How to quantify correlation in correlated electron system

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Collaboration

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Aim of this talk

CORRELATION

- What is it?
- How to quantify it?

Correlation

- Correlation [lat.]: con+relatio ("with relation")

- Mathematics, Statistics, Natural Science:

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

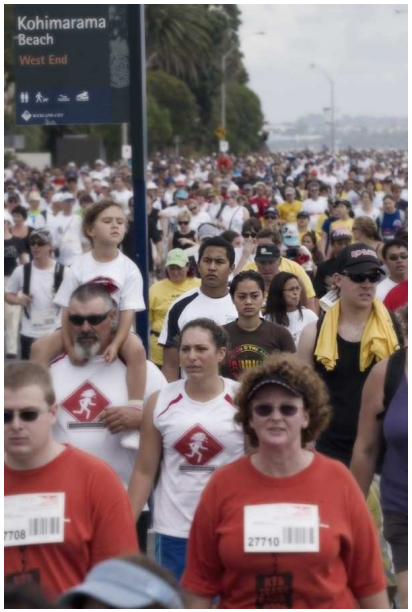
  The term correlation stems from mathematical statistics and means that two distribution functions, $f(x)$ and $g(y)$, are not independent of each other.

- 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 .....

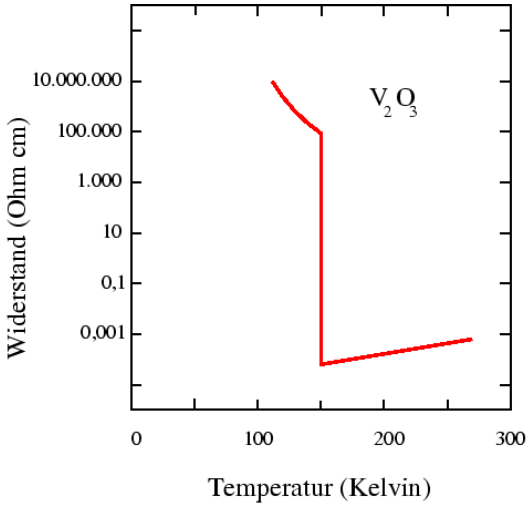


Abb. 3: Beispiel eines Metall-Isolator-Übergangs: Bei Abkühlung unter eine Temperatur von ca. 150 Kelvin erhöht sich der elektrische Widerstand von metallischem Vanadiumoxid (V_2O_3) schlagartig um das Einhundertmillionenfache (Faktor 10^8) – das System wird zum Isolator.

Spatial and temporal correlations neglected

time/space average insufficient

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

Boeing 757 and Tupolev 154 collided at 35,400ft. in 2001

Pilot of Tupolev received at the same time two conflicting (uncorrelated) instructions

Spatial and temporal correlations neglected

Local density approximation (LDA) disaster in HTC

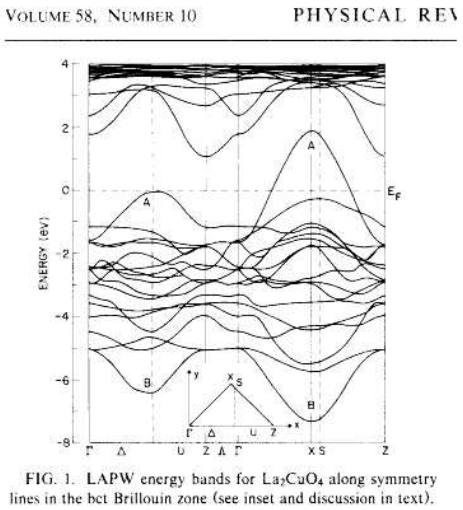
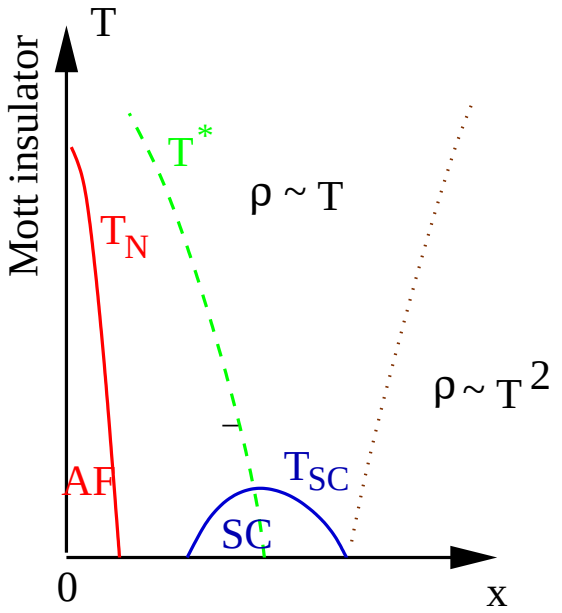


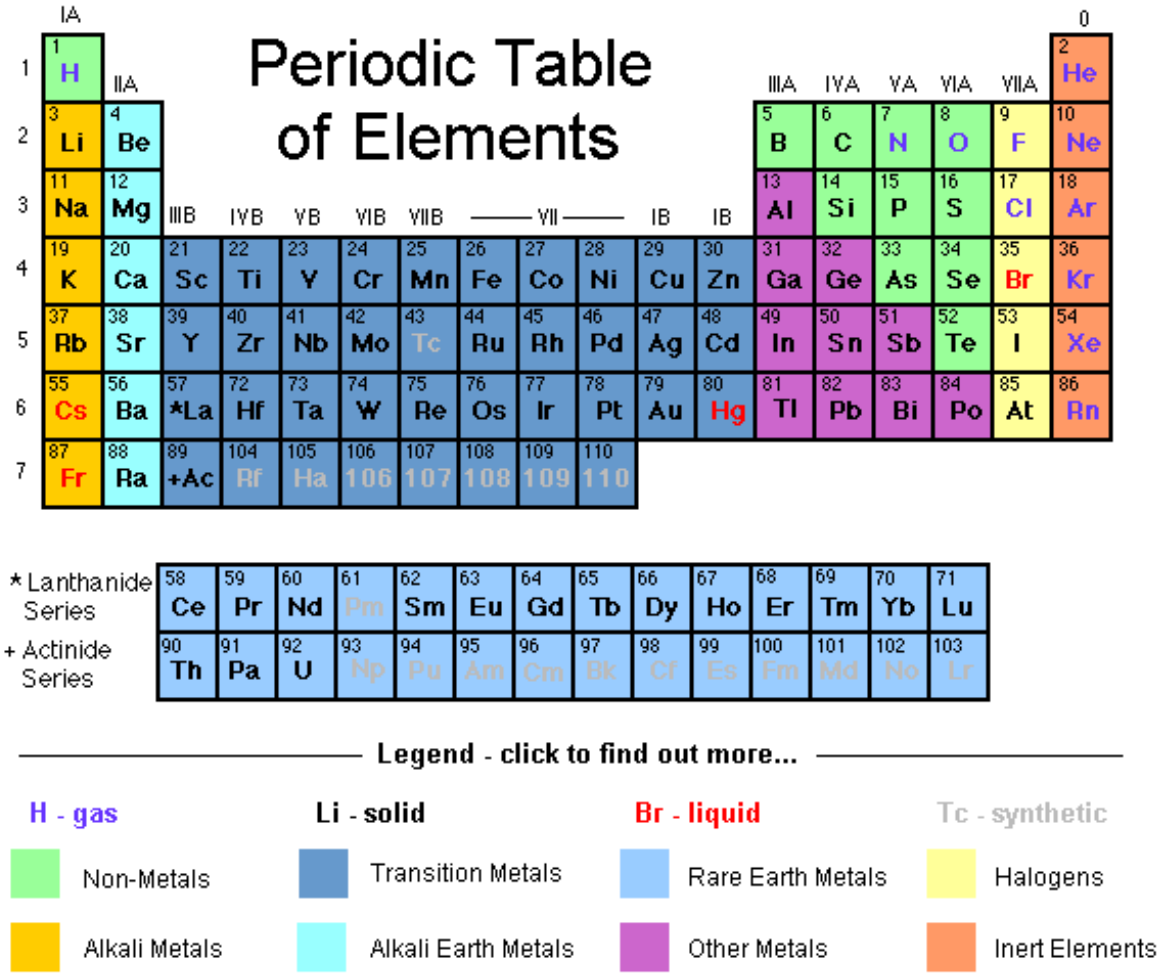
FIG. 1. LAPW energy bands for La_2CuO_4 along symmetry lines in the bct Brillouin zone (see inset and discussion in text).



$LaCuO_4$ Mott (correlated) insulator predicted to be a metal

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

Correlated electrons

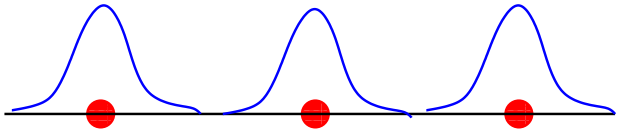


Narrow d,f-orbitals/bands $\rightarrow$ strong electronic correlations

Electronic bands in solids

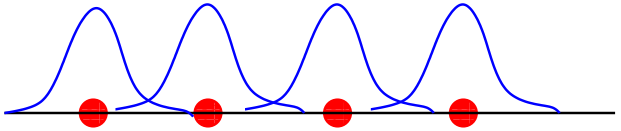
Wave function overlap $\sim t_{ij} = \langle i|\hat{T}|j\rangle \rightarrow |E_{\mathbf{k}}| \sim$ bandwidth W

Band insulators, e.g. NaCl



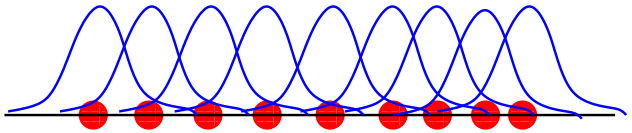
Atomic levels, localized electrons $|\mathbf{R}_i\sigma\rangle$

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

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

$$\text{Heisenberg principle} \quad W\tau \sim \hbar$$

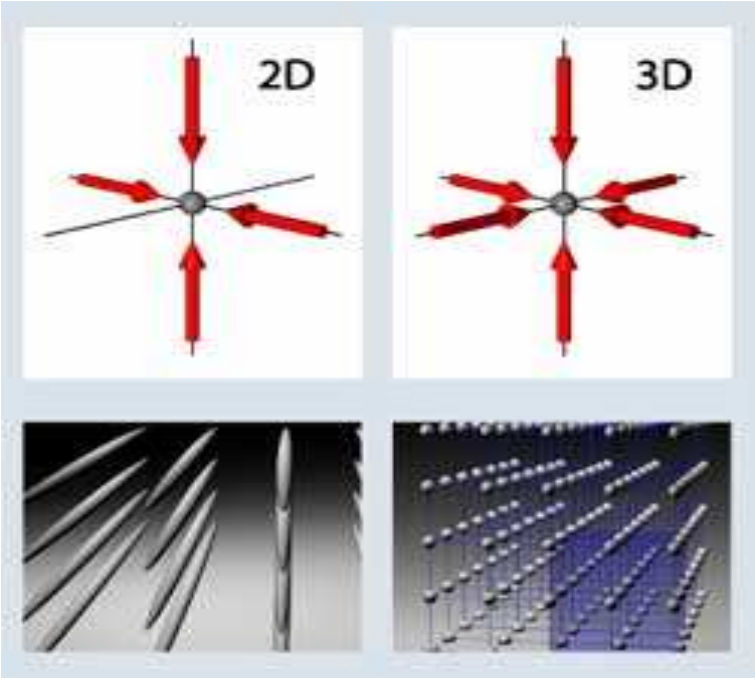
$$\frac{a}{\tau} \sim \frac{aW}{\hbar} \Longrightarrow \tau \sim \frac{\hbar}{W}$$

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 $a \sim 400 - 500nm$

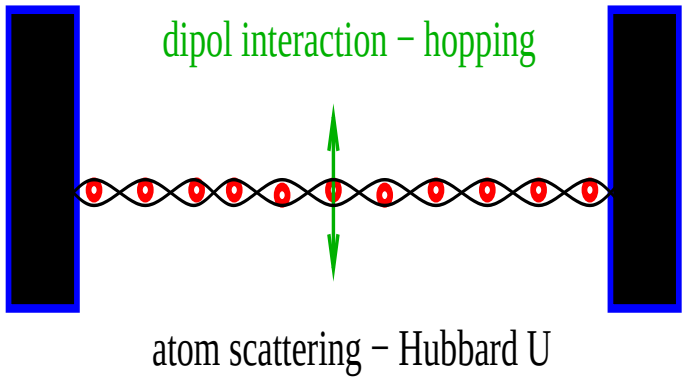


alkali atoms with ns^1 electronic state $J = S = 1/2$

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

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

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



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

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

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

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

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

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

Asymptotic distiguishability

Quantum Sanov theorem:
Probability P_n that a state $\hat{\sigma}$ is not distinguishable from a state $\hat{\rho}$ in n measurements, 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.

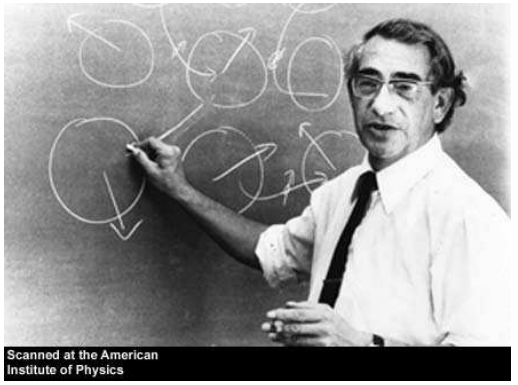
We calculate

- von Neumann entropies and
- relative entropies

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

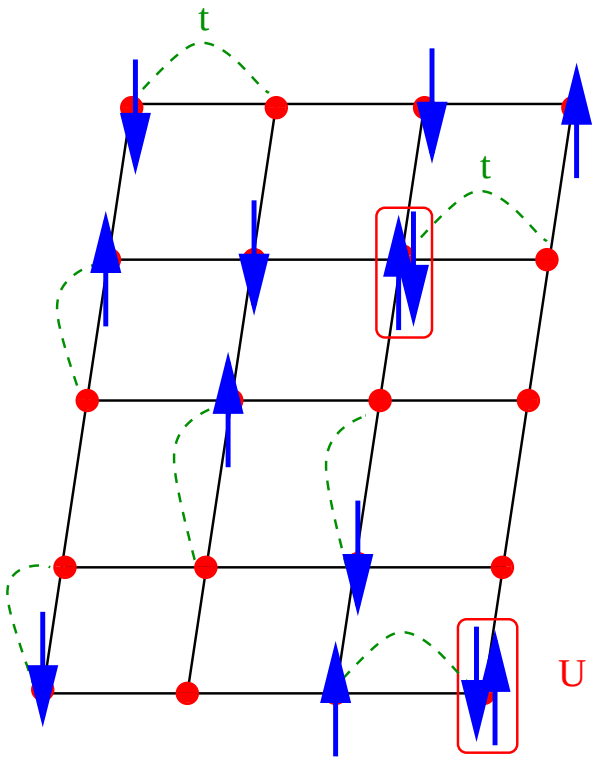
Correlated fermions on crystal and optical lattices

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

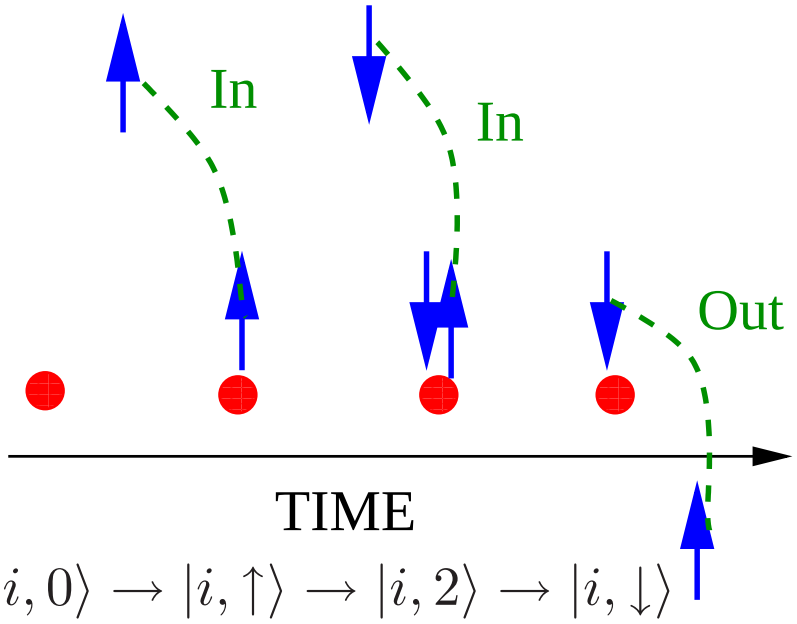


fermionic Hubbard model

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



Local Hubbard physics



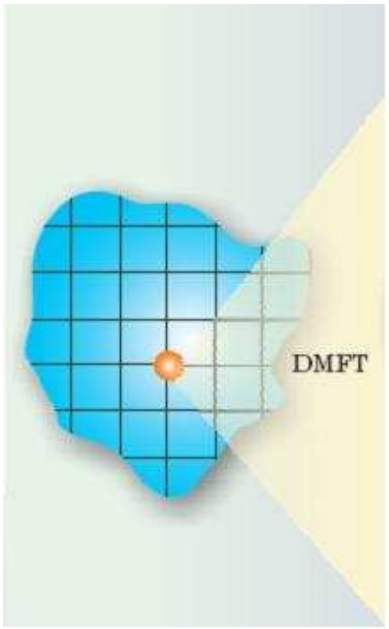
Origin of genuine many-body correlation

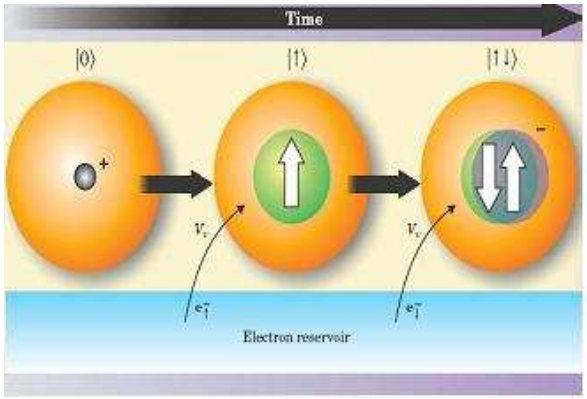
$$H = H^{\text{hopping}} + H^{\text{interaction}}_{\text{loc}}$$

$$\left[H^{\text{hopping}}, H^{\text{interaction}}_{\text{loc}}\right] \neq 0$$

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:

$$\hat{\rho}_i = Tr_{j \neq i} \hat{\rho}$$

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.

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

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

because

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

Calculation details

Trace out the B subsystem, reduced density operator

$$\hat{\rho}_A = Tr_B|\Psi\rangle\langle\Psi| = \sum_\beta \langle\beta|\Psi\rangle\langle\Psi|\beta\rangle = \sum_{\alpha_1,\alpha_2} |\alpha_1\rangle \sum_\beta \Psi_{\alpha_1,\beta}\Psi^\dagger_{\beta,\alpha_2}\langle\alpha_2| = \sum_{\alpha_1,\alpha_2} |\alpha_1\rangle\rho_{\alpha_1,\alpha_2}\langle\alpha_2|.$$

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

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

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.

Calculation details

Local entropy

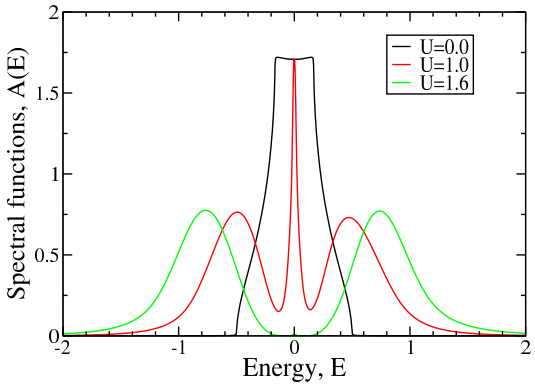
$$S(\hat{\rho}) = -Tr_A \hat{\rho}_A \log \hat{\rho_A} = -\sum_\alpha p_\alpha \log p_\alpha.$$

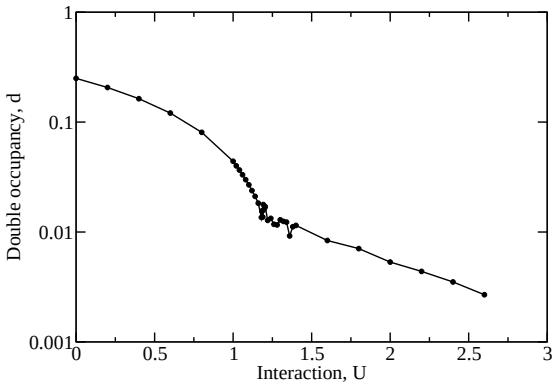
Local relative entropy

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

Correlation and Mott Transition

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





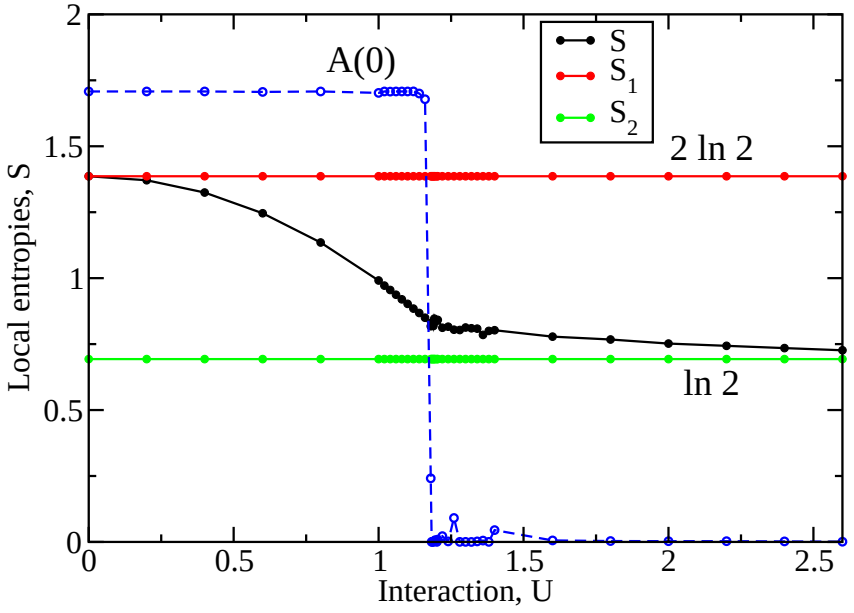
$$S = S(\hat{\rho}_{DMFT})$$
$$S_1 = S(\hat{\rho}_0)$$
$$S_2 = S(\hat{\rho}_a)$$

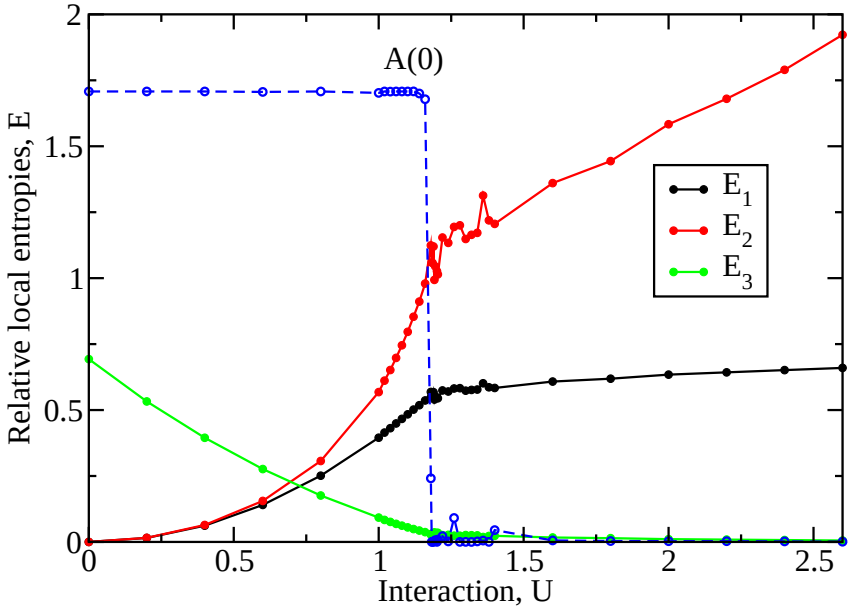
Product (HF) states:

$|0\rangle = \prod_{k\sigma}^{k_F} a^\dagger_{k\sigma}|v\rangle$ - $U = 0$ limit

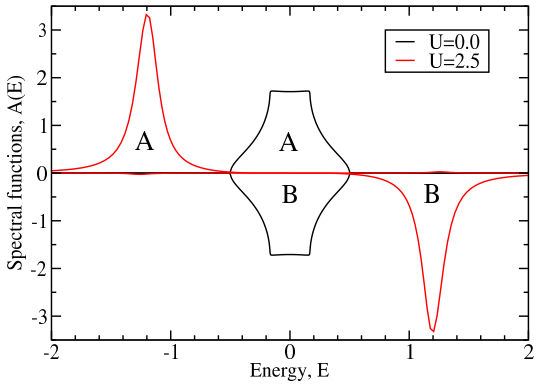
$|a\rangle = \prod_{i}^{N_L} a^\dagger_{i\sigma_i}|v\rangle$ - atomic limit

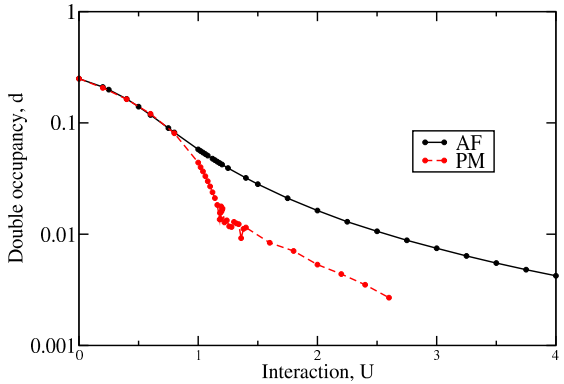
$$E_1 = E(\hat{\rho}_{DMFT}||\hat{\rho}_0)$$
$$E_2 = E(\hat{\rho}_0||\hat{\rho}_{DMFT})$$
$$E_3 = E(\hat{\rho}_a||\hat{\rho}_{DMFT})$$





Correlation and Antiferromagnetic Order





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

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

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

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

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

Product (HF) states:

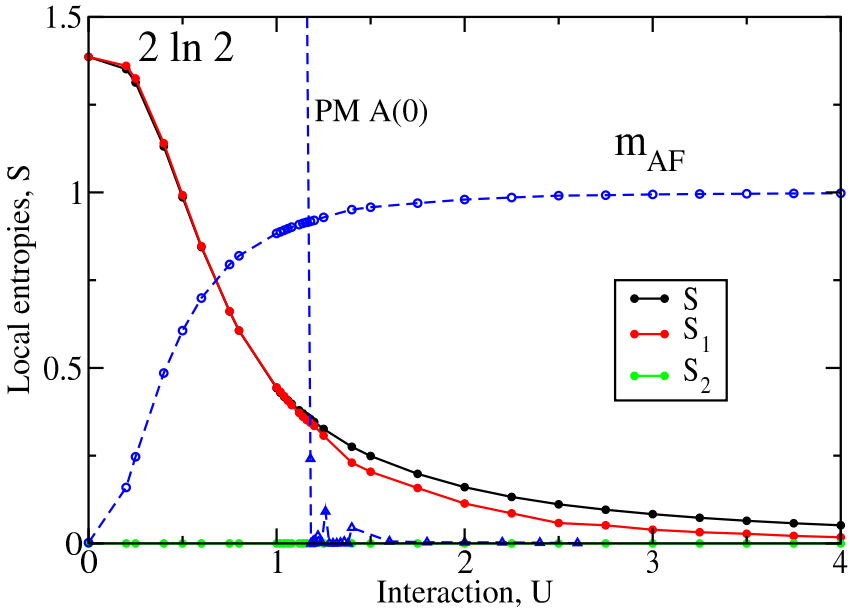
$|0\rangle = \prod_{k\in(A,B)}^{k_F} a^\dagger_{k_A\uparrow} a^\dagger_{k_B\downarrow}|v\rangle$ - Slater limit

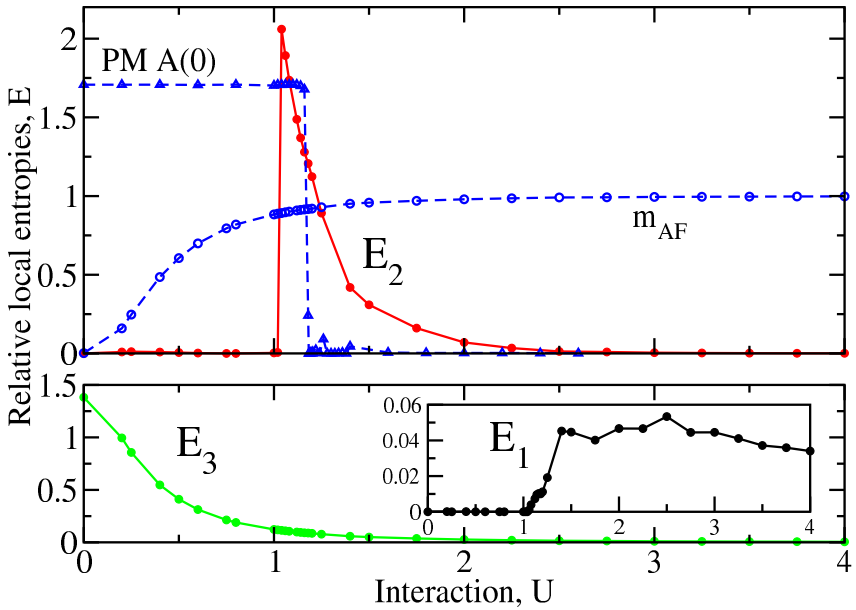
$|a\rangle = \prod_{i\in(A,B)}^{N_L} a^\dagger_{i_A\uparrow} a^\dagger_{i_B\downarrow}|v\rangle$ - Heisenberg limit

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

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

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





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.