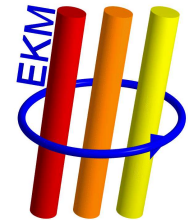
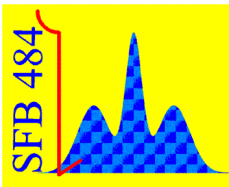


How to quantify correlation in correlated electron system

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Collaboration

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Jan Kunes - Prague, Academy of Sciences

Aim of this talk

CORRELATION

- What is it?
- How to quantify it?

Correlation

- **Correlation** [lat.]: con+relatio (“with relation”)
- Mathematics, Statistics, Natural Science:

$$\langle xy \rangle \neq \langle x \rangle \langle y \rangle$$

The term **correlation** stems from mathematical statistics and means that two distribution functions, $f(x)$ and $g(y)$, **are not independent** of each other.

- In many body physics: **correlations** are effects beyond factorizing approximations

$$\langle \rho(r, t) \rho(r', t') \rangle \approx \langle \rho(r, t) \rangle \langle \rho(r', t') \rangle,$$

as in Weiss or Hartree-Fock mean-field theories

Spatial and temporal correlations everywhere



car traffic

air traffic

human traffic

electron traffic

more

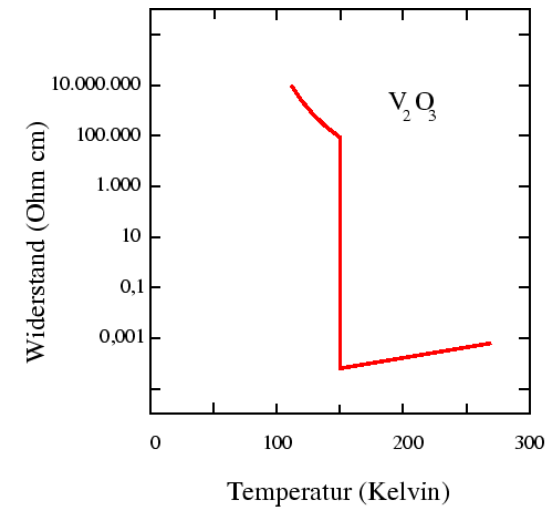


Abb. 3: Beispiel eines Metall-Isolator-Übergangs: Bei Abkühlung unter eine Temperatur von ca. 150 Kelvin erhöht sich der elektrische Widerstand von metallischem Vanadiumoxid (V_2O_3) schlagartig um das Einhundertmillionenfache (Faktor 10^8) – das System wird zum Isolator.

Spatial and temporal correlations neglected

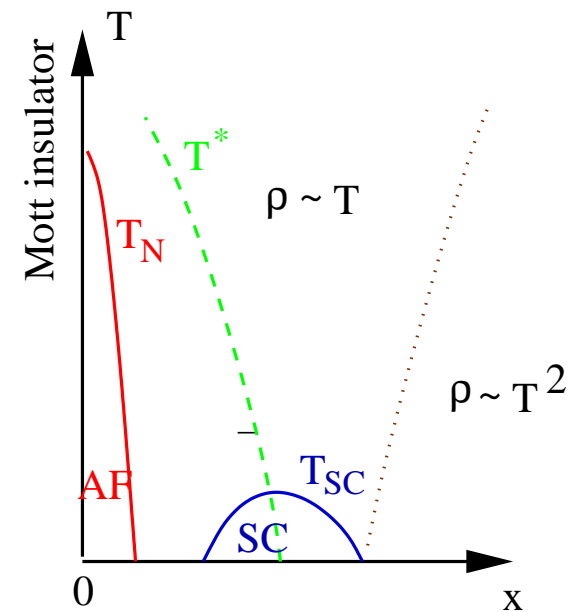
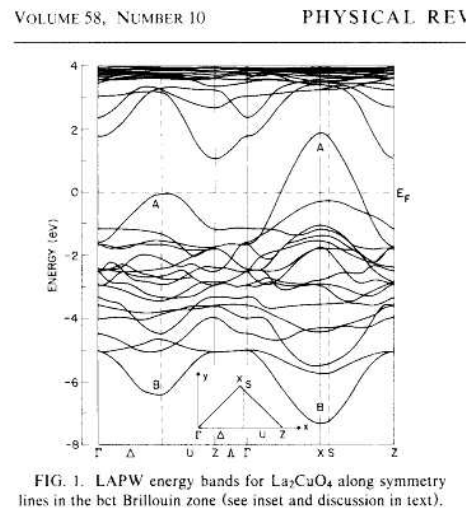
time/space average insufficient

$$\langle \rho(r, t) \rho(r', t') \rangle \approx \langle \rho(r, t) \rangle \langle \rho(r', t') \rangle = \text{disaster!}$$



Spatial and temporal correlations neglected

Local density approximation (LDA) disaster in HTC



LaCuO_4 Mott (correlated) insulator predicted to be a metal

Partially cured by (AF) long-range order ... but correlations are still missed

Correlated electrons

Periodic Table of Elements

1	IA	1	H	IIA	2	He	0																													
2	3	Li	4	Be	5	B	6	C	7	N	8	O	9	F	10	Ne																				
3	11	Na	12	Mg	III B	13	Al	IV B	14	Si	V B	15	P	VI B	16	S	VII B	17	Cl	18	Ar															
4	19	K	20	Ca	21	Sc	22	Ti	23	Y	24	Cr	25	Mn	26	Fe	27	Co	28	Ni	29	Cu	30	Zn	31	Ga	32	Ge	33	As	34	Se	35	Br	36	Kr
5	37	Rb	38	Sr	39	Y	40	Zr	41	Nb	42	Mo	43	Tc	44	Ru	45	Rh	46	Pd	47	Ag	48	Cd	49	In	50	Sn	51	Sb	52	Te	53	I	54	Xe
6	55	Cs	56	Ba	*La	57	Hf	72	Ta	73	W	74	Re	75	Os	76	Ir	77	Pt	78	Au	79	Hg	80	81	Tl	82	Pb	83	Bi	84	Po	85	At	86	Rn
7	87	Fr	88	Ra	+Ac	89	Rf	104	Ha	105	106	107	108	109	110																					









* Lanthanide Series

58	59	60	61	62	63	64	65	66	67	68	69	70	71
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu

+ Actinide Series

90	91	92	93	94	95	96	97	98	99	100	101	102	103
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Legend - click to find out more...

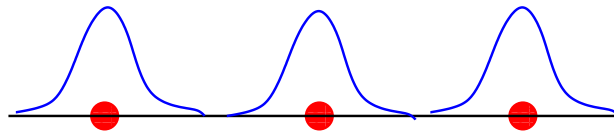
H - gas	Li - solid	Br - liquid	Tc - synthetic
 Non-Metals	 Transition Metals	 Rare Earth Metals	 Halogens
 Alkali Metals	 Alkali Earth Metals	 Other Metals	 Inert Elements

Narrow d,f-orbitals/bands → strong electronic correlations

Electronic bands in solids

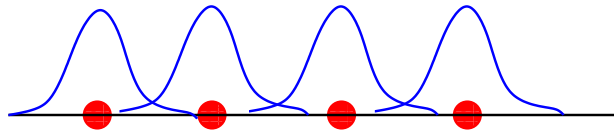
Wave function overlap $\sim t_{ij} = \langle i | \hat{T} | j \rangle \rightarrow |E_{\mathbf{k}}| \sim \text{bandwidth } W$

Band insulators, e.g. NaCl



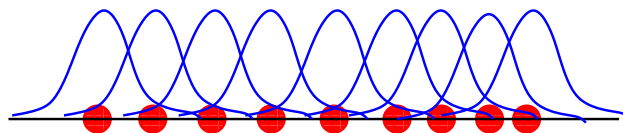
Atomic levels, **localized electrons** $|\mathbf{R}_i\sigma\rangle$

Correlated metals, e.g. Ni, V_2O_3 , Ce



Narrow bands, $|\mathbf{R}_i\sigma\rangle \leftrightarrow |\mathbf{k}\sigma\rangle$

Simple metals, e.g. Na, Al



Broad bands, **extended Bloch waves** $|\mathbf{k}\sigma\rangle$

Electronic bands in solids

Mean time τ spent by the electron on an atom in a solid depends on the band width W

$$\text{group velocity } v_{\mathbf{k}} \approx \frac{\text{lattice spacing}}{\text{mean time}} = \frac{a}{\tau}$$

Heisenberg principle $W\tau \sim \hbar$

$$\frac{a}{\tau} \sim \frac{aW}{\hbar} \implies \tau \sim \frac{\hbar}{W}$$

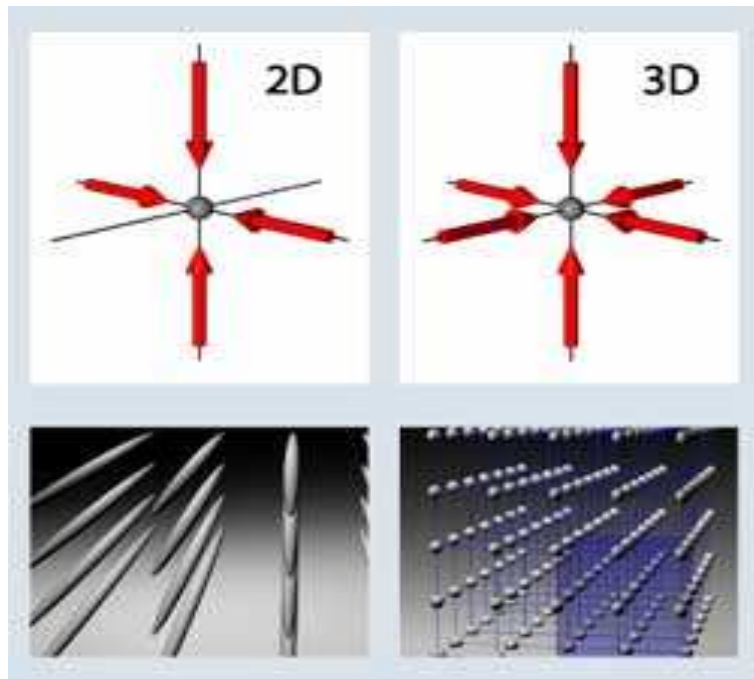
Small W means longer interaction with another electron on the same atom

Strong electronic correlations

Optical lattices filled with bosons or fermions

Greiner et al. 02, and other works

atomic trap and standing waves of light create optical lattices $a \sim 400 - 500nm$

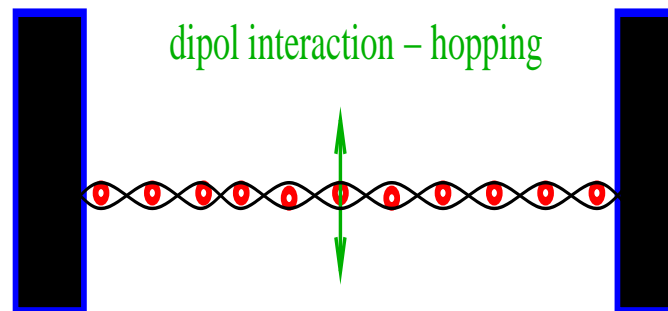


alkali atoms with ns^1 electronic state $J = S = 1/2$

$$\mathbf{F} = \mathbf{J} + \mathbf{I}$$

^{87}Rb , ^{23}Na , ^7Li - $I = 3/2$: effective **bosons**

^6Li - $I = 1$, ^{40}K - $I = 4$: effective **fermions**



atom scattering - Hubbard U

$$E_{int}^{solid} \sim 1 - 4eV \sim 10^4 K, \quad E_{kin}^{solid} \sim 1 - 10eV \sim 10^5 K$$

$$E_{kin}^{optical} \sim E_{int}^{optical} \sim 10kHz \sim 10^{-6} K$$

Quantifying correlations

**How many correlation is there
in correlated electron systems?**

We need information theory tools to address this issue.

Classical vs. Quantum Information Theory

Probability distribution vs. **Density operator**

$$p_k \longleftrightarrow \hat{\rho} = \sum_k p_k |k\rangle \langle k|$$

Shannon entropy vs. **von Neumann entropy**

$$I = -\langle \log_2 p_k \rangle = -\sum_k p_k \log_2 p_k \longleftrightarrow S = -\langle \ln \hat{\rho} \rangle = -Tr[\hat{\rho} \ln \hat{\rho}]$$

Two correlated (sub)systems have **relative entropy**

$$I = I_1 + I_2 - \Delta I \longleftrightarrow S = S_1 + S_2 - E$$

$$\Delta I(p_{kl} || p_k p_l) = -\sum_{kl} p_{kl} \left[\log_2 \frac{p_{kl}}{p_k p_l} \right] \longleftrightarrow E(\hat{\rho} || \hat{\rho}_1 \otimes \hat{\rho}_2) = -Tr[\hat{\rho}(\ln \hat{\rho} - \ln \hat{\rho}_1 \otimes \hat{\rho}_2)]$$

Relative entropy vanishes in the absence of correlations (product states)

Asymptotic distinguishability

Quantum Sanov theorem:

Probability P_n that a state $\hat{\sigma}$ is not distinguishable from a state $\hat{\rho}$ in n measurements on $\hat{\sigma}$, when $n \gg 1$, is

$$P_n \approx e^{-nE(\hat{\rho}||\hat{\sigma})}.$$

Relative entropy $E(\hat{\rho}||\hat{\sigma})$ as a 'distance' between quantum states.

We calculate

- von Neumann entropies and
- relative entropies

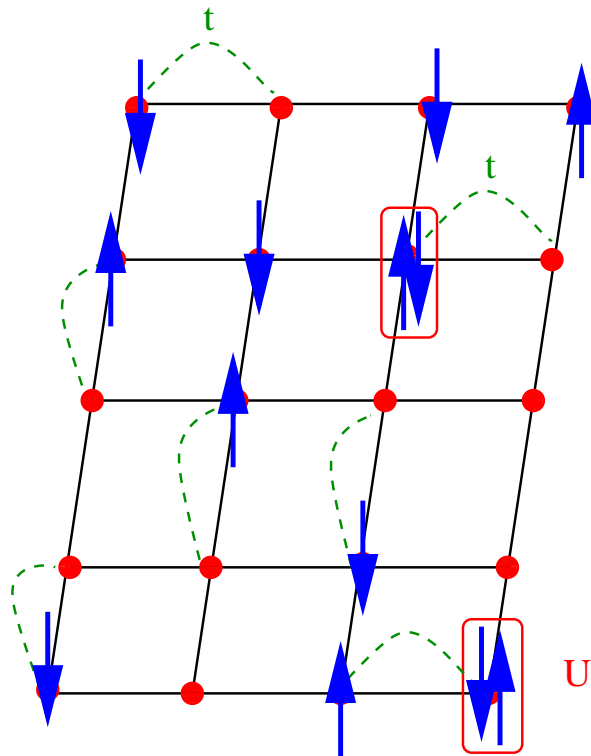
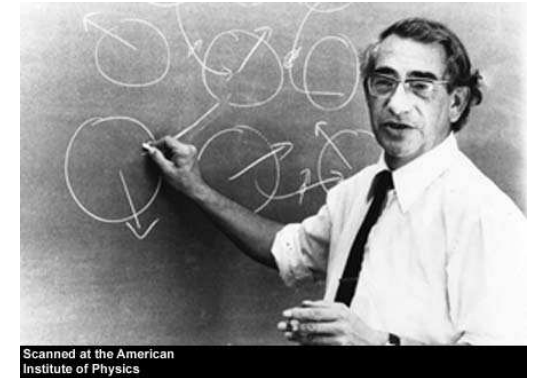
for and between different correlated and uncorrelated (product) states of the Hubbard model.

Correlated fermions on crystal and optical lattices

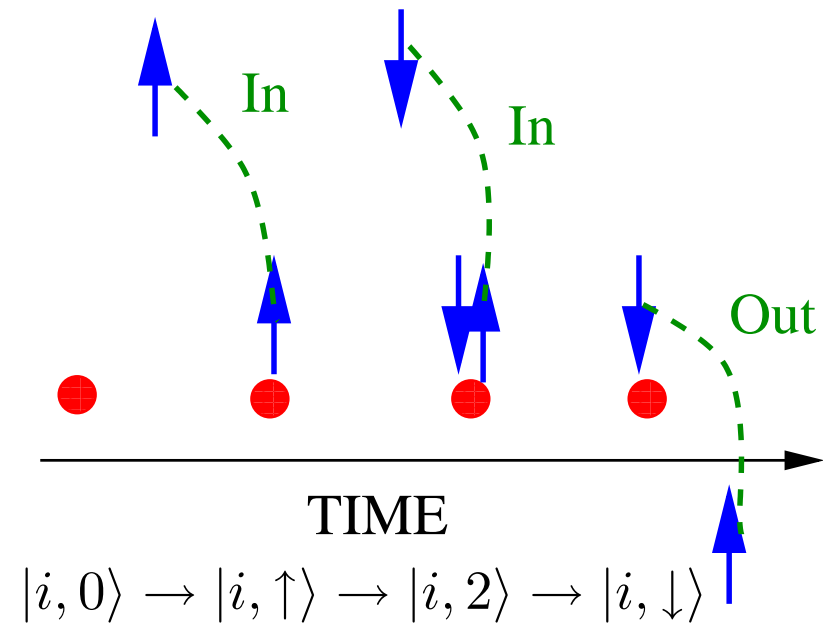
$$H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

fermionic Hubbard model

P.W. Anderson, J. Hubbard, M. Gutzwiller, J. Kanamori, 1960-63



Local Hubbard physics



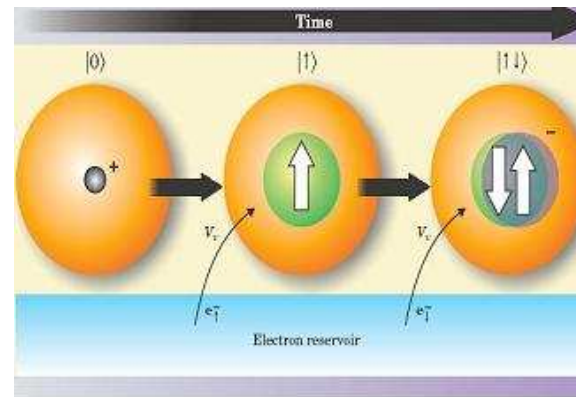
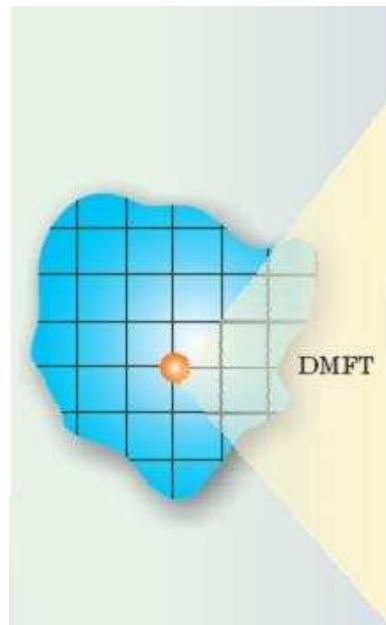
Origin of genuine many-body correlation

$$H = H^{\text{hopping}} + H_{\text{loc}}^{\text{interaction}}$$

$$[H^{\text{hopping}}, H_{\text{loc}}^{\text{interaction}}] \neq 0$$

DMFT for lattice fermions

Replace (map) full many-body lattice problem by a single-site coupled to dynamical reservoir and solve such problem self-consistently



All local dynamical correlations included exactly

Space correlations neglected - mean-field approximation

Local Entropy and Local Relative Entropy

Local density operator:

$$\hat{\rho}_i = \text{Tr}_{j \neq i} \hat{\rho}$$

Local entropy:

$$S[\hat{\rho}_i] = - \sum_{k=1}^4 p_k \ln p_k,$$

where

$$p_1 = \langle (1-n_{i\uparrow})(1-n_{i\downarrow}) \rangle, \quad p_2 = \langle n_{i\uparrow}(1-n_{i\downarrow}) \rangle, \quad p_3 = \langle (1-n_{i\uparrow})n_{i\downarrow} \rangle, \quad p_4 = \langle n_{i\uparrow}n_{i\downarrow} \rangle.$$

A.Rycerz, Eur. Phys. J B **52**, 291 (2006);

D. Larsson and H. Johannesson, Phys. Rev. A **73**, 042320 (2006)

Generalized equations for [local relative entropy](#).

KB, D. Vollhardt, '09

Expectation values for correlated states are determined from DMFT solution and for uncorrelated states from Hartree-Fock solutions.

Local Entropy and Local Relative Entropy

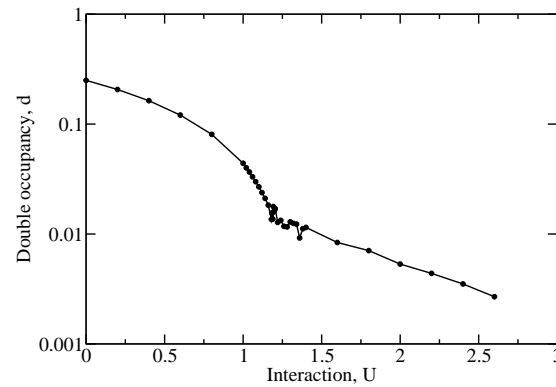
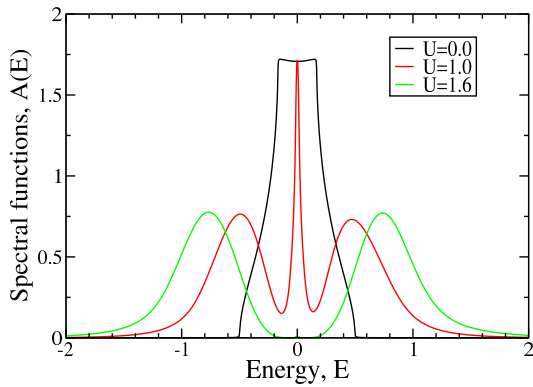
Local entropy

$$S(\hat{\rho}) = -Tr_A \hat{\rho}_A \log \hat{\rho}_A = - \sum_{\alpha} p_{\alpha} \log p_{\alpha}.$$

Local relative entropy

$$E(\hat{\rho}||\hat{\sigma}) = -Tr_A \hat{\rho}_A (\log \hat{\rho}_A - \log \hat{\sigma}_A) = - \sum_{\alpha} p_{\alpha} (\log p_{\alpha} - \log p_{\alpha}^{\sigma}).$$

Correlation and Mott Transition



$$S(\hat{\rho}) = -Tr[\hat{\rho} \ln \hat{\rho}]$$

$$E(\hat{\rho}||\hat{\sigma}) = -Tr[\hat{\rho} \ln \hat{\rho} - \hat{\rho} \ln \hat{\sigma}]$$

$$S = S(\hat{\rho}_{DMFT})$$

$$S_1 = S(\hat{\rho}_0)$$

$$S_2 = S(\hat{\rho}_a)$$

Product (HF) states:

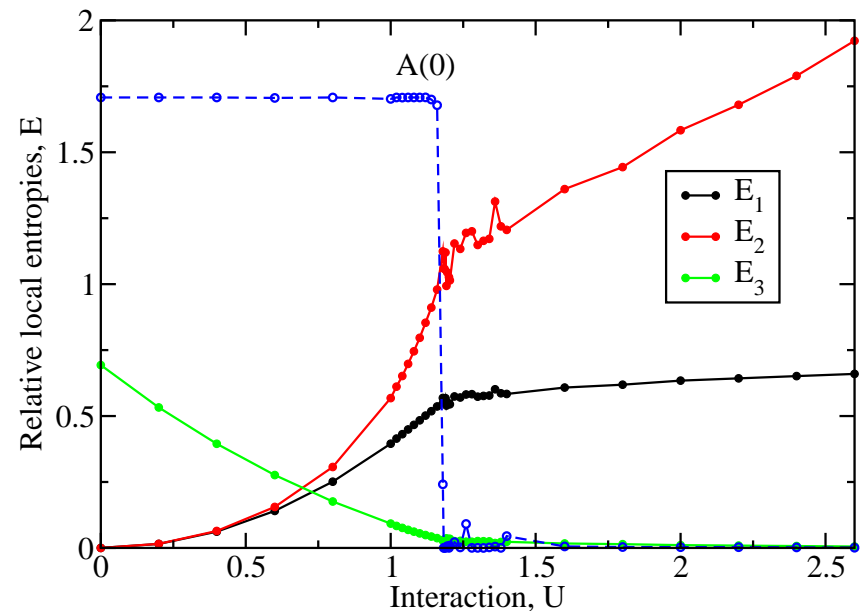
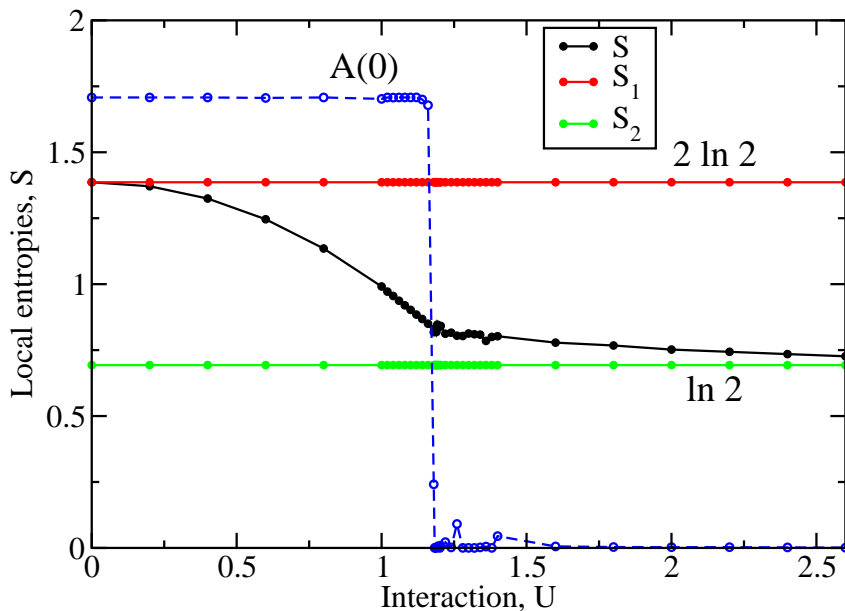
$$|0\rangle = \prod_{k\sigma}^{k_F} a_{k\sigma}^\dagger |v\rangle - U = 0 \text{ limit}$$

$$|a\rangle = \prod_i^{N_L} a_{i\sigma_i}^\dagger |v\rangle - \text{atomic limit}$$

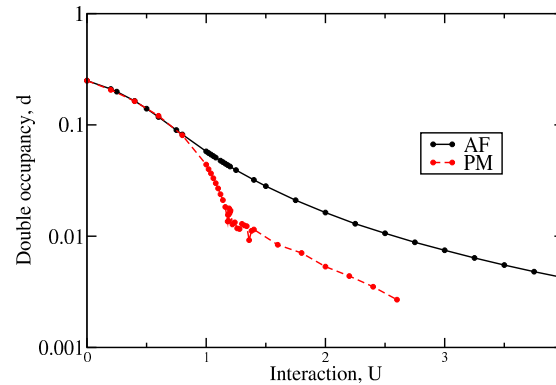
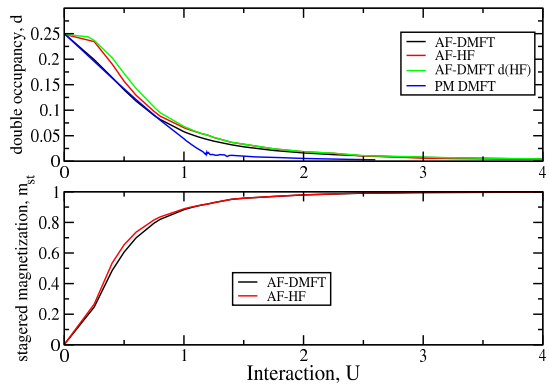
$$E_1 = E(\hat{\rho}_{DMFT}||\hat{\rho}_0)$$

$$E_2 = E(\hat{\rho}_0||\hat{\rho}_{DMFT})$$

$$E_3 = E(\hat{\rho}_a||\hat{\rho}_{DMFT})$$



Correlation and Antiferromagnetic Order



$$S(\hat{\rho}) = -Tr[\hat{\rho} \ln \hat{\rho}]$$

$$E(\hat{\rho}||\hat{\sigma}) = -Tr[\hat{\rho} \ln \hat{\rho} - \hat{\rho} \ln \hat{\sigma}]$$

$$S = S(\hat{\rho}_{DMFT})$$

$$S_0 = S(\hat{\rho}_0)$$

$$S_a = S(\hat{\rho}_a)$$

Product (HF) states:

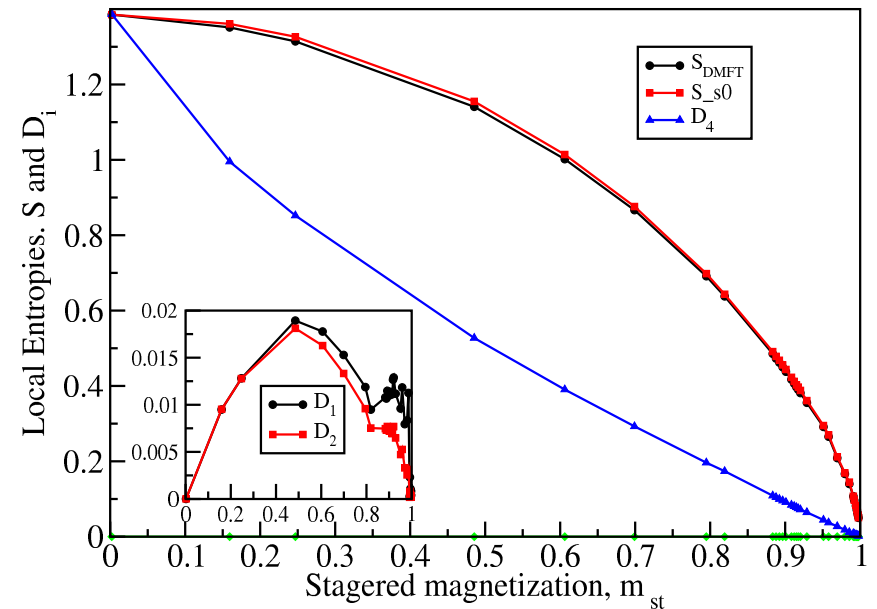
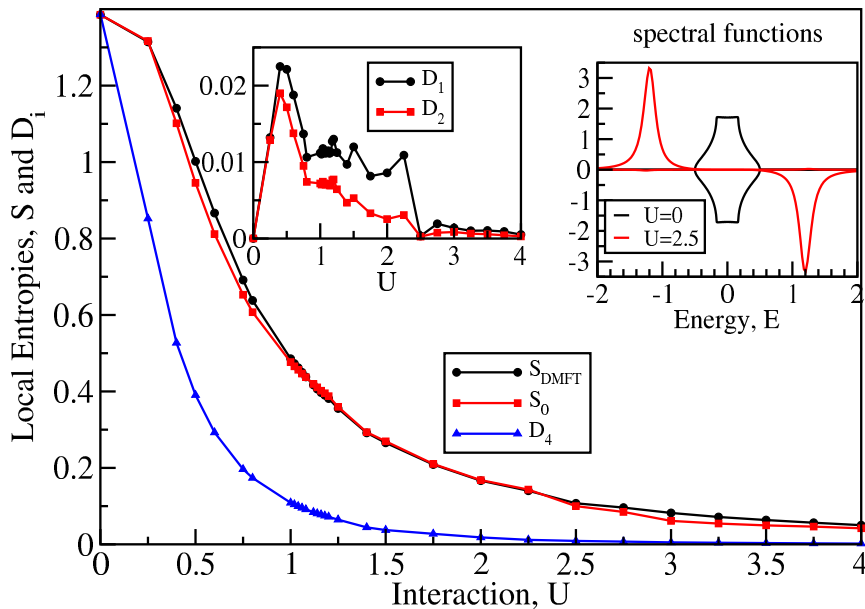
$$|0\rangle = \prod_{k \in (A,B)}^{k_F} a_{k_A \uparrow}^\dagger a_{k_B \downarrow}^\dagger |v\rangle - \text{Slater limit}$$

$$|a\rangle = \prod_{i \in (A,B)}^{N_L} a_{i_A \uparrow}^\dagger a_{i_B \downarrow}^\dagger |v\rangle - \text{Heisenberg limit}$$

$$D_1 = E(\hat{\rho}_{DMFT}||\hat{\rho}_0)$$

$$D_2 = E(\hat{\rho}_0||\hat{\rho}_{DMFT})$$

$$D_4 = E(\hat{\rho}_a||\hat{\rho}_{DMFT})$$



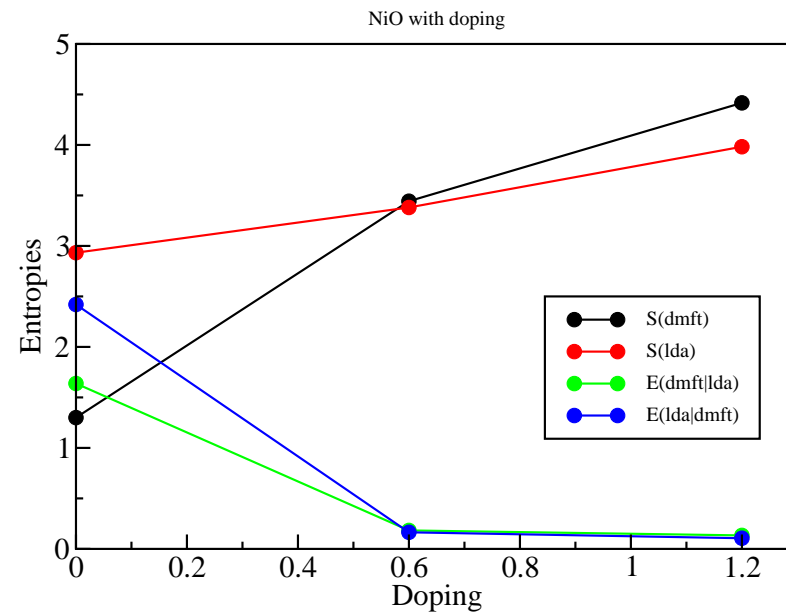
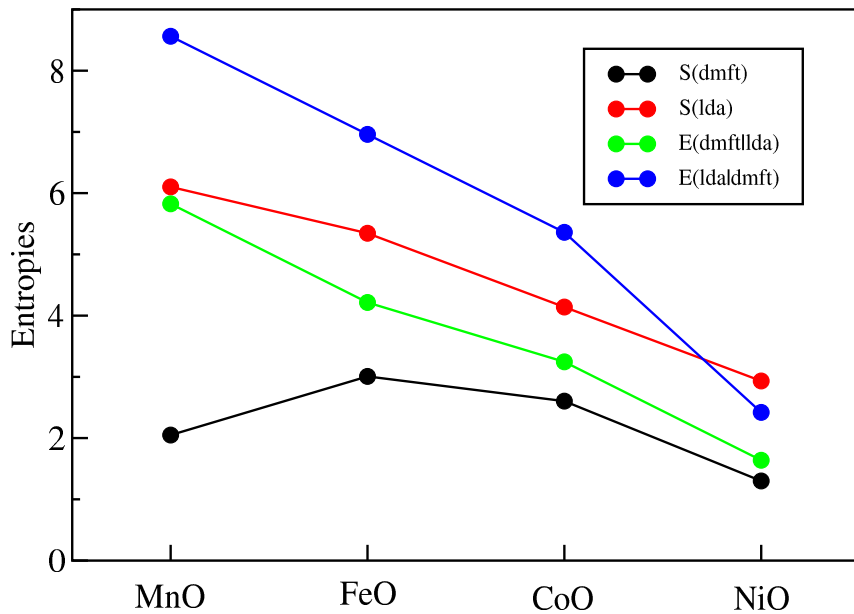
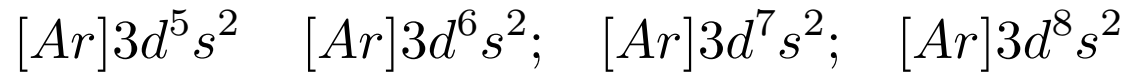
Correlation in Transition Metal-Oxides

MnO

FeO

CoO

NiO



LDA entropy represents number of local states - maximum at d^5

Interaction reduces this number and it becomes almost the same

Non-interacting system chemistry decides how much it is correlated

Doping reduces number of local states in noninteracting system

Summary

- We used **entropy** and **relative entropies** to **quantify in numbers** correlation in correlated electron systems.
- Examples for Hubbard model.
- Different correlations in paramagnetic and in antiferromagnetic cases.
- Different amount of correlation in transition metal oxides: MnO 3 times more correlated than NiO.

Calculation details

Consider a pure state (maximal information)

$$|\Psi\rangle = \sum_{\alpha\beta} \Psi_{\alpha\beta} |\alpha\rangle |\beta\rangle$$

of a system which is composed of two subsystems $A = \{|\alpha\rangle\}$ and $B = \{|\beta\rangle\}$.

Density operator (Schmidt decomposition)

$$\hat{\rho} = \sum_k p_k |k\rangle \langle k| = |\Psi\rangle \langle \Psi|.$$

Entropy

$$S(\hat{\rho}) = -\langle \log \hat{\rho} \rangle = -\text{Tr} \hat{\rho} \log \hat{\rho} = -\sum_k p_k \log p_k = 0,$$

because

$$p_k = \delta_{k,\Psi}.$$

Calculation details

Trace out the B subsystem, reduced density operator

$$\hat{\rho}_A = \text{Tr}_B |\Psi\rangle\langle\Psi| = \sum_{\beta} \langle\beta|\Psi\rangle\langle\Psi|\beta\rangle = \sum_{\alpha_1, \alpha_2} |\alpha_1\rangle \sum_{\beta} \Psi_{\alpha_1, \beta} \Psi_{\beta, \alpha_2}^{\dagger} \langle\alpha_2| = \sum_{\alpha_1, \alpha_2} |\alpha_1\rangle \rho_{\alpha_1, \alpha_2} \langle\alpha_2|.$$

Subsystem A is in a **mixed state** (reduced information).

Introduce projector and transition operators

$$\hat{P}_i = |i\rangle\langle i|, \quad \hat{T}_{ij} = |i\rangle\langle j|,$$

then

$$\rho_{\alpha_1 \alpha_2} = \sum_{\beta} \Psi_{\alpha_1, \beta} \Psi_{\beta, \alpha_2}^{\dagger} = \langle\Psi|\hat{P}_{\alpha_1} \hat{T}_{\alpha_1, \alpha_2} \hat{P}_{\alpha_2} |\Psi\rangle^{\dagger}.$$

Calculation details

Consider a single lattice site (DMFT) as the A subsystem

$$|\alpha\rangle = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\},$$

then

$$\hat{P}_\alpha = \begin{cases} (1 - \hat{n}_\uparrow)(1 - \hat{n}_\downarrow) \\ \hat{n}_\uparrow(1 - \hat{n}_\downarrow) \\ (1 - \hat{n}_\uparrow)\hat{n}_\downarrow \\ \hat{n}_\uparrow\hat{n}_\downarrow, \end{cases}$$

and

$$\hat{T}_{\alpha_1, \alpha_2} = \begin{pmatrix} 1 & c_\uparrow & c_\downarrow & c_\downarrow c_\uparrow \\ c_\uparrow^\dagger & 1 & c_\uparrow^\dagger c_\downarrow & -c_\downarrow \\ c_\downarrow^\dagger & c_\downarrow^\dagger c_\uparrow & 1 & c_\uparrow \\ c_\uparrow^\dagger c_\downarrow^\dagger & -c_\downarrow^\dagger & c_\uparrow^\dagger & 1 \end{pmatrix}.$$

Assuming absence of any off-diagonal order $\langle \Psi | c_\sigma | \Psi \rangle = \langle \Psi | c_\sigma c_{-\sigma} | \Psi \rangle$ the reduced density operator is diagonal

$$\rho_{\alpha_1 \alpha_2} = p_1 |0\rangle \langle 0| + p_2 |\uparrow\rangle \langle \uparrow| + p_3 |\downarrow\rangle \langle \downarrow| + p_4 |\uparrow\downarrow\rangle \langle \uparrow\downarrow|,$$

Calculation details

with matrix elements

$$p_\alpha = \langle \Psi | \hat{P}_\alpha | \Psi \rangle$$

determined with an arbitrary pure state $|\Psi\rangle$ (exact, DMFT, HF, etc.) of the full system.

It is straightforward to derive for an arbitrary mixed state $\hat{\rho}$ of the full system.