Quantification of correlations in quantum many-particle systems

Krzysztof Byczuk

Institute of Theoretical Physics, Faculty of Physics
University of Warsaw

April 13th, 2012

WYDZIAŁ FIZYKI
UNIWERSYTET WARSZAWSKI

EKM

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

FNP
Foundation for Polish Science

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND

www.fuw.edu.pl/byczuk

www.fuw.edu.pl/pmss

Quantification of correlations in quantum many-particle systems

Collaboration

Jan Kuneš - Prague, Academy of Sciences

Walter Hofstetter - Frankfurt University

Dieter Vollhardt - Augsburg University

Phys. Rev. Lett. **108**, *087004 (2012); arXiv:1110.3214*

Aim of this talk

CORRELATION

- What is it?

- Where to look for its effects?

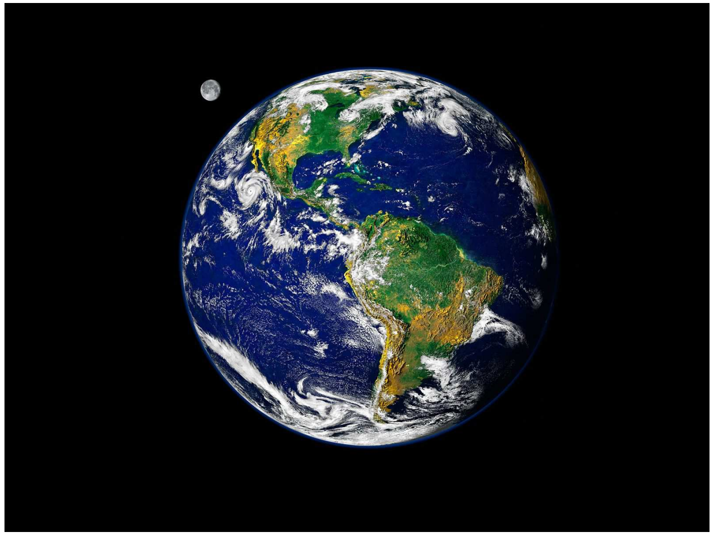
- How to quantify it?

Correlation

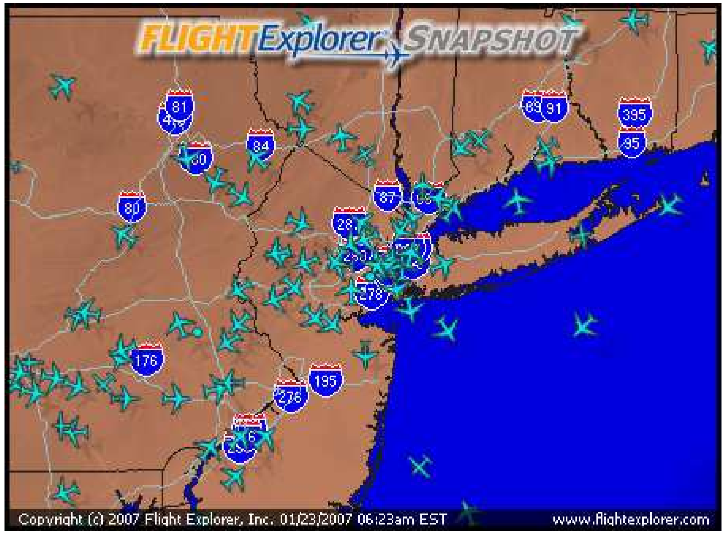
- Correlation [lat.]: con+relatio ("with relation")
  - Two or more objects needed
  - Grammar: either ... or, look for, deal with, ...
  - Many-body physics:

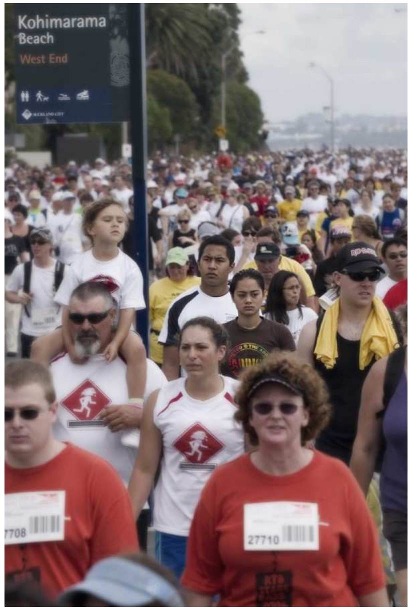
$$\frac{d\mathbf{p}_1}{dt} = \mathbf{F}_1 + \mathbf{F}_{12}, \qquad \mathbf{p}_1 = m_1 \frac{d\mathbf{x}_1}{dt}$$

$$\frac{d\mathbf{p}_2}{dt} = \mathbf{F}_2 + \mathbf{F}_{21}, \qquad \mathbf{p}_2 = m_2 \frac{d\mathbf{x}_2}{dt}$$



Spatial and temporal correlations everywhere





car traffic

air traffic

human traffic

electron traffic

more .....

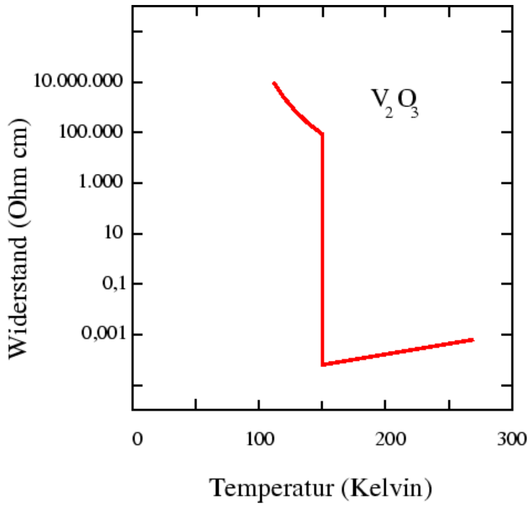


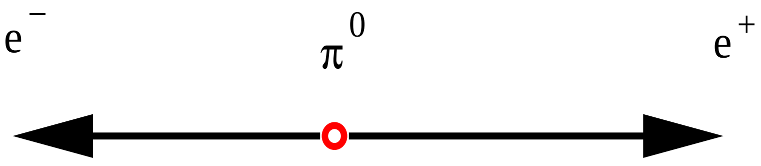
Abb. 3: Beispiel eines Metall-Isolator-Übergangs: Bei Abkühlung unter eine Temperatur von ca. 150 Kelvin erhöht sich der elektrische Widerstand von metallischem Vanadiumoxid (V_2O_3) schlagartig um das Einhundertmillionenfache (Faktor 10^8) – das System wird zum Isolator.

Correlations in quantum mechanics

Einstein, Podolsky, Rosen (1935)

$$\mathcal{H} = \mathcal{H}_+ \otimes \mathcal{H}_-$$

$$|\Psi\rangle = [|\uparrow\rangle_- \otimes |\downarrow\rangle_+ - |\downarrow\rangle_- \otimes |\uparrow\rangle_+]/\sqrt{2}$$



$\pi^0 \to e^+ + e^-$

$S_{\mathrm{tot}} = 0$ and $S^z = 0$ - singlet state (Bohm 1954)

Orthodox (Copenhagen) view:

neither particle had either spin up or spin down until the act of measurement intervented: your measurment of e^- collapsed the wave function, and instanteneusly "produced" the spin of e^+ 20 light years far away

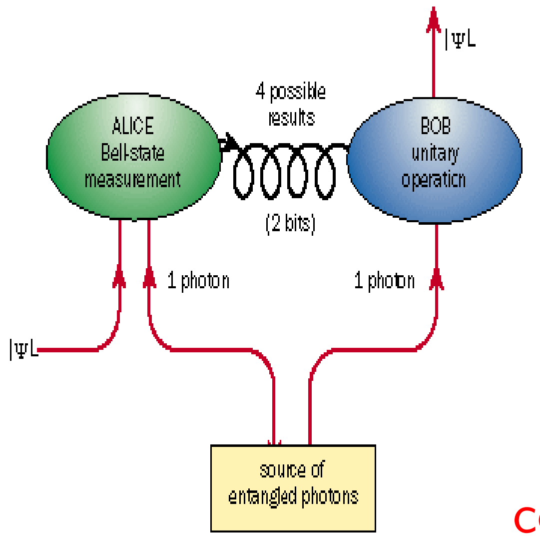
spooky action at a distance, hidden variable, ghost field, ..., to keep locallity

Correlation as resource - quantum teleportation

Bennett *et al.* (1993), photons (1998-2005), atoms (2004)

Alice and Bob share one entangled state, e.g. $|\Phi^+\rangle$. Alice wants to send to Bob all necessary information about the unknown quantum state $|\Phi\rangle = a|0\rangle + b|1\rangle$ she has got such that Bob could recreate this state using a particle he has at hand. This is a task of quantum teleportation. The state at Alice will be destroyed. What about the entangled state they share?

$$|\Phi\rangle|\Phi^+\rangle \sim [|\Phi^+\rangle(a|0\rangle + b|1\rangle) + |\Phi^-\rangle(a|0\rangle - b|1\rangle) + |\Psi^+\rangle(a|1\rangle + b|0\rangle) + |\Psi^-\rangle(a|1\rangle - b|0\rangle)]$$



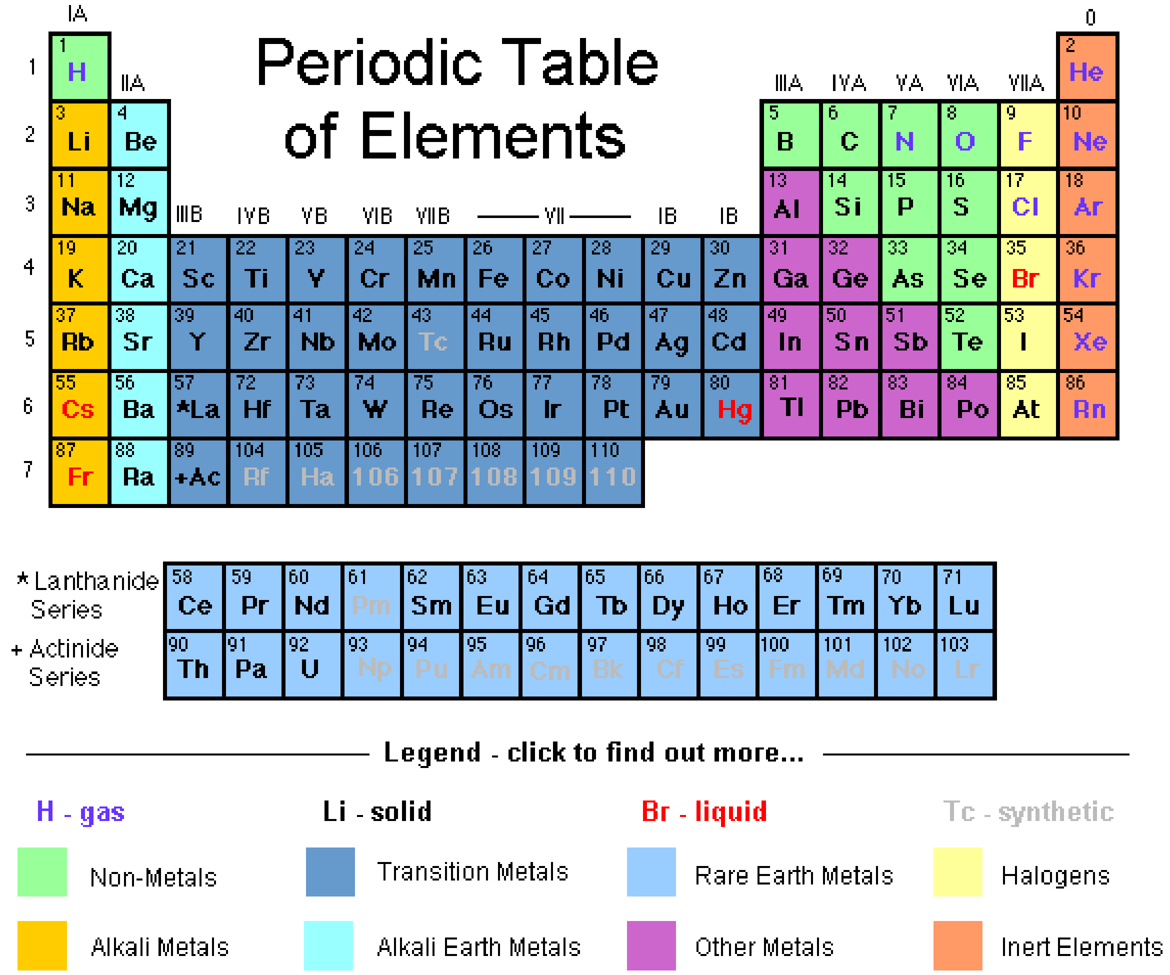
A: performs projective measurement on her 2 qbits - LO

A: call Bob and tells her result (one of 4) - CC

B: depending on A info performs 1 or σ_x or/and σ_z - LO

cost: one Bell state is eatten up

Correlated electrons



Narrow d,f-orbitals/bands → strong electronic correlations

Electronic bands in solids

Mean time τ spent by the electron on an atom in a solid
depends on the band width W

$$\text{group velocity} \quad v_{\mathbf{k}} \approx \frac{\text{lattice spacing}}{\text{mean time}} = \frac{a}{\tau}$$

$$\text{Heisenberg principle} \quad W\tau \sim \hbar$$

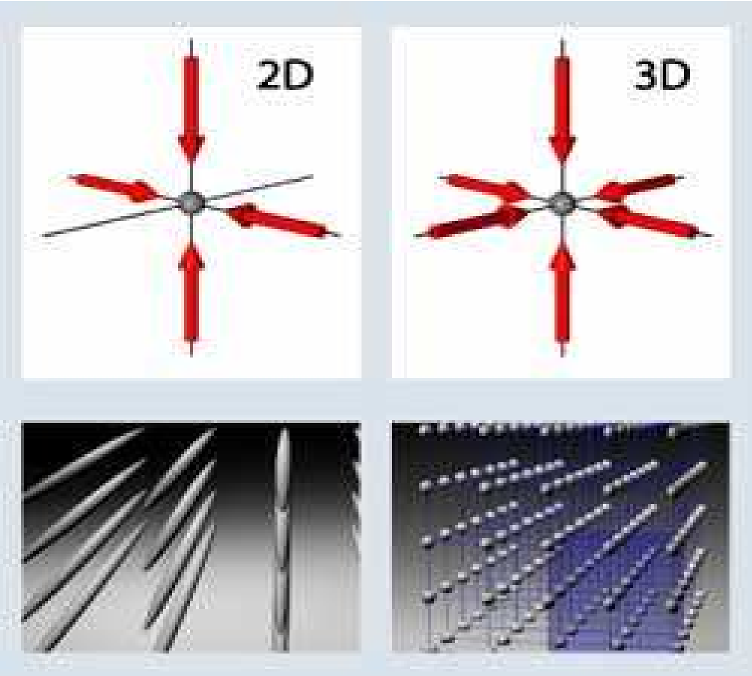
$$\frac{a}{\tau} \sim \frac{aW}{\hbar} \Longrightarrow \tau \sim \frac{\hbar}{W}$$

Small W means longer interaction with another electron on the same atom
Strong electronic correlations

Optical lattices filled with bosons or fermions

Greiner et al. 02, and other works

atomic trap and standing waves of light create optical lattices $a \sim 400 - 500nm$

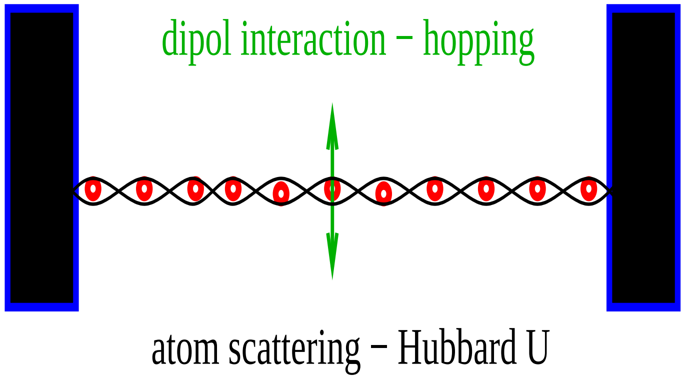


alkali atoms with ns^1 electronic state $J = S = 1/2$

$$\mathbf{F} = \mathbf{J} + \mathbf{I}$$

^{87}Rb, ^{23}Na, ^{7}Li - $I = 3/2$: effective bosons

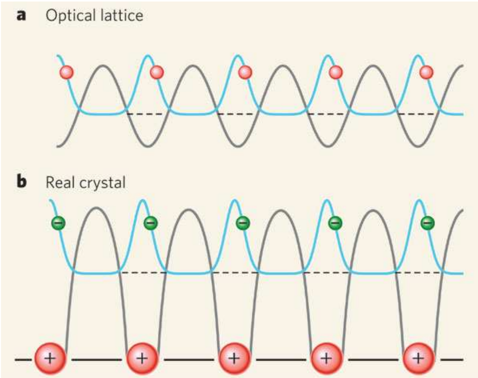
^{6}Li - $I = 1$, ^{40}K - $I = 4$: effective fermions

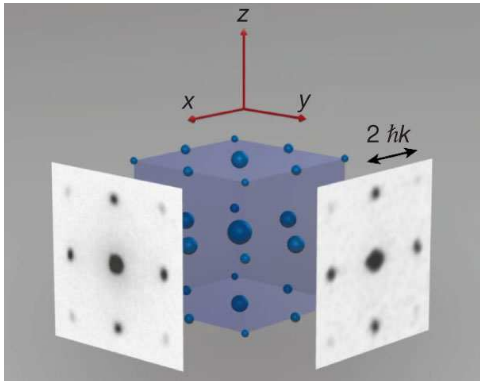


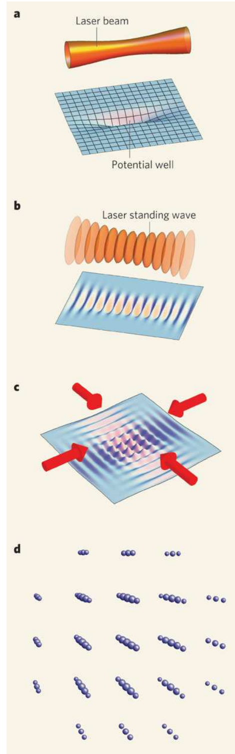
$$E_{int}^{solid} \sim 1 - 4eV \sim 10^4 K, \quad E_{kin}^{solid} \sim 1 - 10eV \sim 10^5 K$$

$$E_{kin}^{optical} \sim E_{int}^{optical} \sim 10kHz \sim 10^{-6} K$$

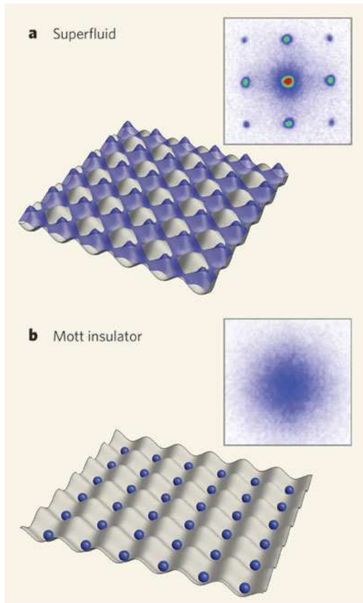
Superfluid-Mott transition - correlated lattice bosons

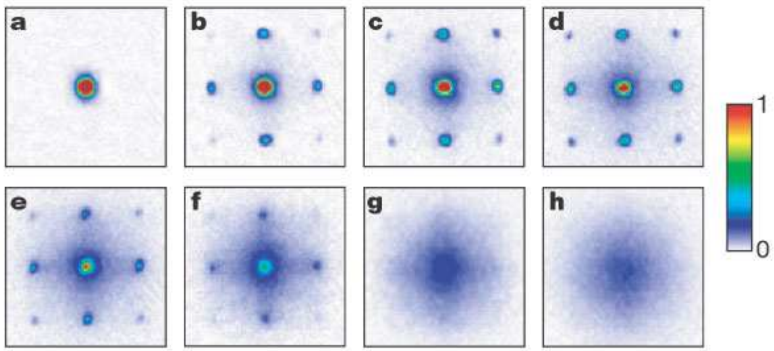






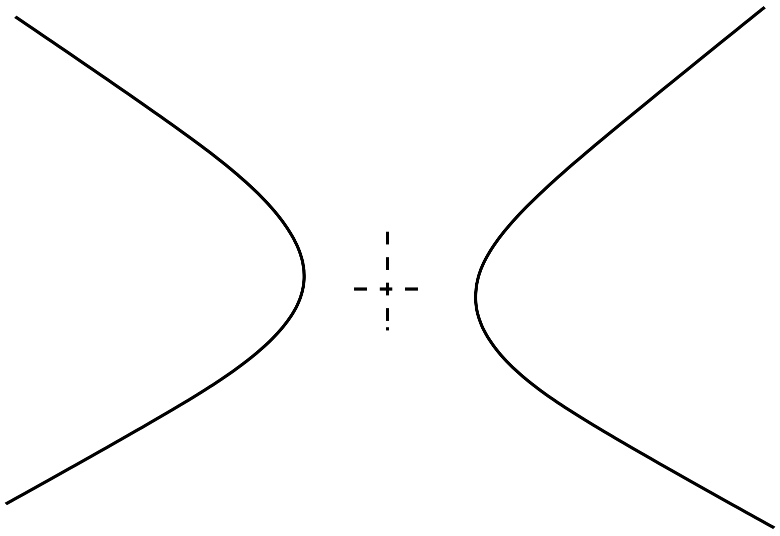
Optical lattices with cold atoms



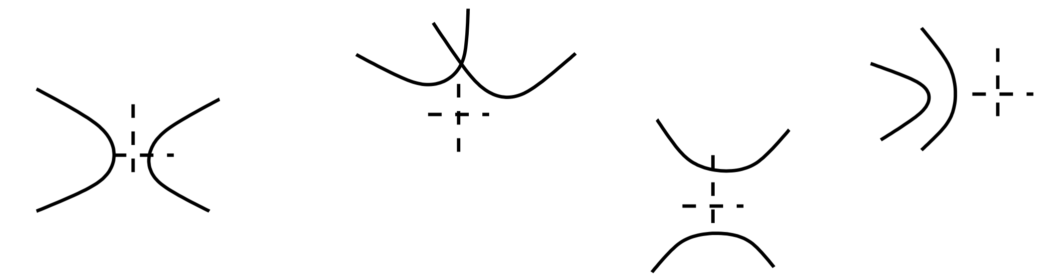


Superfluid-Mott insulator transition, Greiner, Mandel, Esslinger, Hänsch, Bloch, 2002

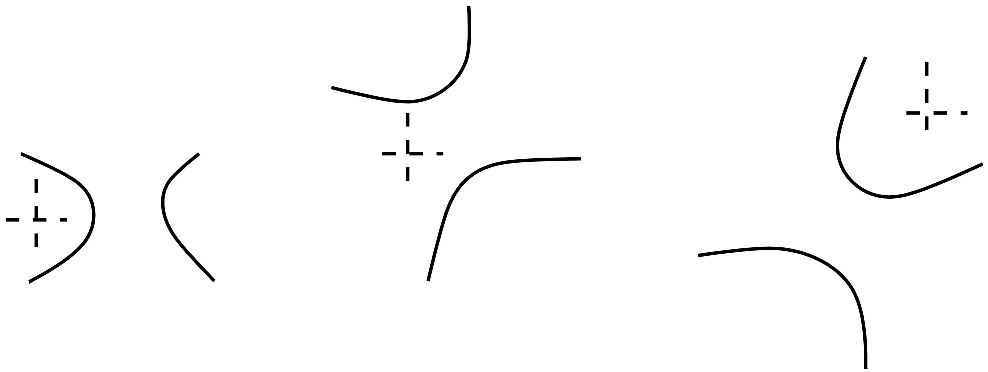
Detecting/describing amount of correlations



Detecting/describing amount of correlations



uncorrelated



correlated

Many trials and statistical analysis

Correlation

- Mathematics, Statistics, Natural Science: "In statistics, dependence refers to any statistical relationship between two random variables or two sets of data. Correlation refers to any of a broad class of statistical relationships involving dependence." (*Wikipedia*)

- Formally: Two random variables are not independent (are dependent) if

$$P(x, y) \neq p(x)p(y),$$

and are correlated if

$$\langle xy \rangle \neq \langle x \rangle \langle y \rangle,$$

$p(x) = \int dy P(x, y)$.

- 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.

Spatial and temporal correlations neglected

time/space average insufficient

$$\langle \rho(r,t)\rho(r',t')\rangle \approx \langle \rho(r,t)\rangle\langle \rho(r',t')\rangle = \text{disaster!}$$

Spatial and temporal correlations neglected

Local density approximation (LDA) disaster in HTC

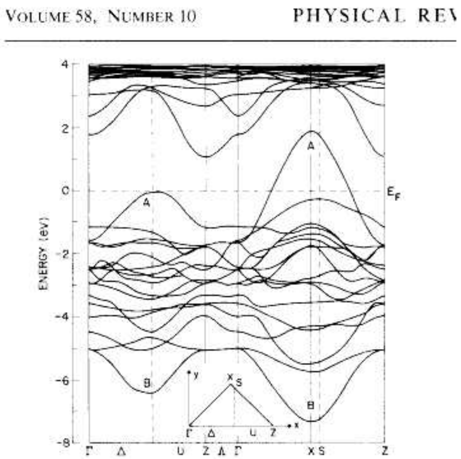
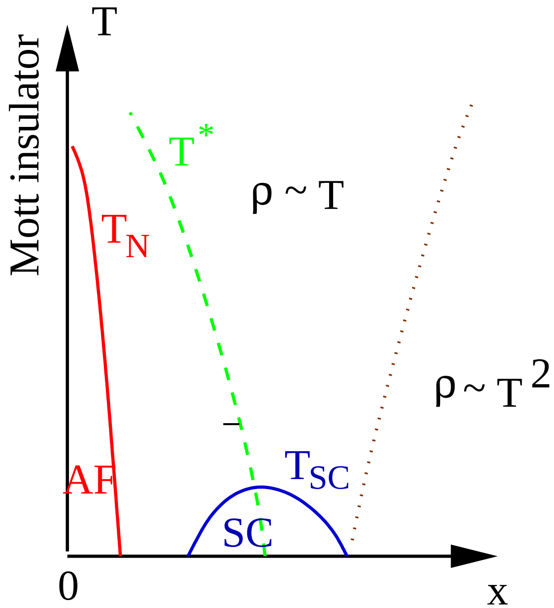


FIG. 1. LAPW energy bands for La_2CuO_4 along symmetry lines in the bct Brillouin zone (see inset and discussion in text).



$LaCuO_4$ Mott (correlated) insulator predicted to be a metal

Partially curred by (AF) long-range order ... but correlations are still missed

Quantifying correlations in many-body systems

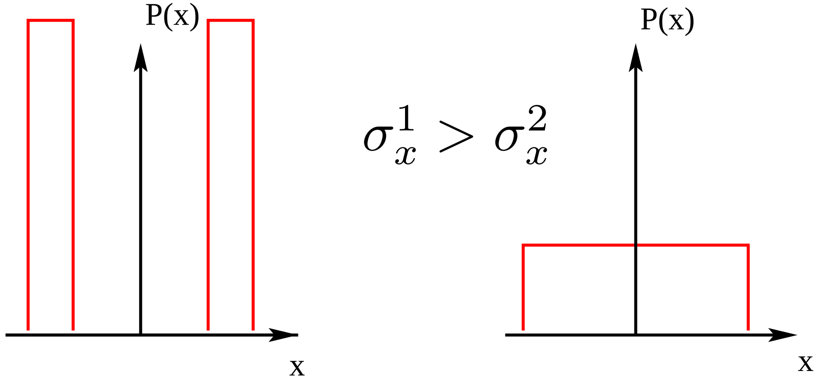
Conventional measures of correlation strength

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

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



$\sigma_x^1 > \sigma_x^2$

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

Single correlation function (variance) is not fully informative
Information theory is needed to address "How many correlations...?"

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...
Many body quantum theory, Quantum chemistry:

$$E_{\mathrm{gs}} = E^0_{gs} + E^{\mathrm{HF}}_{gs} + E^{\mathrm{corr}}_{gs}$$

Correlation energy - all contributions (Feynman diagrams) beyond the Hartree-Fock terms to the ground state energy.

Exact exchange density functional theory:

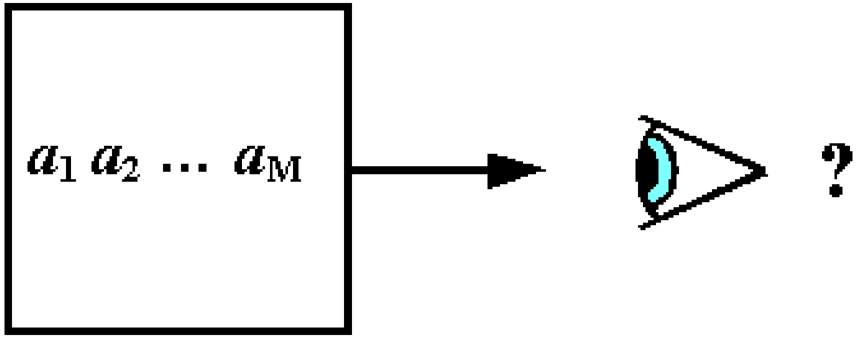
$$E[n] = T[n] + V[n] + E^{Coulomb}[n] + E^x[n] + E^{corr}[n]$$

Correlation (unknown) functional - the functional beyond exactly known, from the non-interacting approximation, terms.

Which correlations? All correlations!

Information theory

C. Shannon, 1916-2001



abstraction from the real (human) meaning of the messages

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

Information entropy

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

positive, monotonic, additive, convex, ...

Information theory - correlation

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

Messages are **correlated** (not independent)

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

i.e.

$$\langle a_i b_j \rangle \neq \langle a_i \rangle \langle b_j \rangle$$

Total correlation

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

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

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

Two correlated (sub)systems have relative entropy

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

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

and generalization to many-body systems.

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

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

e.g., after taking partial integrals or trace

In quantum mechanics the uncorrelated state depends on choosing the base
position-space vs. momentum-space

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.

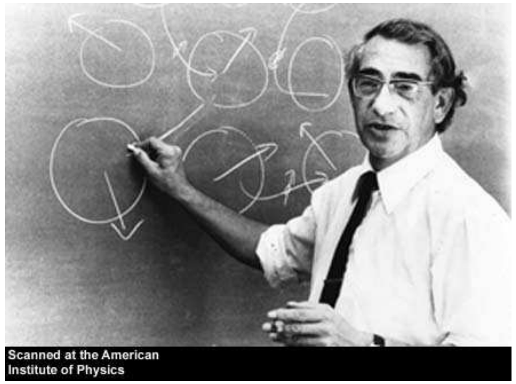
Entropic measure of correlation strength

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

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

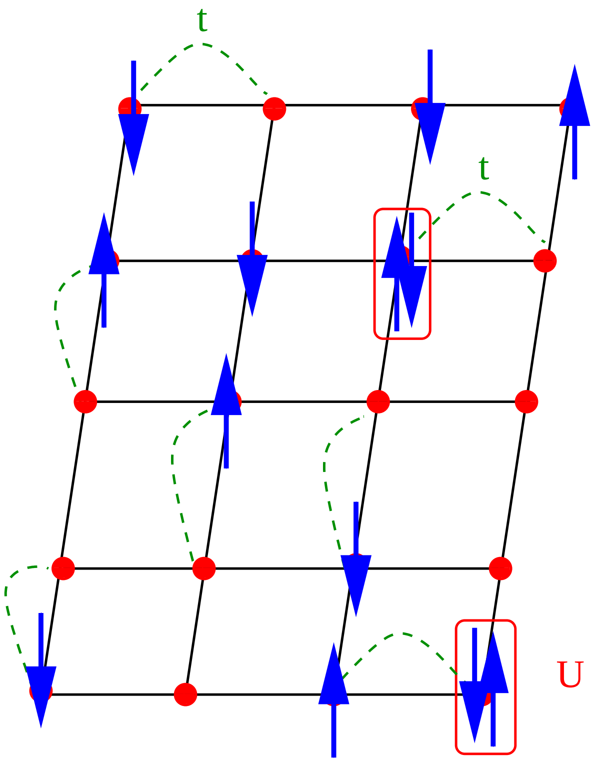
Correlated fermions on lattices

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

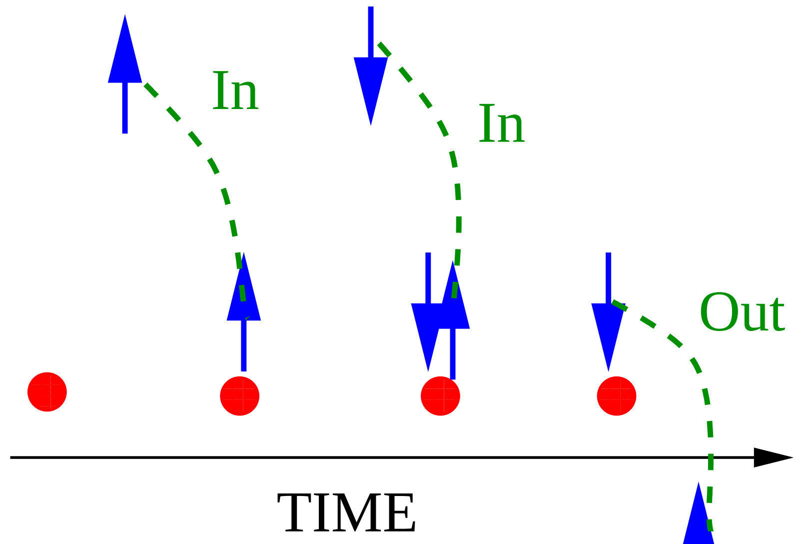


fermionic Hubbard model

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



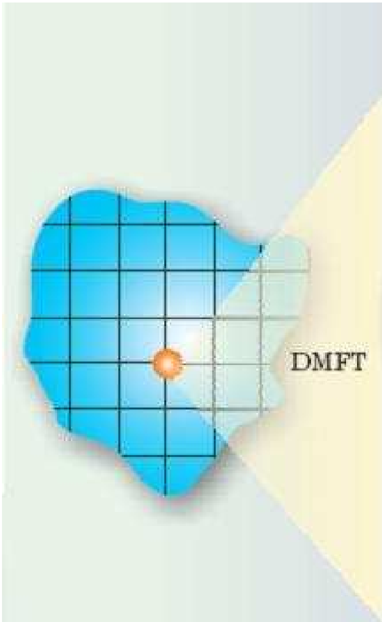
Local Hubbard physics

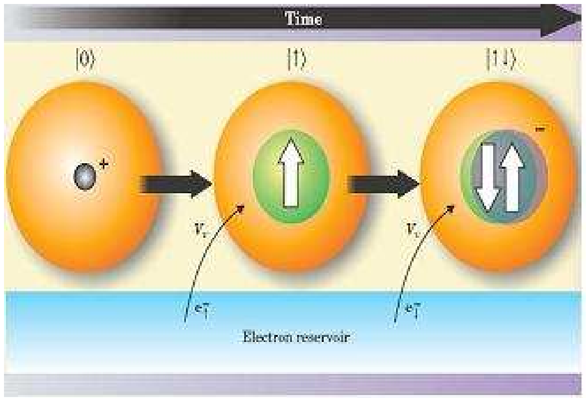


$$|i,0\rangle \rightarrow |i,\uparrow\rangle \rightarrow |i,2\rangle \rightarrow |i,\downarrow\rangle$$

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, (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.

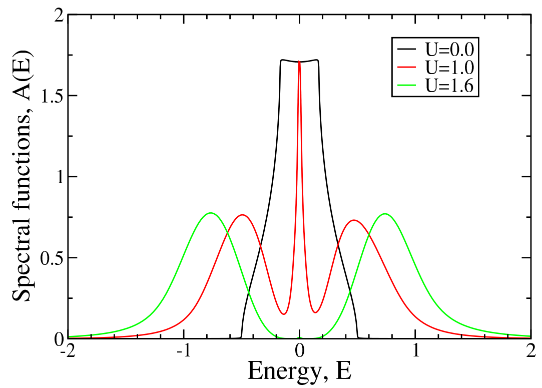
Example 1: Correlation and Mott Transition

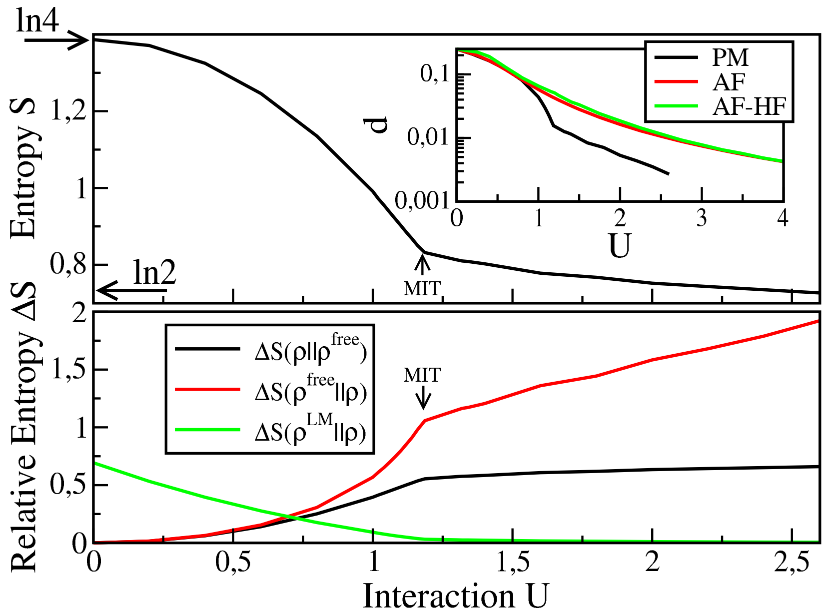
Hubbard model, $n = 1$, $T = 0$, $d = 3$, PM

Uncorrelated product states:

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

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





Correlation strength not linear in U/W

Correlation strength similar in Mott insulators at different U

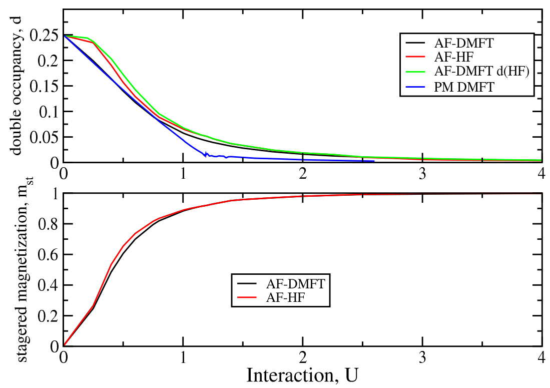
Example 2: Correlation and Antiferromagnetic LRO

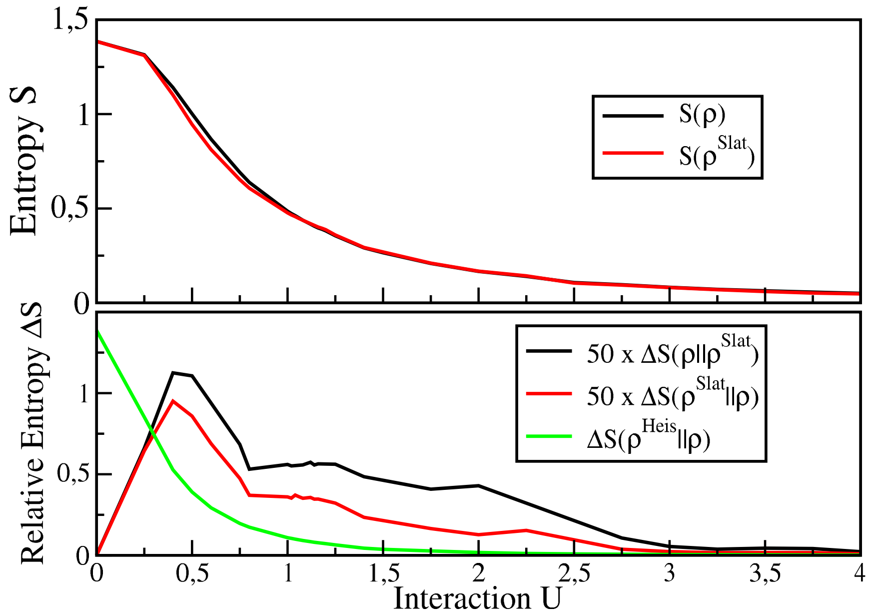
Hubbard model, $n=1$, $T=0$, $d=3$, AF

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



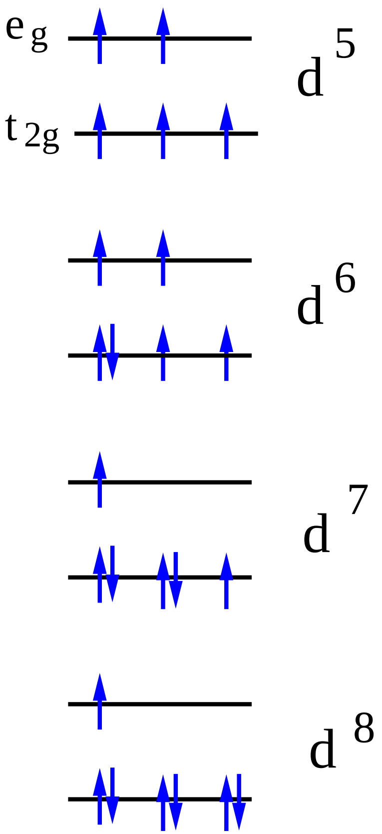


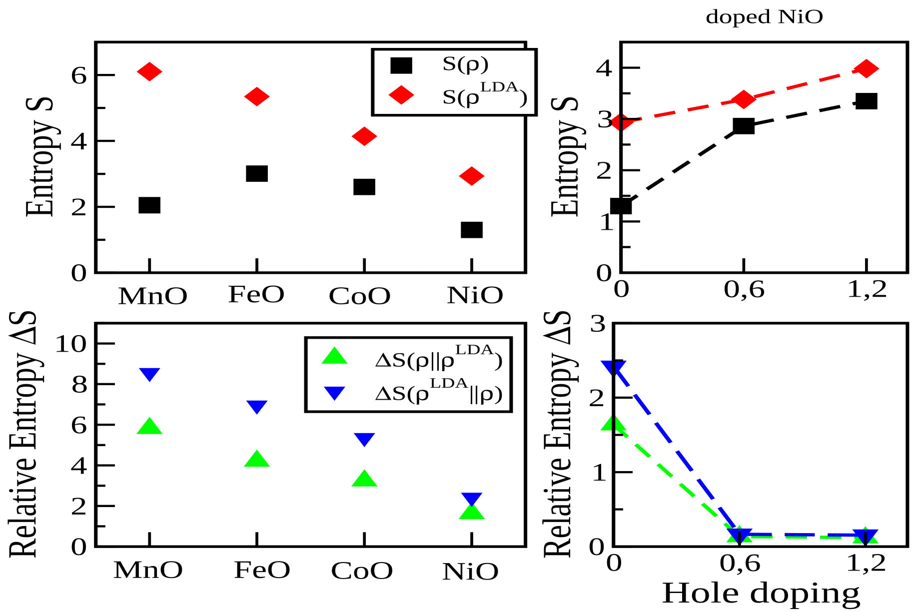
LRO-HF (Slater) states imitates correlations well

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$\rightarrow$FeO$\rightarrow$CoO$\rightarrow$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*.