26th Wien2k Workshop, Vienna, August 14th, 2019

Introduction to Dynamical Mean-Field Theory

Jan M. Tomczak

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Outline

- **Correlated electrons—what are they, and why are they interesting?**
- **Dynamical Mean-Field Theory (DMFT)**
  - a cartoon
  - a few equations
  - applications that (nowadays) are simple
- **DMFT for the Kondo insulator $Ce_3Bi_4Pt_3$**

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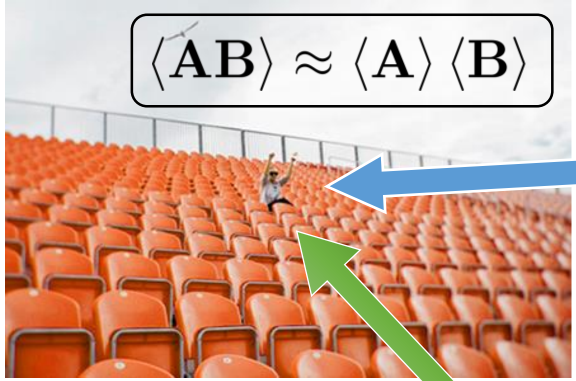
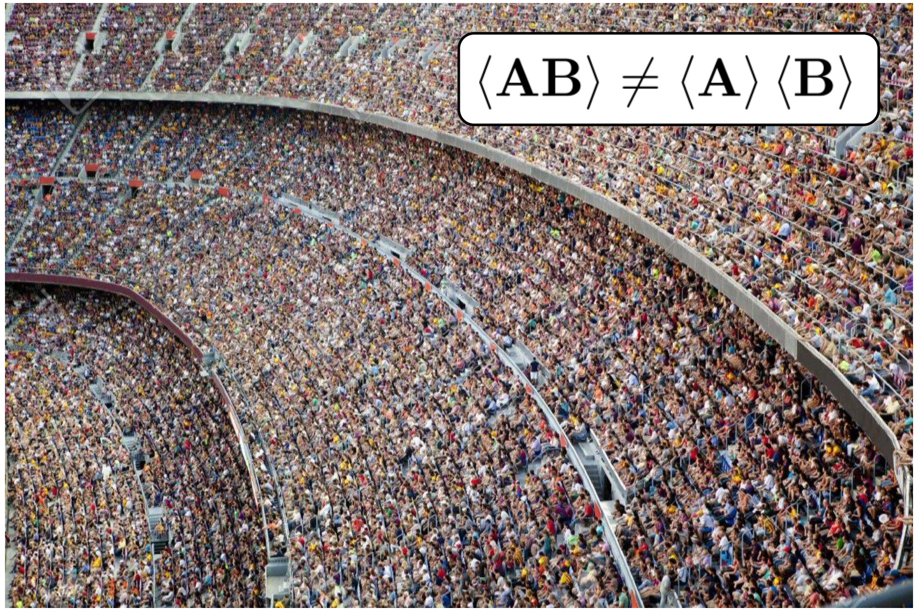
“Correlations”: a not so serious analogy

low density → nearly independent people



intermediate density

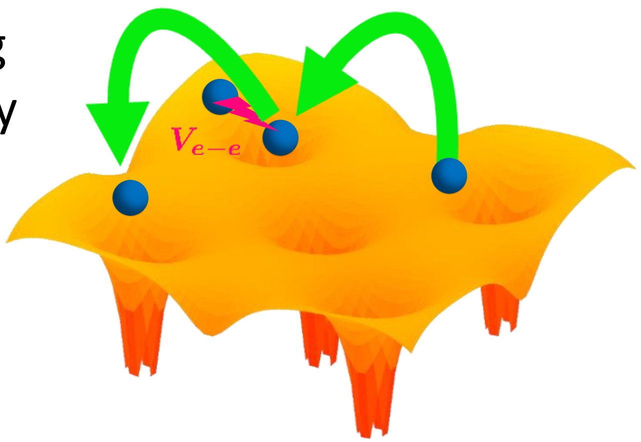


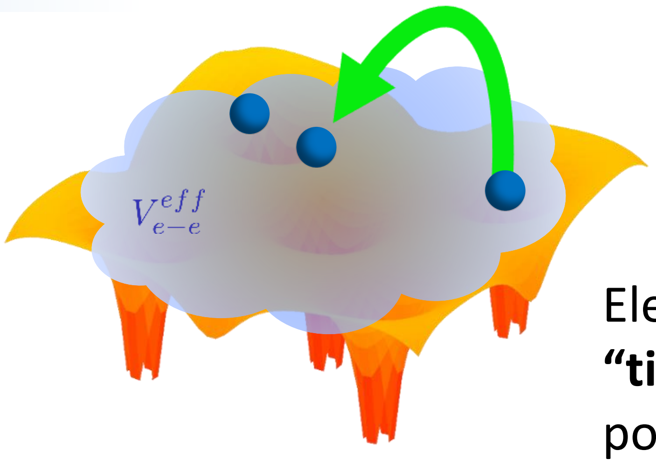
high density → many-people regime

Band theory

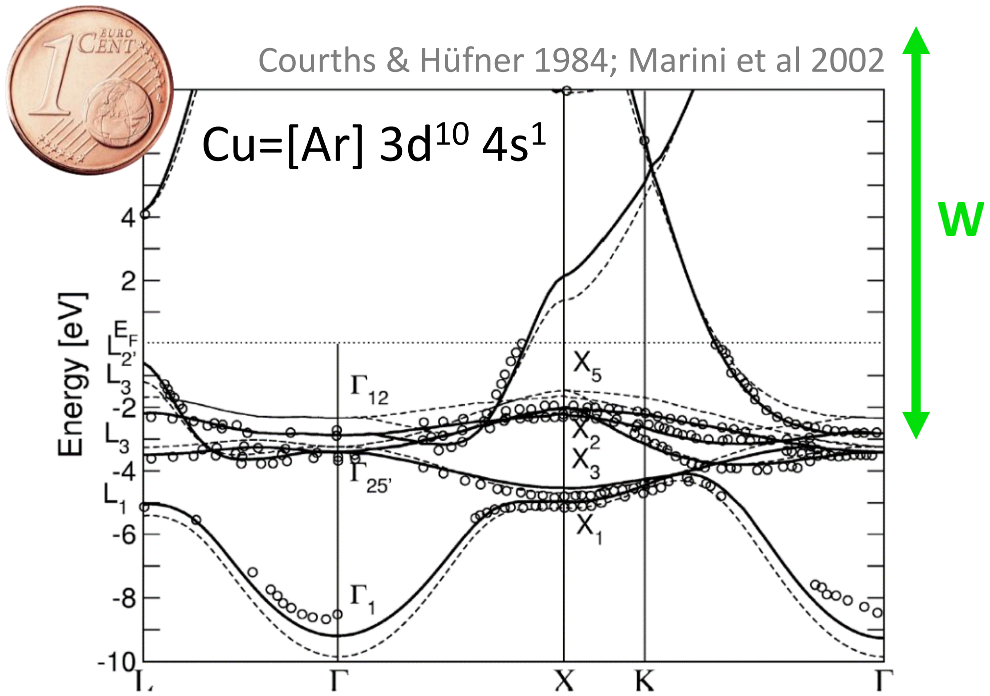
$$\langle \mathbf{AB} \rangle \approx \langle \mathbf{A} \rangle \langle \mathbf{B} \rangle$$

Interacting many-body problem





Electrons in **"time-averaged"** potential



Why does this work?

- **Large kinetic energy** = large bandwidth **W**
- **Screening** reduces bare Coulomb to V_{e-e}

➢ **W** $\gg$ V_{e-e} → <u>one</u> energy scale dominates!

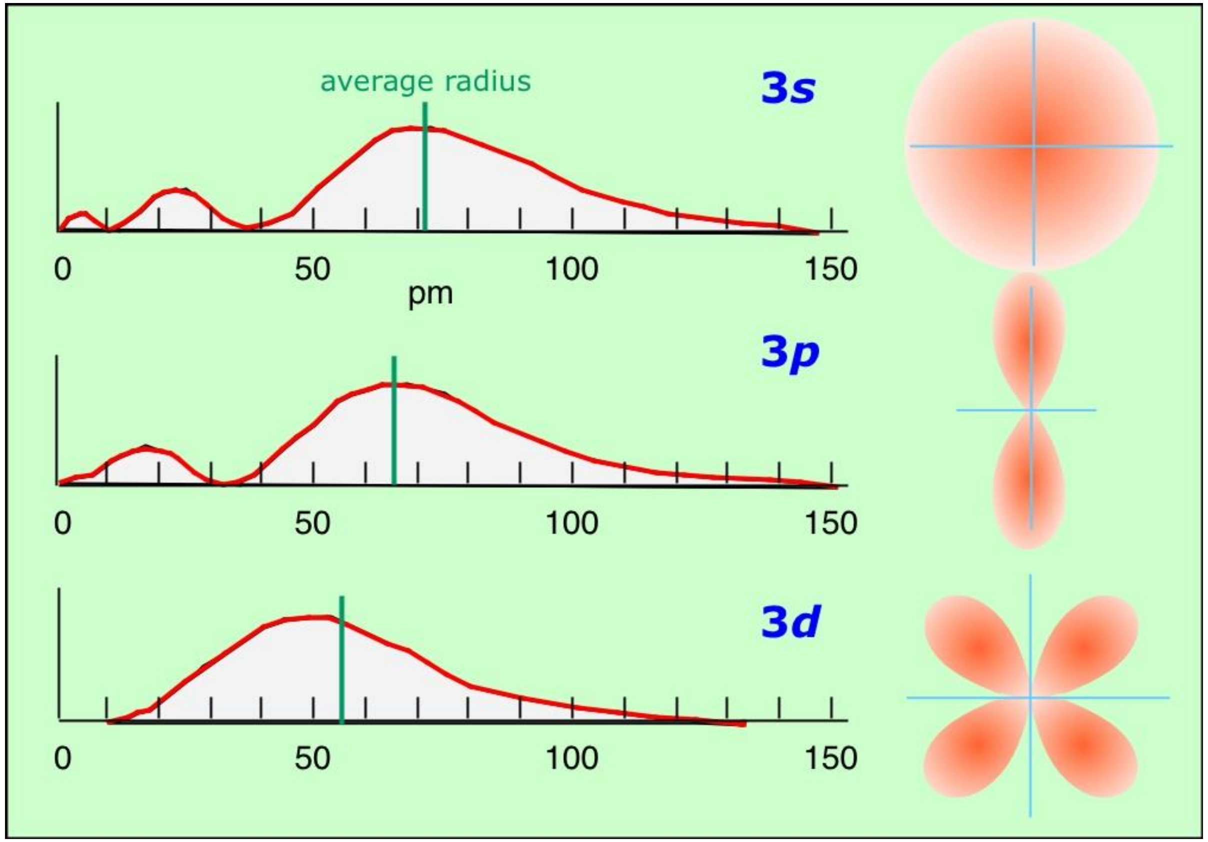
Correlations: a question of orbitals

- extended orbitals: stronger bonding
  - diamond: sp^3 covalent bonding

- orbitals with l = n-1
  most localized
  - in particular: 3d, 4f
  - participate less in bonding
  - more atomic-like characteristics

→ $V_{e\text{-}e}$ / **W** not small → <u>competition</u>

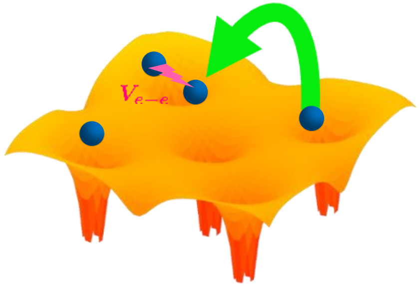
$$\bar{r} = (5.29\text{pm})\,\frac{n^2}{Z}\left[\frac{3}{2} - \frac{l(l-1)}{2n^2}\right]$$



[UC Davis ChemWiki]

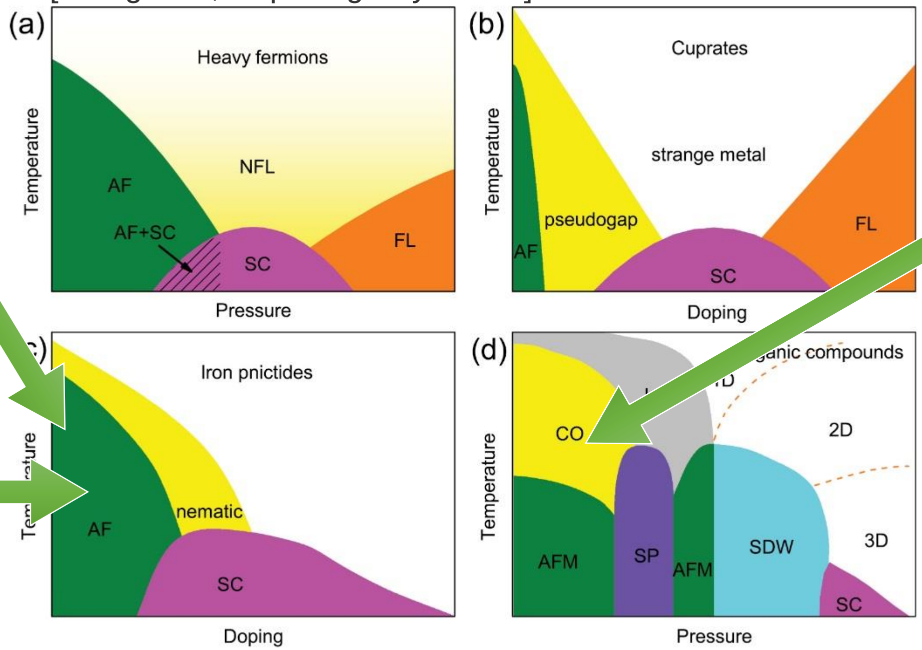
Correlated electrons–phase diagrams

magnons



Band-width W	↔	Coulomb interaction U
Metal		(Mott) insulator
Crystal-field splitting	**↔**	**Hund's rule coupling J**
Low-spin state		High-spin state

[Weng et al, Rep Prog Phys 2016]



competing energy scales → sensitivity to external stimuli

0:1 →

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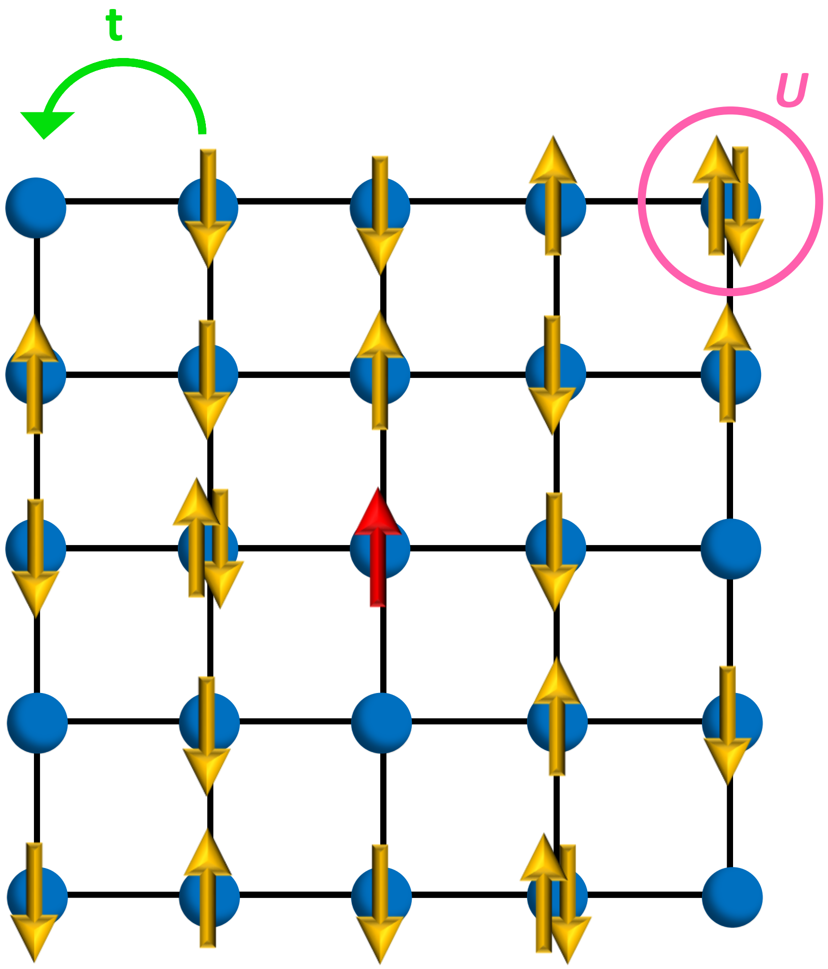
Correlated electrons & DMFT in 1 slide



$t \sim U$ → competing energy scales

Hubbard model

$$H = -\sum_{\mathbf{R}\mathbf{R}'\sigma} t_{\mathbf{R},\mathbf{R}'} \mathbf{c}^{\dagger}_{\mathbf{R}\sigma}\mathbf{c}_{\mathbf{R}'\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow}$$

Long time scales (= low energy)

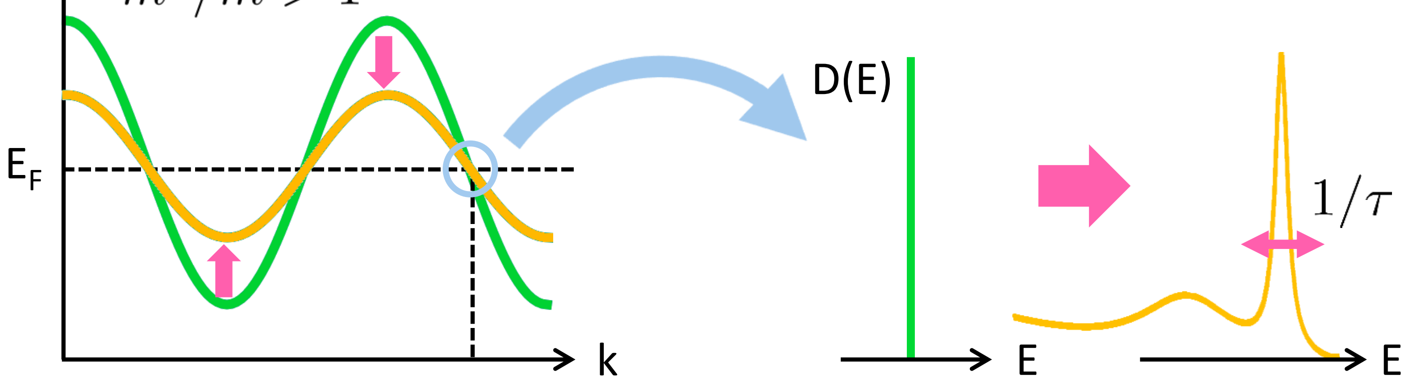
- Delocalized → quasi-particles, "band theory" ($t \gg U$)

Short time scales (= high energy)

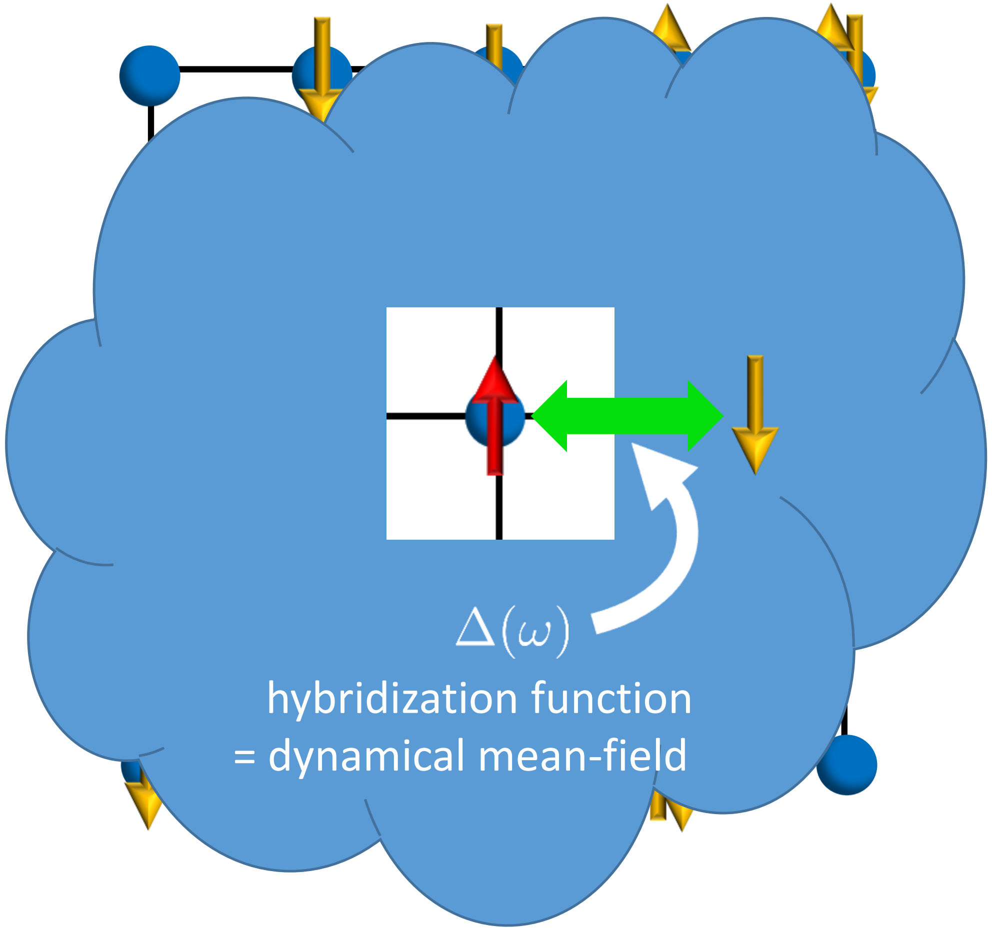
- Localized → atomic characteristics ($U \gg t$)

effective mass $m^*/m > 1$

k not conserved: **finite lifetimes**



Correlated electrons & DMFT in 1 slide



Hubbard model

$$H = -\sum_{\mathbf{RR}'\sigma} t_{\mathbf{R},\mathbf{R}'} \mathbf{c}^\dagger_{\mathbf{R}\sigma} \mathbf{c}_{\mathbf{R}'\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow}$$

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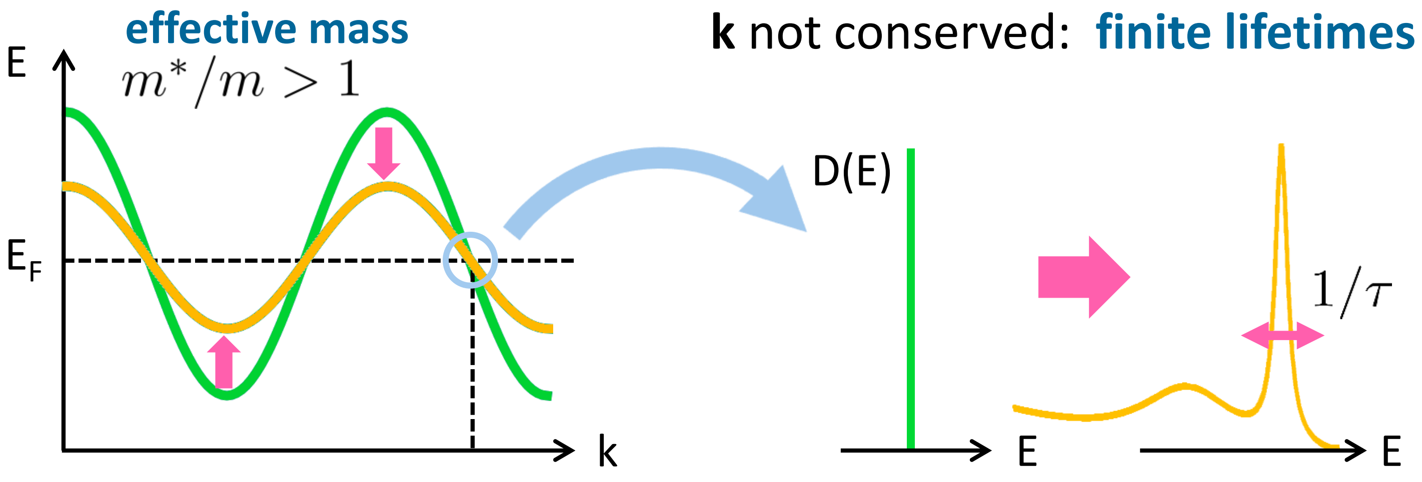


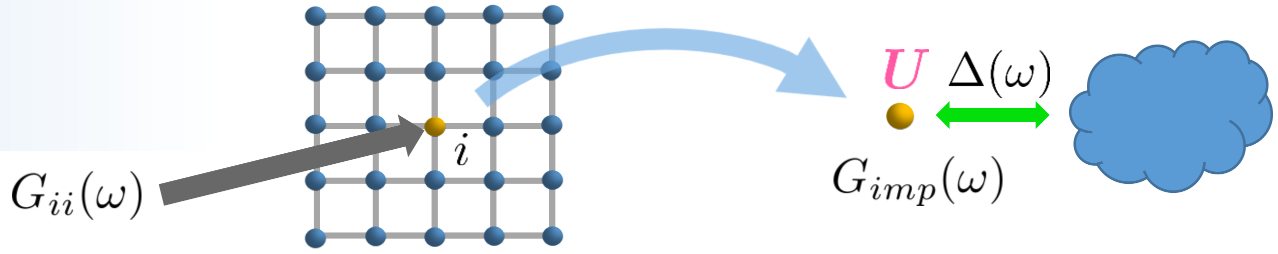
Dynamical mean-field theory (DMFT)

[Vollhardt & Metzner, Georges & Kotliar 1992]

cf. classical mean-field

	Ising model
Hamiltonian	$H = -\sum_{ij} J_{ij} S_i S_j - h \sum_i S_i$
local observable	$m_i = \langle S_i \rangle$
single-site reference system	$H^{eff} = -h^{eff} S$
Weiss field	h^{eff}
self-consistency	$h^{eff} \stackrel{!}{=} \sum_j J_{ij} m_j + h$
solution	$\tanh(\beta h^{eff}[m]) = m$

cf. classical mean-field

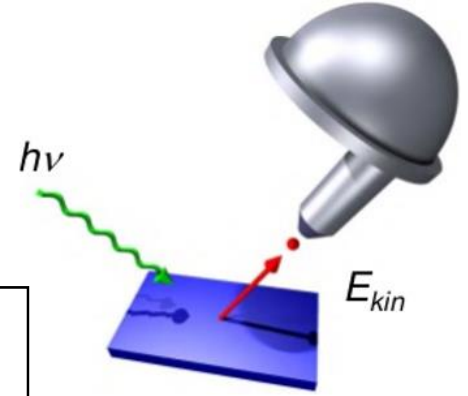


	Ising model	Hubbard model
Hamiltonian	$H=-\sum_{ij} J_{ij} S_i S_j - h\sum_i S_i$	$H=-t\sum_{ij\sigma} \mathbf{c}^{\dagger}_{i\sigma}\mathbf{c}_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$
local observable	$m_i = \langle S_i \rangle$	$G_{ii}(\tau) = -\langle T_\tau \mathbf{c}_i(\tau)\mathbf{c}^{\dagger}_i(0)\rangle$
single-site reference system	$H^{eff} = -h^{eff} S$	$\mathcal{S} = \int d\tau \mathbf{c}^{\dagger}\left(-\frac{\partial}{\partial\tau} + H^{kin}_{loc}\right)\mathbf{c} \; + U d\tau n_\uparrow n_\downarrow$ $+\int d\tau \int d\tau' \mathbf{c}^{\dagger}(\tau)\Delta(\tau-\tau')\mathbf{c}\;(\tau')$
Weiss field	h^{eff}	$\Delta(\omega)$
self-consistency	$h^{eff} \stackrel{!}{=} \sum_j J_{ij} m_j + h$	$G_{imp}(\omega) \stackrel{!}{=} G_{ii}(\omega)$
solution	$\tanh(\beta h^{eff}[m]) = m$	effective Anderson impurity model

Spectrum & self-energy Σ

$$G(k,\tau) = -\left\langle T_\tau \mathbf{c}_k(\tau)\mathbf{c}_k^\dagger(0)\right\rangle$$

$$G(k,\omega) = [\omega + \mu - \epsilon_k - \Sigma(\omega)]^{-1}$$

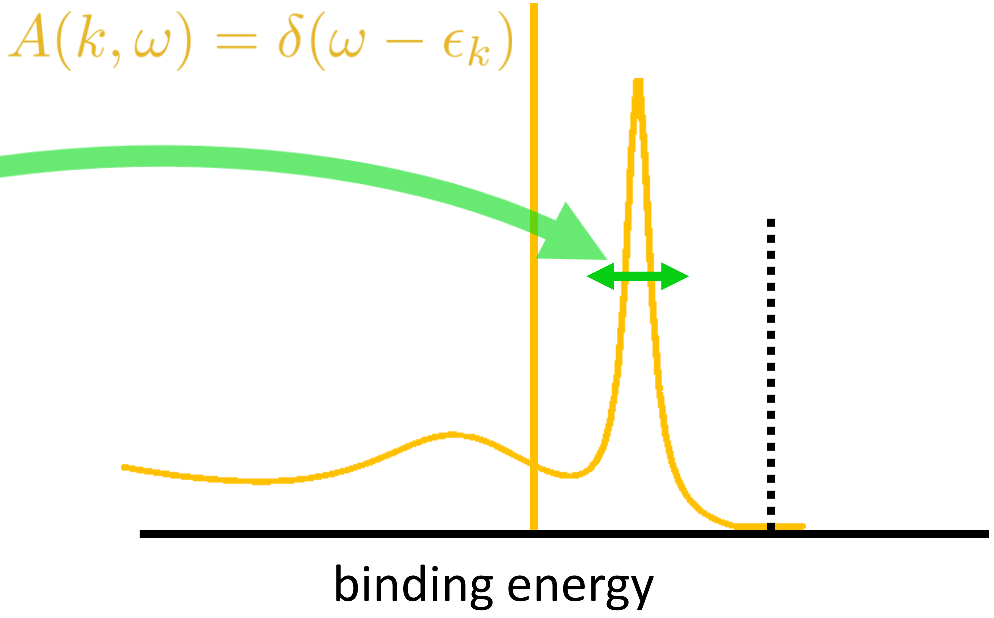


Photoemission spectroscopy

spectral function $$A(k,\omega) = -\frac{1}{\pi}\frac{Im\Sigma}{(\omega - \epsilon_k - Re\Sigma)^2 + (Im\Sigma)^2}$$ renormalized "Lorentzian"

- no correlations: $\Sigma(\omega) = -i0^+$
- Fermi liquid: $\Sigma(\omega) = (1 - Z^{-1})\omega - iB(\omega^2 + (\pi k_B T)^2) + \mathcal{O}(\omega^3)$

$$A(k,\omega) \quad = \quad Z\frac{(Z Im\Sigma/\pi)}{(\omega - Z\epsilon_k)^2 + (Z Im\Sigma)^2} + \cdots$$



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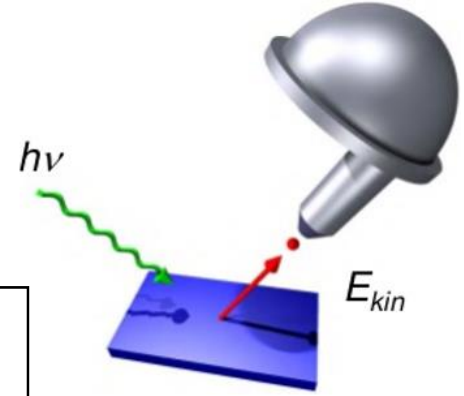

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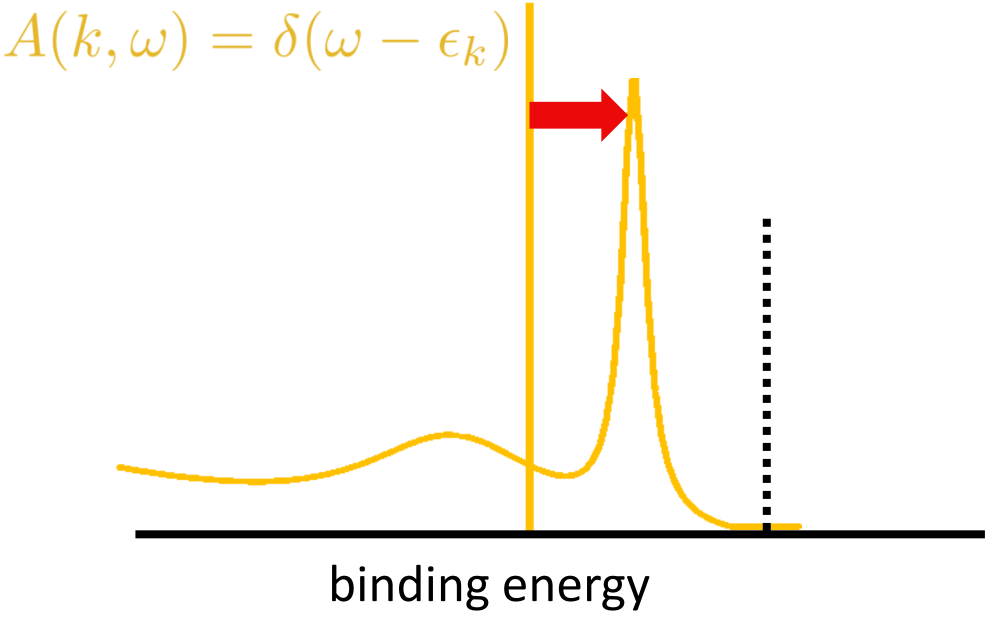

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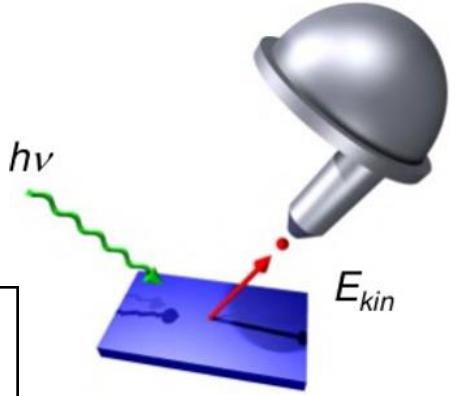

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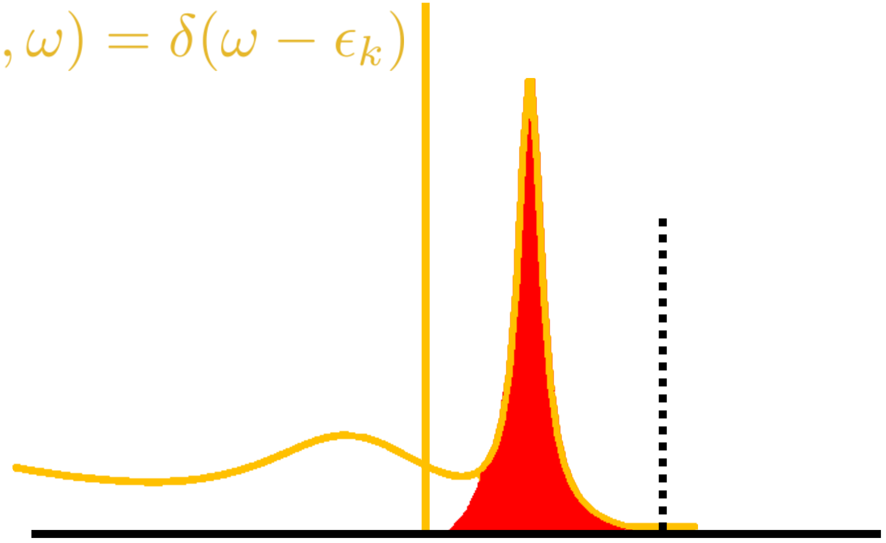
$A(k,\omega) = \delta(\omega - \epsilon_k)$



binding energy

Spectrum & self-energy Σ

$$G(k,\tau) = -\left\langle T_\tau \mathbf{c}_k(\tau)\mathbf{c}_k^\dagger(0)\right\rangle$$

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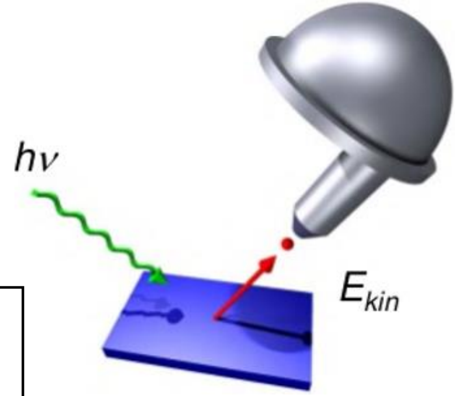

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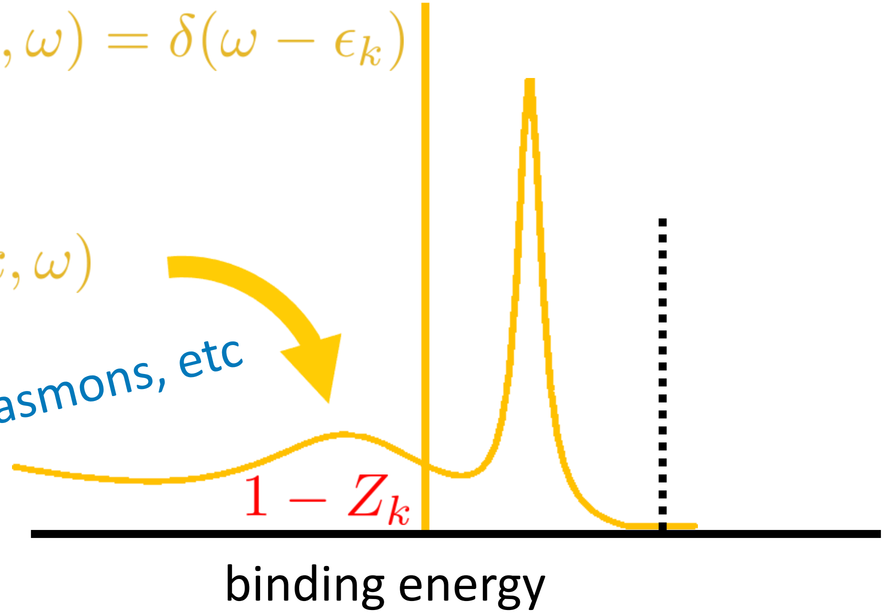
$$A(k,\omega) = Z\frac{(Z Im\Sigma/\pi)}{(\omega - Z\epsilon_k)^2 + (Z Im\Sigma)^2} + \cdots + A_{inc}(k,\omega)$$

Hubbard bands, plasmons, etc



DMFT for the Hubbard model

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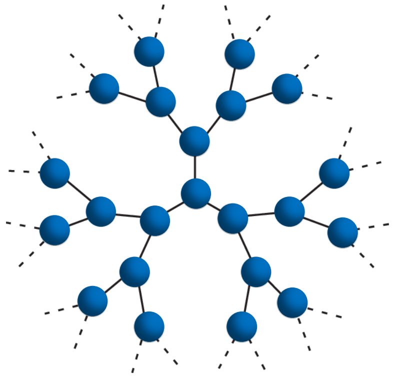
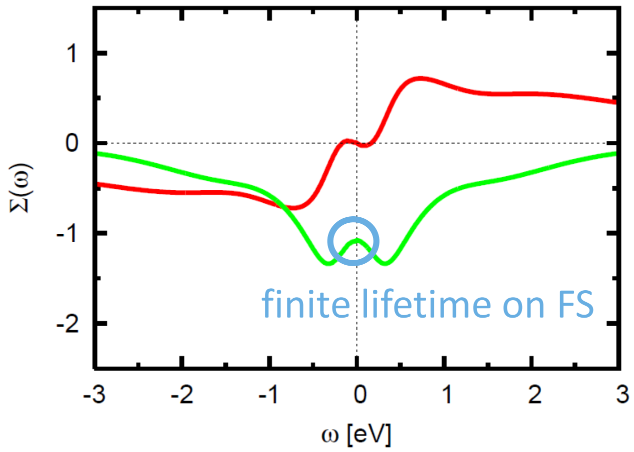
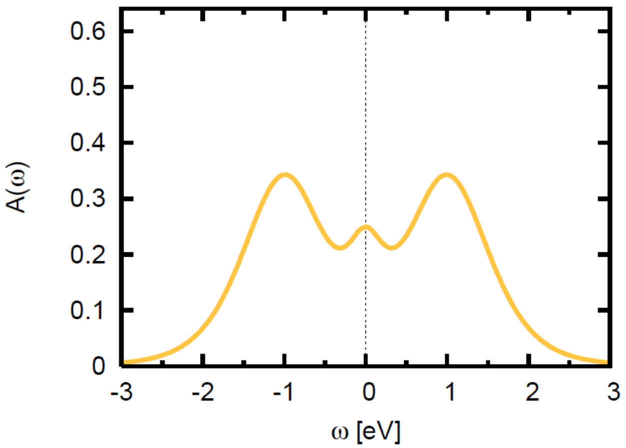
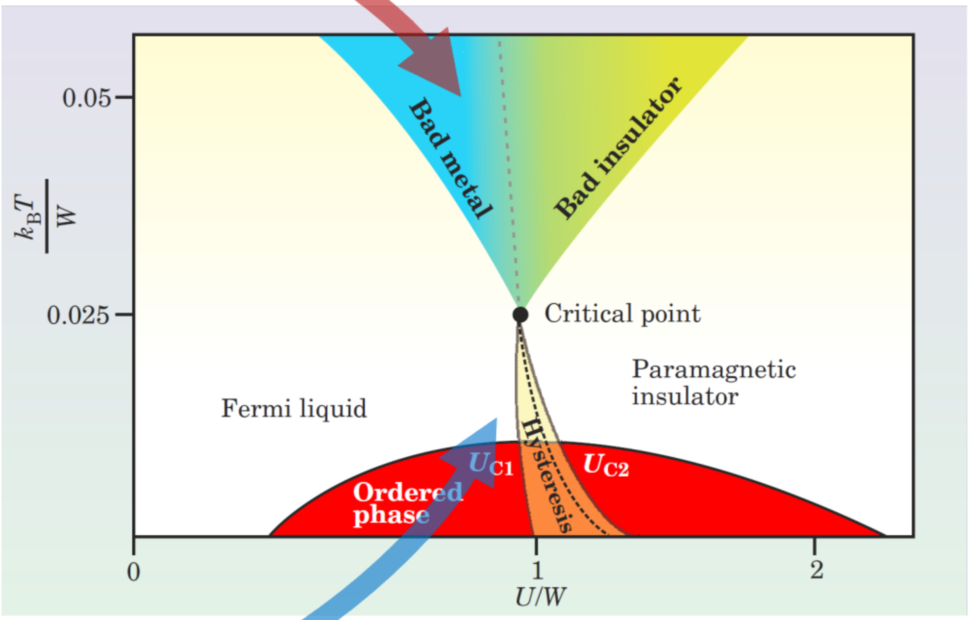


Bethe lattice:
$\Delta = t^2 G$





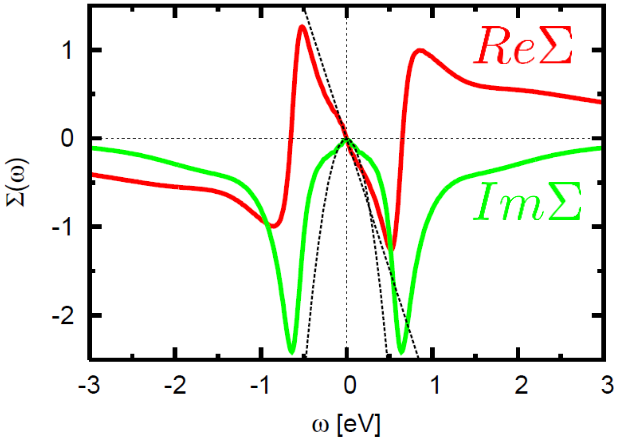


Bethe lattice, 1 band, half-filled

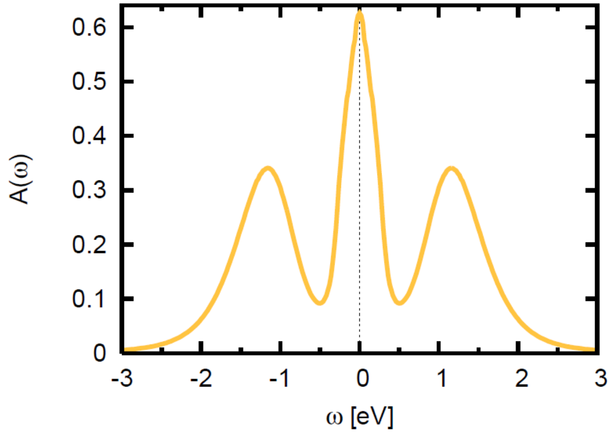
Fermi liquid

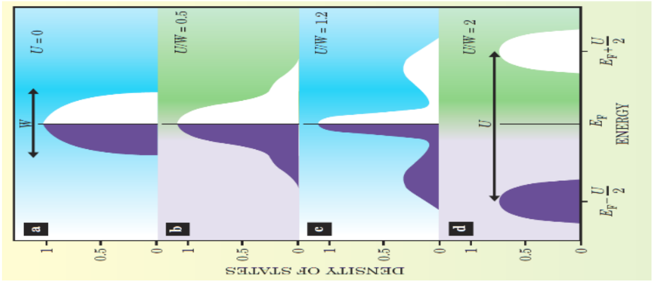
$$\Sigma = (1 - Z^{-1})\omega - iB(\omega^2 + \pi^2 T^2) + \mathcal{O}(\omega^3)$$

self-energy

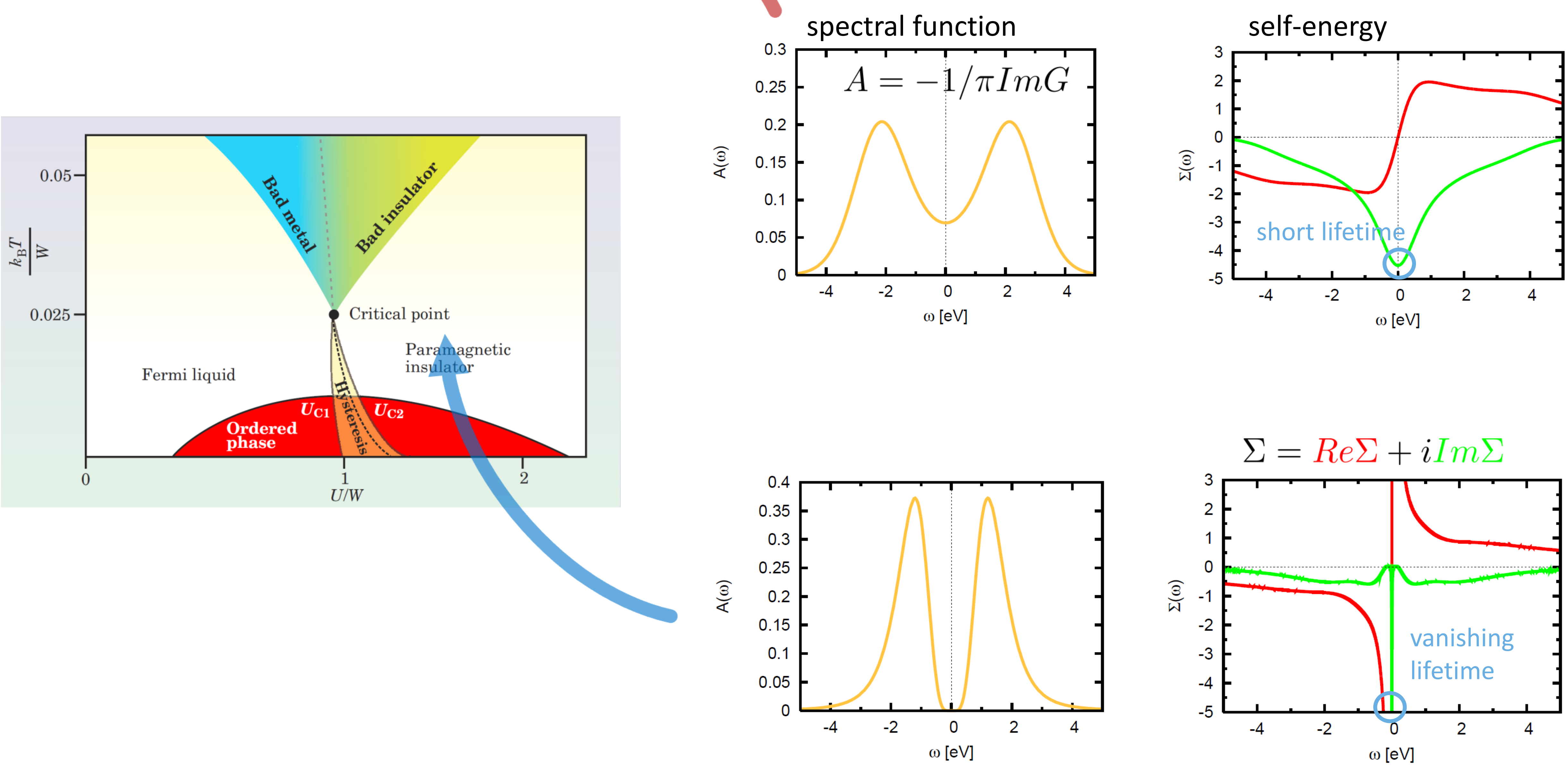


spectral function





DMFT for the Hubbard model



Limits in which DMFT is exact

$$H = -\sum_{\mathbf{R}\mathbf{R}'\sigma} t_{\mathbf{R},\mathbf{R}'} \mathbf{c}^{\dagger}_{\mathbf{R}\sigma}\mathbf{c}_{\mathbf{R}'\sigma} + U\sum_{\mathbf{R}} n_{\mathbf{R}\uparrow}n_{\mathbf{R}\downarrow}$$

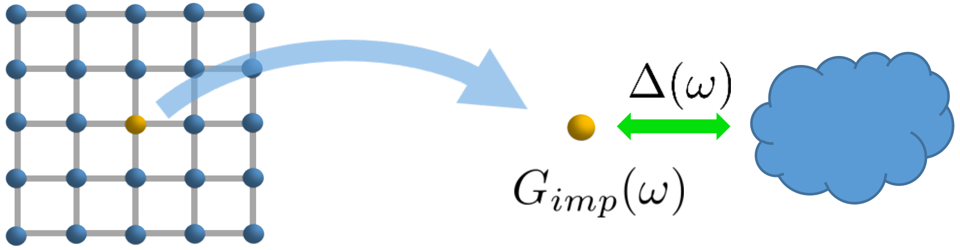
- non-interacting limit $U = 0 \longrightarrow \Sigma = 0$
- atomic limit $t = 0 \longrightarrow \Delta = 0$

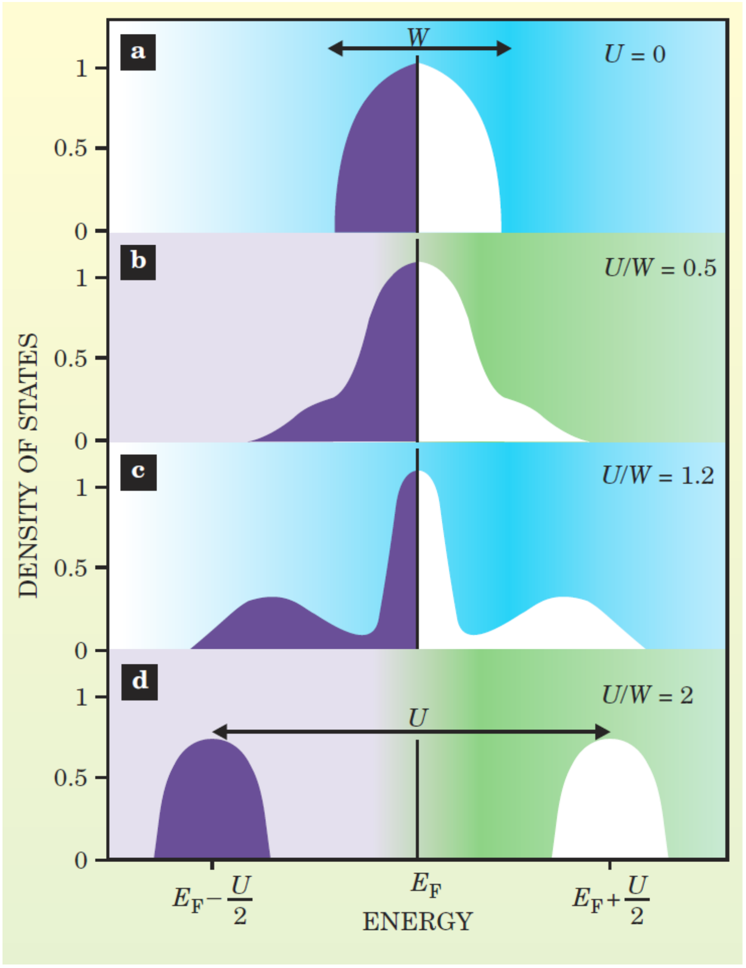
→ non-perturbative: all irreducible diagrams

→"interpolates" between weak and strong coupling

- infinite dimensions/connectivity
  [Metzner & Vollhardt, PRL 62, 324 (1989)]
  [Müller-Hartmann, Z. Phys. B 74, 507 (1989)]

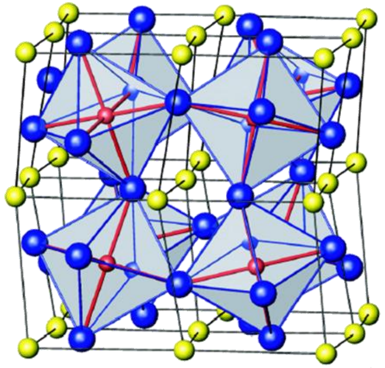
$$D = \infty \longrightarrow \Sigma(\mathbf{k},\omega) = \Sigma(\omega)$$



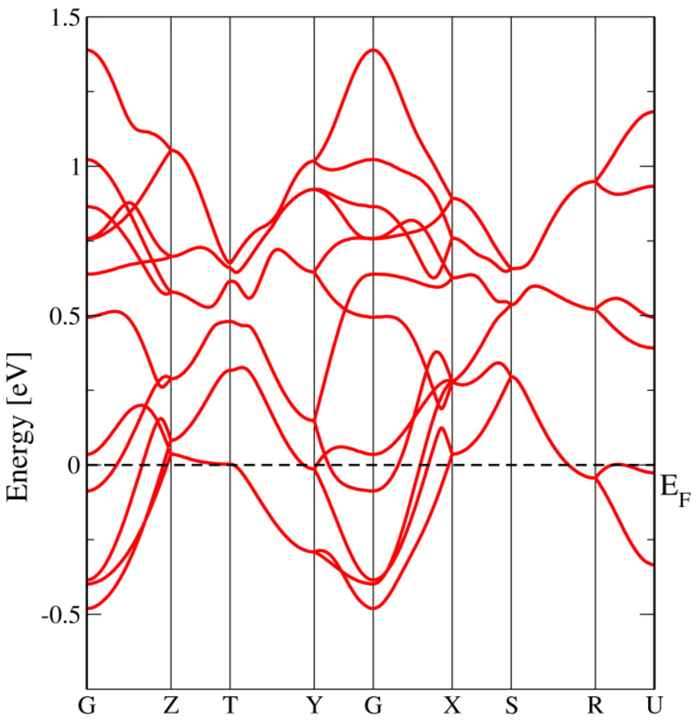


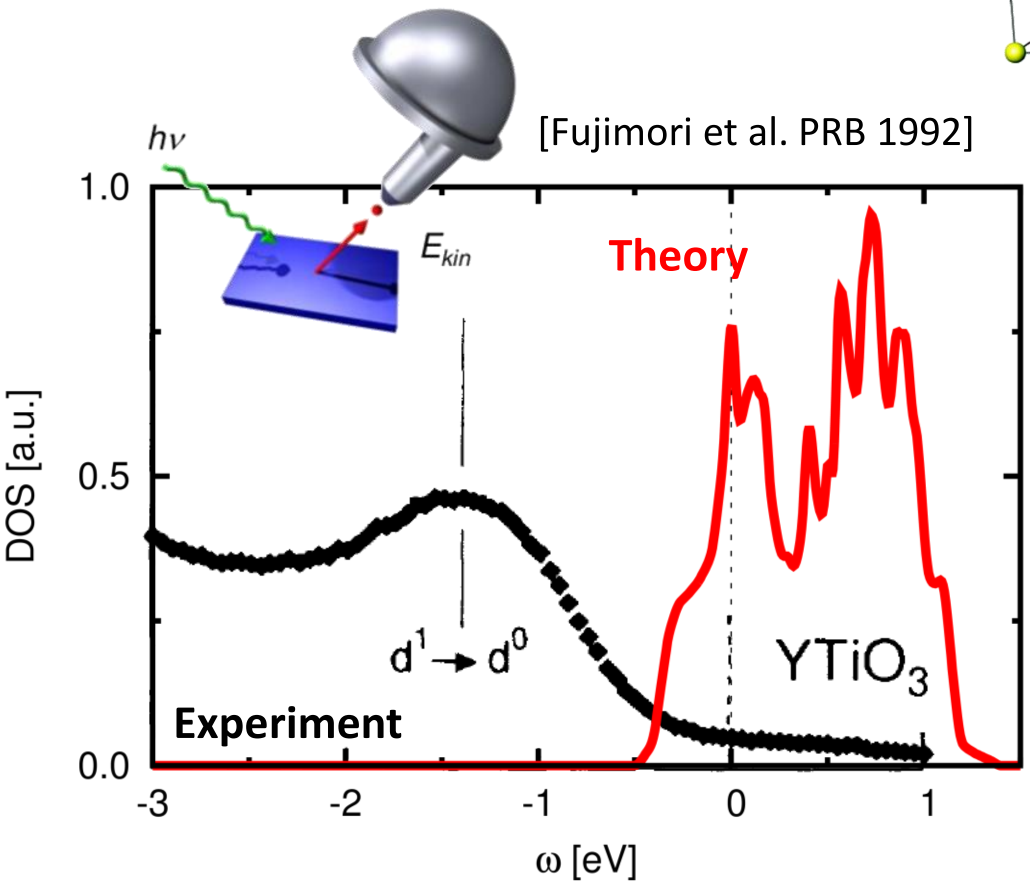
[G. Kotliar & D. Vollhardt, Physics Today 3, 53 (2004)]

Breakdown of band-theory: $YTiO_3$



- distorted perovskite
- Ti $3d^1$
- 4 formula units/cell

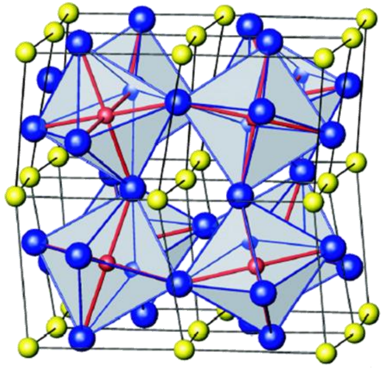




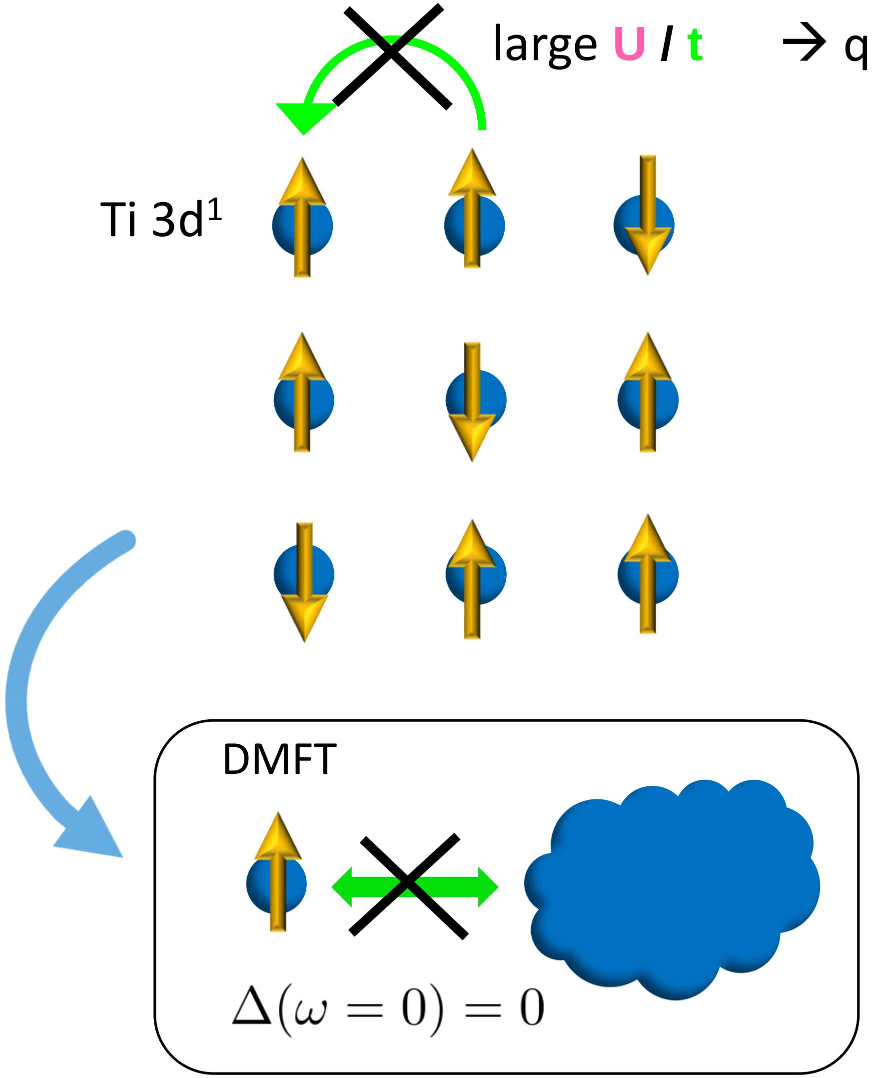
DFT: $YTiO_3$ a metal

reality: a (paramagnetic!) insulator

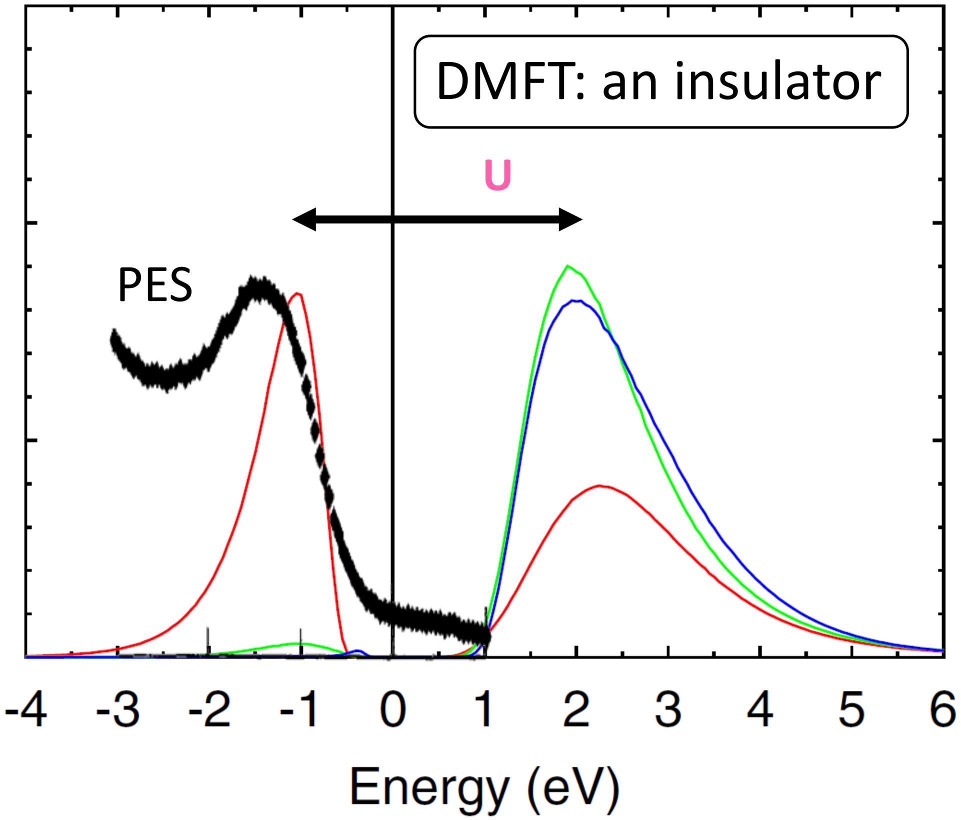
$YTiO_3$: a Mott insulator



large U / t → quasi-particle weight Z = 0 ($m^* \to \infty$)



[Pavarini et al, NJP '05, Fujimori et al, PRB'92]



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https://doi.org/10.1088/1361-648X/aab284

Topical Review

Thermoelectricity in correlated narrow-gap semiconductors

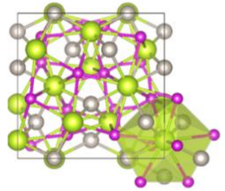
Jan M Tomczak

[Phys.: Condens. Matter 30 183001 (2018)]

& [JMT arXiv:1904.01346]

& [JMT arXiv:1908.00840]

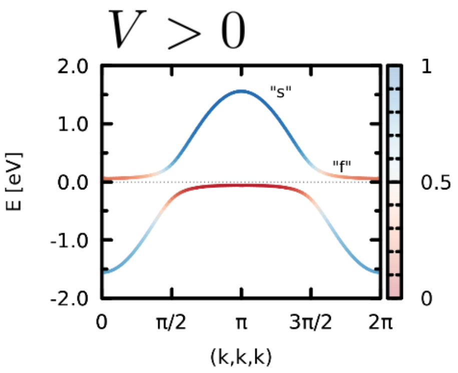
Band theory "$U = T = 0$"

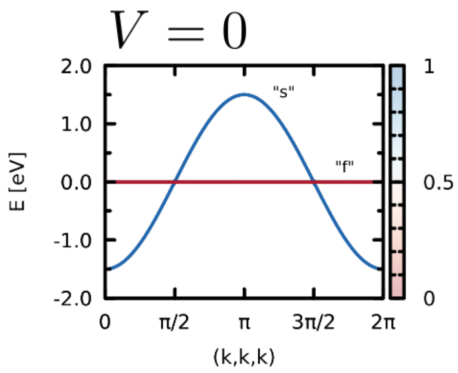


$Ce_3Bi_4Pt_3$

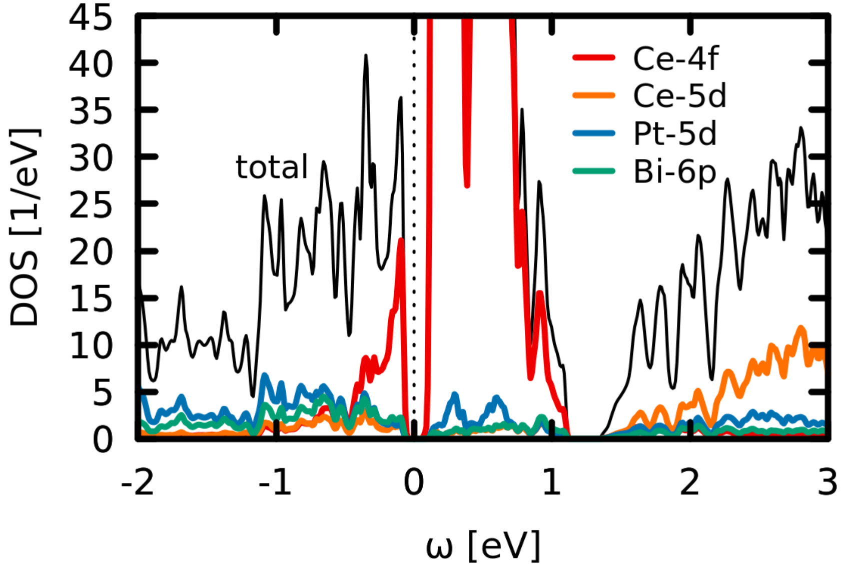
periodic Anderson model

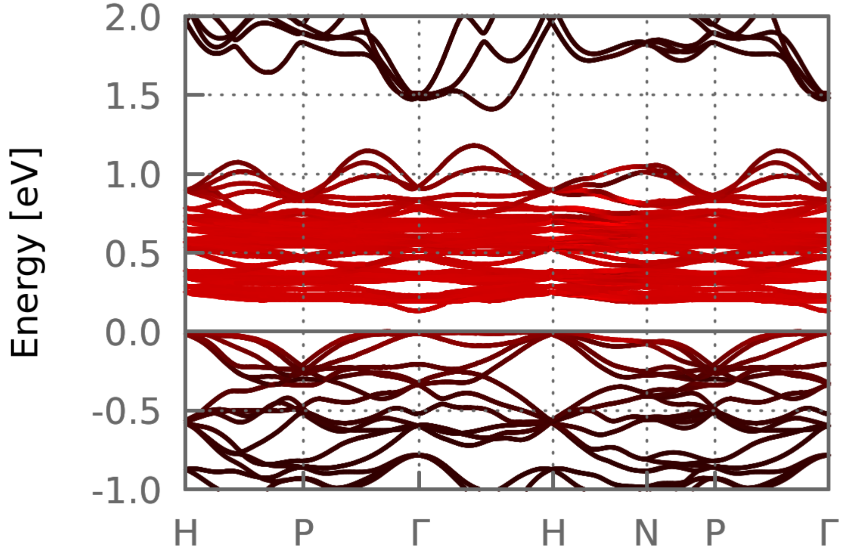
$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \mathbf{c}^{\dagger}_{\mathbf{k}\sigma}\mathbf{c}_{\mathbf{k}\sigma} + \epsilon_f \sum_{i\sigma} f^{\dagger}_{i\sigma} f_{i\sigma} + V \sum_{\mathbf{k}\sigma} (\mathbf{c}^{\dagger}_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + f^{\dagger}_{\mathbf{k}\sigma} \mathbf{c}_{\mathbf{k}\sigma}) + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow}$$





$\Delta_{\text{indir}} \approx$ 130meV





& [JMT arXiv:1908.00840]

[JMT: J. Phys.: Condens. Matter 30 183001 (2018)]

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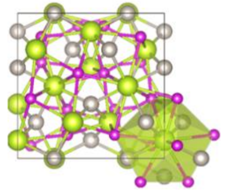
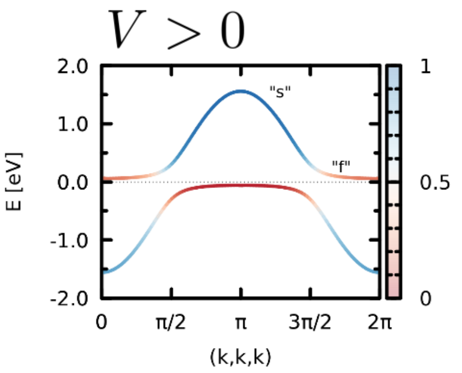
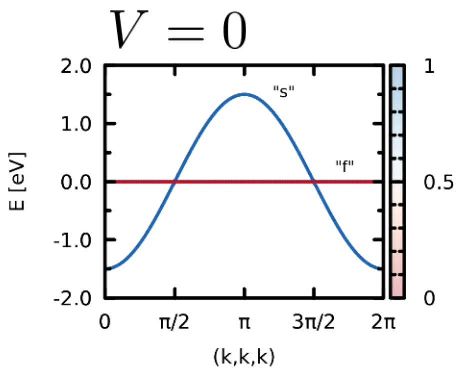


$Ce_3Bi_4Pt_3$

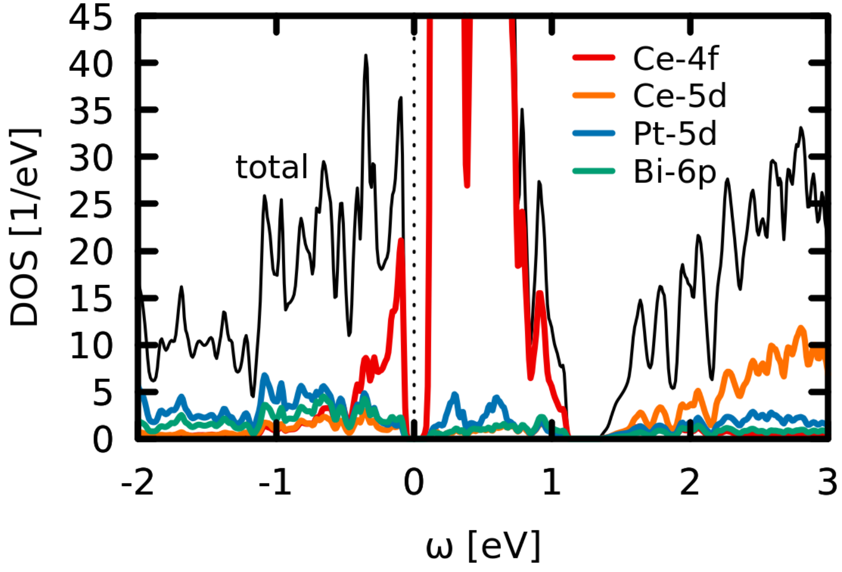
periodic Anderson model

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \mathbf{c}^{\dagger}_{\mathbf{k}\sigma} \mathbf{c}_{\mathbf{k}\sigma} + \epsilon_f \sum_{i\sigma} f^{\dagger}_{i\sigma} f_{i\sigma} + V \sum_{\mathbf{k}\sigma} (\mathbf{c}^{\dagger}_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + f^{\dagger}_{\mathbf{k}\sigma} \mathbf{c}_{\mathbf{k}\sigma}) + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow}$$



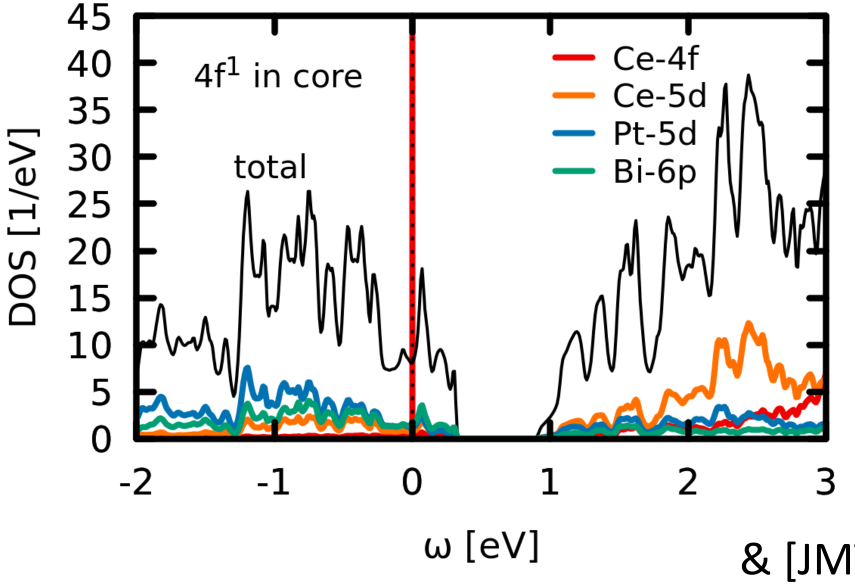


$\Delta_{\text{indir}} \approx 130\text{meV}$



Switch off hybridization of Ce-*4f*

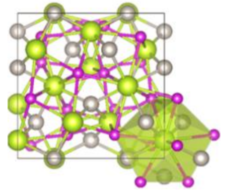
metal



& [JMT arXiv:1908.00840]

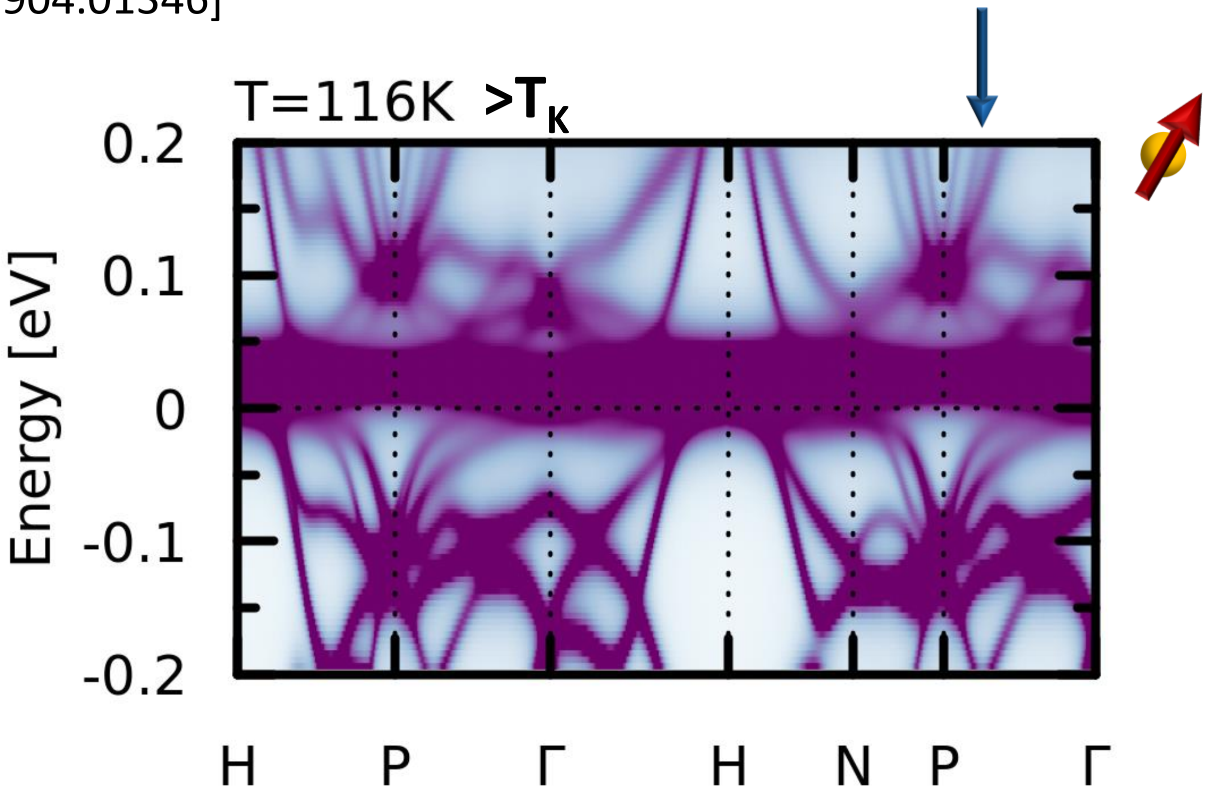
[JMT: J. Phys.: Condens. Matter 30 183001 (2018)]

DMFT “U>0”: spectral properties

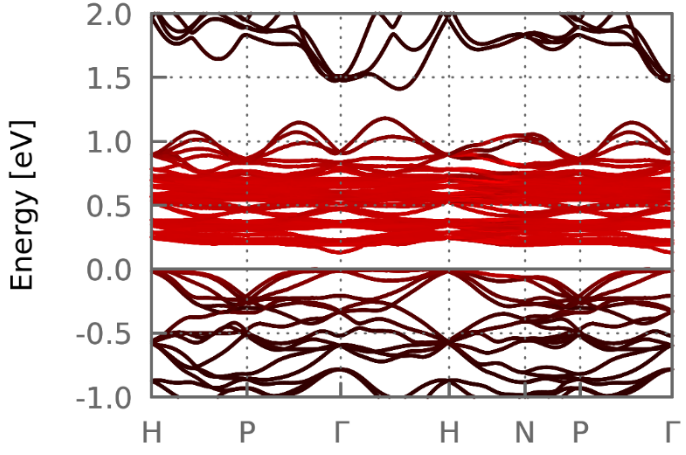


$Ce_3Bi_4Pt_3$

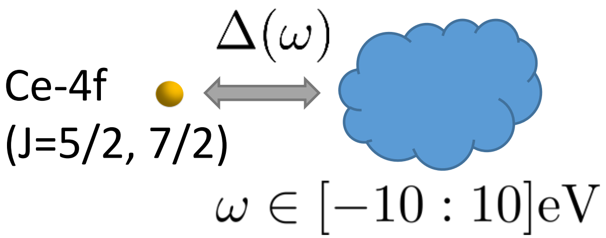
[JMT arXiv:1904.01346]



DFT “U=0”

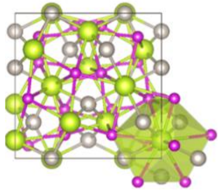


DFT+DMFT



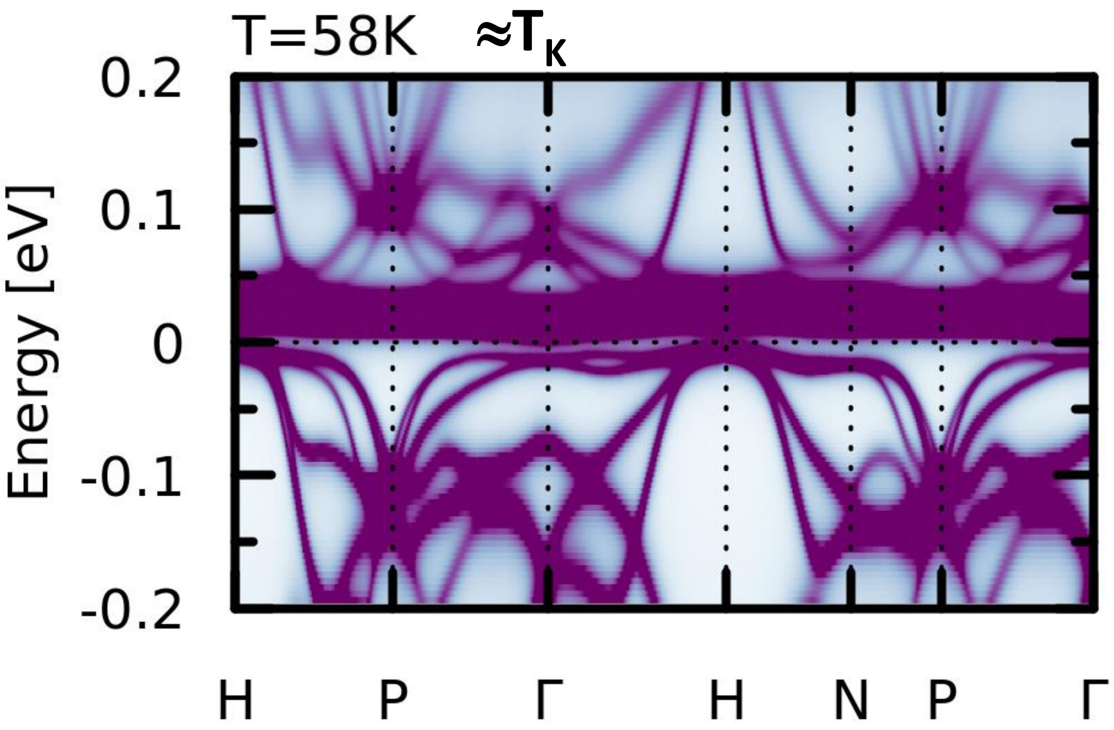
- U=5.5, J=0.68eV, full Coulomb
- ctqmc, charge self-consistency [Haule et al, PRB 2010]

DMFT “U>0”: spectral properties

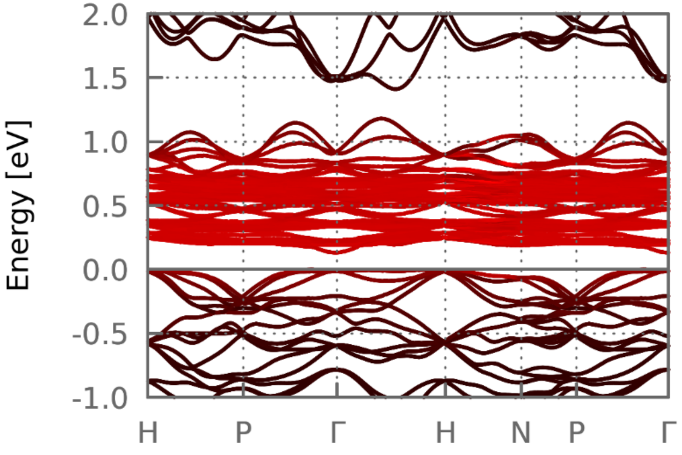


$Ce_3Bi_4Pt_3$

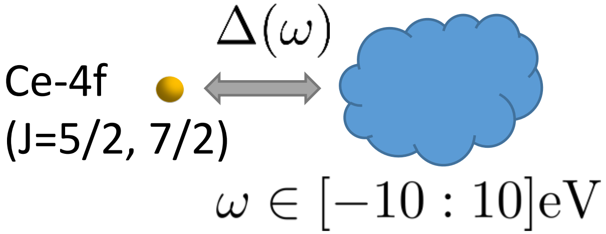
[JMT arXiv:1904.01346]



DFT “U=0”



DFT+DMFT



- U=5.5, J=0.68eV, full Coulomb
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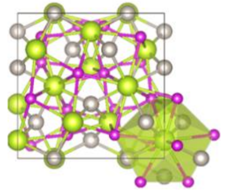
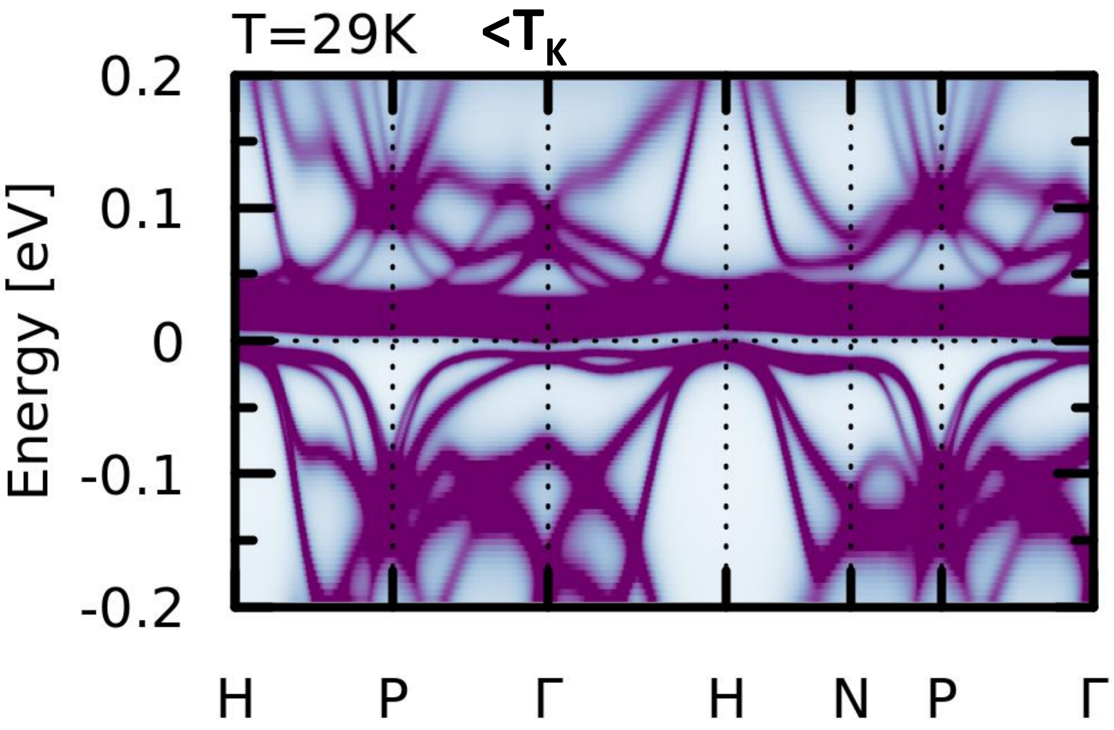
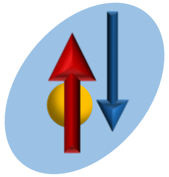
DMFT “U>0”: spectral properties



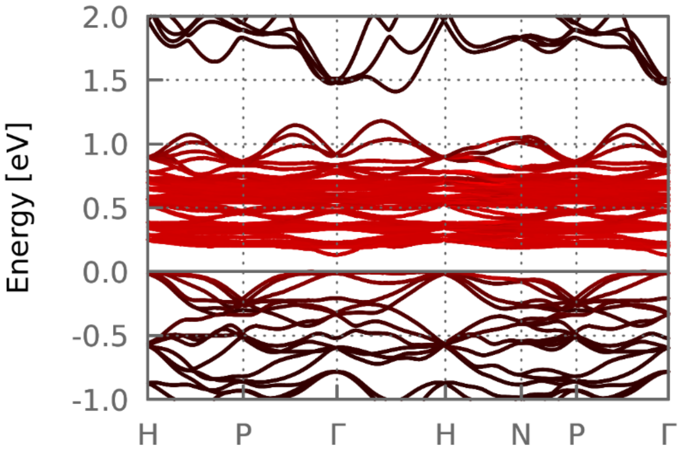
$Ce_3Bi_4Pt_3$

[JMT arXiv:1904.01346]

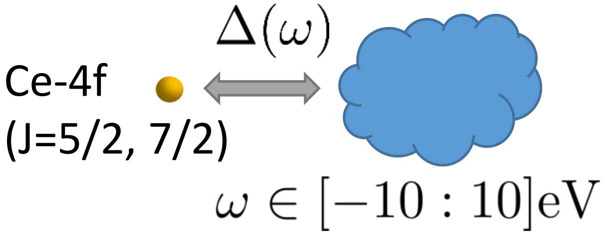




DFT “U=0”



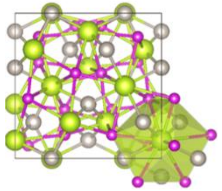
DFT+DMFT



- incoherence-to-coherence crossover ✓
- gap renormalization ($m^*/m_{DFT} = 1/Z \approx 10$) ✓

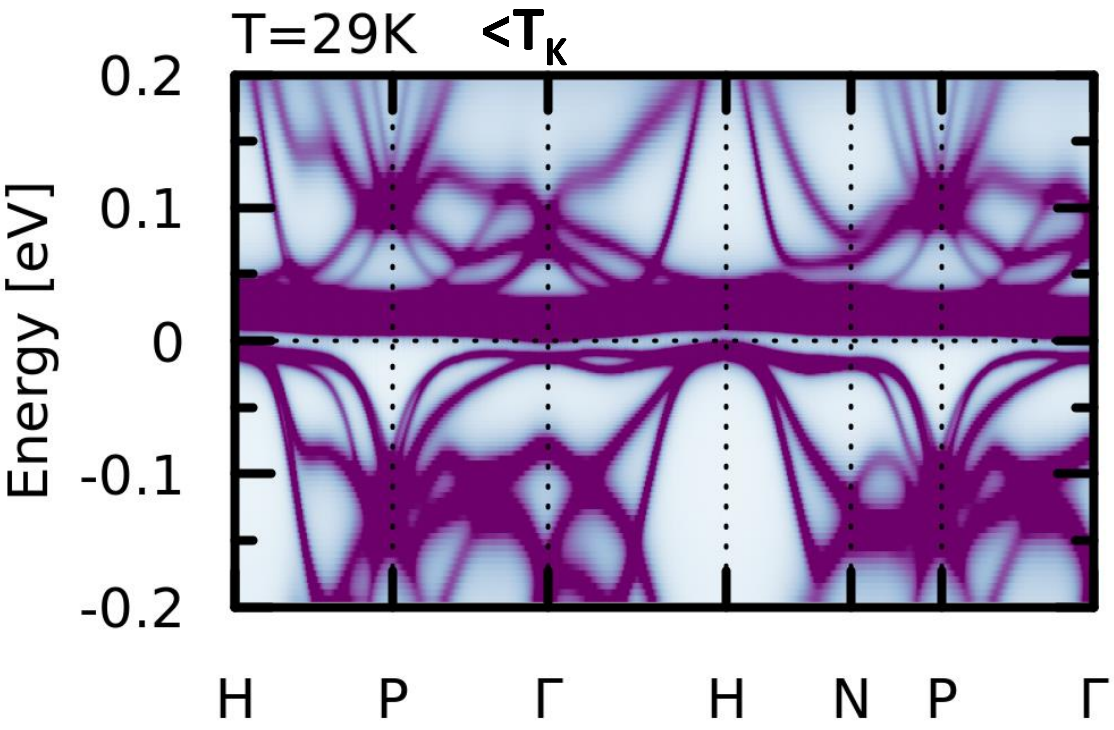
- U=5.5, J=0.68eV, full Coulomb
- ctqmc, charge self-consistency [Haule et al, PRB 2010]

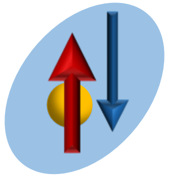
DMFT “U>0”: spectral properties

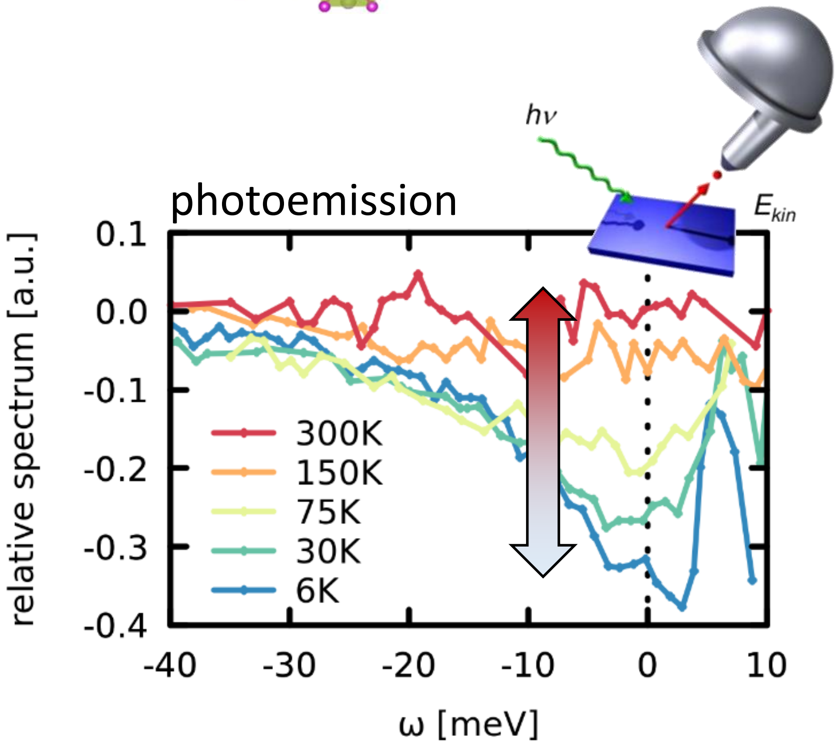


$Ce_3Bi_4Pt_3$

[JMT arXiv:1904.01346]



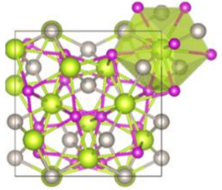




[Takeda et al ’99]

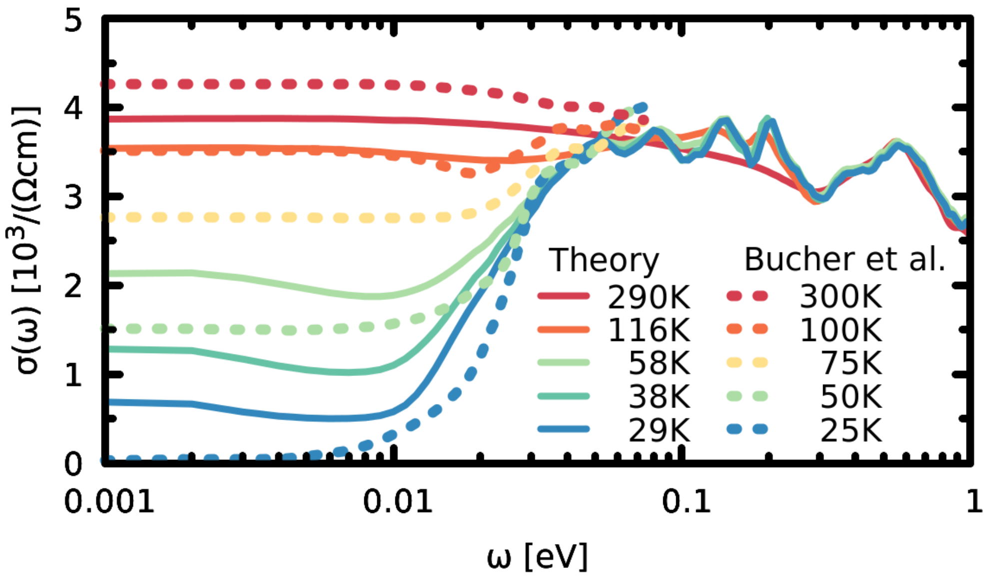
- incoherence-to-coherence crossover ✓
- gap renormalization ($m^*/m_{DFT} = 1/Z \approx 10$) ✓

DMFT: charge & spin observables

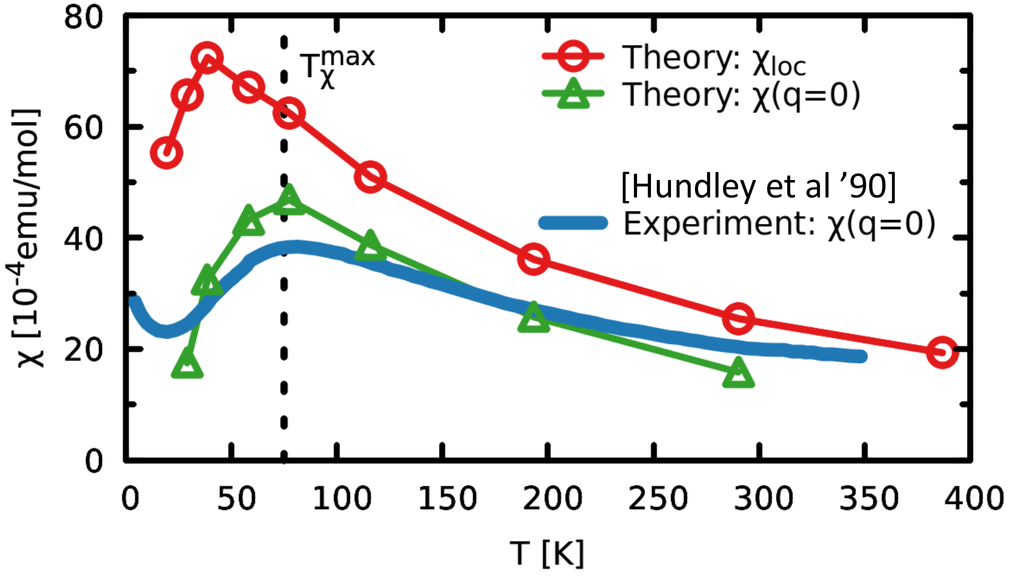


$Ce_3Bi_4Pt_3$

optical conductivity



magnetic susceptibility



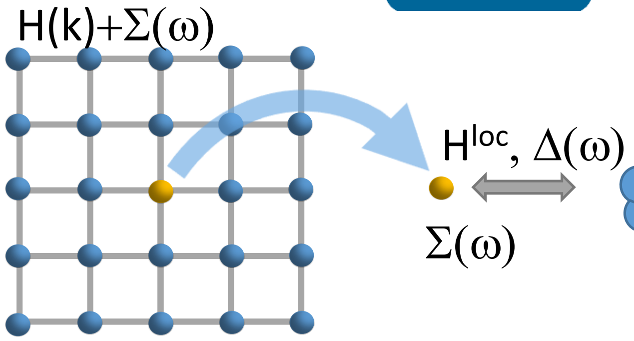
- metallization for $T \ll \Delta/k_B$ through incoherent weight ✓
- transfers of spectral weight over $\Omega \gtrsim 300\mathrm{meV} \gg \Delta$ ✓

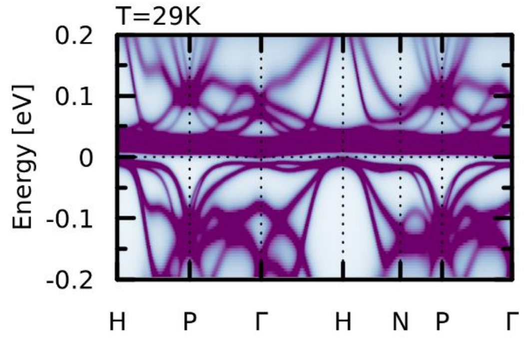
[JMT arXiv:1904.01346]

Summary

➢ dynamical mean-field theory

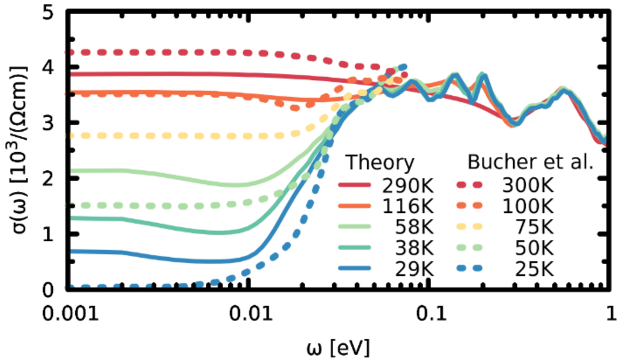
- many-body renormalizations: m*, lifetimes
- excited states
- finite temperatures





➢ introductions to DMFT

- A. Georges: AIP Conf Proc 715, 3 (2004) [arXiv:cond-mat/0403123]
- Juelich School Lecture Notes: www.cond-mat.de/events/correl18/



➢ public codes (with wien2k interfaces, e.g., wien2wannier)

- w2dynamics [Wuerzburg+Wien]
- DFT+Embedded DMFT Functional [K. Haule, Rutgers] → Ce3Bi4Pt3
- TRIQS [O. Parcollet et al, Paris]
- ALPS [Switzerland], …

[arXiv:1904.01346]

[arXiv:1908.00840]

[Phys.: Condens. Matter 30, 183001 (2018)]