Center for Electronic Correlations and Magnetism
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Quantification of correlations in quantum many-particle systems

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Supported by DFG

TRR 80

FOR 1346

12th Japanese-German Symposium
Emergent Phenomena in Novel Quantum Phases of Condensed Matter
July 15, 2012; Shuzenji, Japan

Outline:

- Classical information theory
  - information entropy
  - relative entropy
  - mutual information, correlations
- Generalization to quantum information theory
- Relative entropy: an unbiased measure of correlation strength
- Applications:
  - Hubbard model (para, antiferro)
  - Transition-metal oxide series MnO, FeO, CoO, NiO

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PRL **108**, 087004 (2012)
arXiv:1110.3214

Correlation strength

Weakly, moderately, highly, strongly, extremely correlated electrons

Conventional quantitative measures of correlation strength:

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

Very specific quantities

Related to the uncorrelated state: Correlations are relative

Is there a more objective way to
- quantify correlations of a many-body system?
- compare correlation strength of different systems?

(Quantum) information theory

e.g., Ziesche, Smith, Ho, Rudin, Gersdorf, Taut (1999)
Gottlieb, Mauser (2005, 2007)

Classical Information Theory

$a = \{a_1, a_2, \ldots, a_M\}$ set of random variables (events, signals, coin toss, spin direction...)

$p(a)$ probability distribution of a

$p(a_i)$ probability of event a_i

$$I(a_i) := -\ln p(a_i) \geq 0$$

gain in information ("surprise") due to a_i

$$S(p(a)) := \langle I(a_i) \rangle_{p(a)} = -\sum_i p(a_i) \ln p(a_i)$$

average gain in information

Information ("Shannon") entropy

Usually $\ln \rightarrow \log_2$ (bit)

Discrimination between two probability distributions

Two sets of random variables (events, signals, ...):

$$a = \{a_1, a_2, \ldots, a_M\}$$

$p(a)$ prob. distrib. of a

Example: True (or exact, known) distrib. of events

$$b = \{b_1, b_2, \ldots, b_M\}$$

$p(b)$ prob. distrib. of b

Example: Model or approximate distrib. of events

How to quantify their (dis)similarity?

Distinction between two probability distributions

Relative entropy ("Kullbach-Leibler distance/divergence/measure")
of the prob. distrib. $p(a)$ w.r.t. $p(b)$:

$$\Delta S(p(a)\|p(b)) := \langle I(b_i) - I(a_i)\rangle_{p(a)}$$

$$= \sum_i p(a_i)[\ln p(a_i) - \ln p(b_i)] \quad \begin{cases} > 0, & p(a) \neq p(b) \\ = 0, & p(a) = p(b) \end{cases}$$

Quantifies the "dissimilarity" between the distributions $p(a)$ and $p(b)$

$\Delta S(p(a)\|p(b)) \neq \Delta S(p(b)\|p(a))$ → not a metric or distance

<u>Example</u>

- Ising spin without field H=0/fair coin: $p(a) = (\frac{1}{2}, \frac{1}{2})$
- Ising spin with $H = \infty$/completely unfair coin: $p(b) = (1, 0)$

$$\Rightarrow \Delta S(H=0\|H=\infty) = \frac{1}{2}(\ln\frac{1}{2} - \ln 0) + \frac{1}{2}(\ln\frac{1}{2} - \ln 1) = \infty$$

$$\Delta S(H=\infty\|H=0) = 1(\ln 1 - \ln\frac{1}{2}) + 0(\ln 0 - \ln\frac{1}{2}) = \ln 2$$

Mutual information

Two sets of random variables (events, signals, ...):

$$a = \{a_1, a_2, \ldots, a_M\}$$
$$b = \{b_1, b_2, \ldots, b_M\}$$

with joint prob. distrib. $p(a,b)$, $\sum_{i,j} p(a_i, b_j) = 1$

Marginal distrib. $p(a_i) := \sum_j p(a_i, b_j)$

$$p(b_j) := \sum_i p(a_i, b_j)$$

In general $p(a_i, b_j) \neq p(a_i)\, p(b_j)$

→ the random variables are correlated

Mutual information $I_S(a:b) := S(p(a)) + S(p(b)) - \underbrace{S(p(a,b))}_{\text{joint entropy}}$

$$= \Delta S(p(a,b) \| p(a)\, p(b))$$ = relative entropy

= "dissimilarity" between *p(a,b)* (correlated) and *p(a)p(b)* (uncorrelated)

From Classical to Quantum Information Theory

Classical probability distribution $p(a)$

→ statistical operator/density matrix $\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

↑ probab. for $|\psi_i\rangle$

- maximal information about quantum state
- includes classical and quantum correlations (entanglement)

Product state $\hat{\rho}^{PS}$ (uncorrelated)

Example: Two subsystems (e.g., 2 quantum particles)

$$\hat{\rho}^{PS} = \hat{\rho}_1 \otimes \hat{\rho}_2$$

How to compare $\hat{\rho}$ with $\hat{\rho}^{PS}$?

Information theory

classical	quantum
• prob. distrib. $p(a)$	• statistical operator $\hat{\rho} = \sum_i p_i \lvert\psi_i\rangle\langle\psi_i\rvert$
• probability of event a_i: $p(a_i)$	• prob. for state $\lvert\psi_i\rangle$: p_i
• Shannon entropy	• von Neumann entropy
$S(p(a)) := -\langle \ln p(a_i) \rangle_{p(a)} = -\sum_i p(a_i) \ln p(a_i)$	$S(\hat{\rho}) = -\langle \ln \hat{\rho} \rangle_{\hat{\rho}} = -Tr(\hat{\rho} \ln \hat{\rho})$

Relative entropy

classical	quantum
$\Delta S(p(a) \Vert p(b)) = \sum_i p(a_i)[\ln p(a_i) - \ln p(b_i)]$	$\Delta S(\hat{\rho} \Vert \hat{\sigma}) = Tr\hat{\rho}(\ln \hat{\rho} - \ln \hat{\sigma})$

$\Rightarrow$

classical	quantum
$\Delta S(p(a,b) \Vert p(a)p(b)) = \sum_{i,j} p(a_i,b_j)[\ln p(a_i,b_j) - \ln p(a_i) - \ln p(b_j)]$	$\Delta S(\hat{\rho} \Vert \hat{\rho}_1 \otimes \hat{\rho}_2) = Tr\hat{\rho}[\ln \hat{\rho} - \ln(\hat{\rho}_1 \otimes \hat{\rho}_2)]$
	Quantifies dissimilarity between $\hat{\rho}$ and uncorrelated product state $\hat{\rho}_1 \otimes \hat{\rho}_2$

Application: Quantum version of Sanov's theorem (1957)

Hiai, Petz (1991)
Bjelković (2005)

How to distinguish between two states $\hat{\rho}, \hat{\sigma}$ of a quantum system Q ?

Given N identically prepared copies of Q

Probability for wrongly identifying $\hat{\sigma}$ with $\hat{\rho}$ after N experiments:

$$P_N(\hat{\rho}) \xrightarrow{N \to \infty} e^{-N \Delta S(\hat{\rho} \| \hat{\sigma})}$$

$$\neq P_N(\hat{\sigma} | \hat{\rho})$$

Schumacher, Westmoreland (2000)
Vedral (2002)

Quantification of correlations in quantum many-particle systems

Calculate relative entropy $\Delta S(\hat{\rho}\|\hat{\rho}^{PS})$

$\uparrow$ correlated state

$\uparrow$ uncorrelated product state

- Accounts for all possible correlation functions generated by $\hat{\rho}$
- Provides unbiased quantification of correlations
- Enables comparison of ΔS for different systems

Application to correlated many-electron systems

I. Hubbard model

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

d=3: Cubic lattice (W=1), NN hopping

Not exactly solvable
→ employ DMFT to compute relative entropy
→ only the local correlations of the exact solution are included

DMFT → reduced statistical operator $\hat{\rho}_{\mathrm{i}}$

Site i : $|a\rangle = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |2\rangle\}$

$$\rightarrow \hat{\rho}_i = Tr_{j\neq i}\hat{\rho} = \sum_a p_a |a\rangle\langle a|$$

Rissler, Noack, White (2006)
Rycerz (2006)
Franca, Capelle (2006)
Larsson, Johannesson (2006)

$$p_0 = 1 - n + d$$
$$p_\sigma = \frac{1}{2}(n + \sigma m) - d$$
$$p_2 = d$$

DMFT ⇒

Local von Neumann entropy $S(\hat{\rho}_i) = \sum_a p_a \ln p_a$

Relative entropy $\Delta S(\hat{\rho}_i \| \hat{\rho}_i^{PS}) = \sum_a p_a (\ln p_a - \ln p_a^{PS})$

Drop index i: $\hat{\rho}_{\mathrm{i}} \equiv \hat{\rho}$

Paramagnetic ground state $|PM\rangle$

Uncorrelated reference states:

$$|HF\rangle = \prod_{k,\sigma}^{k_F} a^{\dagger}_{k\sigma} |0\rangle$$ product state in **k** space $(U = 0 \Rightarrow d^{HF} = \frac{1}{4})$
(Hartree-Fock)

$$|LM\rangle = \prod_{i}^{N} a^{\dagger}_{i\sigma_i} |0\rangle$$ product state in position space $(U = \infty \Rightarrow d^{LM} = 0)$
(Local Moment)

$$n = 1, m = 0 \Rightarrow S(\hat{\rho}) = -2[d \ln d + (\frac{1}{2} + d)\ln(\frac{1}{2} + d)]$$ determined by *d(U)*

$$S_{HF} = \ln 4$$

$$S_{LM} = \ln 2$$

Correlated state $|PM\rangle$ can be distinguished from $|HF\rangle, |LM\rangle$ by:

$\Delta S(\hat{\rho} \| \hat{\rho}^{HF})$

$\Delta S(\hat{\rho}^{HF} \| \hat{\rho})$

$\Delta S(\hat{\rho} \| \hat{\rho}^{LM})=\infty$ for $U < \infty$ since $d^{LM} = 0 \Rightarrow$ perfectly distinguishable

$\Delta S(\hat{\rho}^{LM} \| \hat{\rho})$

Paramagnetic ground state $|PM\rangle$

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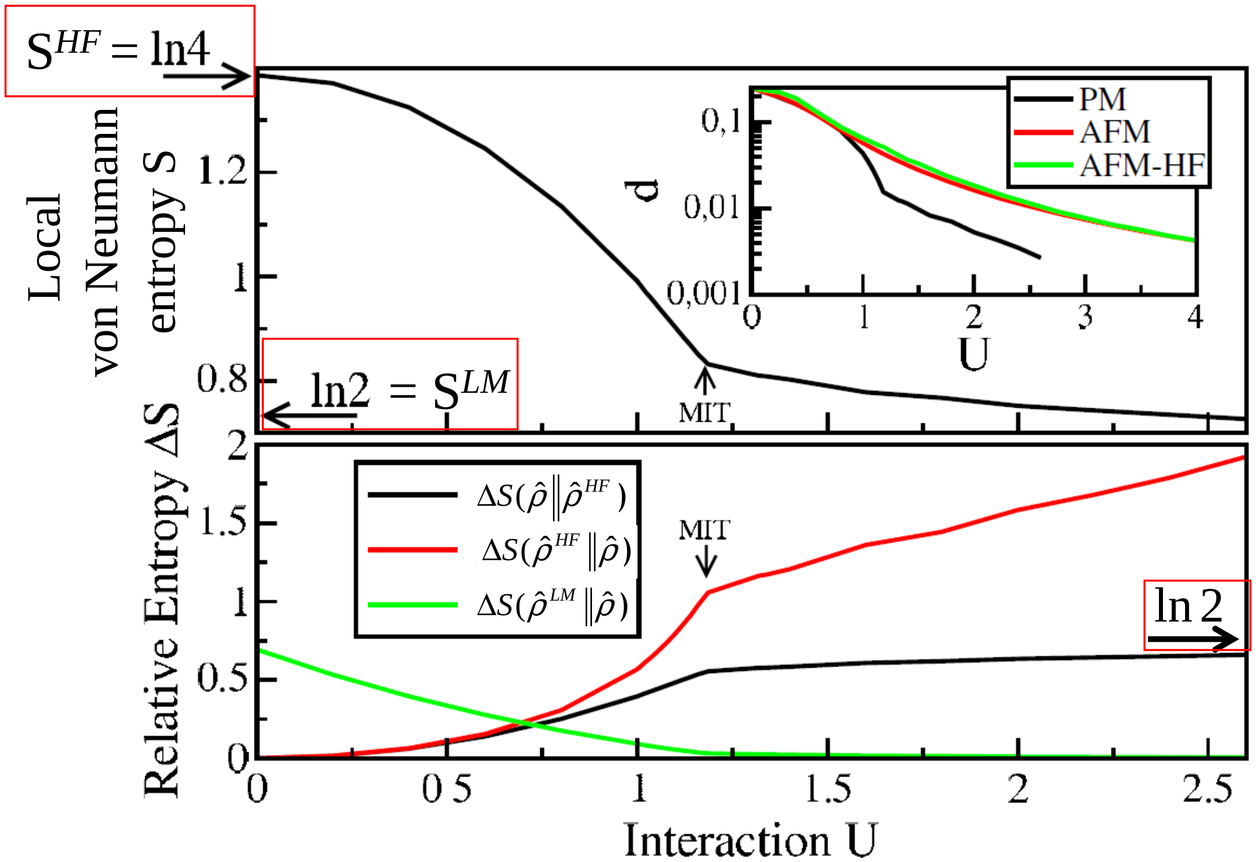
(Local Moment)



$U_{MIT} \simeq 1.225$

$\Delta S(\hat\rho \| \hat\rho^{HF}) = \ln 4 - S(\hat\rho)$

weak increase in Mott phase

Antiferromagnetic ground state $|AF\rangle$

Uncorrelated reference states:

$$|Slat\rangle = \prod_{k\in(A,B)} a^{\dagger}_{k_A\uparrow} a^{\dagger}_{k_B\downarrow} |0\rangle$$ Slater spin-density product state in **k** space

$$|Heis\rangle = \prod_{i\in(A,B)}^{N_L} a^{\dagger}_{i_A\uparrow} a^{\dagger}_{i_B\downarrow} |0\rangle$$ Neél-type product ("Heisenberg") state in position space $(m^{stag} = 1, d^{Heis} = 0)$

Correlated state $|AF\rangle$ can be distinguished from $|Slat\rangle, |Heis\rangle$ by:

$\Delta S(\hat{\rho} \| \hat{\rho}^{Slat})$

$\Delta S(\hat{\rho}^{Slat} \| \hat{\rho})$

$\Delta S(\hat{\rho} \| \hat{\rho}^{Heis}) = \infty$ since $d^{Heis} = 0 \Rightarrow$ perfectly distinguishable

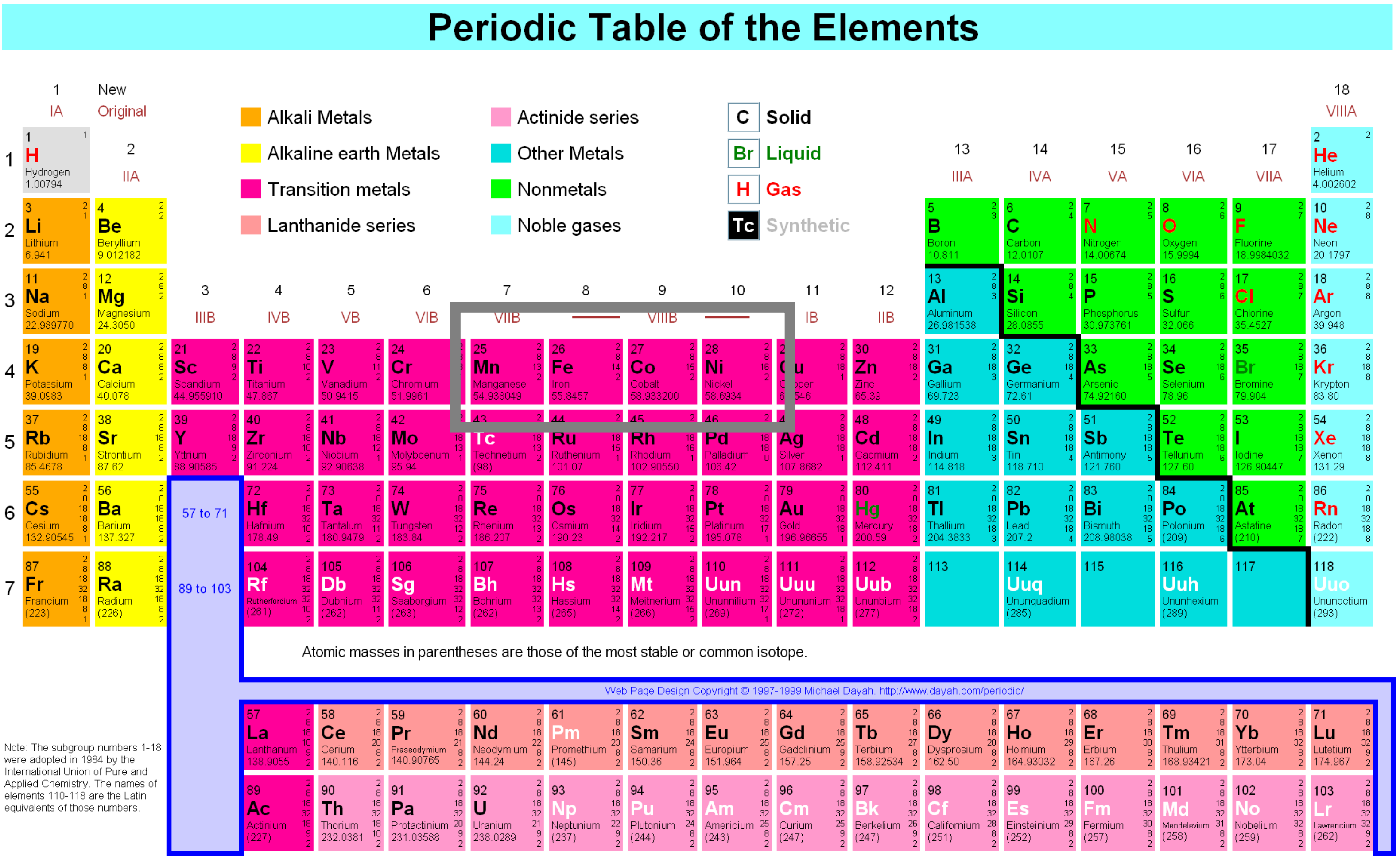
$\Delta S(\hat{\rho}^{Heis} \| \hat{\rho})$

Long range ordered Hartree-Fock (Slater) state mimics correlations well

II. Correlations in materials

Example:

Late transition-metal monoxides TMO: TM=Mn, Fe, Co, Ni



II. Correlations in materials

Example:
Late transition-metal monoxides TMO: TM=Mn, Fe, Co, Ni

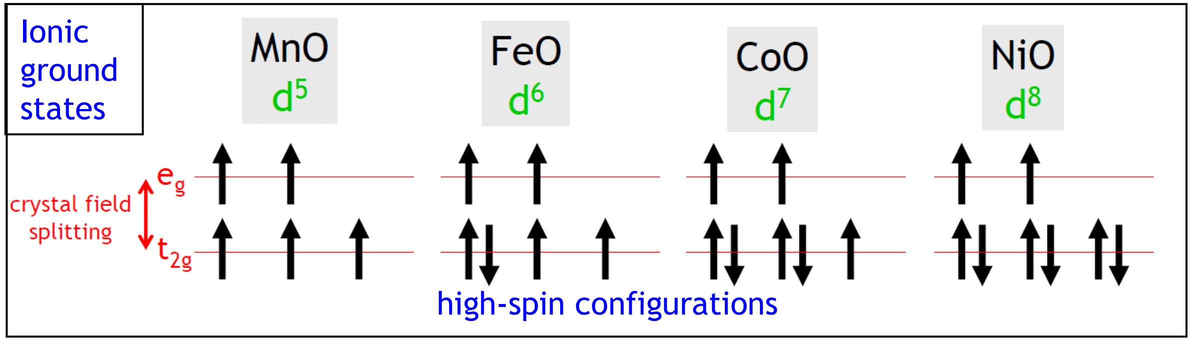
- Correlated 3d electrons → 5x2=10 orbitals
- Projection onto Wannier functions →
  TM-3d and O-2p Hamiltonian (8-bands)

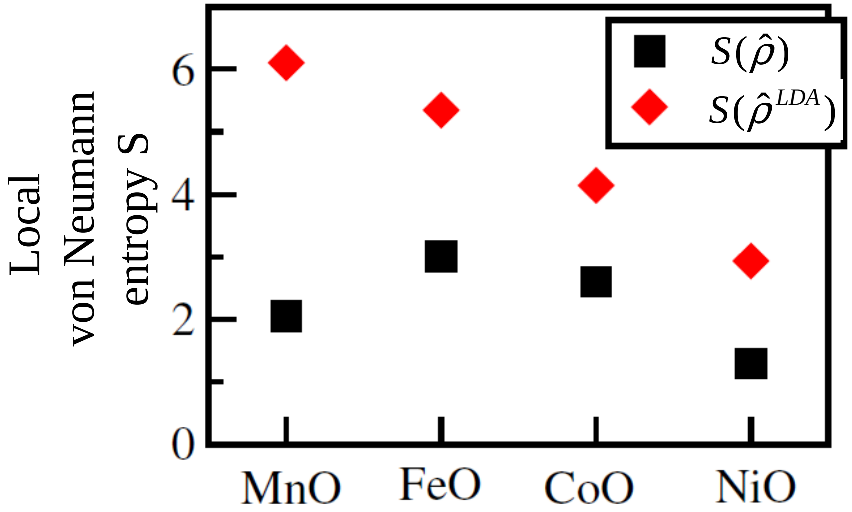
Kuneš *et al.* (2007,2008)

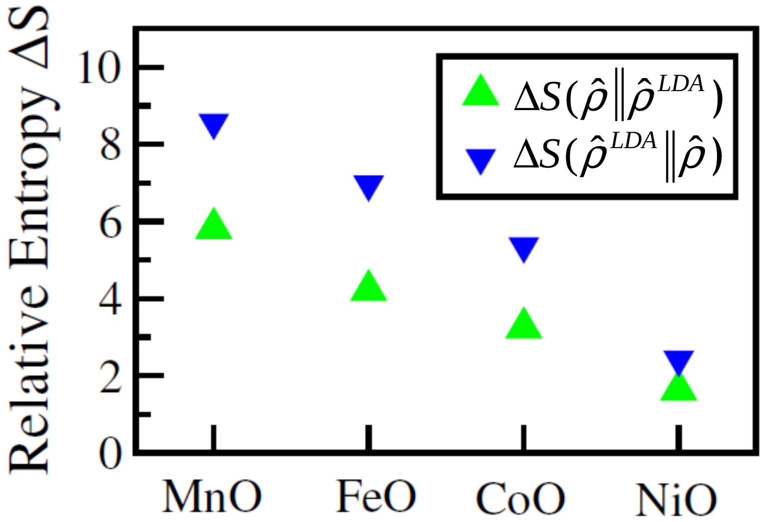
Correlated state:	$\lvert TMO\rangle$
Uncorrelated reference state:	$\lvert LDA\rangle$

$$\left.\begin{array}{l}\Delta S(\hat{\rho}\|\hat{\rho}^{LDA}) \\ \Delta S(\hat{\rho}^{LDA}\|\hat{\rho})\end{array}\right\}$$ computed with LDA+DMFT(CT-QMC)

Correlations in TMO





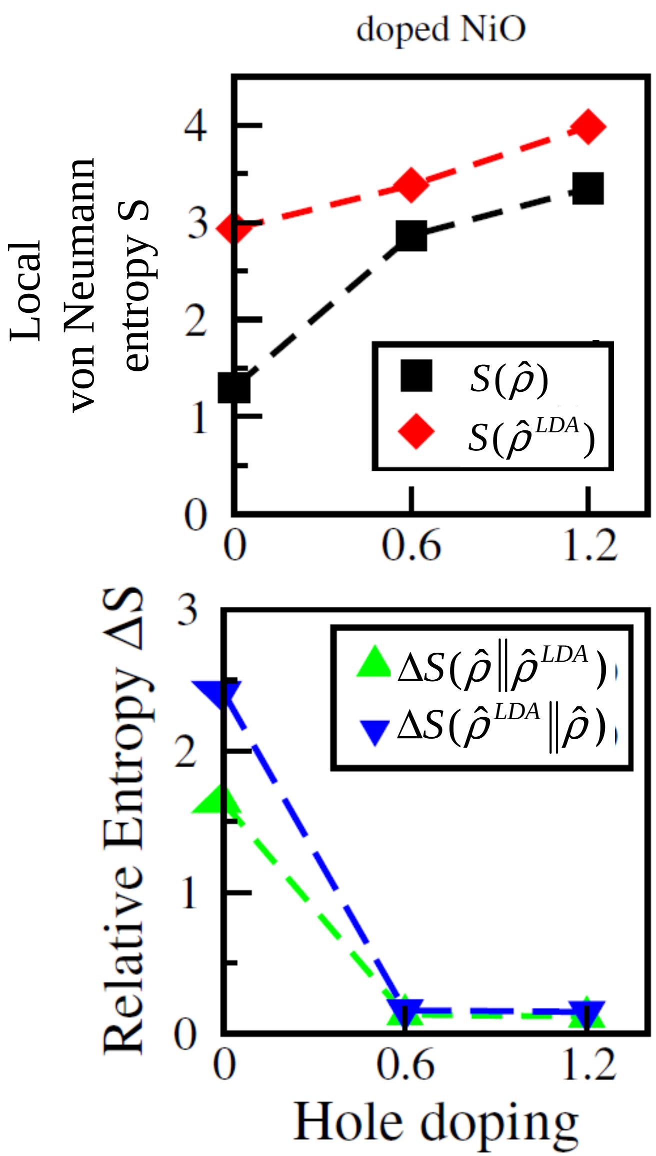


$S(\hat{\rho}^{LDA})$: # possibilities to distribute 5,6,7,8 electrons among 10 orbitals → decreases

$S(\hat{\rho})$: strong reduction of # local many-body state due to correlations

Correlation strength decreases from MnO to NiO

Effect of hole doping in NiO



Hole doping increases # local states

$$\underbrace{d^8(t_{2g}^6 e_g^2)}_{\text{stoichiometric}} \rightarrow \underbrace{\boxed{d^7(t_{2g}^6 e_g^1)} \leftrightarrow d^8(t_{2g}^6 e_g^2) \leftrightarrow \boxed{d^9(t_{2g}^6 e_g^3)}}_{\text{hole doped}}$$

→ increases local entropy

Relative entropy decreases with # holes

Doping → substantial decrease of correlations

Summary

- Unbiased method to quantify correlations in quantum many-particle systems

Compute relative von Neumann entropy $\Delta S(\hat{\rho} \| \hat{\rho}^{PS})$

- Applications: 1. Correlations in the Hubbard model

Use DMFT to compute reduced statistical operator $\hat{\rho}_{\mathrm{i}}$

$$\Rightarrow \Delta S(\hat{\rho}_{\mathrm{i}} \| \hat{\rho}_{\mathrm{i}}^{PS})$$

paramagnetic sol.: $|PS\rangle = |HF\rangle, |LM\rangle$
antiferromagnetic sol.: $|PS\rangle = |Slat\rangle, |Heis\rangle$

2. Correlations in transition metal monoxides

$$\Rightarrow \Delta S(\hat{\rho}_{\mathrm{i}} \| \hat{\rho}_{\mathrm{i}}^{LDA})$$

Correlations decrease MnO → FeO → CoO → NiO

- Perspective: include non-local spatial correlations