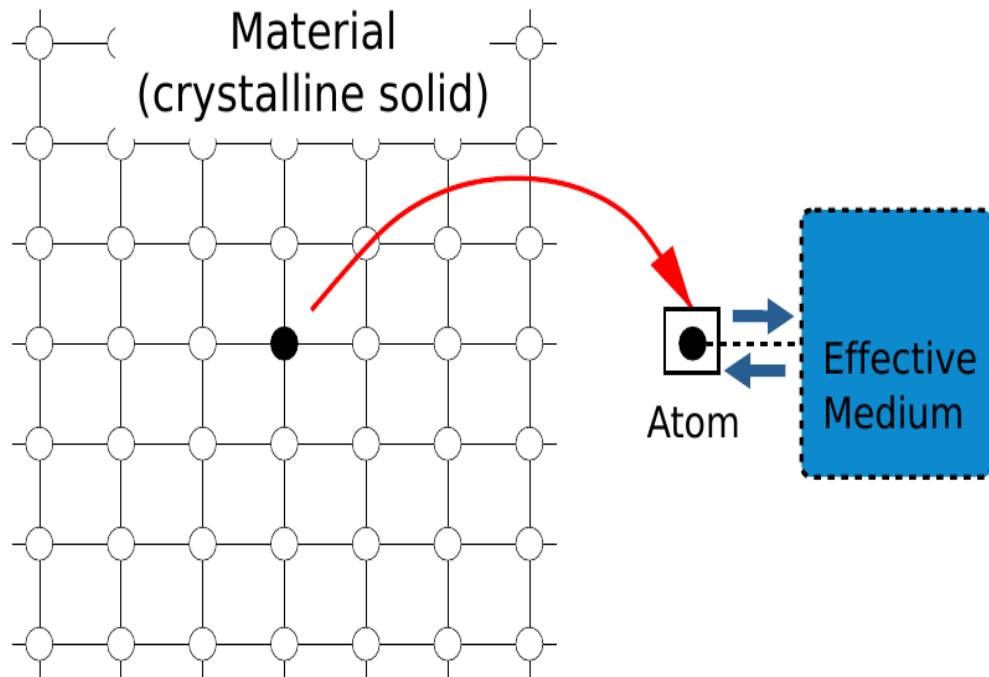


Fig. 6: *The Dynamical Mean-Field Theory (DMFT) concept. A solid is viewed as an array of atoms exchanging electrons, rather than as a gas of interacting electrons moving in a periodic potential. DMFT replaces the solid by a single atom exchanging electrons with a self-consistent medium and takes into account local many-body correlations on each site.*

$$G_{\text{imp}}^{(i\omega)} = \frac{1}{i\omega + \mu - \Delta - \Sigma(i\omega)}$$

$$G(\mathbf{k}, i\omega) = \frac{1}{i\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, i\omega)}$$

$$G_{\text{imp}}^{(i\omega)} = \sum_{\mathbf{k}} G(\mathbf{k}, i\omega)$$

$$G_{\text{imp}}[i\omega_n, \Delta] = \sum_{\mathbf{k}} \frac{1}{G_{\text{imp}}[i\omega_n; \Delta]^{-1} + \Delta(i\omega_n) - \epsilon_{\mathbf{k}}}$$

DMFT: When does it work?

The single-site DMFT construction becomes exact in the following limits.

- In the atomic limit $t_{ij} = 0$, by construction (then, $\Delta = 0$).
- In the non-interacting limit $U = 0$. Indeed, in this case the self-energy $\Sigma = 0$, so that it is trivially \mathbf{k} -independent.
- Hence, both the limit of a non-interacting band and that of isolated atoms are correctly reproduced by DMFT, which provides an interpolating scheme between these extreme cases.
- In the limit of infinite lattice coordination (infinite number of spatial dimensions), first introduced for fermions in the pioneering work of Metzner and Vollhardt [23]. The hopping must be scaled as $t_{ij} = t/\sqrt{d}$ for this limit to be properly defined and non-trivial.
- Being an exact solution of Hubbard-like models in the limit of infinite dimensions, it is thus guaranteed that DMFT preserves all sum-rules and conservation laws.

DMFT: Let's simplify one step further

TABLE 1. Correspondance between the mean-field theory of a classical system and the dynamical mean-field theory of a quantum system.

Quantum Case	Classical Case	
$-\sum_{ij\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + \sum_i H_{atom}(i)$	$H = -\sum_{(ij)} J_{ij} S_i S_j - h \sum_i S_i$	Hamiltonian
$G_{ii}(i\omega_n) = -\langle c_i^+(i\omega_n) c_i(i\omega_n) \rangle$	$m_i = \langle S_i \rangle$	Local Observable
$H_{eff} = H_{atom} + \sum_{l\sigma} \tilde{\epsilon}_l a_{l\sigma}^+ a_{l\sigma} + \sum_{l\sigma} V_l (a_{l\sigma}^+ c_{\sigma} + h.c)$	$H_{eff} = -h_{eff} S$	Effective single-site Hamiltonian
$\Delta(i\omega_n) = \sum_l \frac{ V_l ^2}{i\omega_n - \epsilon_l}$ $\mathcal{G}_0^{-1}(i\omega_n) \equiv i\omega_n + \mu - \Delta(i\omega_n)$	h_{eff}	Weiss function/Weiss field
$\sum_{\mathbf{k}} [\Delta(i\omega_n) + G(i\omega_n)^{-1} - \epsilon_{\mathbf{k}}]^{-1} = G(i\omega_n)$	$h_{eff} = \sum_j J_{ij} m_j + h$	Self-consistency relation

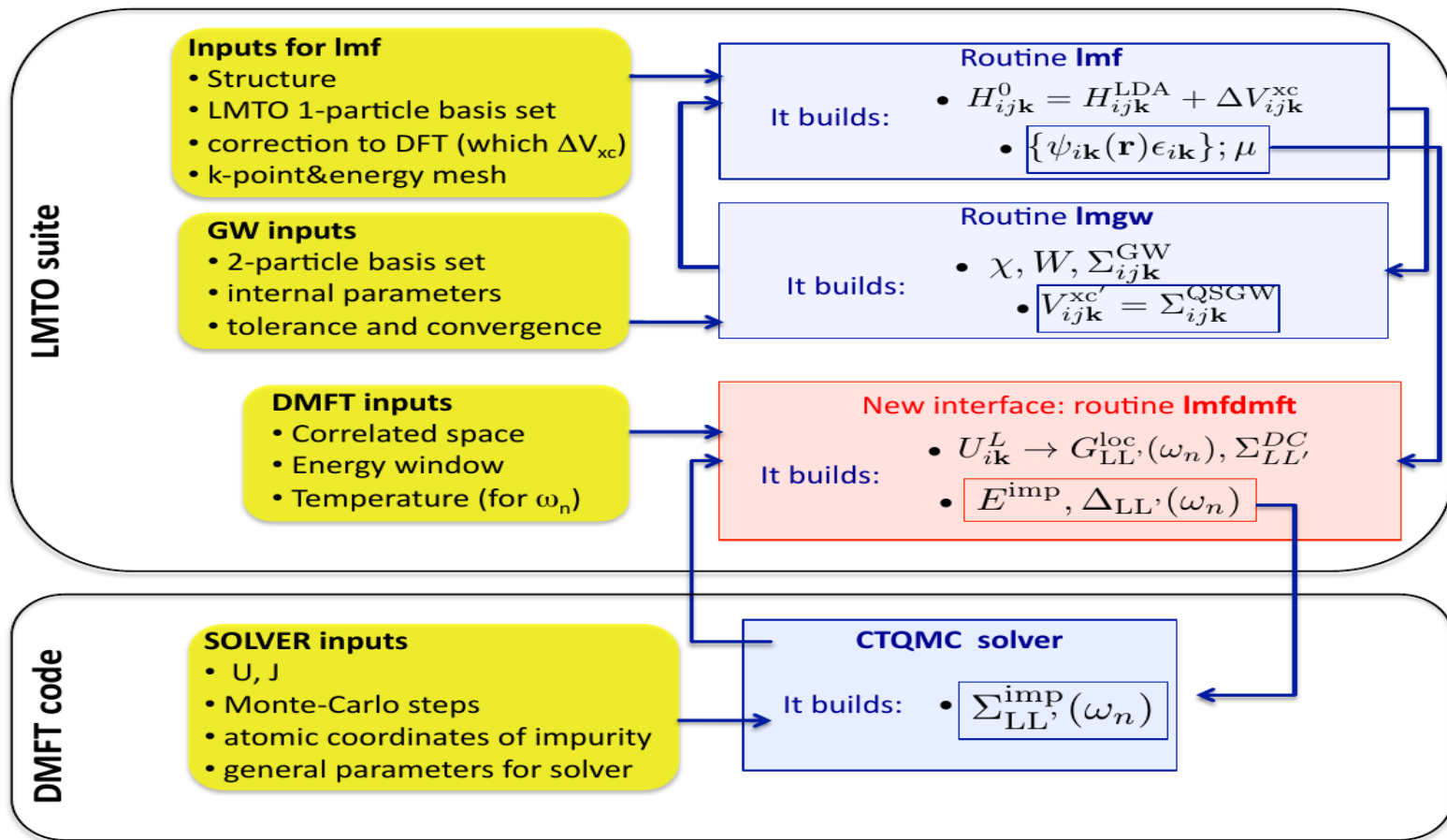
TABLE 2. Comparison of theories based on functionals of a local observable

Theory	MFT	DFT	DMFT
Quantity	Local magnetization m_i	Local density $n(x)$	Local GF $G_{ii}(\omega)$
Equivalent system	Spin in effective field	Electrons in effective potential	Quantum impurity model
Generalised Weiss field	Effective local field	Kohn-Sham potential	Effective hybridisation

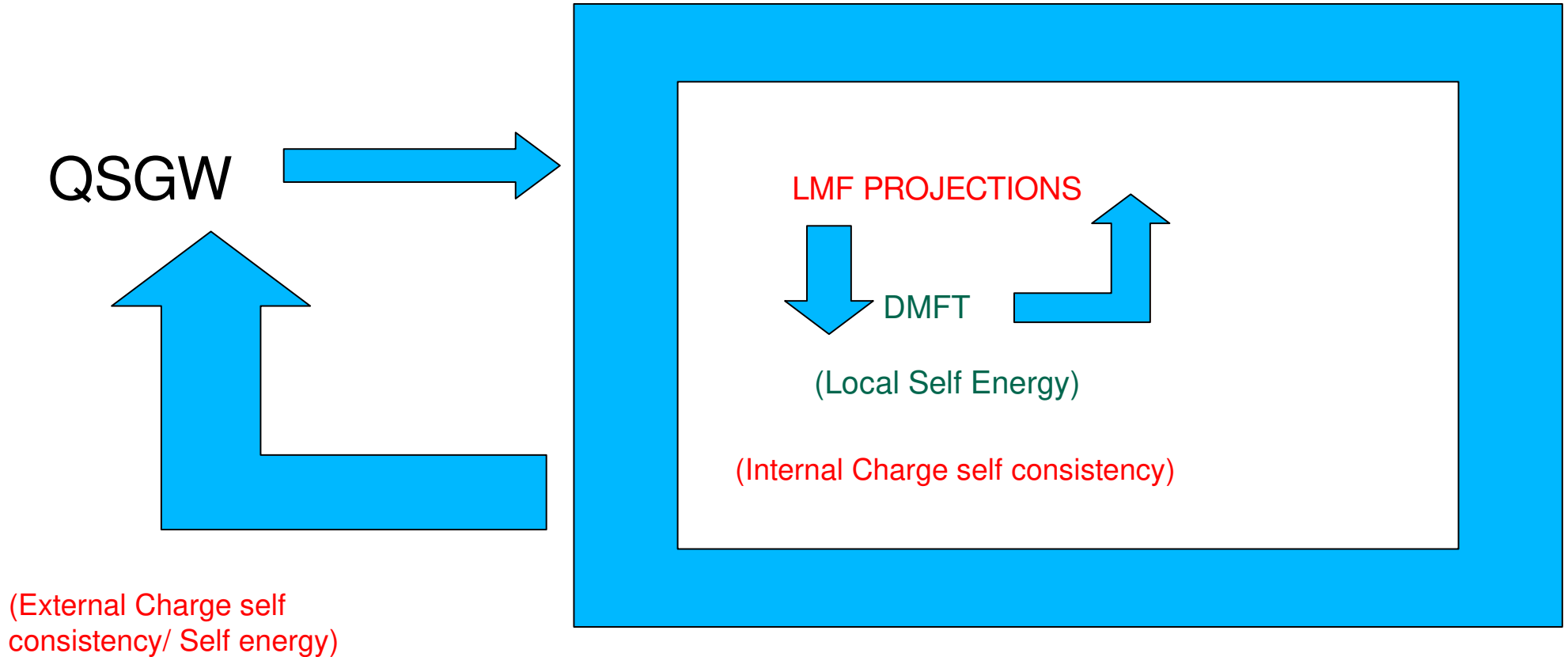
DMFT in our implementation

Need to build the impurity Hamiltonian and the hybridization of the impurity with the bath

Pisanti, Thesis,
KCL



DMFT Self Consistency: in our implementations



Systems with $T_N < \Delta_g$: Magnetic ordering is not source of Metal-Insulator transition

La_2CuO_4 : $T_N = 312 \text{ K}$ (26 meV), $\Delta_g = 2.1 \text{ eV}$

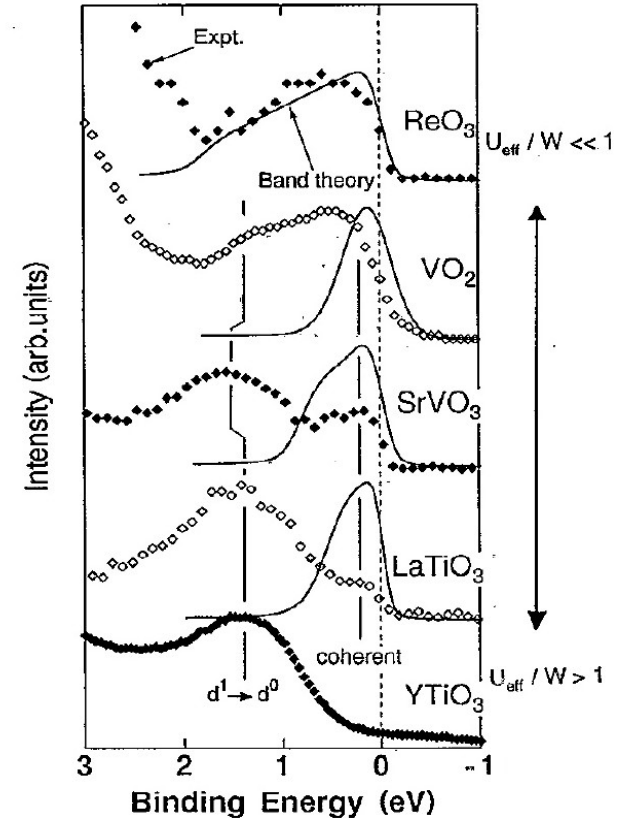
YTiO_3 : $T_C = 30 \text{ K}$ (3 meV), $\Delta_g = 1.0 \text{ eV}$

LaTiO_3 : $T_N = 140 \text{ K}$ (12 meV), $\Delta_g = 0.2 \text{ eV}$

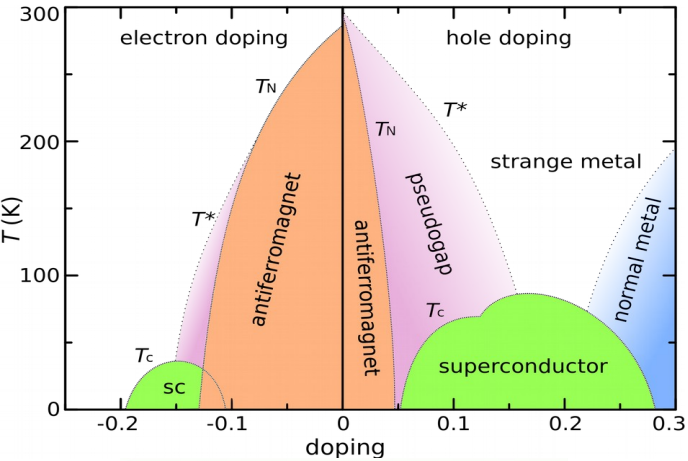
$\Delta_g > T > J$ these systems are paramagnetic insulator

----- Don't need magnetic ordering to become insulator

----- Mott insulators ----- charge blocking---suppress double occupancy



Single and two-particle response in La_2CuO_4



Cu- d_z^2 , O- p_z and Cu-4s are suppressed significantly in QSGW

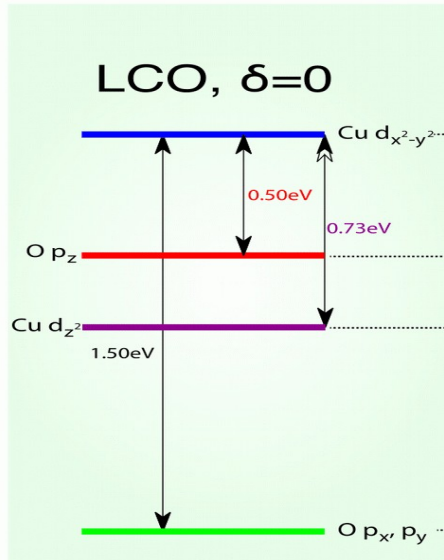


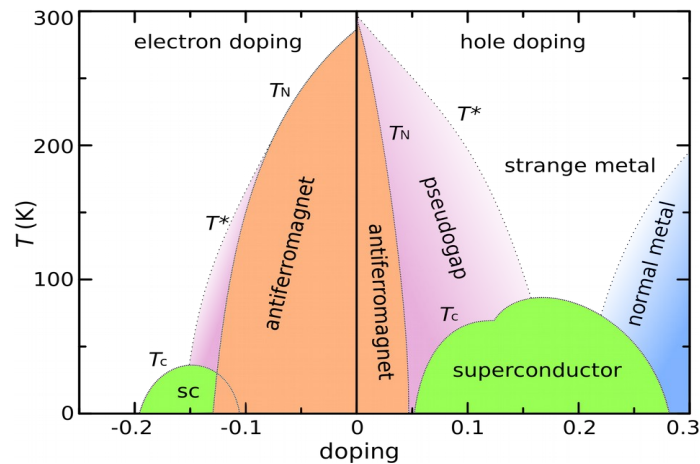
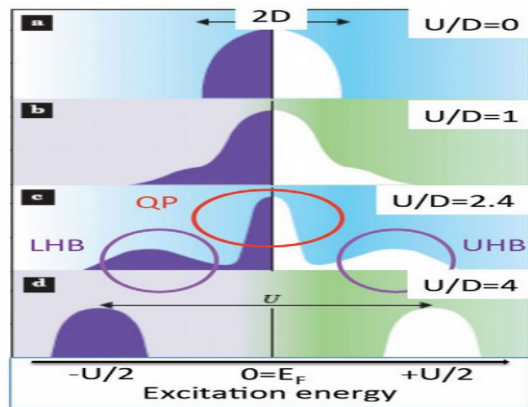
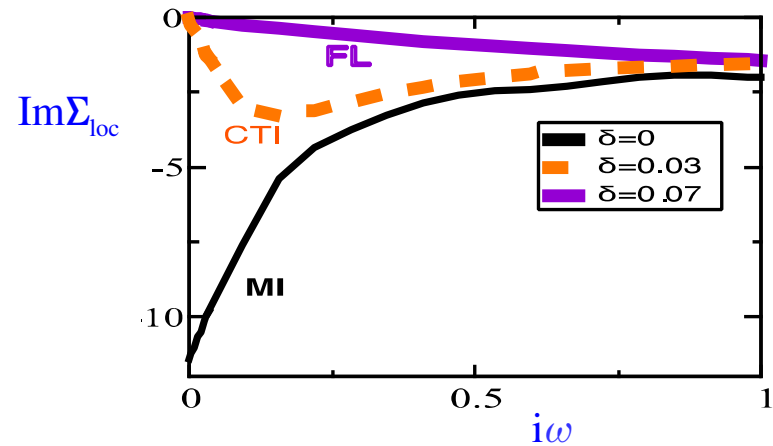
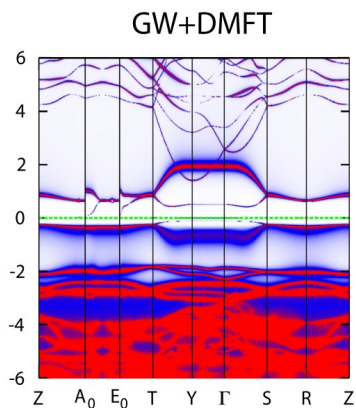
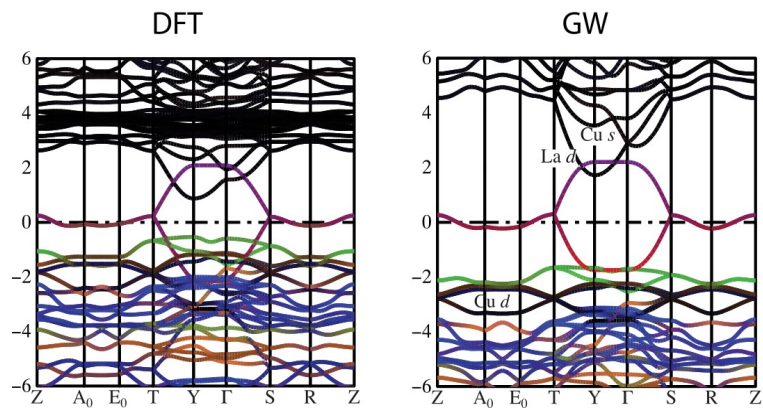
Table								
Compound	Z	Γ in eV	Δ_x in eV	T_c^{max} in K	Δ in eV	Cu $d_{x^2-y^2}$	Axial orbitals	O- p_{xy}
LCO ($\delta = 0$) QSGW	0.00	11.4	-1.53	34	0.78	0.5437	0.108	0.2630
LCO ($\delta = 0.03$) QSGW	0.02	0.41	-1.49	79	1.0	0.5454	0.105	0.2615
LCO ($\delta = 0.05$) QSGW	0.08	10^{-4}	-1.45	53	0	0.5471	0.092	0.2607
LCO ($\delta = 0.09$) QSGW	0.41	10^{-9}	-1.37	11	0	0.5507	0.086	0.2591
LCO ($\delta = 0$) LDA						0.40067	0.22	0.2798
NCO QSGW	0.44	10^{-6}	-0.97	25	0	0.63007	0.033	0.2520

Swagata Acharya et al.,
Phys. Rev. X 8, 021038 (2018)

Cu- d_z^2 , O- p_z and Cu-4s are huge in LDA

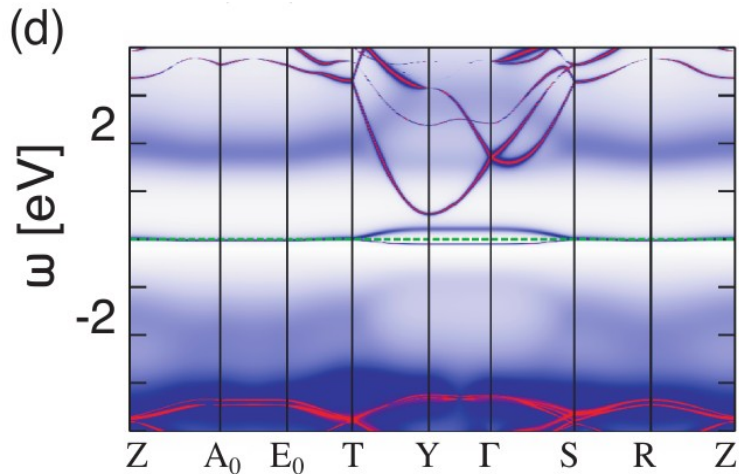
Hyowon Park PhD thesis, Rutgers Lib. (2012)

Single and two-particle response in La_2CuO_4

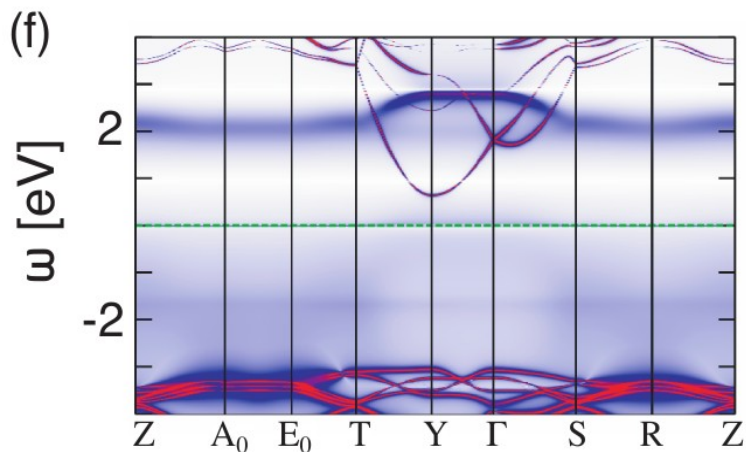


Swagata Acharya et al.,
 Phys. Rev. X 8, 021038
 (2018)

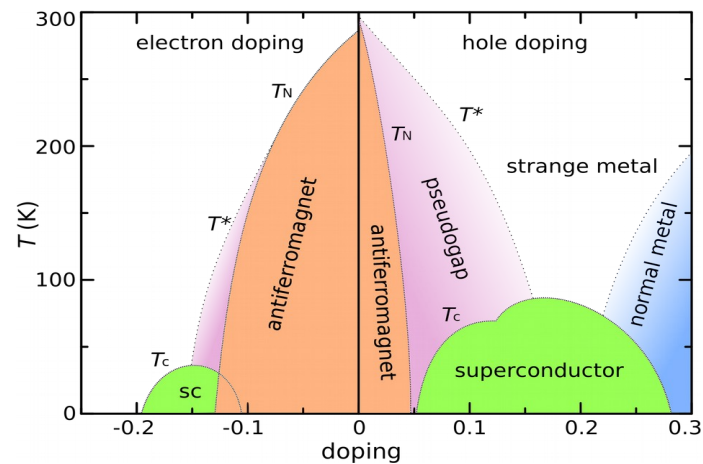
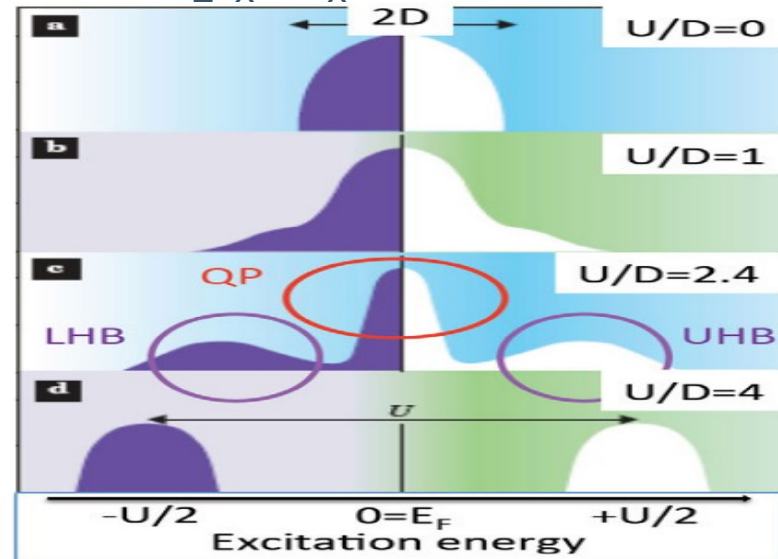
Single-particle response in doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$



$X=0.06$

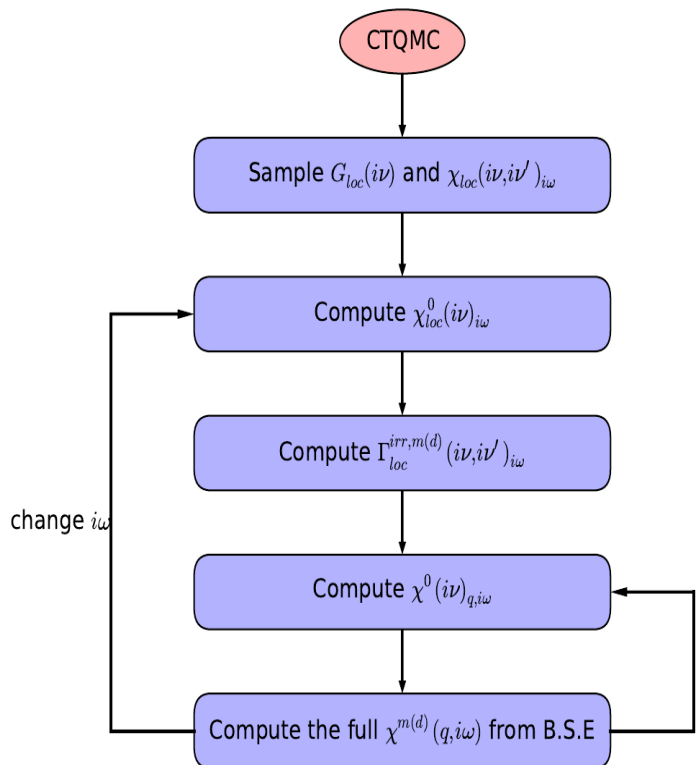


$X=0.02$

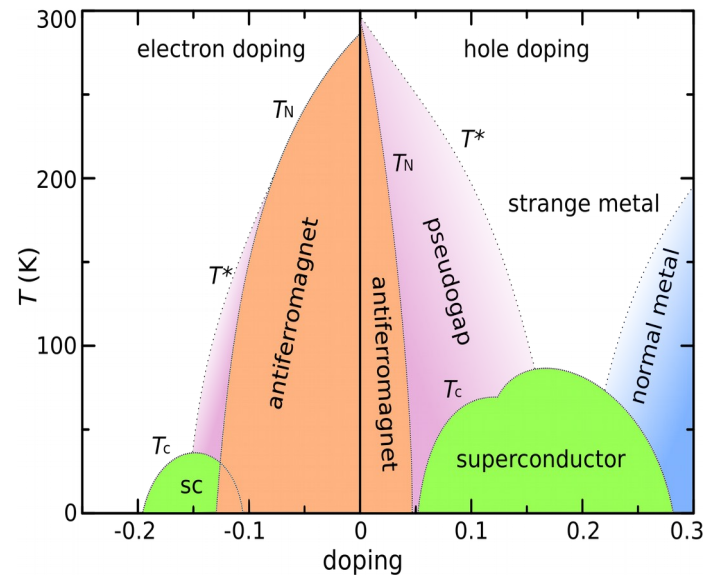


Spin and Charge Susceptibilities in La_2CuO_4

$$\begin{array}{c}
 \begin{array}{ccc}
 \overleftarrow{iv, \alpha'_1 \alpha_1} & \overleftarrow{iv', \alpha_2 \alpha'_2} & \\
 \chi^{m(d)} & & \\
 \overrightarrow{iv + i\omega, \alpha_3 \alpha'_3} & \overrightarrow{iv' + i\omega, \alpha'_4 \alpha_4} & \\
 \end{array}
 = \chi^0 + \begin{array}{ccc}
 \overleftarrow{iv, \alpha'_1 \alpha_1} & \overleftarrow{iv', \alpha_2 \alpha'_2} & \\
 \chi^0 & \Gamma_{loc}^{irr} & \chi^{m(d)} \\
 \overrightarrow{iv + i\omega, \alpha_3 \alpha_4} & \overrightarrow{iv + i\omega, \alpha_3 \alpha'_3} & \overrightarrow{iv' + i\omega, \alpha'_4 \alpha_4} \\
 \end{array}
 \end{array}$$

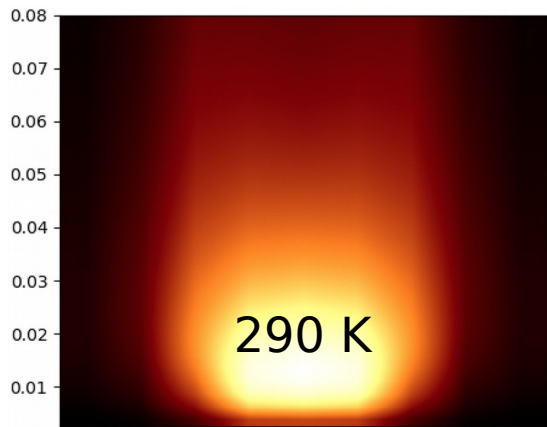


Swagata Acharya et al.,
Phys. Rev. X 8, 021038 (2018)

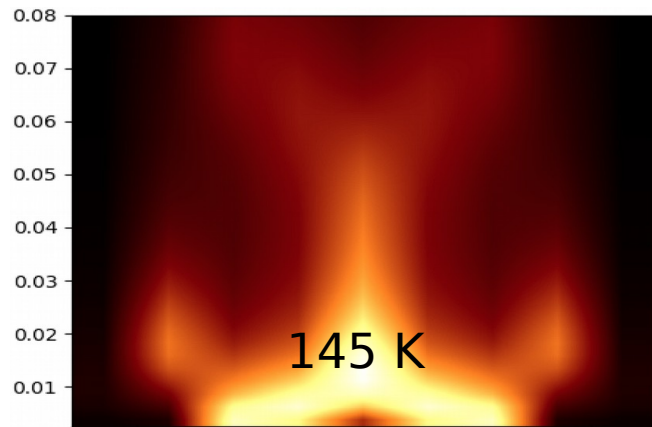


Hyowon Park PhD thesis, Rutgers Lib. (2012)

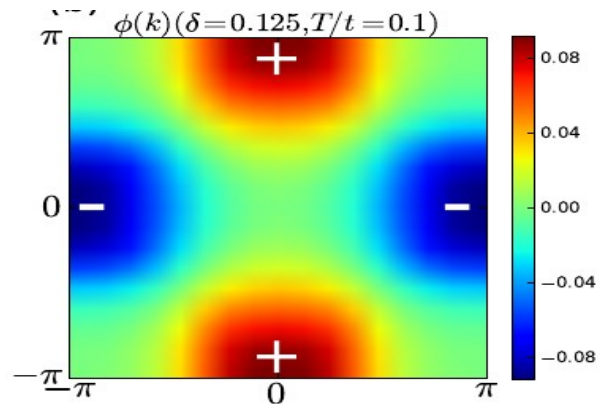
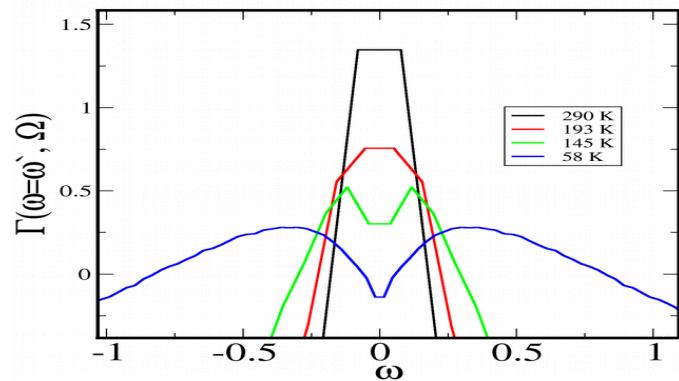
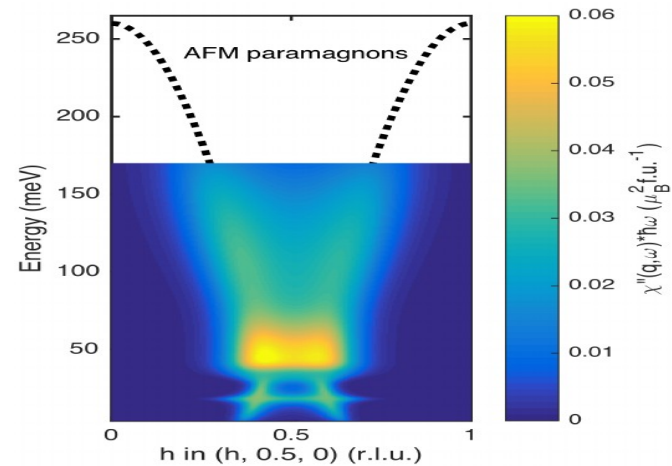
Single and two-particle response in $\text{La}_{1.88}\text{Sr}_{0.12}\text{CuO}_4$



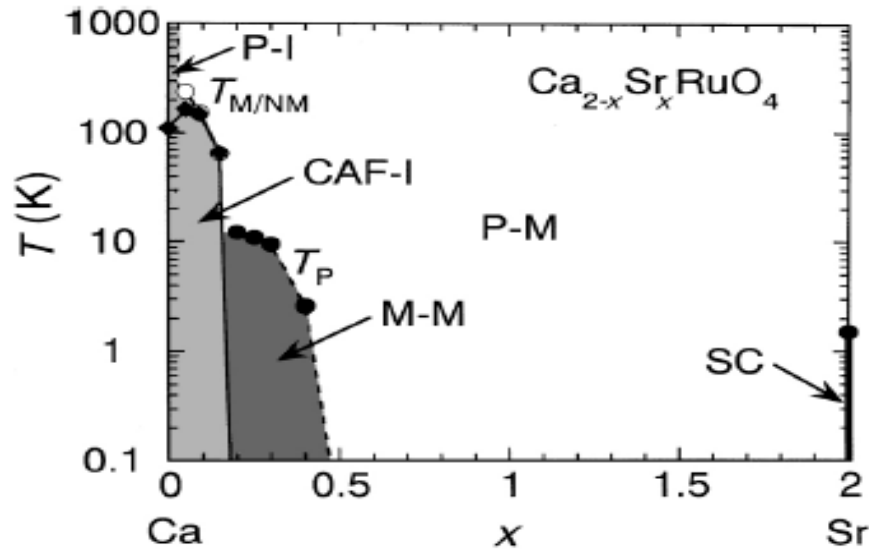
h in $(h, 0.5, 0)$



h in $(h, 0.5, 0)$

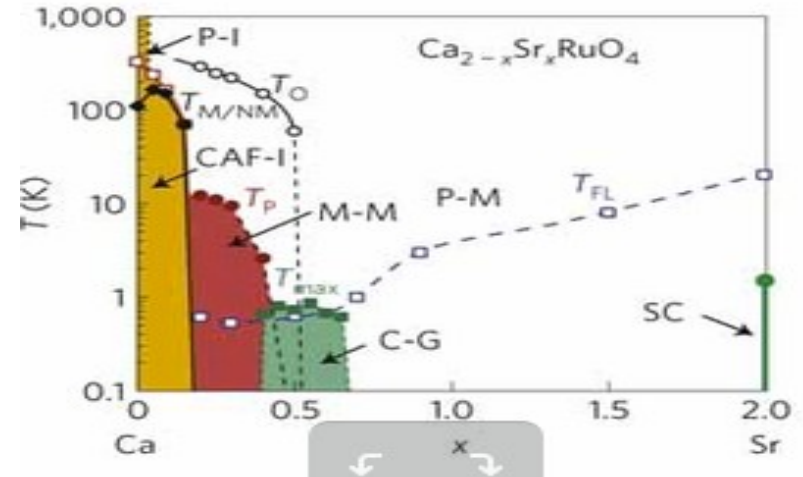


Experimental Phase Diagram : $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$



Carlo et al., Nature (2013)

S. Nakatsuji et al. PRB (2000).



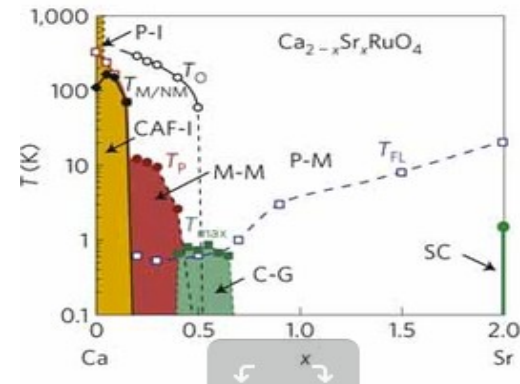
Outstanding issues at $x = 2.0$

- Incoherence-coherence crossover at 25 K
Resistivity crosses from $\sim T$ to $\sim T^2$

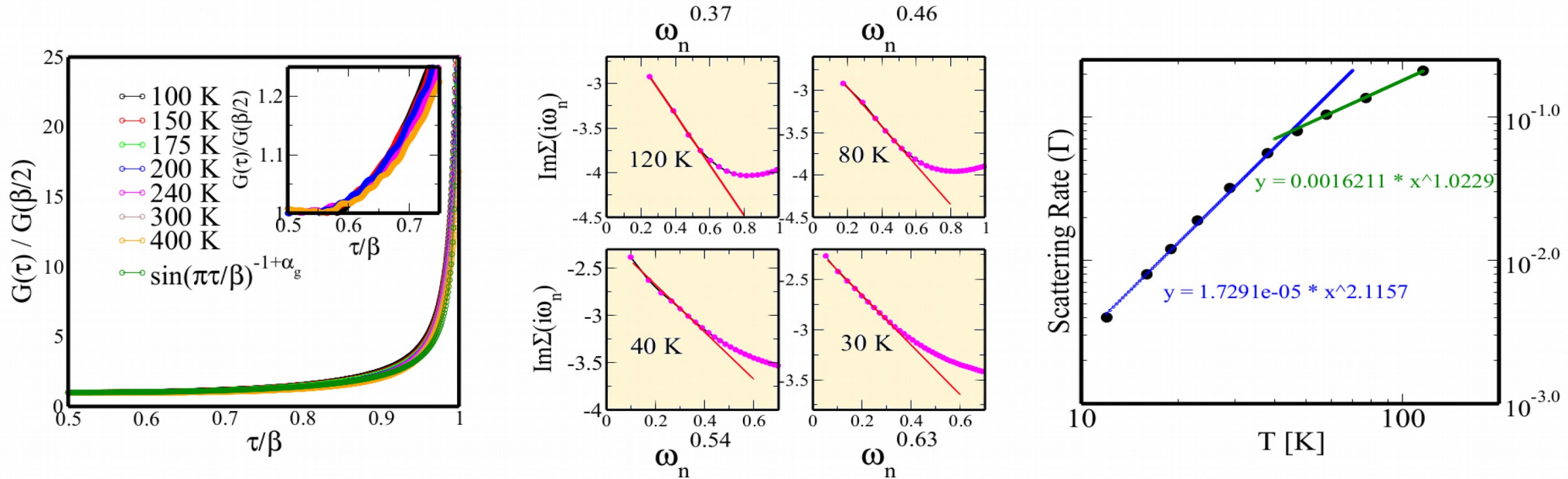
Susceptibility crosses from T^{-1} (Curie-Weiss) to T^0 (Pauli)

S. Acharya et al. Scientific Reports 7, 43033 (2017)

Instabilities of a FL : triplet unconventional superconductivity
(below 1.5 K)



Single-particle Response of Sr_2RuO_4



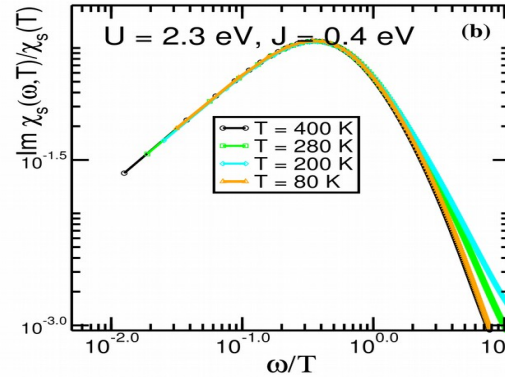
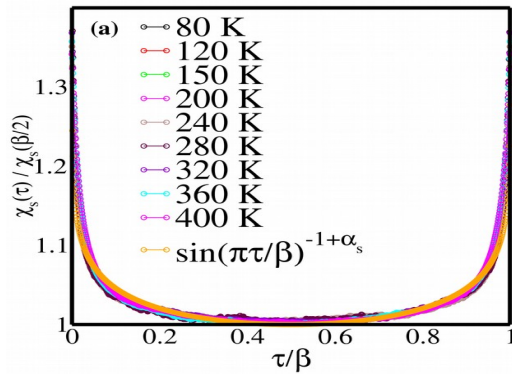
S. Acharya et al. Scientific Reports 7, 43033 (2017)

41 K : Scattering rate $\sim T$ to $\sim T^2$ crossover

30 K: Resistivity $\sim T$ to $\sim T^2$ crossover (Maeno et al. 2004)

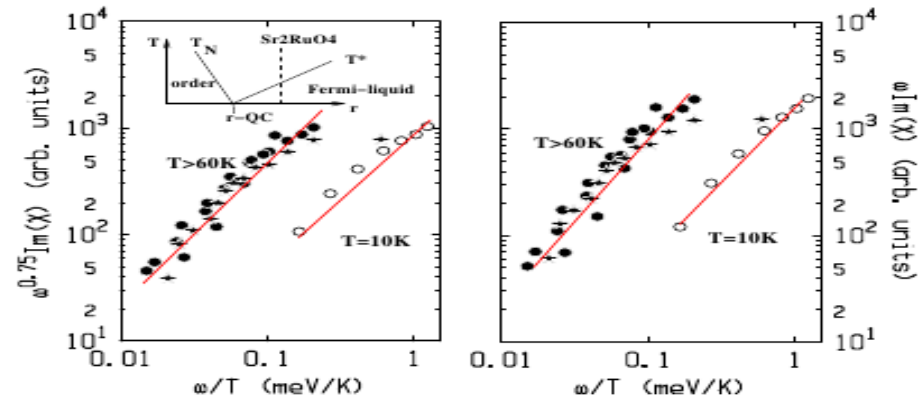
Thermal Scaling of Local Spin Susceptibilities

S. Acharya et al. Scientific Reports 7, 43033 (2017)

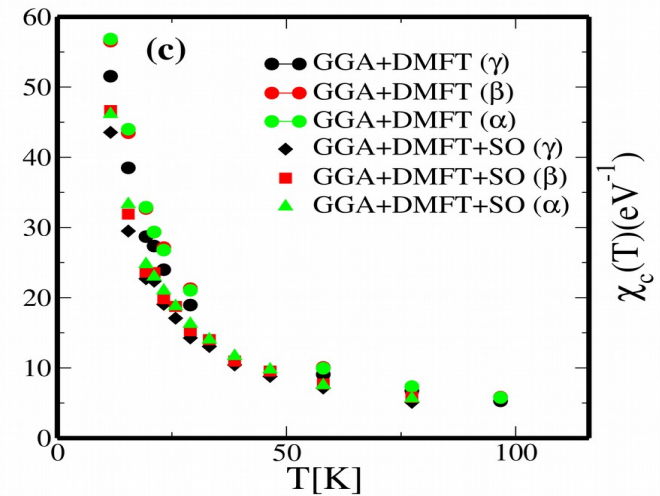
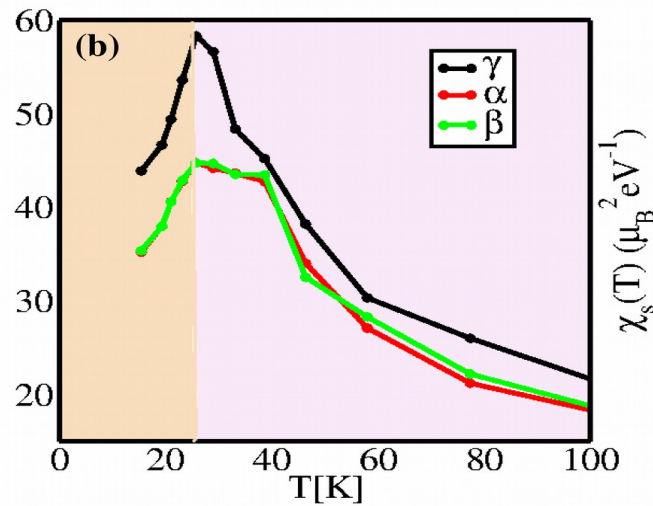
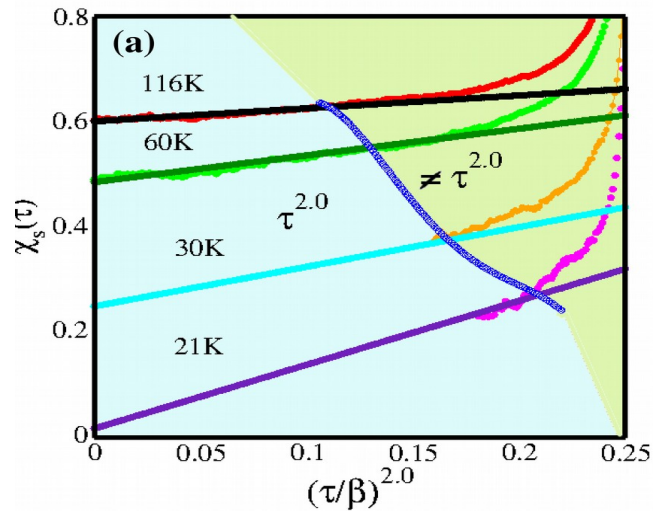


Critical thermal scaling collapse of dynamic local spin susceptibilities

Braden et al. 2002 (PRB)

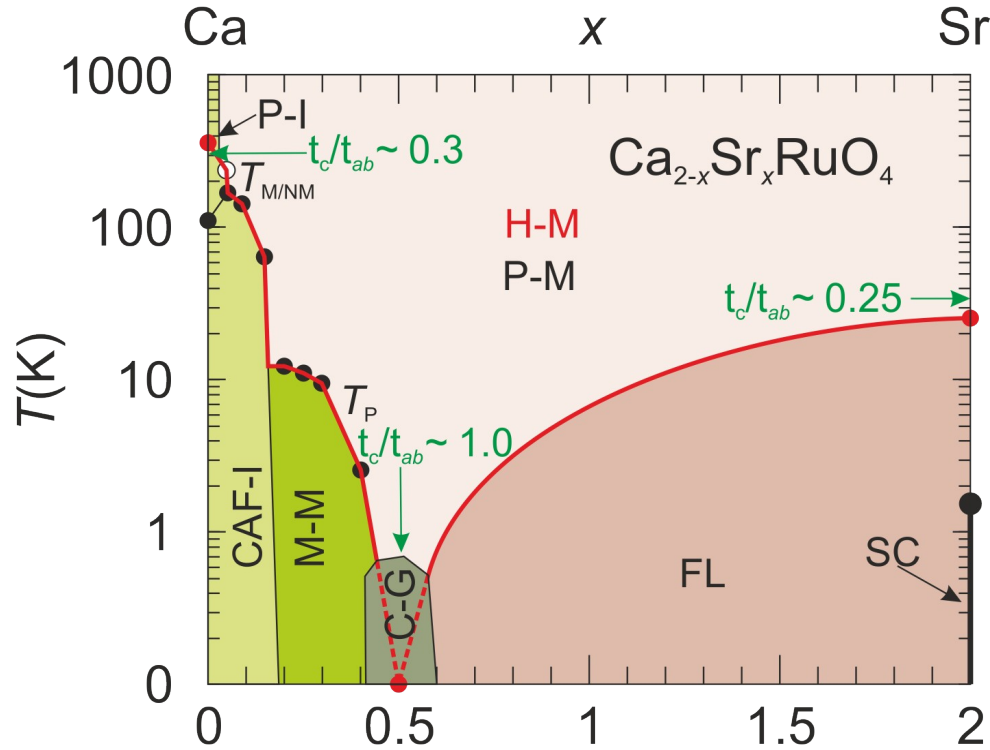


Two-particle Response: Sr_2RuO_4

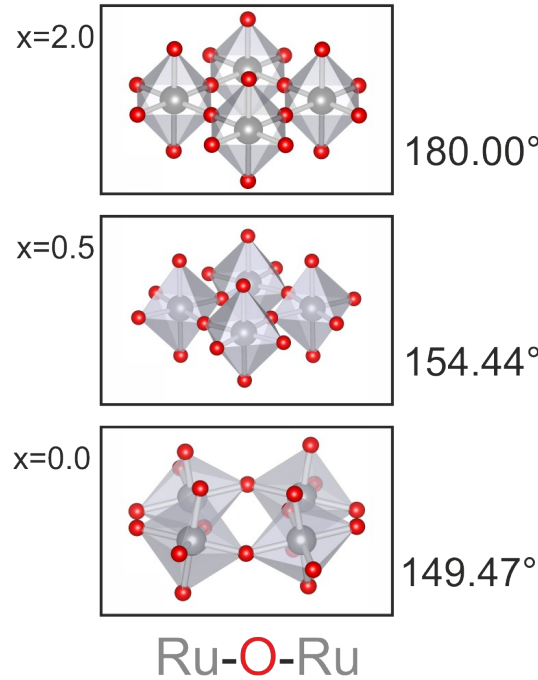


Local moment quenches around 25 K
Charge susceptibility is singular down to 12 K

Phase diagram for the iso-electronic series $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$



[S.Acharya et al. JPC, 2, 075004 \(2018\).](#)



$I4/mmm$ $a=3.8606 \text{ \AA}$,
 $c=12.70658 \text{ \AA}$

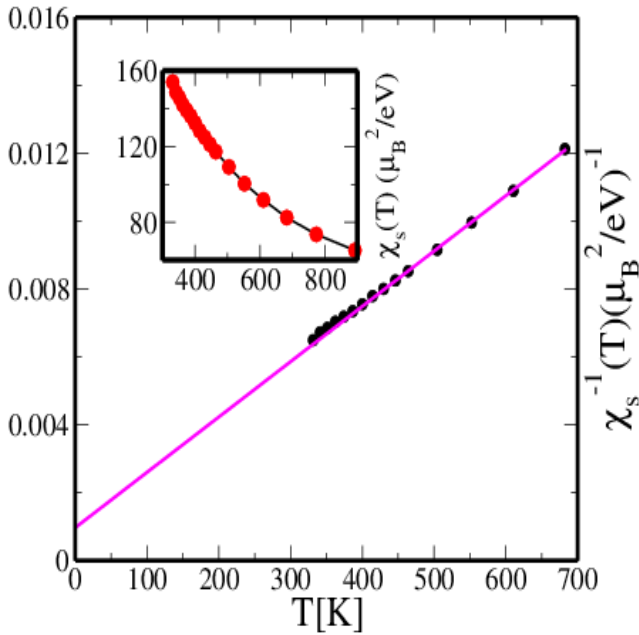
$I4_1/acd$, $a=7.52 \text{ \AA}$ and
 $c=24.1645 \text{ \AA}$

L-Pbca,
 $a=5.3869 \text{ \AA}$
 $b=5.6334 \text{ \AA}$
 $c=11.7349 \text{ \AA}$

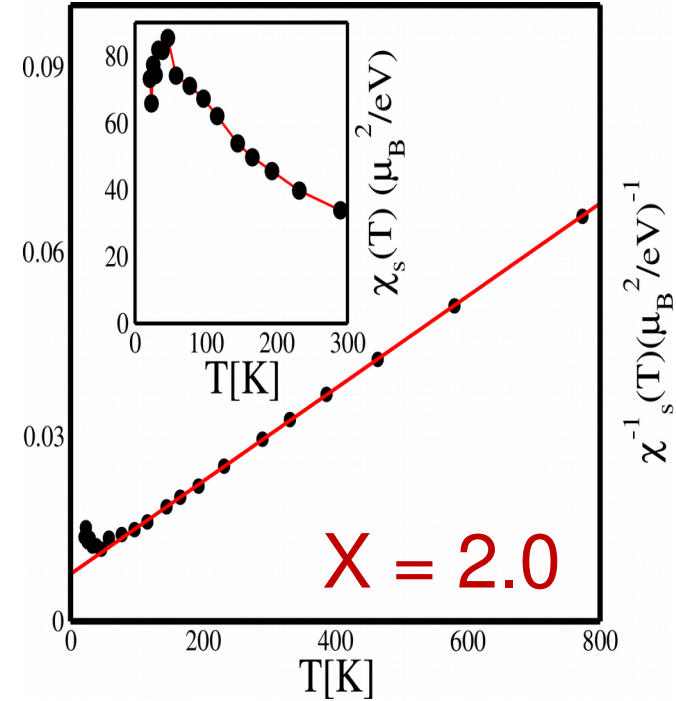
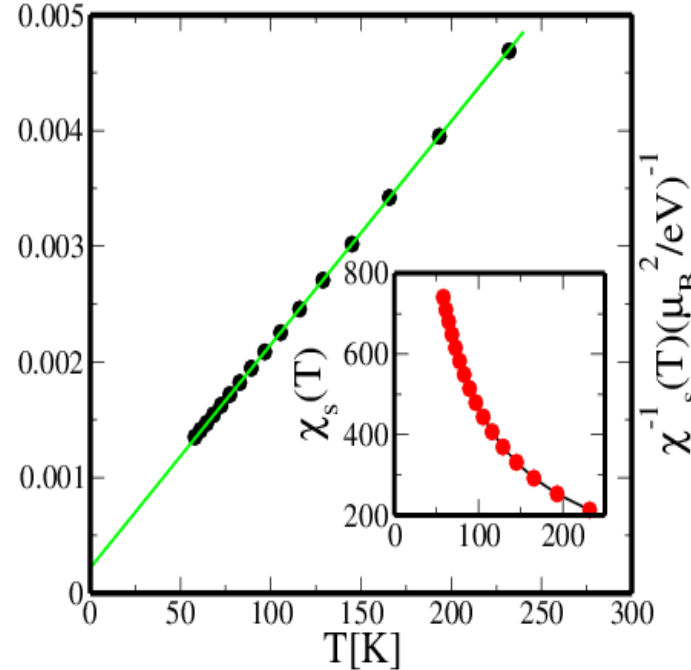
Local Static Spin Susceptibilities: $x = 0, 0.5, 2.0$

$X=0.5$

[S.Acharya et al. JPC. 2, 075004 \(2018\).](#)

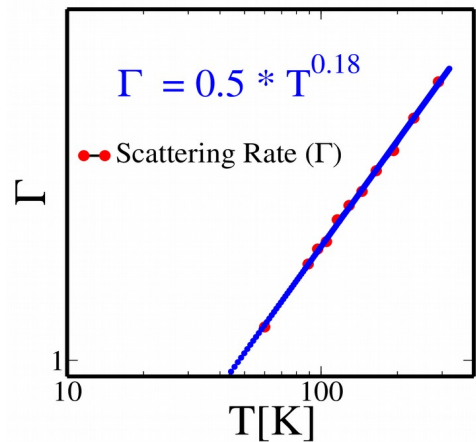
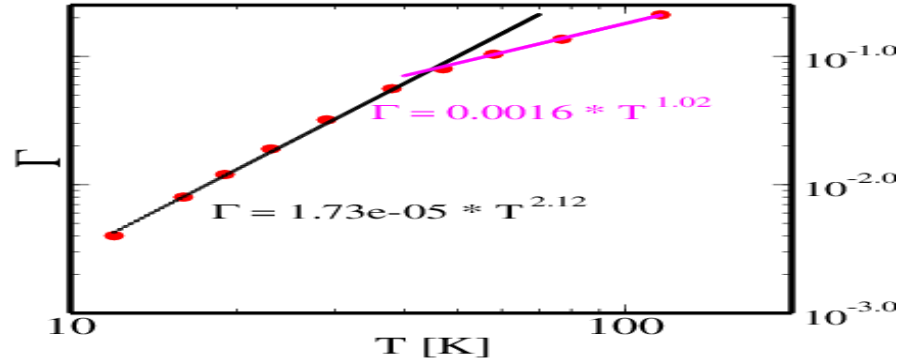
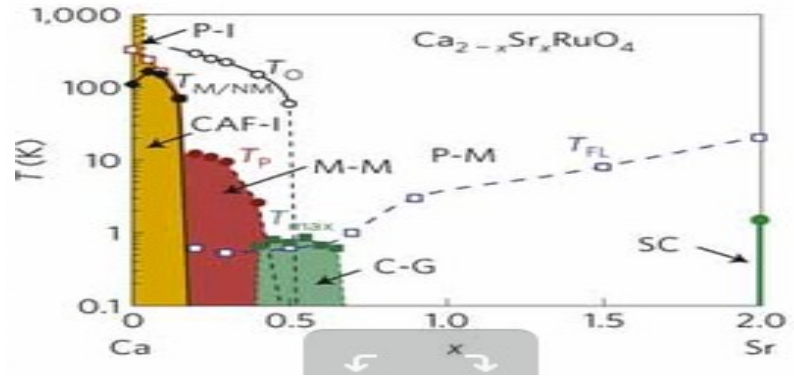


$X = 0.0$



$X = 2.0$

Scattering rates: FL and NFL

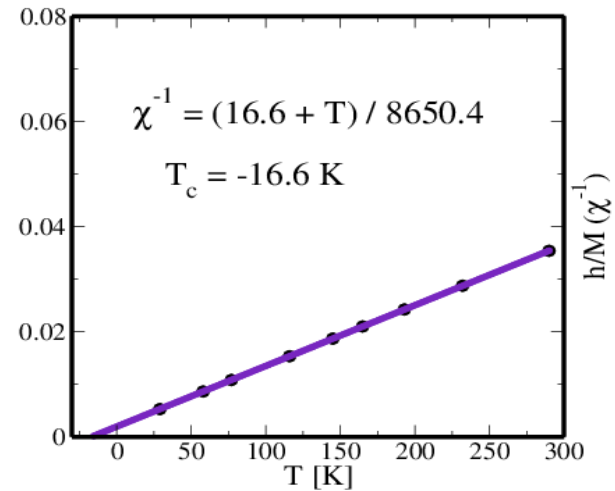
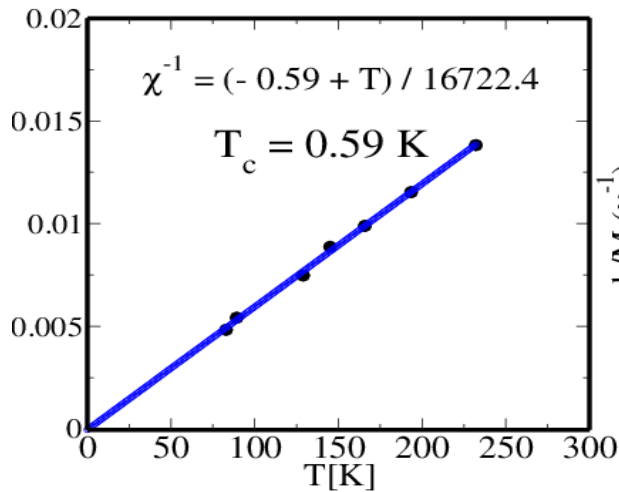
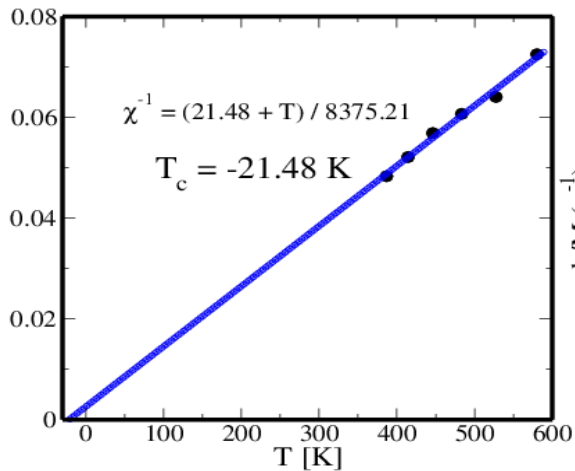


[S.Acharya et al. JPC, 2, 075004 \(2018\).](#)

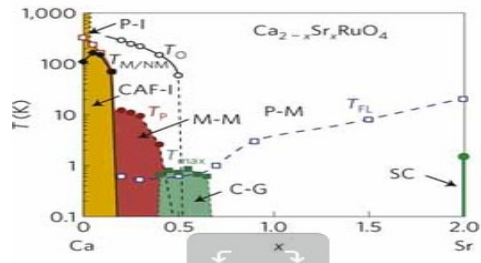
FL to NFL crossover
across 40 K for X = 2.0

Nearly incoherent
spin-frozen state x= 0.5

Uniform Spin Susceptibilities: $x = 2.0, 0.5, 0.0$



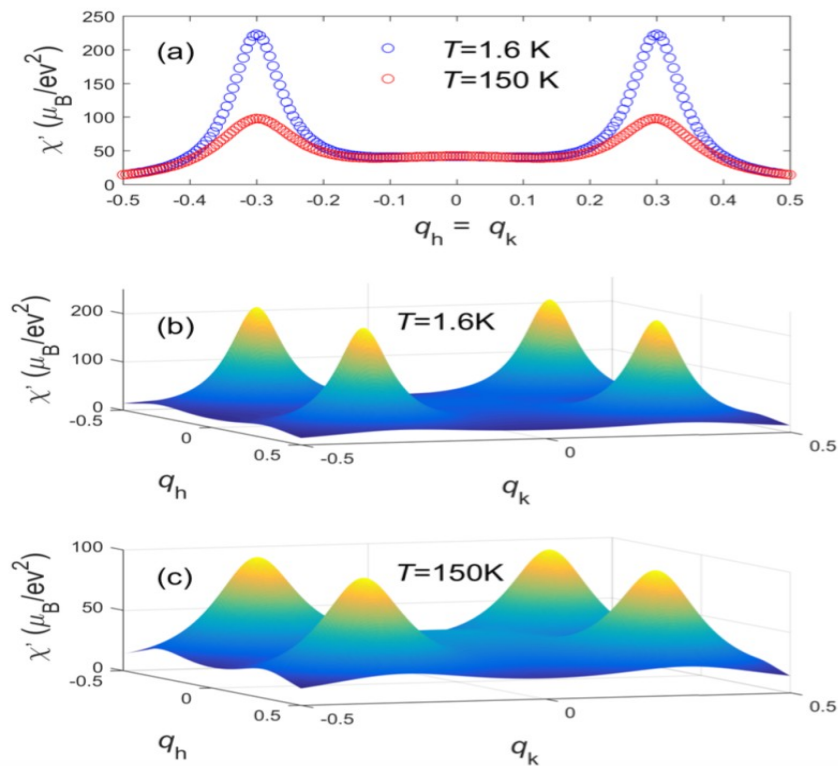
$X = 0.0$
AFM



$X = 0.5$
FM

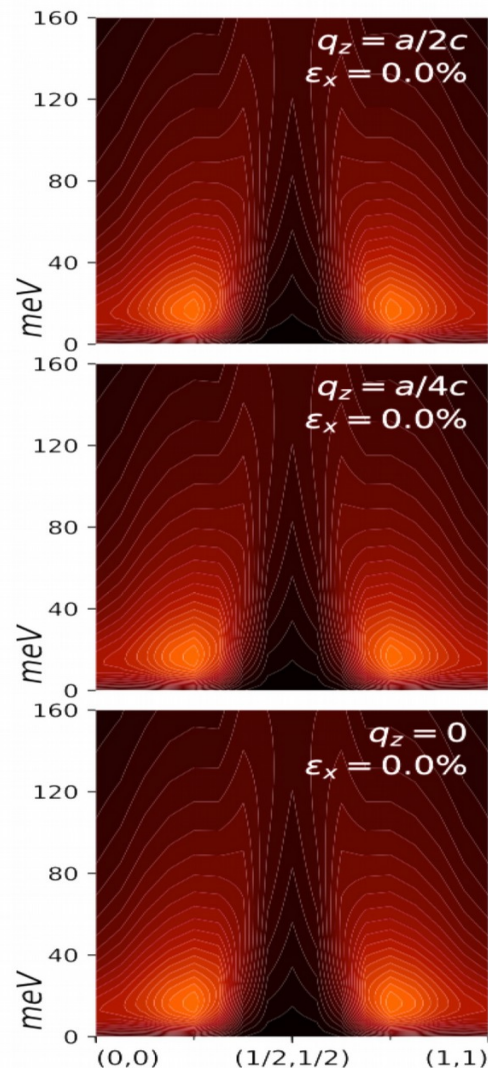
$X = 2.0$
AFM

Spin susceptibility



Inelastic neutron scattering shows strong peaks at incommensurate $q = q^* = (0.3, 0.3, 0)$ with $\omega_{\text{max}} \approx 10\text{ meV}$.

QSGW+DMFT result for χ^s is **nearly identical**. Peaks do not derive from the nesting as in Cr: **proper treatment of vertex is essential!**

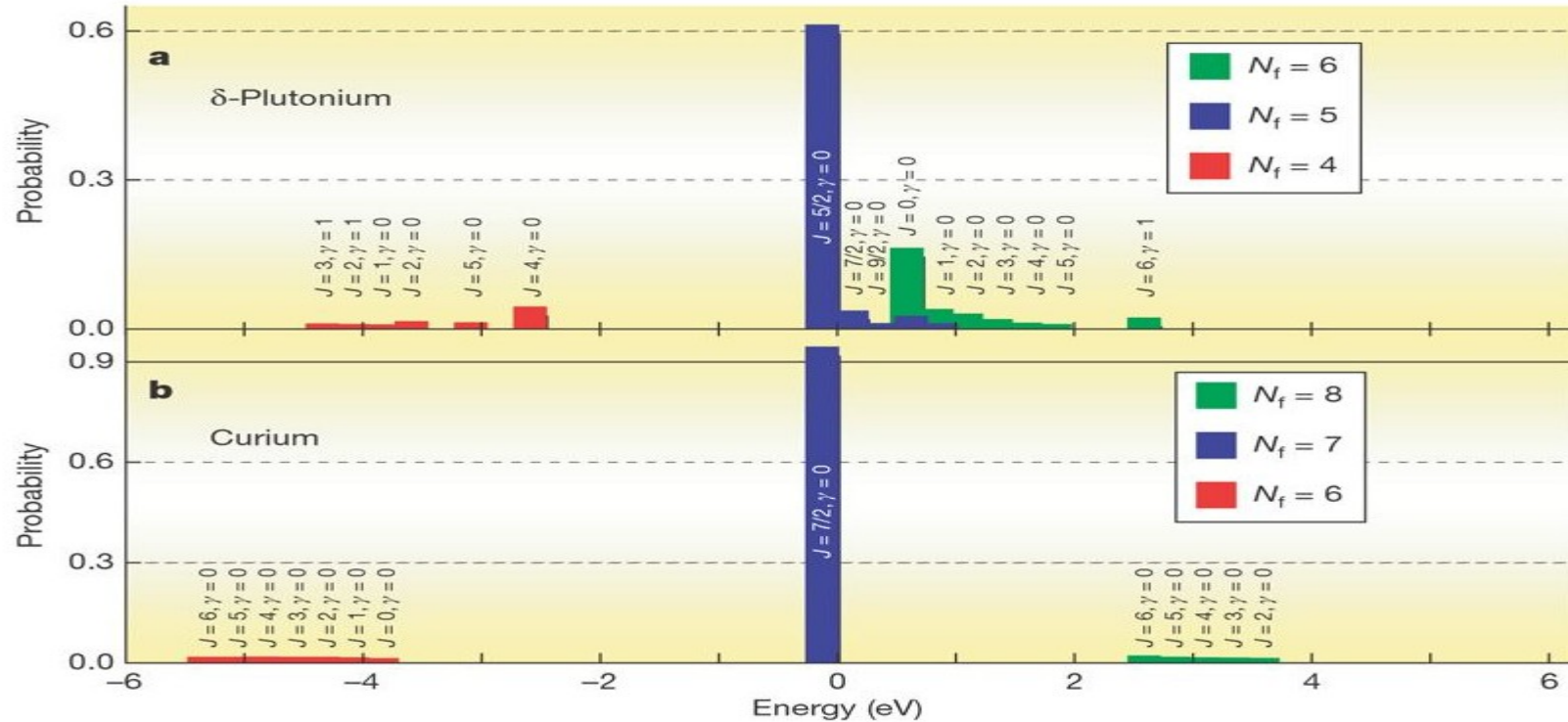


P. Steffens et al,
arXiv:1808.05855

arXiv:1811.05143

Valence fluctuations: Atomic Multiplets

Plutonium is in ideal f^5 state and curium is f^7 state



Shim, Kristjan, Gabi, Nature volume446, pages513-516 (29 March 2007)

QSGW+DMFT+BSE

Lattice parameters,
atomic co-ordinates

➤ **QSGW** (low level theory, all electron bath) (long range Coulomb interactions treated perturbatively but nearly sufficiently!)

➤ **QSGW+DMFT (CT-QMC)** (high level theory, only subspace)

QSGW+DMFT+BSE

What diagrams missing?

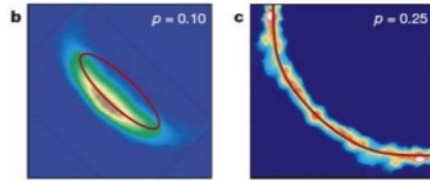
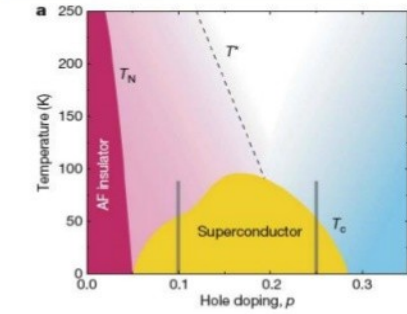
Ladders in charge (e-h) + spin fluctuations (local + non-local)

Spin, charge, sc-pairing
Susceptibilities,
gap symmetries

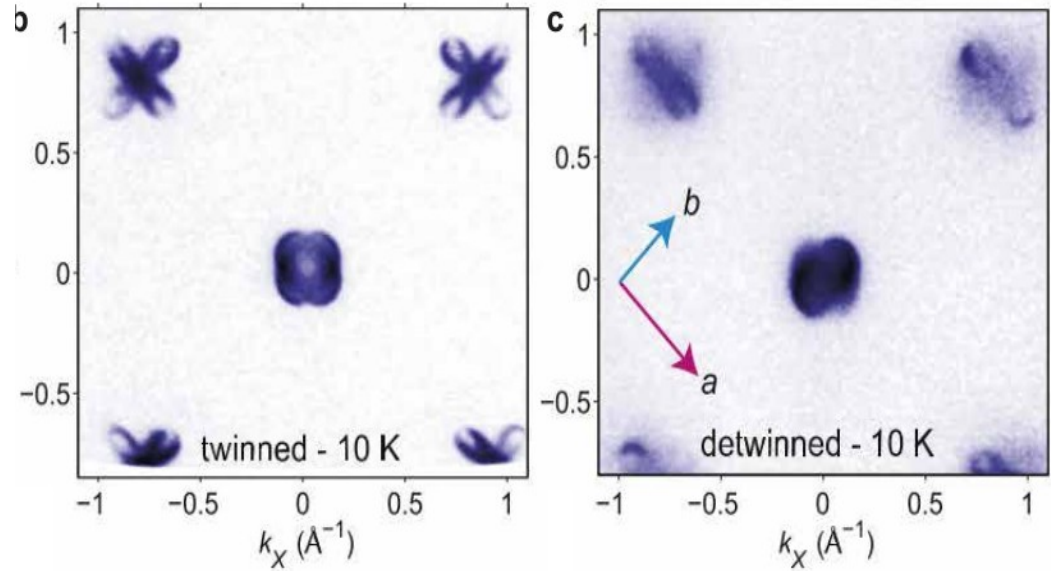
Brian's **QSGW+BSE (ladders in W, sc)** (high level theory, all electron)

What you don't expect from DMFT

Evolution of the Fermi surface with doping



Doiron-Leyraud *et al*
Nature (2007)



Single-site DMFT does not have --Momentum dependent incoherence--
 $\text{Im}\Sigma(\omega)$ ---- one needs momentum dependent life time effect $-\text{Im}\Sigma(\mathbf{k}, \omega)$ ----Dual Fermions, Cluster
 DMFT. Diagrammatic QMC