Dynamical mean-field theory of strongly correlated electron systems

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Universität Mainz

Outline

Motivation

Introduction

Dynamical Mean-field Theory

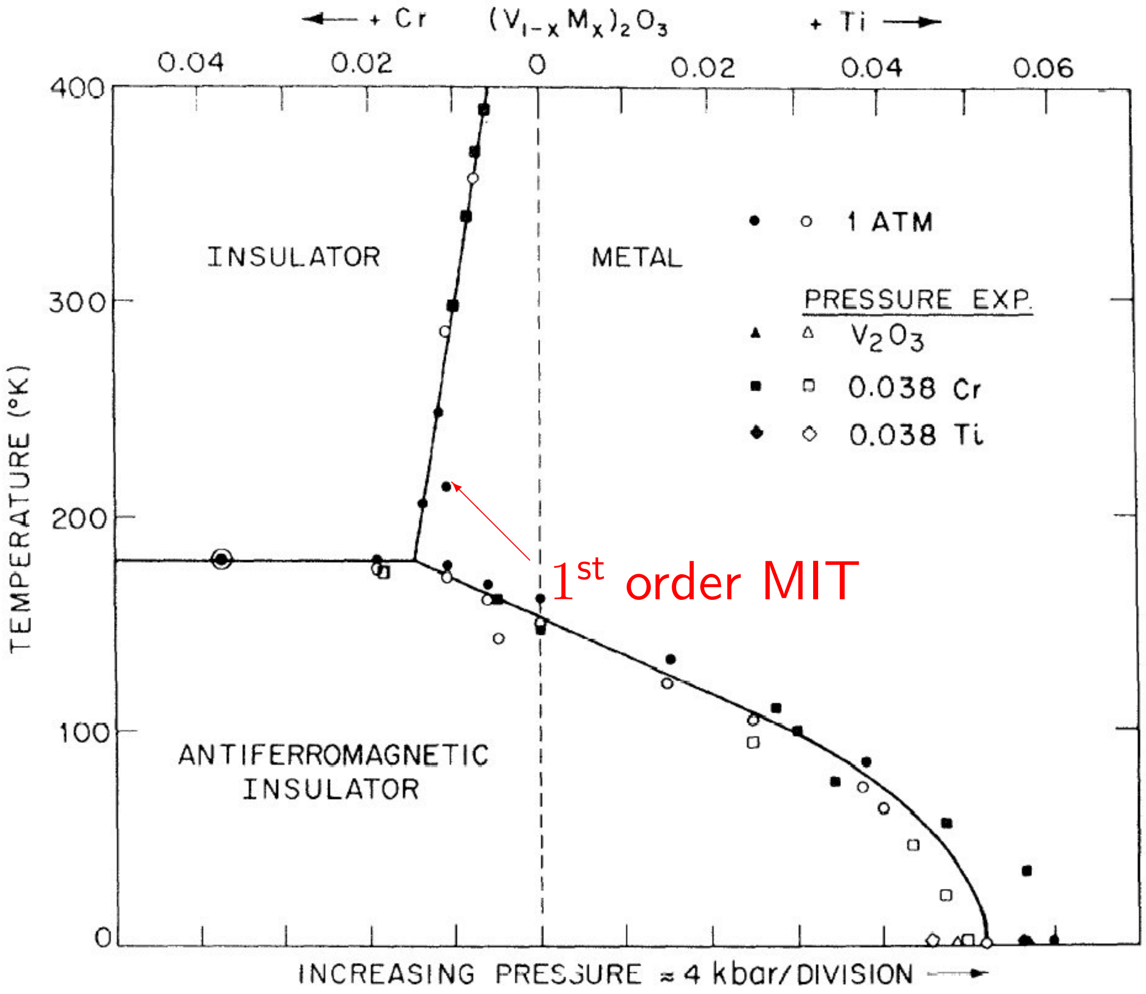
Mott Transition, Mott Insulator

LDA+DMFT(QMC) for $La_{1-x}Sr_xTiO_3$

Future Projects

Motivation

Metal-insulator transition (MIT) in V_2O_3



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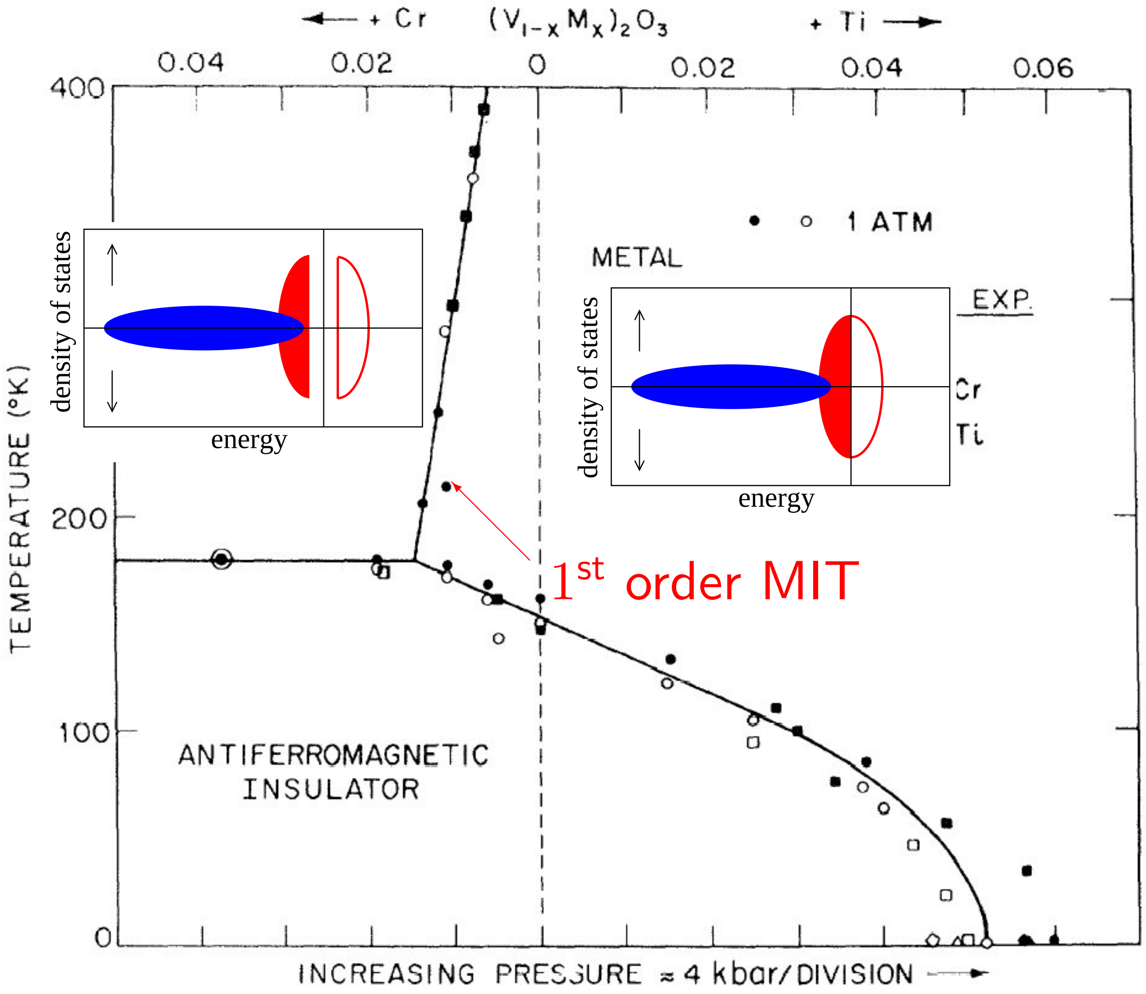

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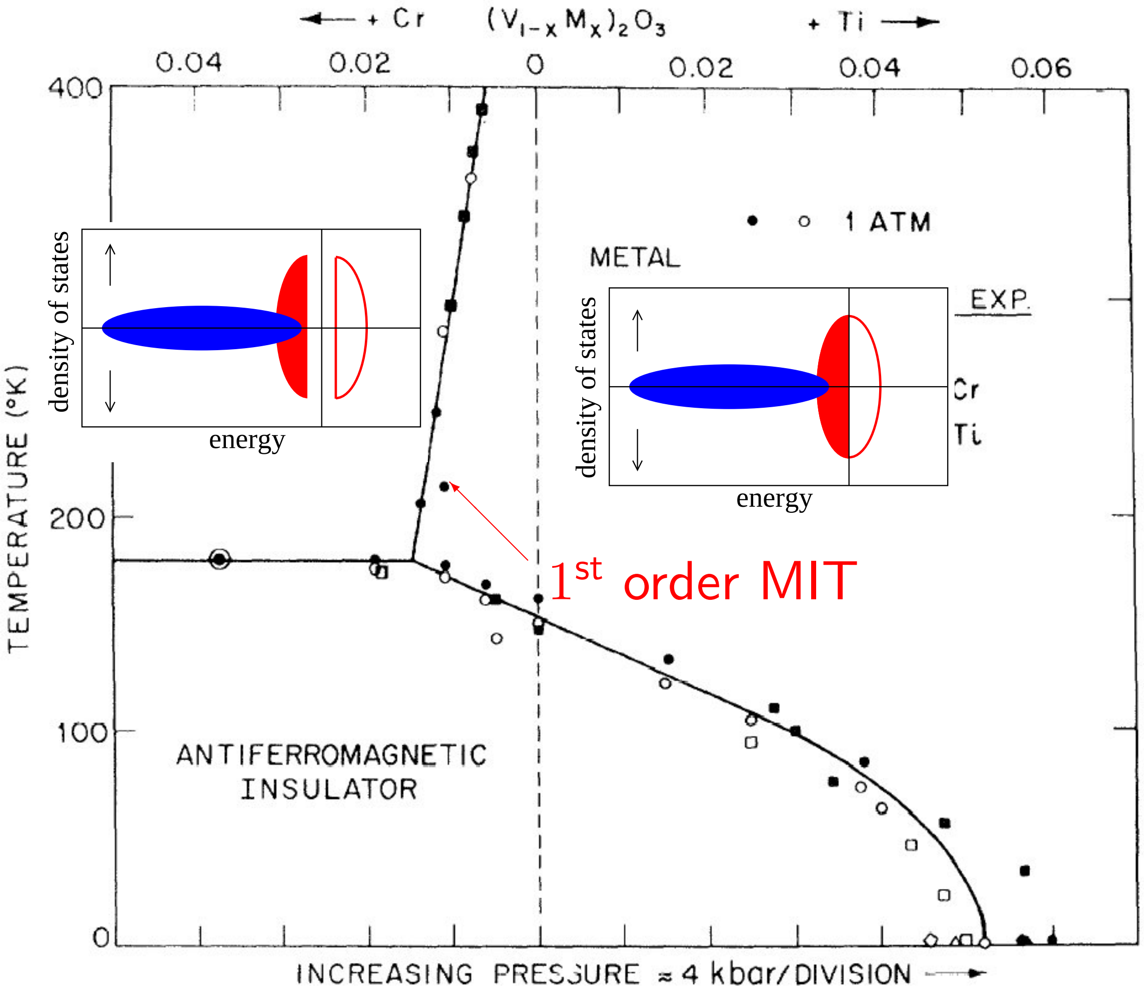

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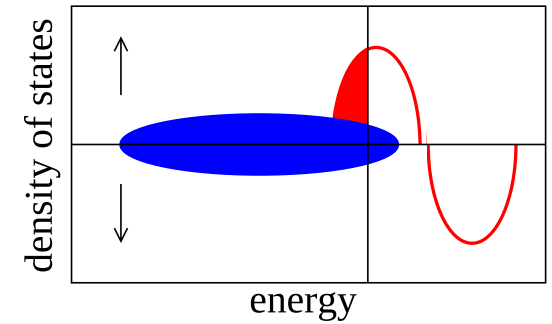
Itinerant ferromagnetism



High-T_c superconductivity

Introduction

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

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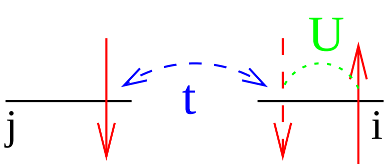

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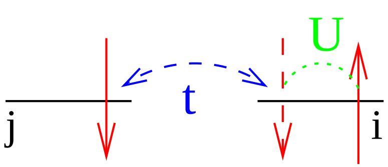

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← **density functional theory (DFT)**

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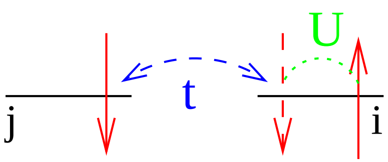

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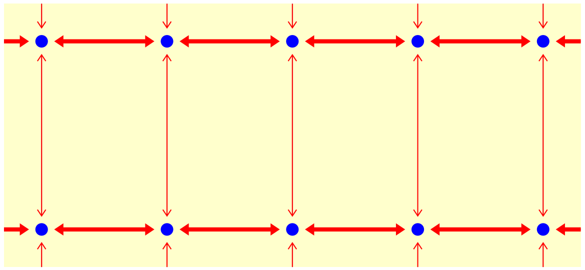
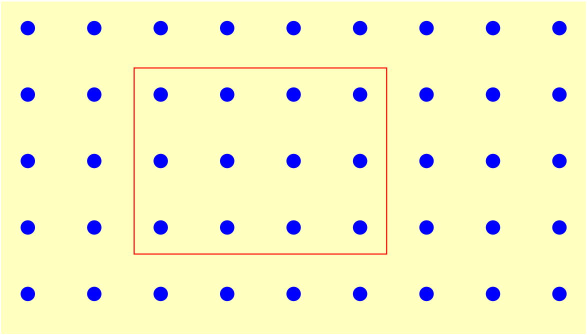
$d = 1$: Bethe ansatz, DMRG



Perturbation theory:

- $U \longrightarrow 0$: Hartree-Fock (uncorrelated)
- $t \longrightarrow 0$: half filling ($n = 1$) $\rightsquigarrow$ Heisenberg model
- $T \longrightarrow \infty$, $n \longrightarrow 0$
- ($V_{\text{ion}} \longrightarrow 0 \rightsquigarrow$ jellium model $\rightsquigarrow$ LDA)

finite clusters: ED, QMC



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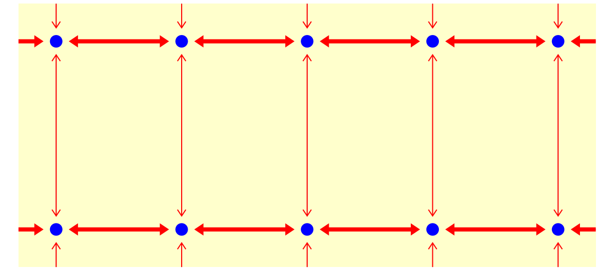

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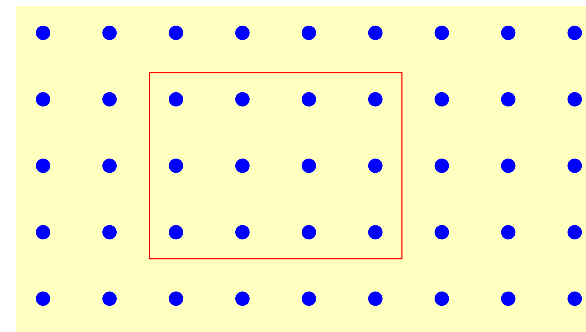

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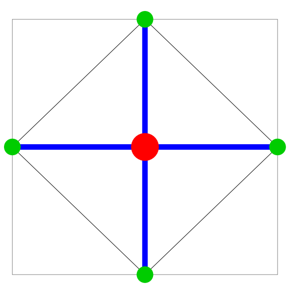
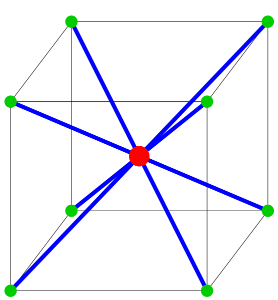
Dynamical mean-field theory (DMFT):

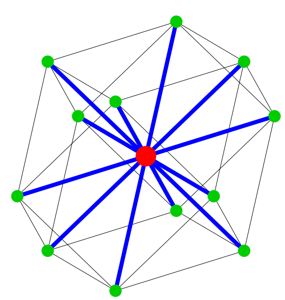
- exact for $Z \longrightarrow \infty$
- dynamical on-site correlations preserved
- non-perturbative ⇝ valid at MIT
- thermodynamic limit



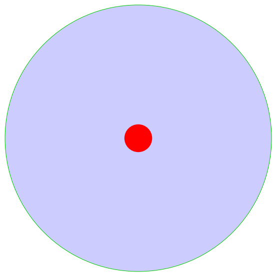
d=2: $Z = 4$



bcc: $Z = 8$



fcc: $Z = 12$



DMFT: $Z = \infty$

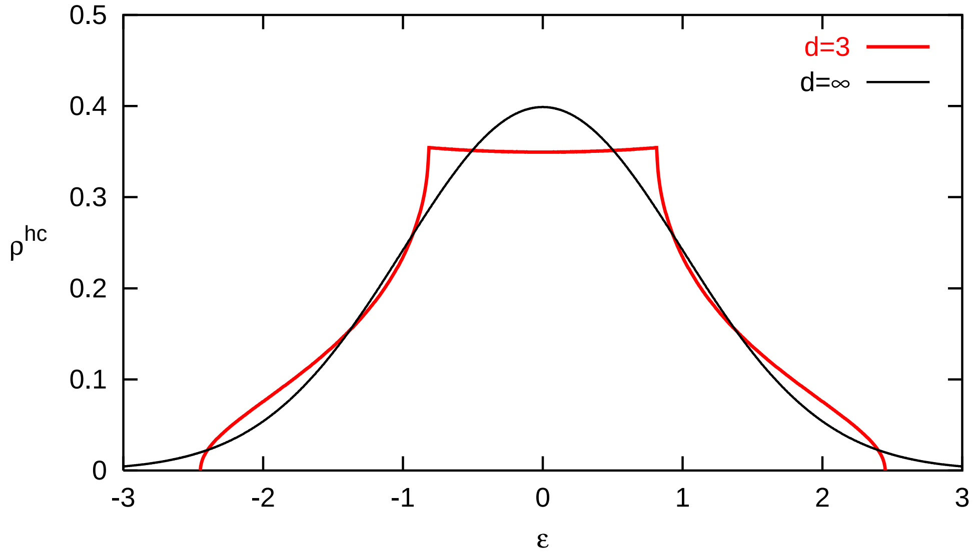
Dynamical mean-field theory

1989 Metzner/Vollhardt: $d \to \infty$ nontrivial for fermions if $t = t^*/\sqrt{2d}$

Gutzwiller approximation exact

Müller-Hartmann: local self-energy: $\Sigma(\boldsymbol{q}, \omega) \to \Sigma(\omega)$

Brandt/Mielsch: exact solution of Falicov-Kimball model for $d = \infty$



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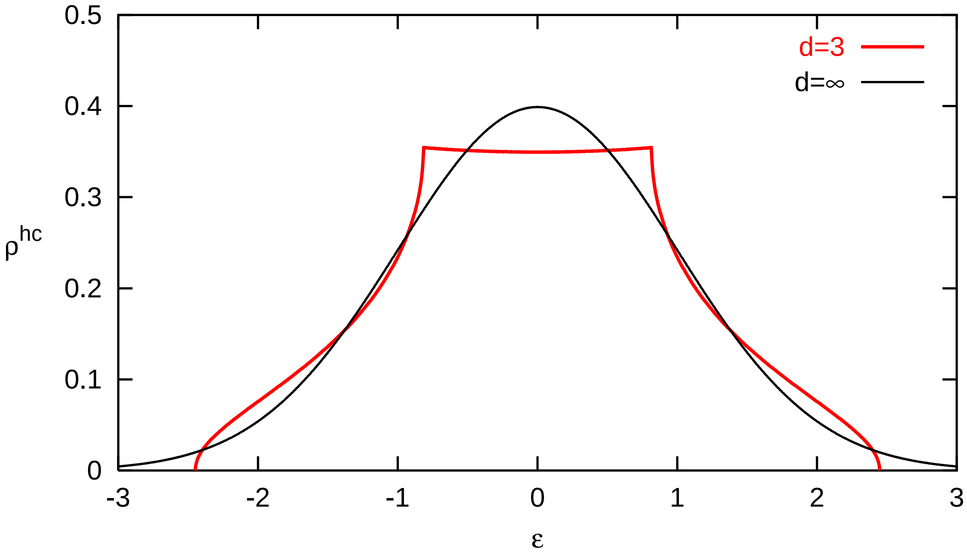

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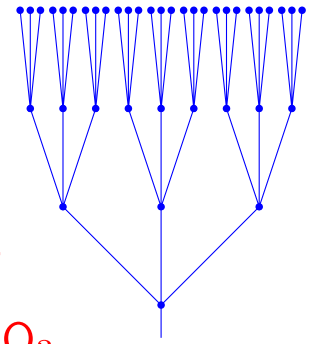

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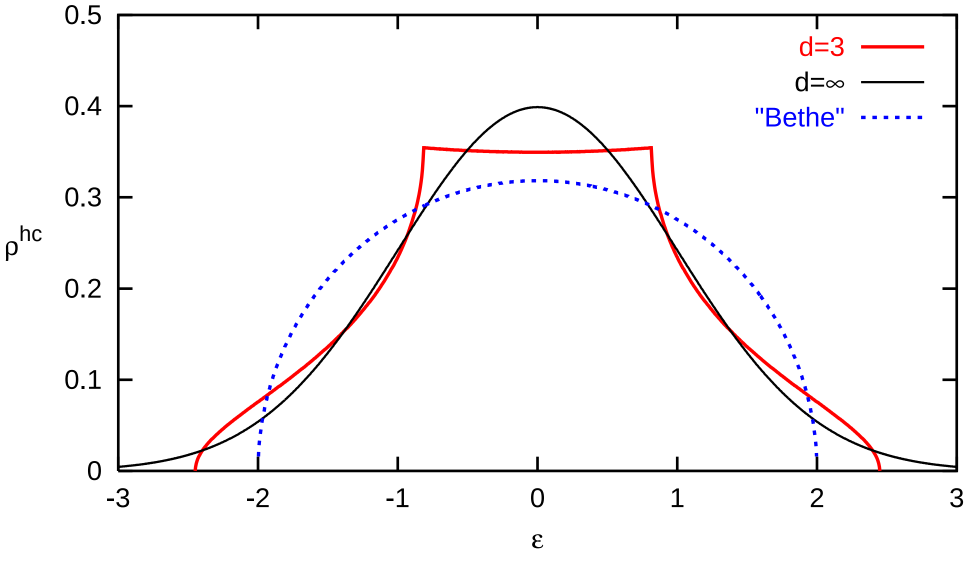

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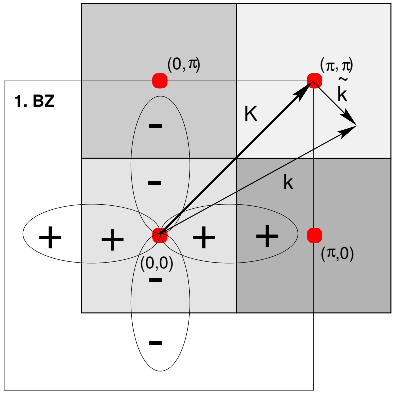

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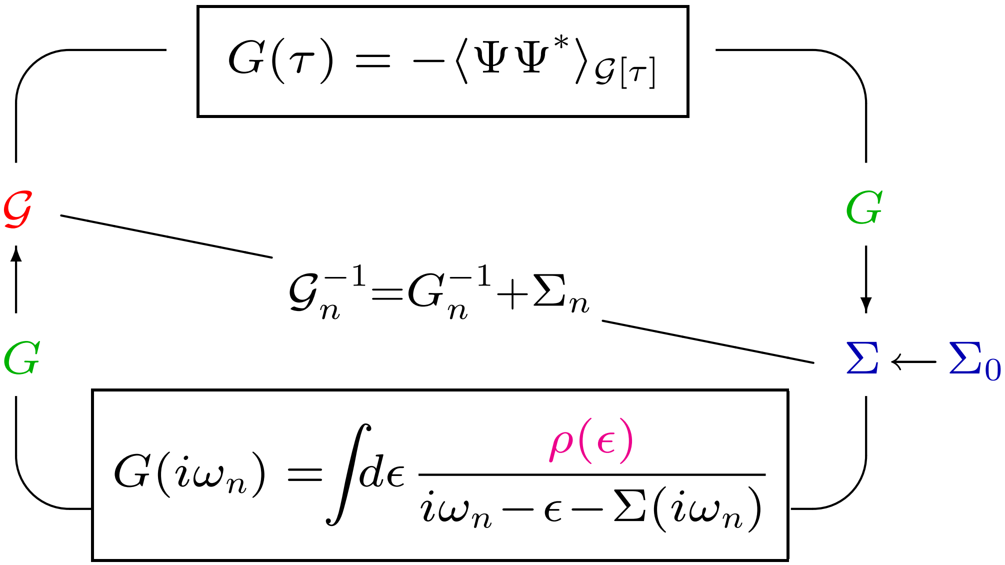
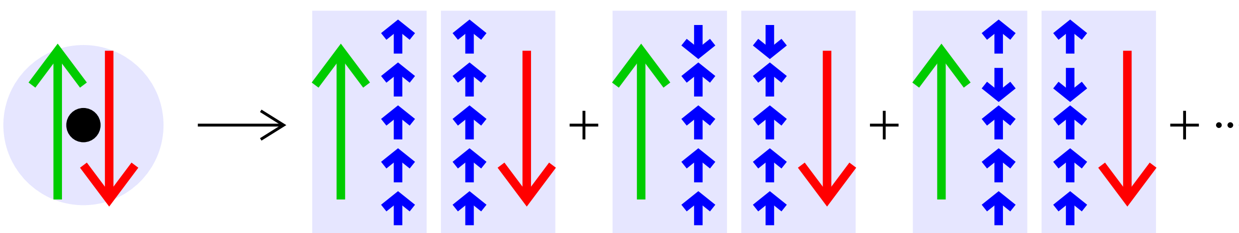
2004 **Physics Today** article; lecture notes; conferences "beyond LDA" etc.

Future: **complete understanding of abstract models (within DMFT)**
realistic calculations (LDA+DMFT)
cluster methods (DCA, CDMFT)

Iterative solution of DMFT equations



QMC algorithm: discretization $\beta = \Lambda \, \Delta\tau$, discrete 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, $50 \lesssim \Lambda \lesssim 400$

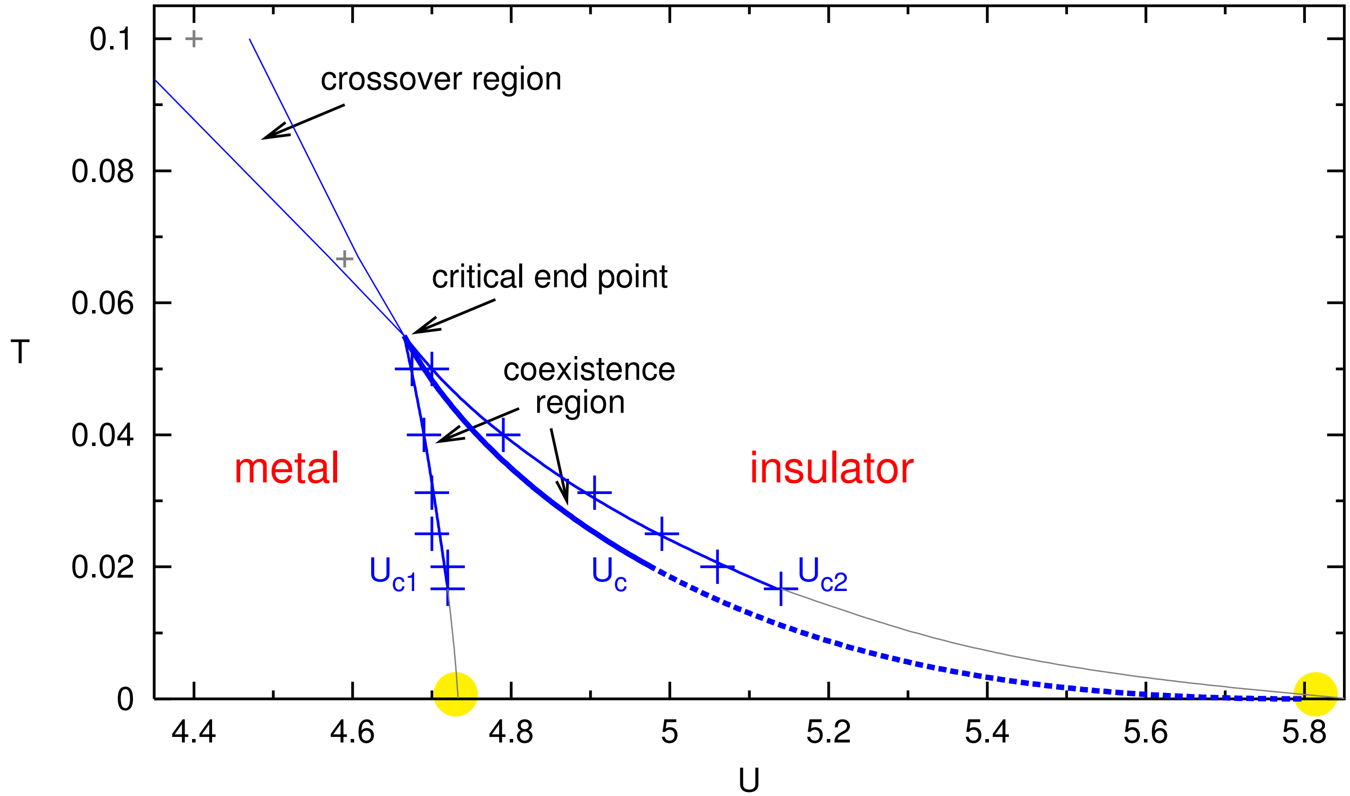
+ nonperturbative, numerically exact

− effort scales as T^{-3}

− no information for $\omega \gtrsim \omega_{\text{Nyquist}}$

Mott transition

1-band frustrated Hubbard model, semi-elliptic DOS, $n = 1$



Georges and Krauth (1993)

Rozenberg, Kotliar, Zhang (1994)

Georges et al. (RMP, 1996)

Schlipf et al. (1999)

Rozenberg, Chitra, Kotliar (1999)

Krauth (2000)

Bulla (1999, 2001)

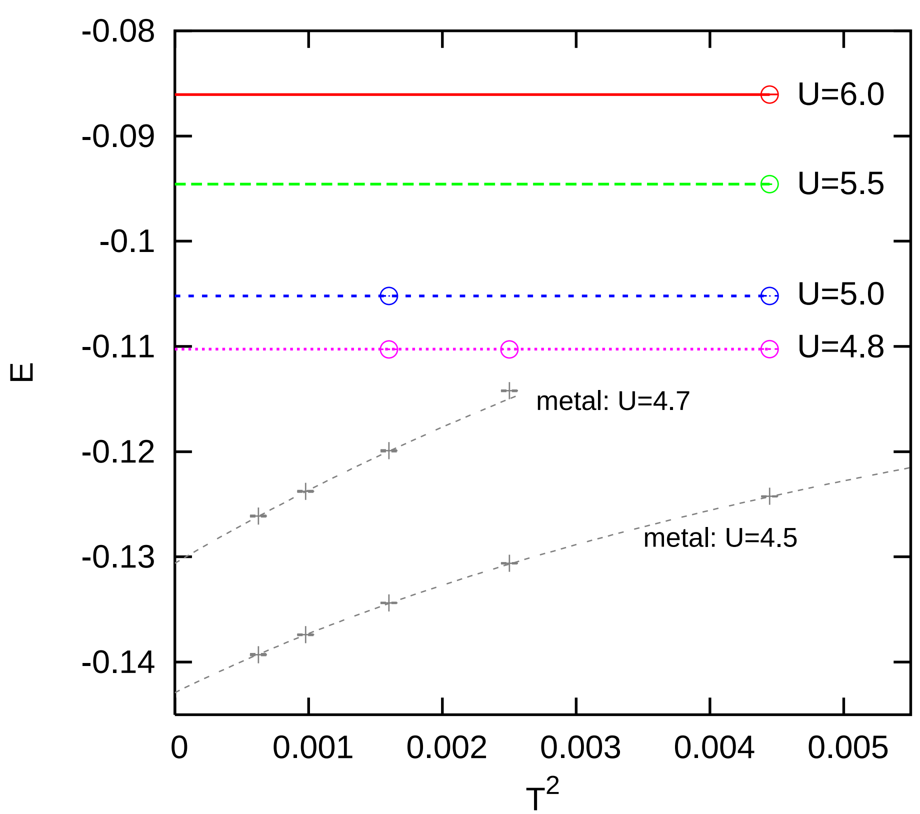
Joo, Oudovenko (2001)

Tong (2001)

Blümer (2000, 2002)

low-T energetics?

Energy: QMC and Perturbation Theory



Quantum Monte Carlo

40×10^7 sweeps

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

$0.1 \leq \Delta\tau \leq 0.25$

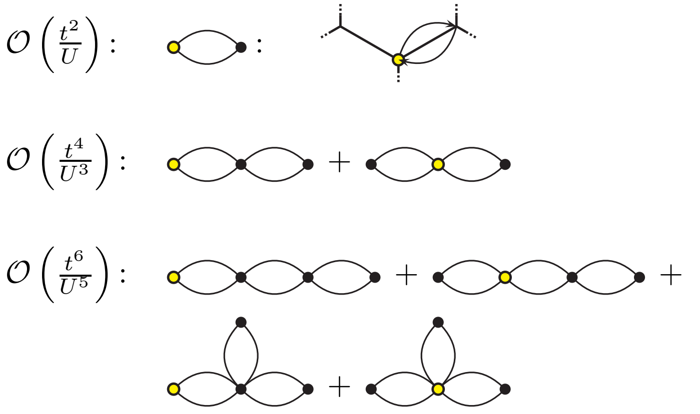
$\Delta E \approx 10^{-5}$

$\Delta D \approx 10^{-5}$

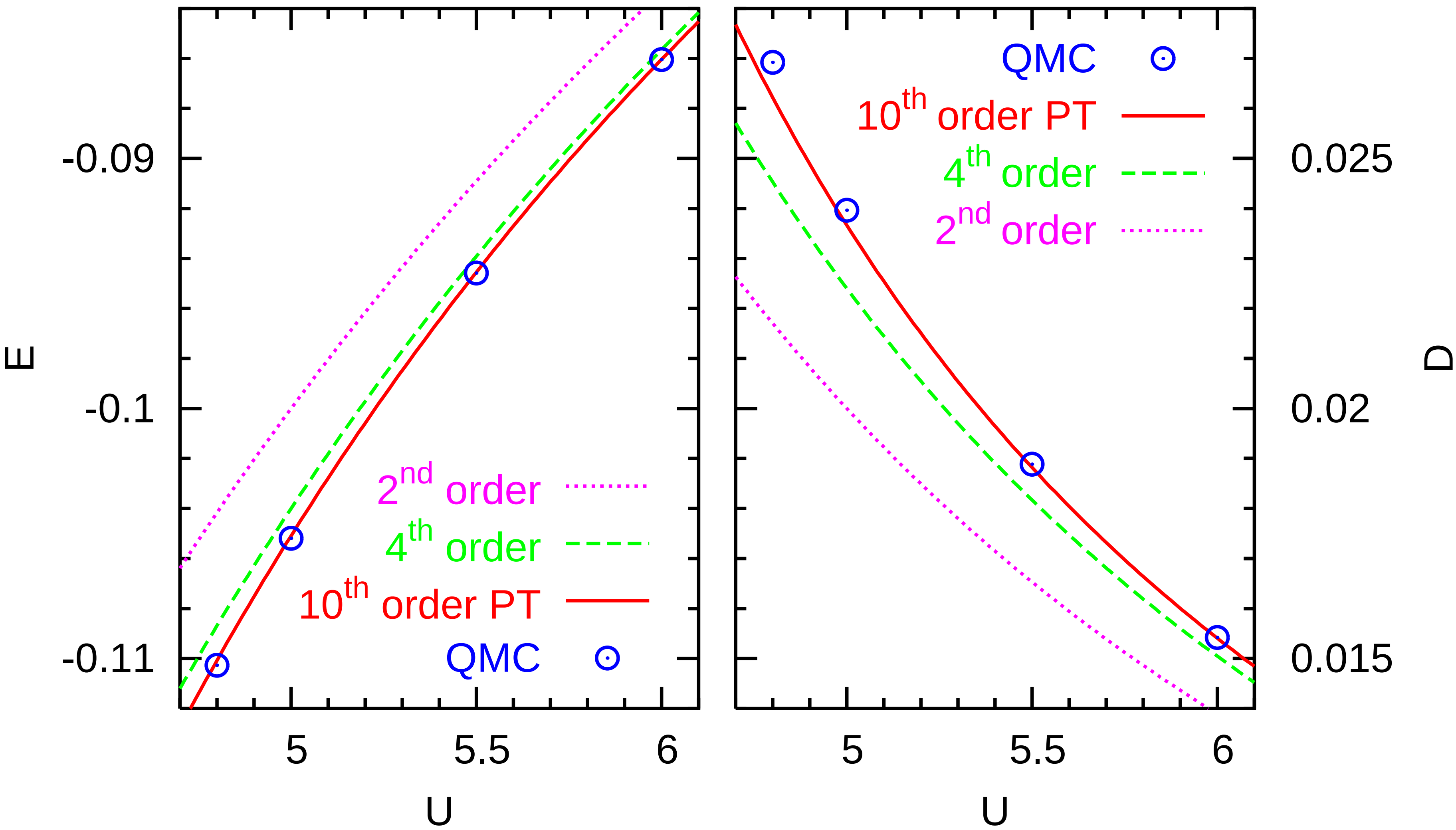
Kato-Takahashi perturbation theory at $T = 0$ $(t^* = 1)$:

$$E_{\text{PT}}(U) = -\frac{1}{2U} - \frac{1}{2U^3} - \frac{19}{8U^5} - \frac{593}{32U^7} - \frac{23877}{128U^9}$$

$$D_{\text{PT}}(U) = dE_{\text{PT}}(U)/dU$$



Mott insulator: double occupancy + energy



Excellent agreement at $U = 6.0$.

continuous fit + critical behavior?

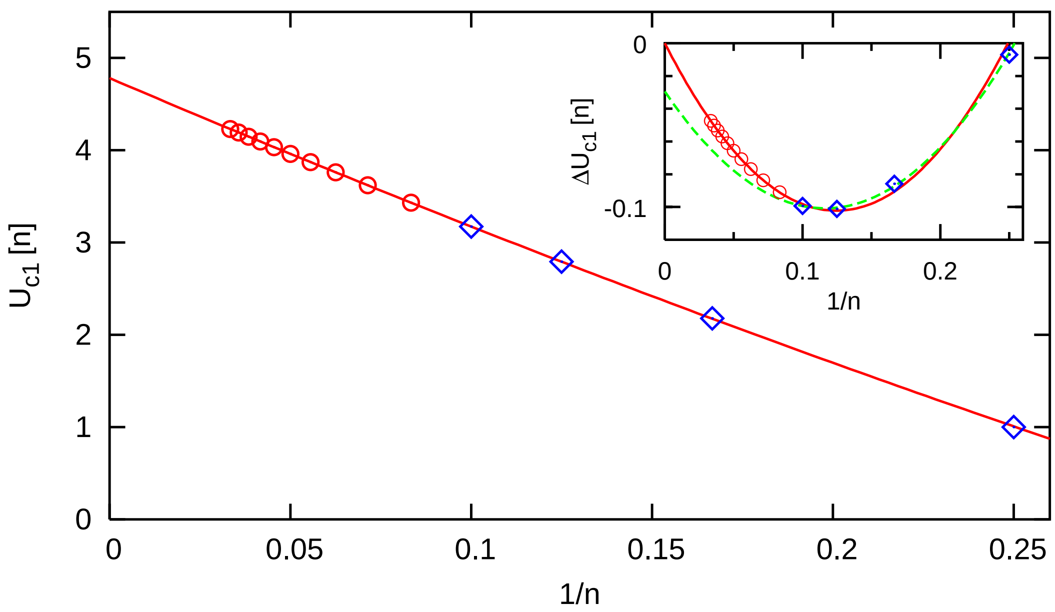
ePT: numerical extension of PT to infinite orders

Idea: extrapolate PT coefficients in

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

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

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



Consequences:

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

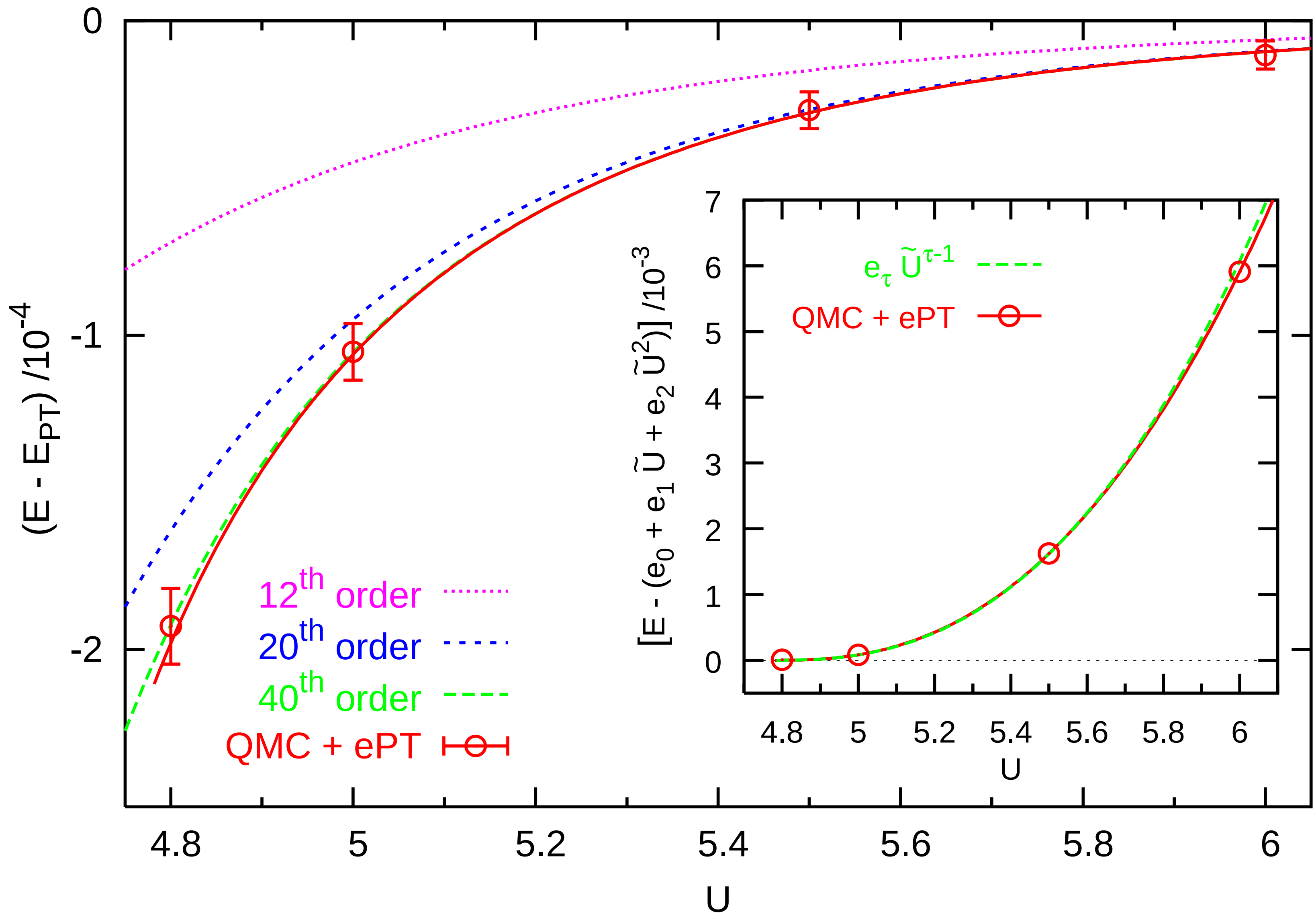
$$a_n \;\propto\; n^{\tau}\, U_{c1}^{n}$$

$$E_{\text{critical}}(U) \;=\; e_{\tau}\,(U - U_{c1})^{\tau-1}$$

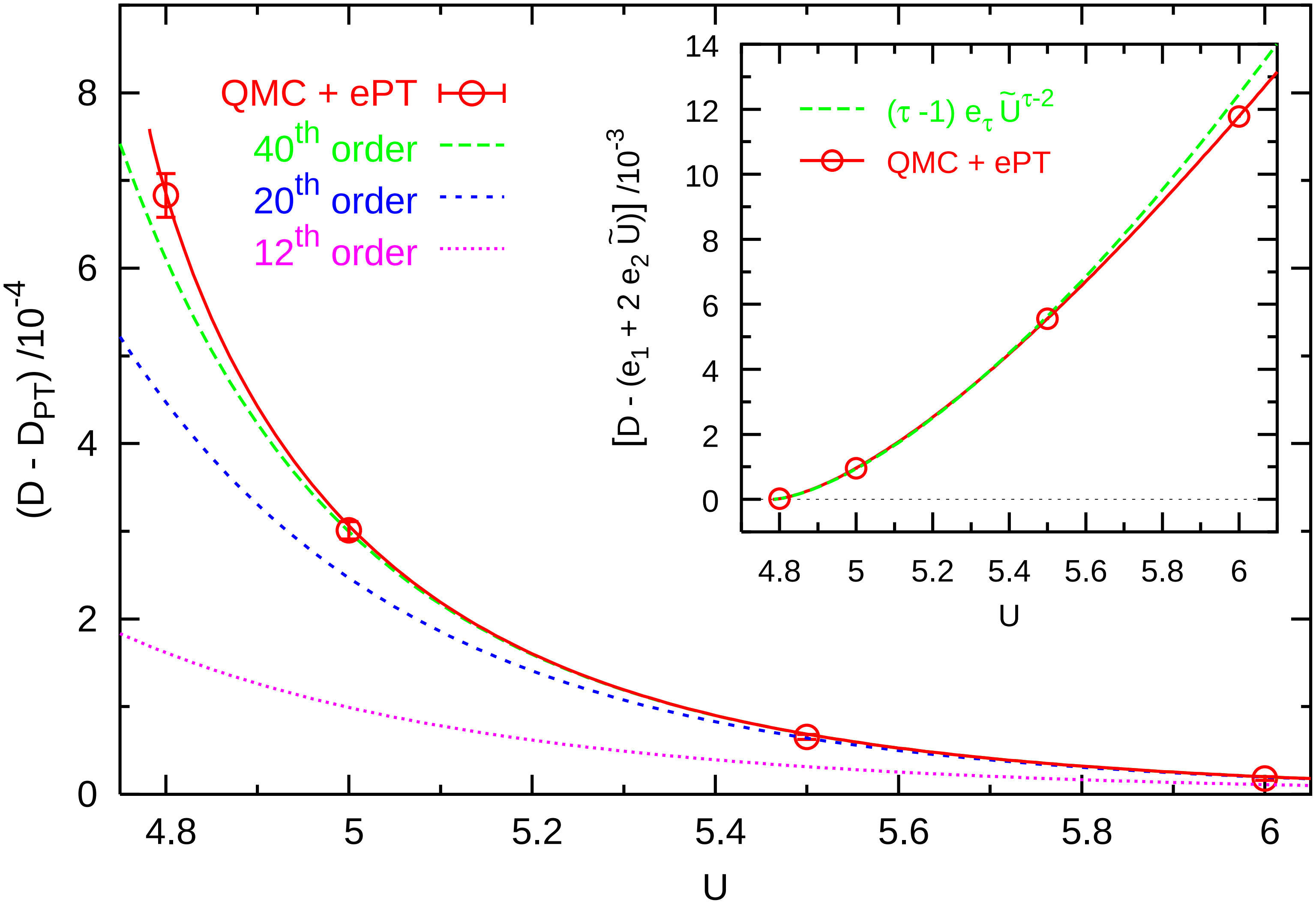
$$D_{\text{critical}}(U) \;=\; (\tau - 1)\, e_{\tau}\,(U - U_{c1})^{\tau-2}$$

$\tau \approx 3.44 \approx 3.5, \quad U_{c1} = 4.782 \quad$ (unrestricted: $U_{c1} = 4.75$)

Energy



Double occupancy

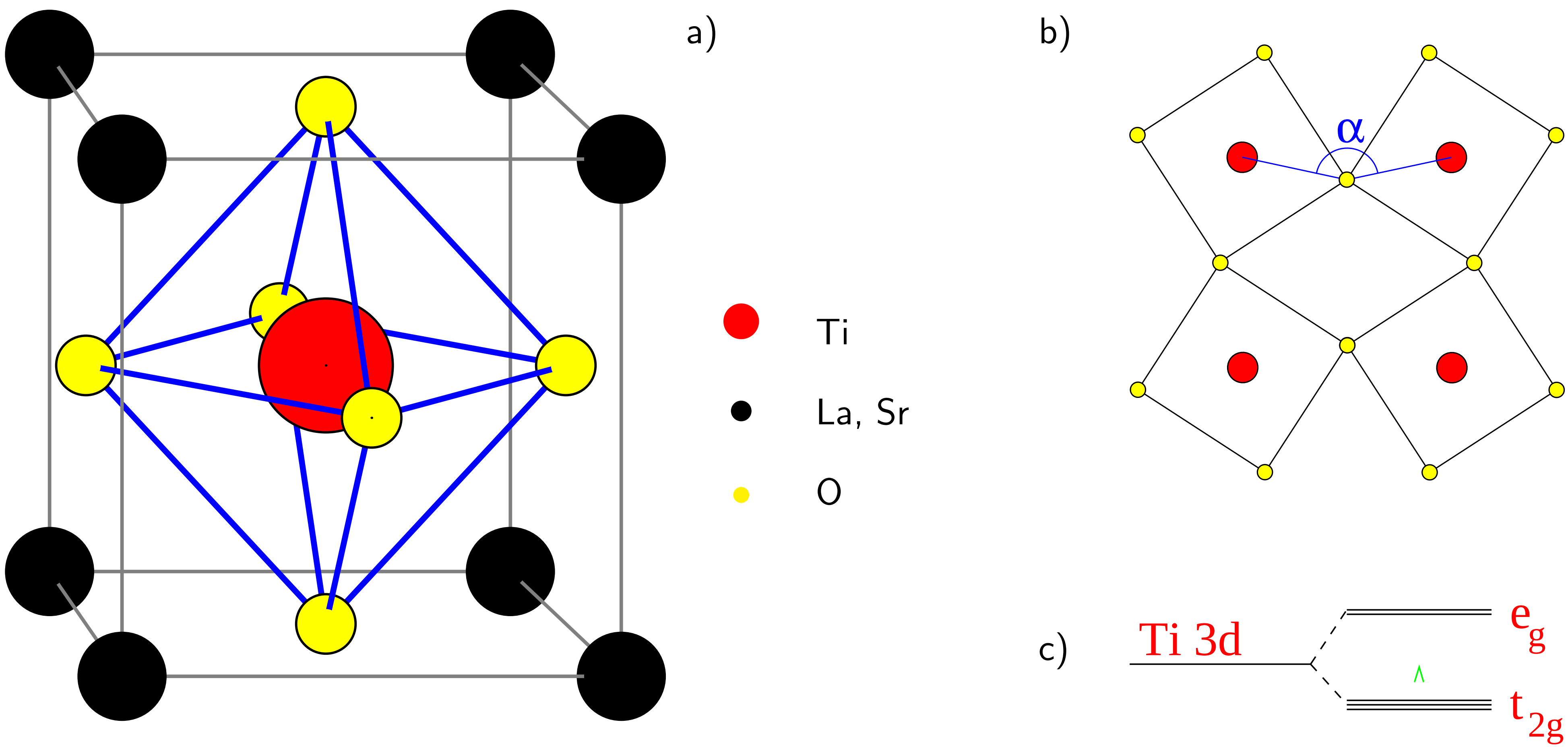


Mott insulator: new estimate of lower stability edge U_{c1}, critical exponents

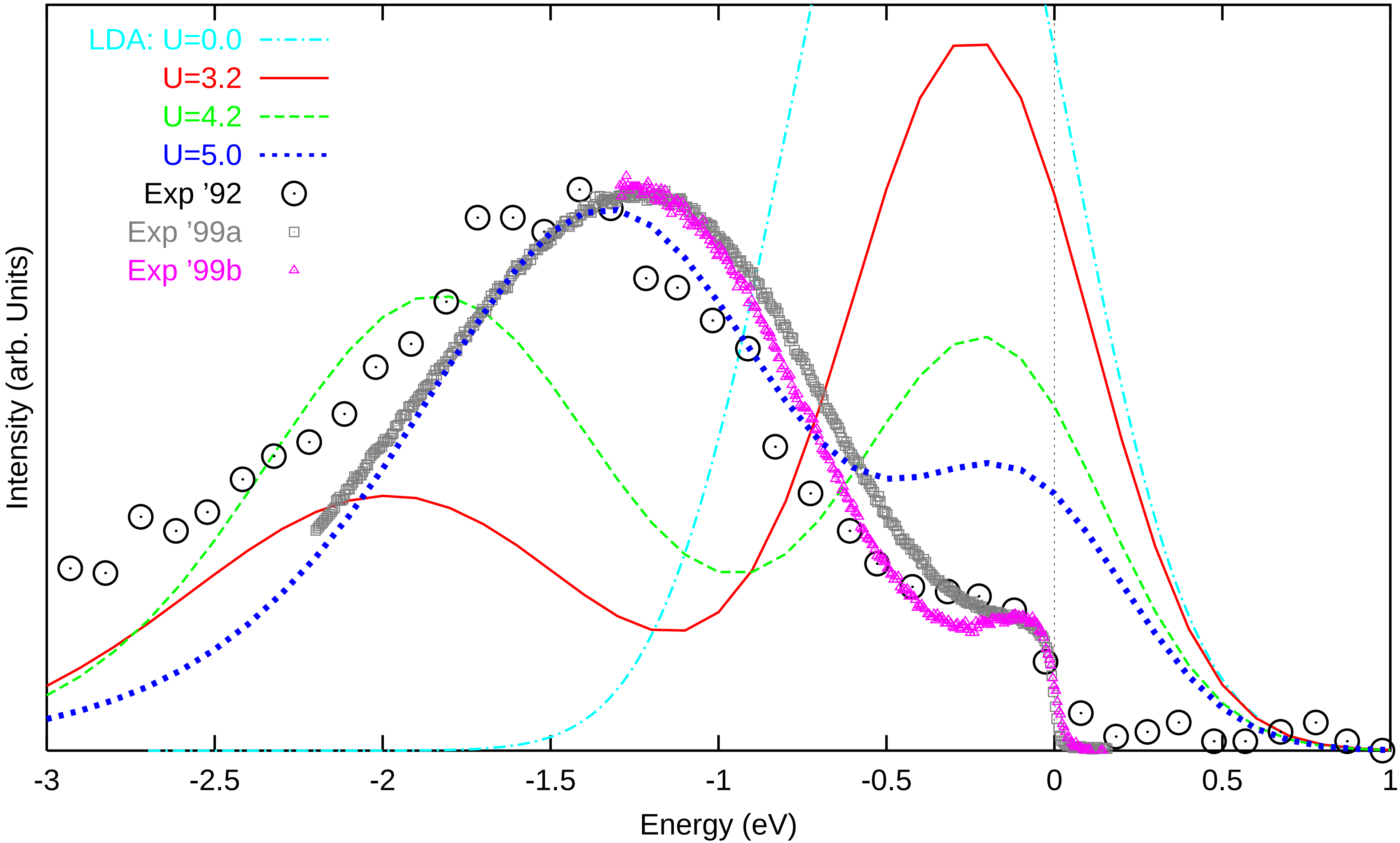
high-precision results for E, D at all U (parametrizations available)

$\rightsquigarrow$ low-T parameter for $U_c(T)$, benchmark for old and new methods

Realistic LDA+DMFT(QMC) calculations



Photoemission spectra for $La_{1-x}Sr_xTiO_3$ (x=0.6)



Forschergruppe “Neue Materialien mit hoher Spinpolarisation”

Heusler-Verbindungen (z.B. $Co_2Cr_{1-x}Fe_xAl$)

Doppelperowskite (z.B. Sr_2FeMoO_6, Sr_2FeReO_6)

1	Felser	Synthese: Heusler-Verbindungen
2	Jacob, Adrian	Dünne Schichten
3	Jourdan, Jacob, Adrian	Tunnelspektroskopie
4	Tremel	Synthese: Doppelperowskite
5	Elmers	Grenzflächenmagnetisierung
6	Blümer, van Dongen	Theorie der Doppelperowskite: LDA+DMFT(QMC)
7	Schönhense, Felser	Spinaufgelöste Photoemission und DFT
8	Ksenofontov, Felser	Mößbauer Spektroskopie
9	Demokritov, Hillebrands	Brillouin-Lichtstreuspektroskopie
10	Aeschlimann, Bauer	Spektroskopie unbesetzter Zustände (2PPE)