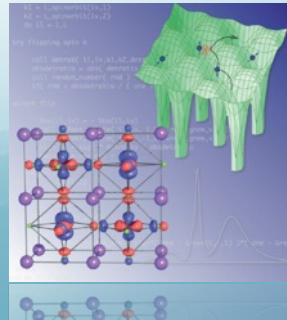
Electron Structure and Magnetism

Alexander Lichtenstein
University of Hamburg

In collaboration with

M. Harland, E. Stepanov, S. Brener,
A. Rubtsov and M. Katsnelson



Outline

- Correlation effects and magnetism
- DFT+DMFT: Reference System
- Realistic DMFT for Fe and Ni
- Double-Bethe Lattice: AFM-VBS transition
- Triple-Bethe Lattice: SL ?
- Magnetism and Superconductivity in Quadro-Bethe

Heisenberg Model

$$\widehat{H} = -\sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

1932

Zur Theorie des Ferromagnetismus.

Von **W. Heisenberg** in Leipzig.

Mit 1 Abbildung. (Eingegangen am 20. Mai 1928.)

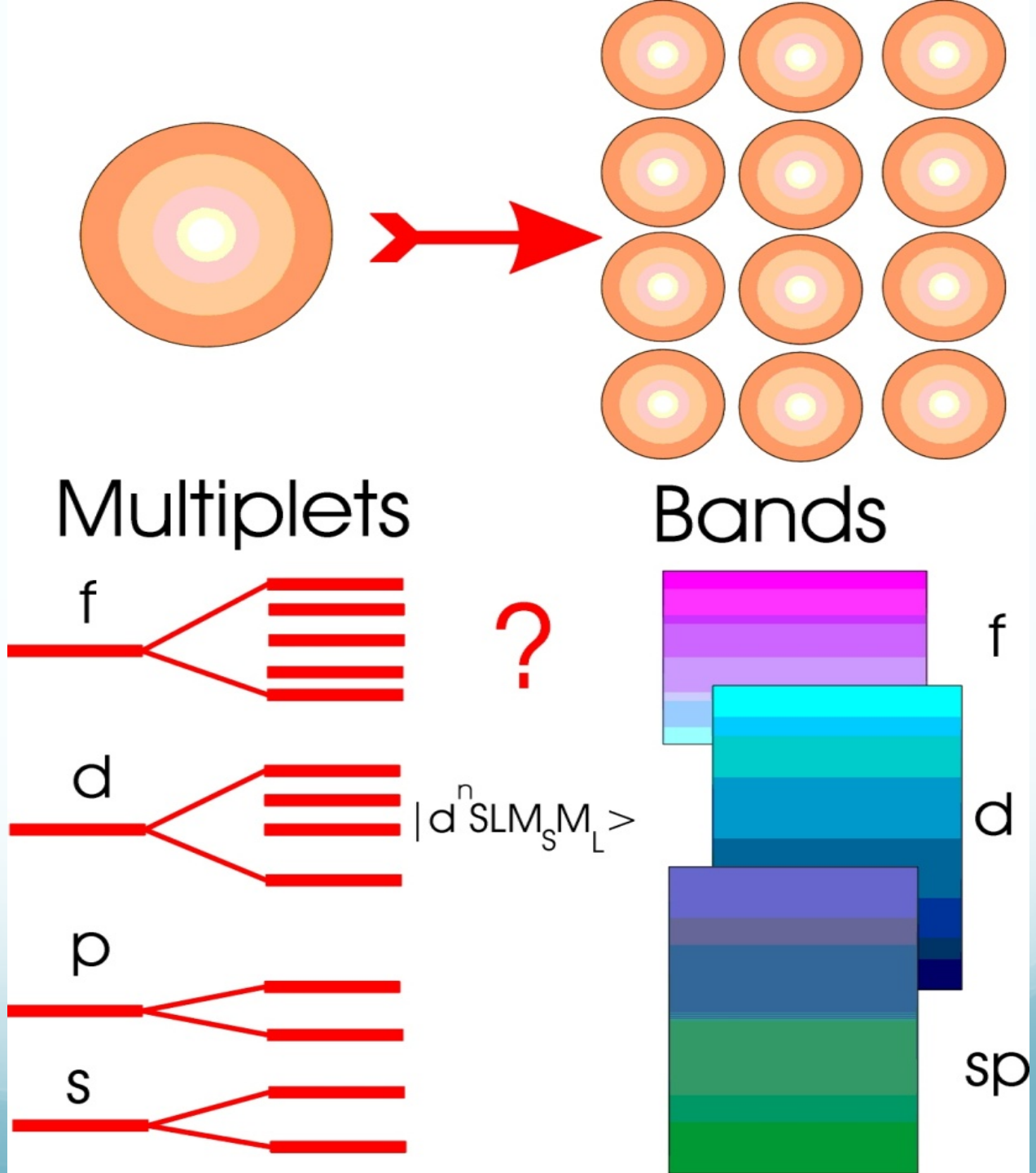
Methode I. Nach Pauli

1945

Quantum Mechanics:
Ferromagnetism = “Exchange Interactions’ =
Coulomb interactions + Pauli Principle

$$J_{(kl)} = \frac{1}{2}\int \psi_k^z \psi_k^\lambda \psi_l^z \psi_l^\lambda \left(\frac{2e^2}{r_{kl}} + \frac{2e^2}{r_{z\lambda}} - \frac{e^2}{r_{zk}} - \frac{e^2}{r_{zl}} - \frac{e^2}{r_{\lambda k}} - \frac{e^2}{r_{\lambda l}}\right) d\tau_k d\tau_l$$

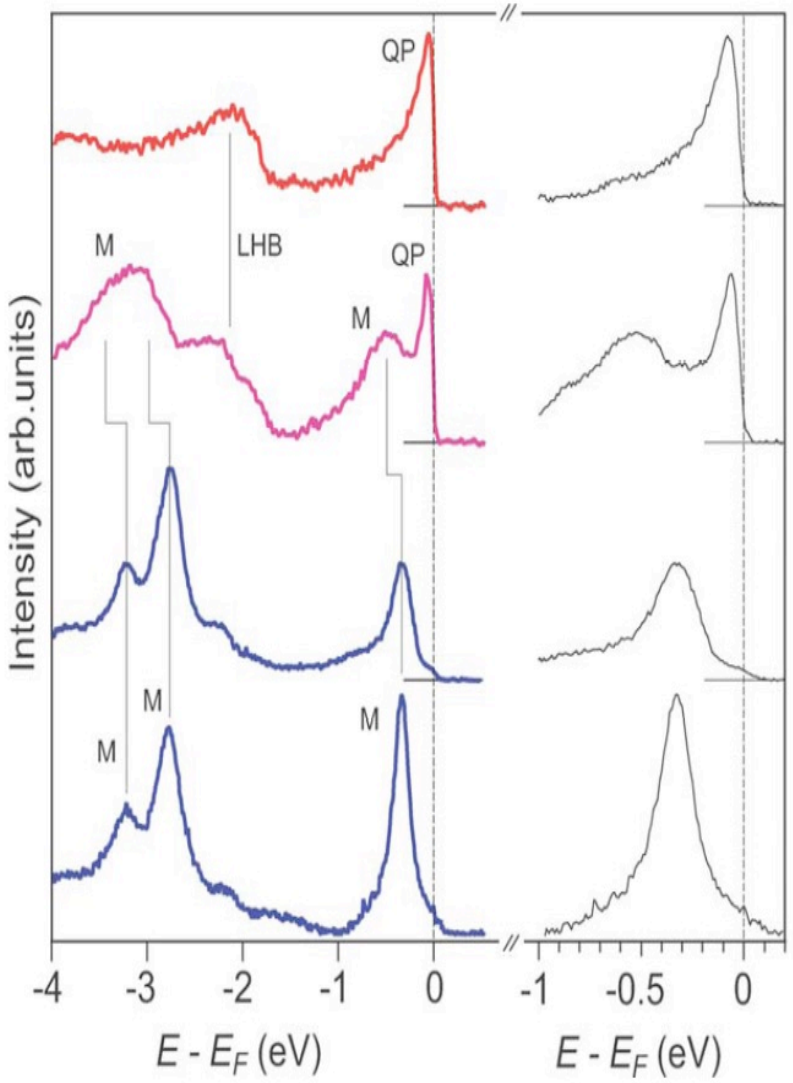
From Atom to Solids

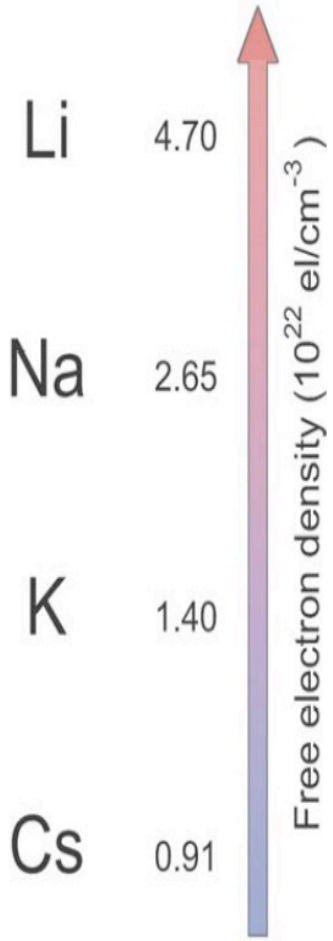


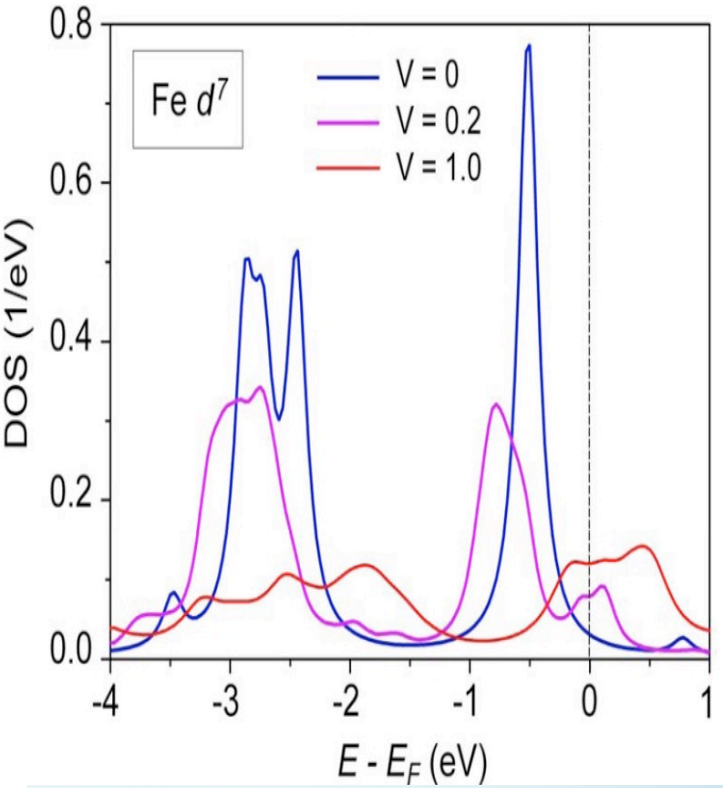
Disolving Multiplets: Fe in alkali system

PES

SIAM: 5-band in 1-bath

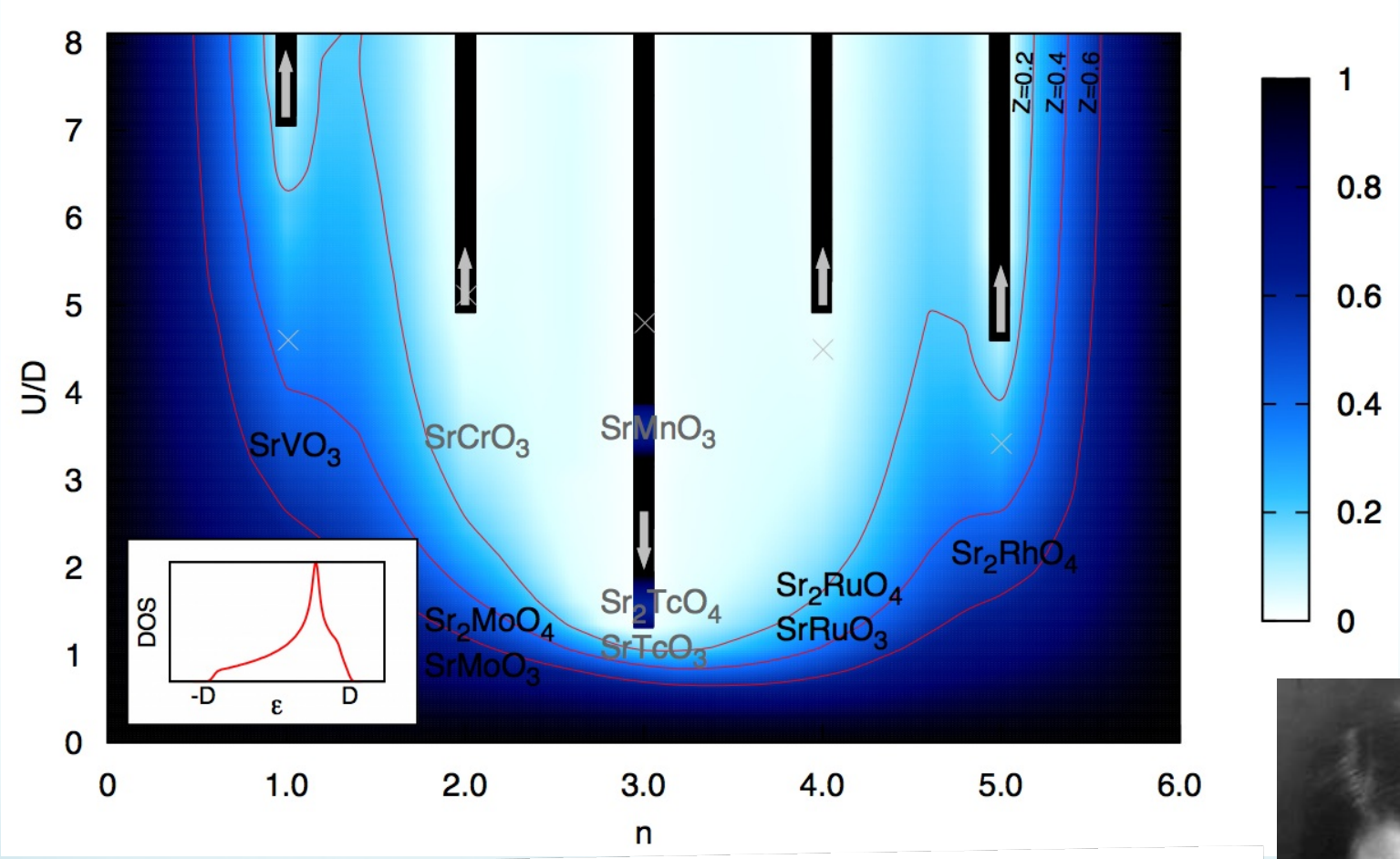






C. Carbone (Trieste),
O. Rader (BESSY), *et al*
PRL (2010)

J - Hund's Materials



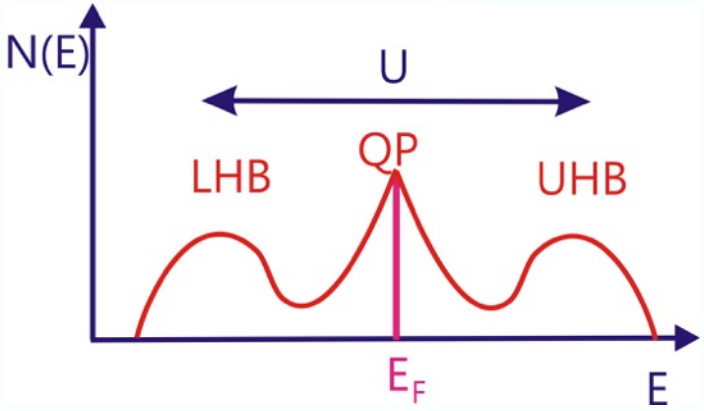
$$H_{t_{2g}} = (U - 3J)\,\frac{\hat{N}(\hat{N}-1)}{2} - 2J\,\vec{S}^2 - \frac{J}{2}\vec{L}^2 + \frac{5}{2}J\,\hat{N}$$

A. Georges et.al, PRL (2012)

Correlated Materials

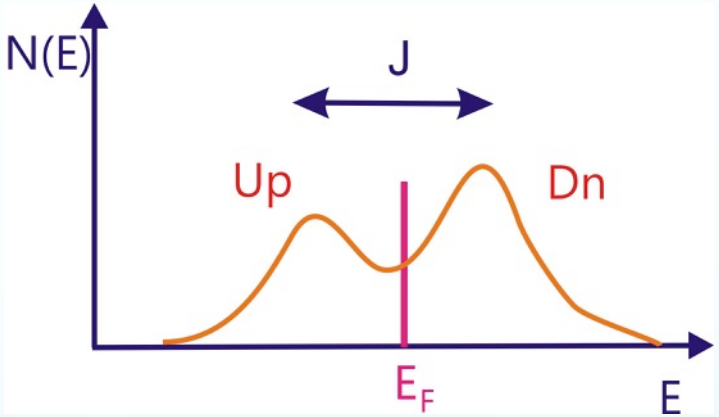
Hubbard-metal

(correlations due to U)
Single-band DMFT



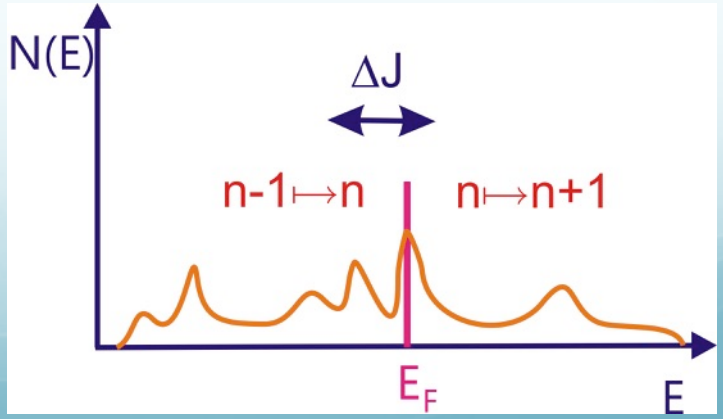
Hunds-metal

(correlations due to J)
Fe-based HTSC



Racah-metal

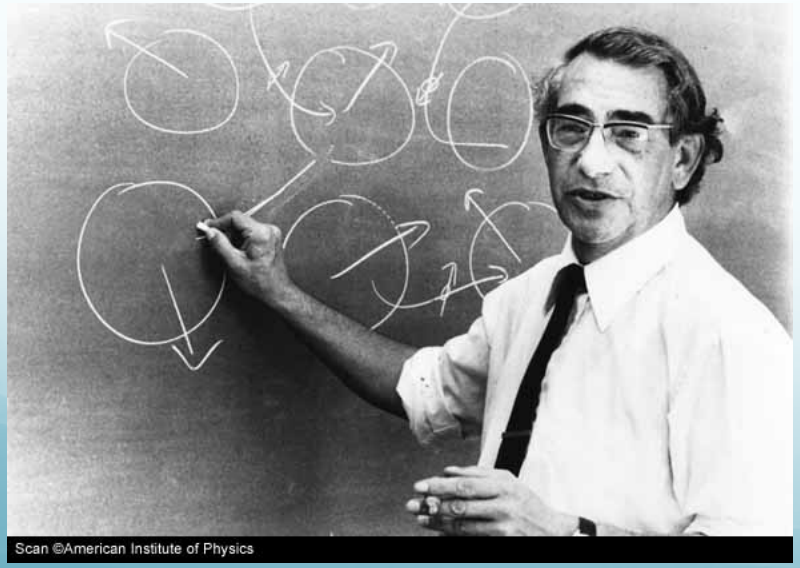
(correlations due to F_k)
f-compounds

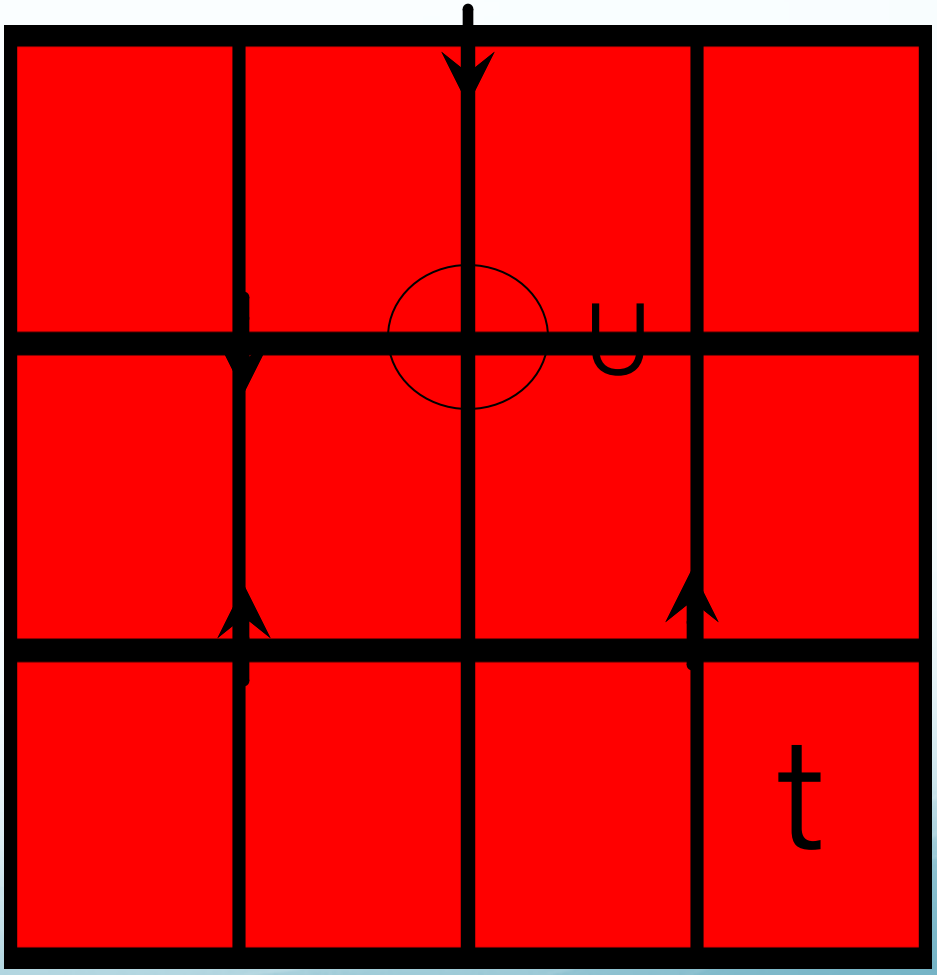


Hubbard model for correlated electrons

$$H = \sum_{ij} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

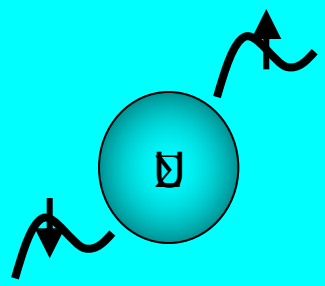
- U/t
- Chemical potential





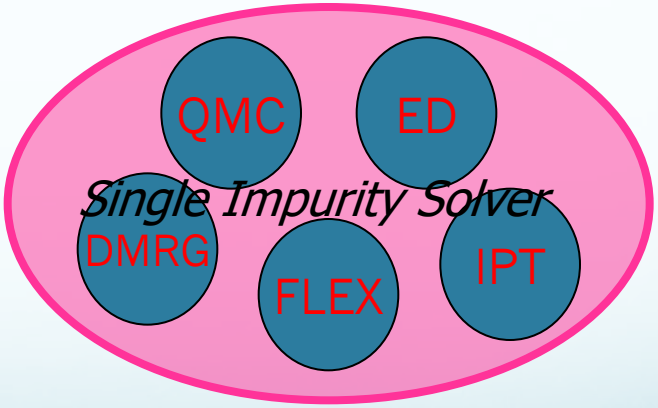
Dynamical Mean Field Theory

$$\mathcal{G}_0(\tau-\tau')$$



$$\hat{G}(i\omega_n)=\frac{1}{\Omega}\sum_{\vec{k}}^{BZ}\hat{G}(\vec{k},i\omega_n)$$

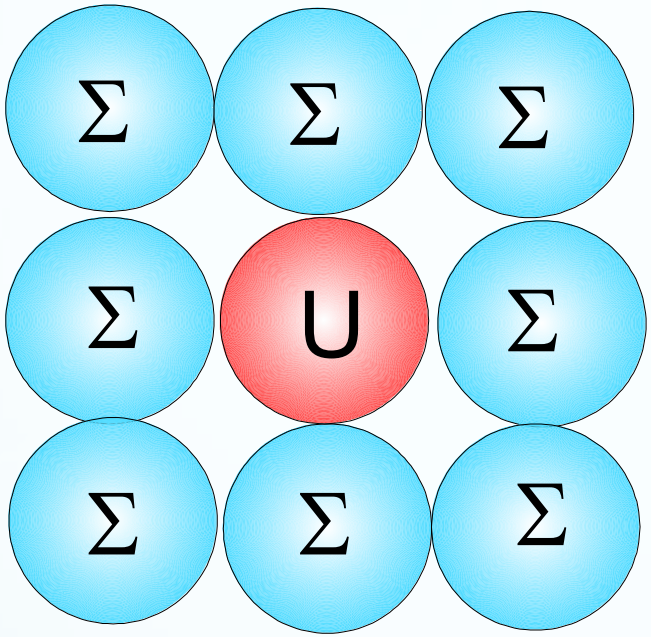
$$\hat{\mathcal{G}}_0^{-1}(i\omega_n)=\hat{G}^{-1}(i\omega_n)+\hat{\Sigma}(i\omega_n)$$

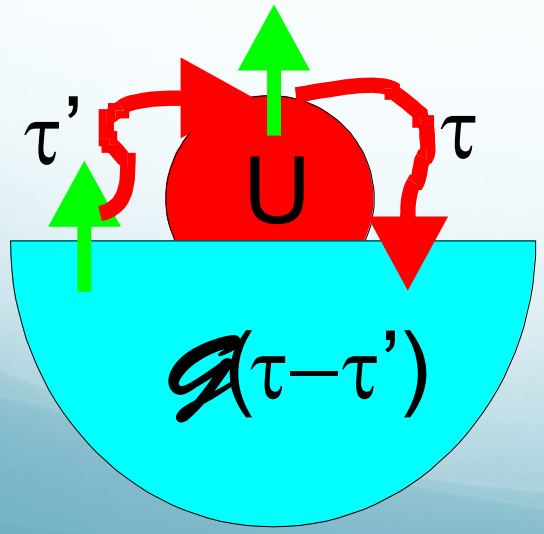


$$\hat{\Sigma}_{new}(i\omega_n)=\hat{\mathcal{G}}_0^{-1}(i\omega_n)-\hat{G}^{-1}(i\omega_n)$$

V. Metzner and D. Vollhardt (1987)
A. Georges and G. Kotliar (1992)

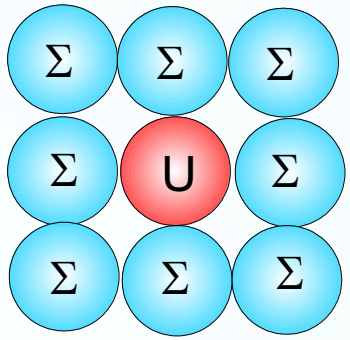
Quantum Impurity Solver





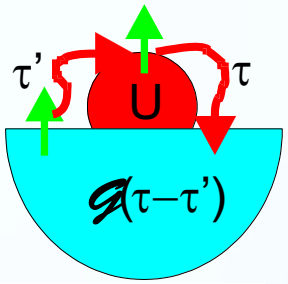
What is a best scheme?
Quantum Monte Carlo !

Continuous Time Quantum Monte Carlo



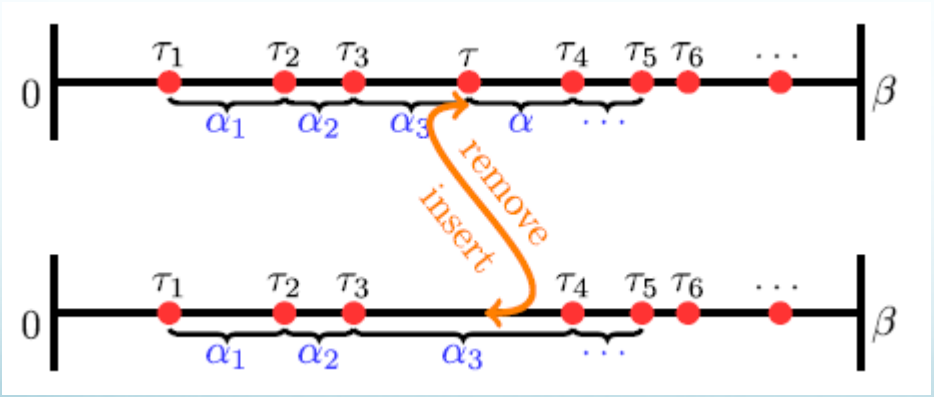
Partition function: $H = H_0 + V$

$$Z = \mathrm{Tr}\left[e^{-\beta H_0} \mathbf{T}_\tau e^{-\int_0^\beta d\tau V(\tau)}\right]$$



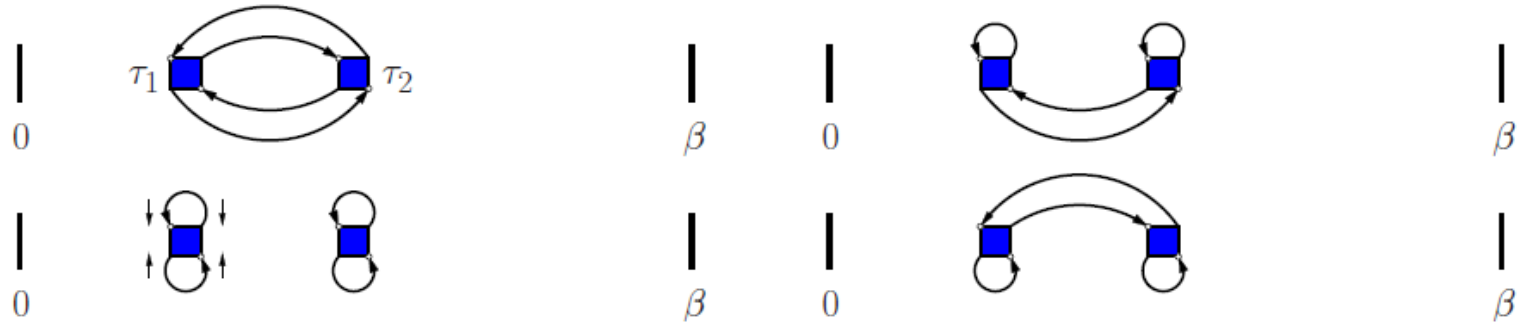
Continuous Time Quantum Monte Carlo (CT-QMC)

$$Z = \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \ldots \int_{\tau_{k-1}}^\beta d\tau_k \mathrm{Tr}\left[e^{-\beta H_0} e^{-\tau_k H_0}(-V)\ldots e^{-(\tau_2-\tau_1)H_0}(-V) e^{-\tau_1 H_0}\right]$$



E. Gull, A. Millis, A.L., A. Rubtsov, M. Troyer, Ph. Werner, Rev. Mod. Phys. **83**, 349 (2011)

Weak coupling QMC: CT-INT



$$\mathcal{Z}_{\text{imp}} = \int e^{-S_0[c^*,c]+U\int_0^\beta n_\uparrow(\tau)n_\downarrow(\tau)}\mathcal{D}[c^*,c]$$

$$= \int e^{-S_0[c^*,c]} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} U^k \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k \, c_\uparrow^*(\tau_1)c_\uparrow(\tau_1)$$

$$\times c_\downarrow^*(\tau_1)c_\downarrow(\tau_1)\ldots c_\uparrow^*(\tau_k)c_\uparrow(\tau_k)c_\downarrow^*(\tau_k)c_\downarrow(\tau_k)\,\mathcal{D}[c^*,c]$$

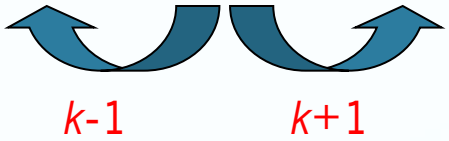
$$= \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} U^k \int d\tau_1 \ldots \int d\tau_k \text{sgn}(\det \hat{G}) \underbrace{|\det \hat{G}|}_{P(k)}$$

$$\hat{G}_{ij} = g_0(\tau_i - \tau_j)$$

A. Rubtsov and A.L., JETP Lett. 80, 67 (2004)

CT-INT: random walks in the *k* space

$Z = \ldots Z_{k-1} + Z_k + Z_{k+1} + \ldots$

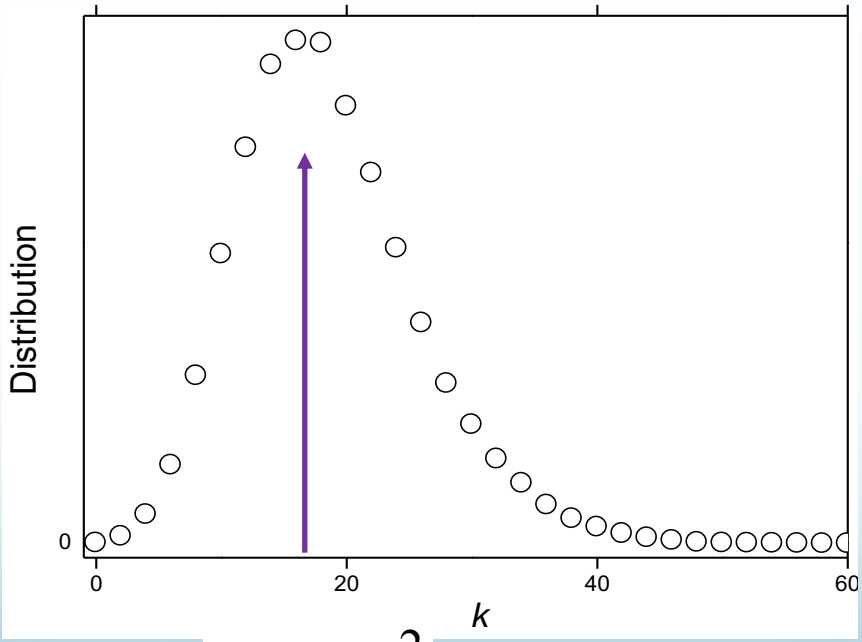


Acceptance ratio

decrease

Step *k*-1

$$\frac{k}{|w|}\frac{D^{k-1}}{D^k}$$



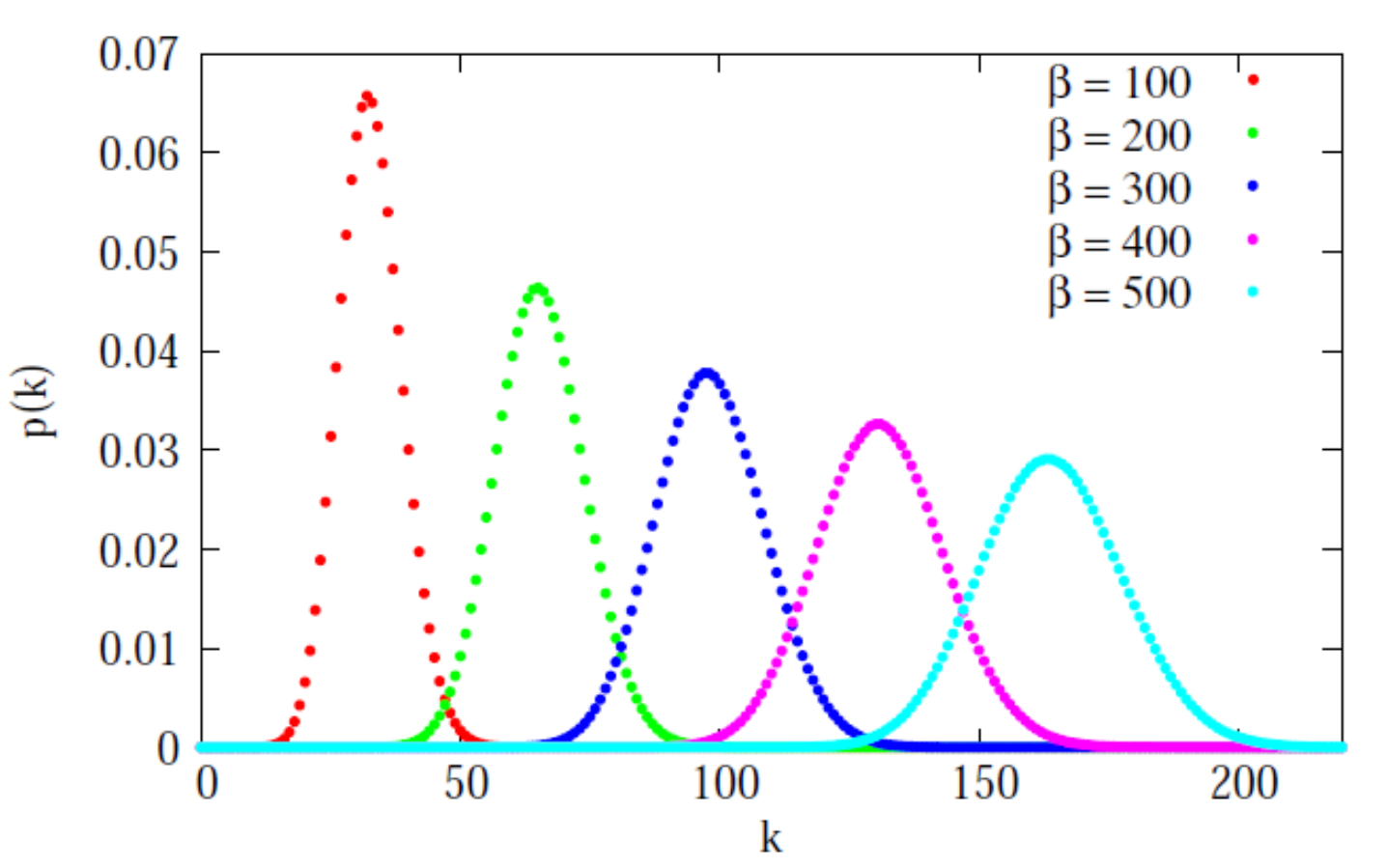
increase

Step *k*+1

$$\frac{|w|}{k+1}\frac{D^{k+1}}{D^k}$$

Maximum at βUN^2

Convergence with Temperature: CT-INT



Maximum: βUN^2

Impurity solver: miracle of CT-QMC

$$S = \sum_{\sigma\sigma'} \int_0^\beta d\tau \int_0^\beta d\tau [-G_0^{-1}(\tau-\tau')c_\sigma^+(\tau)c_\sigma(\tau') + \frac{1}{2}U\delta(\tau-\tau')c_\sigma^+(\tau)c_{\sigma'}^+(\tau)c_{\sigma'}(\tau')c_\sigma(\tau')]$$

$$G_0^{-1}(\tau-\tau') = \delta(\tau-\tau')[\frac{\partial}{\partial\tau} + \mu] - \Delta(\tau-\tau')$$

Interaction expansion CT-INT: A. Rubtsov et al, JETP Lett (2004)

$$Z = Z_0 \sum_{k=0}^{\infty} \frac{(-U)^k}{k!} Tr\,\det[G_0(\tau-\tau')]$$

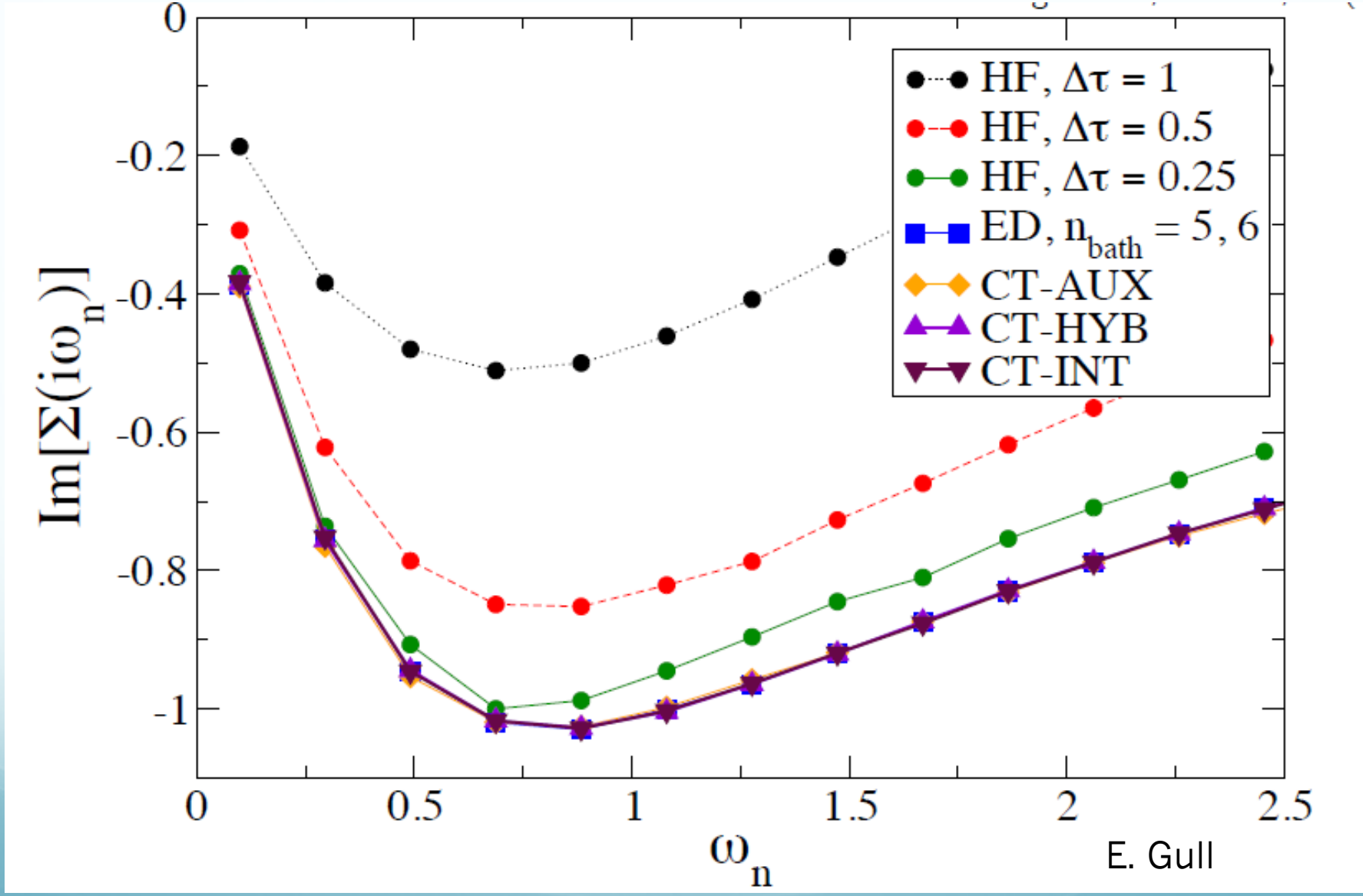
Hybridization expansion CT-HYB: P. Werner et al, PRL (2006)

$$Z = Z_0 \sum_{k=0}^{\infty} \frac{1}{k!} Tr \left\langle c_\sigma^+(\tau)c_\sigma(\tau')...c_{\sigma'}^+(\tau)c_{\sigma'}(\tau') \right\rangle_0 \det[\Delta(\tau-\tau')]$$

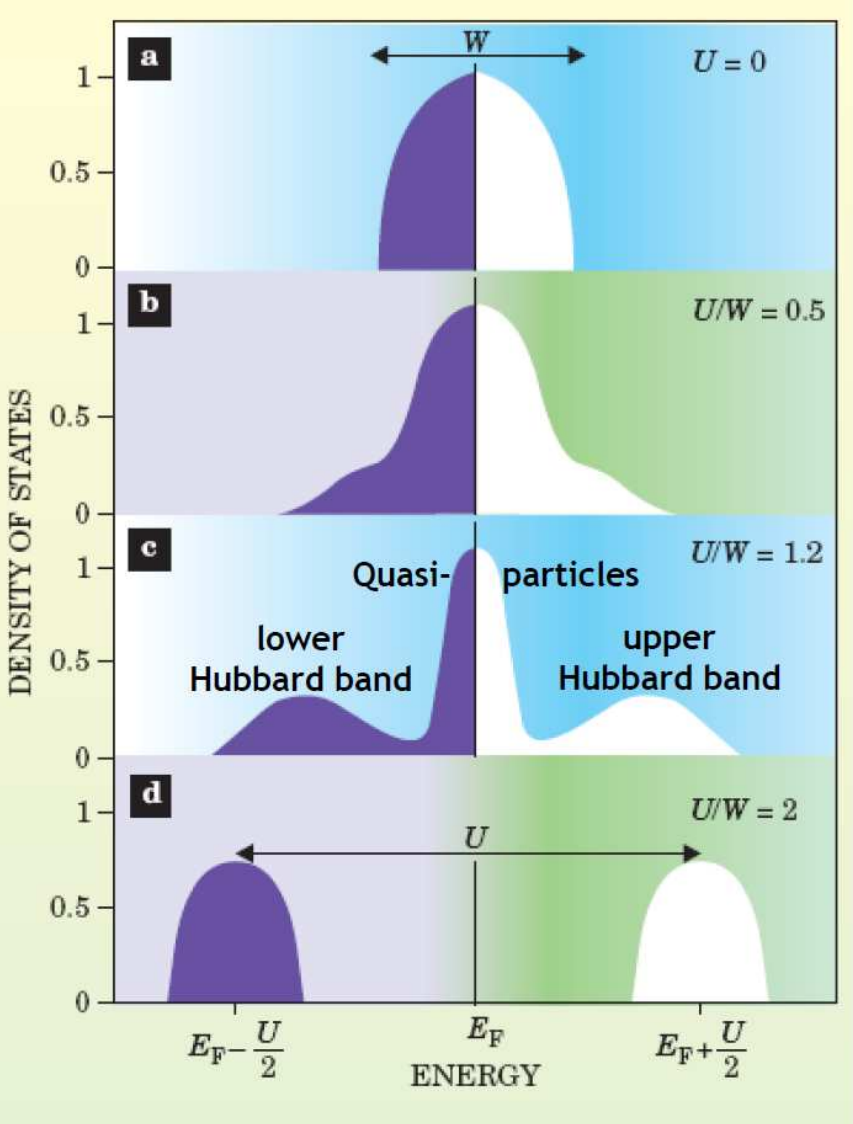
Efficient Krylov scheme: A. Läuchli and P. Werner, PRB (2009)

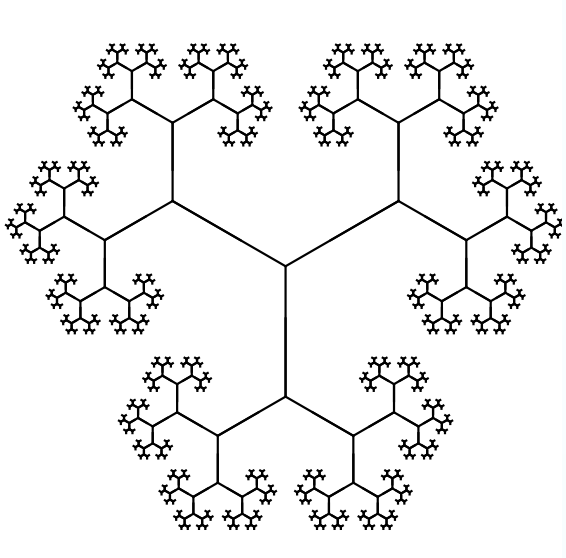
E. Gull, et al, RMP **83**, 349 (2011)

Benchmark for CT-QMC

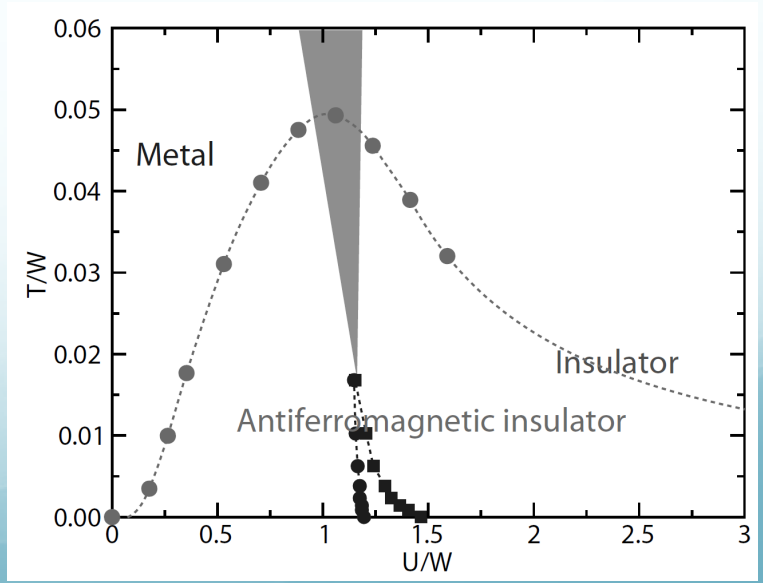


DMFT: Metal-Insulator Transition





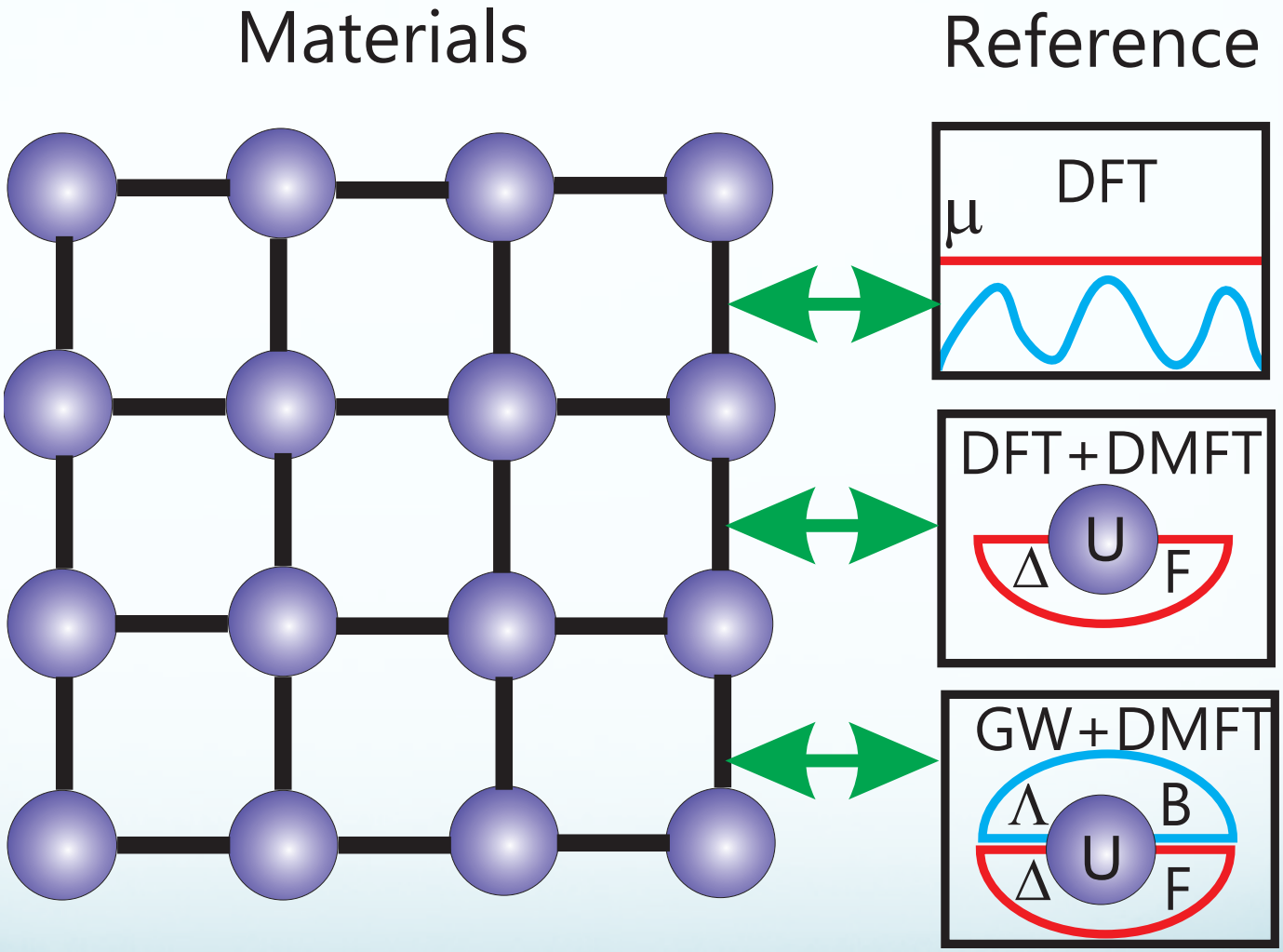
Bethe Lattice (Z=3)



$Z \rightarrow \infty$

G. Kotliar and D. Vollhardt, Phys. Today **3,** 53 (2004)

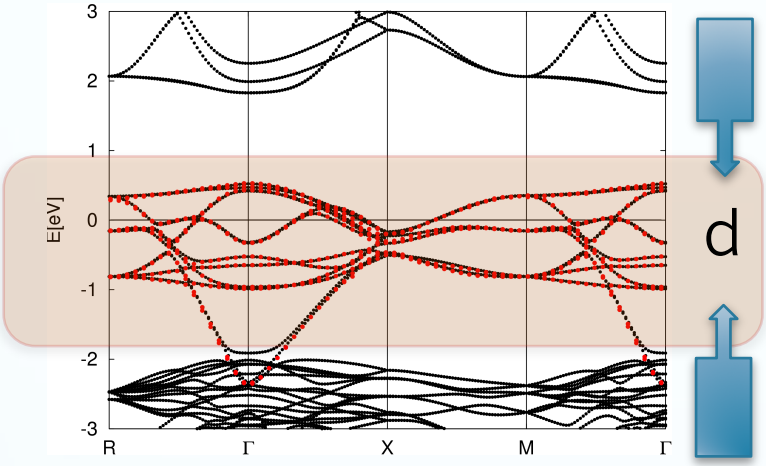
Real Materials: Reference Systems



Reference system is important: Archimedes
„Give me the place to stand, and I shall move the earth.“

Non-local screened interactions

F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, A. L. PRB 70, 195104 (2004).



c-RPA screening

χ_0^t

χ_0^r

Interaction	C_2F	C_2H
U_{00}	5.16	4.69
U_{01}	2.46	2.19
U_{02}	1.66	1.11
U_{03}	1.46	0.85
J_{01}^F (screened)	0.018	0.034
J_{01}^F (bare)	0.044	0.099

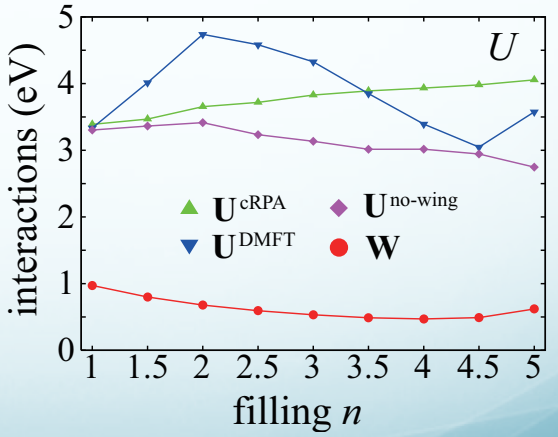
V. Mazurenko, et al, PRB 94, 214411 (2016)

$$\bar{W} = (1 - v\chi_0^r)^{-1} v \qquad W = (1 - \bar{W}\chi_0^t)^{-1} \bar{W}$$

$$U_{ij} = \left\langle ij \middle| \bar{W} \middle| ij \right\rangle$$

$$J_{ij} = \left\langle ij \middle| \bar{W} \middle| ji \right\rangle$$

Non-local Coulomb and Exchange



C-RPA in Wannier basis:
Y. Nomura, M. Kaltak, K. Nakamura, C. Taranto, S. Sakai, A. Toschi, R. Arita, K. Held, G. Kresse, M. Imada, PRB **86**, 085117 (2012)

Constrained GW calculations of U

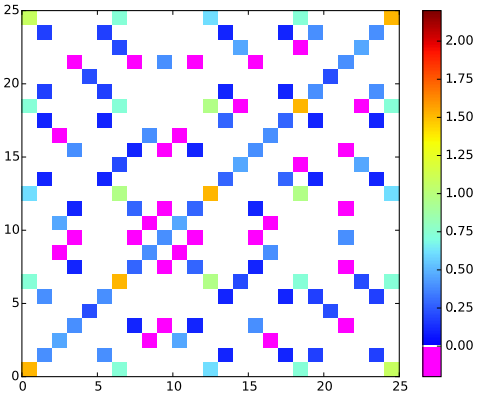
PHYSICAL REVIEW B **70**, 195104 (2004)

Frequency-dependent local interactions and low-energy effective models from electronic structure calculations

F. Aryasetiawan,[1] M. Imada,[2,3] A. Georges,[4,5] G. Kotliar,[6] S. Biermann,[4] and A. I. Lichtenstein[7]

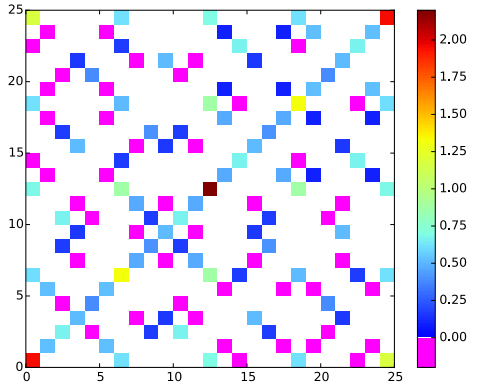
$$U_{nn',mm'}(\tau-\tau') \doteq \int d^3r d^3r' \, \phi_n^*(\mathbf{r})\phi_{n'}(\mathbf{r}) W_r(\mathbf{r},\mathbf{r}';\tau-\tau')\,\phi_m^*(\mathbf{r}')\phi_{m'}(\mathbf{r}')$$

3d



Slater

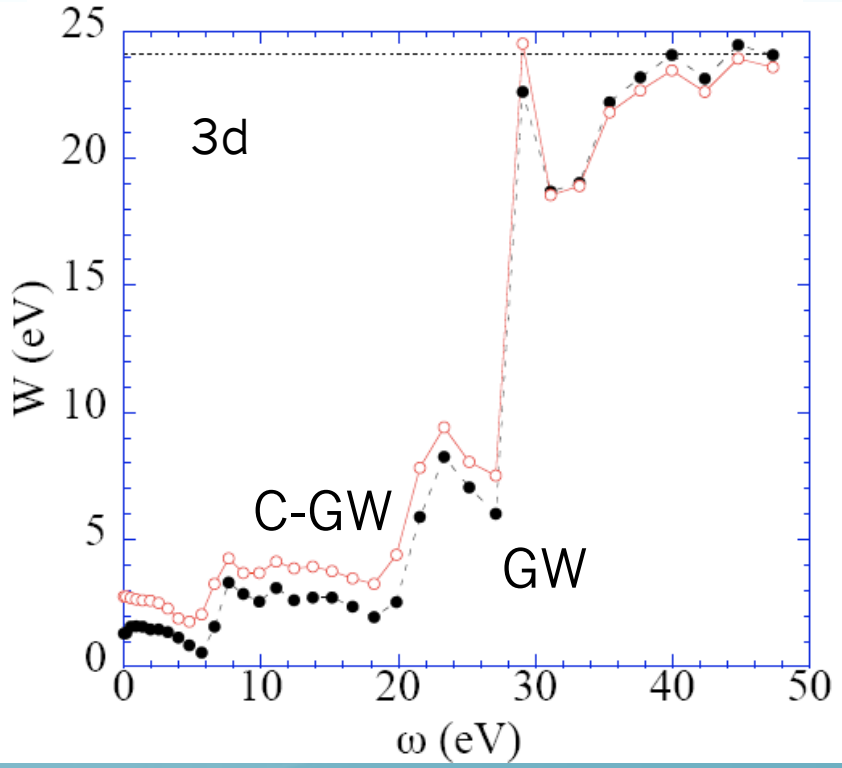
Spher. Sym.



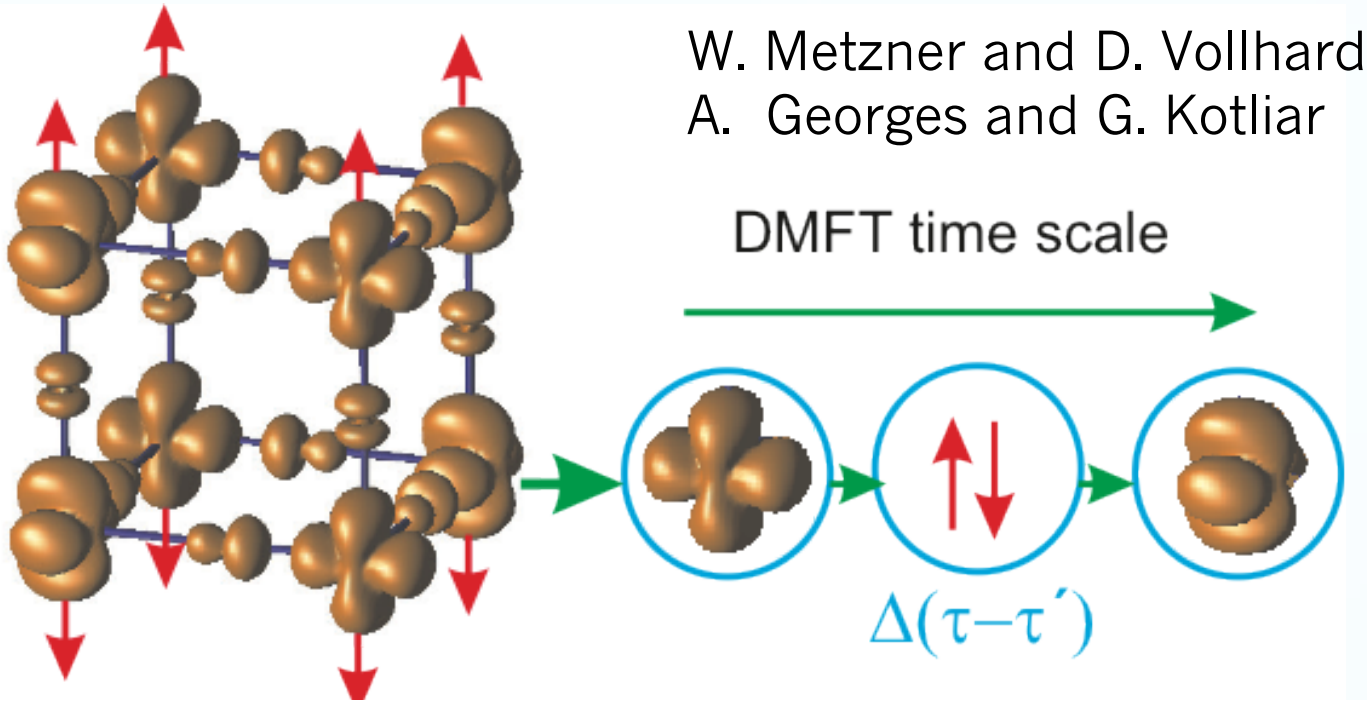
C-RPA

Cubic. Sym.

$$W_r(\omega) = [1 - vP_r(\omega)]^{-1} v$$



Realistic DMFT: Charge+Spin+Orbital Fluctuations



W. Metzner and D. Vollhardt (1987)
A. Georges and G. Kotliar (1992)

$$S[c^*,c] = -\sum_{\omega \mathbf{k}\sigma\, mm'} c^*_{\omega \mathbf{k}\sigma m}\left[(i\omega+\mu)\mathbf{1} - t^{mm'}_{\mathbf{k}\sigma}\right] c_{\omega \mathbf{k}\sigma m'} + \sum_i S_{\mathrm{U}}[c^*_i, c_i]$$

$$S_{\mathrm{loc}}[c^*,c] = -\sum_{\omega\,\alpha\beta} c^*_{\omega\alpha}\left[(i\omega+\mu)\mathbf{1} - \Delta^{\alpha\beta}_{\omega}\right] c_{\omega\beta} + S_{\mathrm{U}}[c^*,c]$$

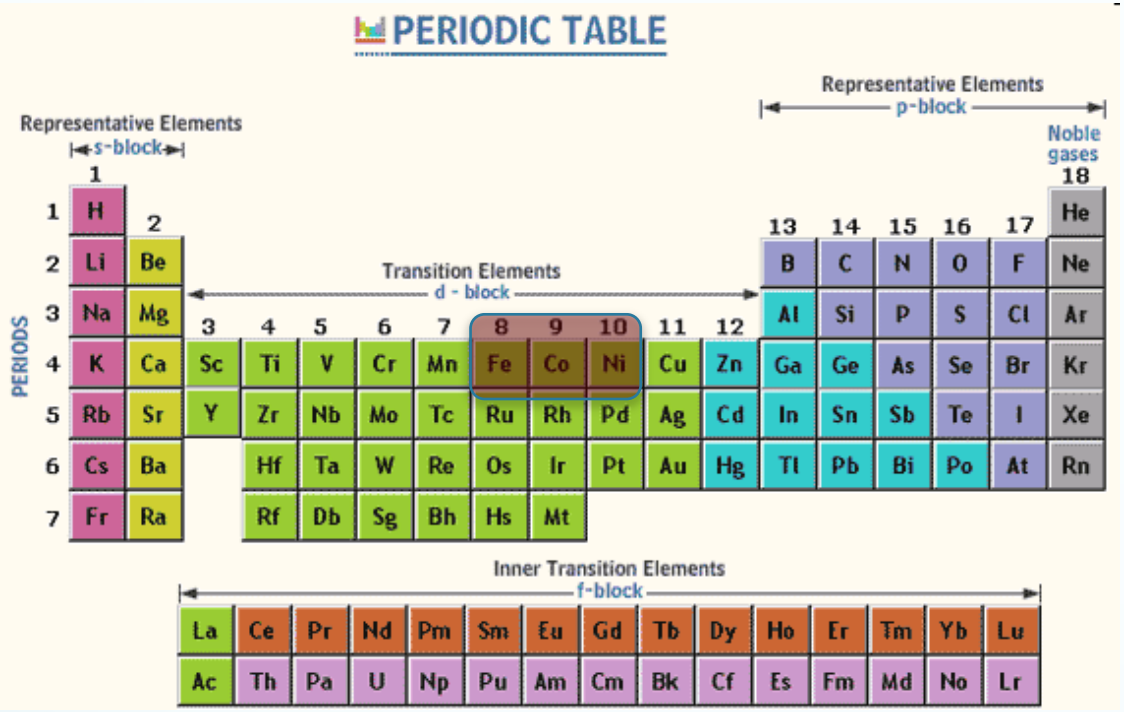
$$g_{12} = -\langle c_1 c_2^* \rangle_{\mathrm{loc}}$$

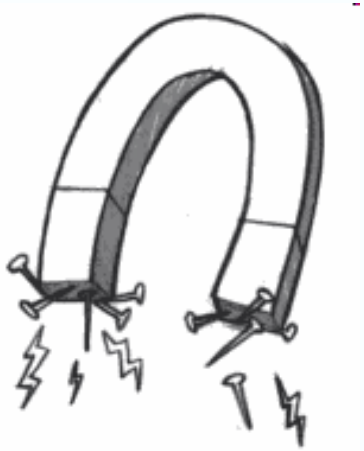
$$\sum_{\mathbf{k}} \left[g^{-1}_{\omega} + \Delta_{\omega} - t_{\mathbf{k}}\right]^{-1} = g_{\omega}$$

DMFT
self-consistensy

DMFT
Impurity solver
TRIQS, ALPS

Magnetism of Fe, Co, Ni





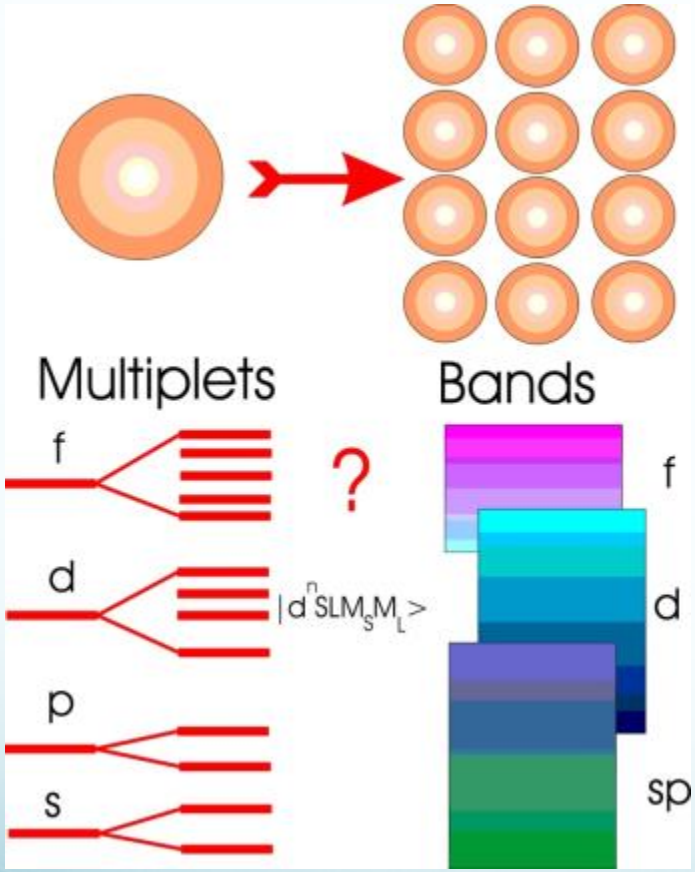
Ferromagnetism of iron is known from ancient times
Hippocrates – 440 BC
Lucretius – 100 BC

Iron (T_c=1041 K)

Cobalt (T_c=1394 K)

Nickel (T_c=633 K)

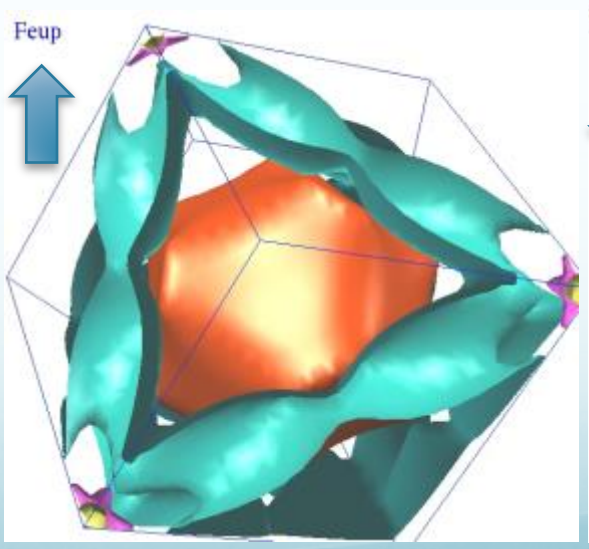
Coexistence of localized and itinerant behavior

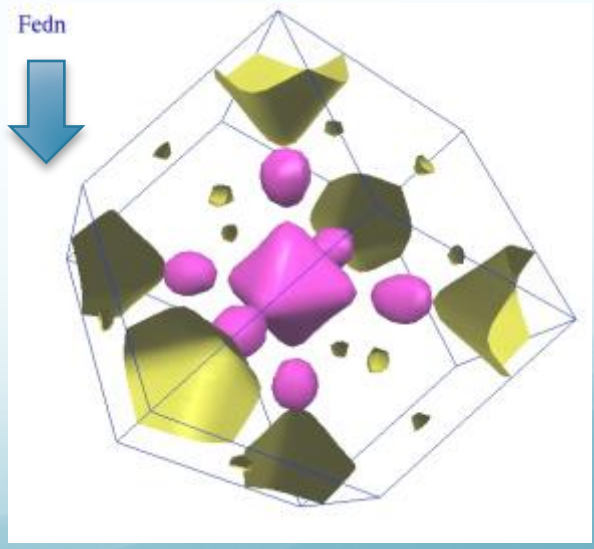


Local magnetic moments exists above T_C
- Curie-Weiss law, spectroscopy, neutrons

d electrons are itinerant
- FS, chemical bonding, transport

Iron Fermi Surface



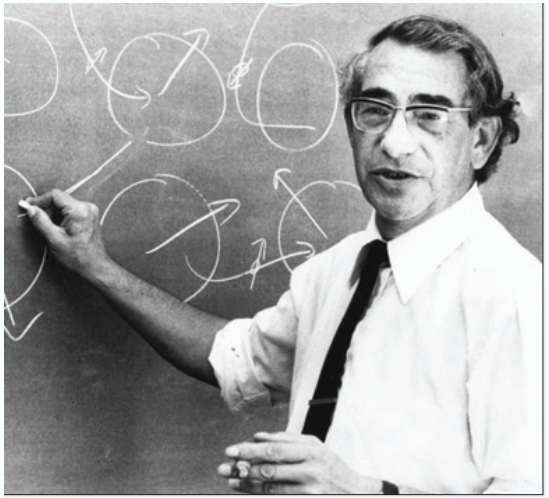


S. Hershfield **http://www.phys.ufl.edu/fermisurface**

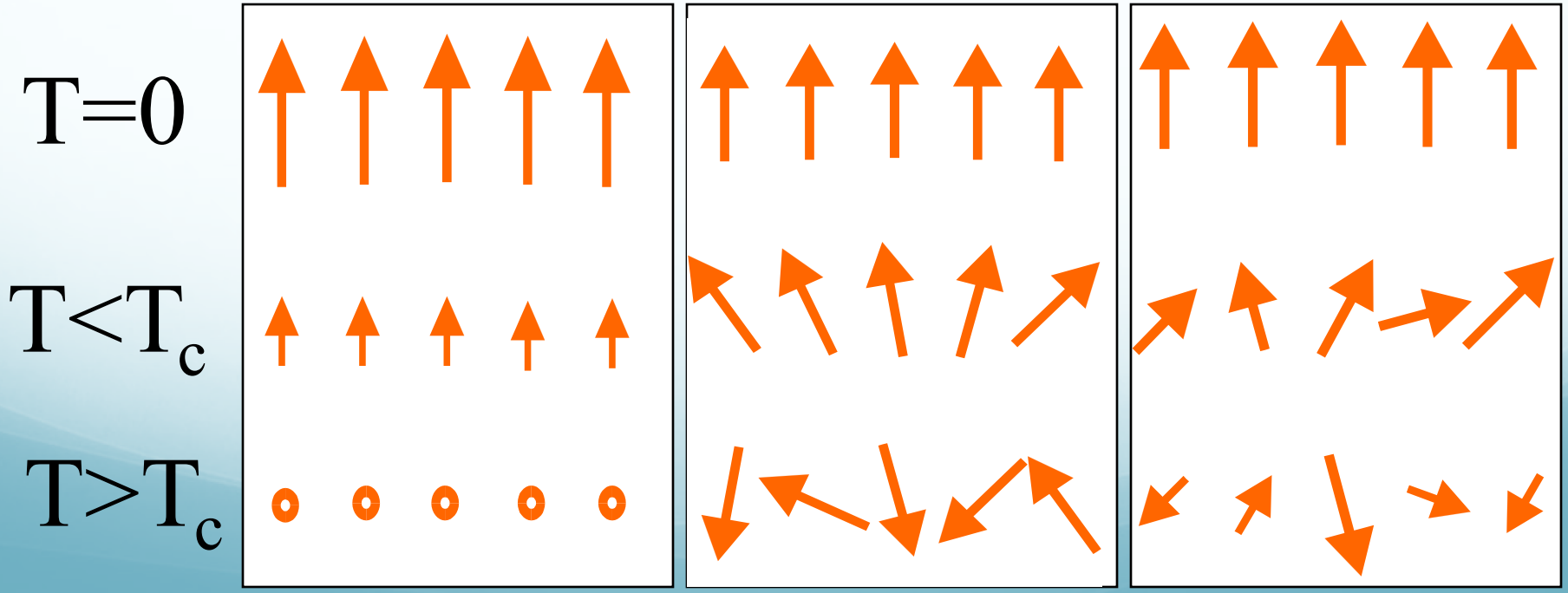
Itinerant ferromagnetism

Stoner

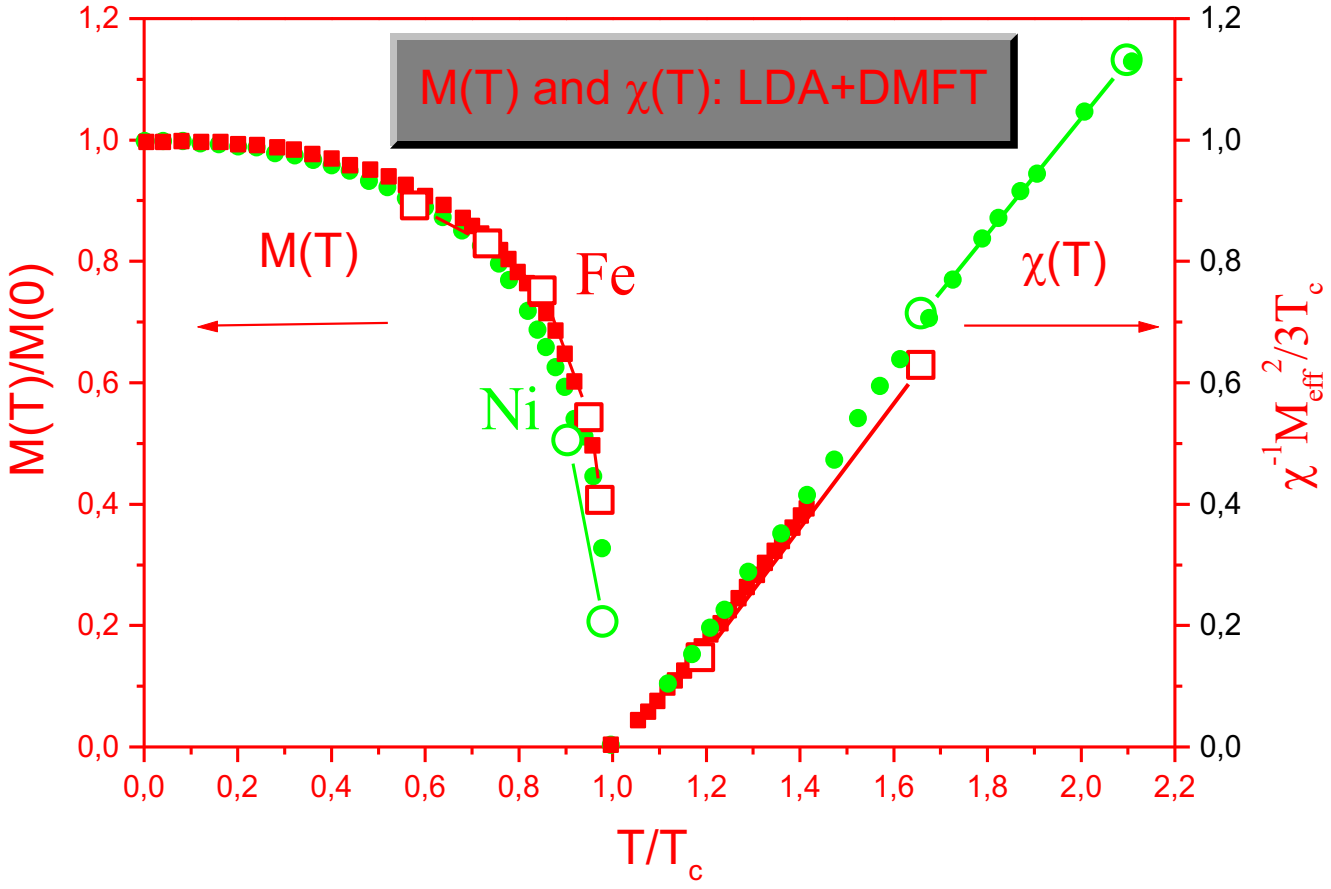
Heisenberg



Hubbard

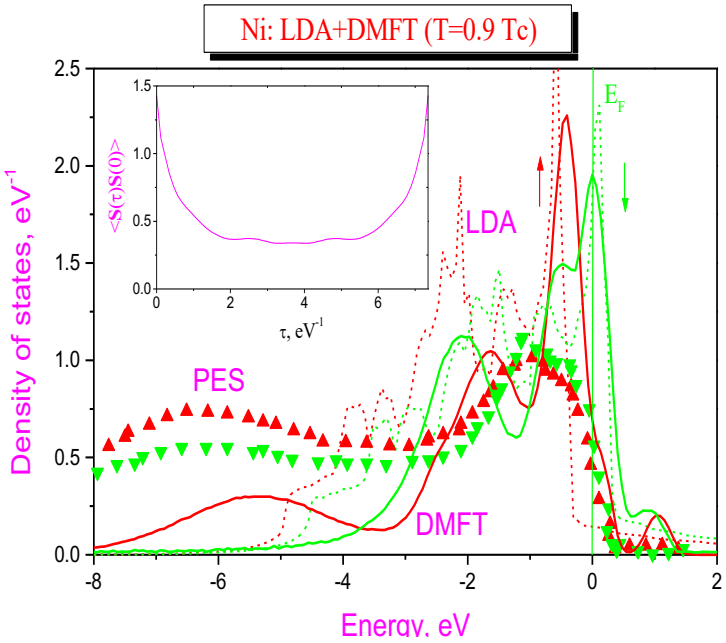


Magnetism of metals: LDA+DMFT



A. L., M. Katsnelson and G. Kotliar, PRL(2001)

PES: satellite structure in Ni



PES (LDA)

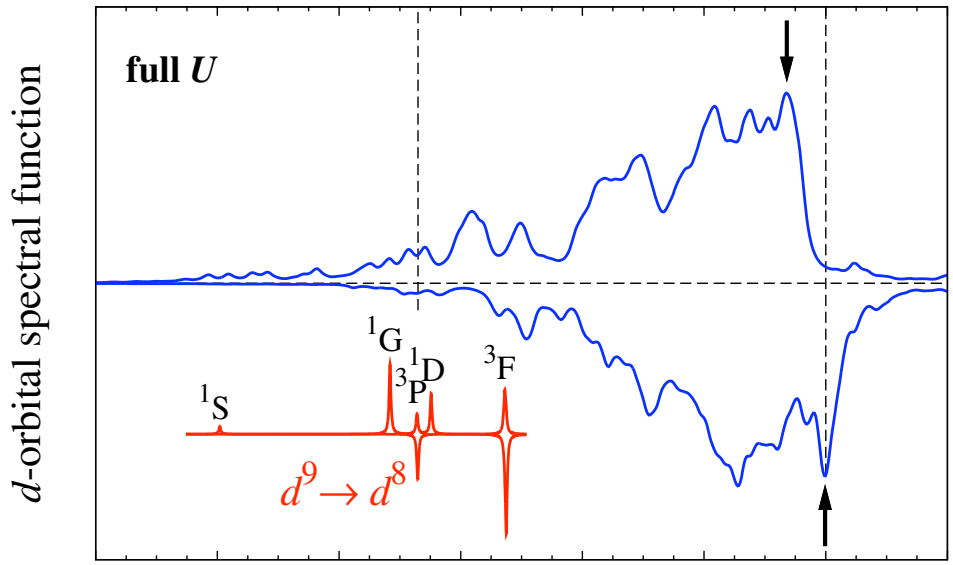
$$W_{band} = 3(4)\ \text{eV}$$

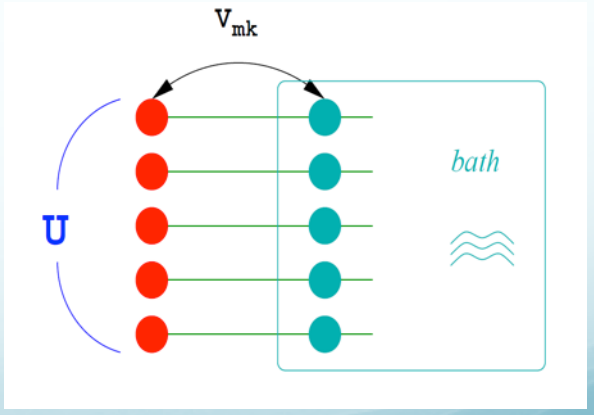
$$\Delta E_{ex} = 0.3(0.6)\ \text{eV}$$

$$E_{sat} = -6(?)\ \text{eV}$$

LDA+DMFT+QMC

A. L., M. Katsnelson and G. Kotliar, PRL (2001)





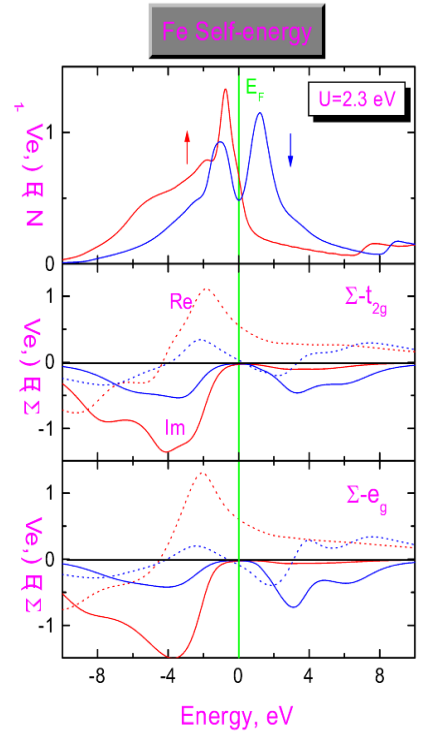
T-Lanczos (5d+10k)

J. Kolorenč et al, PRB 85, 235136 (2012)

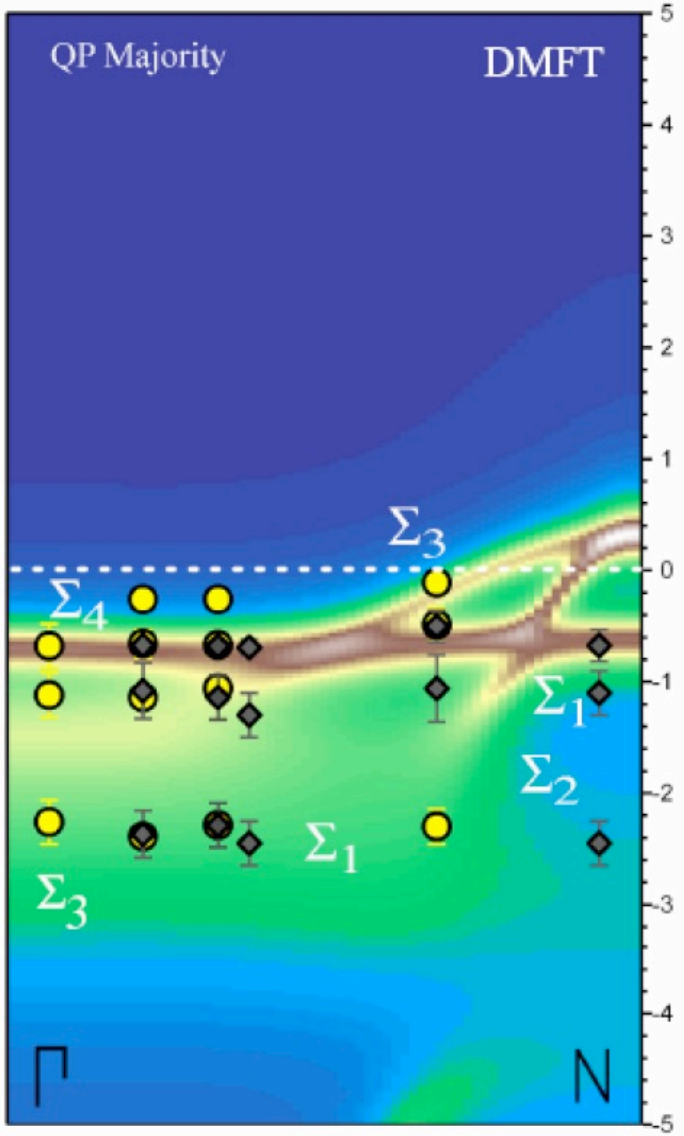
Spectral Function Fe: ARPES vs. DMFT

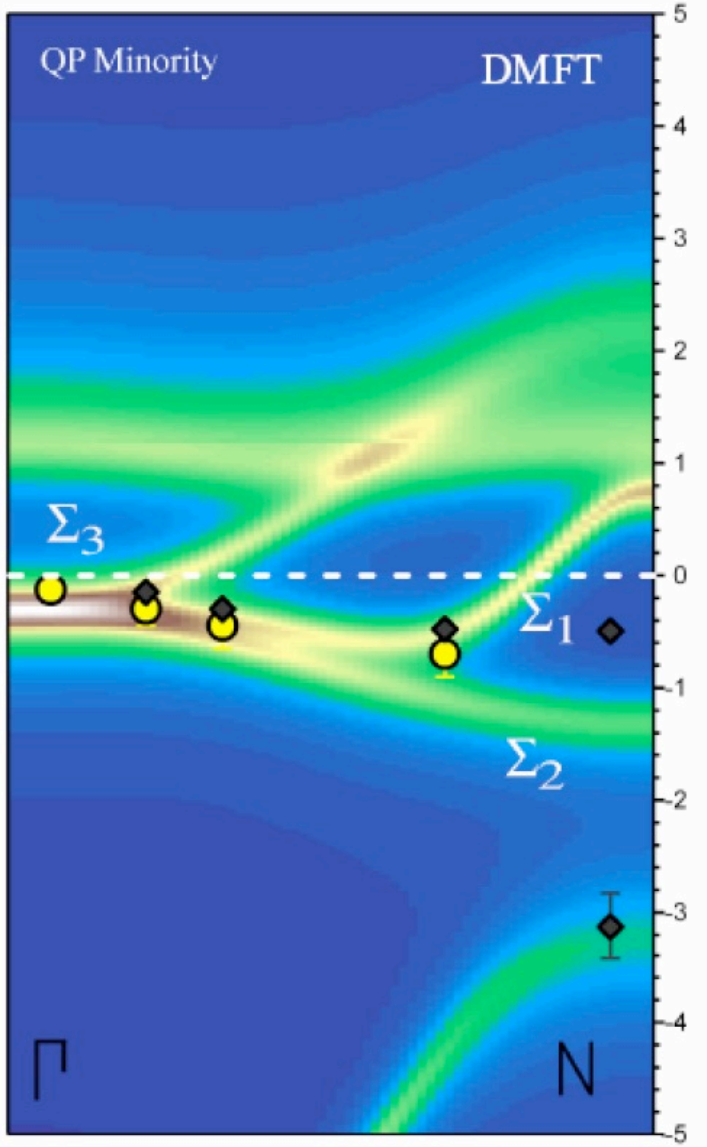
Vertical Pol.

Horizontal Pol.

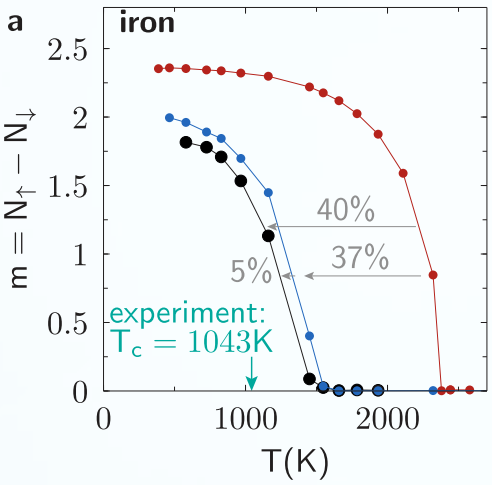


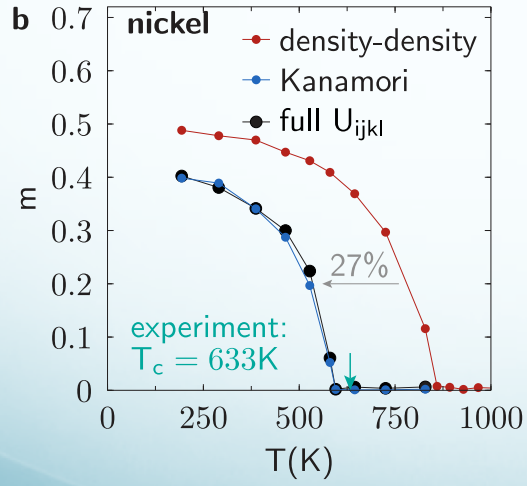
SP-ARPES (BESY)
J. Sánchez-Barriga, et al, PRL (2010)

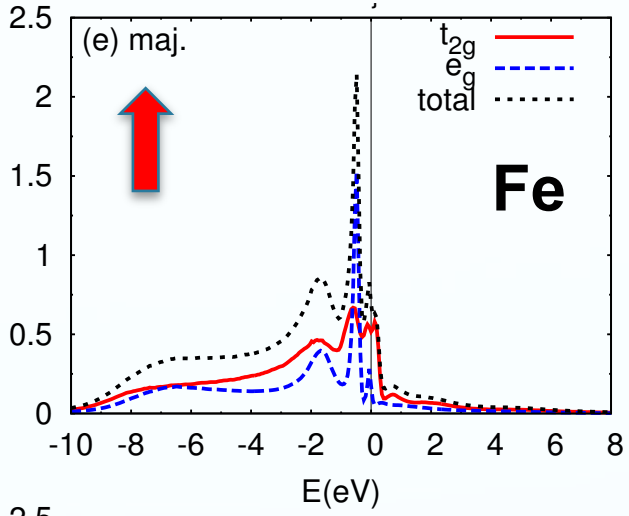


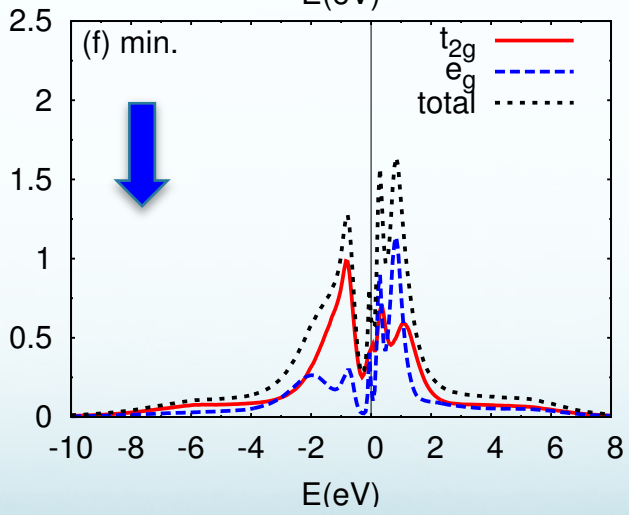


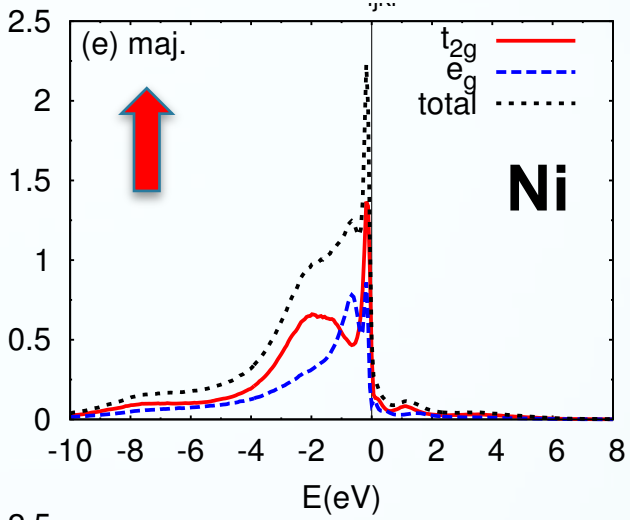
CT-QMC with full U

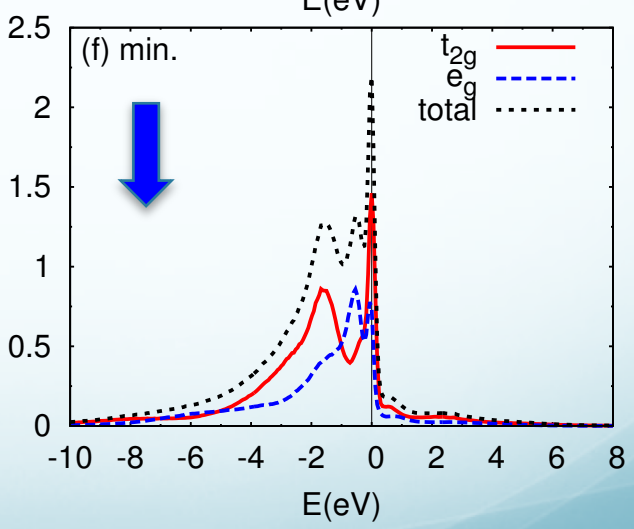










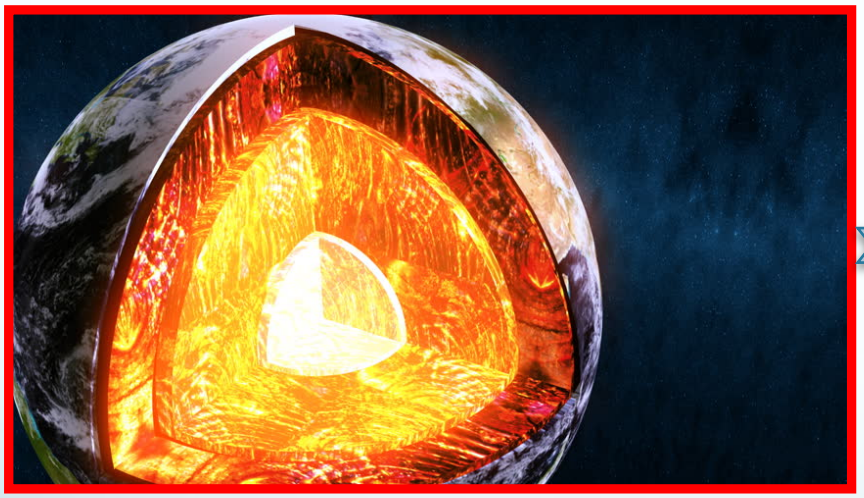


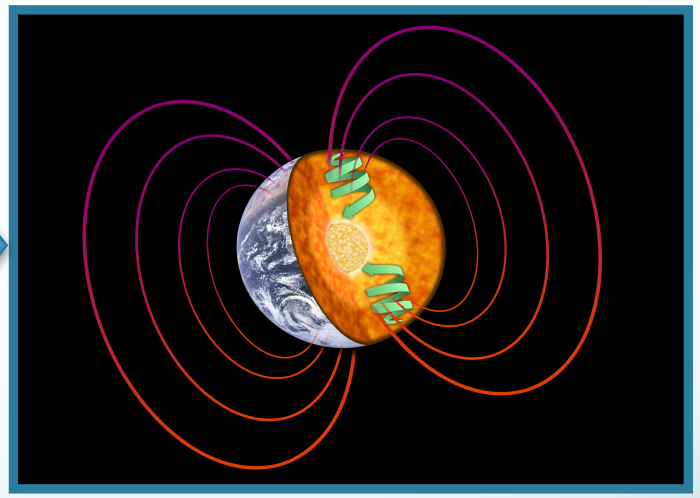
A. Hausoel, et al Nat. Comm. (2017)

$$H_{\text{int}} = \frac{1}{2}\sum_{m,\sigma} U_{mm'm''m'''} c^{+}_{m\sigma} c^{+}_{m'\sigma'} c_{m'''\sigma'} c_{m''\sigma}$$

3d-Magnets at high pressure

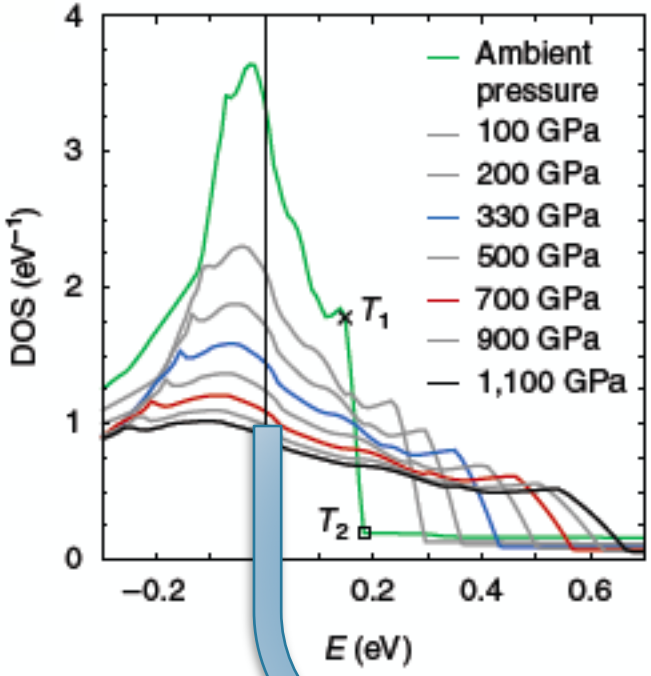
Fe and **Ni** and their **alloys** under pressure
from ambient to **Earth ‘s core** condition





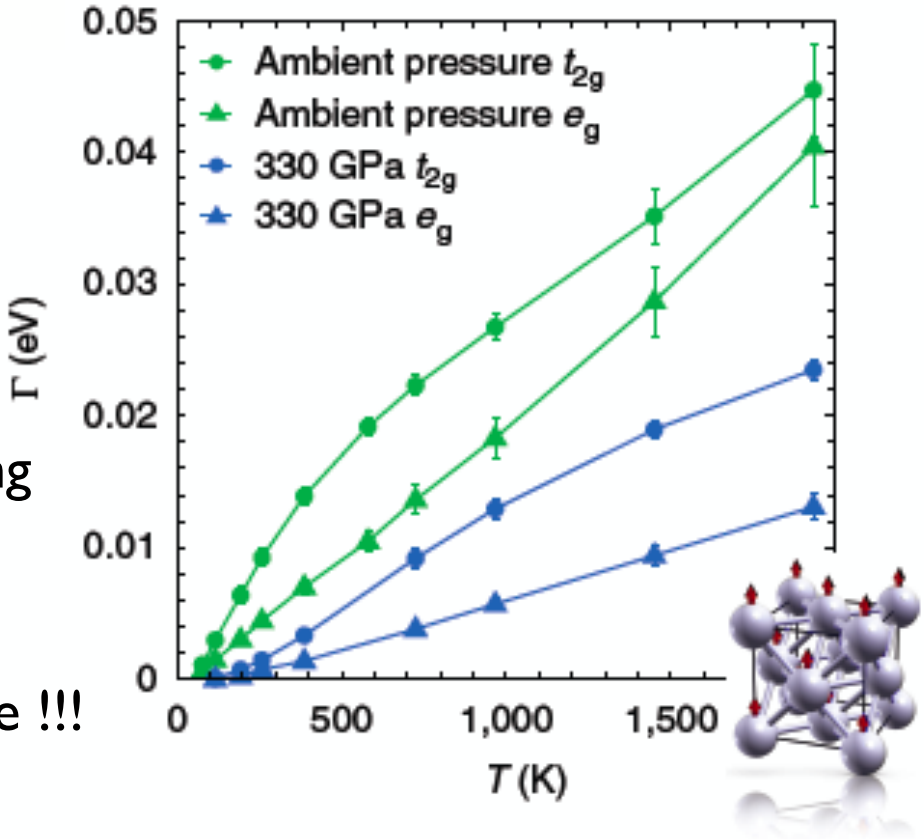
Earth‘s magnetism

What about Nickel ?



❖ **A.Hausoel, M. Karolak, E. Sasioglu, A.I. Lichtenstein, K. Held, A.A. Katanin, AT and G. Sangiovanni , Nat. Comm. (2017)**

DOI: 10.1038/ncomms16062



✧ comparable el-el scattering as in Fe

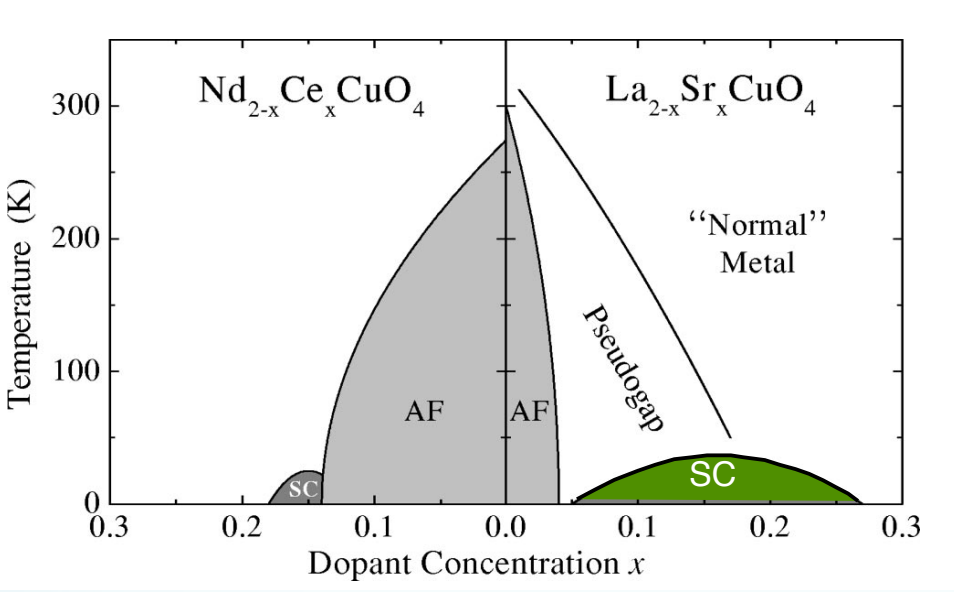
BUT

✧ much less Fermi-liquid-like !!!

(no T^2 –behavior visible)

30 years of HTSC: d-wave superconductivity

Damascelli *et al.*, Rev. Mod. Phys 75, 2 (2003)



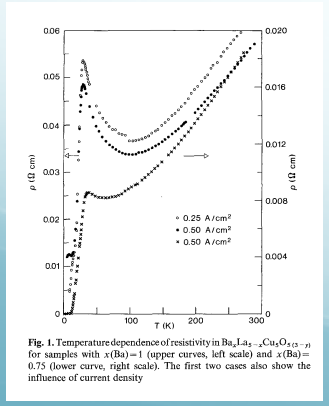
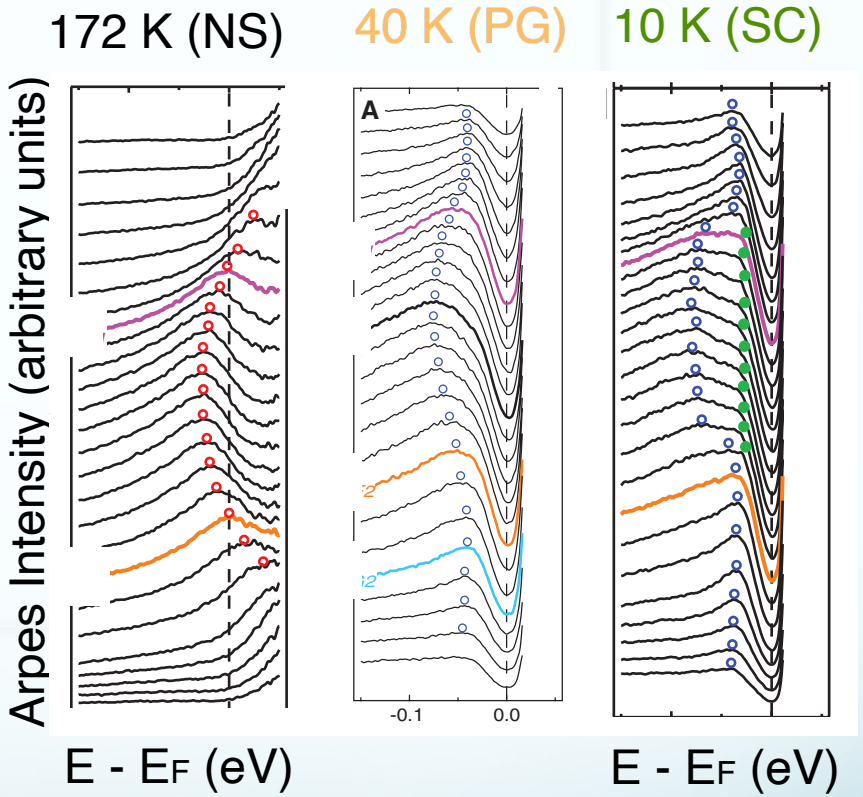


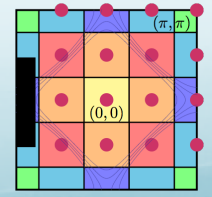
Fig. 1. Temperature dependence of resistivity in $Ba_xLa_{5-x}Cu_5O_{5(3-y)}$ for samples with $x(Ba)=1$ (upper curves, left scale) and $x(Ba)=0.75$ (lower curve, right scale). The first two cases also show the influence of current density

Bednorz and Müller

Zeitschrift für Physik B 64, 189 (1986)

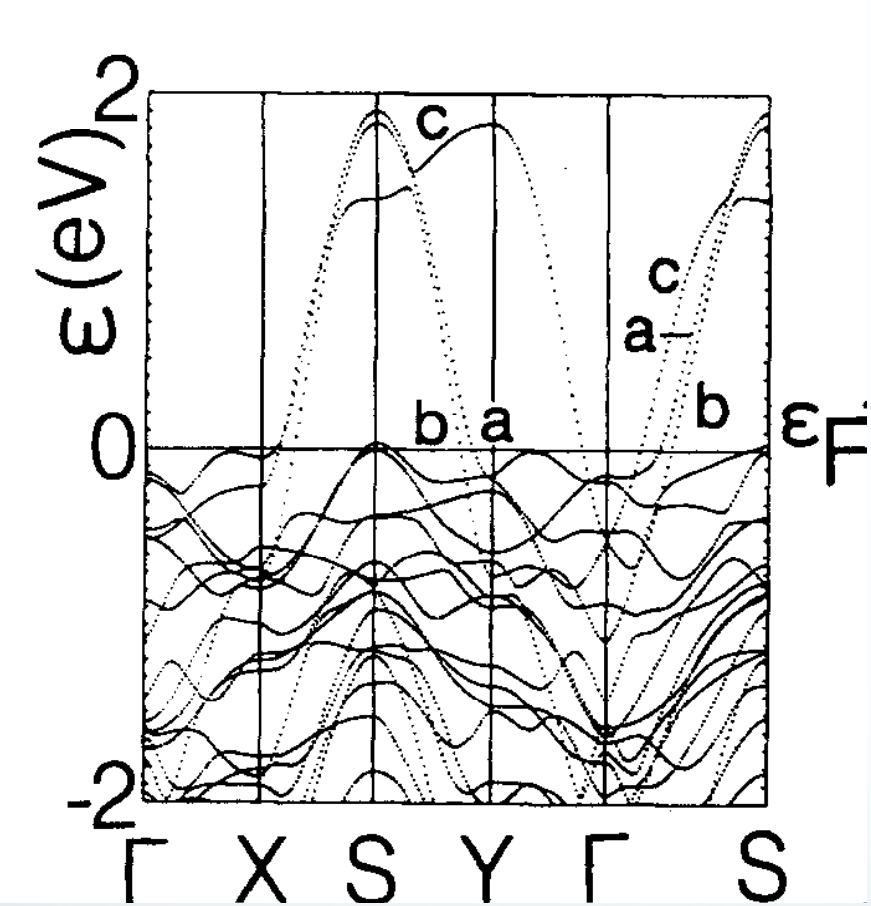
He *et al.*, Science 331, 1579 (2011)



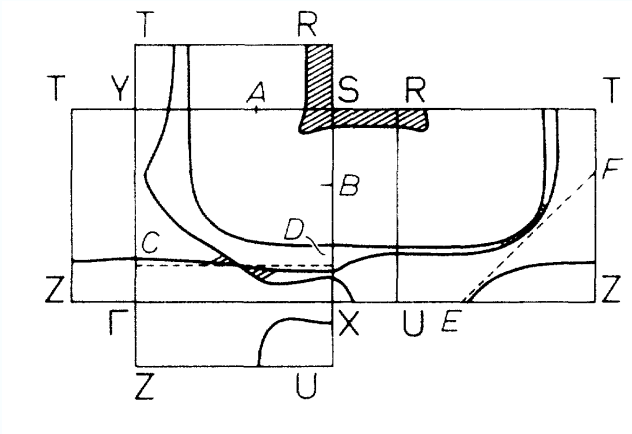


Arpes EDC for cuts along Brillouin-zone boundary (near (π,0)), almost optimally doped Pb-Bi2201 with T_c of 38K, T* of 132K

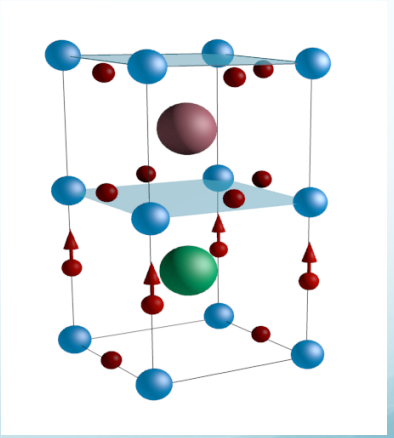
Electronic Structure YBCO



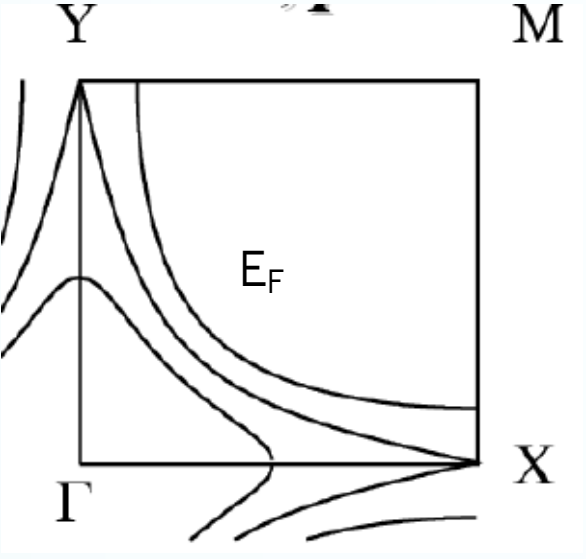
O. K. Andersen et al, JPCS (1995)



I.Mazin, et al PRB (1992)



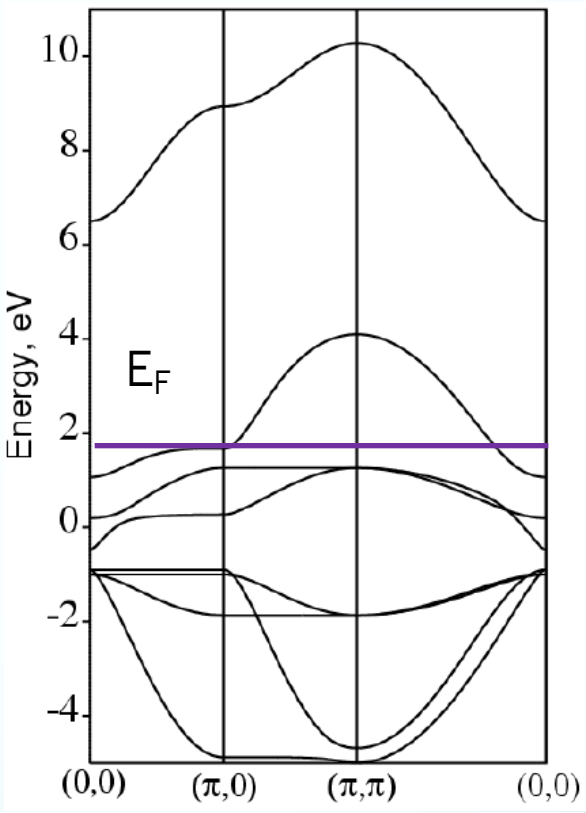
HTSC: from LDA to 1-band model



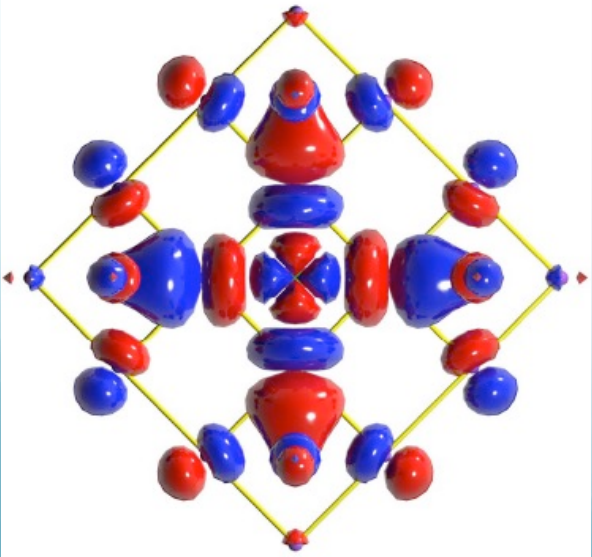
From LDA "Chemistry"
to
Low-energy TB-model

t'/t= -0.3 for YBCO

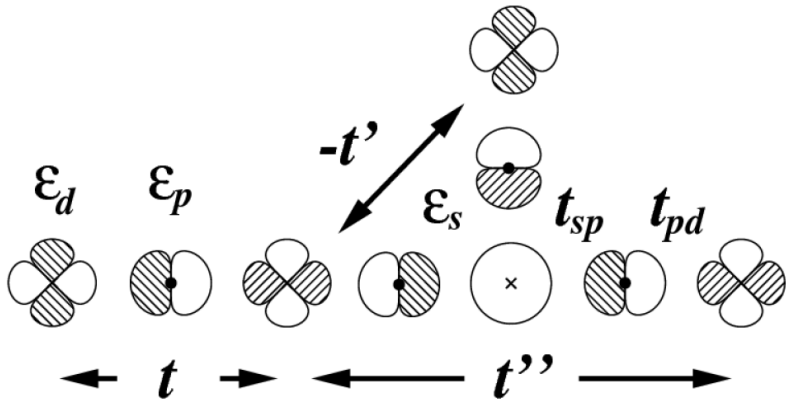
O.K. Andersen, *at al*
J. Phys. Chem. Solids
56, 1573 (1995)



La_2CuO_4

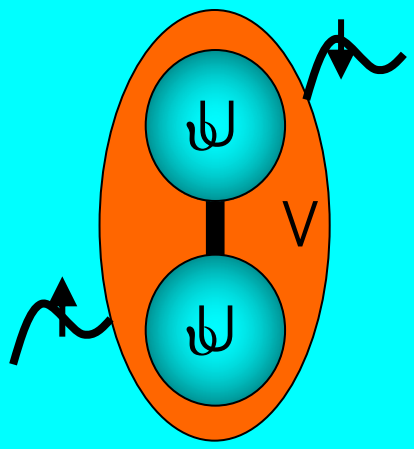


NMTO-orbitals
O.K. Andersen, *et al*
Phys. Rev. B
62, R16219 (2000)

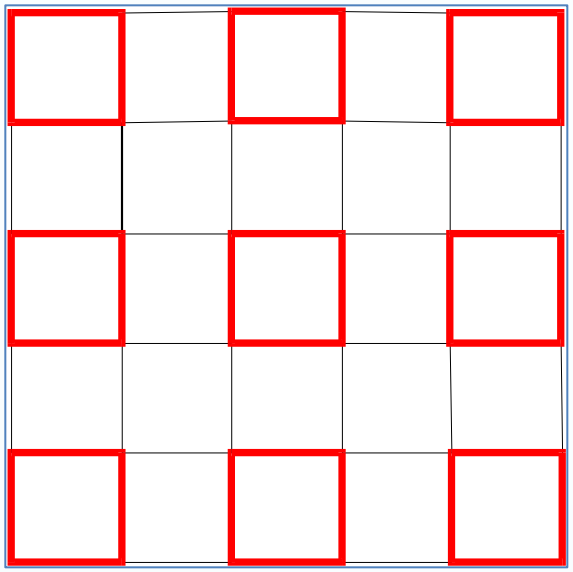


Cluster DMFT

$$\mathcal{G}_0(\tau - \tau')$$



Cluster DMFT scheme

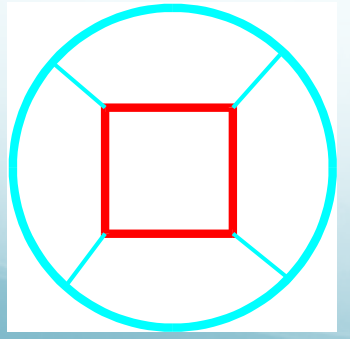


$$\hat{G}(i\omega_n) = \frac{1}{\Omega}\sum_{k}^{BZ}\left[\hat{I}(\mu + i\omega_n) - \hat{H}_0(k) - \hat{\Sigma}(i\omega_n)\right]^{-1}$$

$$\hat{\mathcal{G}}_0^{-1}(i\omega_n) = \hat{G}^{-1}(i\omega_n) + \hat{\Sigma}(i\omega_n)$$

$$S_{eff} = -\iint d\tau d\tau' c_{I\sigma}^{+}(\tau)\mathcal{G}_{IJ}^{-1}(\tau - \tau')c_{J\sigma}(\tau') + \int d\tau U n_{I\uparrow}(\tau)n_{J\downarrow}(\tau)$$

Mapping



$$\hat{G}_{IJ}(\tau - \tau') = -\frac{1}{Z}\int D[c, c^{+}]c_I(\tau)c_J^{+}(\tau')e^{-S_{eff}}$$

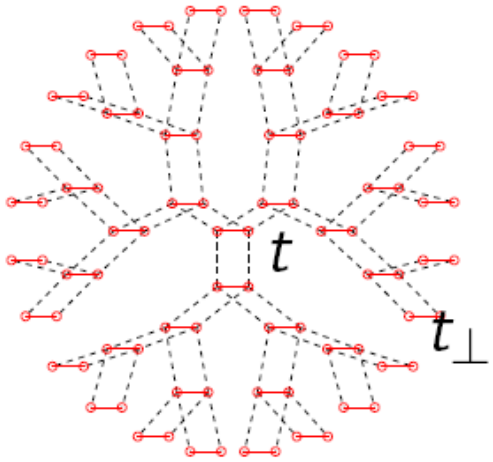
$$\hat{\Sigma}_{new}(i\omega_n) = \hat{\mathcal{G}}_0^{-1}(i\omega_n) - \hat{G}^{-1}(i\omega_n)$$

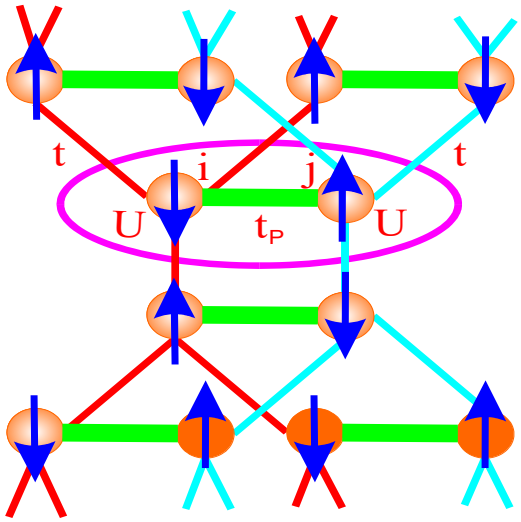
A.L., M. Katsnelson, PRB ***62****, R928368, (2000)*
G. Kotliar, et al RMP ***78****, 865 (2006)*

Double-Bethe Lattice: exact C-DMFT

bilayer Hubbard model on the Bethe lattice
(for coordination $z = 3$)

A. Ruckenstein
PRB (1999)

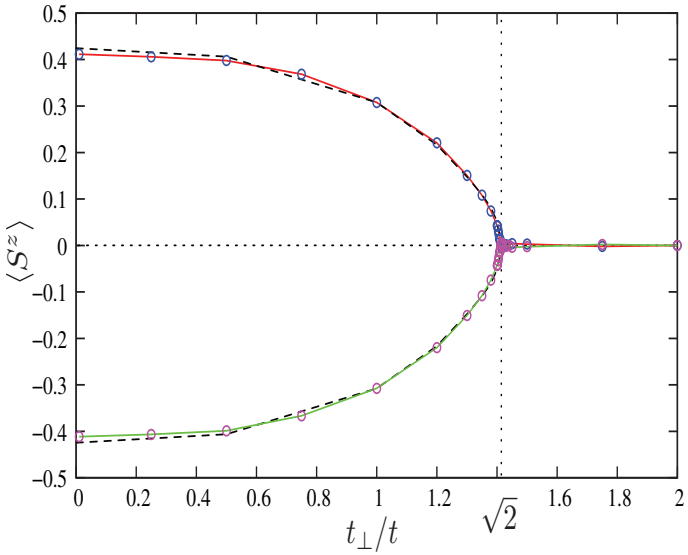


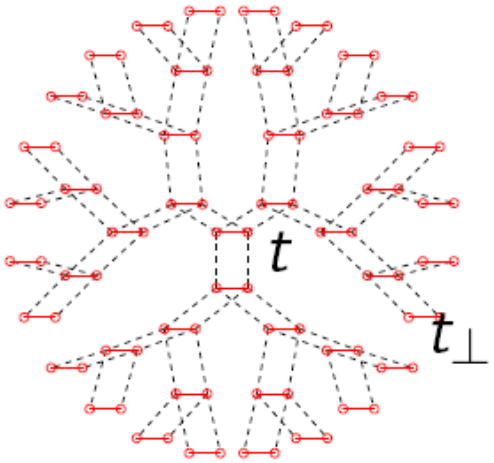


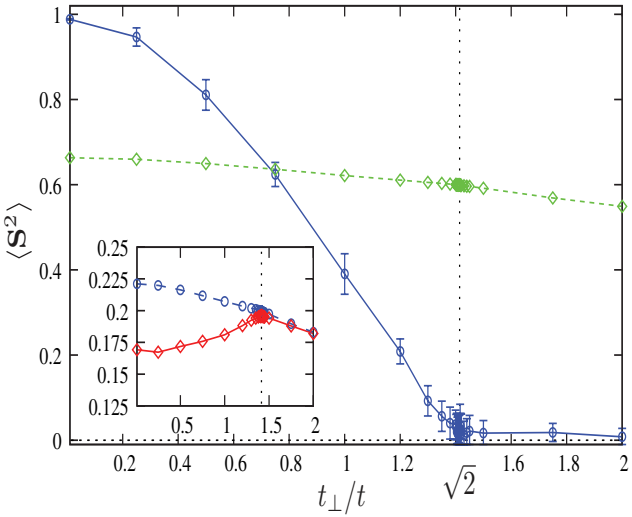
$$H = -t \sum_{\langle ij \rangle, \sigma} (a^\dagger_{i\sigma} a_{j\sigma} + b^\dagger_{i\sigma} b_{j\sigma}) - t_\perp \sum_{i\sigma} (a^\dagger_{i\sigma} b_{i\sigma} + b^\dagger_{i\sigma} a_{i\sigma})$$

$$+ U \sum_{i\sigma} (n_{ai\uparrow} n_{ai\downarrow} + n_{bi\uparrow} n_{bi\downarrow})$$

Self-consistent condition: C-DMFT





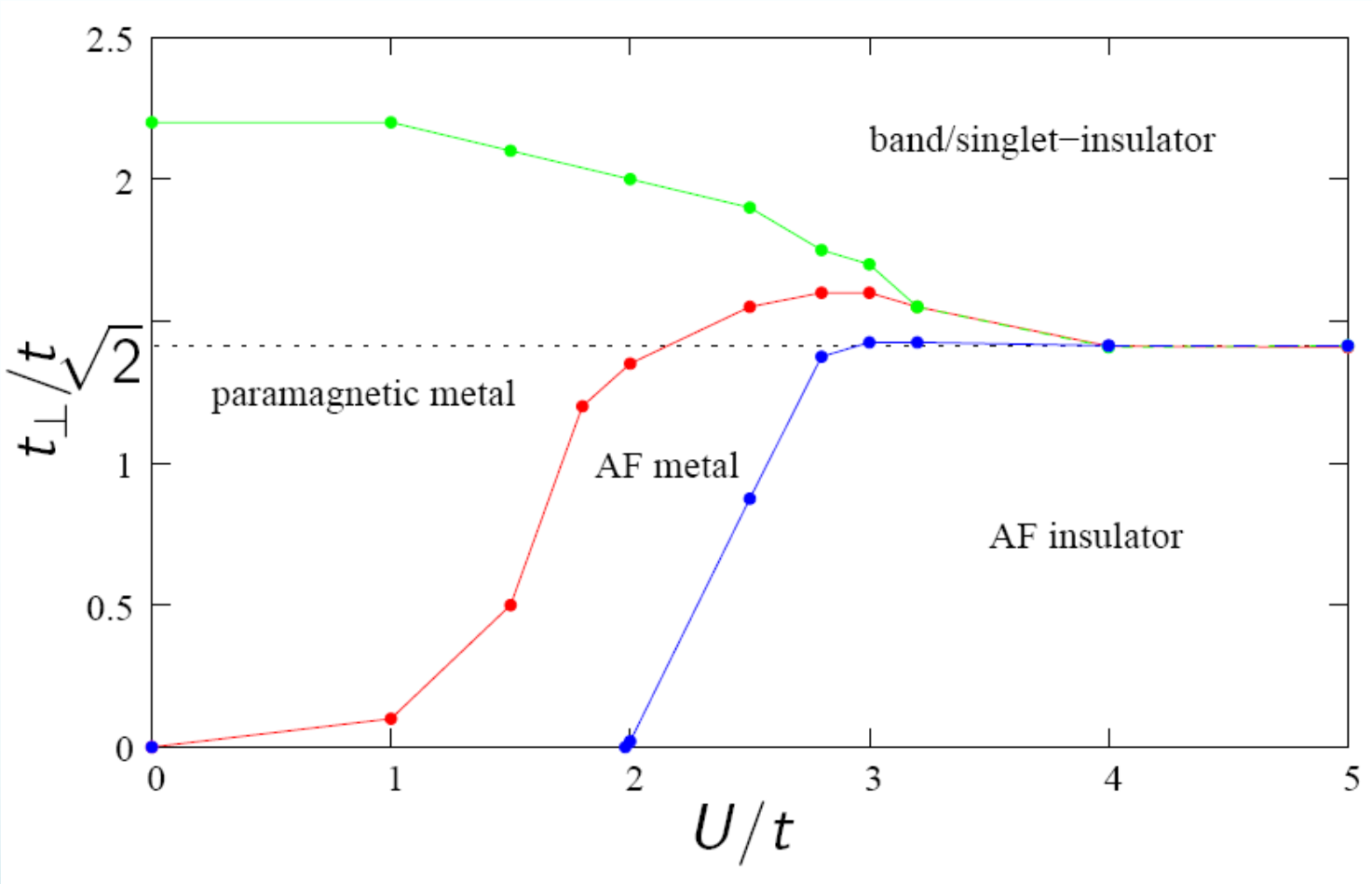


$$\mathcal{G}_\sigma^{-1}(i\omega_n) = \begin{pmatrix} i\omega_n + \mu - h\sigma & -t_\perp \\ -t_\perp & i\omega_n + \mu + h\sigma \end{pmatrix} - t^2 \mathbf{G}_{-\sigma}(i\omega_n) \ ,$$

AF-between plane

AF-plane

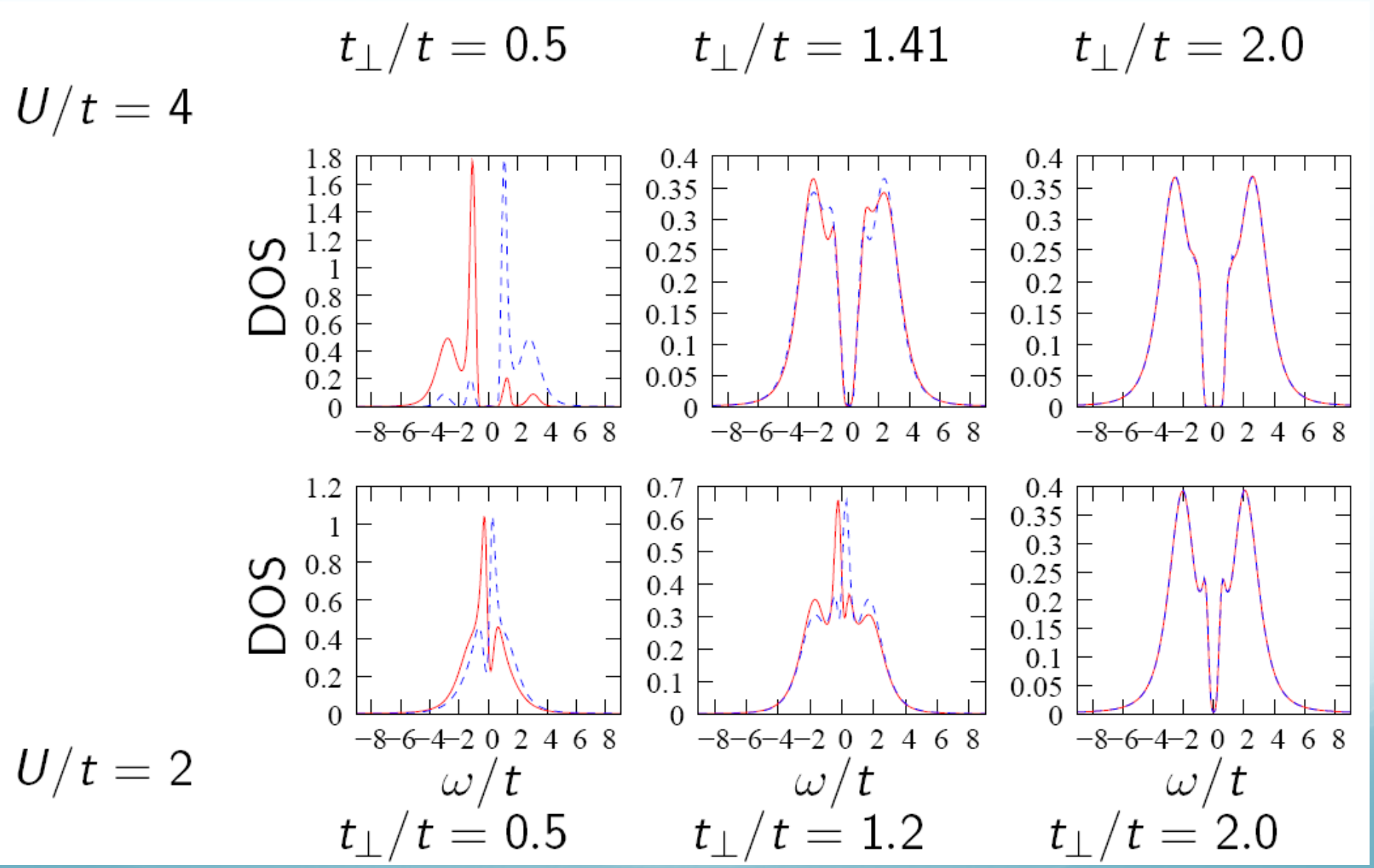
Finite temperature phase diagram



- order-disorder transition at $t_\perp / t=\sqrt{2}$ for large U
- MIT for intermediate U

H. Hafermann, M. Katsnelson and A.L., EPL, **85,** 37006 (2009)

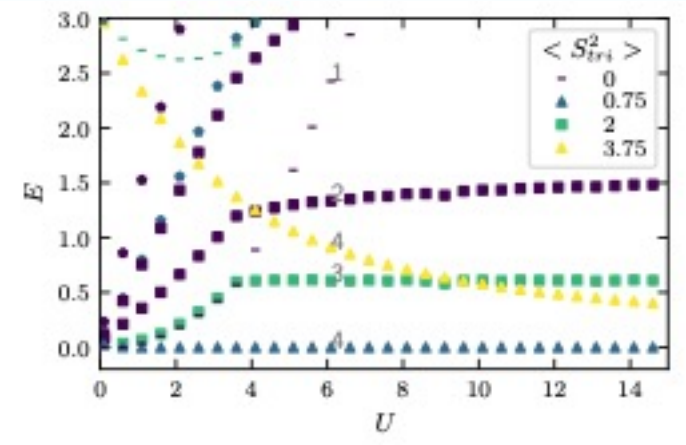
Density of States: large U



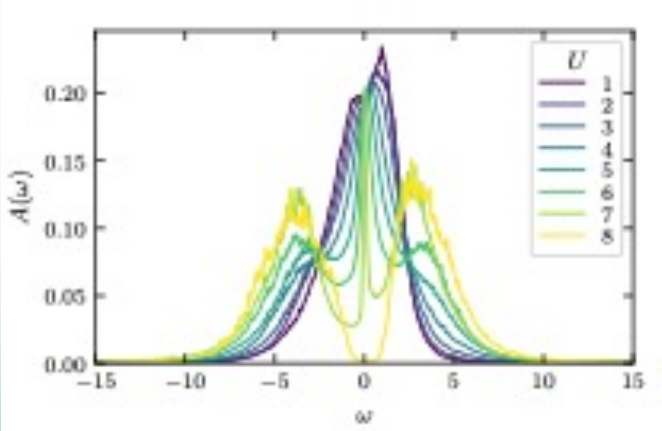
Exotic Magnetism: Triple Bethe lattice

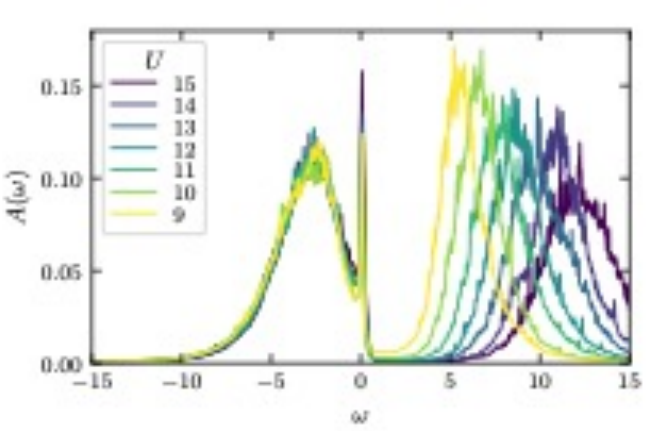
$$\underline{t} = \begin{pmatrix} 0 & -t_t & -t_t \\ -t_t & 0 & -t_t \\ -t_t & -t_t & 0 \end{pmatrix}$$

TB-triangula-hoppings



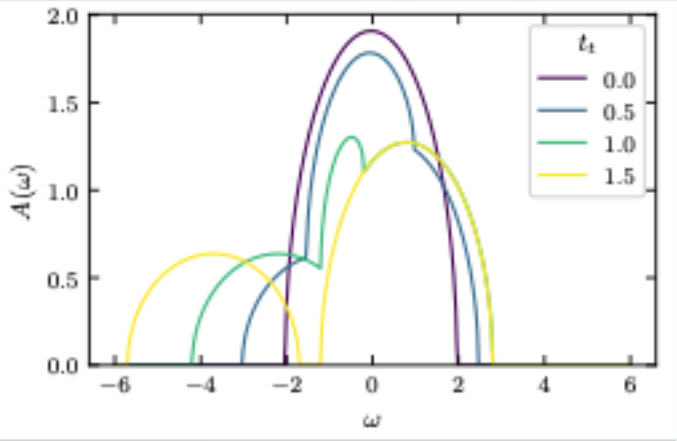
Low-States energies as function of U



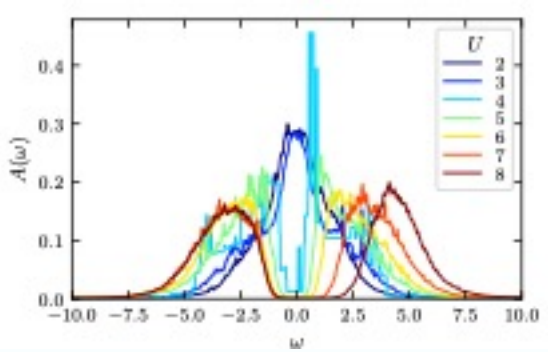


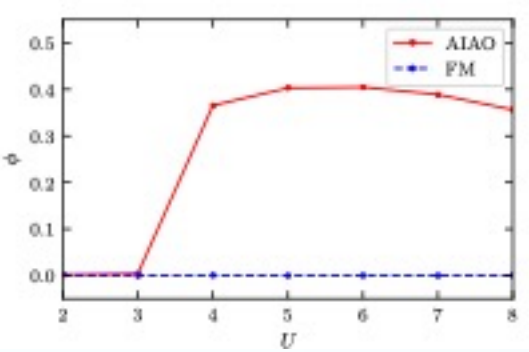
Different triple Bethe DOS

Exotic Magnetism: Triple Bethe lattice

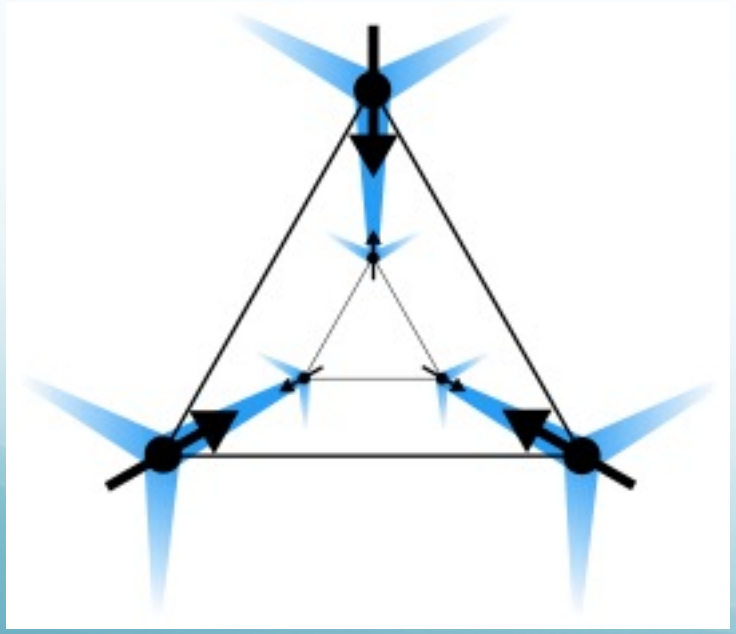


U=0 DOS

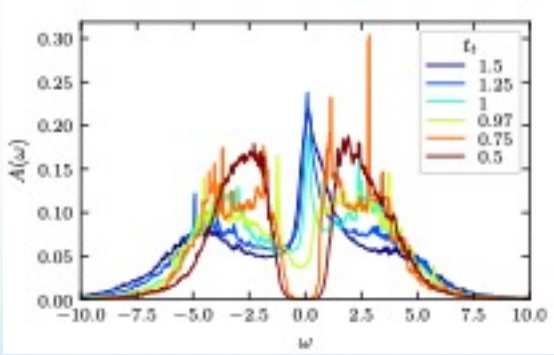


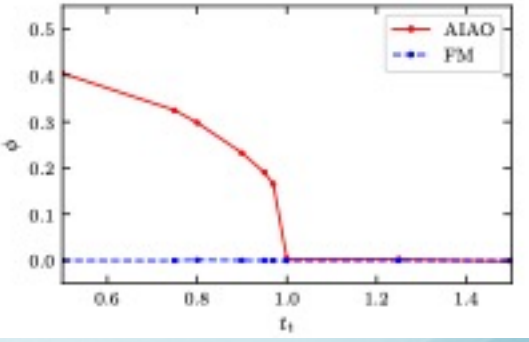


different Hubbard interactions U
at β = 10, t = 0.5 and half-filling



120-grad AIAO (all-in/all-out) state



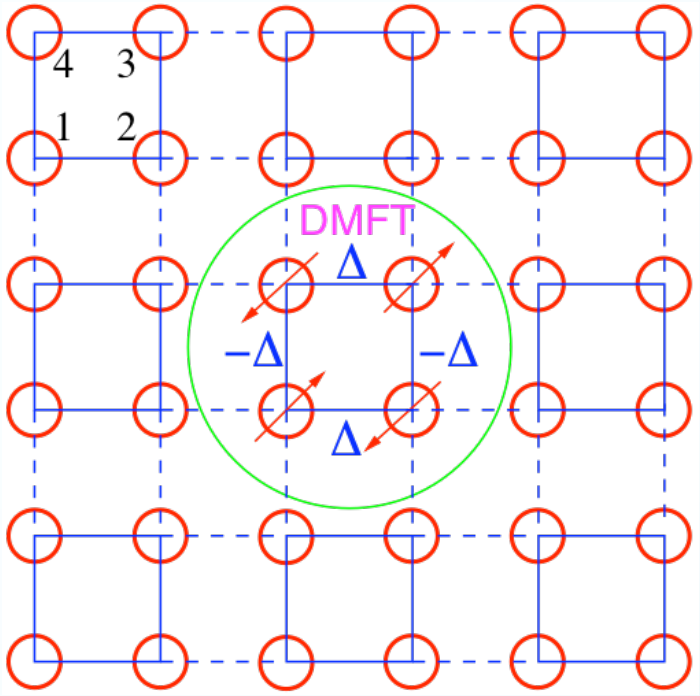


different triangle hoppings t
at β = 10, U = 6 and half-filling

Cluster-DMFT

Plaquette hopping matrix

$$T_{I,J}(\mathbf{K}) = \begin{pmatrix} 0 & t_x K_x^+ & 0 & t_y K_y^+ \\ t_x K_x^- & 0 & t_y K_y^+ & 0 \\ 0 & t_y K_y^- & 0 & t_x K_x^- \\ t_y K_y^- & 0 & t_x K_x^+ & 0 \end{pmatrix}$$



where $K_{x(y)}^{\pm} \equiv 1 + \exp\left(\pm i K_{x(y)} a\right)$

Supercell Green Function

$$G(\mathbf{K}, i\omega) = \left[(i\omega + \mu)\,\mathbf{1} - T(\mathbf{K}) - \Sigma(i\omega)\right]^{-1}$$

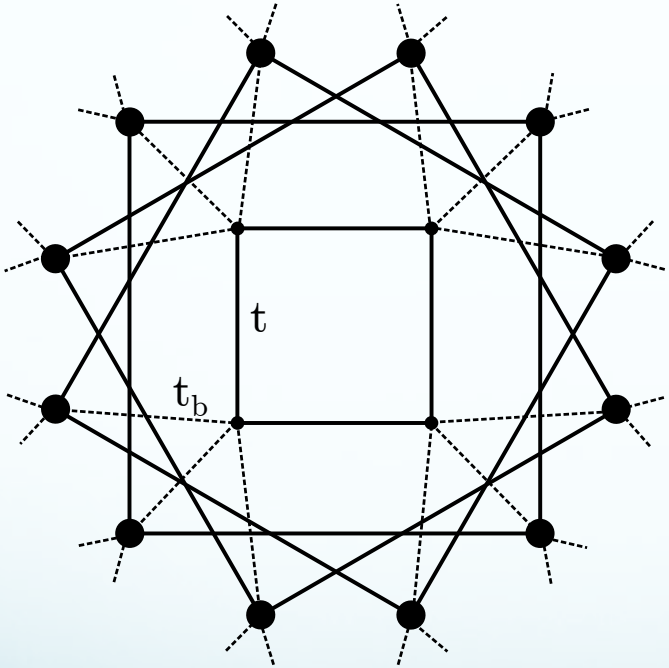
Where Self-energy matrix for plaquette has the form:

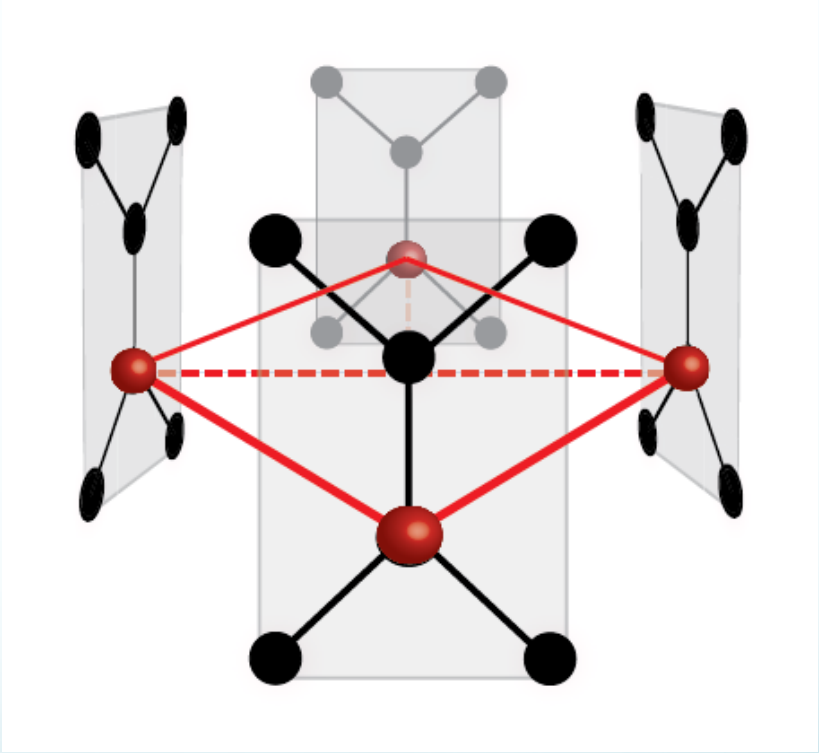
$$\mathcal{G}^{-1}(i\omega) - G^{-1}(i\omega) = \begin{pmatrix} \Sigma_{\uparrow}(i\omega) & S(i\omega) \\ S(i\omega) & \Sigma_{\downarrow}^{*}(-i\omega) \end{pmatrix},$$

GF in superconducting state:

$$G(i\omega) = \begin{pmatrix} G_{\uparrow}(i\omega) & F(i\omega) \\ F(i\omega) & G_{\downarrow}^{*}(-i\omega) \end{pmatrix}$$

Quadruple Bethe lattice



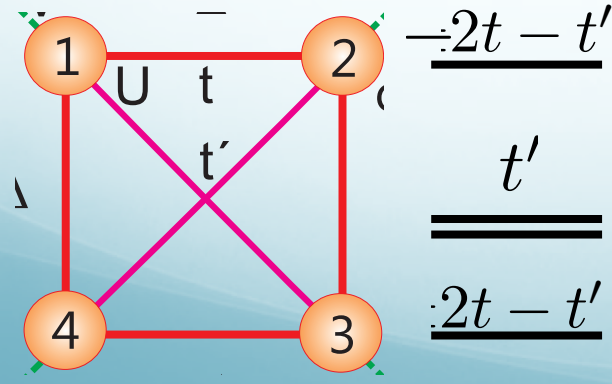


Single Plaquette

M. Harland, M. Katsnelson, A.L. Phys. Rev. B **94**, 125133 (2016)

$$H_p = \sum_{(i,j)=1..4} h^0_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i=1..4} U n_{i\uparrow} n_{i\downarrow}$$

$$-\hat{h}_0 = \begin{pmatrix} \mu & t & t' & t \\ t & \mu & t & t' \\ t' & t & \mu & t \\ t & t' & t & \mu \end{pmatrix}$$

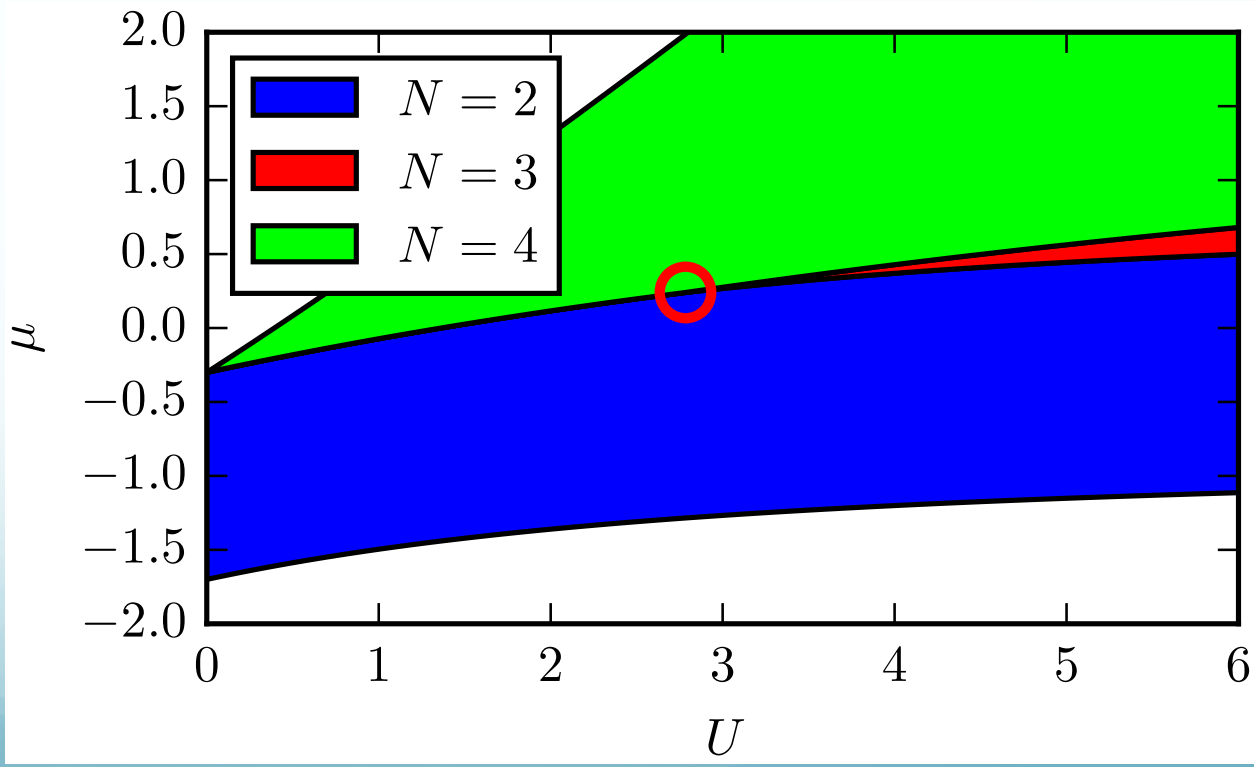


$-2t - t'$

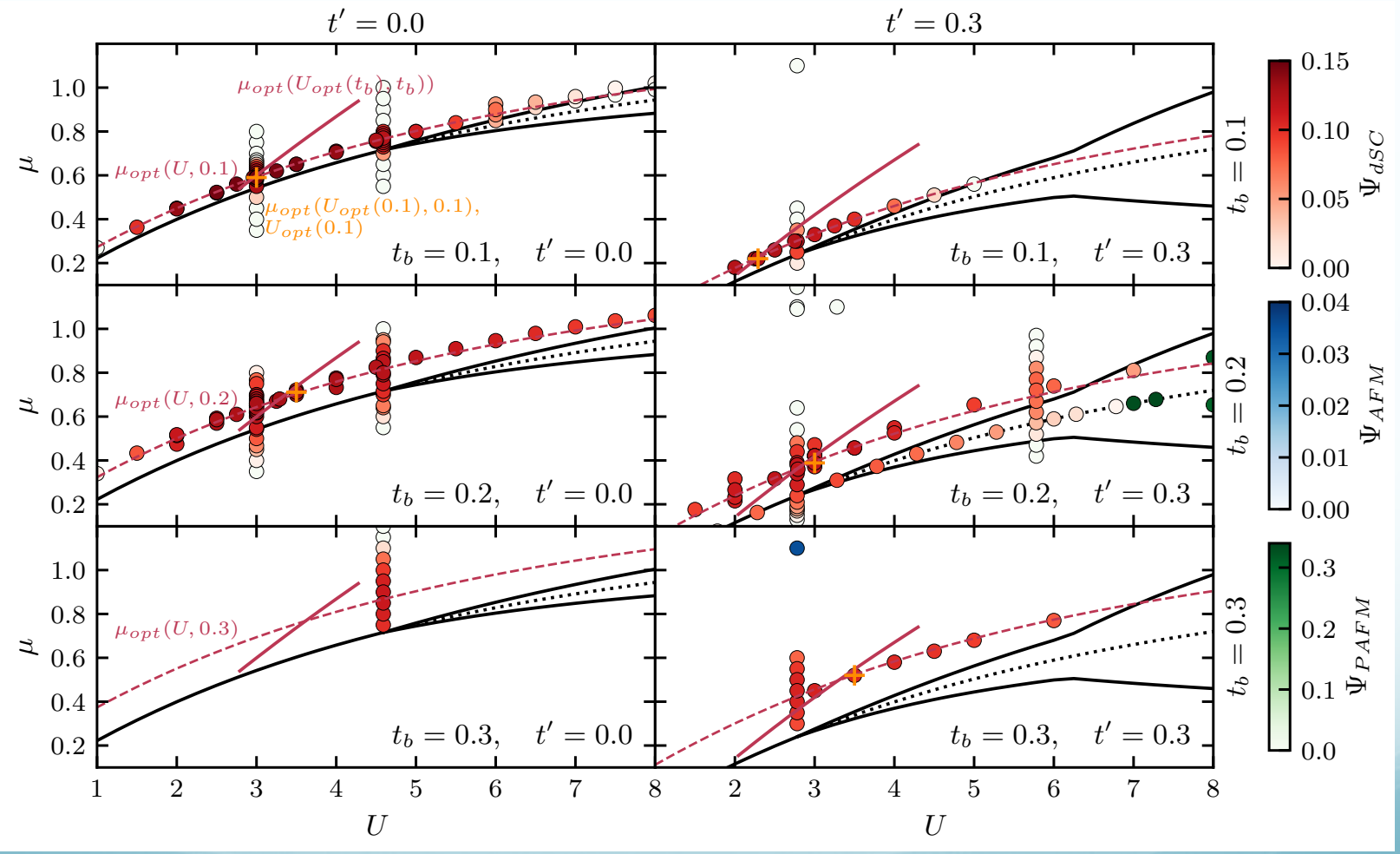
t'

$2t - t'$

„Plaquette Quantum Critical Point“

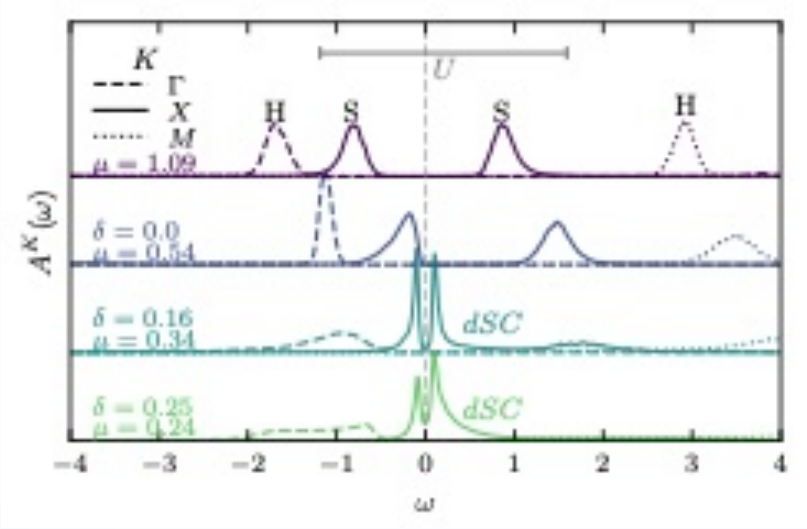


Phase Diagramm of 4-Bethe

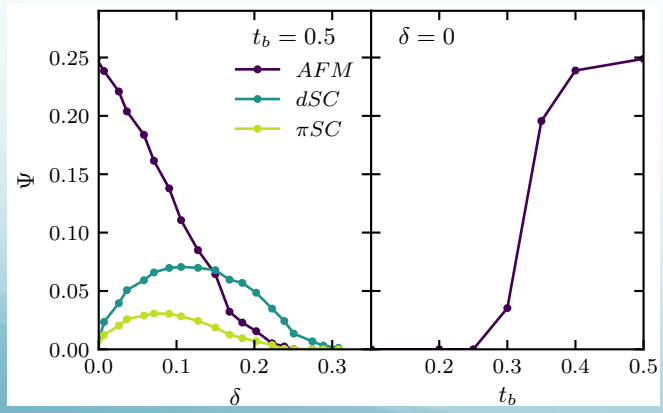


M. Harland, et al, arXiv:1905.12610

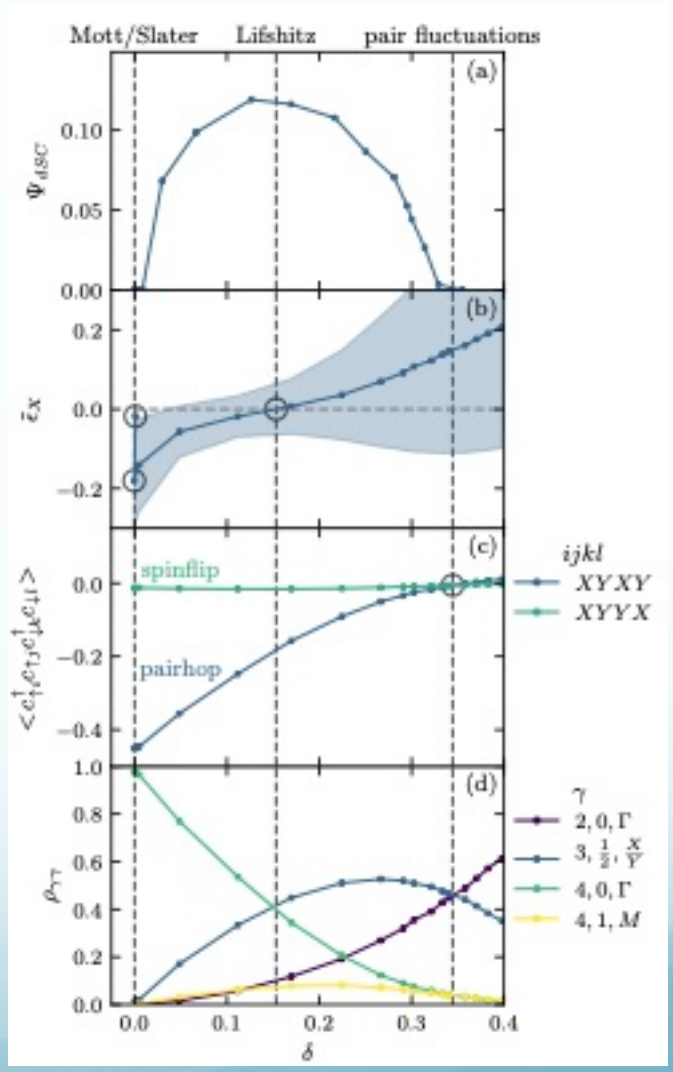
d-wave Superconductivity



Dopping dependence of Spectral function

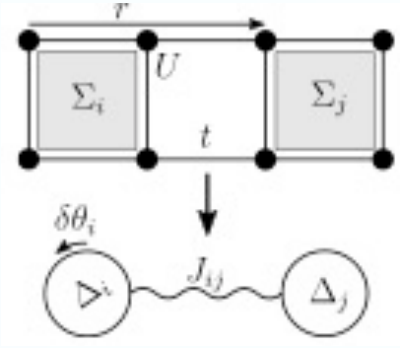


Magnetism and Superconductivity



d-wave order parameter

Josephson lattice model for dSC phase fluctuations



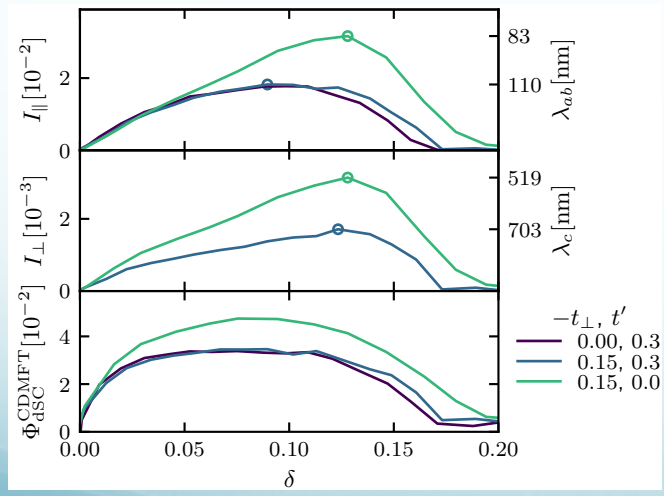
Effective Josephson couplings:

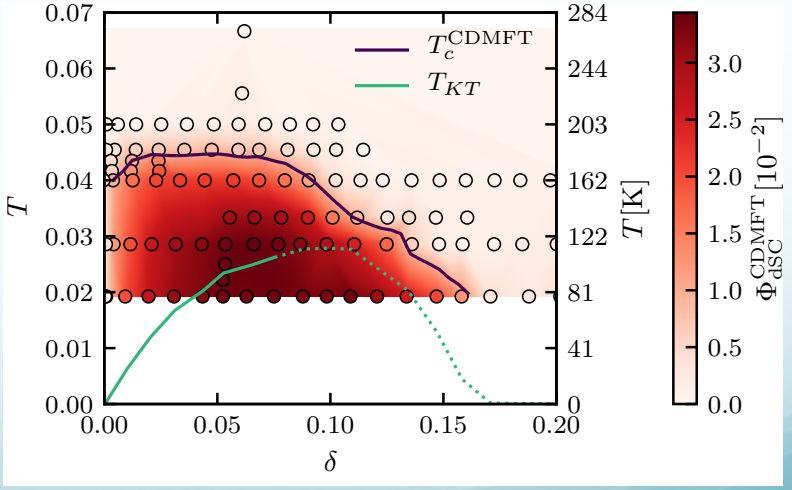
$$H_{\rm eff} = -\sum_{ij} J_{ij} \cos\left(\theta_i - \theta_j\right)$$

Related with Anomalous Self-energy (S)

$$\begin{pmatrix} G^{p\uparrow} & F \\ F & G^{h\downarrow} \end{pmatrix}^{-1}_{ij} = \begin{pmatrix} G_0^{p\uparrow} & \\ & G_0^{h\downarrow} \end{pmatrix}^{-1}_{ij} - \delta_{ij} \begin{pmatrix} \Sigma^{p\uparrow} & S \\ S & \Sigma^{h\downarrow} \end{pmatrix}_i$$

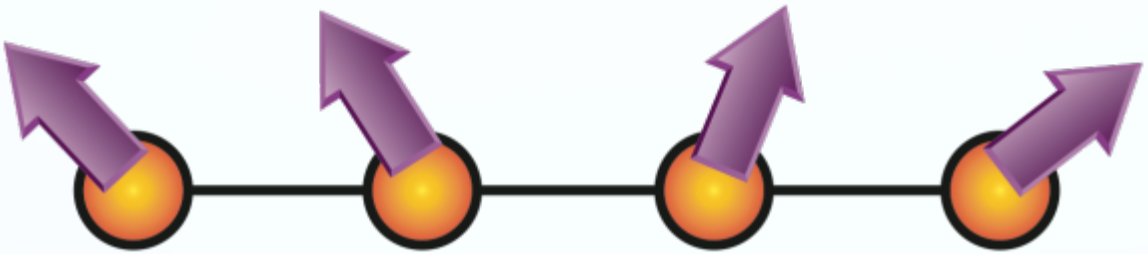
$$J_{ij} = T\,\mathrm{Tr}_{\omega\alpha}\left(F_{ij}S_jF_{ji}S_i - G^{p\uparrow}_{ij}S_jG^{h\downarrow}_{ji}S_i\right)$$



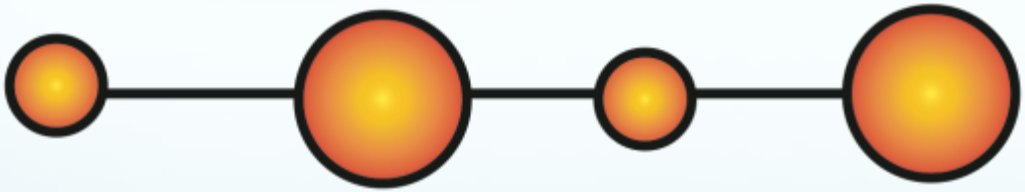


M. Harland, et al, arXiv:1810.12986

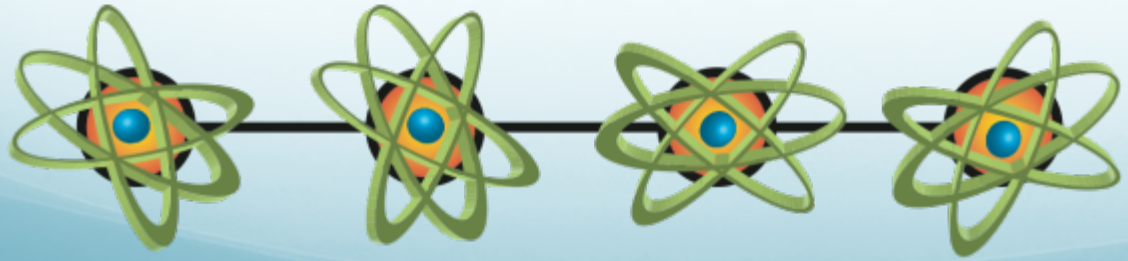
Interaction of electrons with collective excitations



Magnons



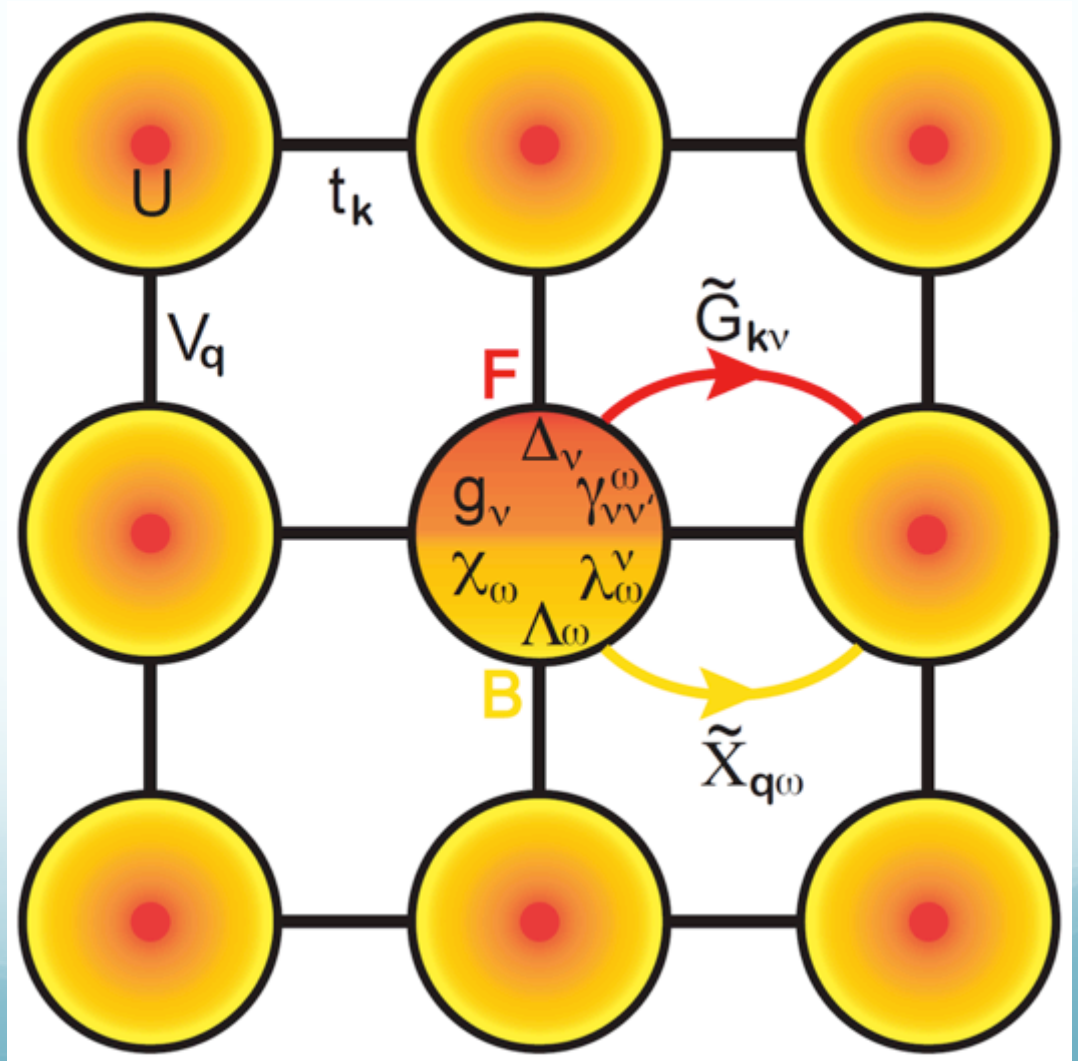
Plasmons



Orbitons

Dual Boson: General Idea

$$S_{imp} = \iint_0^\beta d\tau d\tau' \left[-\sum_\sigma \mathcal{G}^{-1}_{\tau\tau'} c^*_{\tau\sigma} c_{\tau'\sigma} + \frac{1}{2}\left(U + \Lambda^c_{\tau\tau'}\right) n_\tau n_{\tau'} + \frac{1}{2}\Lambda^s_{\tau\tau'}\, \vec{s}_\tau \cdot \vec{s}_{\tau'} \right]$$

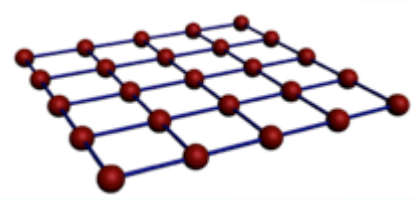


HTSC

$$\Lambda_\omega \sim J_{\tau\tau'} \vec{S}_\tau \cdot \vec{S}_{\tau'}$$

G. Rohringer, et al
RMP **90**, 025003 (2018)

Beyond DMFT: Dual DB/DF scheme



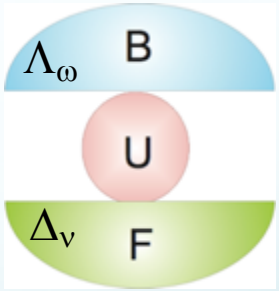
General Lattice Action: $U_{\mathbf{q}} = U + V_{\mathbf{q}}$

$$S = -\sum_{\mathbf{k}\nu\sigma} c^{+}_{\mathbf{k}\nu\sigma}[i\nu + \mu - \varepsilon_{\mathbf{k}}]c_{\mathbf{k}\nu\sigma} + \frac{1}{2}\sum_{\mathbf{q}\omega} U_{\mathbf{q}}\, n^{*}_{\mathbf{q}\omega} n_{\mathbf{q}\omega}$$

$$n_{\mathbf{q}\omega} = \sum_{\mathbf{k}\nu\sigma}(c^{*}_{\mathbf{k}\nu} c_{\mathbf{k}+\mathbf{q},\nu+\omega} - \langle c^{*}_{\mathbf{k}\nu} c_{\mathbf{k}\nu}\rangle \delta_{\mathbf{q}\omega})$$

Reference system: Local Action with hybridization Δ_ν and Λ_ω

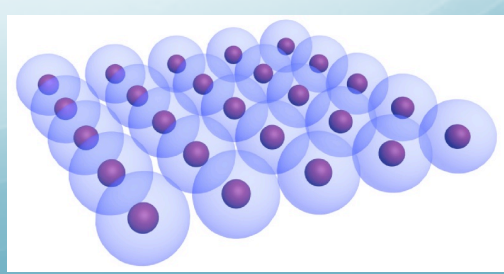
$$S_{\mathrm{ref}} = -\sum_{\nu\sigma} c^{+}_{\nu\sigma}[i\nu + \mu - \Delta_\nu]c_{\nu\sigma} + \frac{1}{2}\sum_{\omega} \mathcal{U}_\omega\, n^{*}_{\omega} n_{\omega}$$



Lattice-Impurity connection: $S = \sum S^{(i)}_{\mathrm{ref}} + \Delta S$

$$\Delta S = \sum_{\nu\mathbf{k}\sigma} c^{+}_{\nu\mathbf{k}\sigma}[\varepsilon_{\mathbf{k}} - \Delta_\nu]c_{\nu\mathbf{k}\sigma} + \frac{1}{2}\sum_{\mathbf{q}\omega}(U_{\mathbf{q}} - \mathcal{U}_\omega)\, n^{*}_{\mathbf{q}\omega} n_{\mathbf{q}\omega}$$

$\mathcal{U}_\omega = U + \Lambda_\omega$ $\qquad$ $U_{\mathbf{q}} - \mathcal{U}_\omega = V_{\mathbf{q}} - \Lambda_\omega$



A. Rubtsov, M. Katsnelson, A.L., Ann. Phys. 327, 1320 (2012)

Dual Transformation

$$\Sigma_{k\nu} = \Sigma^{ref}_{\nu} + \bar{\Sigma}_{k\nu}$$

$$\bar{\Sigma}^{-1}_{k\nu} = \tilde{\Sigma}^{-1}_{k\nu} + G^{ref}_{\nu}$$

Fermionic Hubbard-Stratanovich transformation

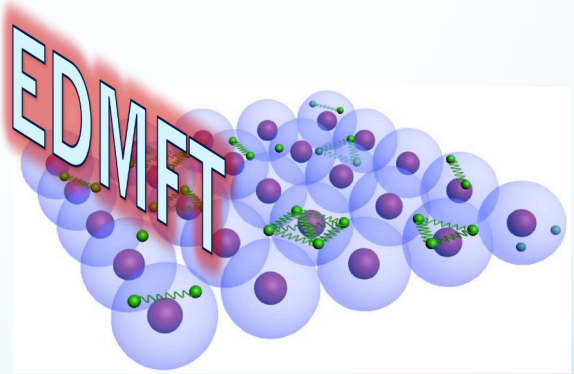
$$e^{\sum_{\mathbf{k}\nu\sigma} c^*_{\mathbf{k}\nu\sigma}[\Delta_{\nu\sigma}-\varepsilon_{\mathbf{k}}]c_{\mathbf{k}\nu\sigma}} = \det[\Delta_{\nu\sigma}-\varepsilon_{\mathbf{k}}]\int D[f^*,f]\, e^{-\sum_{\mathbf{k}\nu\sigma}\left\{f^*_{\mathbf{k}\nu\sigma}[\Delta_{\nu\sigma}-\varepsilon_{\mathbf{k}}]^{-1}f_{\mathbf{k}\nu\sigma}+c^*_{\nu\sigma}f_{\nu\sigma}+f^*_{\nu\sigma}c_{\nu\sigma}\right\}}$$

Bosonic Hubbard-Stratanovich transformation

$$\sqrt{\det[\Lambda_\omega - V_{\mathbf{q}}]}\, e^{\frac{1}{2}\sum_{\mathbf{q}\omega} n^*_{\mathbf{q}\omega}[\Lambda_\omega - V_{\mathbf{q}}]n_{\mathbf{q}\omega}} = \int D[\phi]\, e^{-\frac{1}{2}\sum_{\mathbf{q}\omega}\left\{\phi^*_{\mathbf{q}\omega}[\Lambda_\omega - V_{\mathbf{q}}]^{-1}\phi_{\mathbf{q}\omega}+n^*_\omega\phi_\omega+\phi^*_\omega n_\omega\right\}}$$

Dual action

$$\tilde{S} = -\sum_{\mathbf{k}\nu} f^*_{\mathbf{k}\nu}\tilde{G}_0^{-1}f_{\mathbf{k}\nu} - \frac{1}{2}\sum_{\mathbf{q}\omega}\phi^*_{\mathbf{q}\omega}\tilde{W}_0^{-1}\phi_{\mathbf{q}\omega} + \ldots$$



$$\tilde{G}_0 = [G^{-1}_{\mathrm{ref},\nu} + \Delta_\nu - \varepsilon_{\mathbf{k}}]^{-1} - G^{\mathrm{ref}}_\nu = G_{\mathrm{E}} - G^{\mathrm{ref}}_\nu$$

$$\tilde{W}_0 = \alpha^{-1}_\omega \left[[U_{\mathbf{q}} - \mathcal{U}_\omega]^{-1} - \chi_\omega\right]^{-1}\alpha^{-1}_\omega = W_{\mathrm{E}} - \mathcal{W}^{\mathrm{ref}}_\omega$$

Augmentation:

$$\alpha_\omega = \mathcal{W}_\omega/\mathcal{U}_\omega = (1+\mathcal{U}_\omega\chi_\omega)$$

$$\mathcal{U}_\omega \rightarrow \mathcal{W}_\omega \leftarrow \tilde{W}_{\mathbf{q}\omega}$$

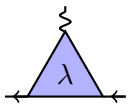
Dual Potential

Effective Interactions:

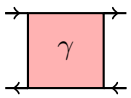
$$\tilde{V} = \frac{1}{4}\sum_{\nu\nu'\omega} \gamma_{\nu\nu'\omega}\, f^*_{\nu} f^*_{\nu'} f_{\nu+\omega} f_{\nu'-\omega} + \sum_{\nu\omega} \left(\lambda_{\nu\omega}\, f^*_{\nu} f_{\nu+\omega} \phi^*_{\omega} + h.c.\right)$$

Definition of correlation functions

$$G_{\mathbf{k}\nu}/G^{\mathrm{ref}}_{\nu} = -\left\langle c \;\; c^{+}\right\rangle_{\mathbf{k}\nu/\nu\,\mathrm{ref}},$$
$$X_{\mathbf{q}\omega}/\chi_{\omega} = -\left\langle n \;\; n^{*}\right\rangle_{\mathbf{q}\omega/\omega\,\mathrm{ref}},$$
$$\mathcal{W}_{\omega} = \mathcal{U}_{\omega} + \mathcal{U}_{\omega}\chi_{\omega}\mathcal{U}_{\omega},$$



$$\lambda_{\nu\omega} = g^{-1}_{\nu} g^{-1}_{\nu+\omega} \alpha^{-1}_{\omega} \left\langle c_{\nu} c^{*}_{\nu+\omega} n_{\omega}\right\rangle_{\mathrm{loc}}$$



$$\gamma_{\nu\nu'\omega} = g^{-1}_{\nu} g^{-1}_{\nu'} g^{-1}_{\nu'-\omega} g^{-1}_{\nu+\omega} \left[\left\langle c_{\nu} c_{\nu'} c^{*}_{\nu'-\omega} c^{*}_{\nu+\omega}\right\rangle - g_{\nu} g_{\nu'} \left(\delta_{\omega} - \delta_{\nu',\nu+\omega}\right)\right]$$

DB: Full impurity vertex $\gamma_{\nu\nu'\omega}$ with $\tilde{G}_{\mathbf{k}\nu}$

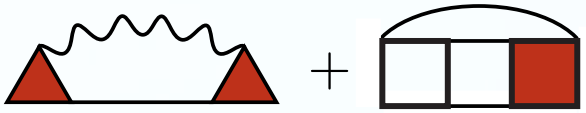
is equivalent to Bare irreducible vertex $\overline{\gamma}^{\mathrm{2PI}\,\varsigma}_{\nu\nu''\omega}$ and $G_{\nu}(\mathbf{k})$

in normal Ladder-perturbation theory

Lattice GF and SCF-condition

Lattice two-point correlation functions

$$G^{-1}_{\mathbf{k}\nu} = G^{-1}_{\mathrm{E}} - \tilde{\Sigma}_{\mathbf{k}\nu}(1 + G^{\mathrm{ref}}_{\nu}\tilde{\Sigma}_{\mathbf{k}\nu})^{-1} \qquad \tilde{\Sigma}_{\mathbf{k}\nu} =$$



$$W^{-1}_{\mathbf{q}\omega} = W^{-1}_{\mathrm{E}} - \tilde{\Pi}_{\mathbf{q}\omega}(1 + \mathcal{W}^{\mathrm{ref}}_{\omega}\tilde{\Pi}_{\mathbf{q}\omega})^{-1} \qquad \tilde{\Pi}_{\mathbf{q}\omega} =$$

Self-consistent conditions:

$$\sum_{\mathbf{k}} G_{\mathbf{k}\nu} = G^{\mathrm{ref}}_{\nu},$$

$$\sum_{\mathbf{q}} W_{\mathbf{q}\omega} = \mathcal{W}^{\mathrm{ref}}_{\omega}. \qquad \text{vs.} \qquad \sum_{\mathbf{q}} X_{\mathbf{q}\omega} = \chi_{\omega}$$

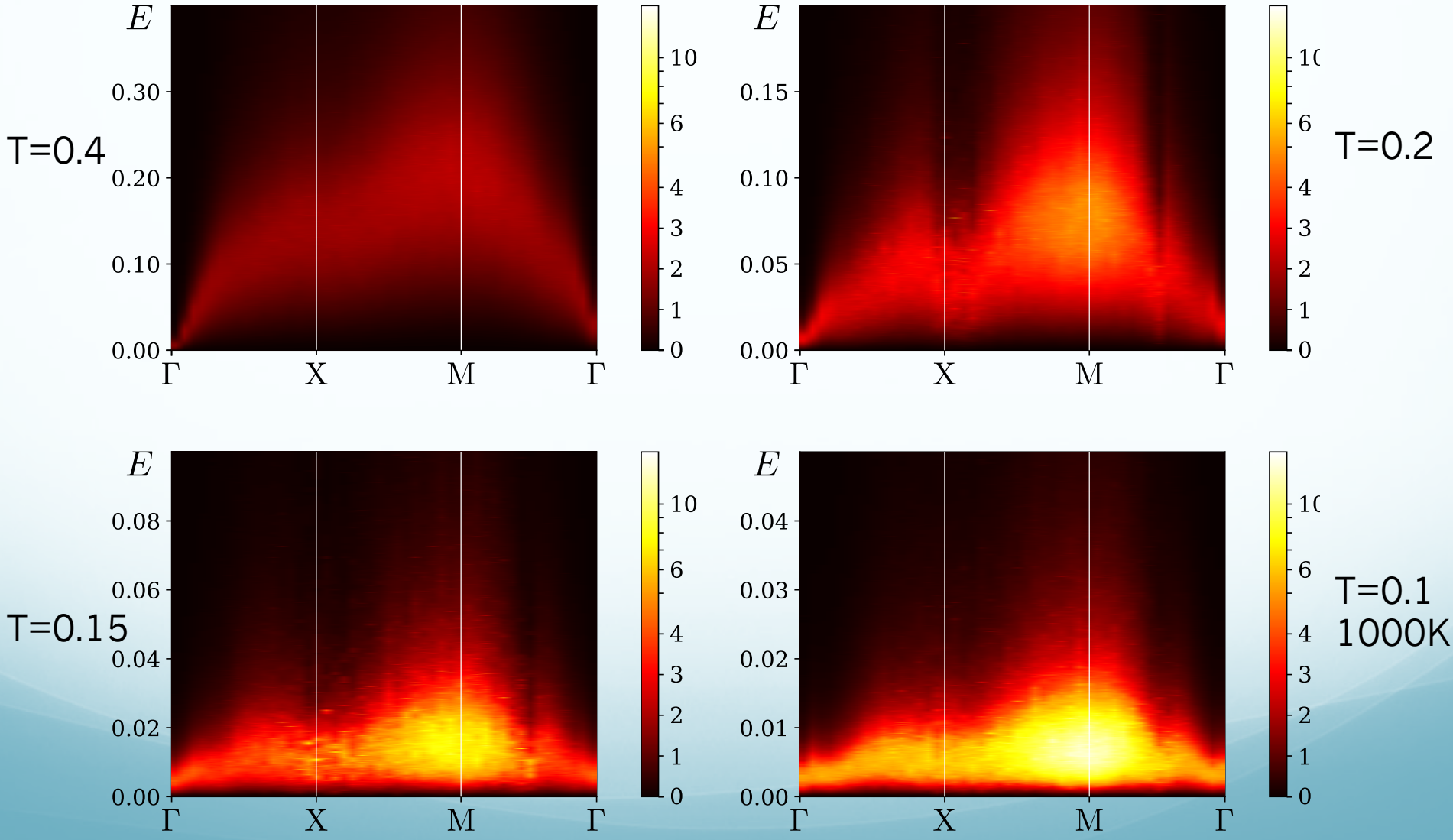
Lattice susceptibility

$$X_{\mathbf{q}\omega} = \tilde{U}^{-1}_{\mathbf{q}\omega}\alpha^{-1}_{\omega}\tilde{W}_{\mathbf{q}\omega}\alpha^{-1}_{\omega}\tilde{U}^{-1}_{\mathbf{q}\omega} - \tilde{U}^{-1}_{\mathbf{q}\omega}$$

Undoped Cuprates

E. Stepanov et al, NPJ Quantum Materials 3, 54 (2018)

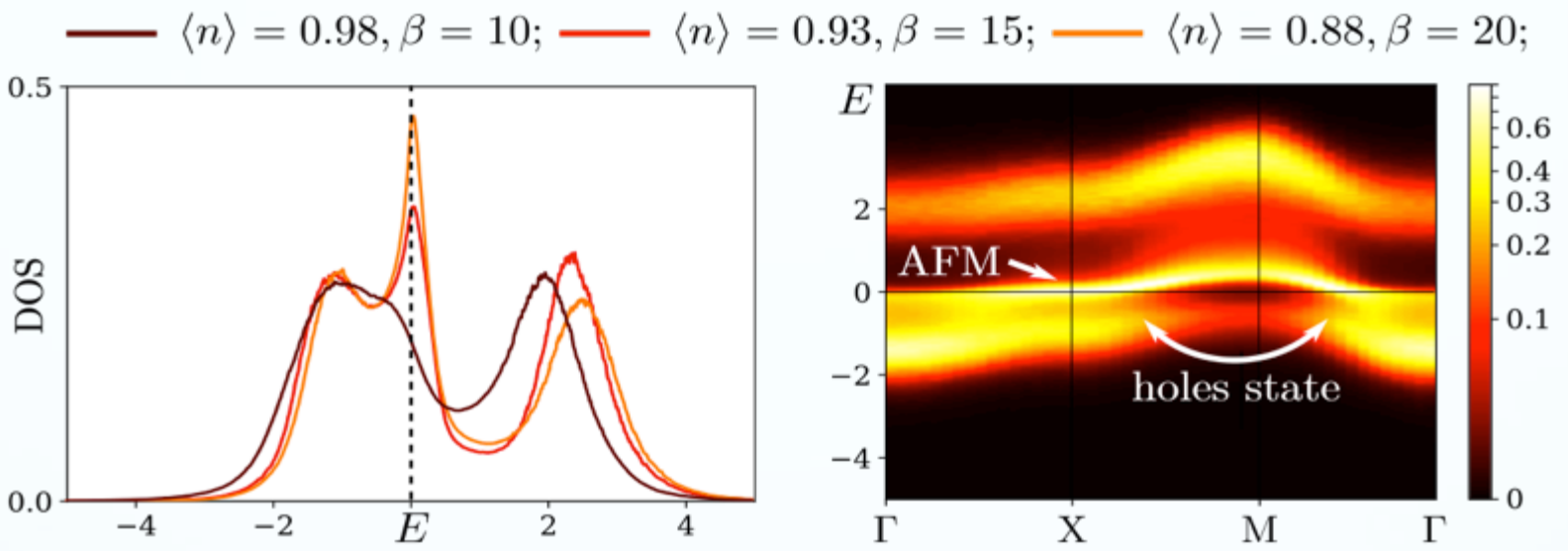
Temperarture dependence of magnetic susceptibilities



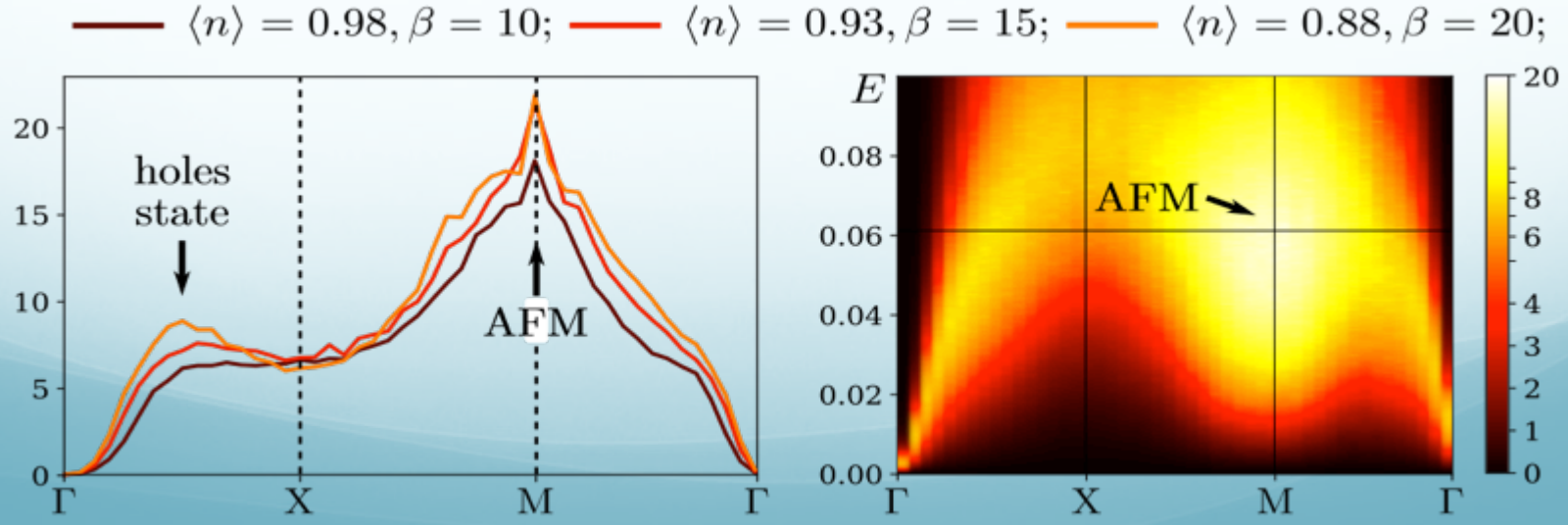
Spin-fluctuations in cuprate

E. Stepanov et al, NPJ Quantum Materials 3, 54 (2018)

Extended Hubbard model: t=0.3, t'=-0.15t, U=3, V=0.5, J_d=0.01



Magnetic Susceptibilities in Ladder-DB: $\left[X^{\text{ladd}}_{\mathbf{q}\omega}\right]^{-1} = J^{\text{d}}_{\mathbf{q}} + \Lambda + \left[X^{\text{DMFT}}_{\mathbf{q}\omega}\right]^{-1}$

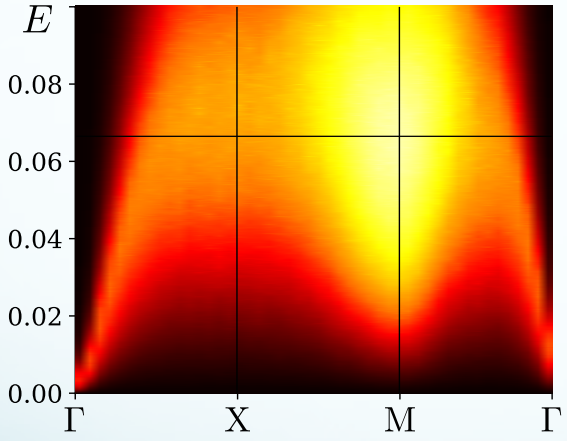


Stability of Resonance mode

Doping and Temperature dependent magnetic susceptibilility

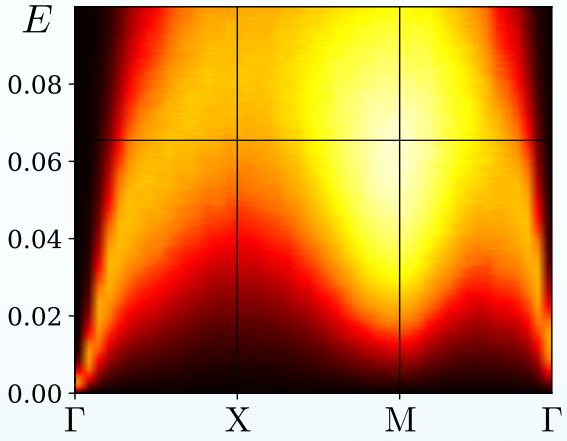
x=0.02

$\langle n \rangle = 0.98, \beta = 10;$



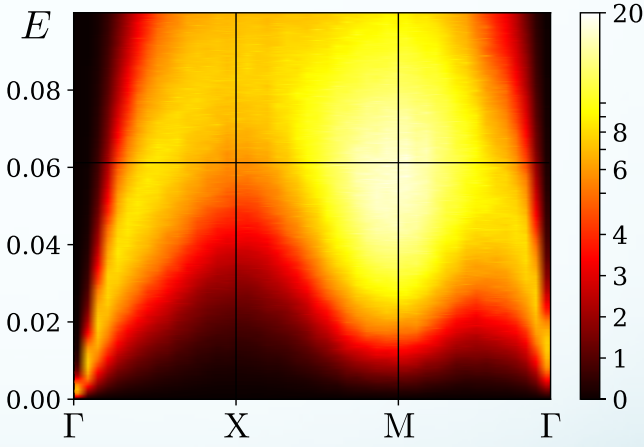
x=0.07

$\langle n \rangle = 0.93, \beta = 15;$

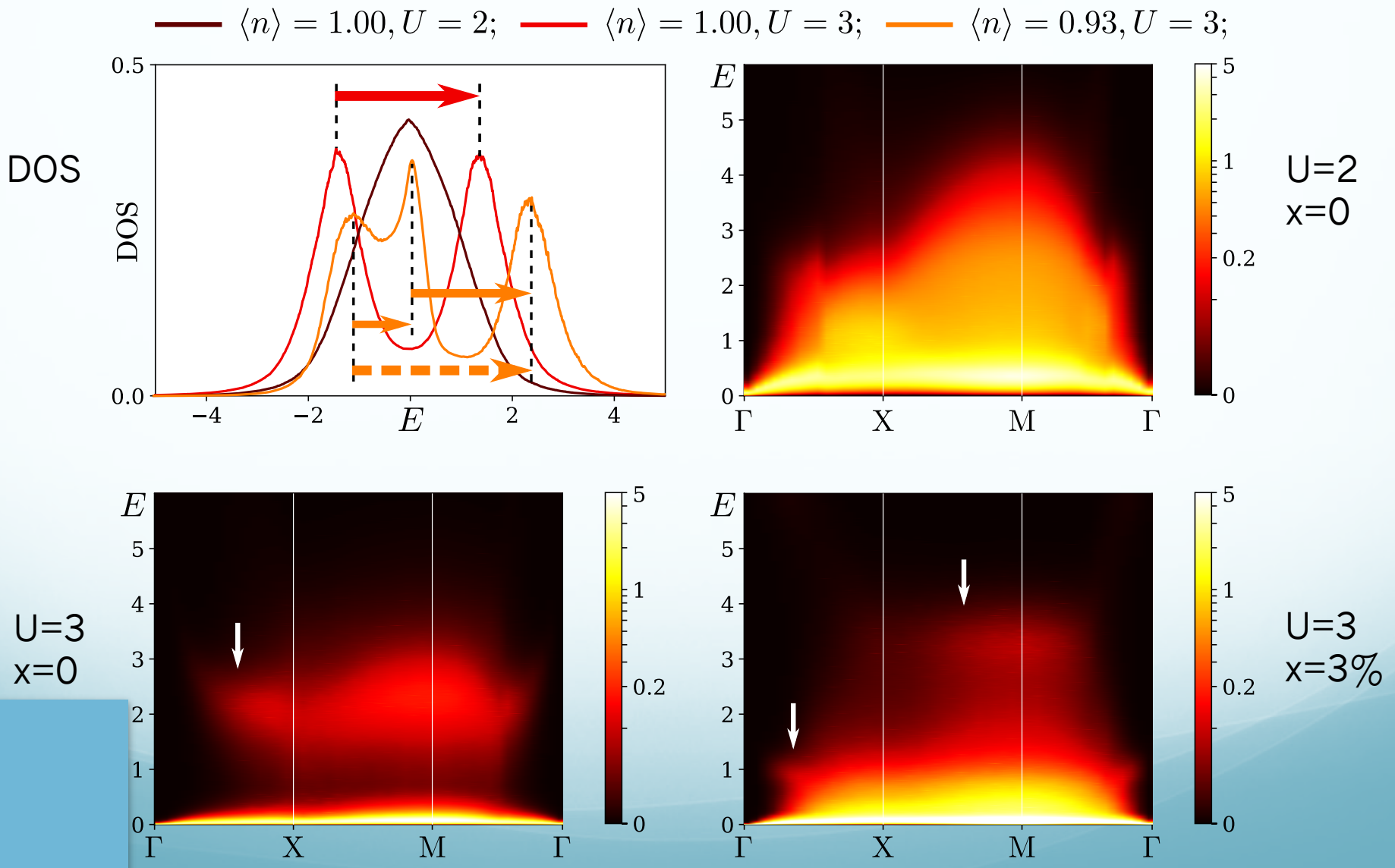


x=0.12

$\langle n \rangle = 0.88, \beta = 20;$

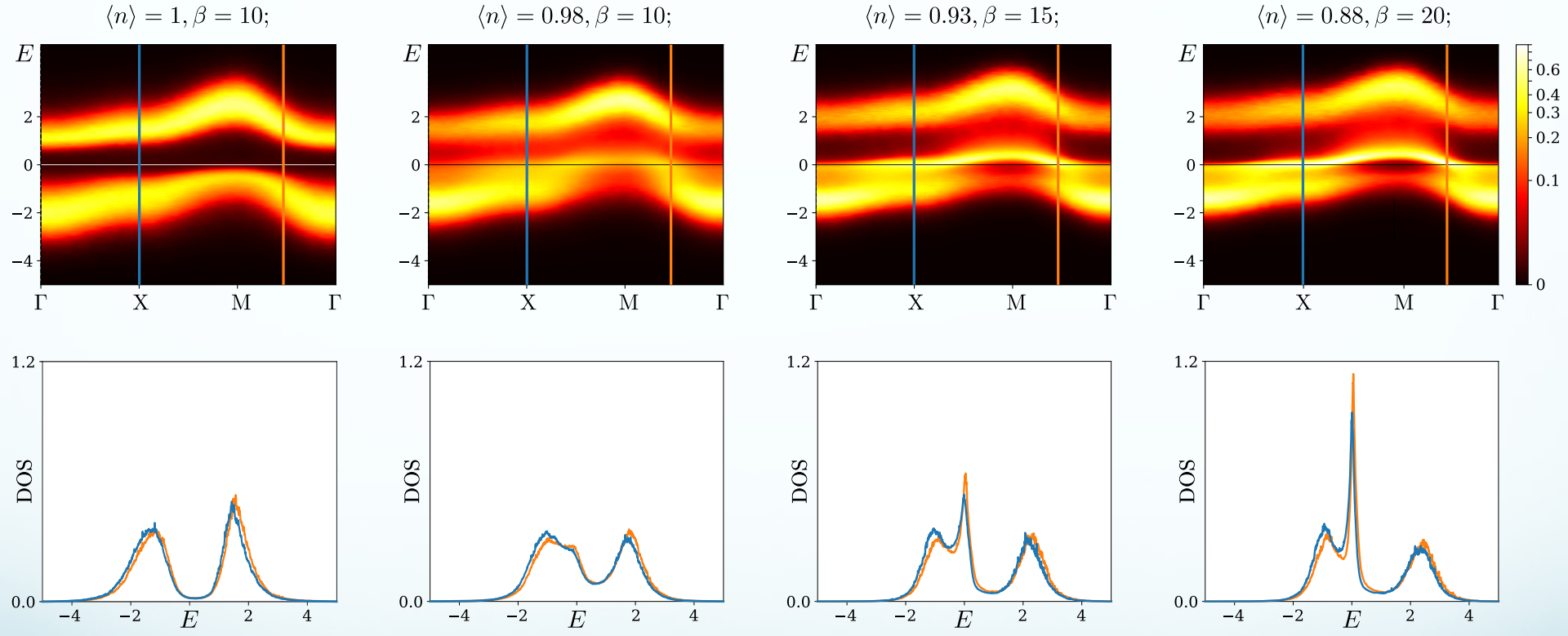


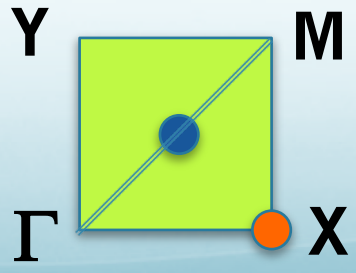
High-energy spin-excitations



Doping dependent Spectral Function

x=0.0 x=0.02 x=0.07 x=0.12





E. Stepanov et al, NPJ Quantum Materials 3, 54 (2018)

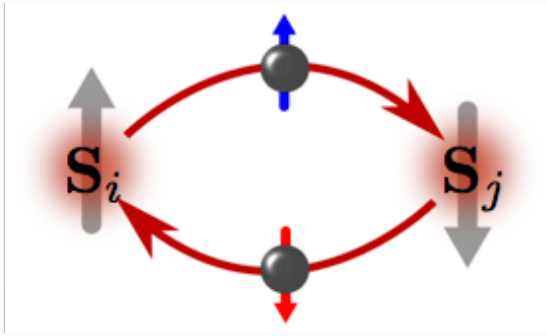
Exchange interactions in DB

From Ladder susceptibility

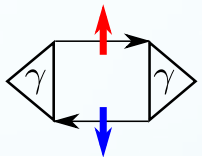
$$X^{\text{ladd}}_{\mathbf{q}\omega} = \text{Tr}\left\{\hat{X}^0_{\mathbf{q}\omega}\left[I + \left(\hat{\bar{\gamma}}^{\text{2PI}}_{\omega} + I\left[J^{\text{D}}_{\mathbf{q}} + \Lambda\right]\right)\hat{X}^0_{\mathbf{q}\omega}\right]^{-1}\right\}$$

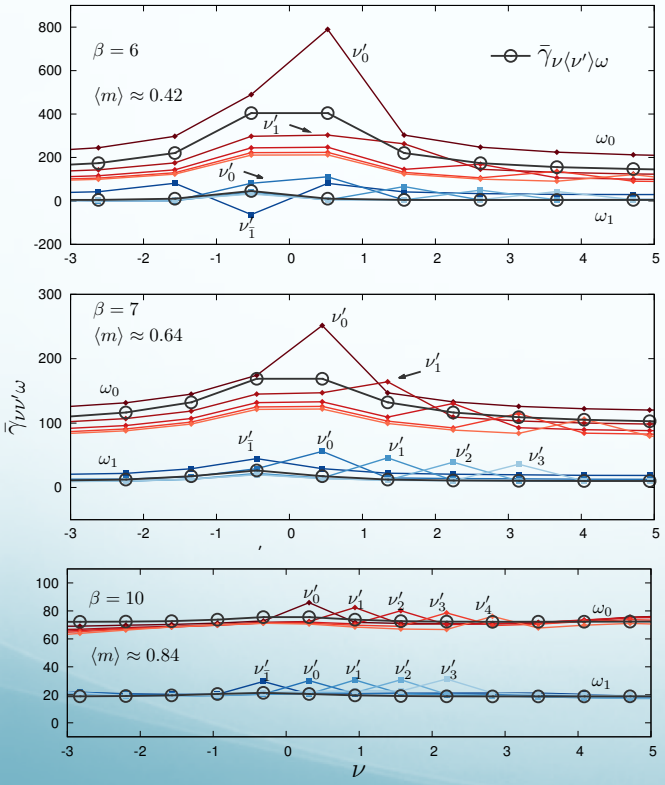
Effective Heisenberg Model

$$J_{ij} = J^{\text{d}}_{ij} -$$

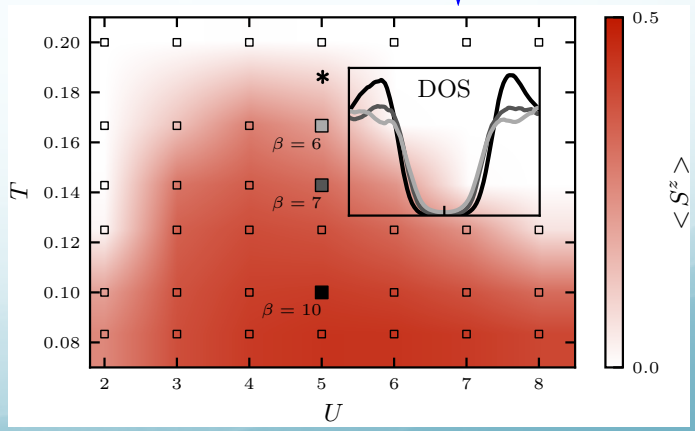


$$J_{\mathbf{q}} = J^{\text{d}}_{\mathbf{q}} - \sum_{\mathbf{k},\nu} \gamma^{-}_{\nu,\omega=0}\, \tilde{G}_{\mathbf{k}+\mathbf{q},\nu\uparrow} \tilde{G}_{\mathbf{k}\nu\downarrow}\, \gamma^{+}_{\nu,\omega=0} \quad :$$





Results from AFM hypercubic lattice



E.Stepanov, S. Brener, F. Krien, M. Harland, A.L., M. Katsnelson, Phys. Rev. Lett. 121, 037204 (2018)

Summary

- DFT+DMFT is a perfect scheme for magnetic materials
- New playground of N-Bethe lattice
- Local correlations exactly computed within CT-QMC impurity solver
- DF/DB is an efficient approach for non-local corrections beyond DMFT
- Exchange interactions and Vertex Corrections