Entangelment and relative local entropies: Introducing a quantitative measure of correlations in correlated electron systems

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Collaboration

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Problem

How many correlations are 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 distigushable 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.

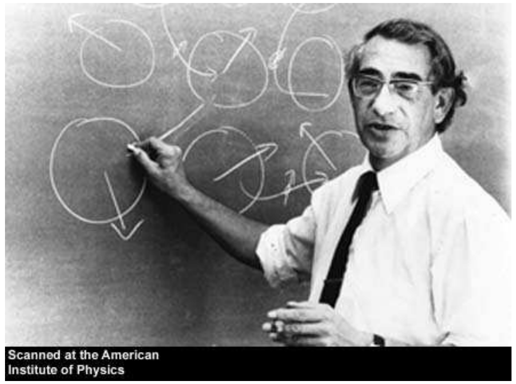
We calculate

- von Neumann entropies and
- relative entropies

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

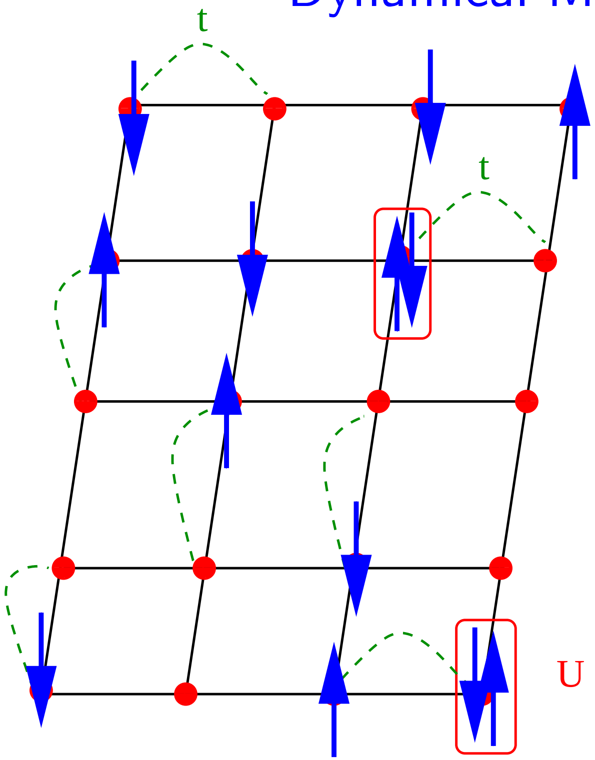
Hubbard Model and DMFT

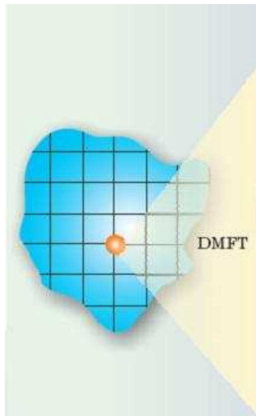
$$H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

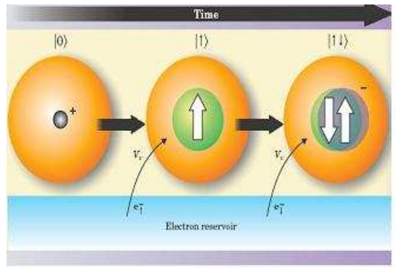


fermionic Hubbard model, 1963

Dynamical Mean-Field Theory -Metzner, Vollhardt '89, Georges, *et al.*, RMP '96







$$|i,0\rangle \rightarrow |i,\uparrow\rangle \rightarrow |i,2\rangle \rightarrow |i,\downarrow\rangle$$

Exact local correlations

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

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

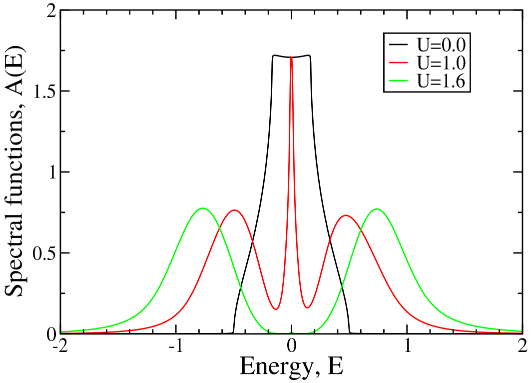
A.Rycerz, Eur. Phys. J B **52**, 291 (2006);
D. Larsson and H. Johannesson, Phys. Rev. A **73**, 042320 (2006)

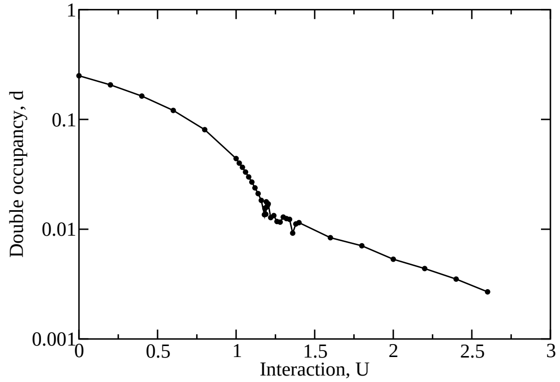
Generalized equations for local relative entropy.
KB, D. Vollhardt, '09

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

Correlations and Mott Transition

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





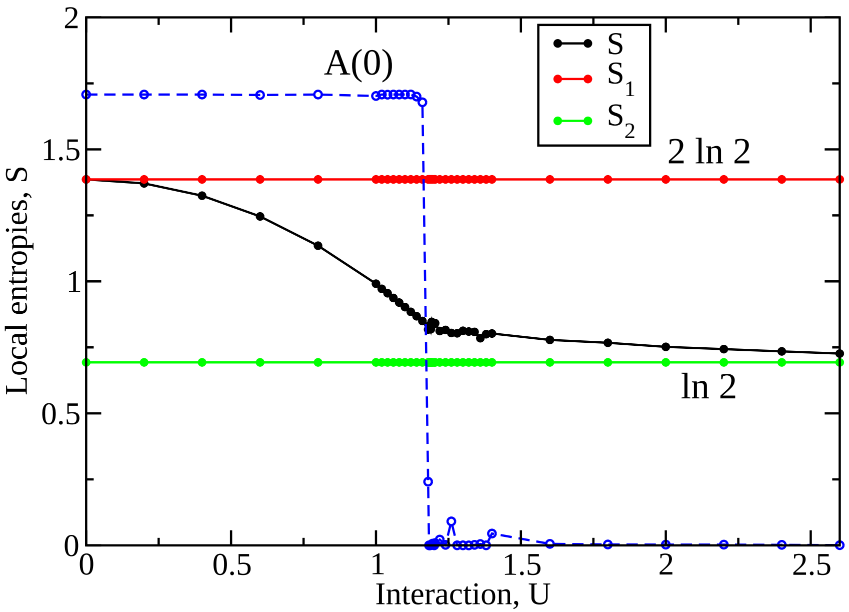
$$S = S(\hat{\rho}_{DMFT})$$
$$S_1 = S(\hat{\rho}_0)$$
$$S_2 = S(\hat{\rho}_a)$$

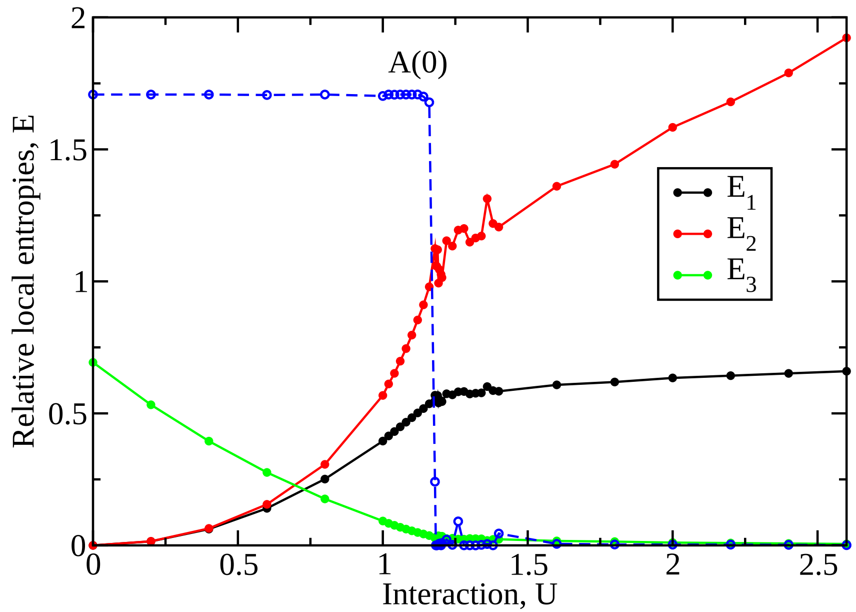
Product (HF) states:

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

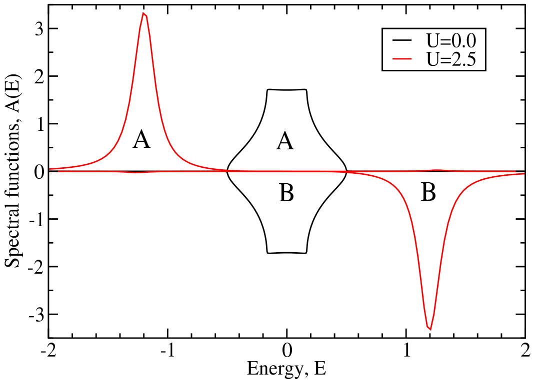
$|a\rangle = \prod_{i}^{N_L} a^\dagger_{i\sigma_i}|v\rangle$ - atomic limit

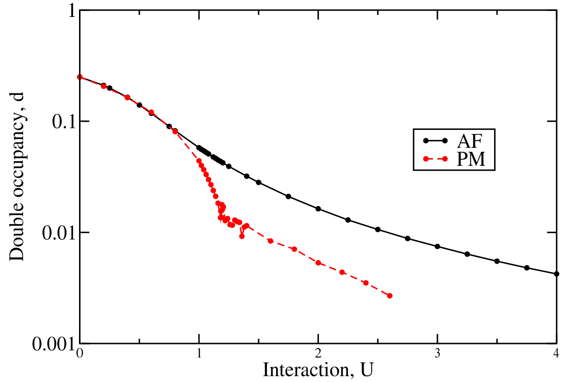
$$E_1 = E(\hat{\rho}_{DMFT}||\hat{\rho}_0)$$
$$E_2 = E(\hat{\rho}_0||\hat{\rho}_{DMFT})$$
$$E_3 = E(\hat{\rho}_a||\hat{\rho}_{DMFT})$$





Correlations 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:

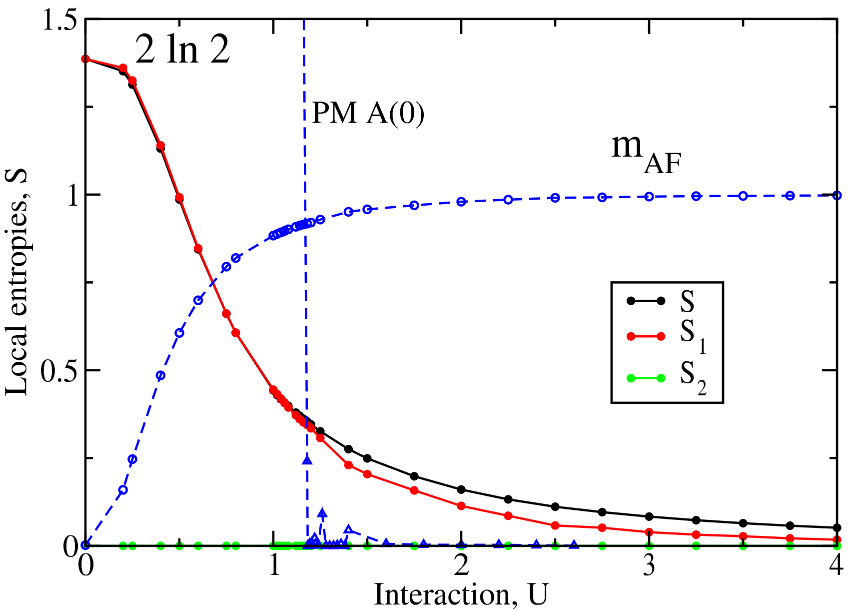
$|0\rangle = \prod_{k\in(A,B)}^{k_F} a^\dagger_{k_A\uparrow} a^\dagger_{k_B\downarrow} |v\rangle$ - Neel limit

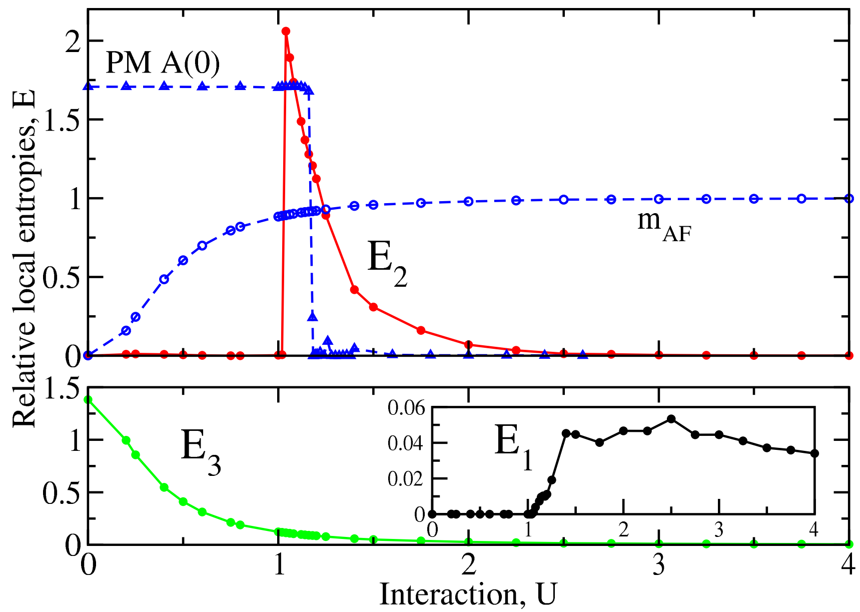
$|a\rangle = \prod_{i\in(A,B)}^{N_L} a^\dagger_{i_A\uparrow} a^\dagger_{i_B\downarrow} |v\rangle$ - Heisenberg limit

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

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

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





Summary

- Introducing entropy and relative entropies to quantify in numbers correlations in correlated electron systems.

- Examples for Hubbard model.

- Different correlations in paramagnetic and in antiferromagnetic cases.