Quantification of correlations in correlated electron systems

Krzysztof Byczuk

Institute of Theoretical Physics, Faculty of Physics
University of Warsaw
and
Center for Electronic Correlations and Magnetism, Institute of Physics,
Augsburg University

September 15th, 2011

www.physik.uni-augsburg.de/theo3/kbyczuk

www.fuw.edu.pl/pmss

Very recent history ...

Happy Birthday to You Dieter!

Quantification of correlations in correlated electron systems

Collaboration

Walter Hofstetter - Frankfurt University

Jan Kuneš - Prague, Academy of Sciences

Dieter Vollhardt - Augsburg University

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

Quantifying correlations

How many correlation is there in correlated electron systems?

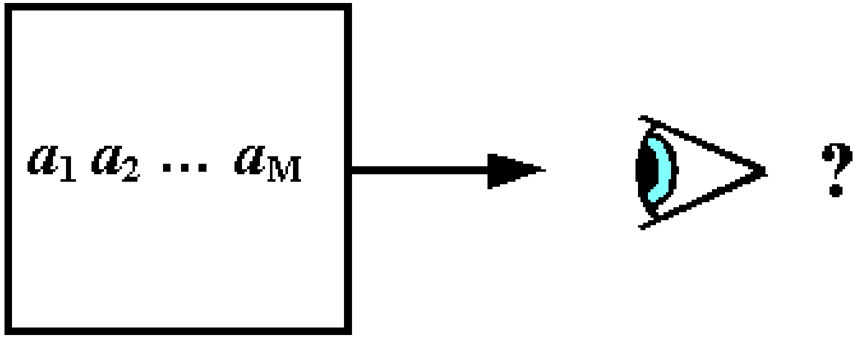
Correlation functions (double occupancy, effective mass, Z- factor, conductance(vity), susceptibilities, ...) are very useful for particular cases when we know what to look at:

R. Grobe, K. Rzążewski, and J.H. Eberly, J. Phys. B: At. Mol. Opt. Phys. **27**, L503 (1994),
A.M. Oleś, F. Pfirsch, P. Fulde, and M.C. Böhm, Z. Phys. B - Condensed Matter **66**, 359 (1987),
P. Ziesche, V.H. Smith, Jr. and M. Ho, S.P. Rudin, P. Gersdorf, and M. Taut, J. Chem. Phys. **110**, 6135 (1999),
A.D. Gottlieb and N.J. Mauser, Phys. Rev. Lett. **95**, 123003 (2005),
J.E. Harriman, Phys. Rev. A **75**, 032513 (2007),
....

However, we need information theory tools to address this issue in general.

Information theory

C. Shannon, 1916-2001



abstraction from the real (human) meaning of the messages

$I(a) = -\ln p(a)$ - surprise

Information entropy

$S(a) = \langle I(a) \rangle = -\langle \ln p(a) \rangle = -\sum_a p(a) \ln p(a)$ - average surprise, **information**

positive, monotonic, additive, convex, ...

Information theory - correlation

Two sources of messages with distribution $p(a,b)$, total information
$S(a,b) = -\langle \ln p(a,b) \rangle$
marginal distributions - $p(a) = \sum_b p(a,b)$, etc.

Messages are **correlated** (not independent)

$$p(a,b) \neq p(a)p(b),$$

i.e.

$$\langle ab \rangle \neq \langle a \rangle \langle b \rangle$$

Total correlation

$$\Delta S(a||b) = S(a,b) - S(a) - S(b) = -\left\{ \sum_{ab} p(a,b) \left[\ln p(a,b) - \ln p(a)p(b) \right] \right\}$$

Relative entropy (Kullback - Leibler divergence) vanishes in the absence of correlations (product distribution)

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

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

Two correlated (sub)systems have relative entropy

$$S = S_1 + S_2 - \Delta S \longleftrightarrow S = S_1 + S_2 - \Delta S$$

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

Asymptotic distinguishability

Quantum version of Sanov's theorem:
Let $\hat{\rho}$ and $\hat{\sigma}$ are two states of quantum system Q, and we are provided with N identically prepared copies of Q. A measurement is made to determine if the prepared state is $\hat{\rho}$. The probability that the state $\hat{\sigma}$ passes this test (i.e. is confused with $\hat{\rho}$) is

$$P_N \approx e^{-N\Delta S(\hat{\rho}||\hat{\sigma})}.$$

as $N \to \infty$ and the optimal strategy is known and depend only on $\hat{\rho}$.
Relative entropy $\Delta S(\hat{\rho}||\hat{\sigma})$ as a 'distance' between quantum states.

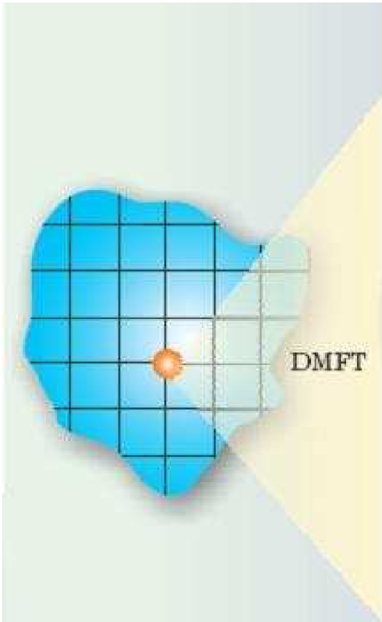
Correlation measure

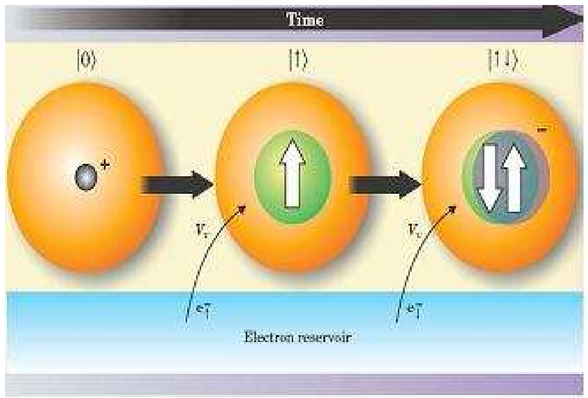
relative entropy between correlated $|\mathrm{corr}\rangle$ and uncorrelated (product) $|\mathrm{prod}\rangle$ states

$$\Delta_{\mathrm{corr}->\mathrm{prod}} = \Delta S(\mathrm{corr}||\mathrm{prod})$$

Application: 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

Reduced Entropy and Reduced Relative Entropy

Reduced density operator:

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

$$S(\hat{\rho}_i) = -\sum_{k=1}^{n} p_k \ln p_k, \quad \Delta S(\hat{\rho}_i || \hat{\rho}_i^{\mathrm{prod}}) = -\sum_{k=1}^{n} p_k (\ln p_k - \ln p_k^{\mathrm{prod}})$$

where, e.g. for 1s orbitals

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

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

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

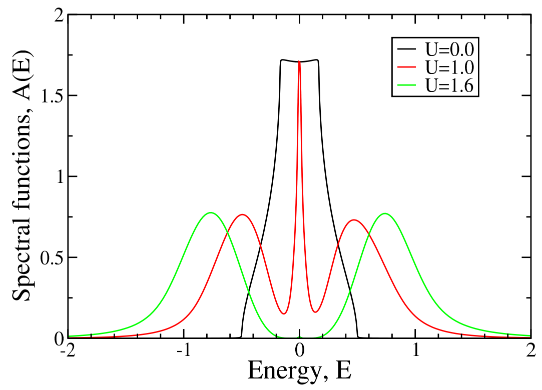
Generalized equations for reduced relative entropy

KB, W. Hofstetter, J. Kuneš, D. Vollhardt, (2011)

Expectation values for correlated states are determined from DMFT solution and for uncorrelated states from product solutions.

Example 1: Correlation and Mott Transition

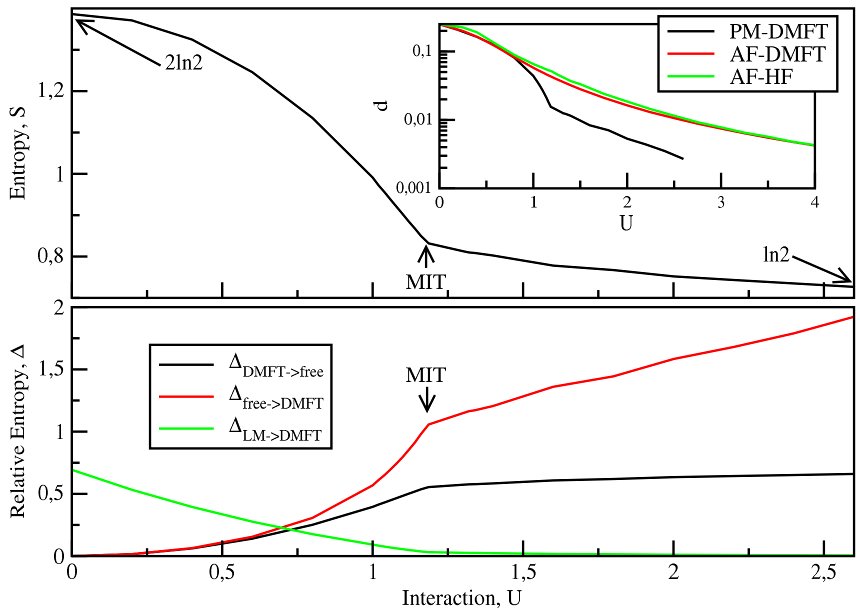
Hubbard model, $n = 1$, $T = 0$, $d = 3$, PM



Uncorrelated product states:

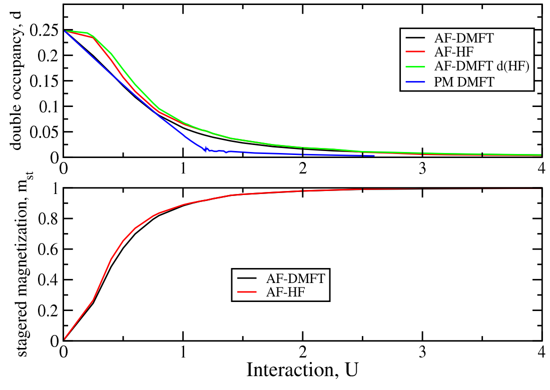
$|\mathrm{free}\rangle = \prod_{k\sigma}^{k_F} a_{k\sigma}^{\dagger}|v\rangle$ - $U = 0$ Hartree-Fock limit

$|\mathrm{LM}\rangle = \prod_{i}^{N_L} a_{i\sigma_i}^{\dagger}|v\rangle$ - local moment limit



Example 2: Correlation and Antiferromagnetic LRO

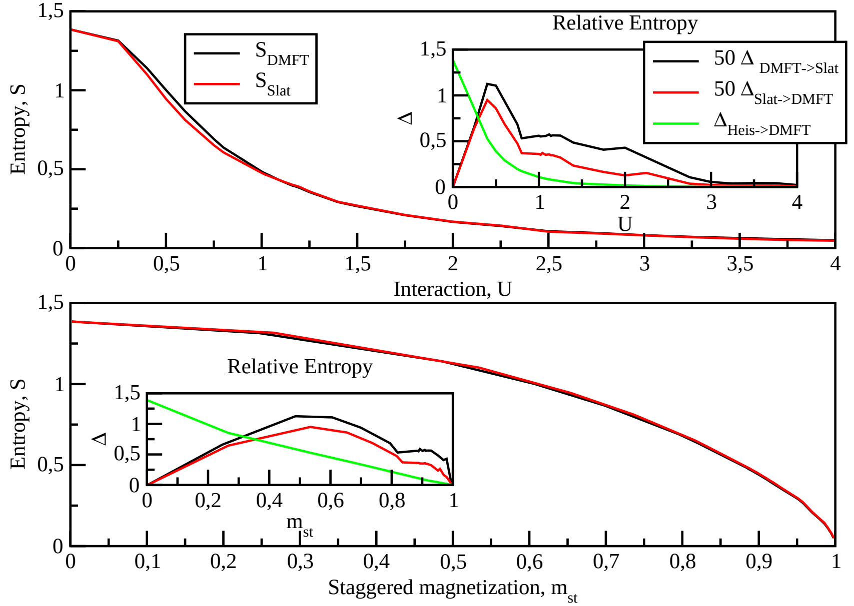
Hubbard model, $n = 1$, $T = 0$, $d = 3$, AF



Uncorrelated product states:

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

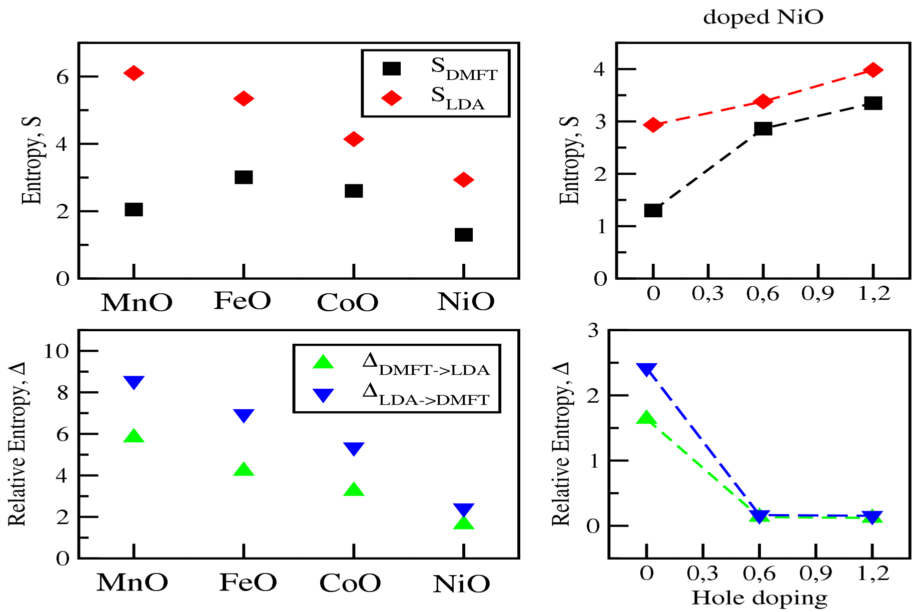
$|\mathrm{Heis}\rangle = \prod_{i\in(A,B)}^{N_L} a^\dagger_{i_A\uparrow} a^\dagger_{i_B\downarrow}|v\rangle$ - Heisenberg limit



Example 3: Correlation in Transition Metal-Oxides

MnO **FeO** **CoO** **NiO**

$$[Ar]3d^5s^2 \quad [Ar]3d^6s^2; \quad [Ar]3d^7s^2; \quad [Ar]3d^8s^2$$



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

Summary

- We used relative entropy to quantify in numbers correlation in interacting many-electron systems.
- Examples for Hubbard model.
- Different correlations in paramagnetic and in antiferromagnetic cases.
- Different amount of correlation in transition metal oxides, e.g., MnO is 3 times more correlated then NiO.