Modeling of strongly correlated electron systems

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Outline

Introduction

Formalism and Methods: DMFT, QMC

Mott Transition, Mott Insulator

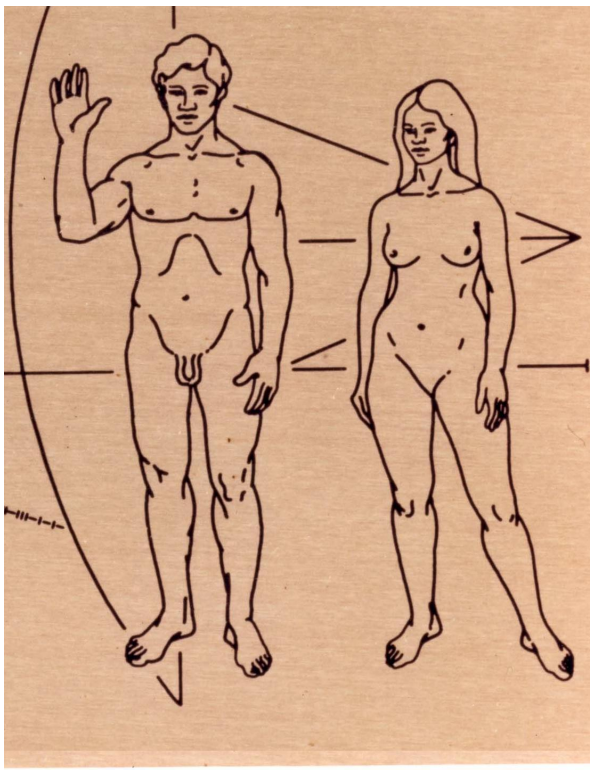
LDA+DMFT(QMC) for $La_{1-x}Sr_xTiO_3$

Outlook: DFG-Forschergruppe

Summary

Prologue: of Mice and Men ("modeling")

Example: models for humans



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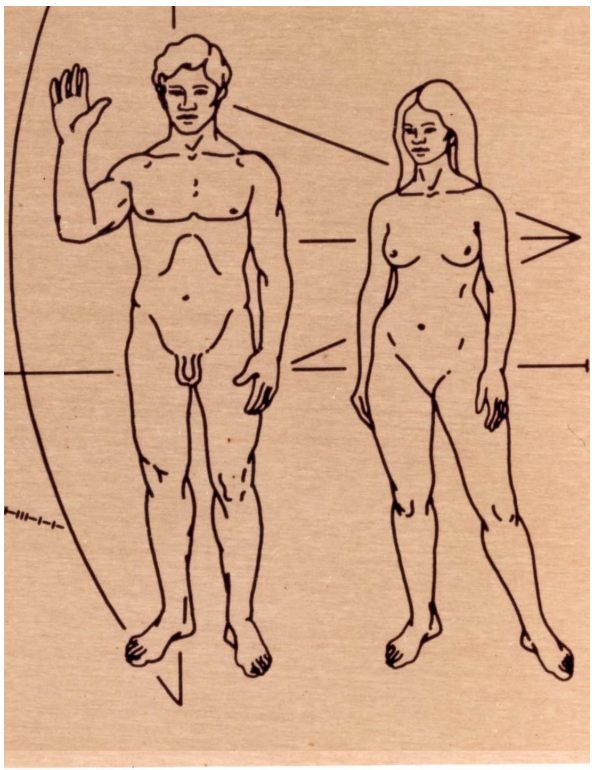

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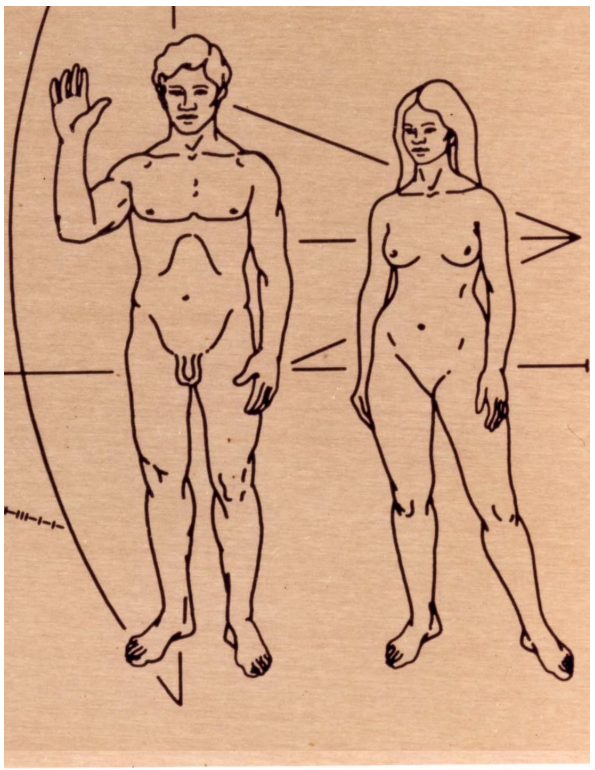
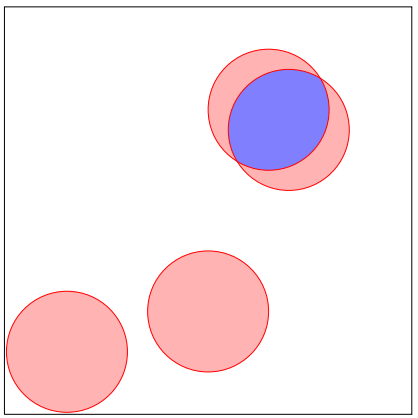


Here: focus on electronic low-energy properties of strongly correlated materials.

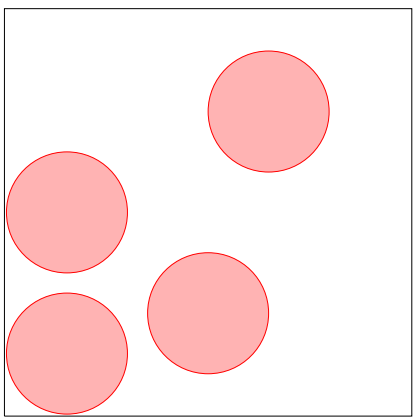
no elastic properties (sound, thermal expansion)
no X-ray physics
(no surface effects)

Interaction induced correlations

classical spheres in 2-d box



noninteracting



hard core interaction

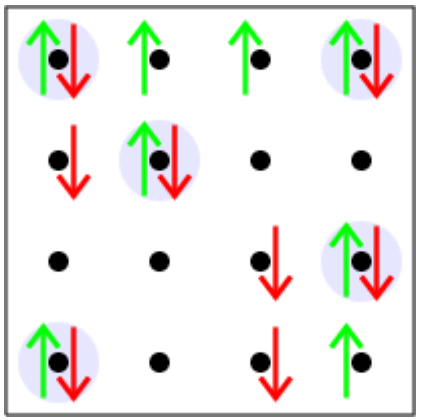
quantum lattice model for electrons (1 band)

Pauli principle:

$D \equiv \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle$

without e-e interaction:

- $D = \langle \hat{n}_\uparrow \rangle \langle \hat{n}_\downarrow \rangle$
- perfect metal



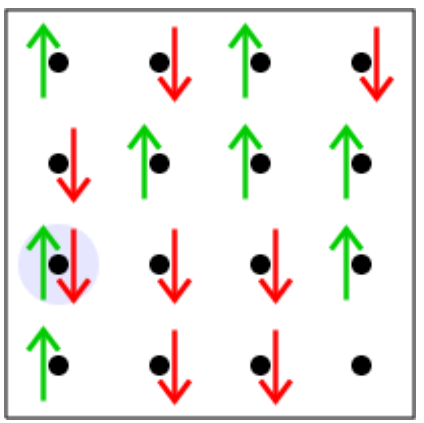
noninteracting ($U = 0$)

Hubbard interaction

$E_{\text{Hub}} = U D$

at strong coupling ($U \to \infty$):

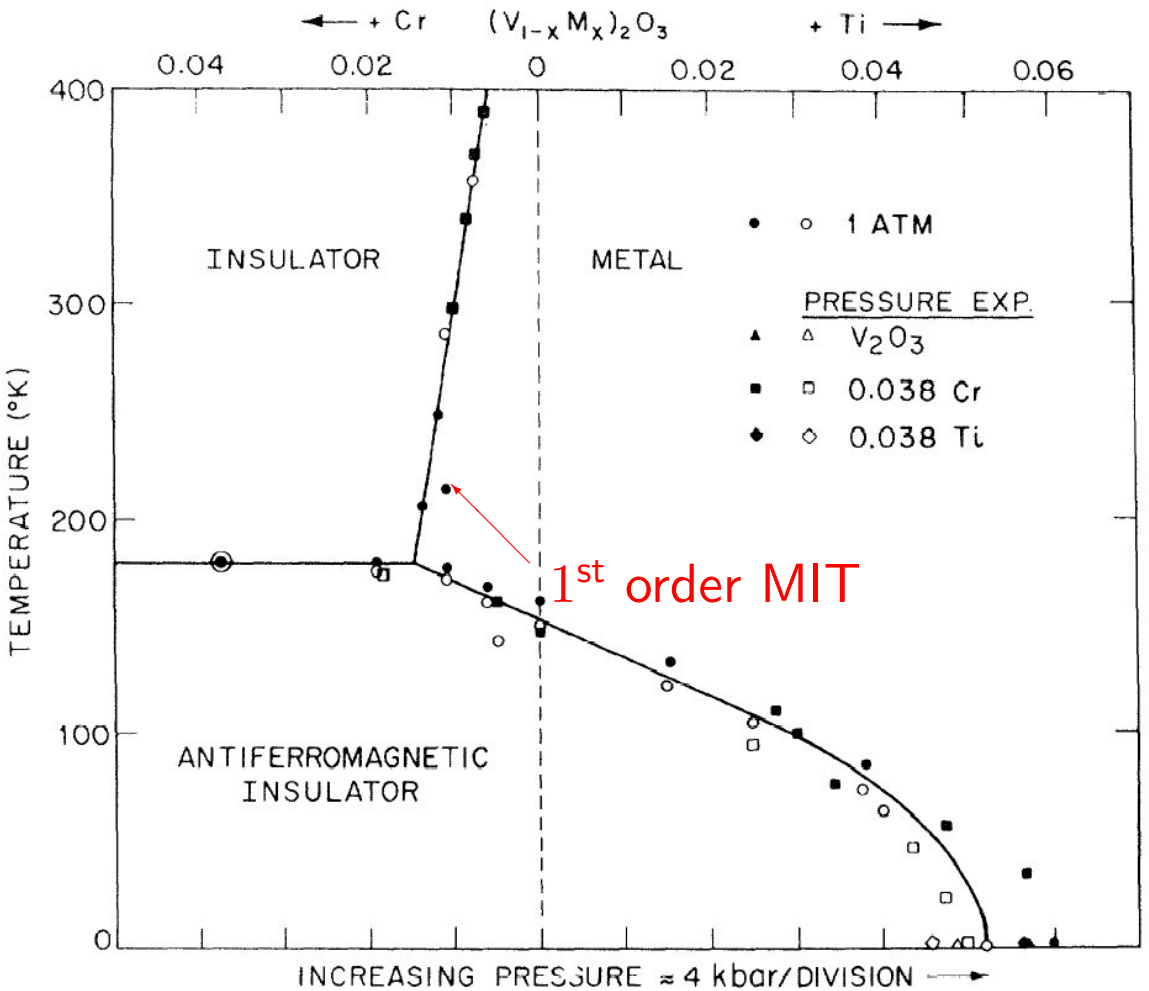
- $D \longrightarrow 0$
- insulator (at $n = 1$)



"hard core" ($U \gtrsim t$)

Strong correlations: materials / phenomena

Mott metal-insulator transition (MIT) in V_2O_3



McWhan et al. (1971)

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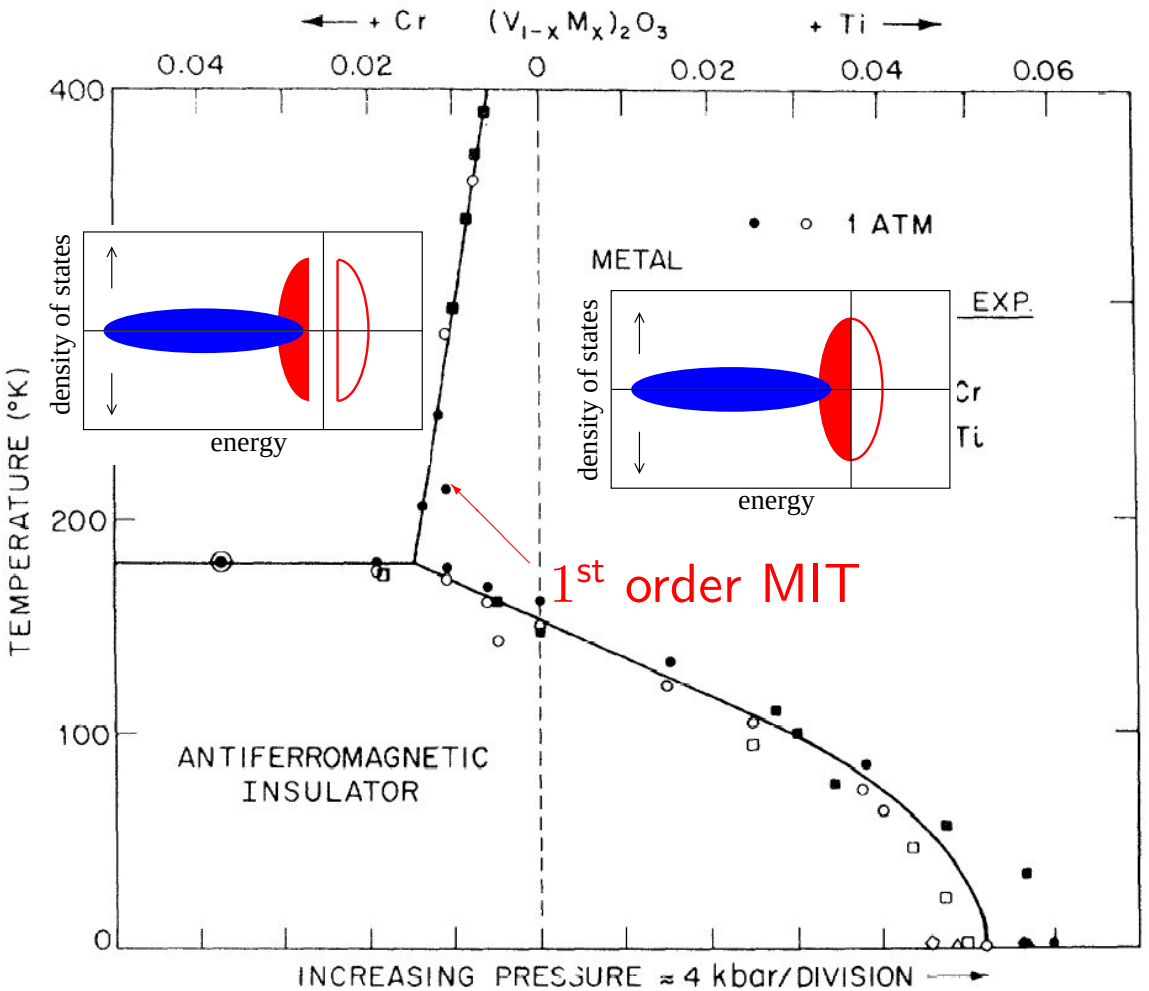

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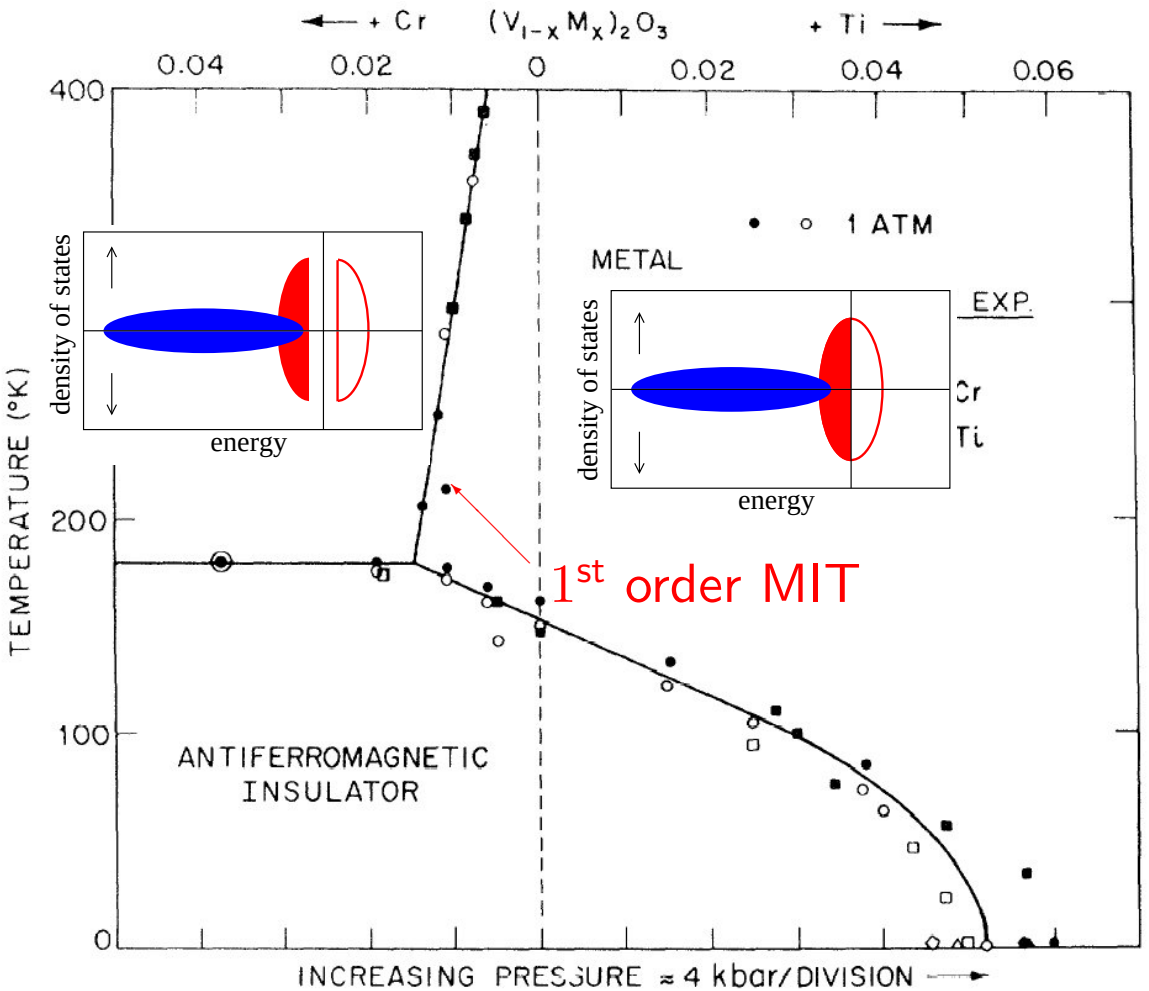

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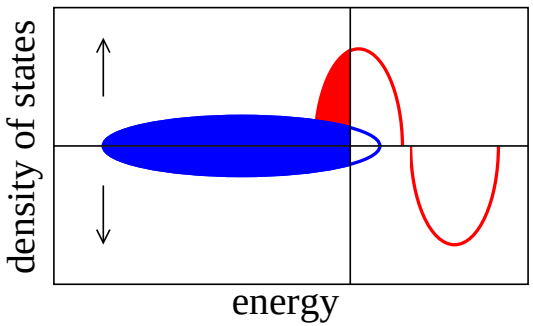
Itinerant ferromagnetism of Fe, Ni, . . .



High-T_c superconductivity

Formalism

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

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Born-Oppenheimer approximation ↓

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

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reduction to valence electrons ↓

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

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occupation number formalism, Wannier orbitals ↓

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

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← **density functional theory (DFT)**

reduction to valence electrons ↓

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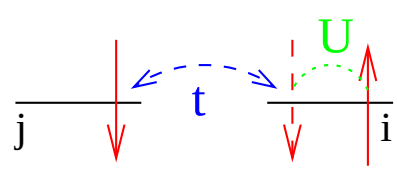
Hubbard model

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



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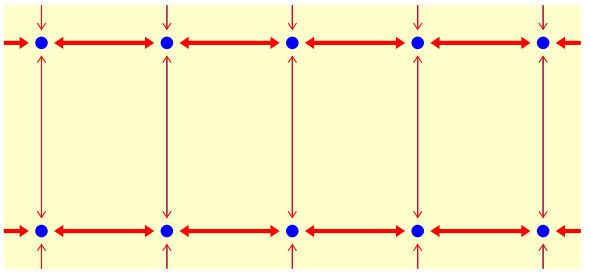
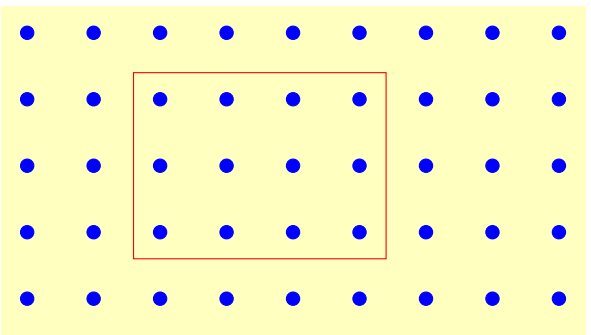
$d = 1$: Bethe ansatz, DMRG



finite clusters: ED, QMC



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)

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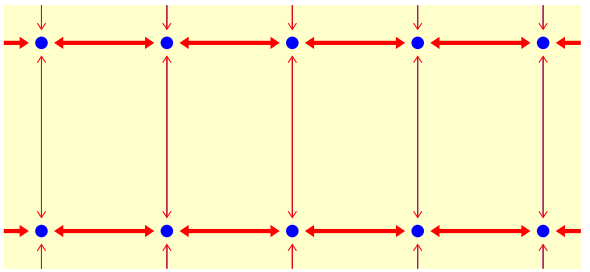

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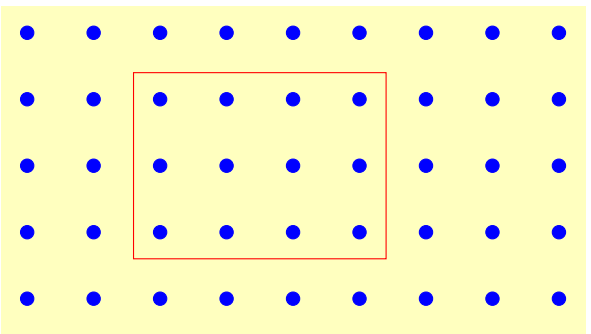

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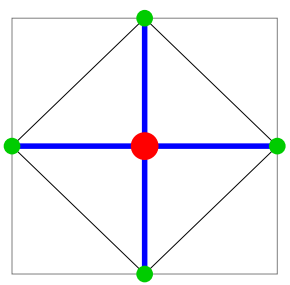
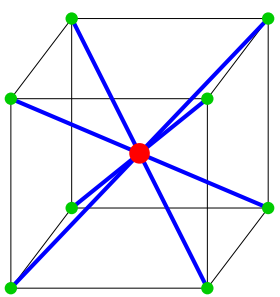
Dynamical mean-field theory (DMFT):

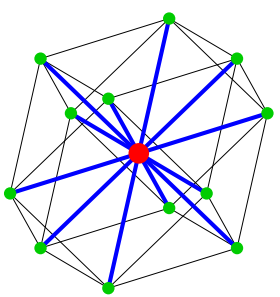
- exact for $Z \longrightarrow \infty$
- dynamical on-site correlations preserved
- non-perturbative $\rightsquigarrow$ valid at MIT
- thermodynamic limit



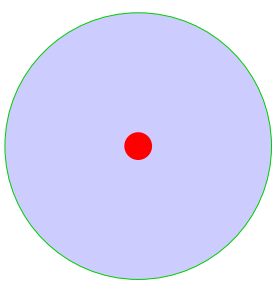
d=2: $Z = 4$



bcc: $Z = 8$

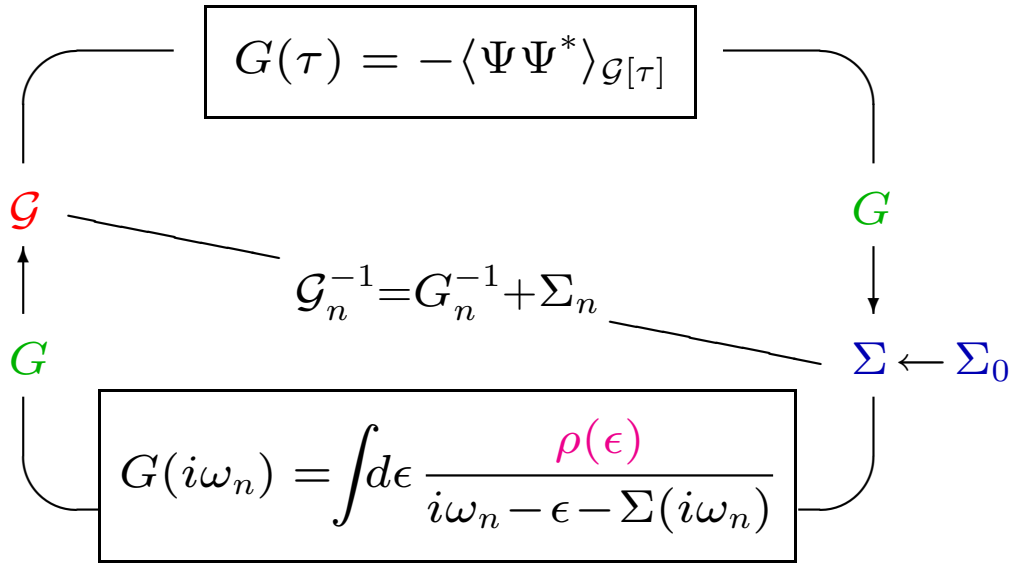


fcc: $Z = 12$

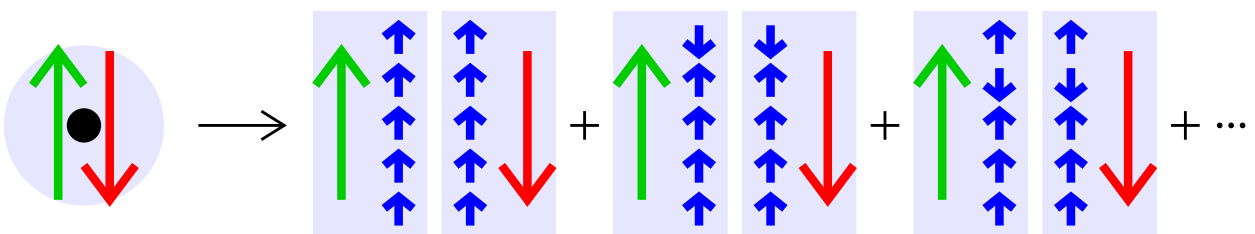


DMFT: $Z = \infty$

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, $50 \lesssim \Lambda \lesssim 400$

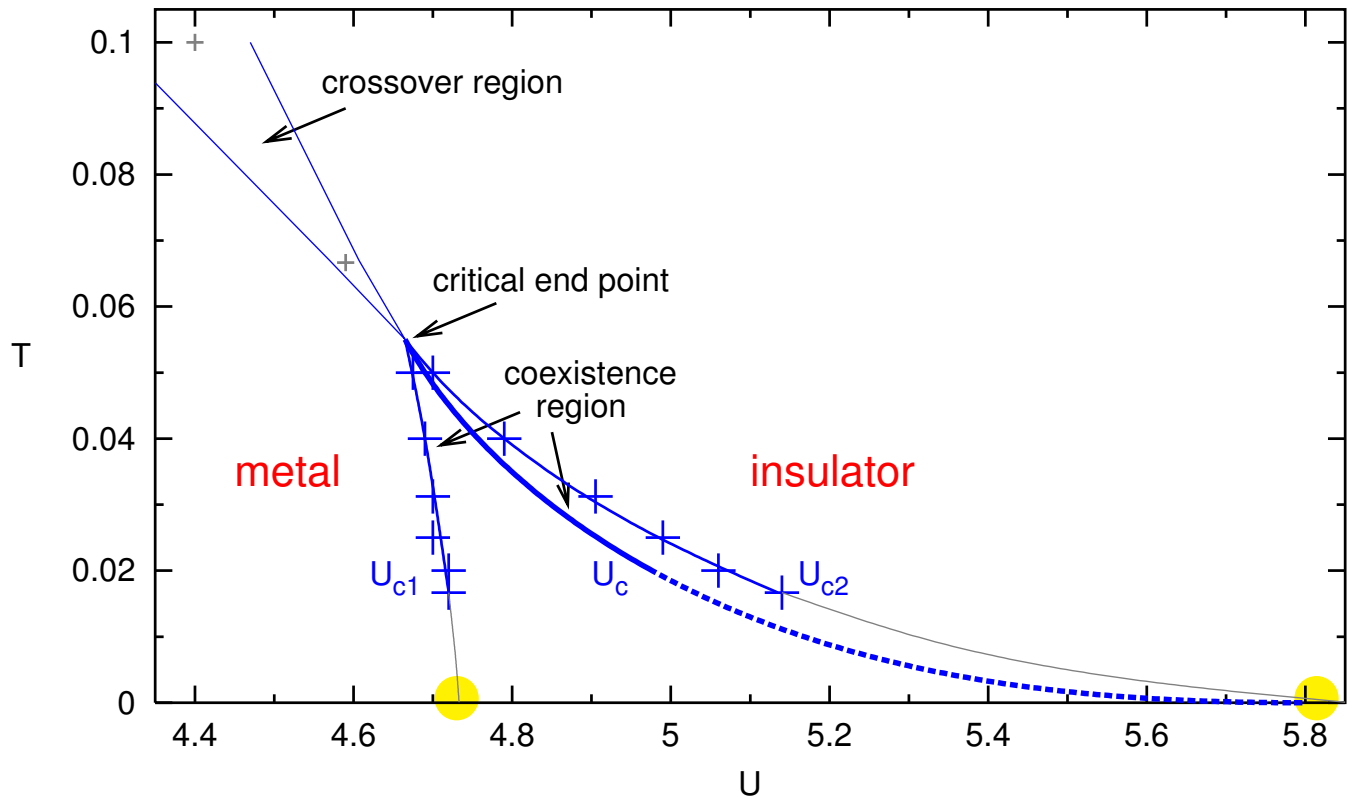
\+ nonperturbative, numerically exact

– effort scales as T^{-3}

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

Mott transition

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



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Bulla (1999, 2001)

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Tong (2001)

Blümer (2000, 2002)

low-T energetics?

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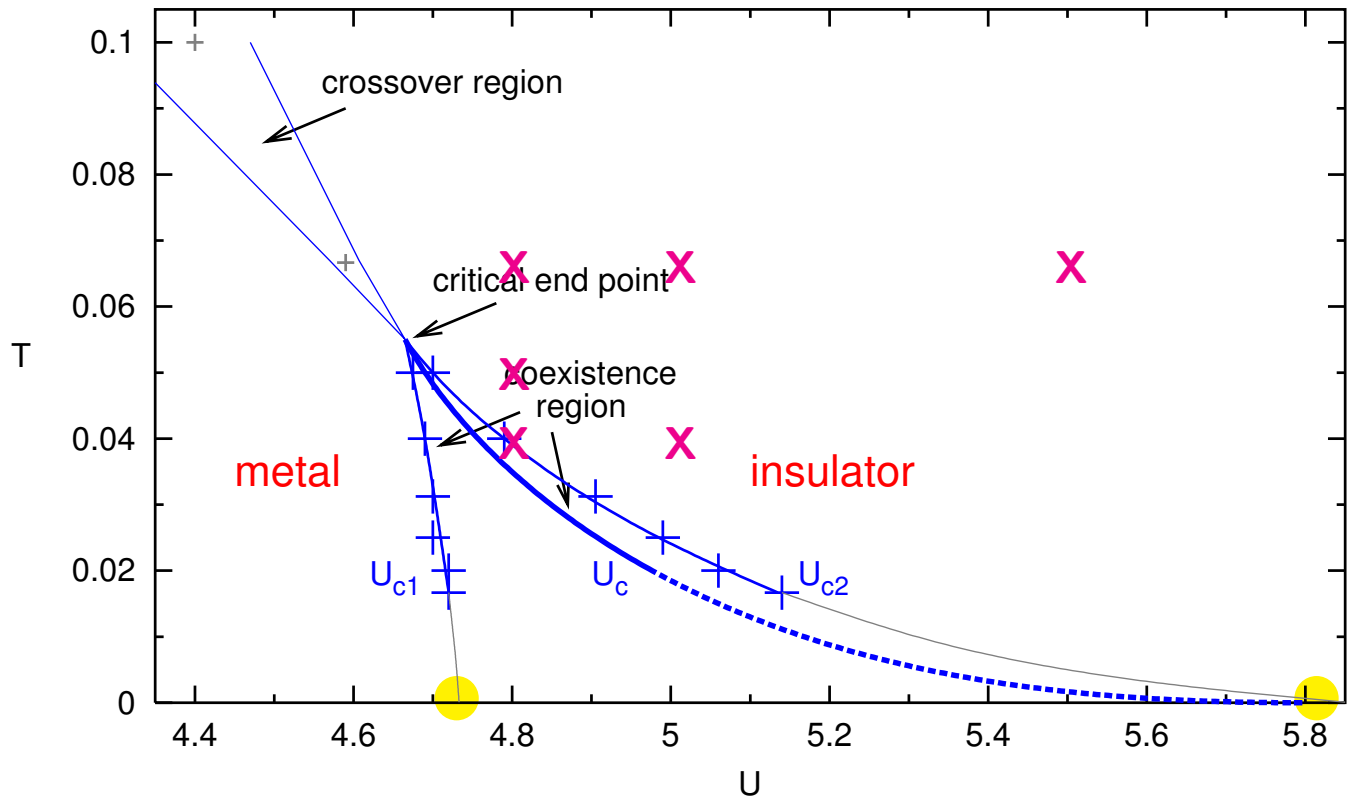

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Energy of Mott insulator: Perturbation Theory (PT) vs. QMC

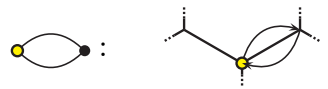
10^{th} order Kato-Takahashi perturbation theory at $T = 0$:

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

accurate at $U \gtrsim 6$: $\Delta E_{\text{PT}} \leq 10^{-5}$, $\Delta D_{\text{PT}} \leq 10^{-5}$

comparison with "old QMC": $\Delta E_{\text{QMC,systematic}} \approx 10^{-3}$

$\mathcal{O}\left(\frac{t^2}{U}\right)$:



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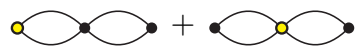
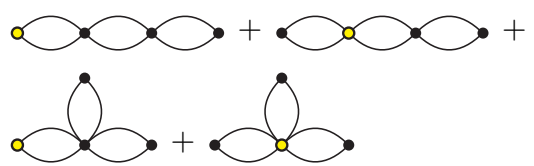


$\mathcal{O}\left(\frac{t^6}{U^5}\right)$:



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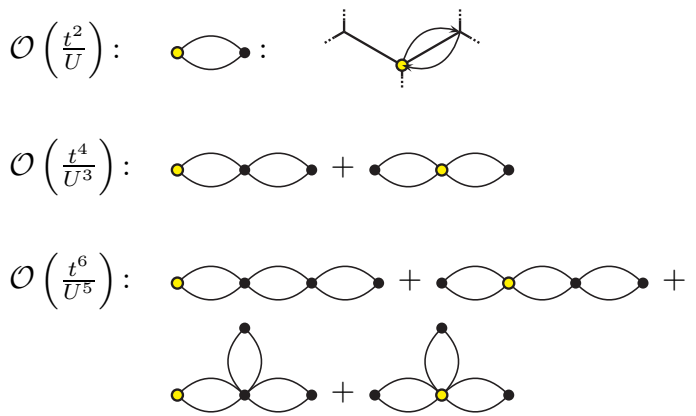

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Quantum Monte Carlo

40×10^7 sweeps

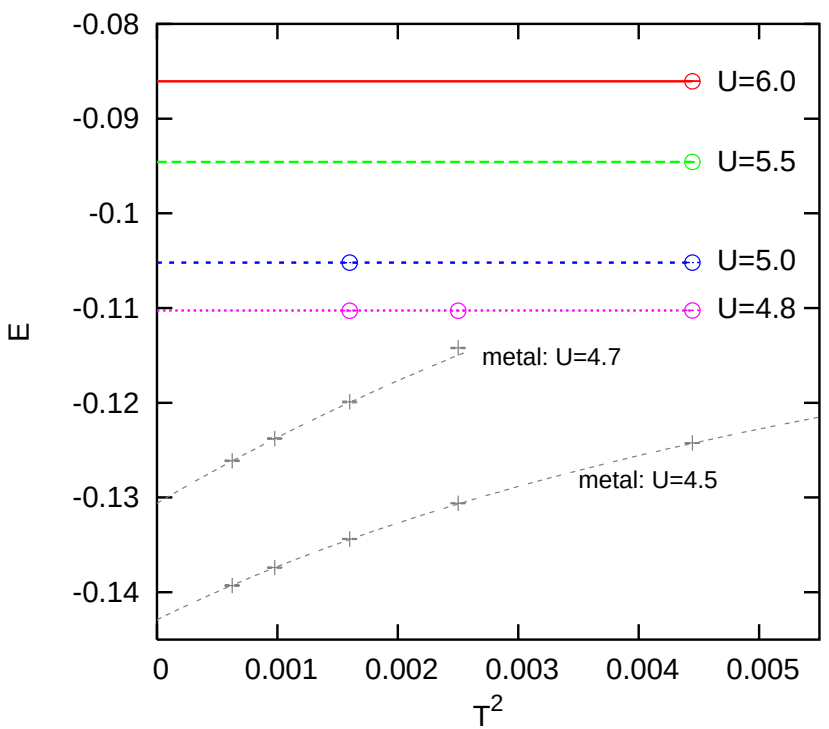
$\Sigma(\omega) = \frac{U^2}{4\omega} + \mathcal{O}(\omega^{-2})$

careful $\Delta\tau$ extrapolation

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

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

[Improved hybrid QMC scheme implemented by Carsten Knecht (see poster)]



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ratios of coefficients: 1 4.8 7.8 10.1

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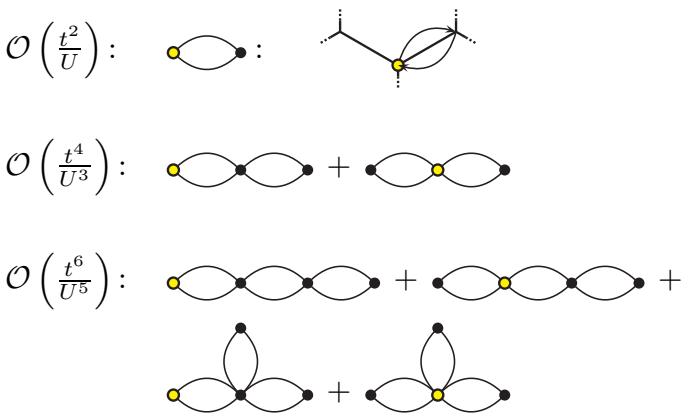

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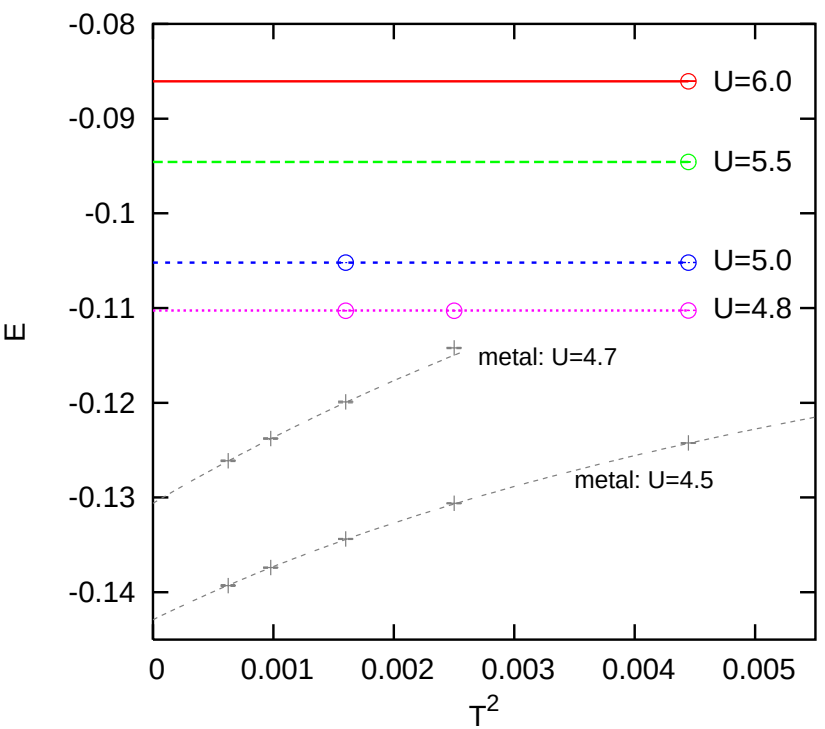
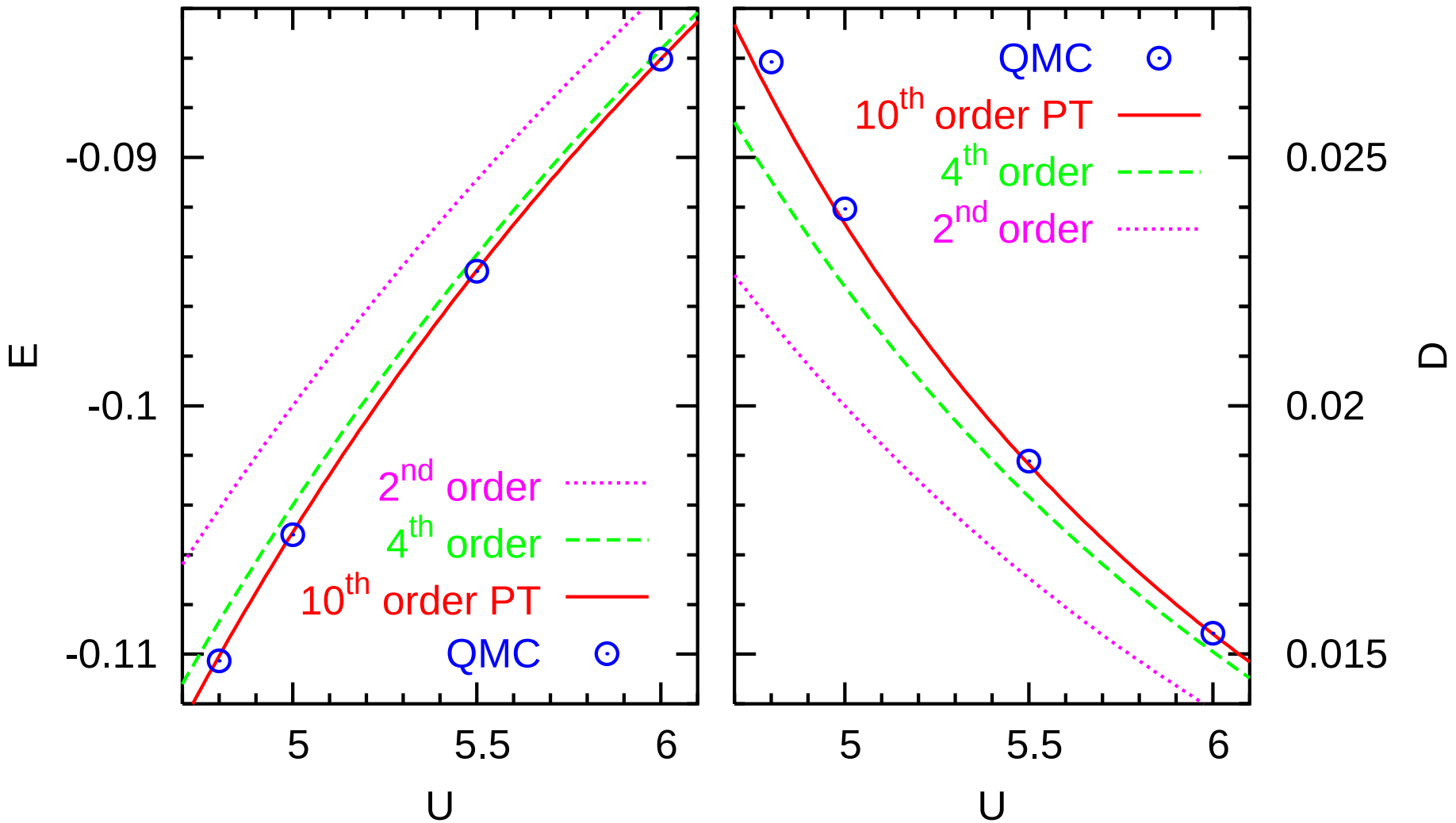
$\Delta D \approx 10^{-5}$

[Improved hybrid QMC scheme implemented by Carsten Knecht (see poster)]



Mott insulator: energy + double occupancy I



Excellent agreement at $U = 6.0$.

continuous fit + critical behavior?

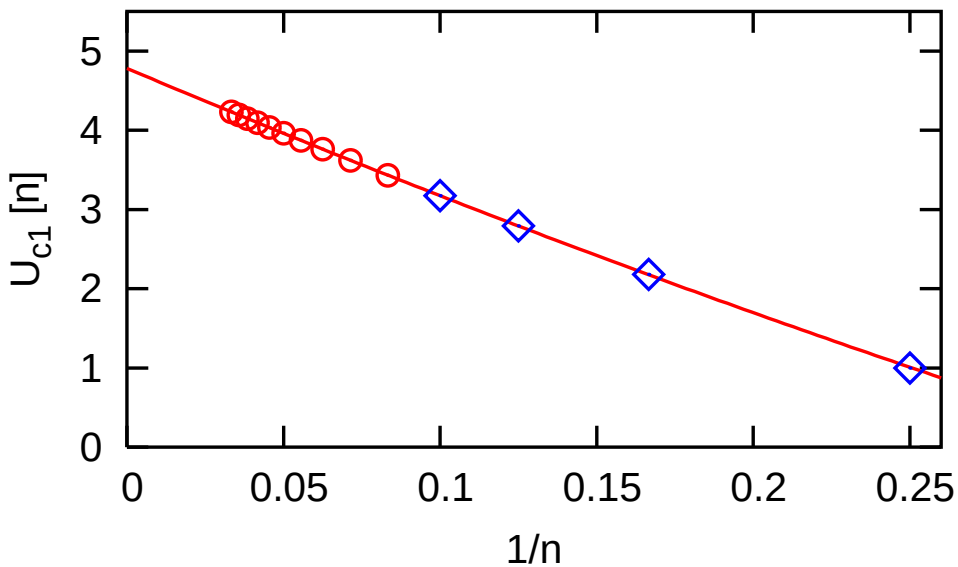
ePT: numerical extension of PT to infinite orders

Idea: extrapolate PT coefficients in

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

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

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



General consequences:

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

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

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

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

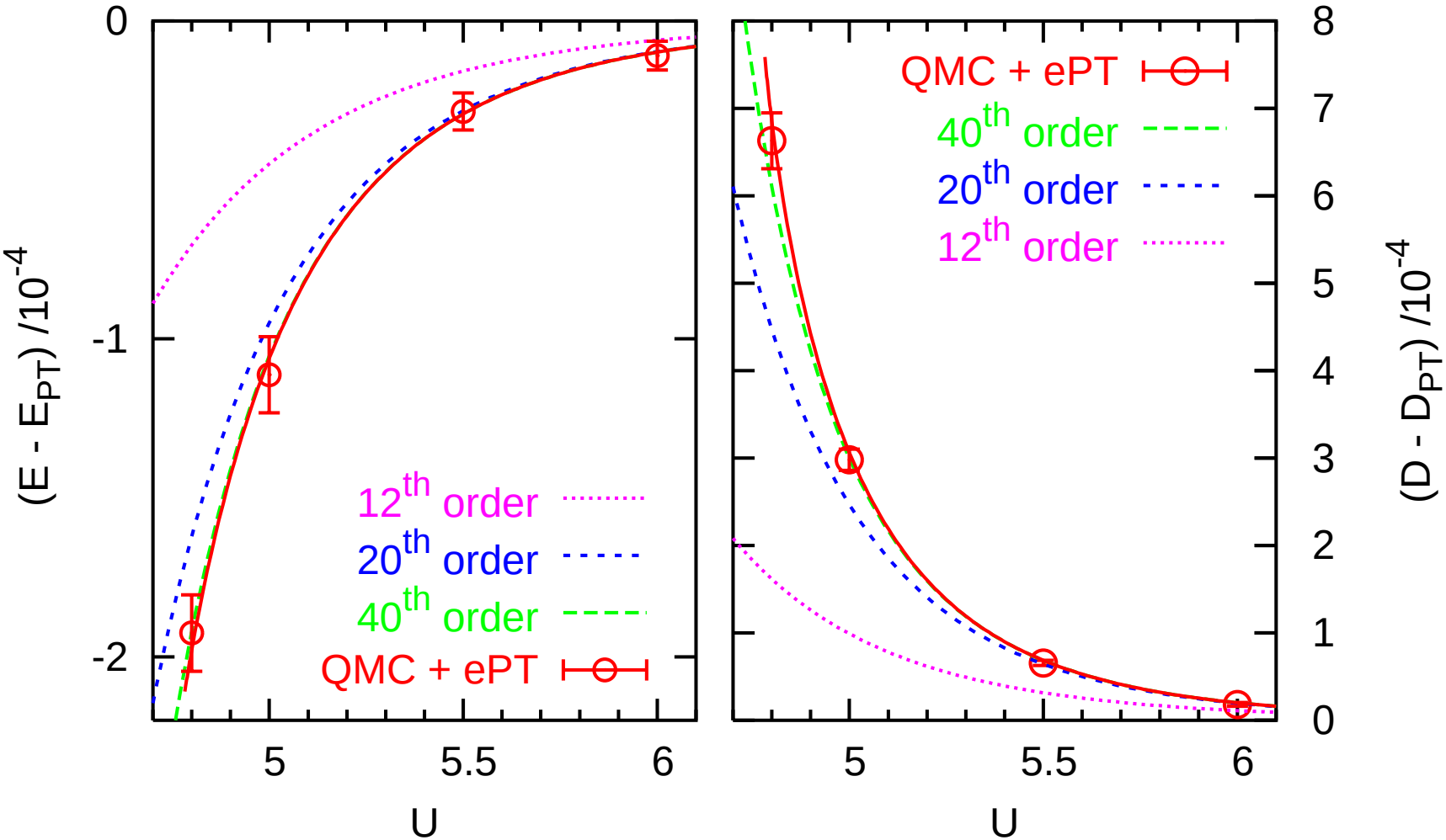
Numerical results of extrapolation:

exponent $\tau \approx 3.44 \overset{QMC}{\longrightarrow} 3.5$

$U_{c1} = 4.782$

$E(U)$, $D(U)$ for all $U \geq U_{c1}$

Mott insulator: energy + double occupancy II



Mott insulator: U_{c1}, critical exponents, low-T parameter for $U_c(T)$

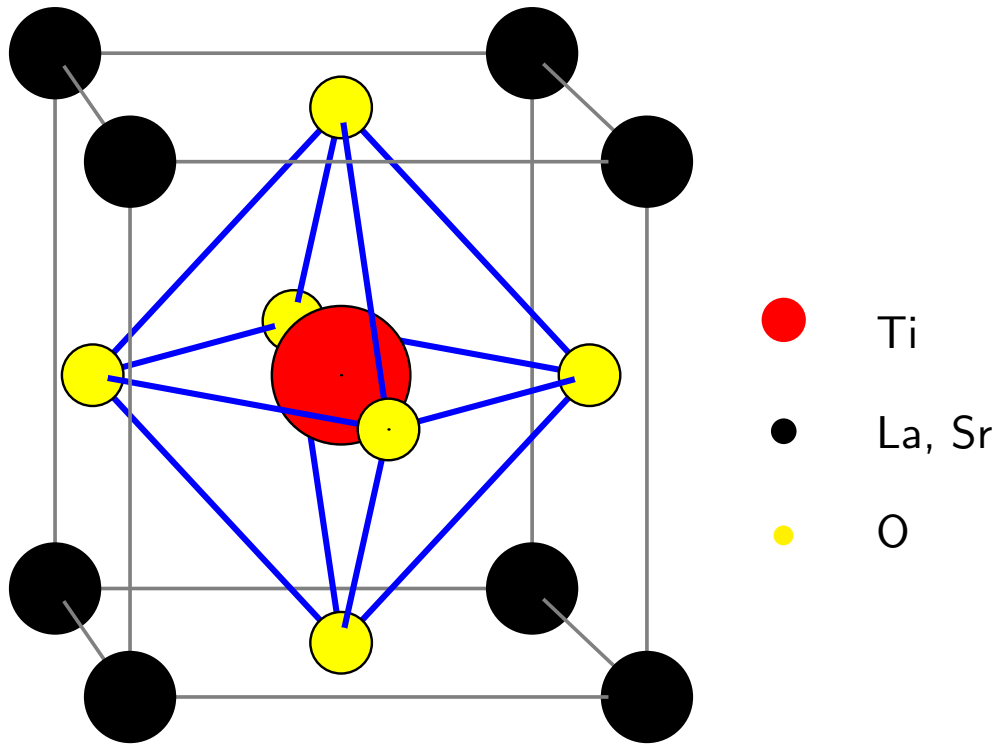
high-precision results for E, D at all U (parametrizations available) $\rightsquigarrow$ benchmark

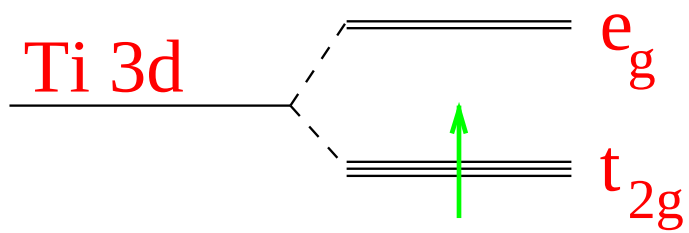
[Blümer, Kalinowski, cond-mat/0404568 (2004)]

Realistic LDA+DMFT(QMC) calculations

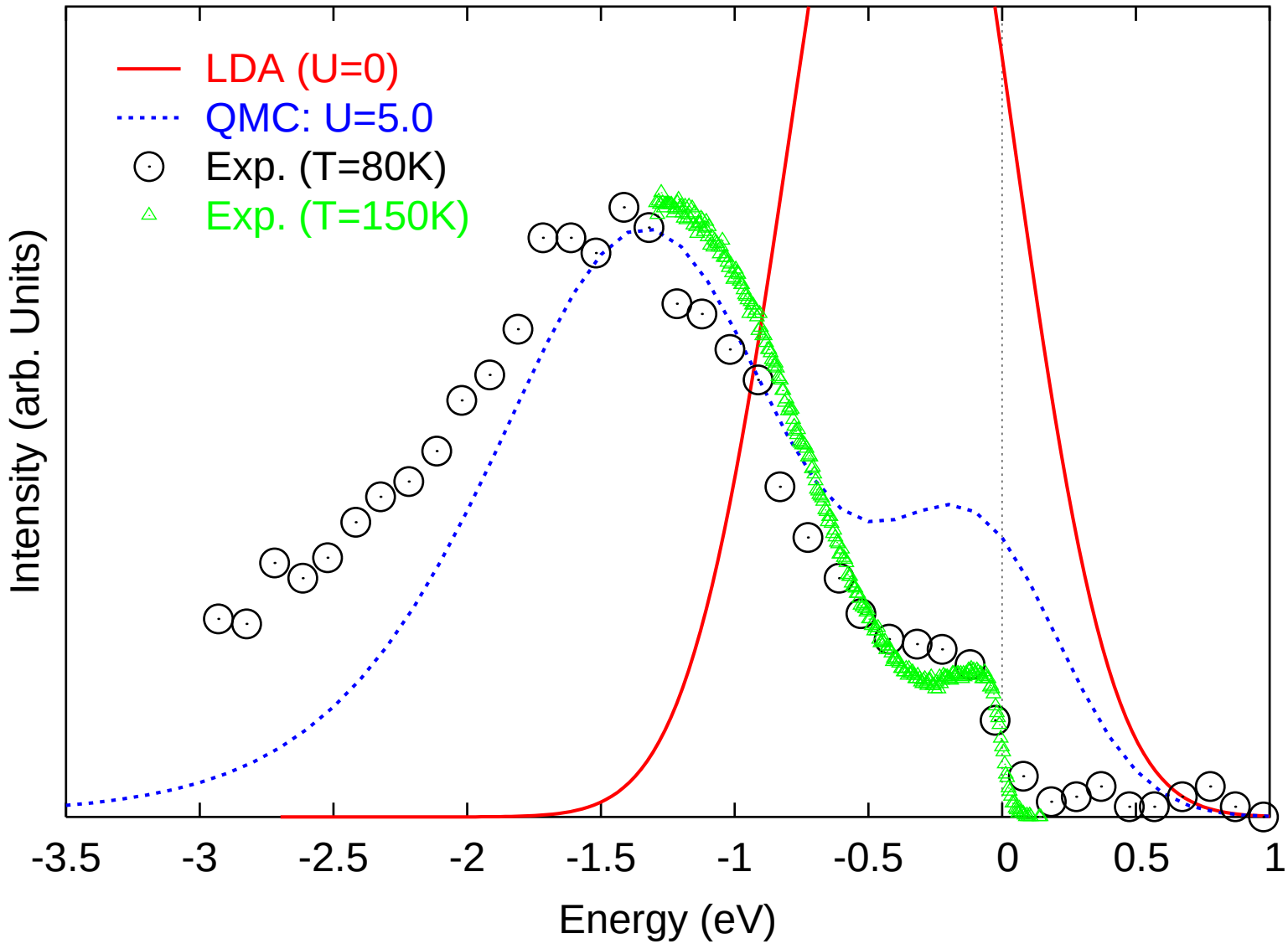
$La_{1-x}Sr_xTiO_3$

- perovskite structure
- $1-x$ t_{2g} electrons per site
- AF for $x \lesssim 0.05$
- strongly correlated metal
- density functional theory (LDA) fails





Photoemission spectra for $La_{1-x}Sr_xTiO_3$ (x=0.06)

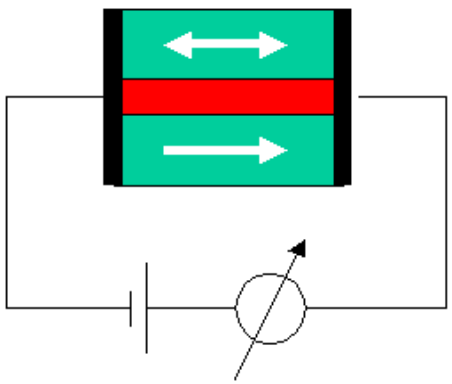


[Nekrasov, Held, Blümer, Poteryaev, Anisimov, Vollhardt, EPJB **18**, 55 (2000)]

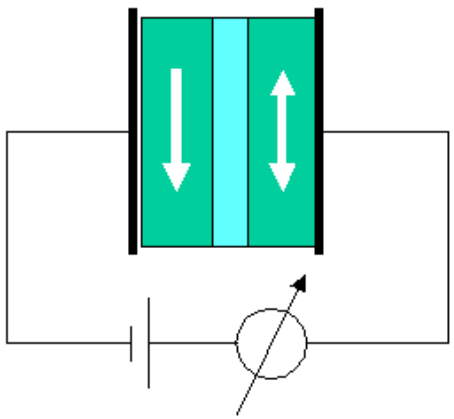
DFG-Forschergruppe “Neue Materialien mit hoher Spinpolarisation” (Mainz – Kaiserslautern)

motivation: spintronics

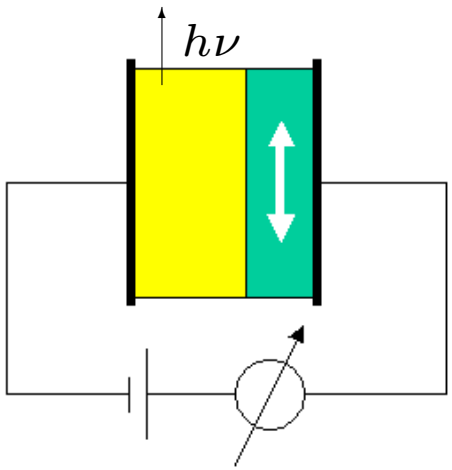
GMR



TMR



Spin injection



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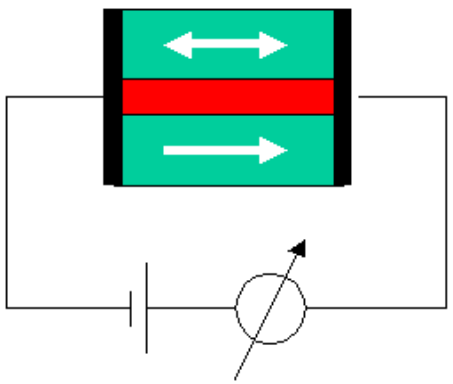
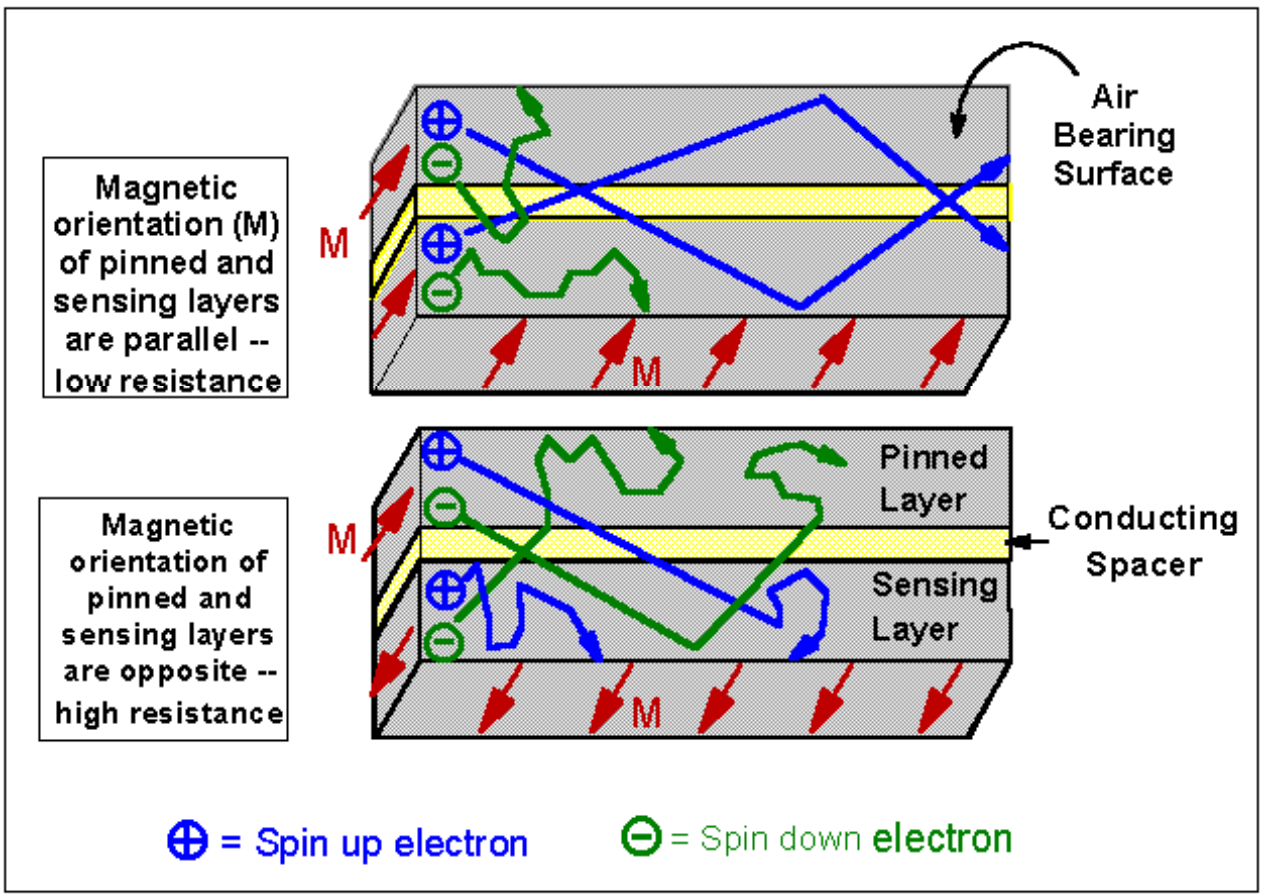


TMR

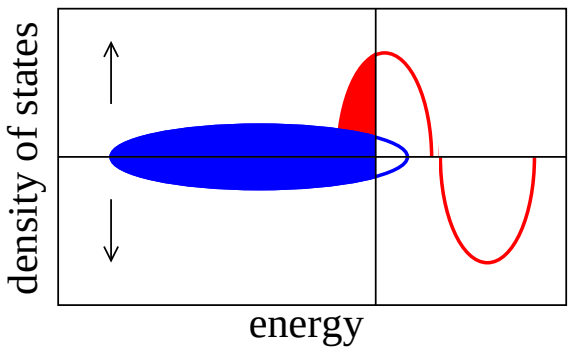
Spin injection

$h\nu$

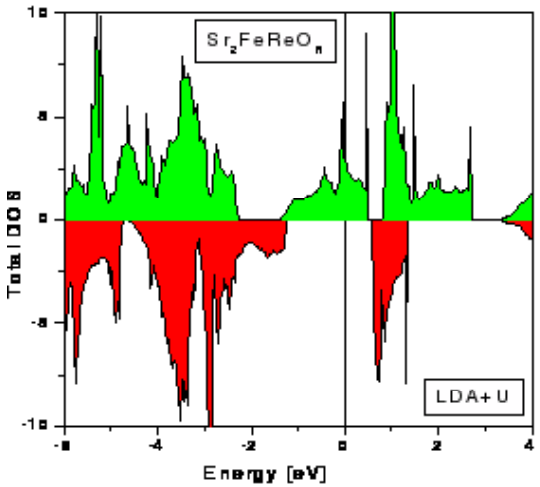


goal: half metallic ferro/ferrimagnets

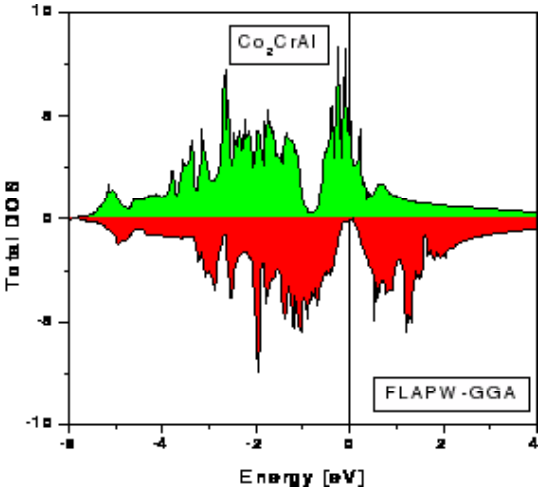
elementary ferromagnet

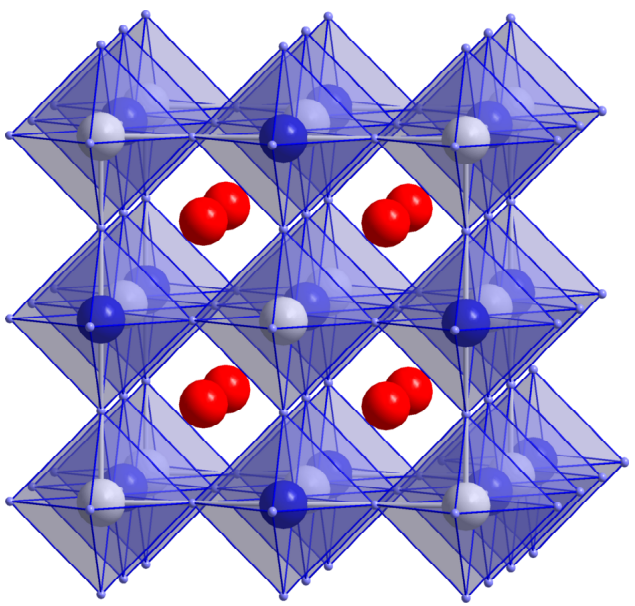


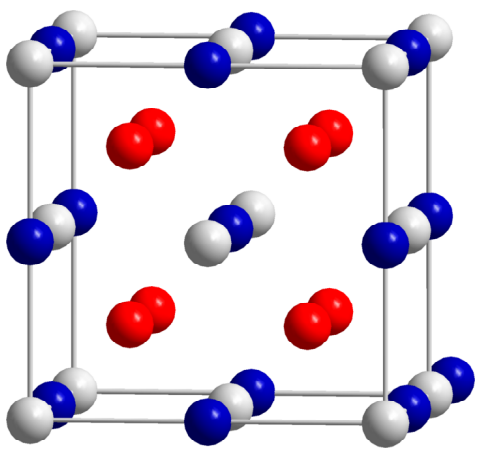
double perovskite



Heusler compound







DFG-Forschergruppe "Neue Materialien mit hoher Spinpolarisation"

Sprecher: Felser (Mainz), Hillebrands (Kaiserslautern)

Aufstellung der Teilprojekte

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(LDA)
8	Ksenofontov, Felser	Mößbauer Spektroskopie
9	Demokritov, Hillebrands	Brillouin-Lichtstreuspektroskopie
10	Aeschlimann, Bauer	Spektroskopie unbesetzter Zustände (2PPE)

Doppelperowskite: z.B. Sr_2FeMoO_6, Sr_2FeReO_6

Summary

Microscopic models for strongly correlated electron systems

Very precise QMC results for "Mott transition", "Mott insulator" (1 band)

New method: ePT

Realistic LDA+DMFT(QMC) calculations for $La_{1-x}Sr_xTiO_3$ (3 bands)

Outlook: increasingly realistic calculations for double perovskites (3-5 bands)

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Not shown:

Transport within DMFT [Blümer, van Dongen]

QMC development, MIT(s) in anisotropic 2 band model [Knecht, Blümer, van Dongen]

Persistent currents in quantum rings [Himmerich, Noack, van Dongen]

Transport in $1d$ systems from DMRG [Jeckelmann]

Multichannel Kondo lattice [Schauerte, Cox, Noack, van Dongen, Batista]

Magnetic domain walls [Lippert, Elmers, van Dongen]