Quantification of correlations in quantum many-particle systems

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Collaboration

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Quantifying correlations in many-body systems

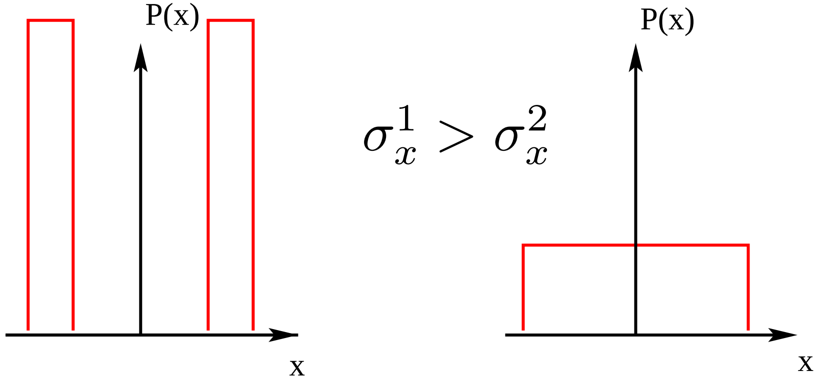
Conventional measures of correlation strength

$$\frac{U}{W}, \quad \frac{m^*}{m}, \quad \frac{E - E_{HF}}{E_{HF}}, \quad \frac{\langle n_{i\uparrow} n_{i\downarrow} \rangle}{\langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle}, \quad .....$$

Correlation is a statistical concept determined relatively to uncorrelated system

R. Grobe, K. Rzążewski, and J.H. Eberly, (1994),
A.M. Oleś, F. Pfirsch, P. Fulde, and M.C. Böhm, (1987),
P. Ziesche, V.H. Smith, Jr. and M. Ho, S.P. Rudin, P. Gersdorf, and M. Taut, (1999),
A.D. Gottlieb and N.J. Mauser, (2005),
J.E. Harriman, (2007), ...

More information
in left distribution



$$\sigma_x^1 > \sigma_x^2 \qquad \sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

Single correlation function (variance) is not fully informative

Quantifying correlations in many-body systems

Many particle systems $i = 1, ..., N = 10^{23}$

$$\langle \mathbf{r}_i \mathbf{r}_j \rangle, \quad \langle \mathbf{r}_i \mathbf{r}_j \mathbf{r}_k \rangle, \quad \langle \mathbf{r}_i \mathbf{r}_j \mathbf{r}_k \mathbf{r}_l \rangle, \quad .....$$

two particle correlations, three particle correlations, ..., 10^{23} particle correlations...

Applying quantum information theory

Probability distribution vs. Density operator

$$p(x_1, ..., x_N) \longleftrightarrow \hat{\rho} = \sum_{k_1, ..., k_N} p_{k_1..k_N} |k_1...k_N\rangle\langle k_1...k_N|$$

Uncorrelated distribution vs. Uncorrelated density operator

$$p(x_1, ..., x_N) = p_1(x_1)...p_N(x_N) \longleftrightarrow \hat{\rho} = \hat{\rho}_1 \otimes ... \otimes \hat{\rho}_N$$

after taking partial integrals or trace

Applying quantum information theory

Shannon entropy vs. von Neumann entropy

$$S(p) = -\sum_{x_1,\ldots,x_N} p(x_1,...,x_N)\ln p(x_1,...,x_N) \longleftrightarrow S(\hat{\rho}) = -Tr[\hat{\rho}\ln\hat{\rho}]$$

Relative entropy of correlated probability distribution or (density operator)

$$\Delta S(p||p_1...p_N) = S(p_1) + ... + S(p_N) - S(p)$$

where

$$\Delta S(p||p_1...p_N) = \sum_{x_1,\ldots,x_N} p(x_1,...,x_N)[\ln p(x_1,...,x_N) - \ln p_1(x_1)...p_N(x_N)]$$

and

$$\Delta S(\hat{\rho}||\hat{\rho}_1 \otimes ... \otimes \hat{\rho}_N) = S(\hat{\rho}_1) + ... + S(\hat{\rho}_N) - S(\hat{\rho})$$

where

$$\Delta S(\hat{\rho}||\hat{\rho}_1 \otimes ... \otimes \hat{\rho}_N) = Tr[\hat{\rho}(\ln\hat{\rho} - \ln\hat{\rho}_1 \otimes ... \otimes \hat{\rho}_N)]$$

Interpretation: Asymptotic distinguishability of states

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.

Entropic measure of correlation strength

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

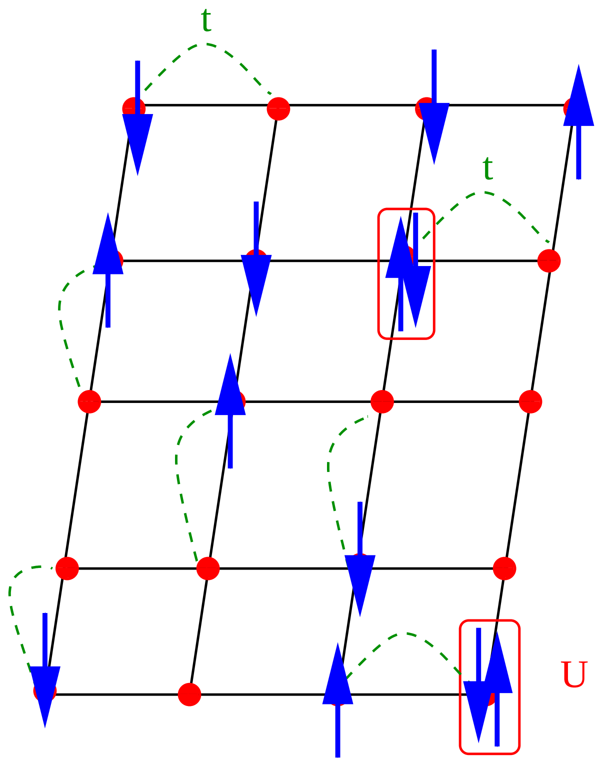
$$\Delta S(\hat{\rho}^{\mathrm{corr}}||\hat{\rho}^{\mathrm{prod}})$$

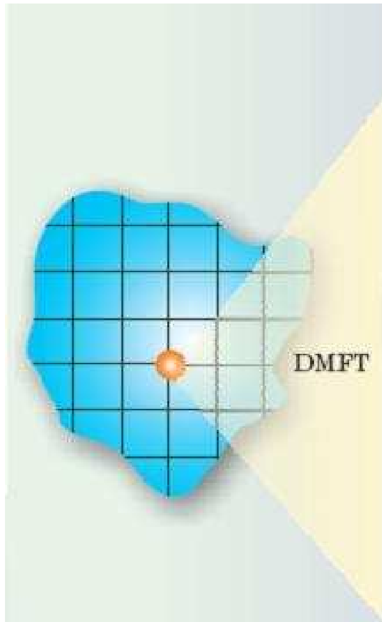
Application: Correlated fermions within DMFT

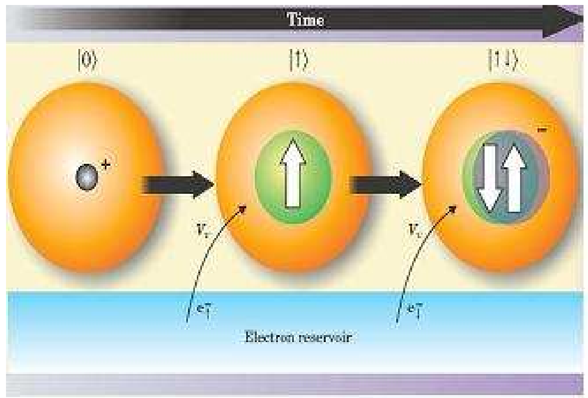
$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

fermionic Hubbard model

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







G. Kotliar and D. Vollhardt (2004)

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

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, (2006); D. Larsson and H. Johannesson, (2006)

Generalized equations for reduced relative entropy

KB, J. Kuneš, W. Hofstetter, and D. Vollhardt, (2012)

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

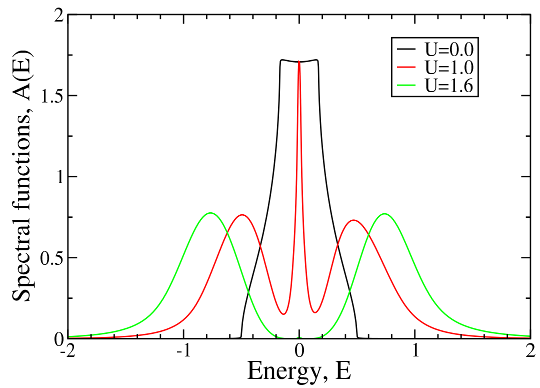
Example 1: Correlation and Mott Transition

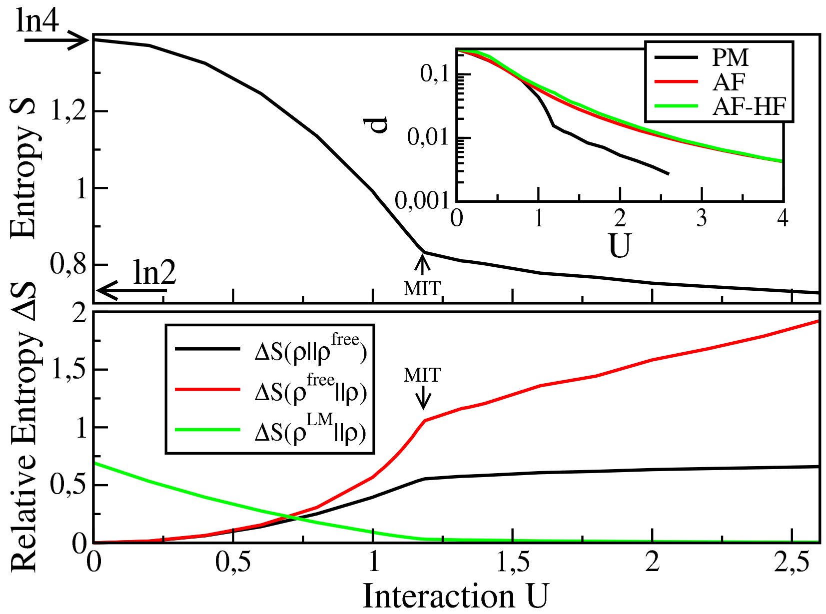
Hubbard model, $n = 1$, $T = 0$, $d = 3$, PM

Uncorrelated product states:

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

$|\text{LM}\rangle = \prod_{i}^{N_L} a^\dagger_{i\sigma_i}|v\rangle$ - local moment limit





Correlation strength not linear in U/W

Correlation strength similar in Mott insulators at different U

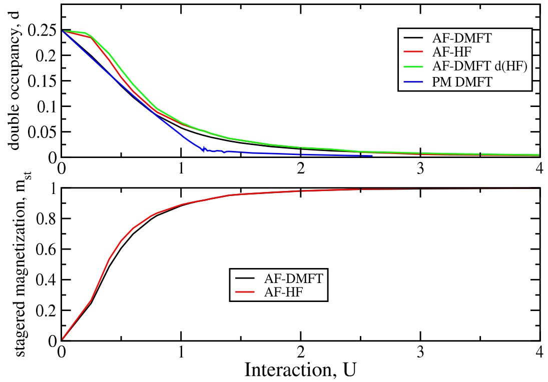
Example 2: Correlation and Antiferromagnetic LRO

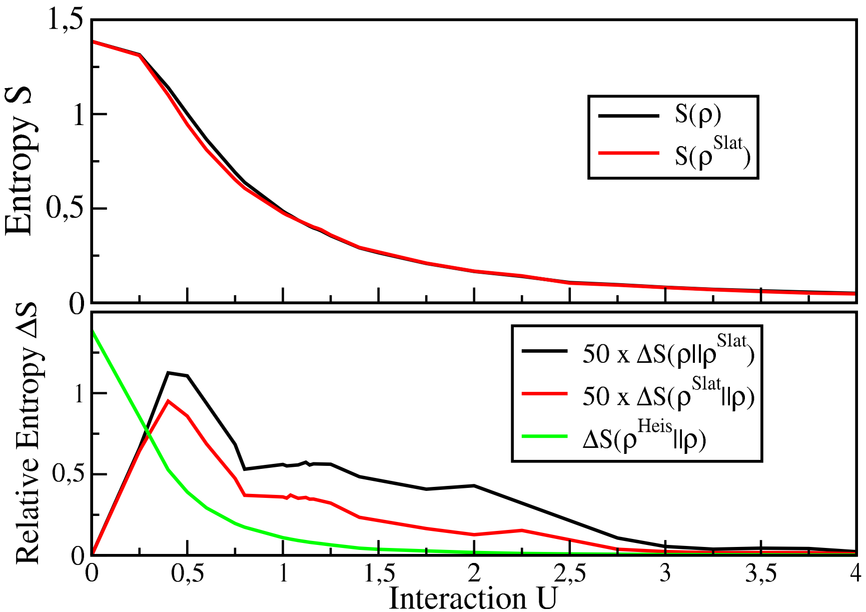
Hubbard model, $n = 1$, $T = 0$, $d = 3$, AF

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

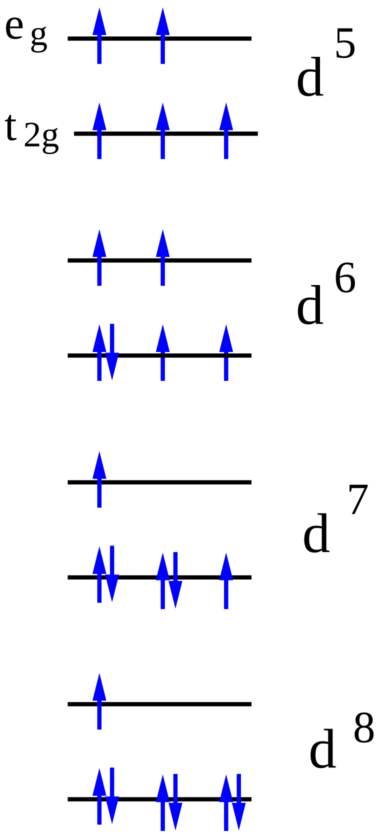




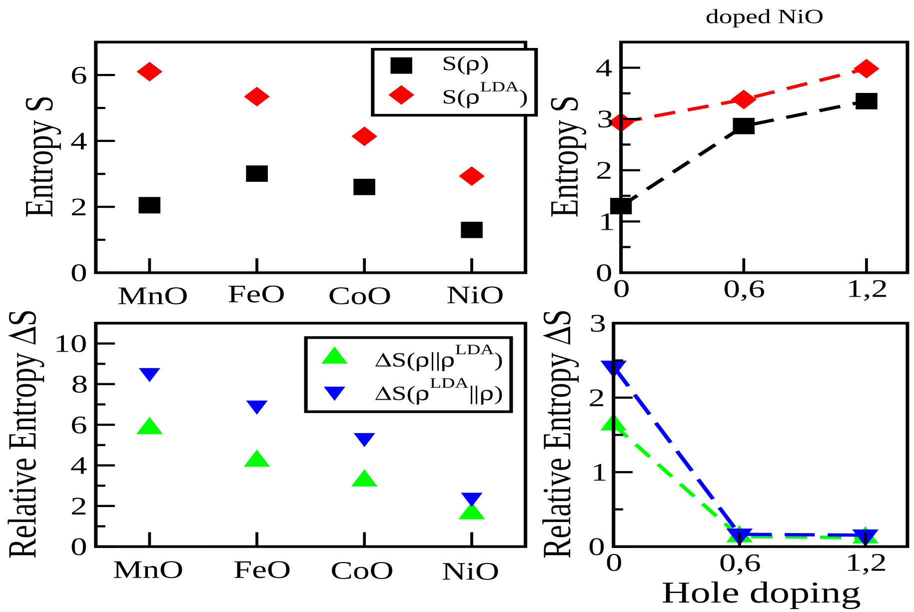
LRO-HF (Slater) states imitates correlations well

Correlation strength very weak in AF insulators at different U

Example 3: Correlation in Transition Metal-Oxides



MnO	**FeO**	**CoO**	**NiO**	paramagnetic
$[Ar]3d^5s^2$	$[Ar]3d^6s^2;$	$[Ar]3d^7s^2;$	$[Ar]3d^8s^2$	



Doping:

$d^8 \rightarrow d^7 + d^9$

Increase $S(\rho)$ and $S(\rho^{LDA})$

Doping reduces correlation

$S(\hat{\rho}^{LDA})$ represents number of local states - maximum at d^5

$S(\hat{\rho})$ decreased since interaction reduces number of states due to multiplet splittings

Non-interacting system chemistry decides how much TMO is correlated

Quantum contribution to correlations in TMO: *P. Thunström, I. Di Marco and O. Eriksson (2012)*

Summary

- Relative entropy to quantify correlations in interacting many-electron systems.
- Examples for Hubbard model and TMO.
  - Different correlations in paramagnetic and in antiferromagnetic cases.
  - Reduction of correlation in paramagnetic TMO: MnO→FeO→CoO→NiO
- "*Quantification of correlations in quantum many-particle systems*",
  K.B., J. Kuneš, W. Hofstetter, and D. Vollhardt,
  Phys. Rev. Lett. **108**, *087004 (2012); arXiv:1110.3214*.