Quantification of correlations in correlated electron systems

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Quantification of correlations in correlated electron systems

Collaboration

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Jan Kuneš - Prague, Academy of Sciences

Dieter Vollhardt - Augsburg University

Aim of this talk

CORRELATION

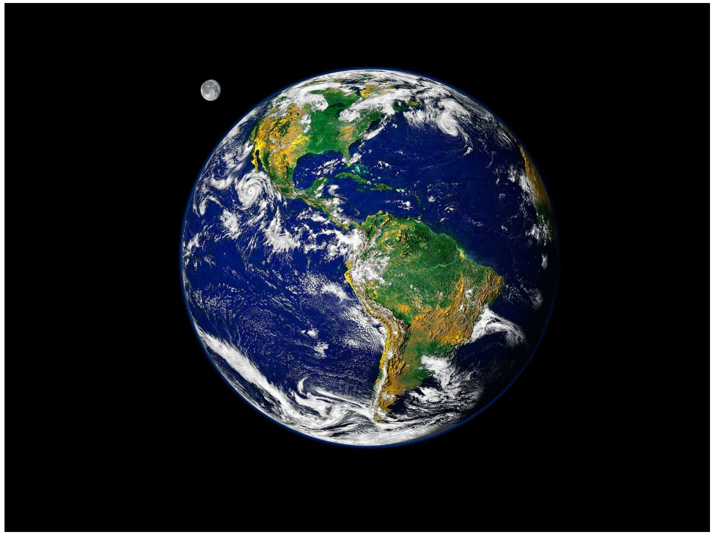
- What is it?
- How to quantify it?

Correlation

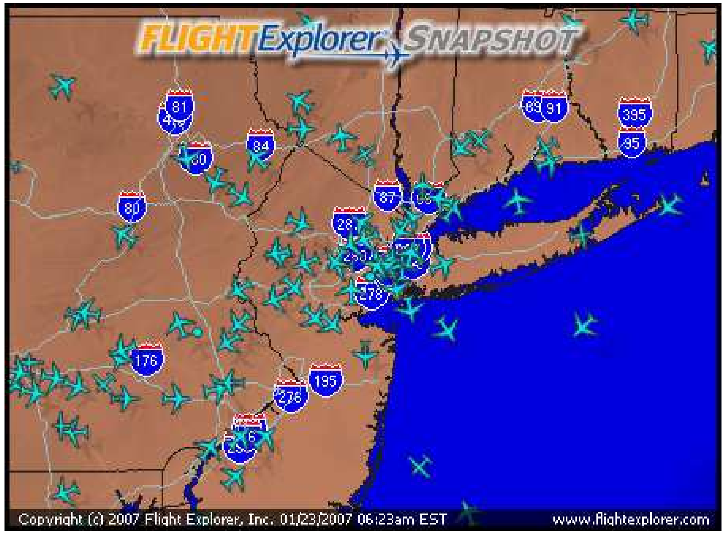
- Correlation [lat.]: con+relatio ("with relation")
  - Two or more objects needed
  - Grammar: either ... or, look for, deal with, ...
  - Many-body physics:

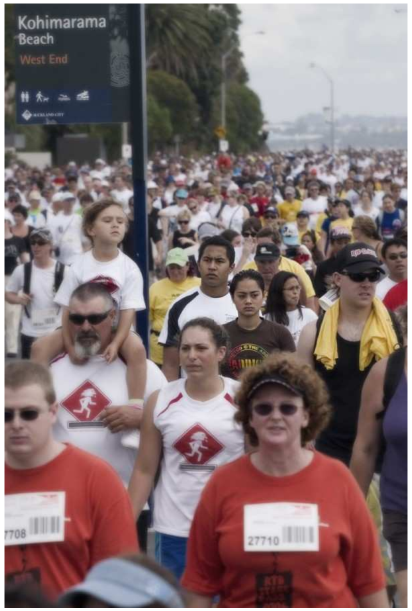
$$\frac{d\mathbf{p}_1}{dt} = \mathbf{F}_1 + \mathbf{F}_{12}, \qquad \mathbf{p}_1 = m_1 \frac{d\mathbf{x}_1}{dt}$$

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



Spatial and temporal correlations everywhere





car traffic

air traffic

human traffic

electron traffic

more .....

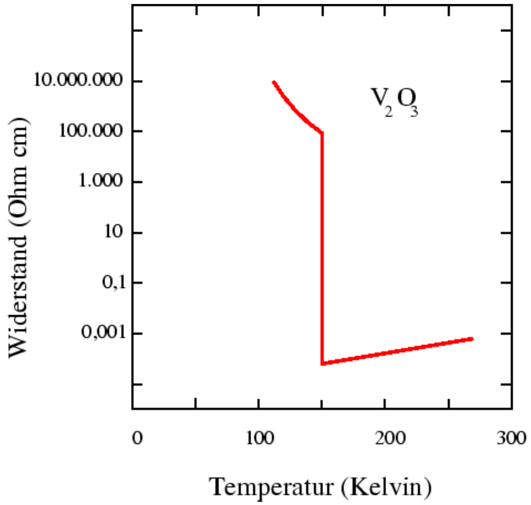


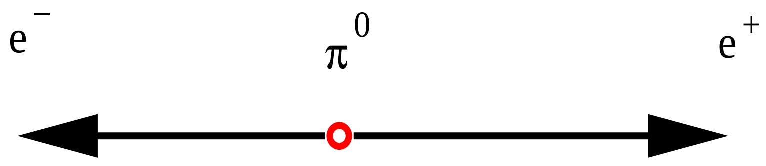
Abb. 3: Beispiel eines Metall-Isolator-Übergangs: Bei Abkühlung unter eine Temperatur von ca. 150 Kelvin erhöht sich der elektrische Widerstand von metallischem Vanadiumoxid (V_2O_3) schlagartig um das Einhundertmillionenfache (Faktor 10^8) – das System wird zum Isolator.

Correlations in quantum mechanics

Einstein, Podolsky, Rosen (1935)

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

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



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

$S_{\rm tot} = 0$ 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

Bipartite pure entanglement

Let $\{|i\rangle_A \otimes |j\rangle_B\} \in \mathcal{H} = \mathcal{H}_\mathcal{A} \otimes \mathcal{H}_\mathcal{B}$ and AB distinguishable.

Any state

$$|\Psi\rangle = \sum_{ij} \gamma_{ij} |i\rangle_A \otimes |j\rangle_B$$

that cannot be represented as a product state is called an entangled state.

- Entanglement is a quantum correlation which does not have a classical counterpart
- Any entangled state cannot be prepared from a product state by local operations (acting on one subsystem) and classical communications (LOCC).

Bell states

- classical two level system (0 or 1) codes one bit of information

- in QM two level system can be both 0 and 1 (spin, polarization, vortex, energy structure, ...)

- it was proposed to call it quantum bit or qbit (read: *qiubit*) in general - Schumacher (1995)

Bell states - maximally entangled states of two qbits

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}\left[|01\rangle - |10\rangle\right]$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}\left[|01\rangle + |10\rangle\right]$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}\left[|00\rangle - |11\rangle\right]$$

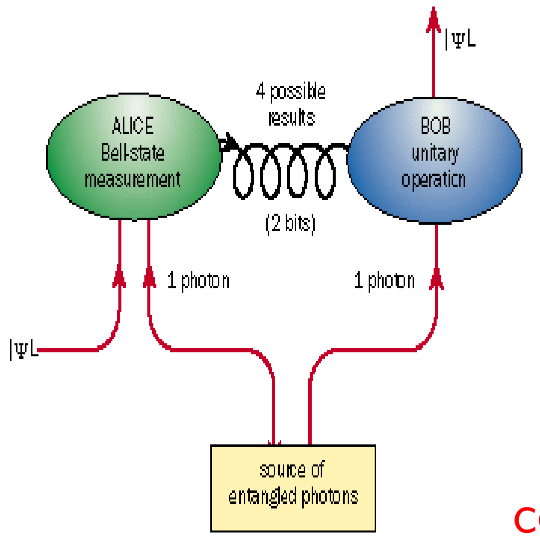
$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left[|00\rangle + |11\rangle\right]$$

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?

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



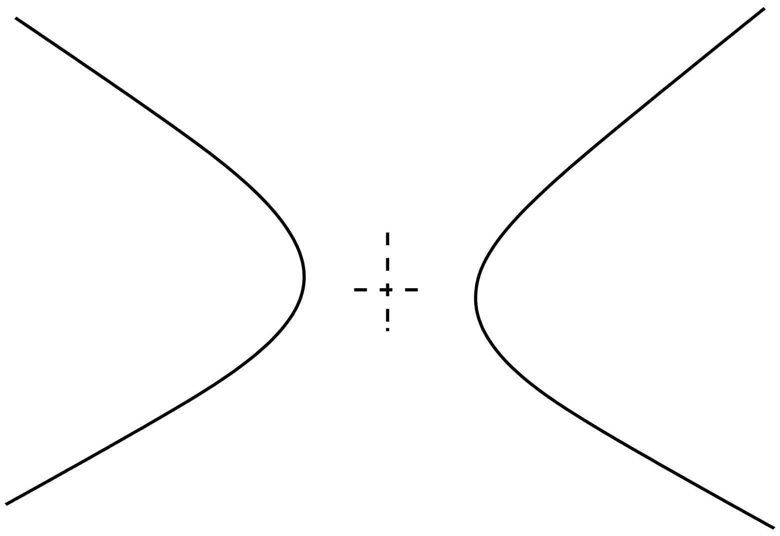
A: performs projective measurement on her 2 qbits - LO

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

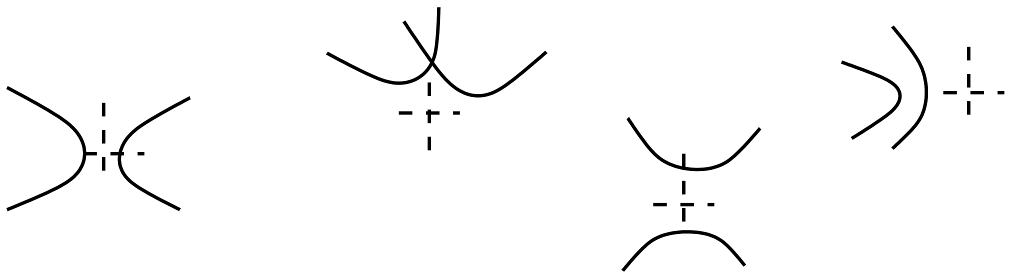
B: depending on A info performs 1 or σ_x or/and σ_z - LO

cost: one Bell state is eatten up

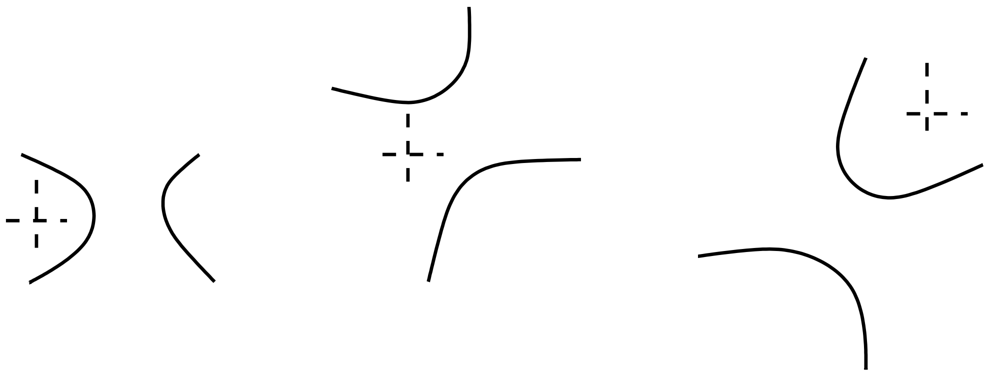
Detecting correlation



Detecting correlation



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

VOLUME 58, NUMBER 10 PHYSICAL REV

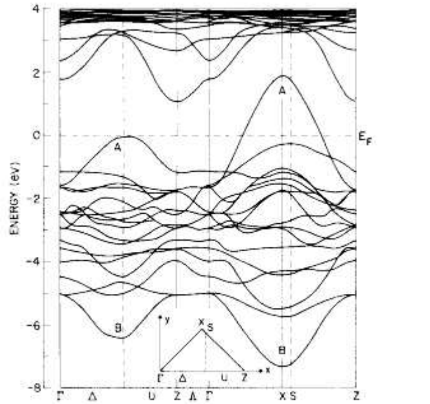
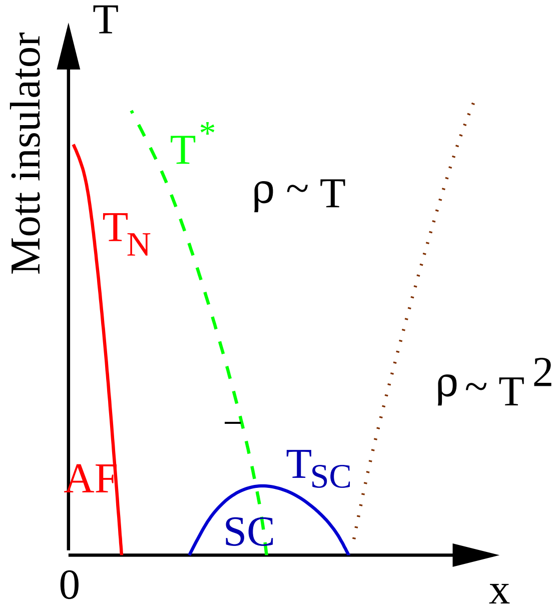


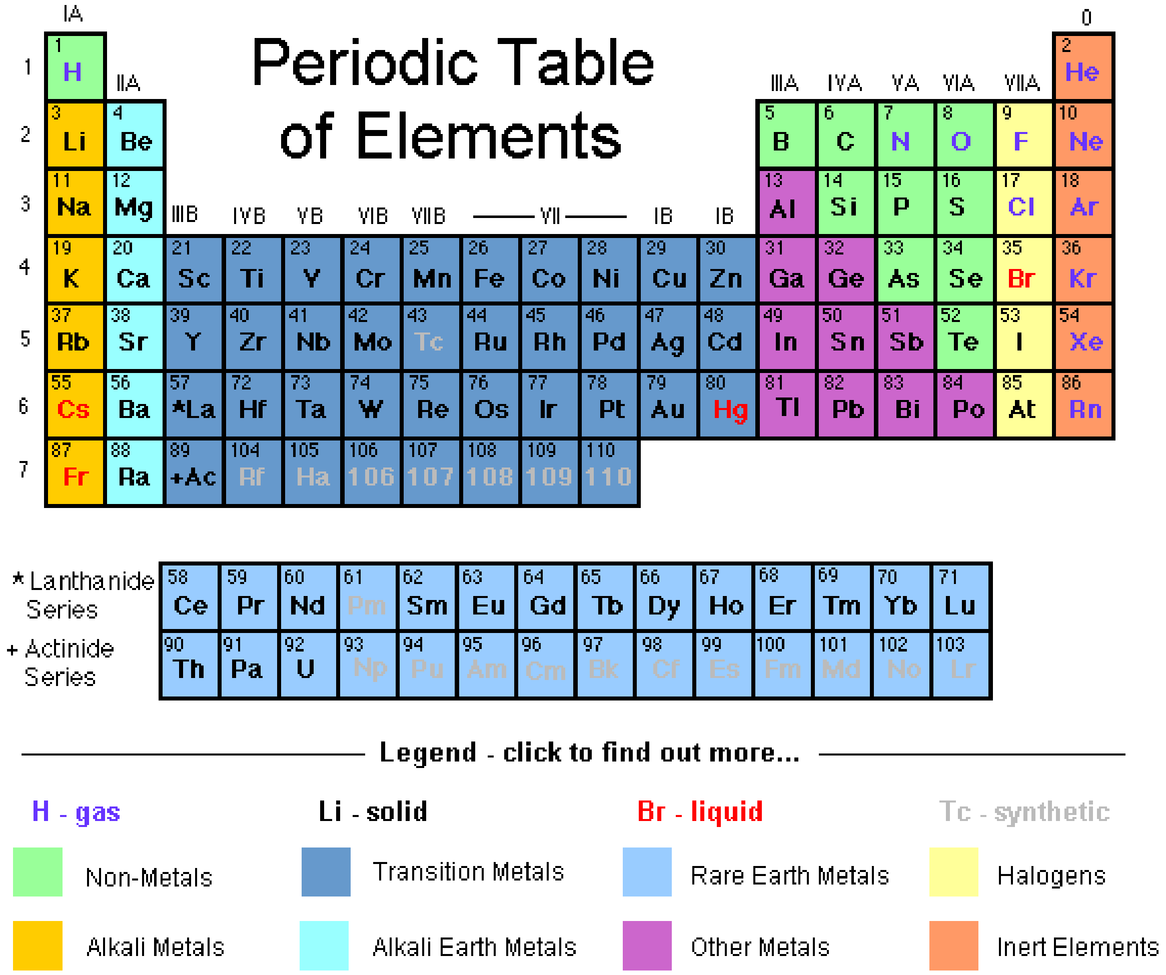
FIG. 1. LAPW energy bands for La_2CuO_4 along symmetry lines in the bct Brillouin zone (see inset and discussion in text).



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

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

Correlated electrons

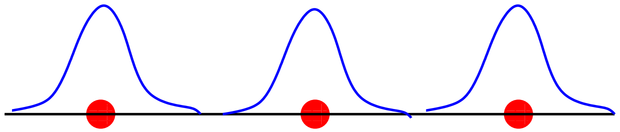


Narrow d,f-orbitals/bands $\rightarrow$ strong electronic correlations

Electronic bands in solids

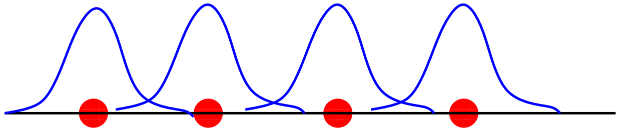
Wave function overlap $\sim t_{ij} = \langle i|\hat{T}|j\rangle \rightarrow |E_{\mathbf{k}}| \sim \mathrm{bandwidth}\, W$

Band insulators, e.g. NaCl



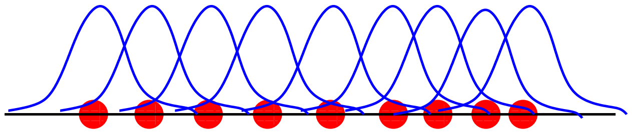
Atomic levels, localized electrons $|\mathbf{R}_i\sigma\rangle$

Correlated metals, e.g. Ni, V_2O_3, Ce



Narrow bands, $|\mathbf{R}_i\sigma\rangle \leftrightarrow |\mathbf{k}\sigma\rangle$

Simple metals, e.g. Na, Al



Broad bands, extended Bloch waves $|\mathbf{k}\sigma\rangle$

Electronic bands in solids

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

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

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

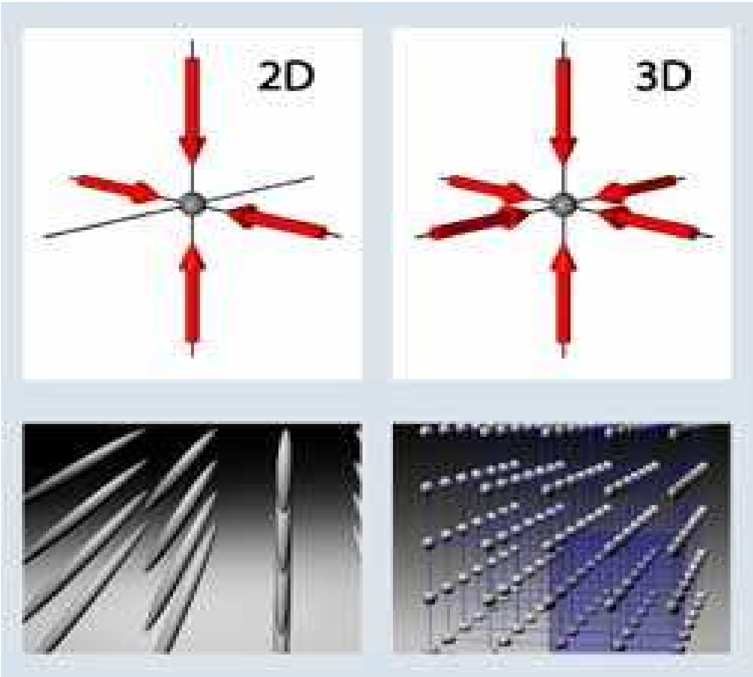
$$\frac{a}{\tau} \sim \frac{aW}{\hbar} \Longrightarrow \tau \sim \frac{\hbar}{W}$$

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 $a \sim 400 - 500nm$

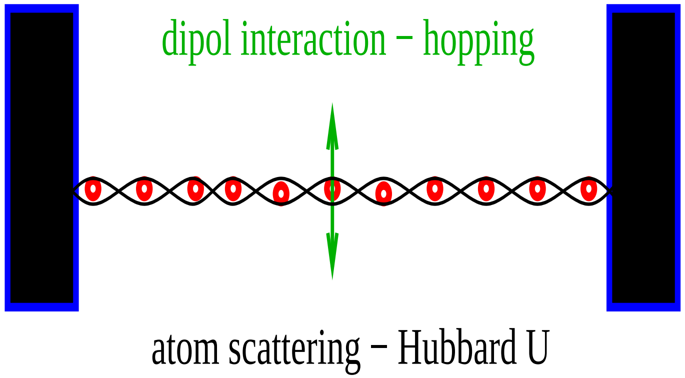


alkali atoms with ns^1 electronic state $J = S = 1/2$

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

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

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



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

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

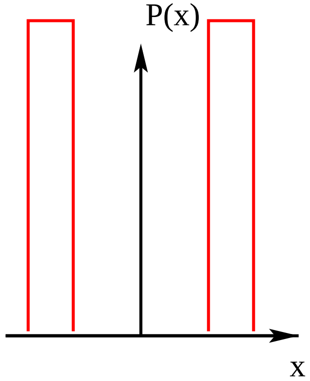
Quantifying correlations

How many correlations is there in correlated electron systems?

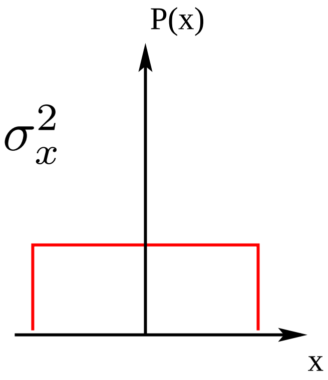
Correlation functions (double occupancy, effective mass, Z- factor, conductance(vity), susceptibilities, ...) are very useful for particular cases when we know what to look at:

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),*
....

More information
in the left distribution

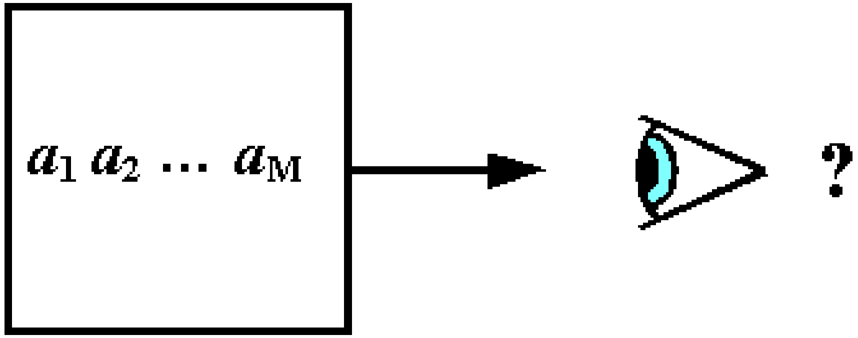


$\sigma_x^1 > \sigma_x^2$



Information theory is needed to address "How many correlations...?"

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.

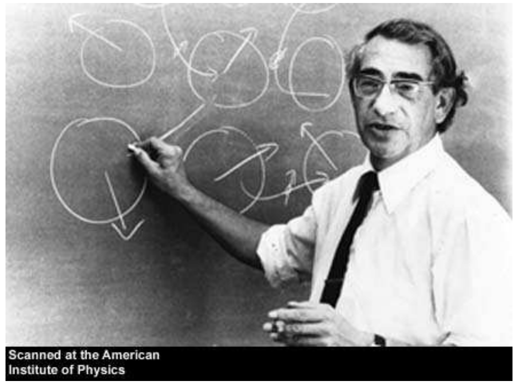
Correlation measure

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

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

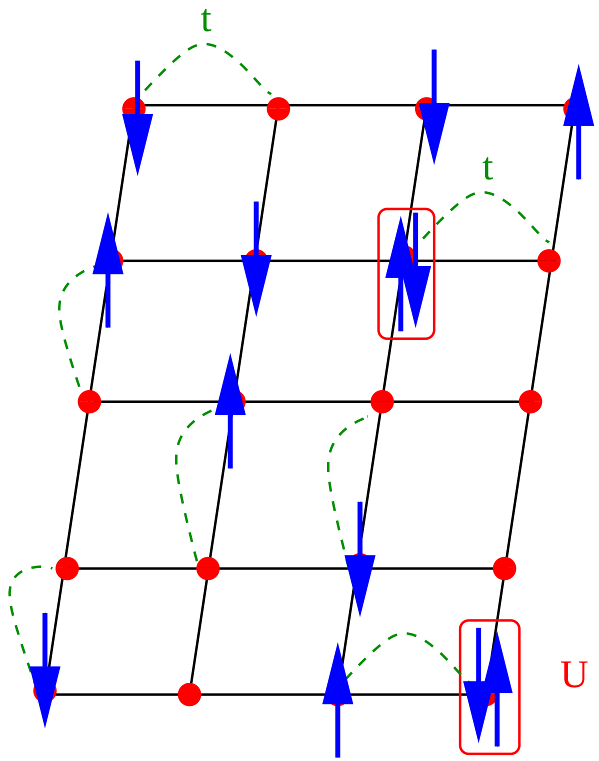
Correlated fermions on lattices

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

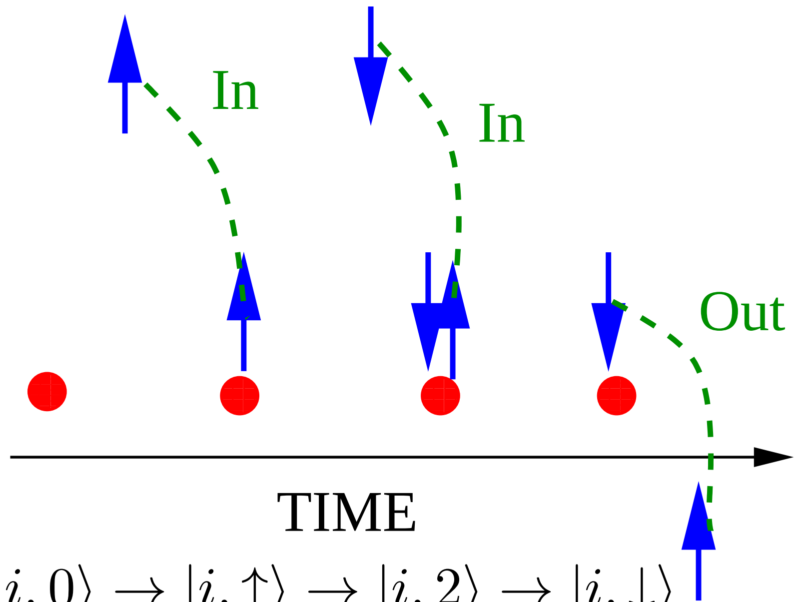


fermionic Hubbard model

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



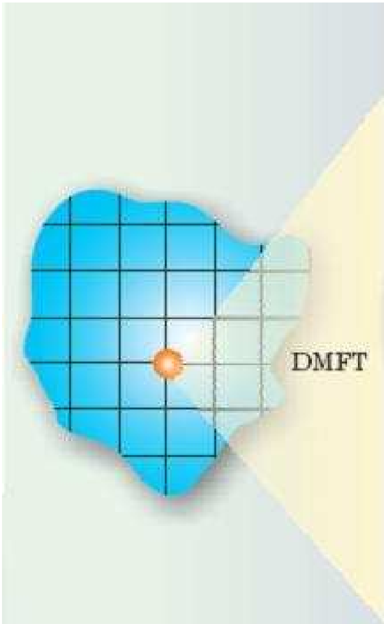
Local Hubbard physics

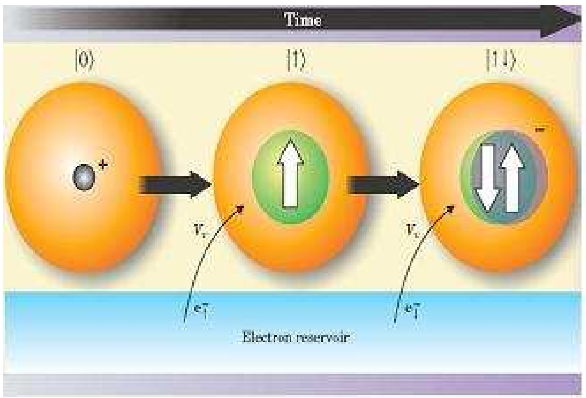


$|i,0\rangle \rightarrow |i,\uparrow\rangle \rightarrow |i,2\rangle \rightarrow |i,\downarrow\rangle$

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:

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

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

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)

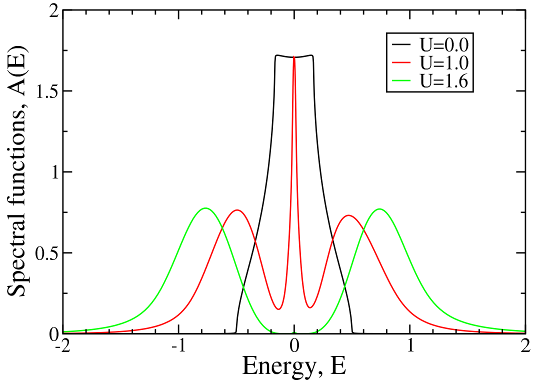
Generalized equations for reduced relative entropy

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

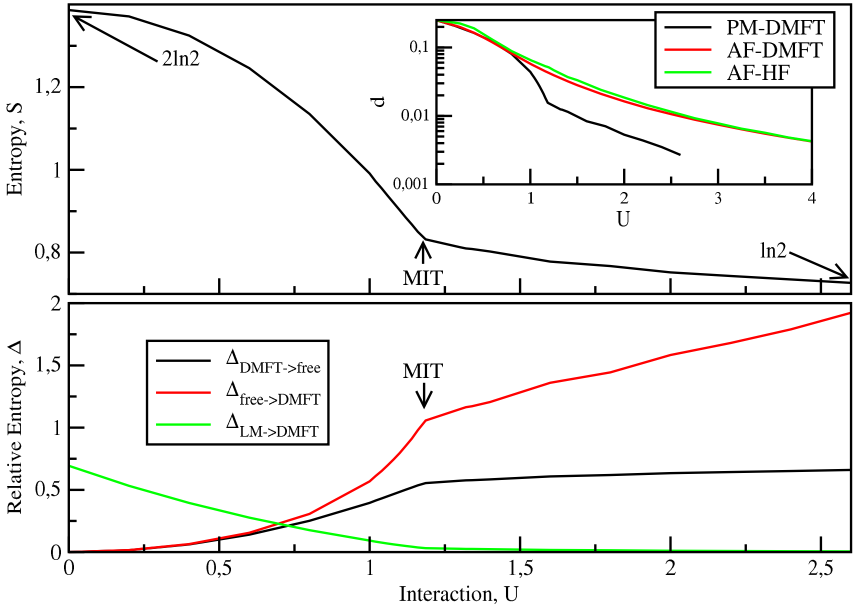
Hubbard model, $n = 1$, $T = 0$, $d = 3$, PM



Uncorrelated product states:

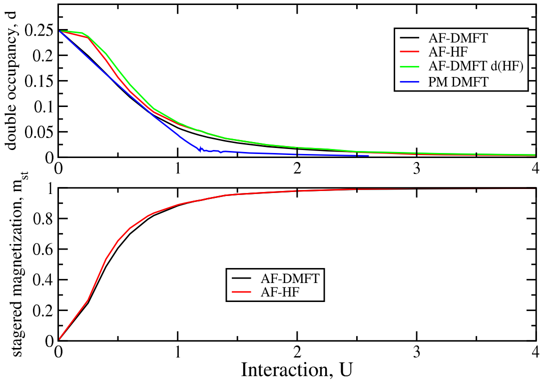
$|\text{free}\rangle = \prod_{k\sigma}^{k_F} a_{k\sigma}^{\dagger}|v\rangle$ - $U = 0$ Hartree-Fock limit

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



Example 2: Correlation and Antiferromagnetic LRO

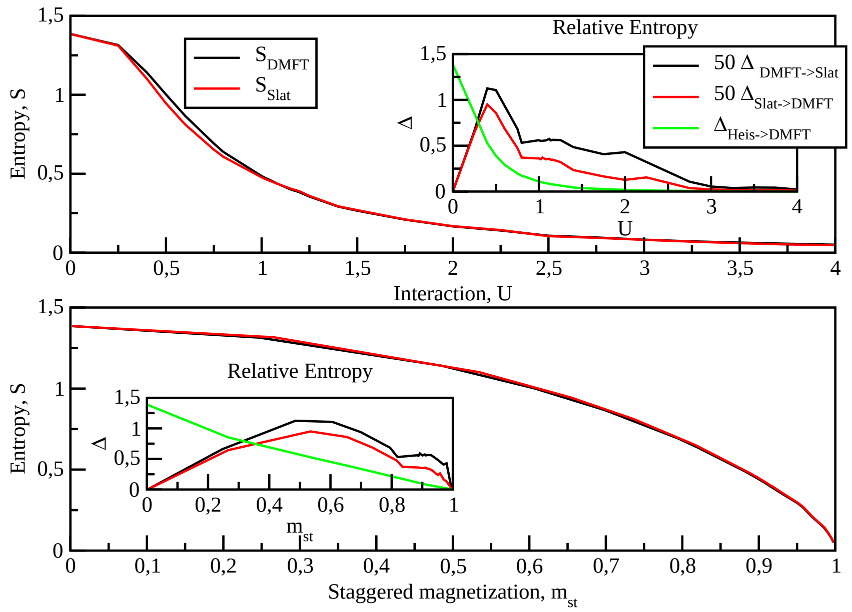
Hubbard model, $n = 1$, $T = 0$, $d = 3$, AF



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

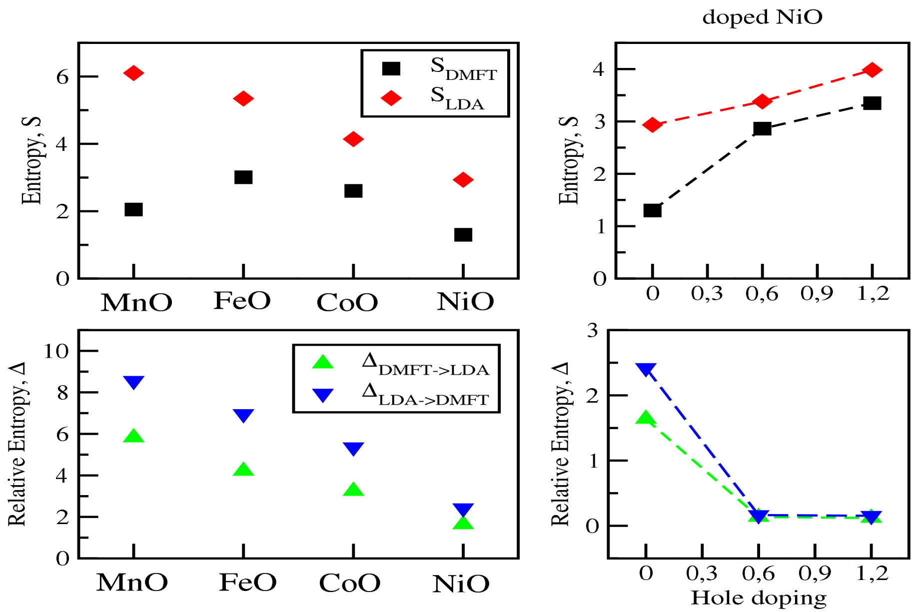
$|\mathrm{Heis}\rangle = \prod_{i\in(A,B)}^{N_L} a^\dagger_{i_A\uparrow} a^\dagger_{i_B\downarrow} |v\rangle$ - Heisenberg limit



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.
- "Quantification of correlations in quantum many-particle systems", K. Byczuk, J. Kunes, W. Hofstetter, D. Vollhardt, arXiv:1110.3214.

Happy New Year!

Calculation details

Consider a pure state (maximal information)

$$|\Psi\rangle = \sum_{\alpha\beta} \Psi_{\alpha\beta} |\alpha\rangle|\beta\rangle$$

of a system which is composed of two subsystems $A = \{|\alpha\rangle\}$ and $B = \{|\beta\rangle\}$.

Density operator (Schmidt decomposition)

$$\hat{\rho} = \sum_k p_k |k\rangle\langle k| = |\Psi\rangle\langle\Psi|.$$

Entropy

$$S(\hat{\rho}) = -\langle \log \hat{\rho} \rangle = -Tr \hat{\rho} \log \hat{\rho} = -\sum_k p_k \log p_k = 0,$$

because

$$p_k = \delta_{k,\Psi}.$$

Calculation details

Trace out the B subsystem, reduced density operator

$$\hat{\rho}_A = Tr_B|\Psi\rangle\langle\Psi| = \sum_{\beta}\langle\beta|\Psi\rangle\langle\Psi|\beta\rangle = \sum_{\alpha_1,\alpha_2}|\alpha_1\rangle\sum_{\beta}\Psi_{\alpha_1,\beta}\Psi^{\dagger}_{\beta,\alpha_2}\langle\alpha_2| = \sum_{\alpha_1,\alpha_2}|\alpha_1\rangle\rho_{\alpha_1,\alpha_2}\langle\alpha_2|.$$

Subsystem A is in a mixed state (reduced information).

Introduce projector and transition operators

$$\hat{P}_i = |i\rangle\langle i|, \quad \hat{T}_{ij} = |i\rangle\langle j|,$$

then

$$\rho_{\alpha_1\alpha_2} = \sum_{\beta}\Psi_{\alpha_1,\beta}\Psi^{\dagger}_{\beta,\alpha_2} = \langle\Psi|\hat{P}_{\alpha_1}\hat{T}_{\alpha_1,\alpha_2}\hat{P}_{\alpha_2}|\Psi\rangle^{\dagger}.$$

Calculation details

Consider a single lattice site (DMFT) as the A subsystem

$$|\alpha\rangle = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\},$$

then

$$\hat{P}_\alpha = \begin{cases} (1-\hat{n}_\uparrow)(1-\hat{n}_\downarrow) \\ \hat{n}_\uparrow(1-\hat{n}_\downarrow) \\ (1-\hat{n}_\uparrow)\hat{n}_\downarrow \\ \hat{n}_\uparrow\hat{n}_\downarrow, \end{cases}$$

and

$$\hat{T}_{\alpha_1,\alpha_2} = \begin{pmatrix} 1 & c_\uparrow & c_\downarrow & c_\downarrow c_\uparrow \\ c_\uparrow^\dagger & 1 & c_\uparrow^\dagger c_\downarrow & -c_\downarrow \\ c_\downarrow^\dagger & c_\downarrow^\dagger c_\uparrow & 1 & c_\uparrow \\ c_\uparrow^\dagger c_\downarrow^\dagger & -c_\downarrow^\dagger & c_\uparrow^\dagger & 1 \end{pmatrix}.$$

Assuming absence of any off-diagonal order $\langle\Psi|c_\sigma|\Psi\rangle = \langle\Psi|c_\sigma c_{-\sigma}|\Psi\rangle$ the reduced density operator is diagonal

$$\rho_{\alpha_1\alpha_2} = p_1|0\rangle\langle 0| + p_2|\uparrow\rangle\langle\uparrow| + p_3|\downarrow\rangle\langle\downarrow| + p_4|\uparrow\downarrow\rangle\langle\uparrow\downarrow|,$$

Calculation details

with matrix elements

$$p_\alpha = \langle \Psi | \hat{P}_\alpha | \Psi \rangle$$

determined with an arbitrary pure state $|\Psi\rangle$ (exact, DMFT, HF, etc.) of the full system.

It is straightforward to derive for an arbitrary mixed state $\hat{\rho}$ of the full system.