Quantum Monte Carlo simulations of strongly correlated electron systems within dynamical mean-field theory

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Outline

Motivation: cooperative phenomena in solids

Approaches for correlated electrons; DFT vs. DMFT

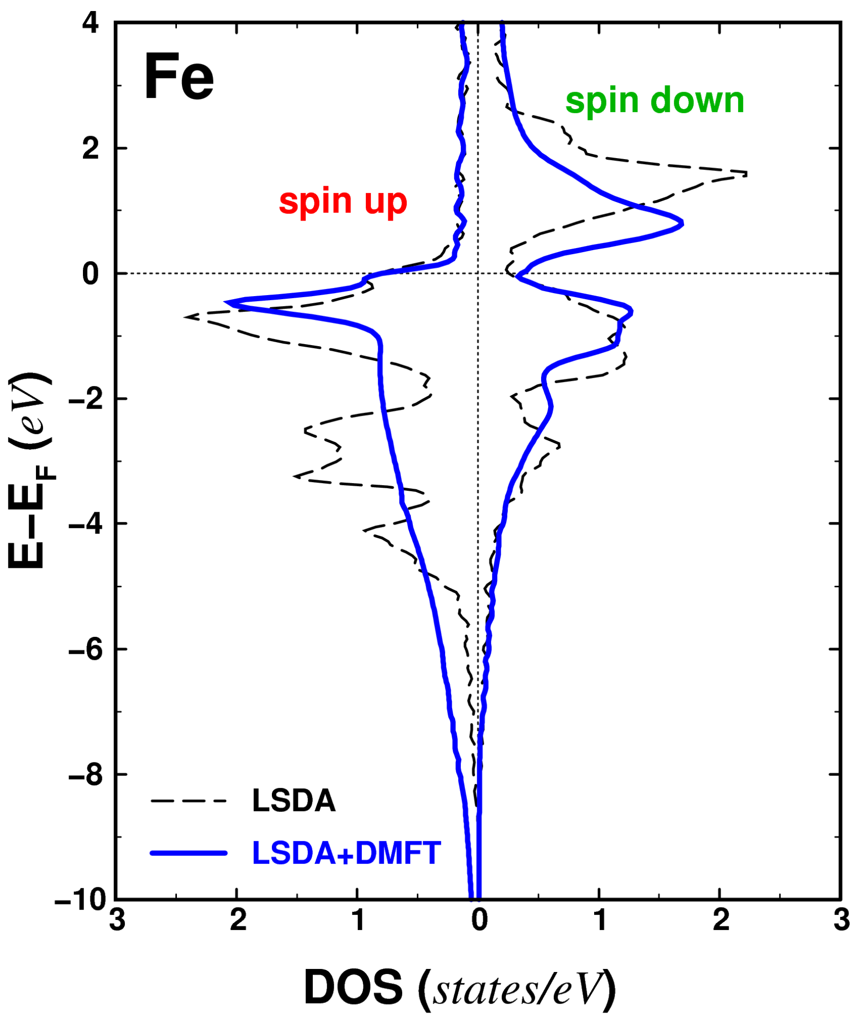
HF-QMC and other DMFT impurity solvers

Orbital-selective Mott transitions

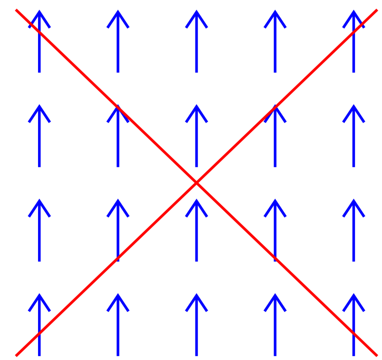
Summary and outlook

Motivation: cooperative phenomena in solids

Itinerant ferromagnetism and half-metallicity

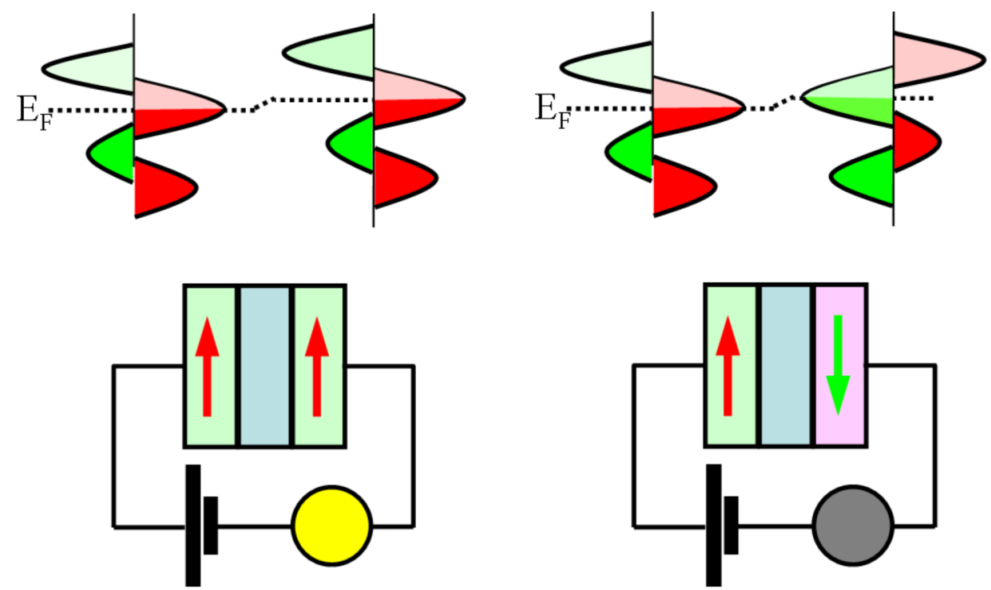


[Chioncel et. al, PRB (2003)]



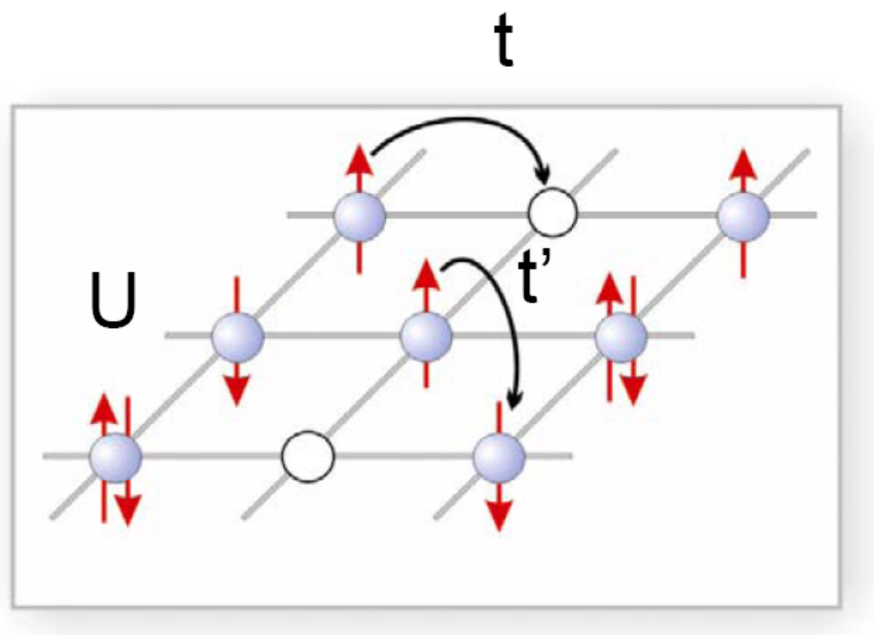
Spin models insufficient

Technological goal: TMR with half metals

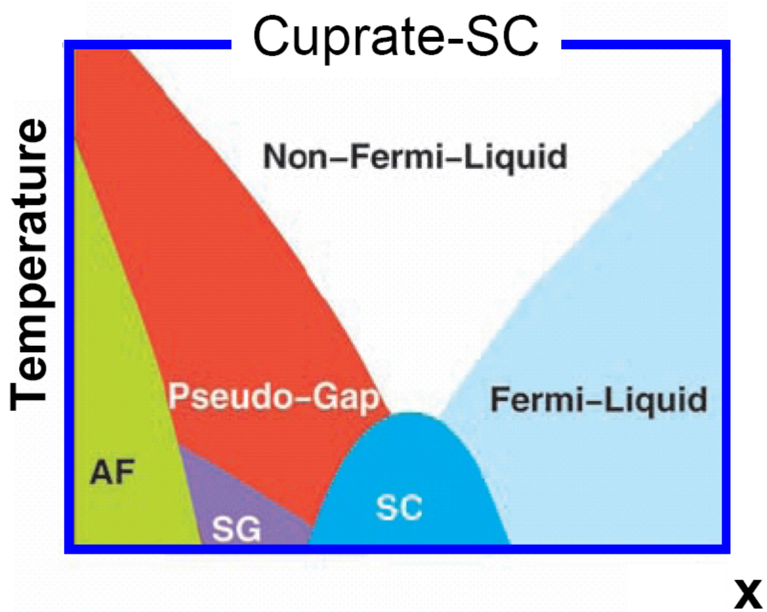


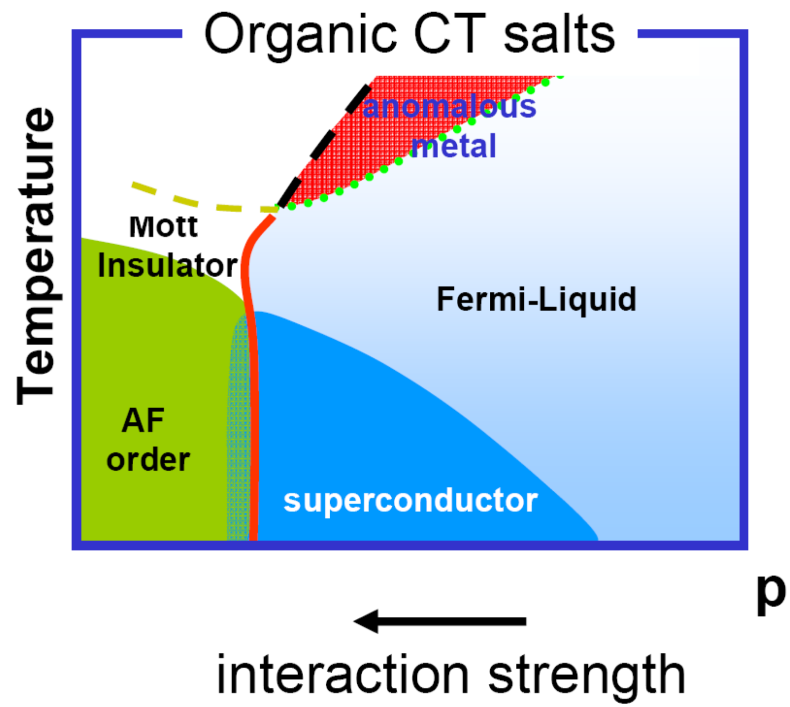
Complex phases of cuprate and organic superconductors

High-T_c physics contained in 2D Hubbard model?



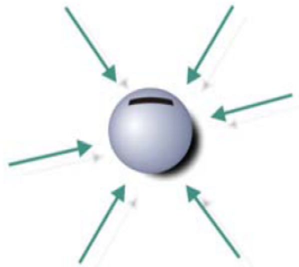
Are antiferromagnetic (AF) and Mott insulating phases essential for superconductivity?



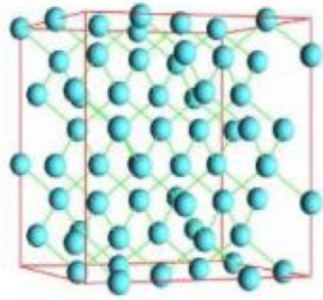


Interplay of multiple degrees of freedom

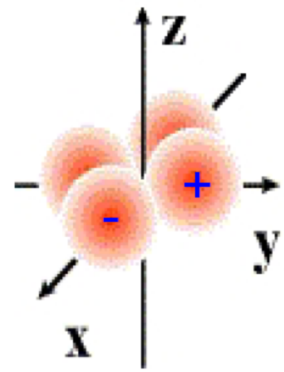
spin



charge

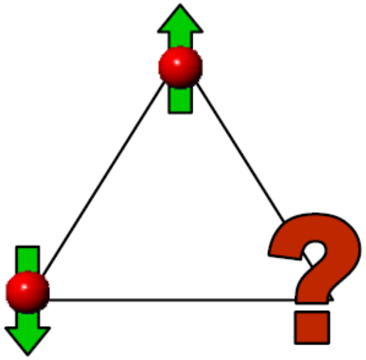


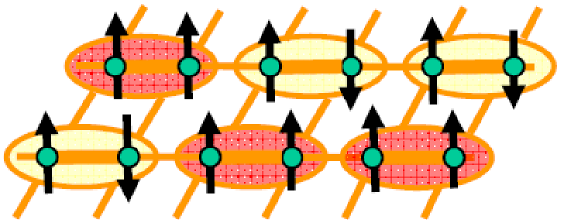
lattice



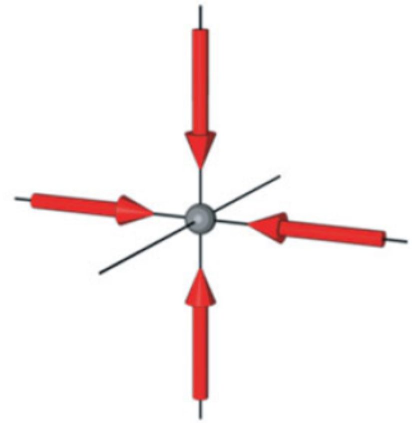
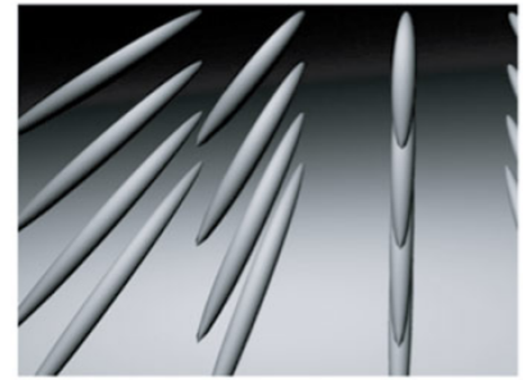
orbital

Frustrated systems, spin liquids, BEC of magnons



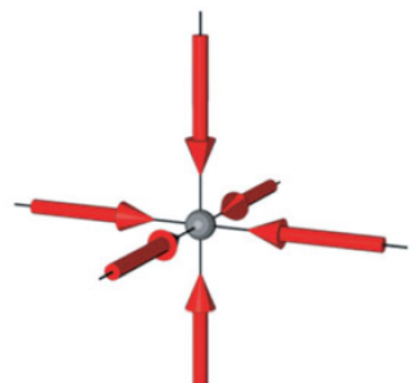
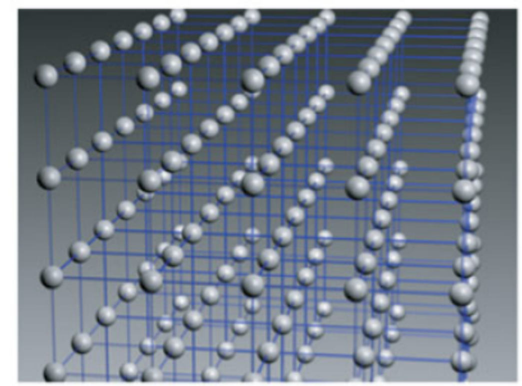


New model systems: ultracold atoms on optical lattices

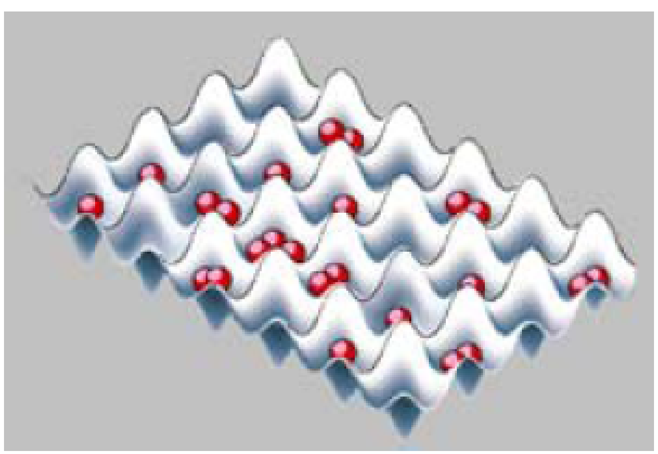



tunable:

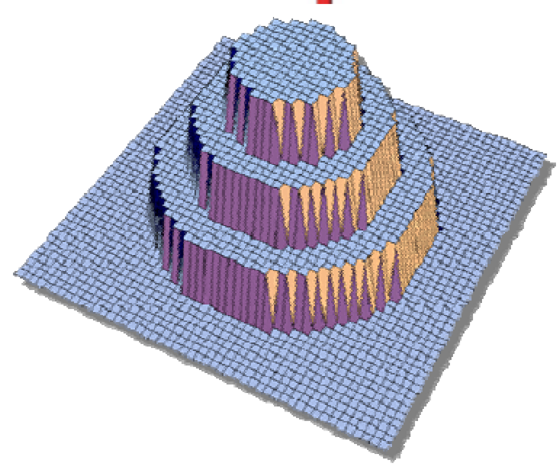
- dimensionality
- statistics
- hopping amplitudes
- interactions

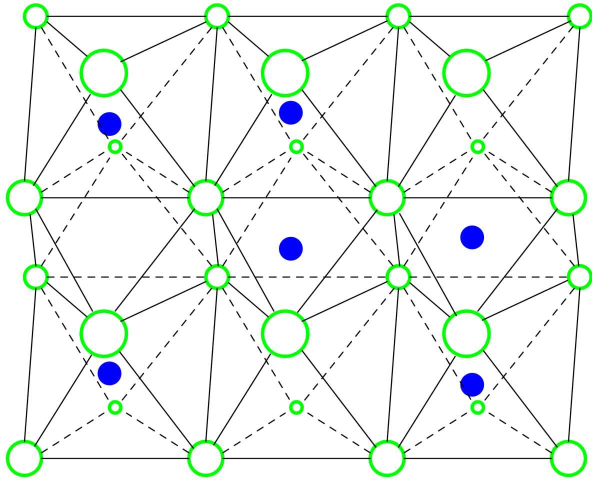
Mott transition (for bosons)



$\stackrel{U}{\Longrightarrow}$



Bandwidth control of metal-insulator transitions

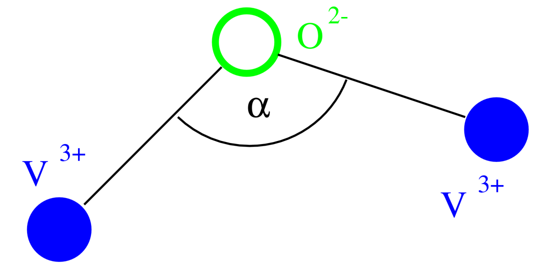


Corundum structure

Hydrostatic pressure or isovalent doping change

- lattice spacings
- bond angles

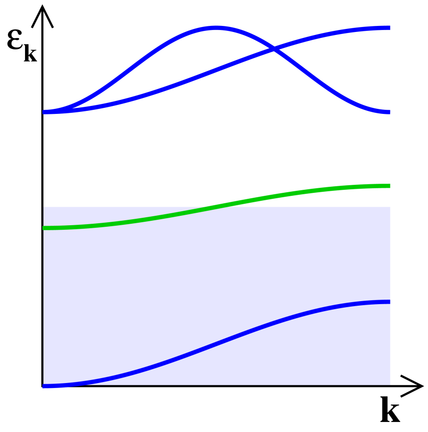
$\rightsquigarrow$ hopping amplitudes

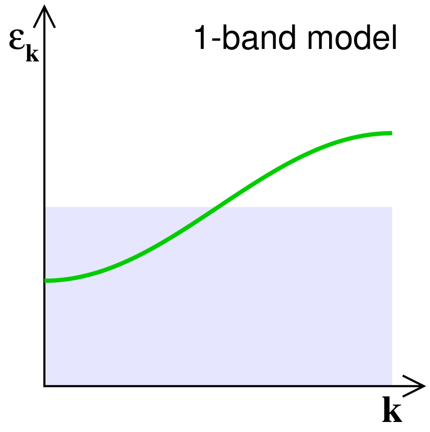


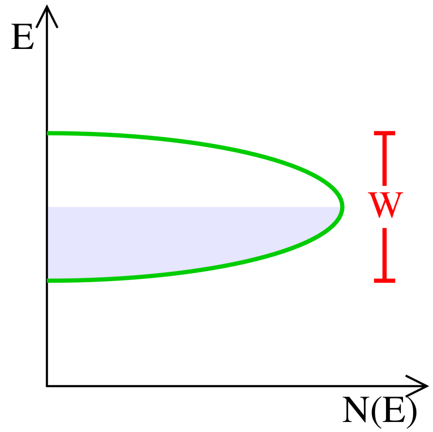
$\alpha_{Cr} < \alpha_V < \alpha_{Ti}$

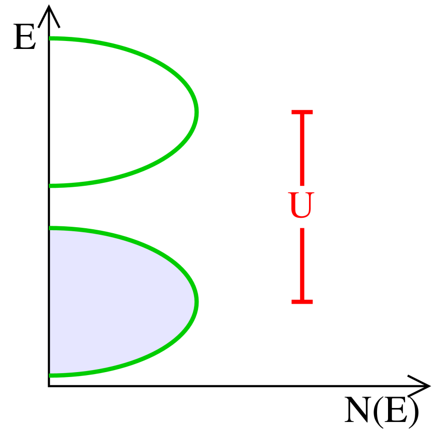
Bond angles for V_2O_3 doped with Cr or Ti

Breakdown of Bloch band description at paramagnetic Mott transition









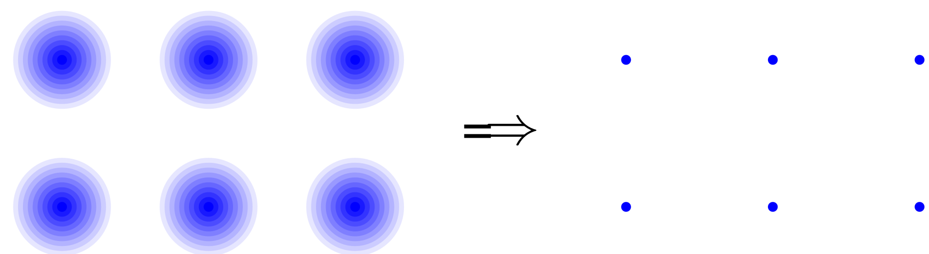
Bloch states near Fermi energy, band-splitting by Coulomb correlations

Microscopic modeling I

General Hamiltonian for nuclei and electrons

$$H = \sum_{i=1}^{N_e} \frac{\mathbf{p}_i{}^2}{2m} + \sum_{k=1}^{L} \frac{\mathbf{P}_k{}^2}{2M_k} + \sum_{k<l} \frac{Z_k Z_l\, e^2}{|\mathbf{R}_k - \mathbf{R}_l|} - \sum_{i,k} \frac{Z_k\, e^2}{|\mathbf{r}_i - \mathbf{R}_k|} + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Born-Oppenheimer approximation (0^{th}order) $\downarrow$



$$H = \sum_{i=1}^{N_e} \frac{\mathbf{p}_i{}^2}{2m} + \sum_{i} V(\mathbf{r}_i) + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Classes of theoretical approaches for electronic problem

- continuum methods (density functional theory, variational+diffusion QMC, ...)
- methods for lattice electrons

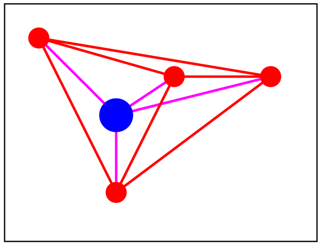
Density functional theory in LDA

Density functional theory (DFT)

- exact ground state approach
- based on electron density $n(\boldsymbol{r})$
- Kohn-Sham equations solve effective single-particle problem

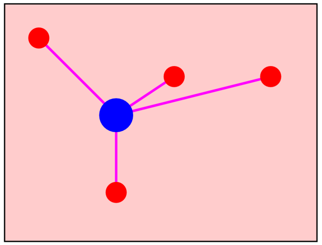
- result: ground state energy + $n(\boldsymbol{r})$
- heuristics: band structure

- problem: exchange-correlation potential unknown

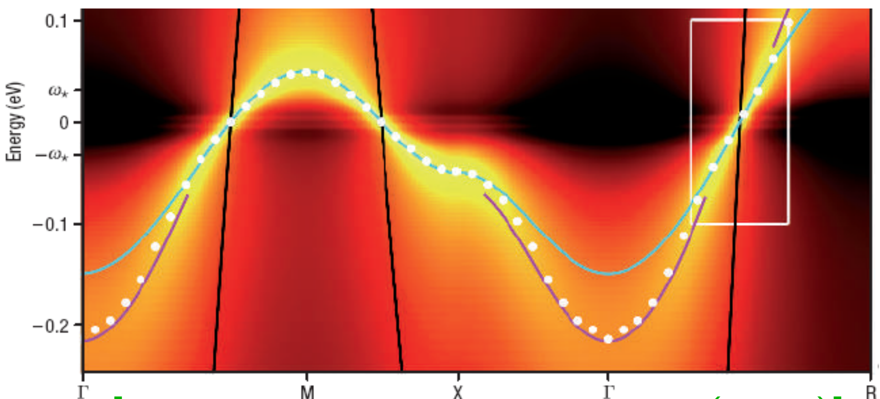


many-body

DFT $\Longrightarrow$



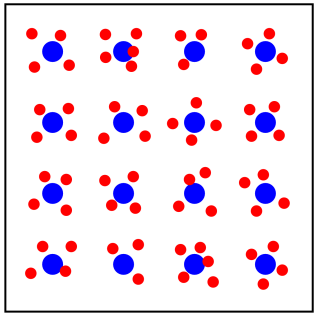
single-particle



[Byzcuk et al., Nature Physics (2006)]

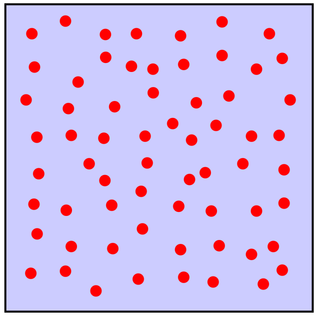
Local density approximation (LDA)

- exchange-correlation potential from jellium model (parametrized QMC)
- not reliable for correlated systems
- often good results
- basis for LDA+U and LDA+DMFT



e^- in solid

LDA $\Longrightarrow$

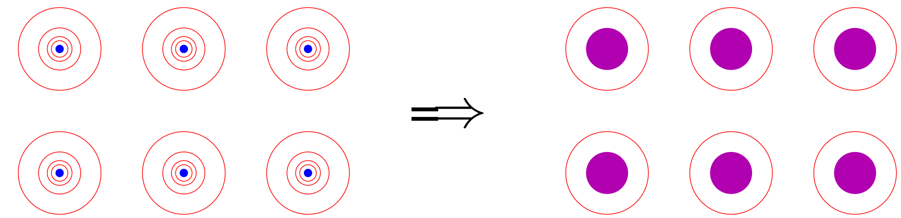


jellium model

Microscopic modeling II

$$H = \sum_{i=1}^{N_e} \frac{\mathbf{p}_i^{\,2}}{2m} + \sum_i V(\mathbf{r}_i) + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

reduction to valence electrons ↓



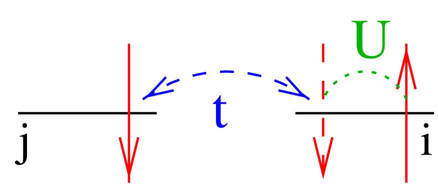
$$H = \sum_{i=1}^{N_v} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N_v} V^{\text{ion}}(\mathbf{r}_i) + \sum_{i=1}^{N_v-1} \sum_{j=i+1}^{N_v} V^{ee}(\mathbf{r}_i, \mathbf{r}_j)$$

occupation number formalism ↓ Wannier orbitals

$$\hat{H} = \sum_{i\nu j\sigma} t_{ij}^{\nu}\, \hat{c}^{\dagger}_{i\nu\sigma}\, \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}_{ijmn}^{\nu\nu'\mu\mu'}\, \hat{c}^{\dagger}_{i\nu\sigma}\, \hat{c}^{\dagger}_{j\nu'\sigma'}\, \hat{c}_{n\mu'\sigma'}\, \hat{c}_{m\mu\sigma}$$

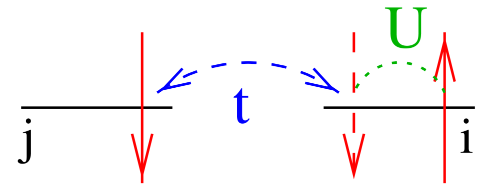
Hubbard model

$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Approaches for Hubbard-type models

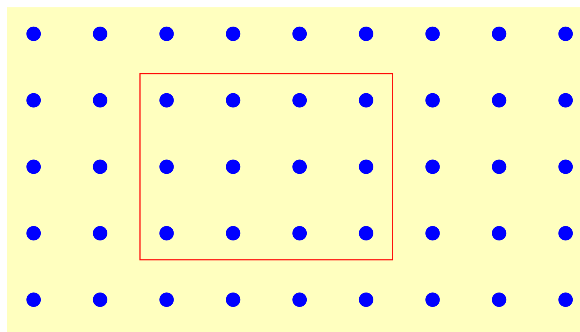
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



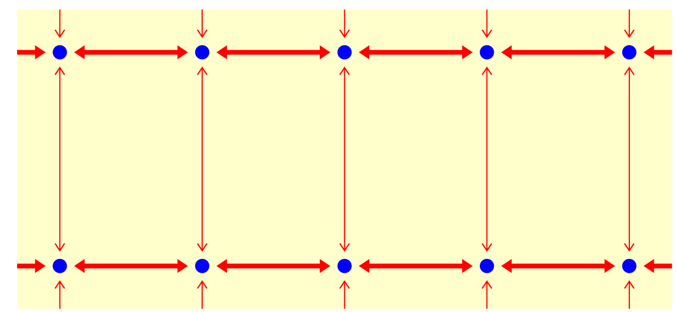
Perturbation theory

- $U \to 0$: Hartree-Fock
  2$^{\text{nd}}$ order PT, . . .
- $t/U \to 0$ (for $n = 1$)
  $\rightsquigarrow$ Heisenberg model

finite clusters: ED, QMC



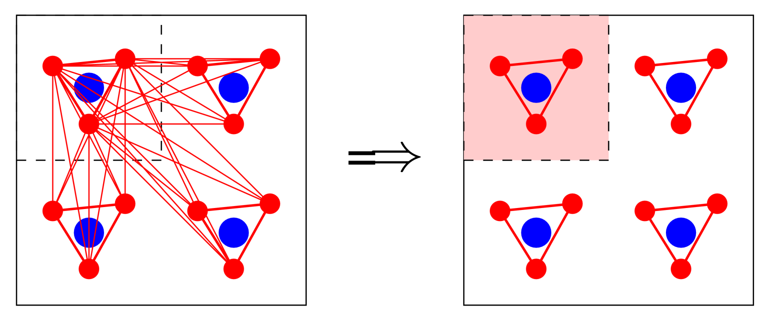
$d \to 1$: Bethe ansatz, DMRG



Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

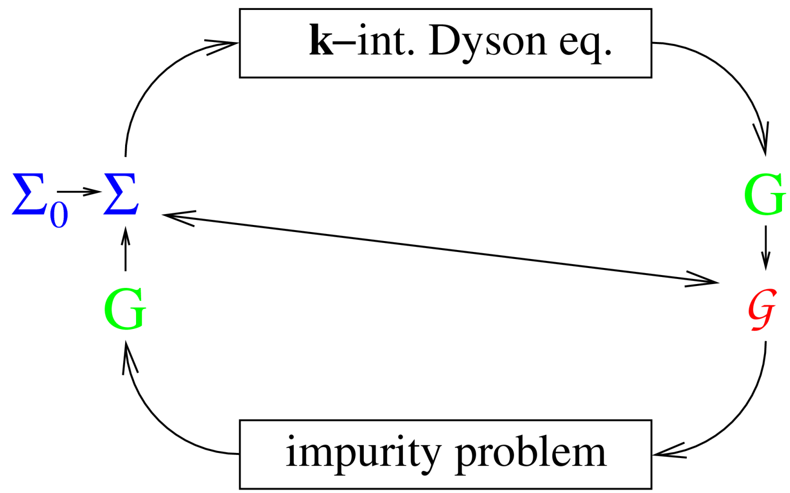
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

+	non-perturbative $\rightsquigarrow$ valid at MIT
+	dynamical on-site correlations preserved
+	in thermodynamic limit
+/−	exact for coordination $Z \to \infty$



Iterative solution of DMFT equations

0. Initialize self-energy
1. Solve Dyson equation
2. Solve single impurity Anderson model (SIAM)

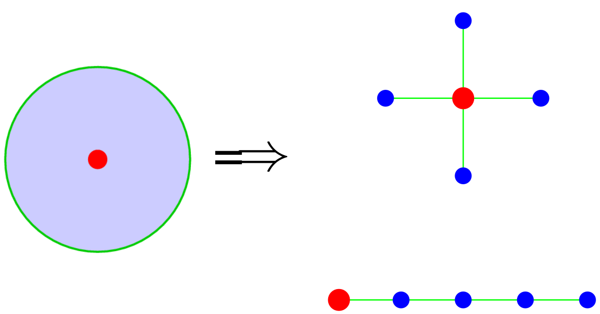


$\longleftarrow$ DOS / t_{ij} / $\epsilon_{\nu \boldsymbol{k}}$

$\longleftarrow$ local interactions

Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
- Quantum Monte-Carlo (QMC)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED



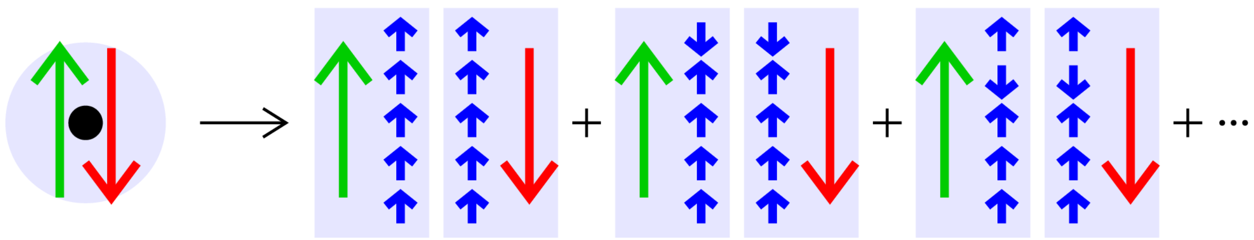
Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

Green-Funktion G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

$$G_\sigma(\tau_2 - \tau_1) \equiv G_\sigma(\tau_1, \tau_2) = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\; \psi_\sigma(\tau_1)\psi^*_\sigma(\tau_2)\; e^{\mathcal{A}},$$

$$\mathcal{A} = \mathcal{A}_0 - \frac{U}{2} \sum_{\sigma\sigma'} \int_0^\beta d\tau\, \psi^*_\sigma(\tau)\psi_\sigma(\tau)\psi^*_{\sigma'}(\tau)\psi_{\sigma'}(\tau)$$

Discretization $\beta = \Lambda\,\Delta\tau$, Trotter decoupling, Hubbard-Stratonovich transformation



Wick theorem:

$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

Metropolis MC importance sampling over auxiliary Ising field, (2^Λ configurations)

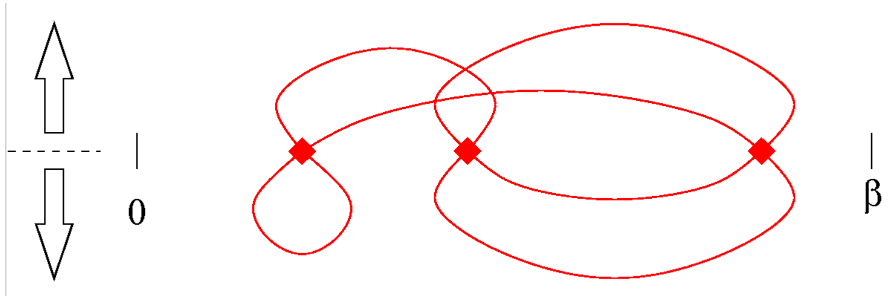
+ numerically exact, − effort scales as T^{-3}, − no info for $\omega \gtrsim \omega_{\text{Nyquist}}$

Recent generalizations: projective QMC (PQMC) [Feldbacher, Held, Assaad (2004)]

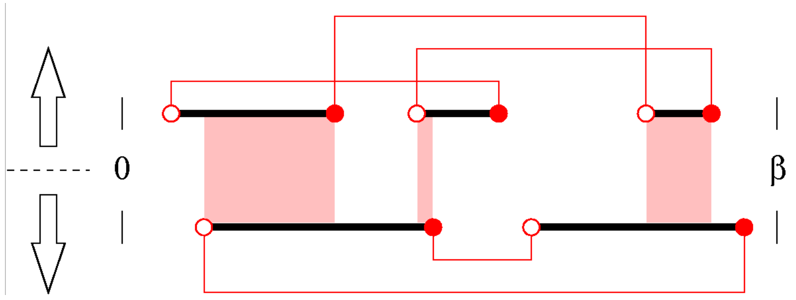
treating Hund rule spin-flip terms without sign problem

New development: continuous-time QMC algorithms

1. weak-coupling expansion
[Rubtsov, Savkin, Lichtenstein, PRB (2005)]



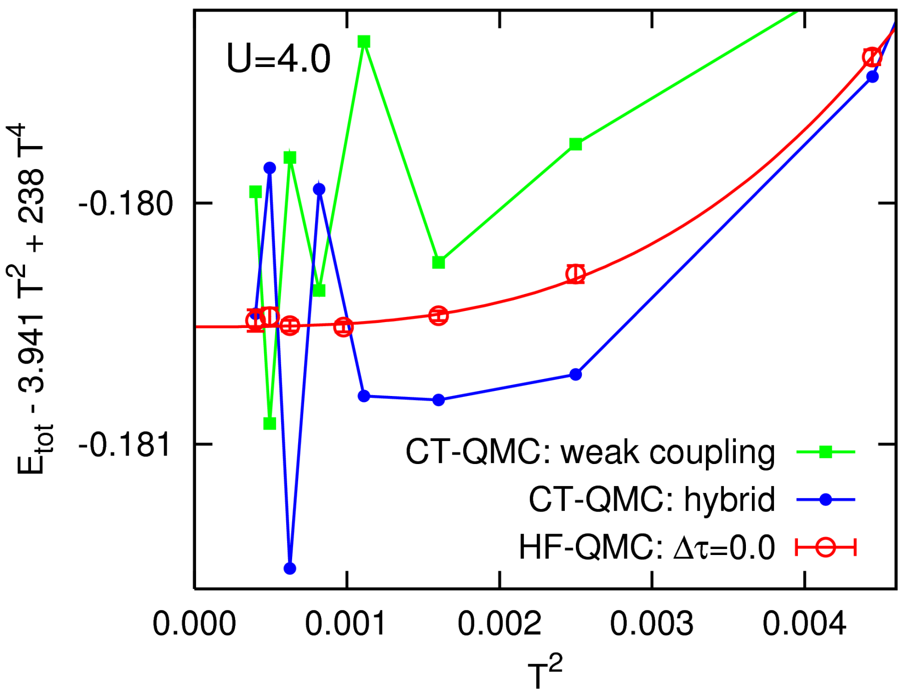
2. hybridization expansion
[Werner et al., PRL (2006)]



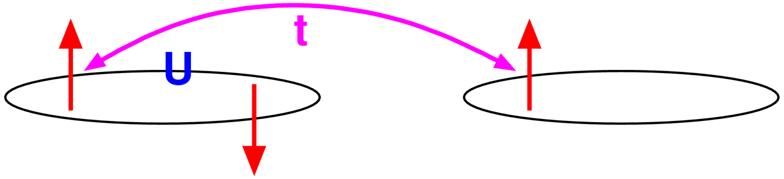
CT-QMC methods: smaller matrices

Claim [Troyer (2006)]: CT-QMC methods are orders of magnitude more efficient than HF-QMC [Gull et al., cond-mat/0609438]

But: high-precision HF-QMC DMFT solver [Knecht, Blümer, van Dongen (2005)] is competitive, at least after extrapolation $\Delta\tau \to 0$ [Blümer, in preparation]

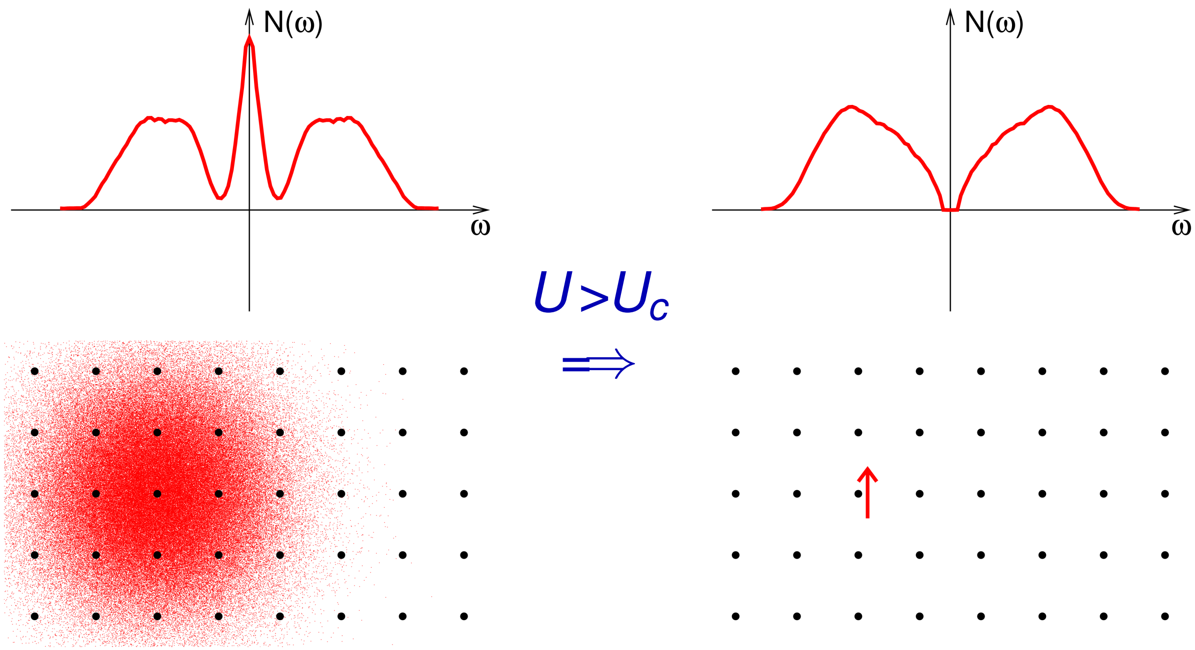


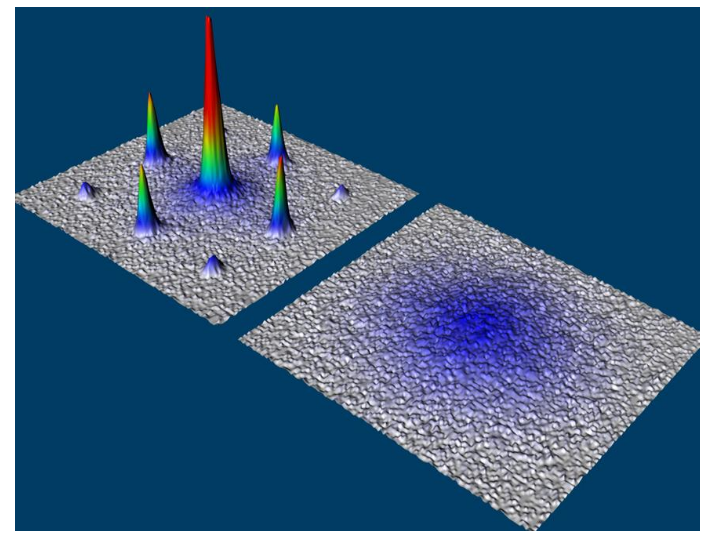
Orbital-selective Mott transitions



Well-known: Mott transition in frustrated 1-band Hubbard model

localization by interactions

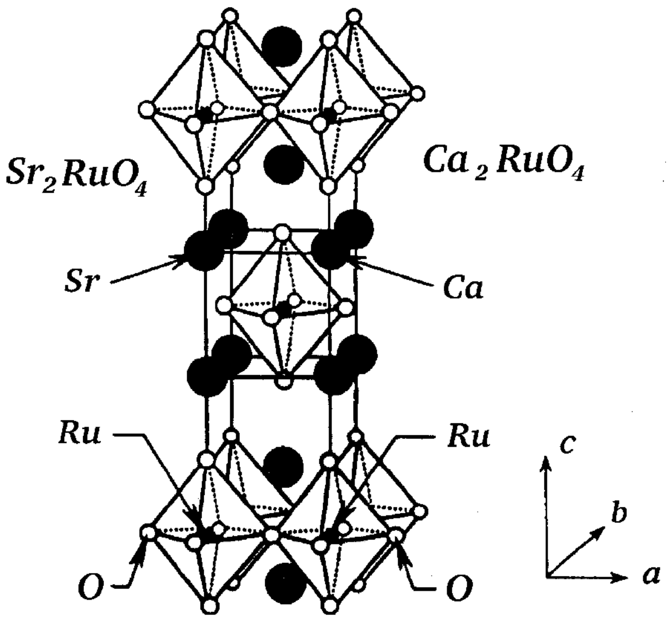




Localization (= decoherence) of ultracold bosons on optical lattice (Bloch group, 2002)

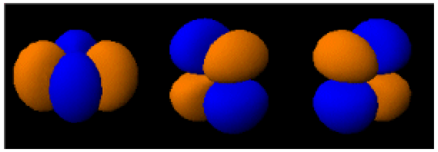
Case of multiple inequivalent orbitals/flavors?

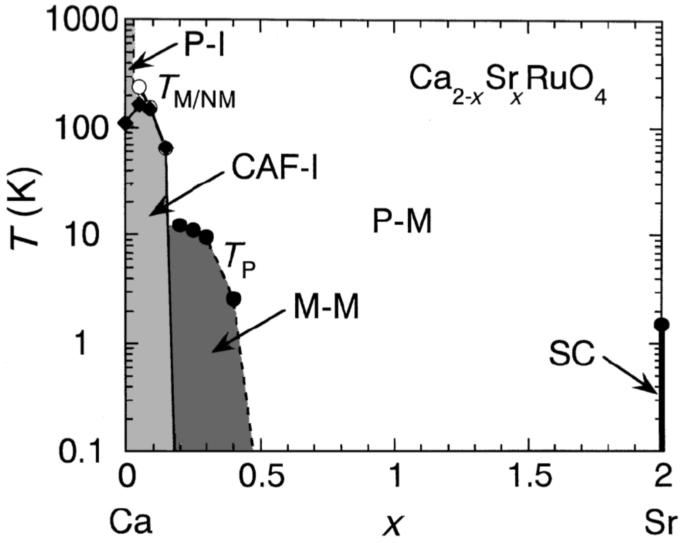
OSMTs in $Ca_{2-x}Sr_xRuO_4$



isostructural to $La_{2-x}Sr_xCuO_4$

4 valence electrons in 3 Ru t_{2g} orbitals





[Nakatsuji, Maeno, PRL (2000)]

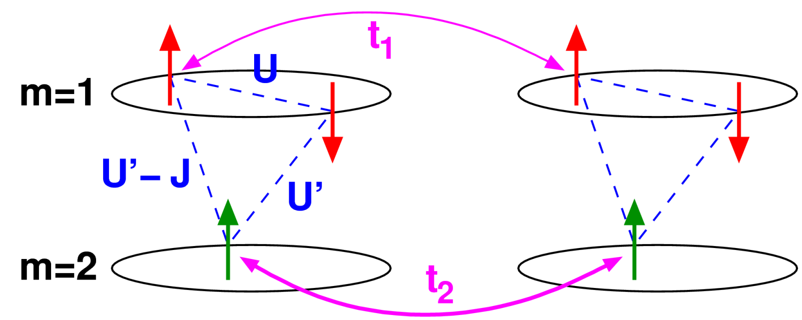
susceptibility, MR $\rightsquigarrow$ $S = 1/2$ system (+ easy axis) for $0.2 < x \lesssim 0.5$ (not $S = 1$)

orbital-selective Mott metal-insulator transitions for $x \approx 0.5$, $x \approx 0.2$?

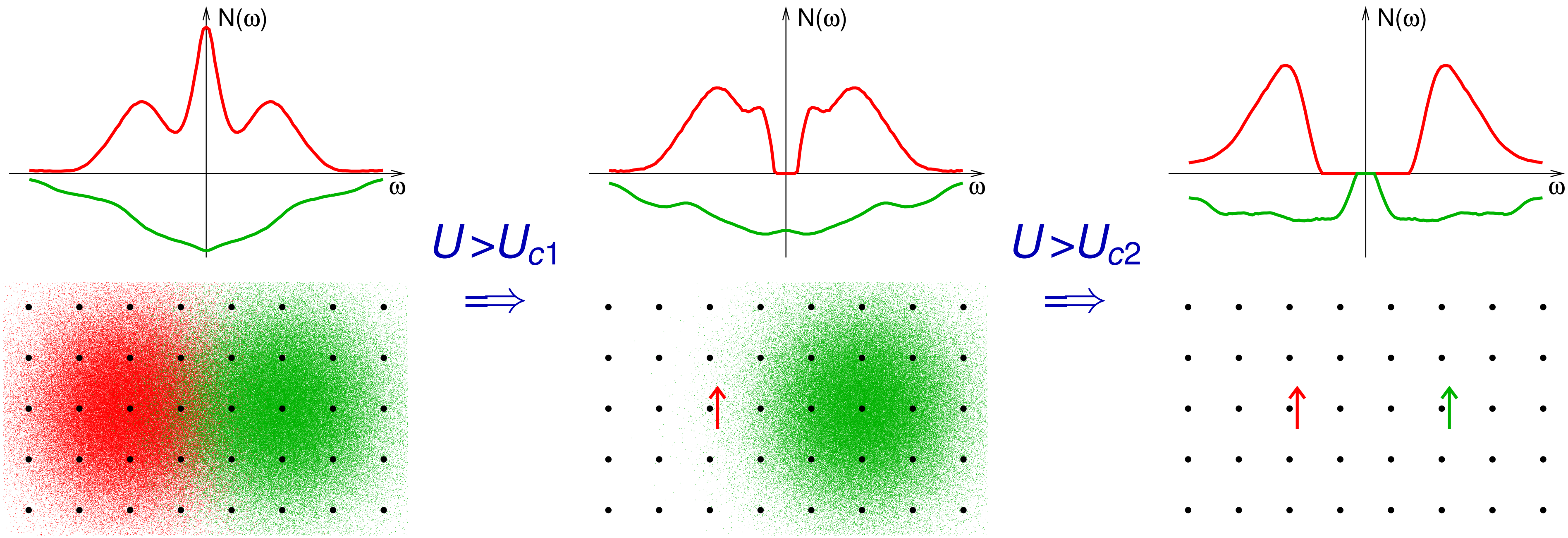
2-band model with orbital-dependent hopping

$$H = \sum_{m=1}^{2} \Big[- \sum_{\langle ij \rangle \sigma} t_m c^{\dagger}_{im\sigma} c_{jm\sigma} + U \sum_i n_{im\uparrow} n_{im\downarrow} \Big]$$

$$+ \sum_{i\sigma\sigma'} (U' - \delta_{\sigma\sigma'} J_z)\, n_{i1\sigma}\, n_{i2\sigma'}$$



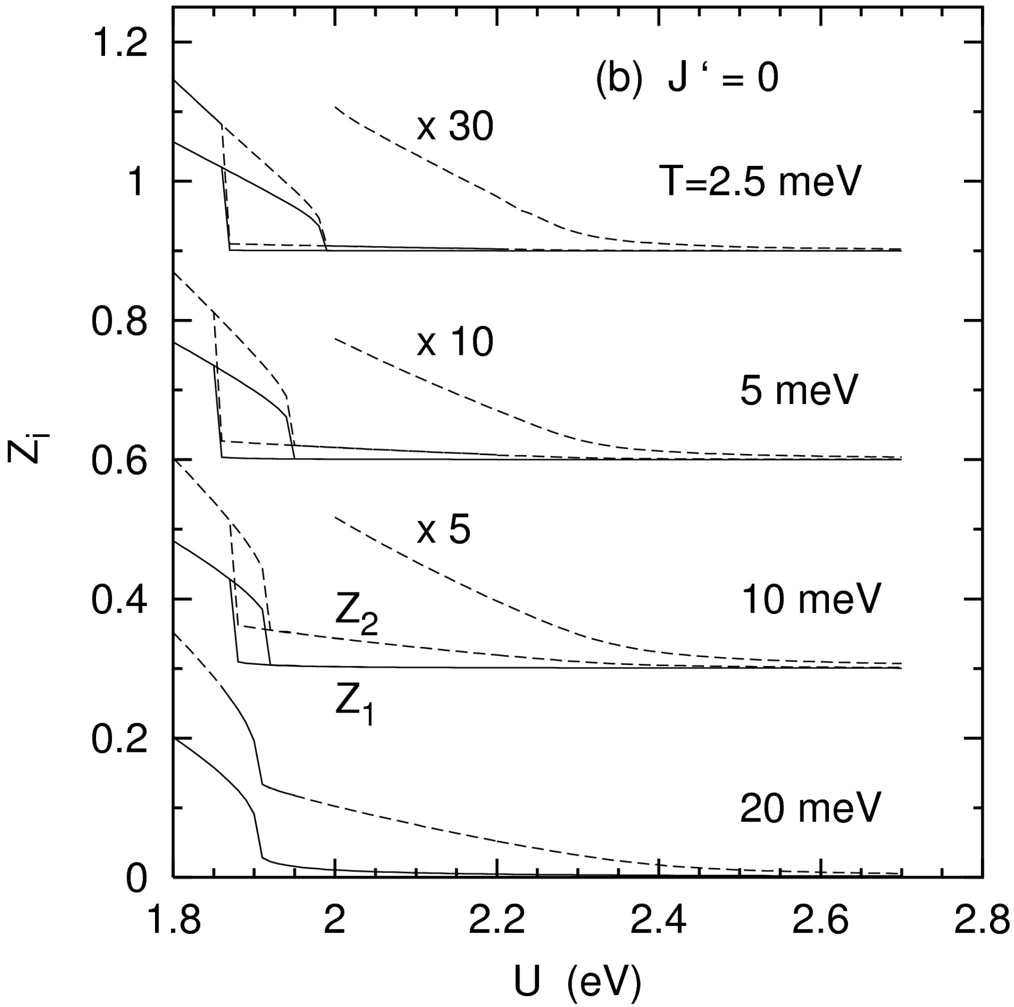
Ising-type Hund couplings with $t_2/t_1 = 2$ and $U' = U/2$, $J_z = U/4$ [Liebsch, PRB (2004)]



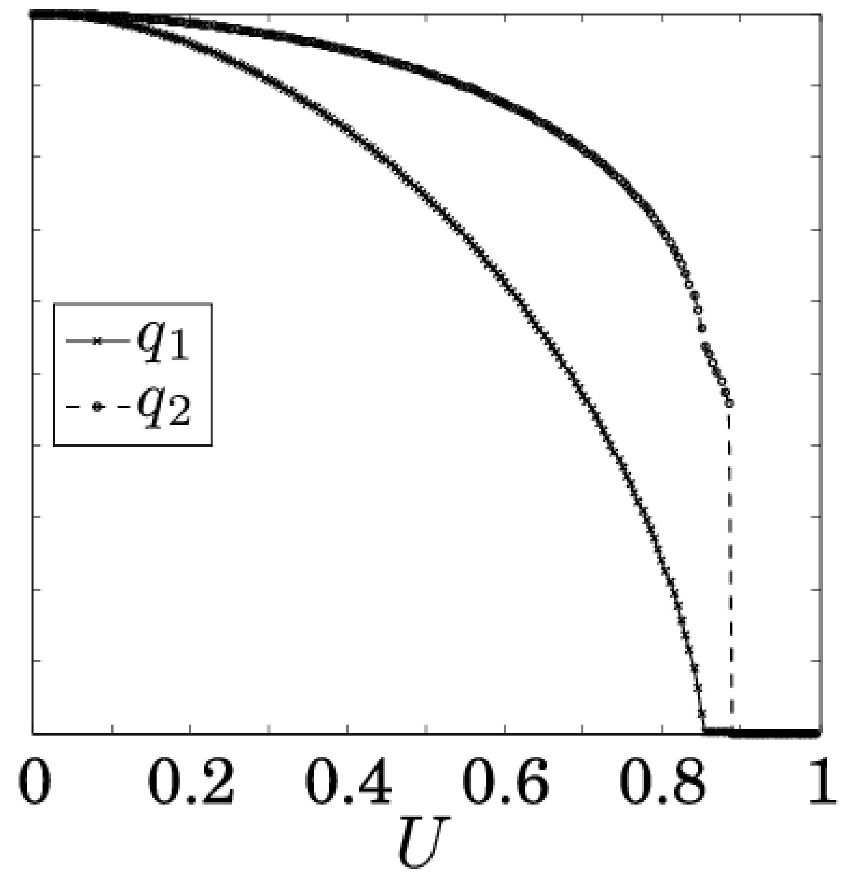
2 phase transitions [Knecht et al. (PRB 2005), de' Medici et al. (PRB 2005), Rüegg et al. (EPJB 2005)]

Character of wide-band transition?

Order of wide-band transition in anisotropic model



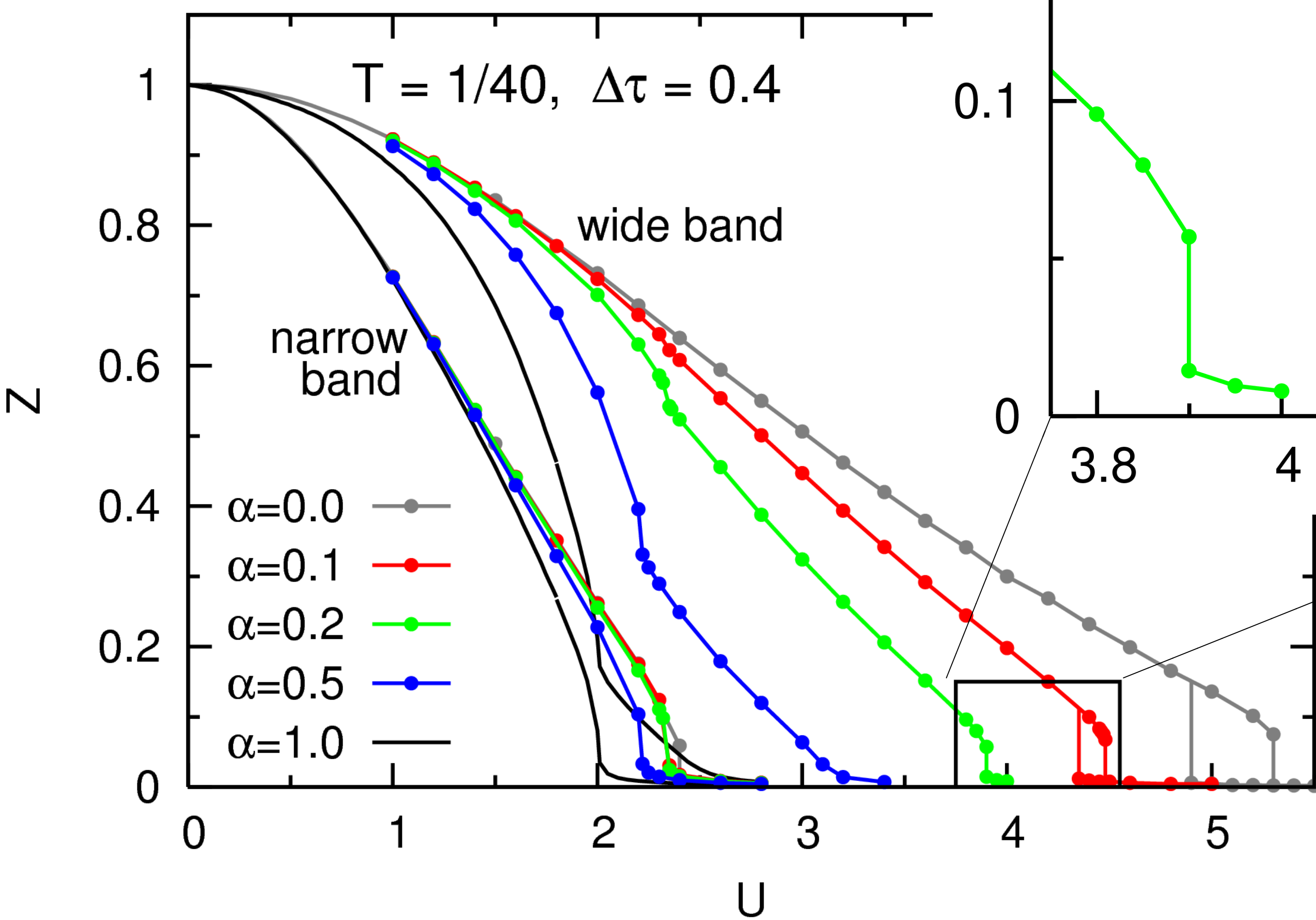
ED $\rightsquigarrow$ no hysteresis at low T for wide-band transition [Liebsch, PRL (2005)]

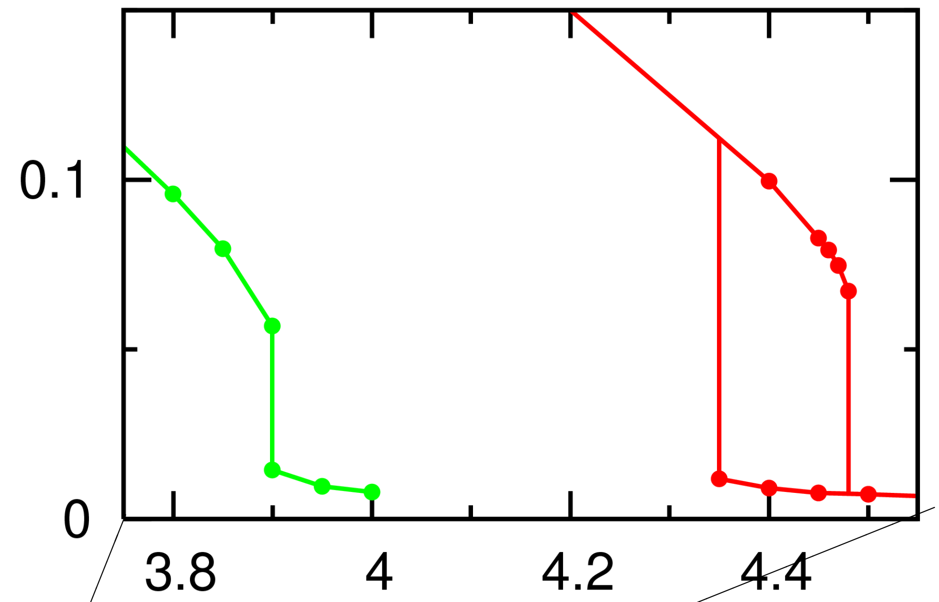


Slave-boson MF $\rightsquigarrow$ 1st order wide-band transition (at $T = 0$) [Rüegg, Indergand, Pilgram, Sigrist, EPJB (2005)]

Systematic study: effect of inter-orbital coupling

$$H = \sum_{m=1}^{2} \Big[-\sum_{\langle ij \rangle \sigma} t_m c^{\dagger}_{im\sigma} c_{jm\sigma} + U \sum_{i} n_{im\uparrow} n_{im\downarrow} \Big] + \alpha \sum_{i\sigma\sigma'} (U/2 - \delta_{\sigma\sigma'} U/4)\, n_{i1\sigma}\, n_{i2\sigma'}$$



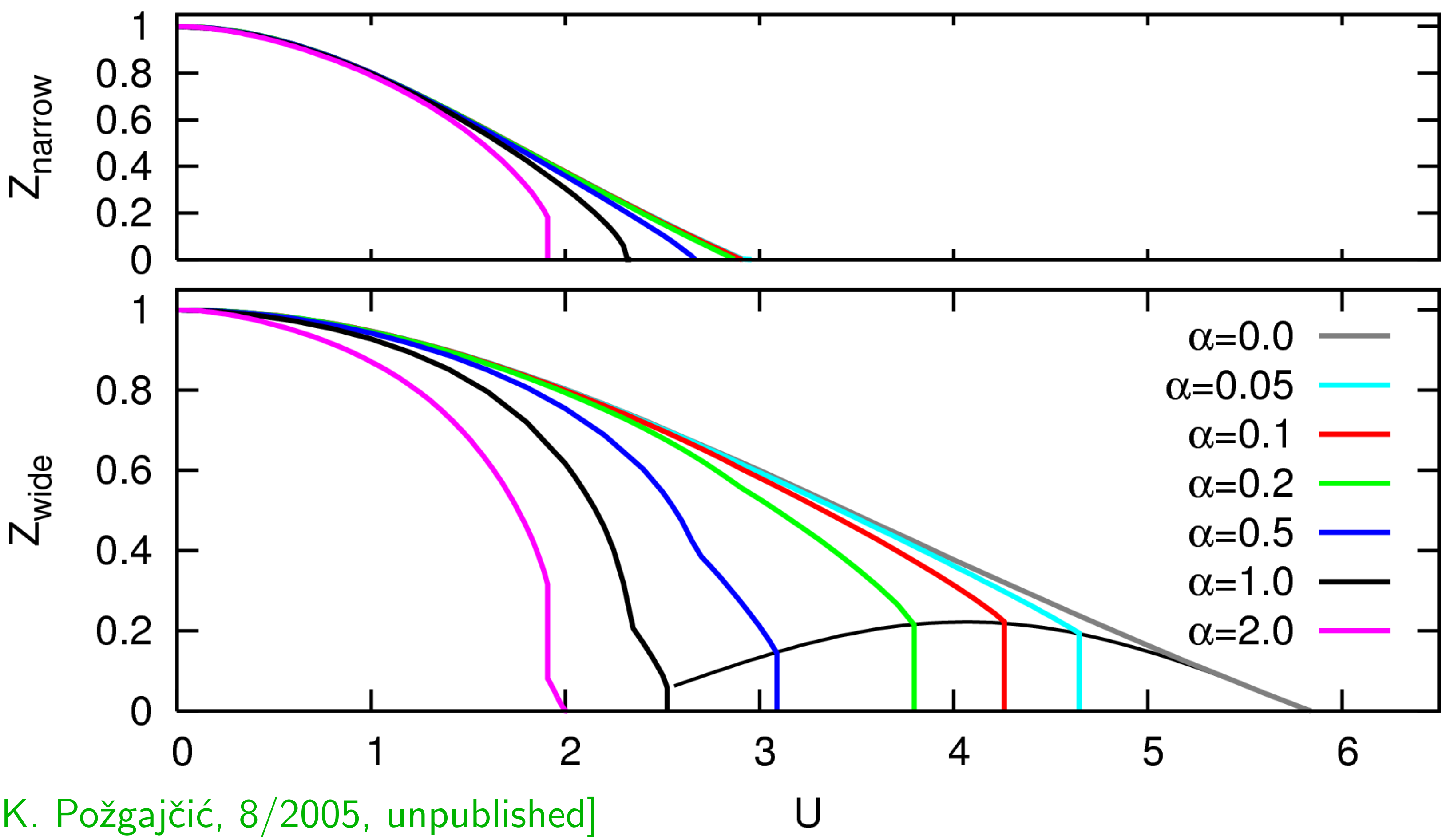


QMC at $T = 1/40$:

wide-band OSMT remains 1st order for small α

1st order at T=0?

Self-energy functional theory (SFT+ED) with 1 bath site per orbital



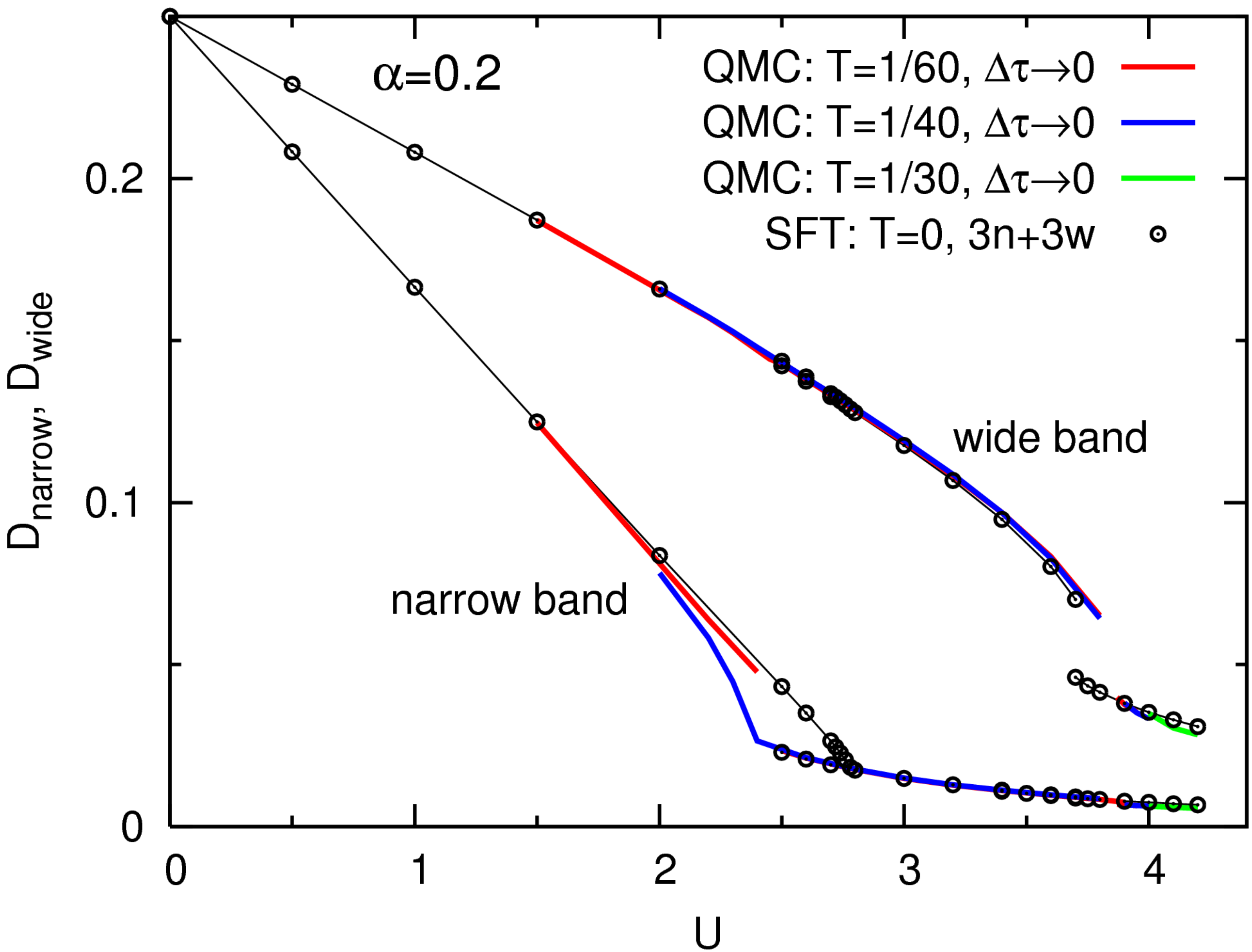
[K. Požgajčić, 8/2005, unpublished]

∘ 1st order wide-band transition for $0 < \alpha \lesssim 1.5$ ∘ larger α: 2nd order ↔ 1st order

Problems: ∘ Low-frequency part of $\Sigma(\omega)$ inconsistent with QMC

∘ Z ill-defined in OSM phase ∘ strong finite-size effects

Double occupancy (1st order derivative of Ω)



Excellent agreement between SFT and QMC

1st order at $T = 0$ (at least) for $0 < \alpha \leq 0.2$

Summary

Cooperative phenomena in correlated electron systems

Theoretical approaches: (multi-band) Hubbard models, DMFT

Numerical solution: Hirsch-Fye QMC, SFT+ED

Application: orbital-selective Mott transitions

Not covered: High-frequency corrections in HF-QMC DMFT solver
Critical exponents from QMC and strong-coupling PT
Theory of half-metallic double perovskites
Realistic material-specific calculations with LDA+DMFT

Outlook

Band structure calculations for correlated systems

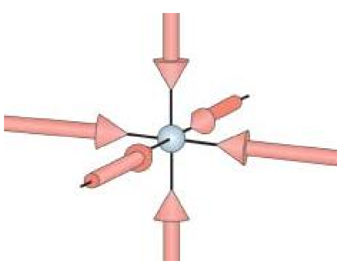
Cluster extensions of DMFT

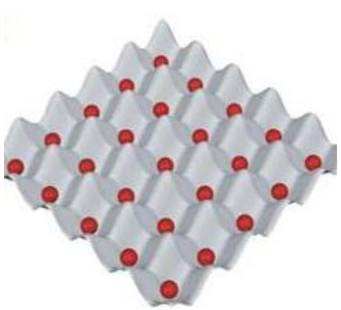
Ultracold quantum gases on optical lattices . . .

Starting in 7/2007: SFB/TRR 49 (Frankfurt - Kaiserslautern - Mainz)
Condensed matter systems with variable many-body interactions

A1 [Bloch] – Ultracold Fermi mixtures in optical lattices
A2 [Kuhr/Bloch] – Spatially addressable quantum gases in optical lattices
A3 [Hofstetter] – Inhomogeneous quantum phases in ultracold gases with strong correlations
A5 [Fleischhauer/Eggert] – Advanced numerical methods for correlated quantum gases
A6 [Blümer] – Flavour-selective Mott transitions of ultracold quantum gases on optical lattices
A7 [Hillebrands/Serha] – Collective effects and instabilities of a magnon gas
A8 [Kopietz] – Interacting magnons and critical behaviour of bosons

project area B: real materials



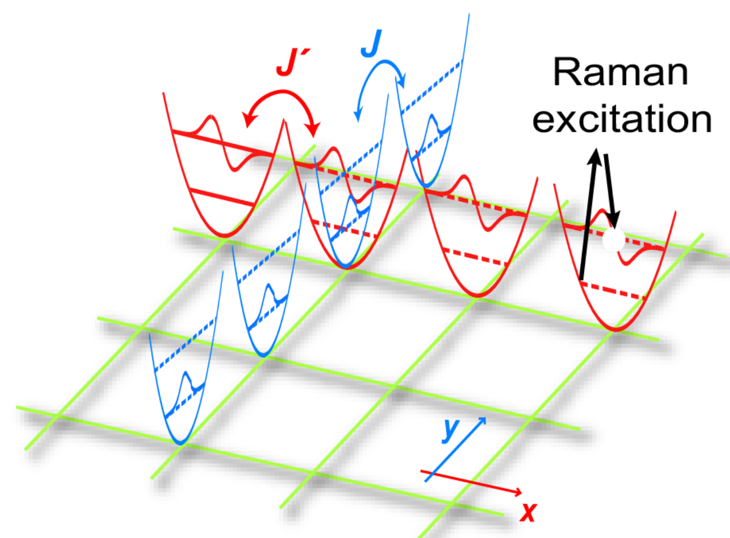


A1 + A6: flavor selectivity in Fermi mixtures of different

- atomic species: ^{6}Li and ^{40}K
- hyperfine states
- vibrational levels

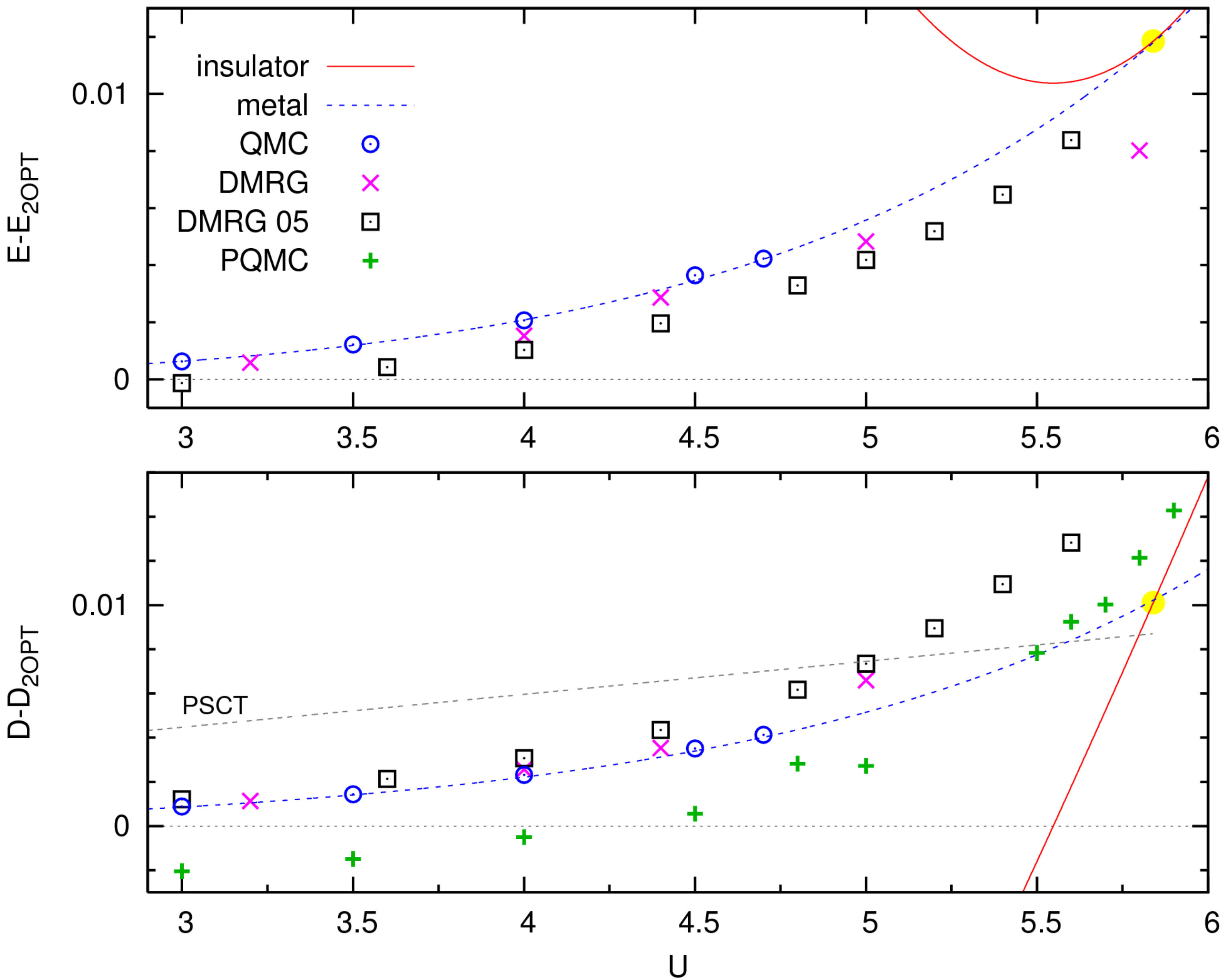
on optical lattices

Hopping amplitudes tunable and flavor-dependent!

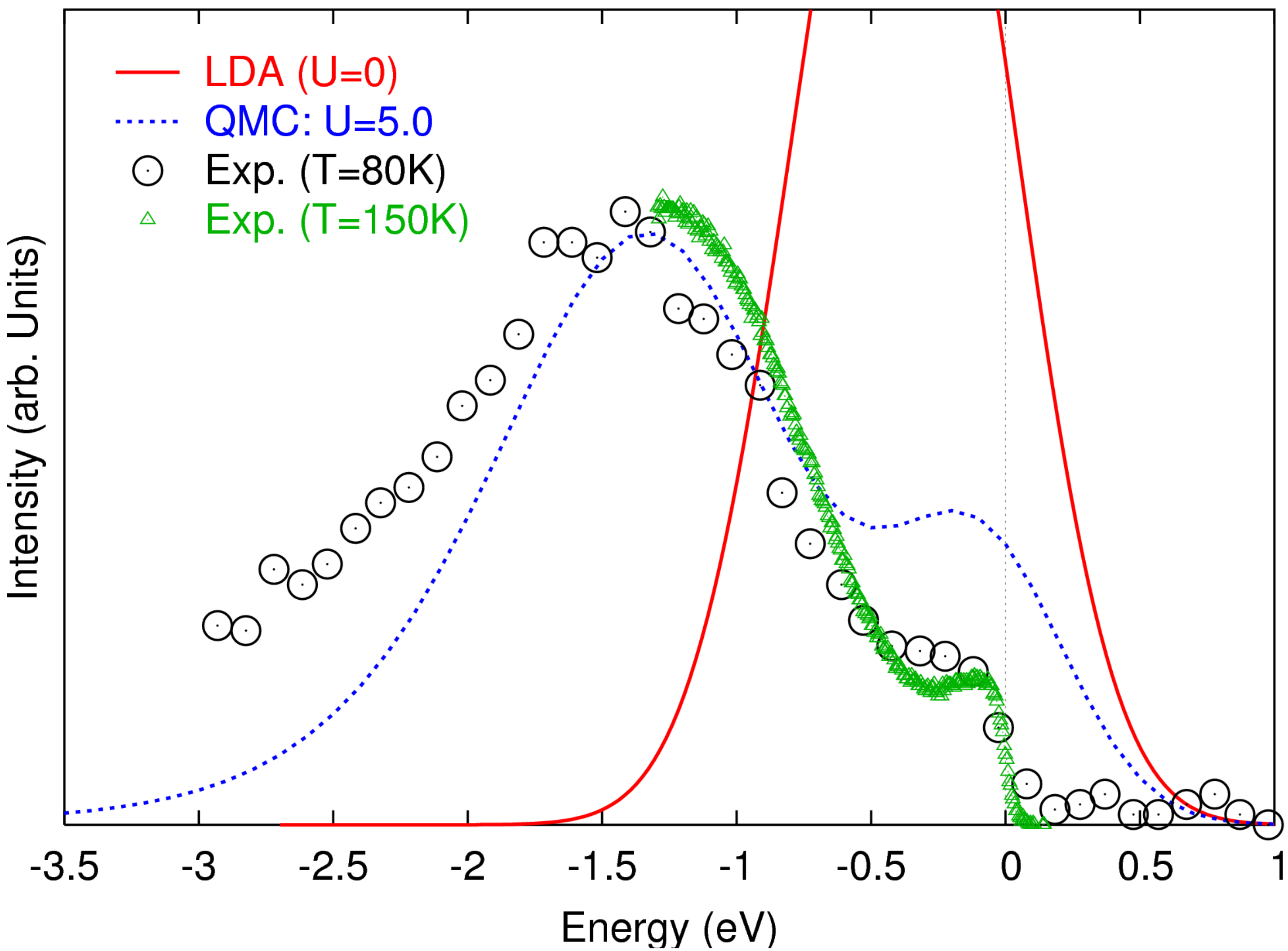


[Müller, Fölling, Widera, Bloch (2007)]

Precision: HF-QMC vs. ground state methods



System near Mott transition: $La_{1-x}Sr_xTiO_3$ – photoemission spectra



[Nekrasov, Held, NB, Poteryaev, Anisimov, Vollhardt (2000)]

LDA+DMFT(QMC): Reasonable accuracy, drastic improvement over LDA

Critical exponents from QMC and ePT

Ground state energy E of 1-band Mott insulator from

1. HF-QMC with $T \to 0$ extrapolation

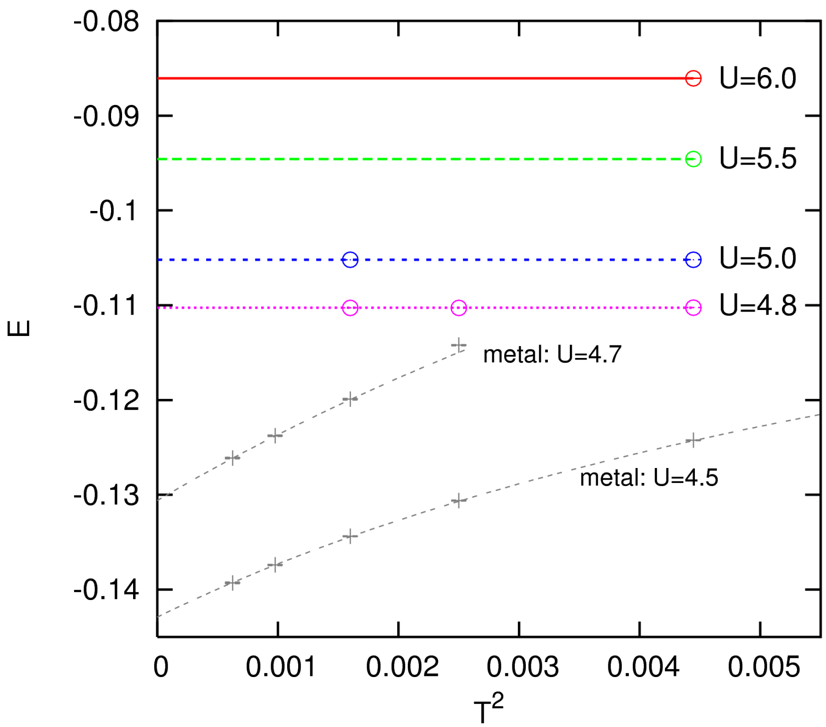
$\Sigma(\omega) = \frac{U^2}{4\omega} + \mathcal{O}(\omega^{-2})$

40×10^7 sweeps

careful $\Delta\tau$ extrapolation

$\Bigg\} \; \Delta E \approx 10^{-5}$

minimal T-dependence for Mott insulator



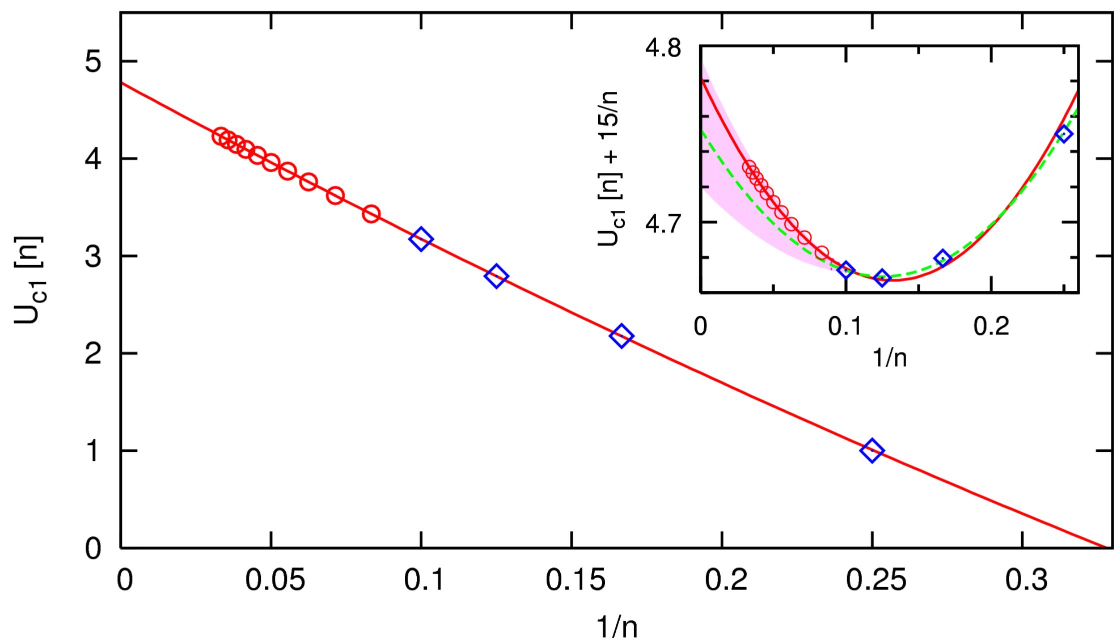
2. $T = 0$ Kato-Takahashi perturbation theory

$$E_{\mathrm{PT}}(U) = -\frac{1}{2\,U} - \frac{1}{2\,U^3} - \frac{19}{8\,U^5} - \frac{593}{32\,U^7} - \frac{23877}{128\,U^9} + \mathcal{O}(U^{-11})$$

coefficient ratios: 1 4.8 7.8 10.1

10^{th}order PT accurate (only) at $U \gtrsim 6$: $\Delta E_{\mathrm{PT}} \leq 10^{-5}$

Extended perturbation theory: ePT



Extrapolate coefficients

in PT series $E_{\text{PT}} = \sum_{i=1}^{\infty} a_{2i}\, U^{1-2i}$

by fitting ratios

$U_{c1}[2i] \equiv \sqrt{a_{2i+2}/a_{2i}}$ to

$$U_{c1}[n] \approx U_{c1} + u_1\, n^{-1} + u_2\, n^{-2}$$

General consequences:

$$U_{c1} = \lim_{i\to\infty} U_{c1}[2i]$$

$$a_n \propto n^{\tau}\, U_{c1}^{n}; \quad \tau = -\frac{u_1}{U_{c1}}$$

$$E(U) \propto (U - U_{c1})^{\tau-1}$$

$$D(U) \propto (U - U_{c1})^{\tau-2}$$

Specifics / numerical results of extrapolation:

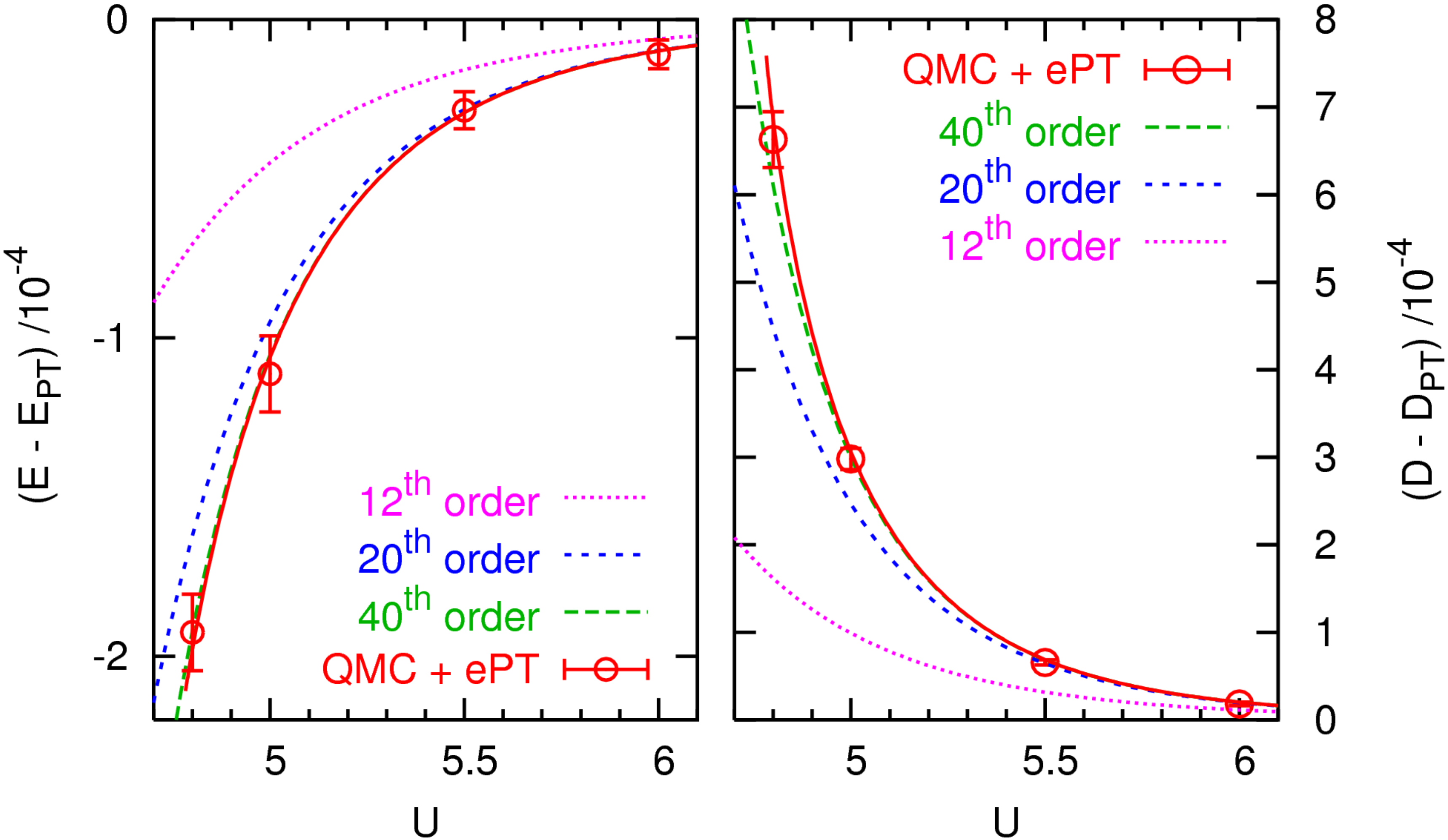
Unrestricted quadratic fit $\rightsquigarrow \tau \approx 3.44,\ U_{c1} \approx 4.75$

Comparisons with QMC $\rightsquigarrow 3.36 \le \tau \le 3.53$

Half-integer exponents likely for mean-field theories

Assume $\tau = 3.5 \rightsquigarrow U_{c1} = 4.782,\ E_{\text{ePT}}(U),\ D_{\text{ePT}}(U)$

Comparisons: energy E and double occupancy $D = dE/dU$



Excellent agreement ⇝ reliable exponents, fully parametrized benchmark results

[Blümer, Kalinowski, Phys. Rev. B **71**, 195102 (2005)]