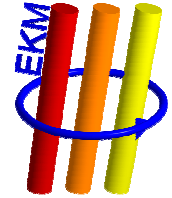




Center for Electronic Correlations and Magnetism
University of Augsburg



Quantification of correlations in quantum many-particle systems

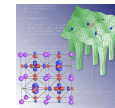
Dieter Vollhardt

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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

In collaboration with
K. Byczuk (Warsaw), J. Kuneš (Prague), W. Hofstetter (Frankfurt)
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

$a = \{a_1, a_2, \dots, a_M\}$ 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, ...):

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

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

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

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

$p(b)$ 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. $p(b)$:

$$\begin{aligned}\Delta S(p(a) \| p(b)) &:= \langle I(b_i) - I(a_i) \rangle_{p(a)} \\ &= \sum_i p(a_i) [\ln p(a_i) - \ln p(b_i)] \quad \begin{cases} > 0, & p(a) \neq p(b) \\ = 0, & p(a) = p(b) \end{cases}\end{aligned}$$

Quantifies the “**dissimilarity**” between the distributions $p(a)$ and $p(b)$

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

Example

- 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, ...):

$$a = \{a_1, a_2, \dots, a_M\} \quad \text{with joint prob. distrib. } p(a, b), \quad \sum_{i,j} p(a_i, b_j) = 1$$
$$b = \{b_1, b_2, \dots, b_M\}$$

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**

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

= “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

- prob. distrib. $p(a)$
- probability of event a_i : $p(a_i)$
- Shannon entropy

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

$$= -\sum_i p(a_i) \ln p(a_i)$$

quantum

- statistical operator $\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$
- prob. for state $|\psi_i\rangle$: p_i
- von Neumann entropy

$$S(\hat{\rho}) = -\langle \ln \hat{\rho} \rangle_{\hat{\rho}} = -\text{Tr}(\hat{\rho} \ln \hat{\rho})$$

Relative entropy

$$\Delta S(p(a) \| p(b))$$

$$= \sum_i p(a_i) [\ln p(a_i) - \ln p(b_i)]$$

$$\Delta S(\hat{\rho} \| \hat{\sigma}) = \text{Tr} \hat{\rho} (\ln \hat{\rho} - \ln \hat{\sigma})$$



$$\Delta S(p(a,b) \| p(a)p(b))$$

$$= \sum_{i,j} p(a_i, b_j) [\ln p(a_i, b_j) - \ln p(a_i) - \ln p(b_j)]$$

$$\Delta S(\hat{\rho} \| \hat{\rho}_1 \otimes \hat{\rho}_2) = \text{Tr} \hat{\rho} [\ln \hat{\rho} - \ln(\hat{\rho}_1 \otimes \hat{\rho}_2)]$$

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:

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

Schumacher, Westmoreland (2000)
Vedral (2002)

Quantification of correlations in quantum many-particle systems

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

↑ ↑
correlated uncorrelated
state 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

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

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 $\hat{\rho}_i$

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

$$\Rightarrow \hat{\rho}_i = \text{Tr}_{j \neq i} \hat{\rho} = \sum_a p_a |a\rangle \langle a|$$

Rissler, Noack, White (2006)

Rycerz (2006)

Franca, Capelle (2006)

Larsson, Johannesson (2006)

$$\left. \begin{aligned} p_0 &= 1 - n + d \\ p_\sigma &= \frac{1}{2}(n + \sigma m) - d \\ p_2 &= d \end{aligned} \right\} \xrightarrow{\text{DMFT}}$$

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: $\hat{\rho}_i \equiv \hat{\rho}$

Paramagnetic ground state $|PM\rangle$

Uncorrelated reference states:

$$|HF\rangle = \prod_{\substack{k_F \\ k, \sigma}} a_{k\sigma}^\dagger |0\rangle \quad \text{product state in } \mathbf{k} \text{ space } (U = 0 \Rightarrow d^{HF} = \frac{1}{4})$$

(Hartree-Fock)

$$|LM\rangle = \prod_i a_{i\sigma_i}^\dagger |0\rangle \quad \text{product state in position space } (U = \infty \Rightarrow d^{LM} = 0)$$

(Local Moment)

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

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

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

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

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

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

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

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

Paramagnetic ground state $|PM\rangle$

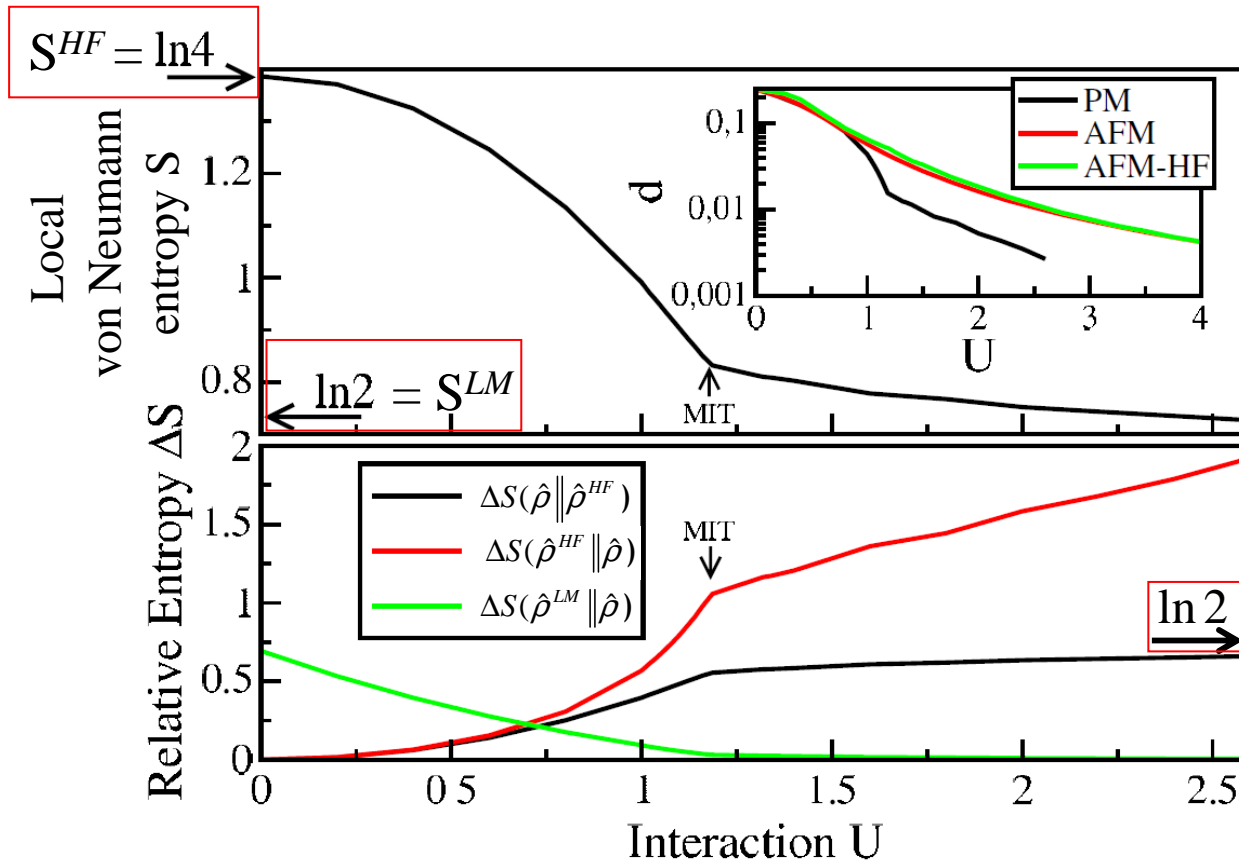
Uncorrelated reference states:

$$|HF\rangle = \prod_{\substack{k \in k_F \\ k, \sigma}} a_{k\sigma}^\dagger |0\rangle \quad \text{product state in } \mathbf{k} \text{ space } (U = 0 \Rightarrow d^{HF} = \frac{1}{4})$$

(Hartree-Fock)

$$|LM\rangle = \prod_i a_{i\sigma_i}^\dagger |0\rangle \quad \text{product state in position space } (U = \infty \Rightarrow d^{LM} = 0)$$

(Local Moment)



$$U_{MIT} \approx 1.225$$

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

weak increase in Mott phase

Antiferromagnetic ground state $|AF\rangle$

Uncorrelated reference states:

$$|Slat\rangle = \prod_{\mathbf{k} \in (A,B)} a_{\mathbf{k}_A \uparrow}^\dagger a_{\mathbf{k}_B \downarrow}^\dagger |0\rangle \quad \text{Slater spin-density product state in } \mathbf{k} \text{ space}$$

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

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

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

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

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

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

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

Periodic Table of the Elements

1 New
IA Original

1 H
Hydrogen
1.00794

2 Li
Lithium
6.941

3 Na
Sodium
22.989770

4 K
Potassium
39.0983

5 Rb
Rubidium
85.4678

6 Cs
Cesium
132.90545

7 Fr
Francium
(223)

2 Be
Beryllium
9.012182

4 Mg
Magnesium
24.3050

12 Ca
Calcium
40.078

20 Sr
Strontium
87.62

38 Ba
Barium
137.327

88 Ra
Radium
(226)

3 Sc
Scandium
44.955910

21 Ti
Titanium
47.867

39 Y
Yttrium
88.90585

57 La
Lanthanum
138.9055

89 Ac
Actinium
(227)

4 Ti
Titanium
47.867

22 V
Vanadium
50.9415

40 Zr
Zirconium
91.224

72 Hf
Hafnium
178.49

90 Th
Thorium
232.0381

5 V
Vanadium
50.9415

23 Cr
Chromium
51.9961

41 Nb
Niobium
92.90638

73 Ta
Tantalum
180.9479

91 Pa
Protactinium
231.03688

6 Cr
Chromium
51.9961

24 Mn
Manganese
54.938049

42 Mo
Molybdenum
95.94

74 W
Tungsten
183.84

92 U
Uranium
238.0289

7 Mn
Manganese
54.938049

25 Fe
Iron
55.8457

43 Tc
Technetium
(98)

75 Re
Rhenium
186.207

93 Np
Neptunium
(237)

8 Fe
Iron
55.8457

26 Co
Cobalt
58.933200

44 Ru
Ruthenium
101.07

76 Os
Osmium
190.23

94 Pu
Plutonium
(244)

9 Co
Cobalt
58.933200

27 Ni
Nickel
58.6934

45 Rh
Rhodium
102.90550

77 Ir
Iridium
192.217

95 Am
Americium
(243)

10 Ni
Nickel
58.6934

28 Cu
Copper
63.546

46 Pd
Palladium
106.42

78 Pt
Platinum
195.078

96 Cm
Curium
(247)

11 Cu
Copper
63.546

29 Zn
Zinc
65.39

47 Ag
Silver
107.8682

79 Au
Gold
196.96655

97 Bk
Berkelium
(247)

12 Zn
Zinc
65.39

30 Ga
Gallium
69.723

48 Cd
Cadmium
112.411

80 Hg
Mercury
200.59

98 Cf
Californium
(251)

13 Al
Aluminum
26.981538

31 Ga
Gallium
69.723

49 In
Indium
114.818

81 Tl
Thallium
204.3833

99 Es
Einsteinium
(252)

14 Si
Silicon
28.0855

32 Ge
Germanium
72.61

50 Sn
Tin
118.710

82 Pb
Lead
207.2

100 Fm
Fermium
(257)

15 P
Phosphorus
30.973761

33 As
Arsenic
74.92160

51 Sb
Antimony
121.760

83 Bi
Bismuth
208.98038

101 Md
Mendelevium
(258)

16 S
Sulfur
32.06

34 Se
Selenium
78.96

52 Te
Tellurium
127.60

84 Po
Polonium
(209)

102 No
Nobelium
(259)

17 Cl
Chlorine
35.4527

35 Br
Bromine
79.904

53 I
Iodine
126.90447

85 At
Astatine
(210)

103 Lr
Lawrencium
(262)

18 He
Helium
4.002602

10 Ne
Neon
20.1797

18 Ar
Argon
39.948

36 Kr
Krypton
83.80

54 Xe
Xenon
131.29

86 Rn
Radon
(222)

118 Uuo
Ununoctium
(293)

Alkali Metals: Orange

Alkaline earth Metals: Yellow

Transition metals: Pink

Lanthanide series: Light blue

Actinide series: Dark pink

Other Metals: Light blue

Nonmetals: Green

Noble gases: Cyan

C Solid

Br Liquid

H Gas

Tc Synthetic

Atomic masses in parentheses are those of the most stable or common isotope.

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57 La Lanthanum 138.9055	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92534	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93032	68 Er Erbium 167.26	69 Tm Thulium 168.93421	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967
89 Ac Actinium (227)	90 Th Thorium 232.0381	91 Pa Protactinium 231.03688	92 U Uranium 238.0289	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

Note: The subgroup numbers 1-18 were adopted in 1934 by the International Union of Pure and Applied Chemistry. The names of elements 110-118 are the Latin equivalents of those numbers.

II. Correlations in materials

Example:

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

- Correlated 3d electrons \rightarrow $5 \times 2 = 10$ orbitals
- Projection onto Wannier functions \rightarrow
TM-3d and O-2p Hamiltonian (8-bands)

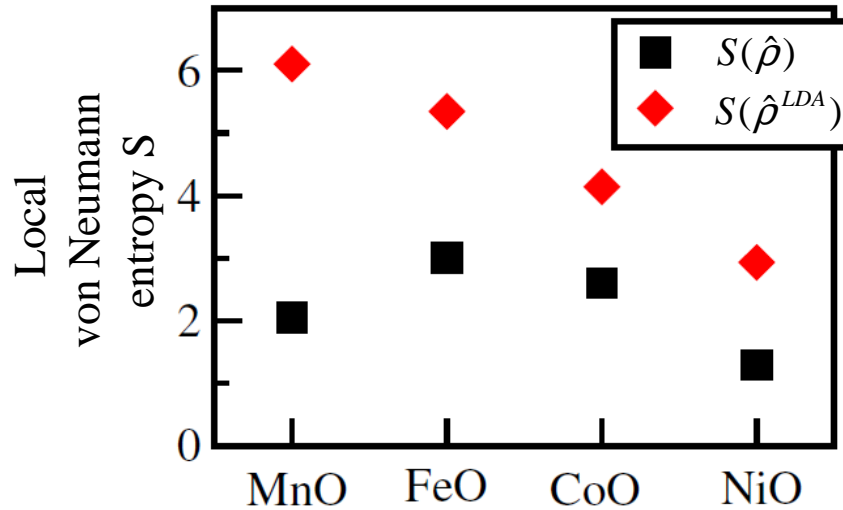
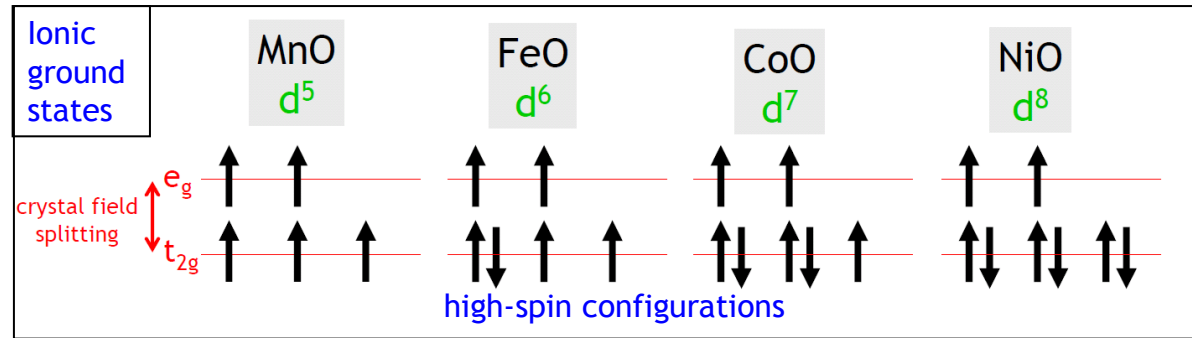
Kuneš et al. (2007,2008)

Correlated state: $|TMO\rangle$

Uncorrelated reference state: $|LDA\rangle$

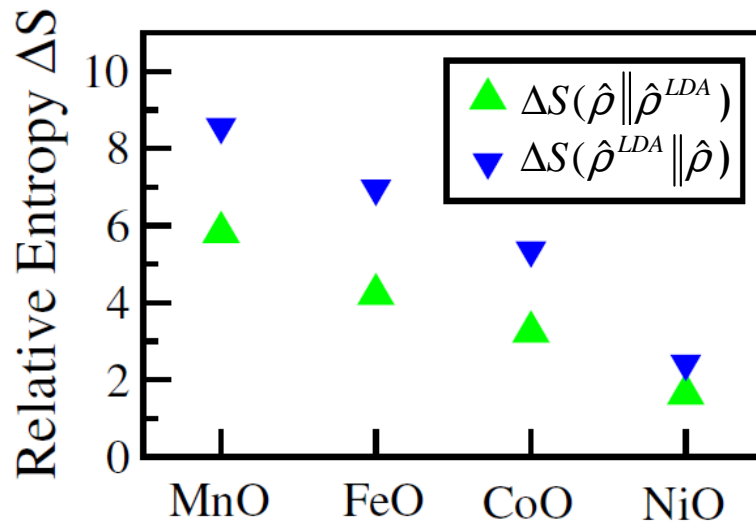
$$\left. \begin{array}{l} \Delta S(\hat{\rho} \parallel \hat{\rho}^{LDA}) \\ \Delta S(\hat{\rho}^{LDA} \parallel \hat{\rho}) \end{array} \right\} \text{ computed with LDA+DMFT(CT-QMC)}$$

Correlations in TMO



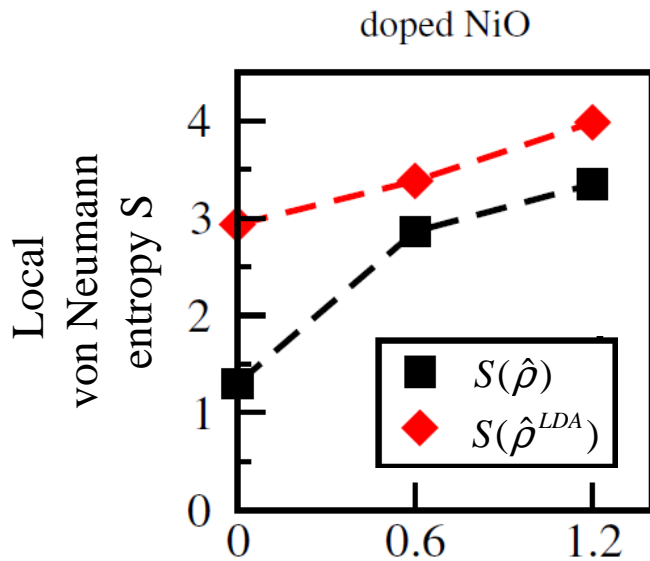
$S(\hat{\rho}^{LDA})$: # possibilities to distribute 5,6,7,8 electrons among 10 orbitals
 → decreases

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

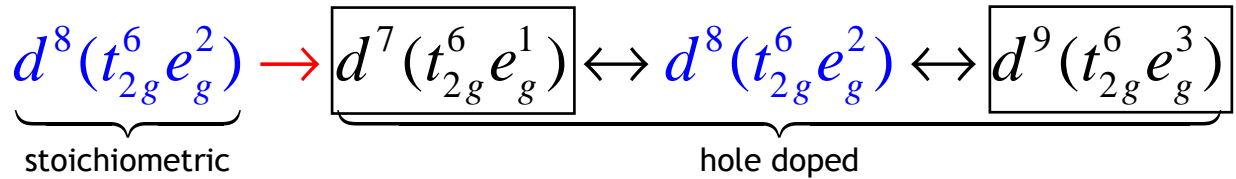


Correlation strength decreases from MnO to NiO

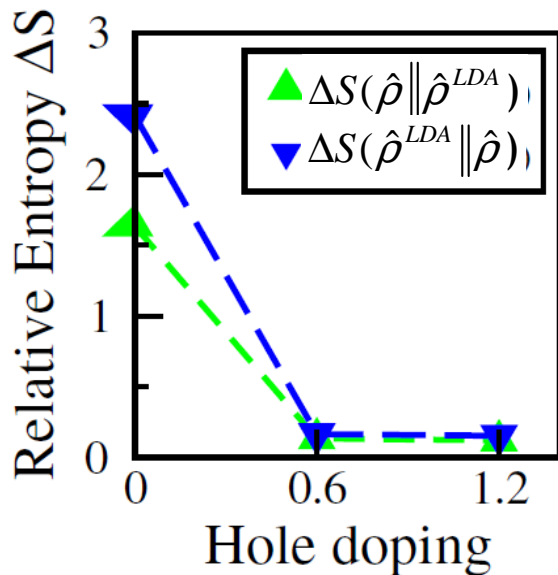
Effect of hole doping in NiO



Hole doping increases # local states



→ 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 $\Delta S(\hat{\rho} \parallel \hat{\rho}^{PS})$

- Applications: 1. Correlations in the Hubbard model

Use DMFT to compute reduced statistical operator $\hat{\rho}_i$

$$\Rightarrow \Delta S(\hat{\rho}_i \parallel \hat{\rho}_i^{PS})$$

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

- 2. Correlations in transition metal monoxides

$$\Rightarrow \Delta S(\hat{\rho}_i \parallel \hat{\rho}_i^{LDA})$$

Correlations decrease $MnO \rightarrow FeO \rightarrow CoO \rightarrow NiO$

- Perspective: include non-local spatial correlations