Electron Correlations in Solids:

From High-Temperature Superconductivity to Half-Metallic Ferromagnetism

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FWF projects n. P18505-N16, P18551-N16,
DFG FOR 538

Outline of the talk

1. Introduction: Correlation in High-Temperature Superconductors

Outline of the talk

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Outline

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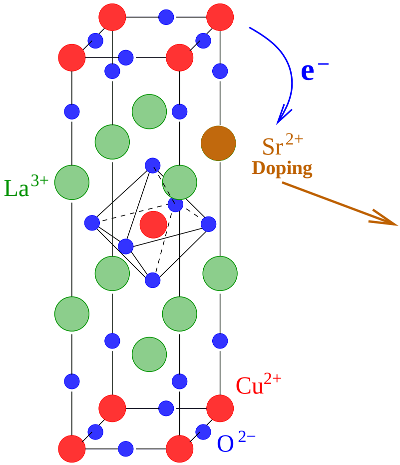
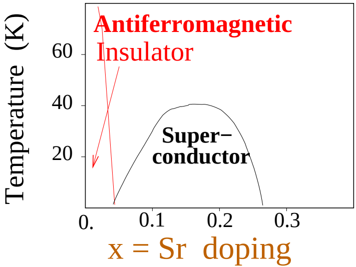
A High−Tc Superconductor



$La_{2-x}Sr_xCuO_4$

Phase diagram



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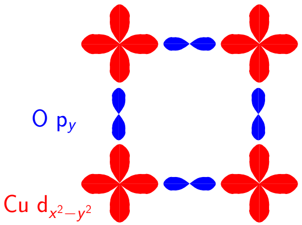
Cu O_2 layer



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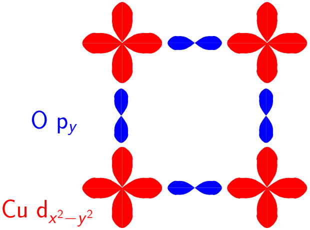
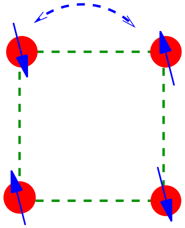


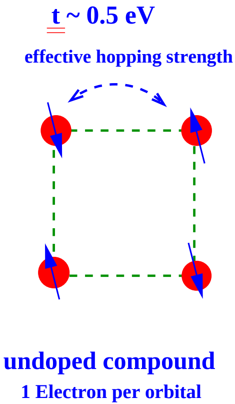
Reduced model

(e.g. Hubbard model)

$t \sim 0.5 eV$

Effective hopping strength





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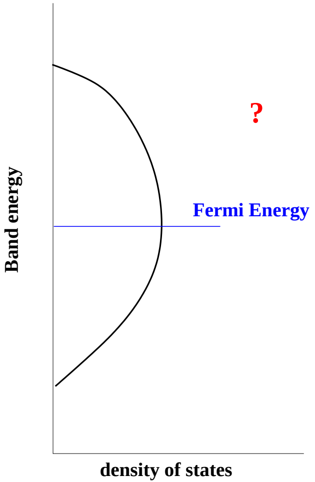
half filled band –> metal ??



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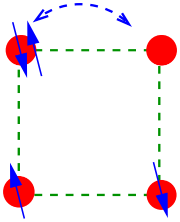
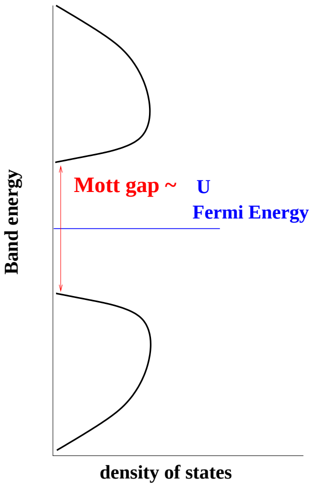


undoped compound

1 Electron per orbital

Mott insulator !



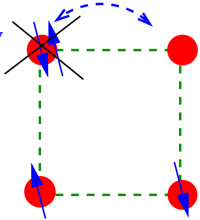
$\underline{\underline{t}} \sim 0.5$ eV

effective hopping strength

Coulomb energy U ~ 4 eV

has to be paid !

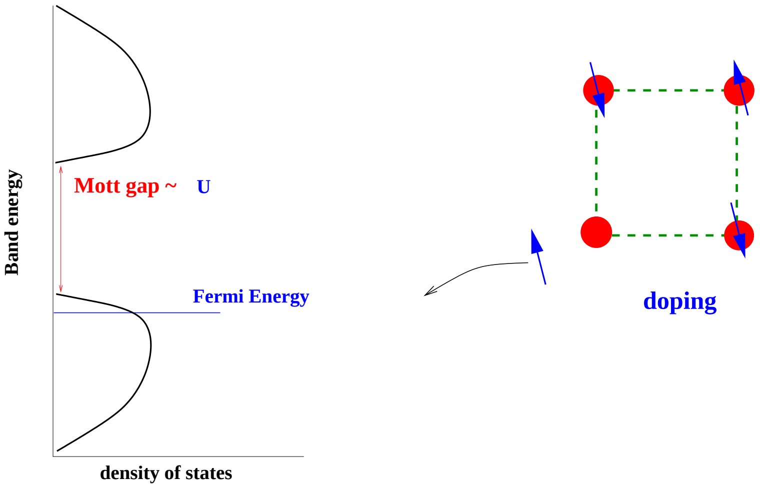
double occupation suppressed !

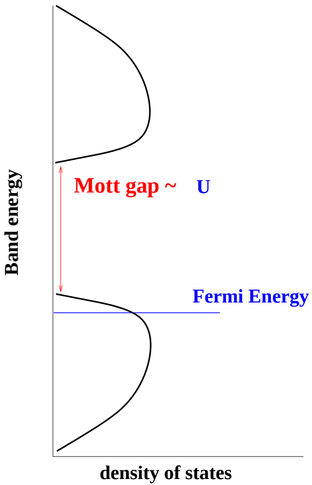


undoped compound

−> insulator

correlation effects are important!


Band energy
Mott gap ~ U
Fermi Energy
density of states
doping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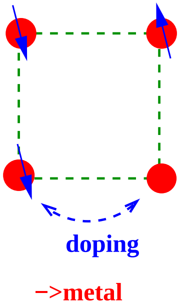
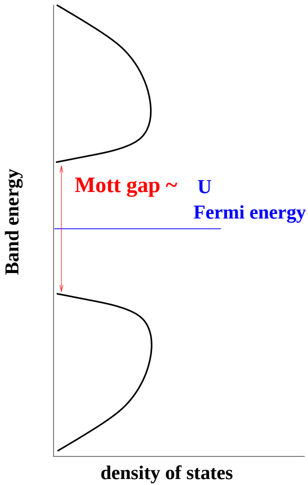
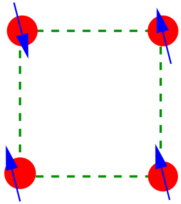

doping
->metal

magnetic properties

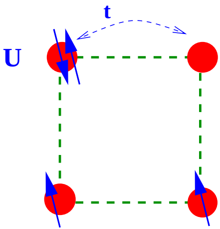




undoped compound

magnetic properties

virtual process
Delocalisation



kinetic energy is reduced
due to $\Delta x \Delta p \geq h$

magnetic properties

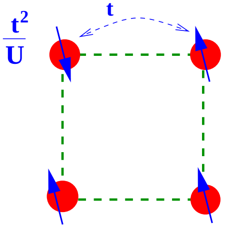
kinetic energy is reduced
due to $\Delta x \Delta p \geq h$

$\Delta E = -J \qquad \textbf{for}(S_1 = -S_2)$

$J \sim t^2/U \sim 150 meV$

Superexchange energy

virtual process
Delocalisation



magnetic properties

not allowed !

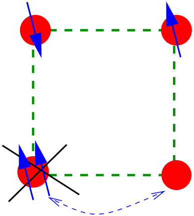
due to Pauli principle

$\Delta E = -J$ **for**$(S_1 = -S_2)$

$\Delta E = 0$ **for**$(S_1 = S_2)$

$J \sim t^2/U \sim 150 meV$

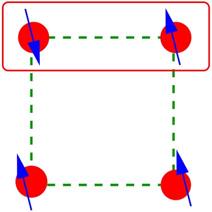
Superexchange energy



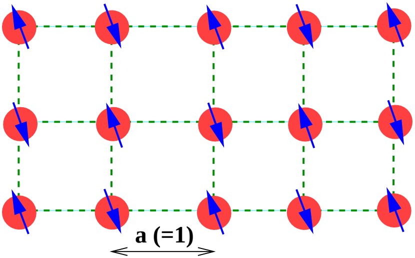
magnetic properties

Superexchange prefers antiparallel spin configuration

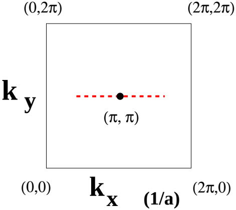
Antiferromagnetism

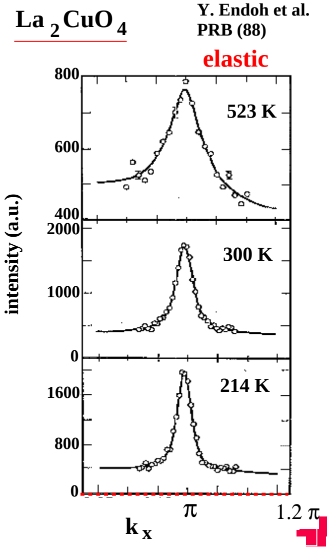


Antiferromagnetism at x=0 (no doping)



neutron scattering:





Outline

1. Introduction: Correlation in High-Temperature Superconductors
2. How do we deal with electron correlation?
   - Variational Cluster Approach (VCA)
   - Combination with *realistic ab initio* methods
3. Application: High-Temperature Superconductors: phase diagram
4. Application: Half-Metallic Ferromagnets
   - Nonquasiparticle states
   - CrO_2
   - VAs: a correlation-induced half-metal ?
5. Summary and Outlook

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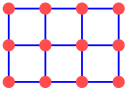
Appropriate numerical treatment of correlations?

1) "Exact" solution for a small cluster:

Quantum Monte Carlo
Exact diagonalisation (Lanczos)



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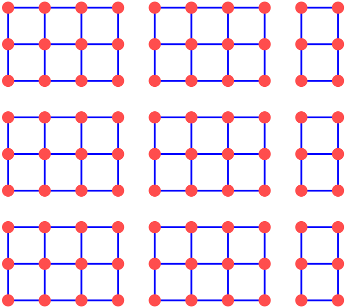


Split infinite lattice into small clusters

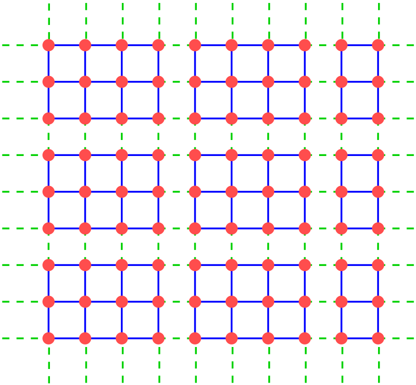
Appropriate numerical treatment of correlations?

1) "Exact" solution for a small cluster:

Quantum Monte Carlo
Exact diagonalisation (Lanczos)

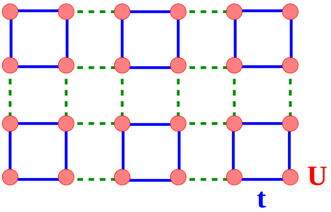
2) Perturbative treatment of intercluster hybridizations

Cluster−perturbation theory (CPT) (Gros,Valenti93; Senechal et al. 2000)



Split infinite lattice into small clusters

Cluster Perturbation Theory (CPT)



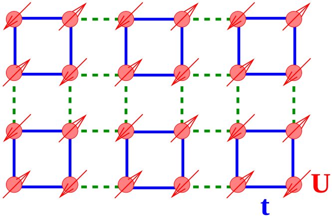
CPT:

$$H = H_{cl} + H_{intercl}$$

$$G_{CPT}^{-1} = G_{cl}^{-1} - T$$

(Gros, Valenti (93), Senechal et al. (00))

Variational Cluster Approach (VCA)



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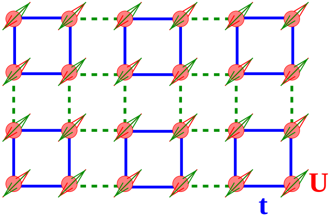
Variational CPT : Treatment of symmetry−broken phases:

$$H'_{cl} = H_{cl} + h_{field}$$

Variational Cluster Approach (VCA)



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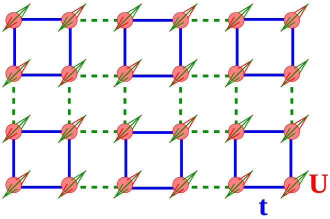

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How is h_{field} determined ?

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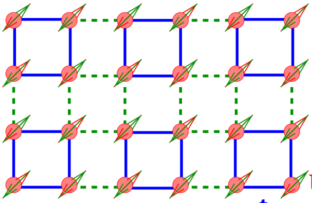

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"Minimisation" of Grand−canonical (SFA) potential

(Potthoff et al .03, Dahnken, Aichhorn, Hanke, Arrigoni,Potthoff 04)

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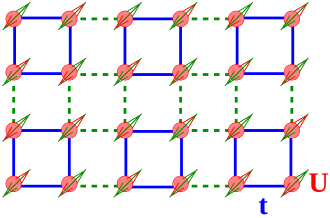

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"Minimisation" of Grand−canonical (SFA) potential

(Potthoff et al .03, Dahnken, Aichhorn, Hanke, Arrigoni,Potthoff 04)

Treatment of superconducting phase:

Senechal et al (05) Aichhorn, Arrigoni(05)
Arrigoni, Aichhorn(06);
Aichhorn,Arrigoni,Potthoff, Hanke (06)

$$h_{SC} = \frac{\Delta}{2} \sum_{R,R'} \eta(R-R')(c_{R,\uparrow} c_{R',\downarrow} + h.c.) ,$$

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Selfenergy Functional Approach (SFA)
(M. Potthoff 2003)

- Many-Body Fermionic Hamiltonian:

$$\boxed{H = H_0[G_0] \text{ (single-particle) } + U \text{ (interaction)}}$$

Selfenergy Functional Approach (SFA)
(M. Potthoff 2003)

- Many-Body Fermionic Hamiltonian: $\boxed{H = H_0[G_0] + U}$
- The Luttinger-Ward functional: $\boxed{\phi[G]}$ is Universal: depends only on U

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$$\Omega_{G_0}[\Sigma] = F[\Sigma] + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$$

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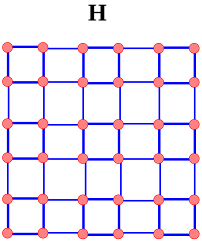
SFA − > Variational Cluster Approach
(M. Pottoff 2003) (C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, M. Potthoff 2004)

- Starting from H



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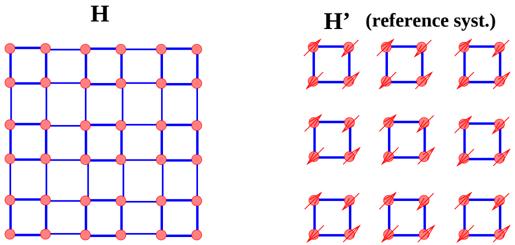
- Consider a Reference system: $\boxed{H' = H_0[G'_0] + U}$ (with the same U)



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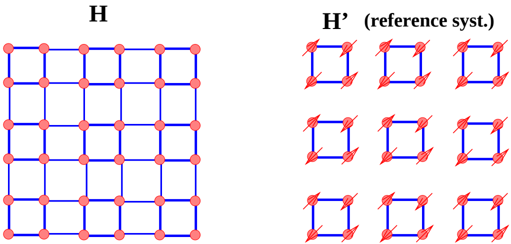
- $F[\Sigma]$ is the same for H' and H (universality)



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  $\Omega_{G'_0}[\Sigma]$ = grand-canonical potential

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- The exact Ω for H is then: (remember $\Omega = F + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$)

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- Caveat: $F[\Sigma]$ can be evaluated only for a restricted subspace of Σ
  e.g. the ones that can be obtained from the cluster (cluster local)

SFA $->$ Variational Cluster Approach

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- Caveat: $F[\Sigma]$ can be evaluated only for a restricted subspace of Σ
- The approximation consists in finding the optimum Σ within this subspace via $\boxed{\delta\Omega_{G_0}[\Sigma]/\delta\Sigma = 0}$

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SFA $->$ Variational Cluster Approach

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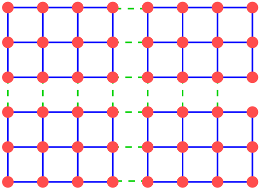
- Consider a Reference system: $H' = H_0[G_0'] + U$ (with the same U)
- $F[\Sigma]$ is the same for H' and H (universality)
- However: $\Omega_{G_0'}[\Sigma]$ (and thus $F[\Sigma]$) can be evaluated exactly for H': $\Omega_{G_0'}[\Sigma]$ = grand-canonical potential
- The exact Ω for H is then: (remember $\Omega = F + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1})$)

$$\Omega_{G_0}[\Sigma] = \Omega_{G_0'}[\Sigma] + \mathrm{Tr}\ln(-(G_0^{-1} - \Sigma)^{-1}) - \mathrm{Tr}\ln(-(G_0'^{-1} - \Sigma)^{-1})$$

- Caveat: $F[\Sigma]$ can be evaluated only for a restricted subspace of Σ
- The approximation consists in finding the optimum Σ within this subspace via $\delta\Omega_{G_0}[\Sigma]/\delta\Sigma = 0$
- This corresponds to the optimisation of the grand-canonical potential discussed before

Model calculations

Problem: models for
strongly correlated systems
are much too simplified:



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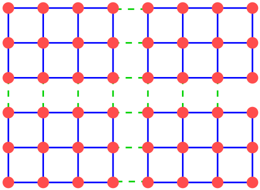

Effort is concentrated on the "big difficulty" electron correlations

phenomenological parameters
(hopping t, interaction U)

Model calculations **vs.** **Ab initio**

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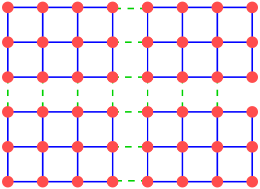

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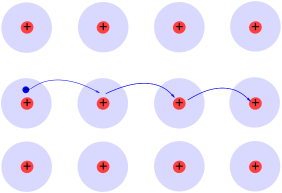
Calculations within density−functional theory (LDA,GGA,..)
(W. Kohn, W. Kohn+ L. J. Sham ... Wien2k)
often very accurate
start from "first principles"



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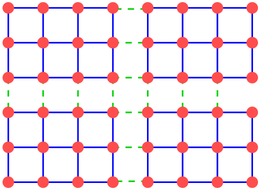

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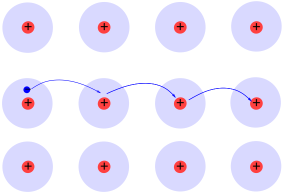

However:

Sometimes fail to explain some phenomena (High−Tc superc., magnetism, Mott−insul.) in which correlations are important

Model calculations vs. Ab initio

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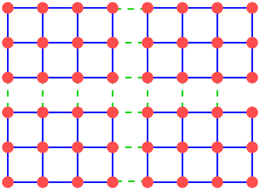

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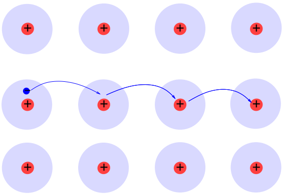


However:
Sometimes fail to explain some phenomena (High−Tc superc., magnetism, Mott−insul.) in which correlations are important

Can one combine the two ideas?

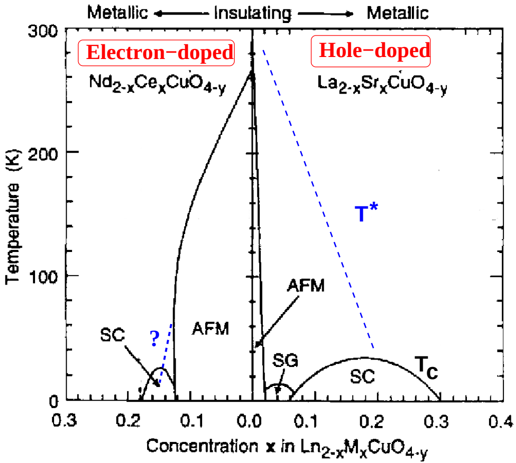
yes ! Combined approach:
LDA+ Dynamical Mean Field Theory
(Anisimov et al., Kotliar+Vollhardt, Held, ...)

Graz University of Technology

Outline

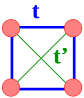
Graz University of Technology

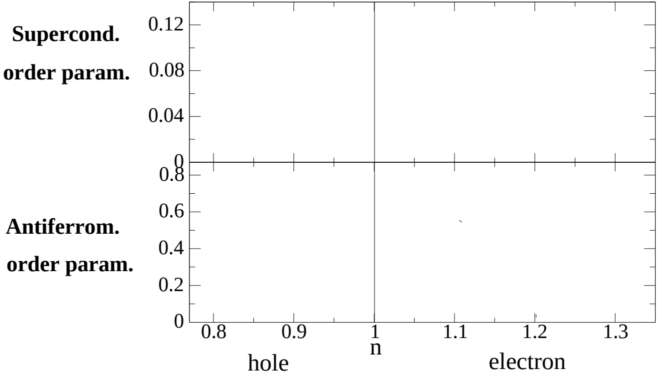
Electron and hole-doped High-Tc Superconductors



Order Parameters

Single−band Hubbard model U/t=8 t'/t = −0.3





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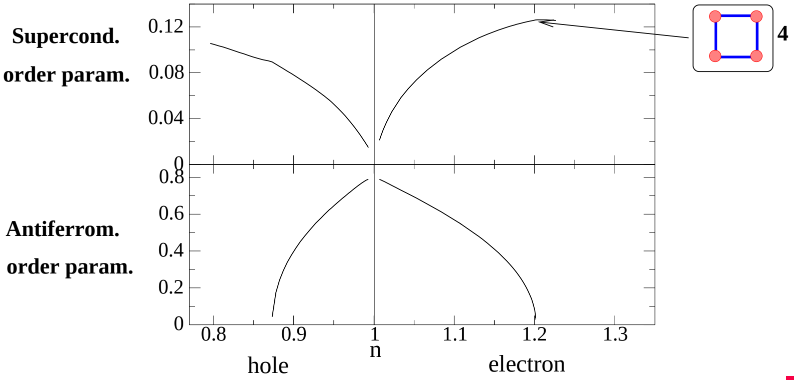

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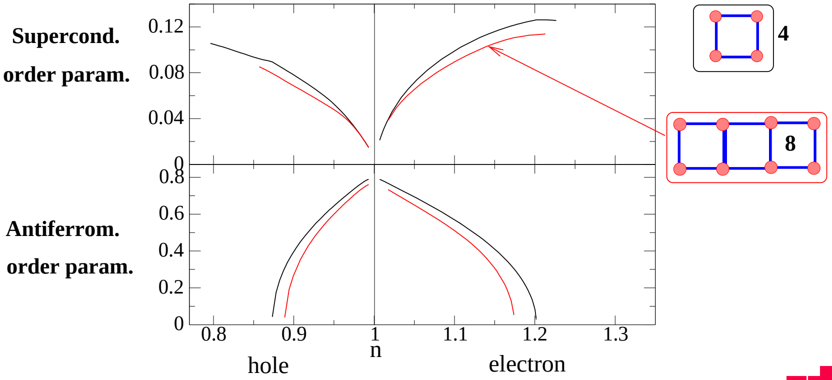
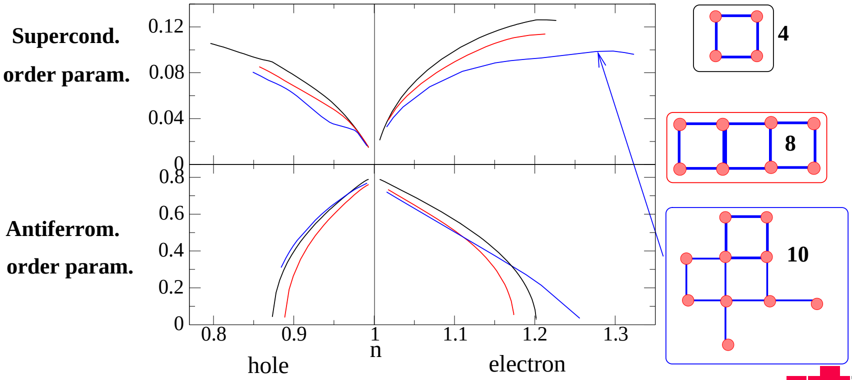


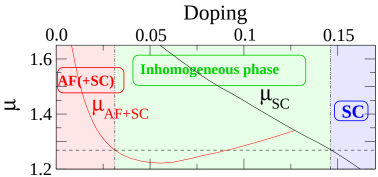
Order Parameters

Weak dependence on size of reference system (cluster)

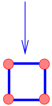


Transition Antiferromagnetism − Superconductivity

Hole doped



Reference System



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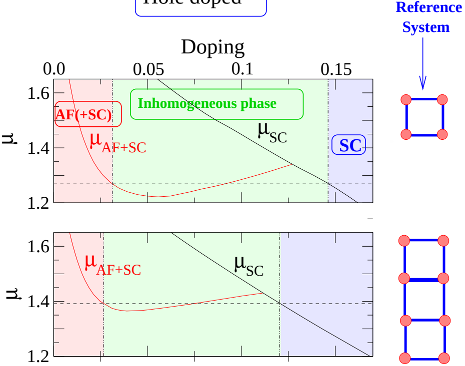

Aichhorn, Arrigoni, Hanke, Potthoff (2006)

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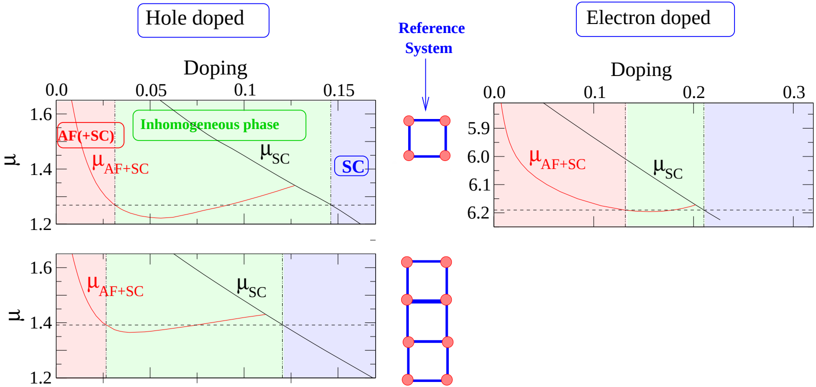

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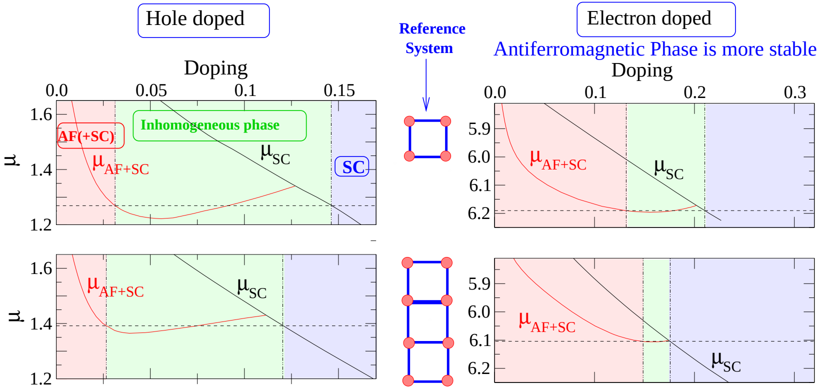
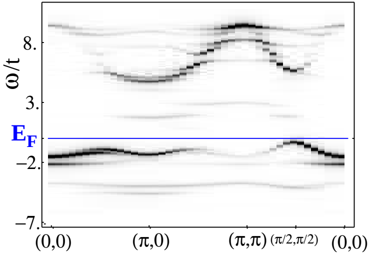


Aichhorn, Arrigoni, Hanke, Potthoff (2006)

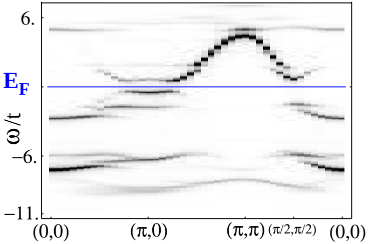
Evolution of single−particle spectrum vs doping

ARPES=Angle−Resolved−Photoemission−Spectroscopy (Aichhorn,Arrigoni EPL 2006)

hole doped x=0.022



electron doped $x=0.13 \sim x_c$



holes first enter at (π/2,π/2)

electron first enter at (π,0)

(In agreement with ARPES results for NdCeCuO Armitage et al. 2001,2002)

(U/t=8, t'/t = −0.3)

Graz University of Technology

Outline

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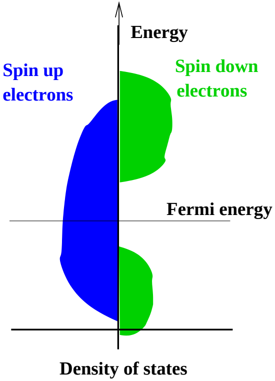
Half−Metallic Ferromagnets



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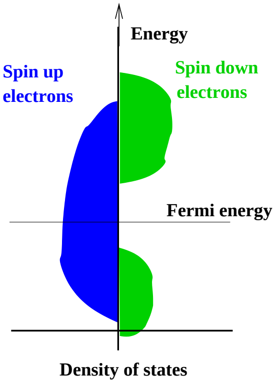
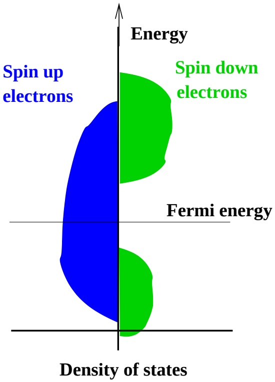


Current is carried by electrons at the Fermi surface

no contribution from spin down electrons!

Half−Metallic Ferromagnets



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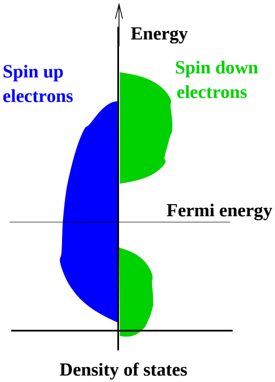
Current is (in principle) 100% spin polarized

Half−Metallic ferromagnets:
(e.g. CrO_2 NiMnSb Sr_2FeMoO_2)

R.A. de Groot el al. (1983)

Half−Metallic Ferromagnets



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Applications in spin electronics
Magnetoresistive devices, Quantum Computer

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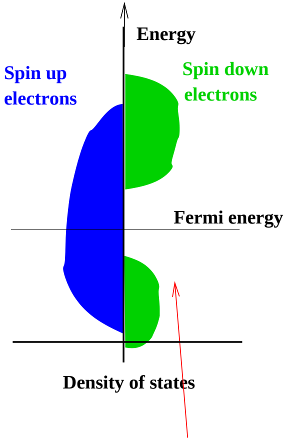

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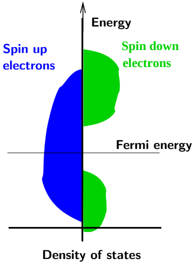
However: these are results obtained by neglecting correlations!

Correlation effects in half-metallic ferromagnets: formation of states within the gap

"non-quasiparticle states"

V. Yu. Irkhin and M. I. Katsnelson (90)
D.M. Edwards and J. A. Hertz (73)



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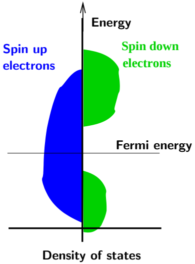

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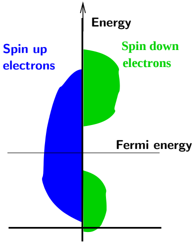

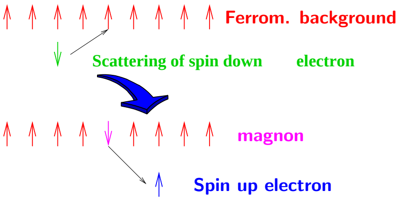

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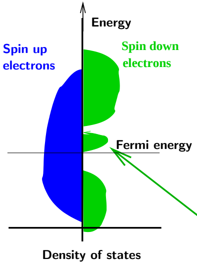

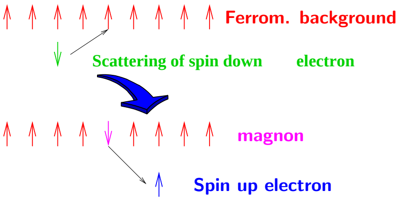

Spin up and spin down electron mix due to scattering with magnons

non−quasiparticle density of states in the gap

Correlation effects in half-metallic ferromagnets: formation of states within the gap

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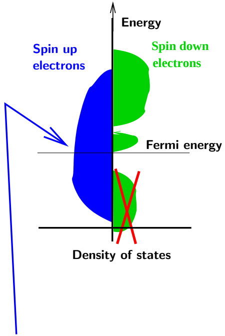

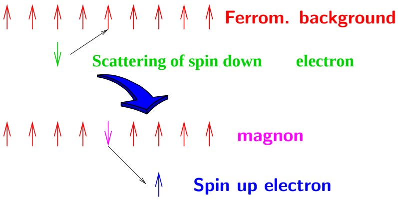

$(N_\uparrow = N+1, N_\downarrow = 0)$ **has spin:** $\boxed{S = \frac{(N+1)}{2}, S_z = S}$

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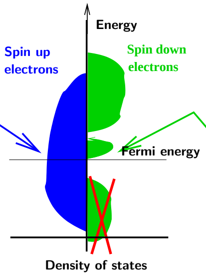
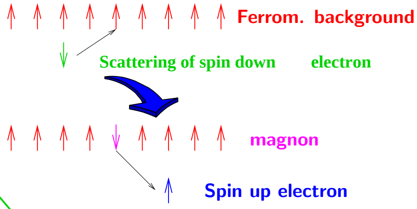


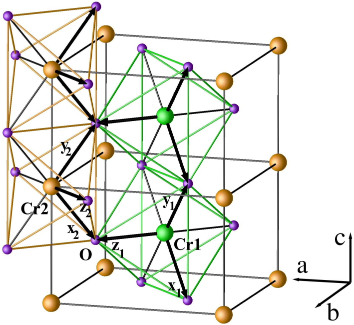


$(N_\uparrow = N+1, N_\downarrow = 0)$ **has spin:** $\boxed{S = \frac{(N+1)}{2}, S_z = S}$

State with $\boxed{S = \frac{(N+1)}{2}, S_z = S - 1}$,

i. e. $(N_\uparrow = N, N_\downarrow = 1)$ **must have the same energy**

CrO$_2$

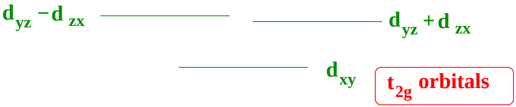


First predicted to be a half-metallic ferromagnet by K.-H. Schwarz, J. Phys. F 19, L211 (1986)

Optics, transport: I. I. Mazin, D. J. Singh, and C. Ambrosch-Draxl, Phys. Rev. B (1999)

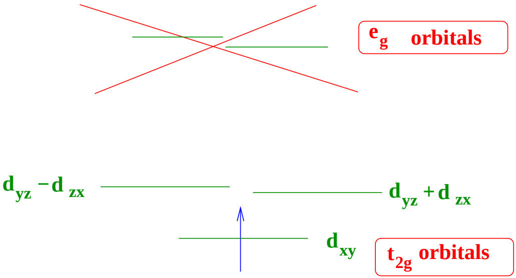
. . . and many others . . .

Building up the model: Relevant orbitals in CrO_2



Cr 3d Orbitals,

Building up the model: Relevant orbitals in CrO$_2$

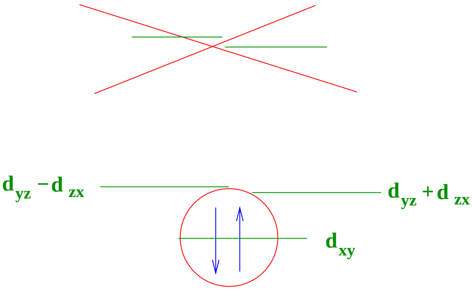


Cr 3d Orbitals, crystal-field splitting

Effective model restricted to t_{2g} orbitals of Cr.
Parameters of the model obtained
AB INITIO by downfolding of LDA bands
downfolding = integrating out high-energy bands

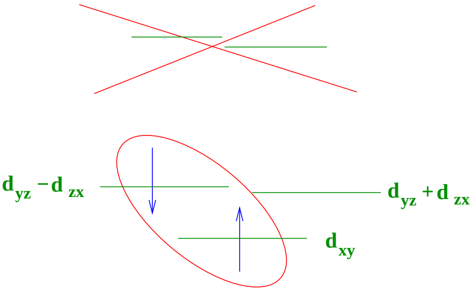
Andersen et al. (2000) ; Yamasaki et al. (2006)

Building up the model: Relevant orbitals in CrO_2



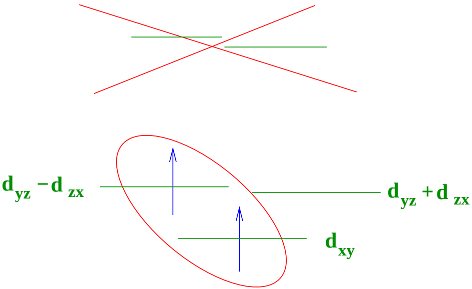
Interaction Energy $U \approx 3eV$

Building up the model: Relevant orbitals in CrO_2



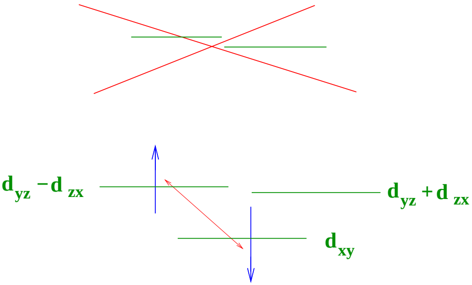
Interaction Energy $U' = U - 2J$

Building up the model: Relevant orbitals in CrO$_2$



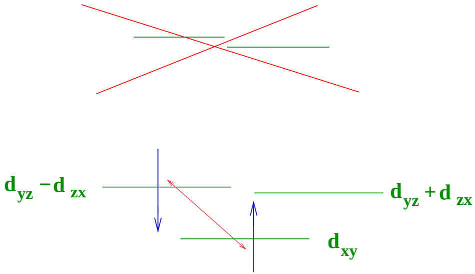
Interaction Energy $U' - J$ (Hund's rule $J \approx 0.9eV$)

Building up the model: Relevant orbitals in CrO$_2$



Spin-flip J: spin-rotation invariance

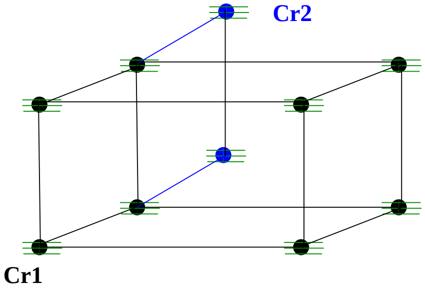
Building up the model: Relevant orbitals in CrO$_2$



Spin-flip J: spin-rotation invariance

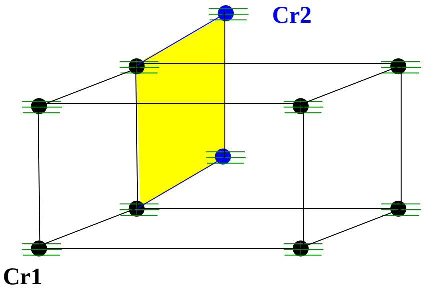
Model

Multi-orbital Hubbard model



Model

Cluster



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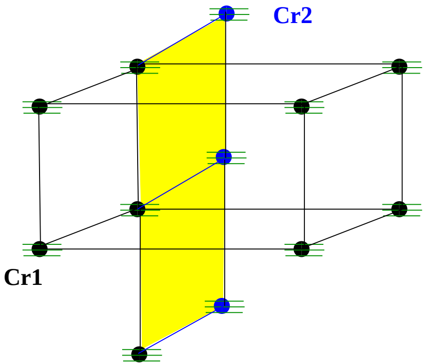
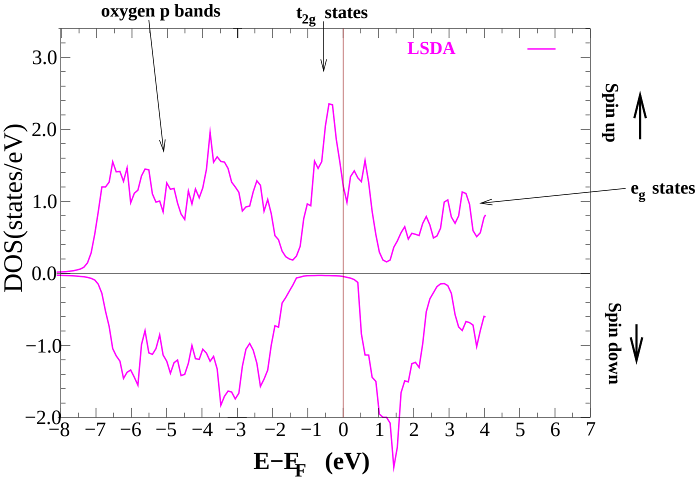


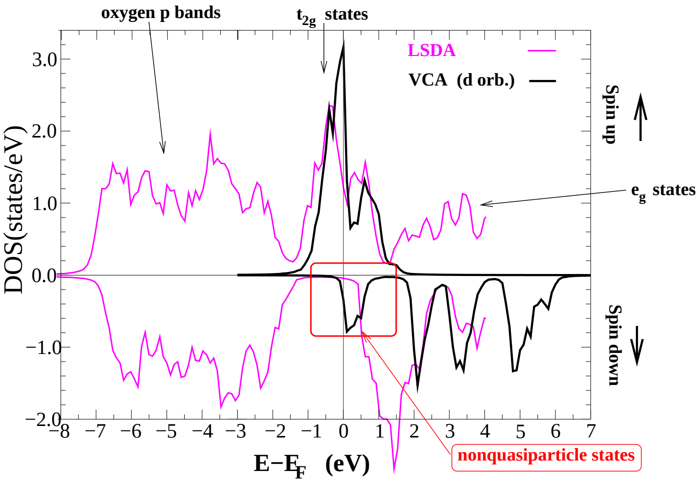
Results: Spin-resolved density of states for CrO_2:

Spin-resolved LDA



Results: Spin-resolved density of states for CrO_2:

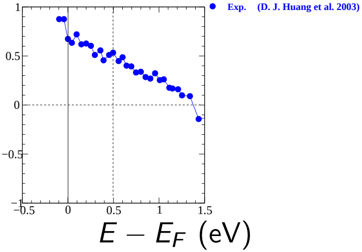
VCA:Our calculation



Energy-Dependent Spin Polarisation

Spin Polarisation

$$\frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$



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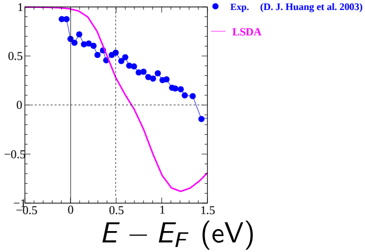

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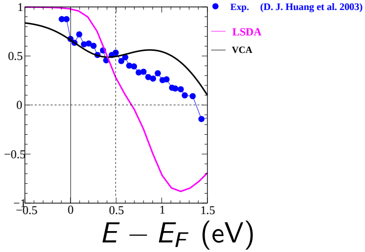

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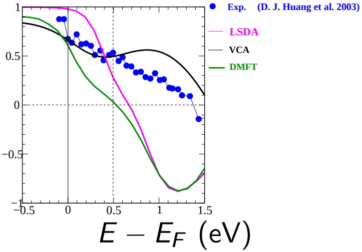
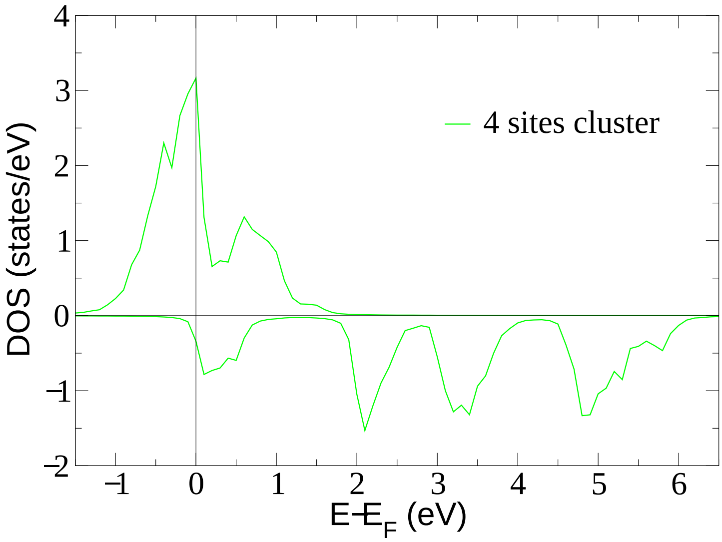


H. Allmaier et al. (Phys. Rev. B 2007)

VCA: Dependence on size of reference system (cluster)



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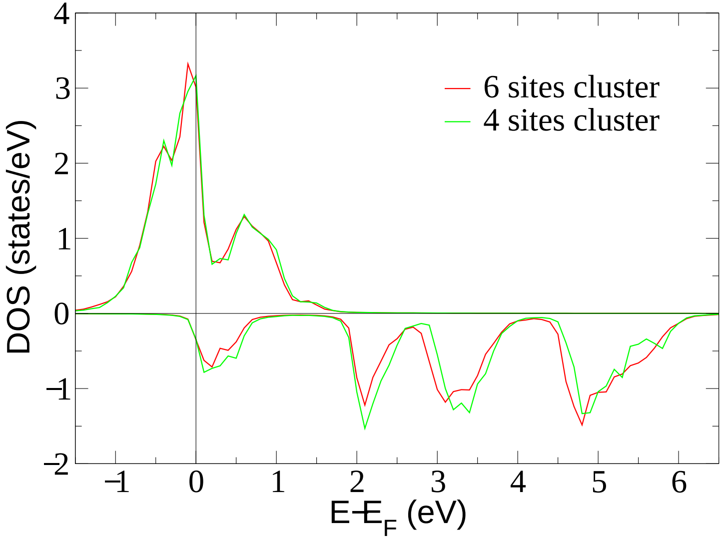

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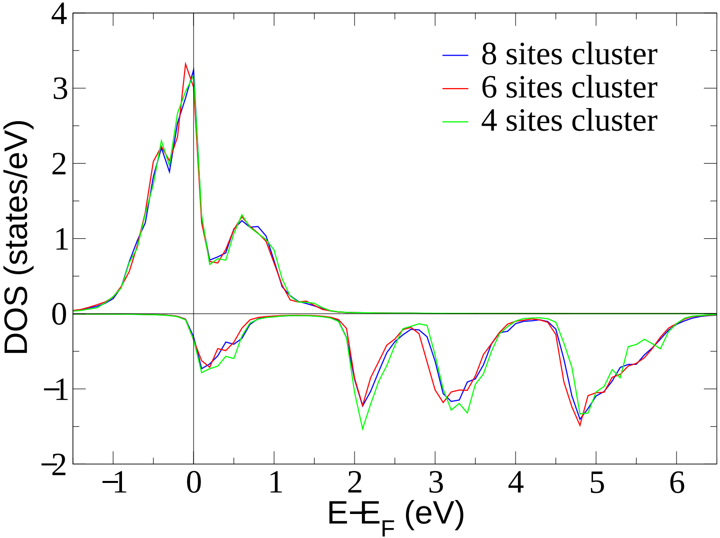

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Electron Correlation is bad for half metallicity?

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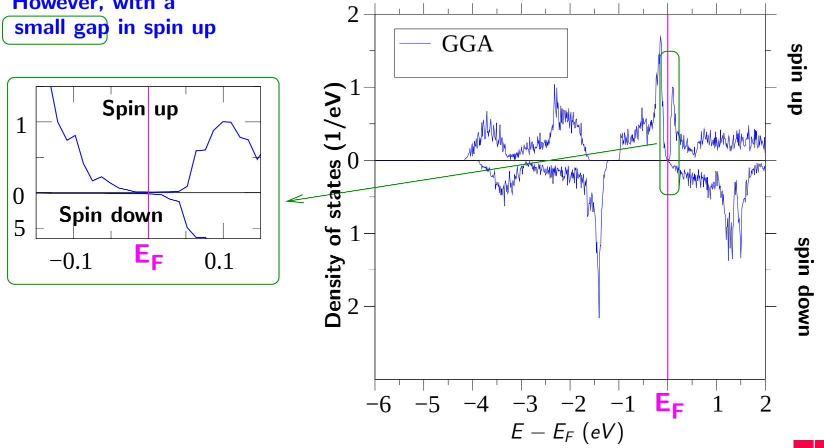

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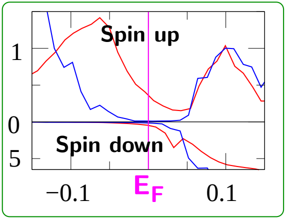

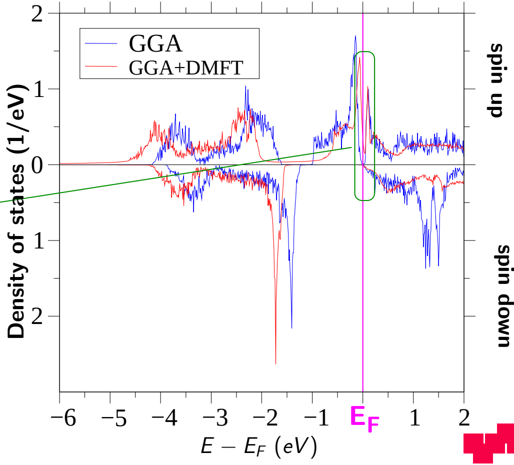

Correlation effects fill the gap in spin up making VAs a half-metallic ferromagnet

Outline

Thanks to

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DFG: FOR 538 “Doping dependence of phase transition and ordering phenomena in copper-oxyde superconductors”

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    - Surface effects (HMF)
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