Basis of dynamical mean-field theory and application to model systems

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Aim of this talk

DYNAMICAL MEAN-FIELD THEORY

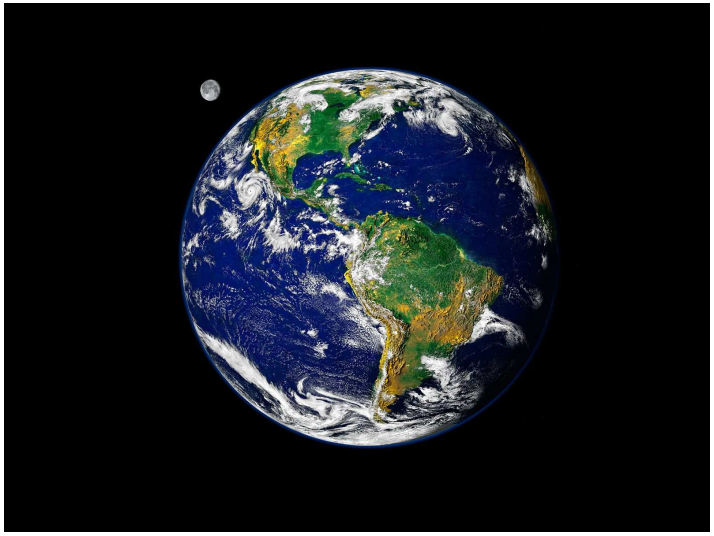
- What is it?
- Why do we need it?
- How to use it?
- Where does it help?

Correlation

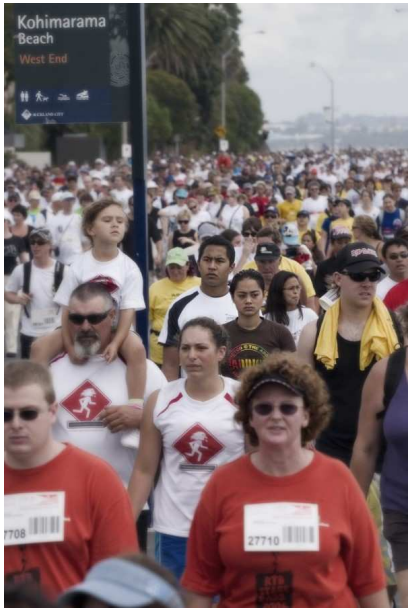
- Correlation [lat.]: con+relatio ("with relation")
  - Two or more objects needed
  - Grammar: either ... or, look for, deal with, ...
  - Many-body physics:

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

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



Spatial and temporal correlations everywhere



car traffic

air traffic

human traffic

electron traffic

more .....

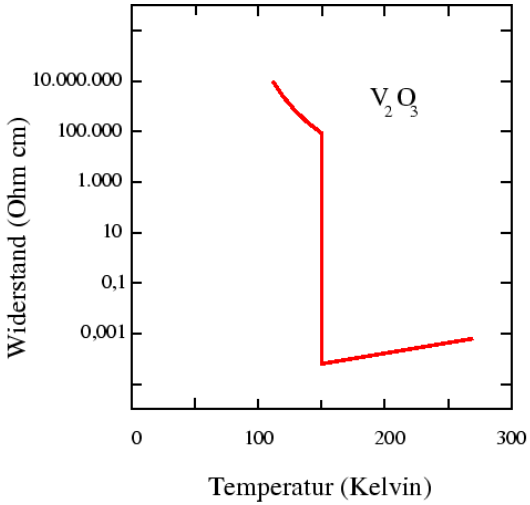


Abb. 3: Beispiel eines Metall-Isolator-Übergangs: Bei Abkühlung unter eine Temperatur von ca. 150 Kelvin erhöht sich der elektrische Widerstand von metallischem Vanadiumoxid (V_2O_3) schlagartig um das Einhundertmillionenfache (Faktor 10^8) – das System wird zum Isolator.

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.

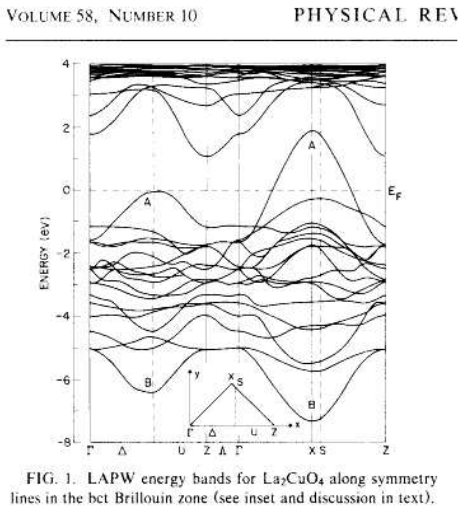
Spatial and temporal correlations neglected

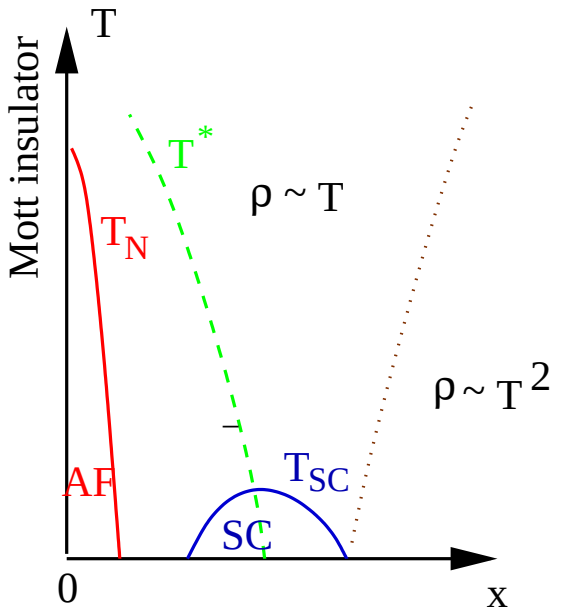
time/space average insufficient

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

Spatial and temporal correlations neglected

Local density approximation (LDA) disaster in HTC

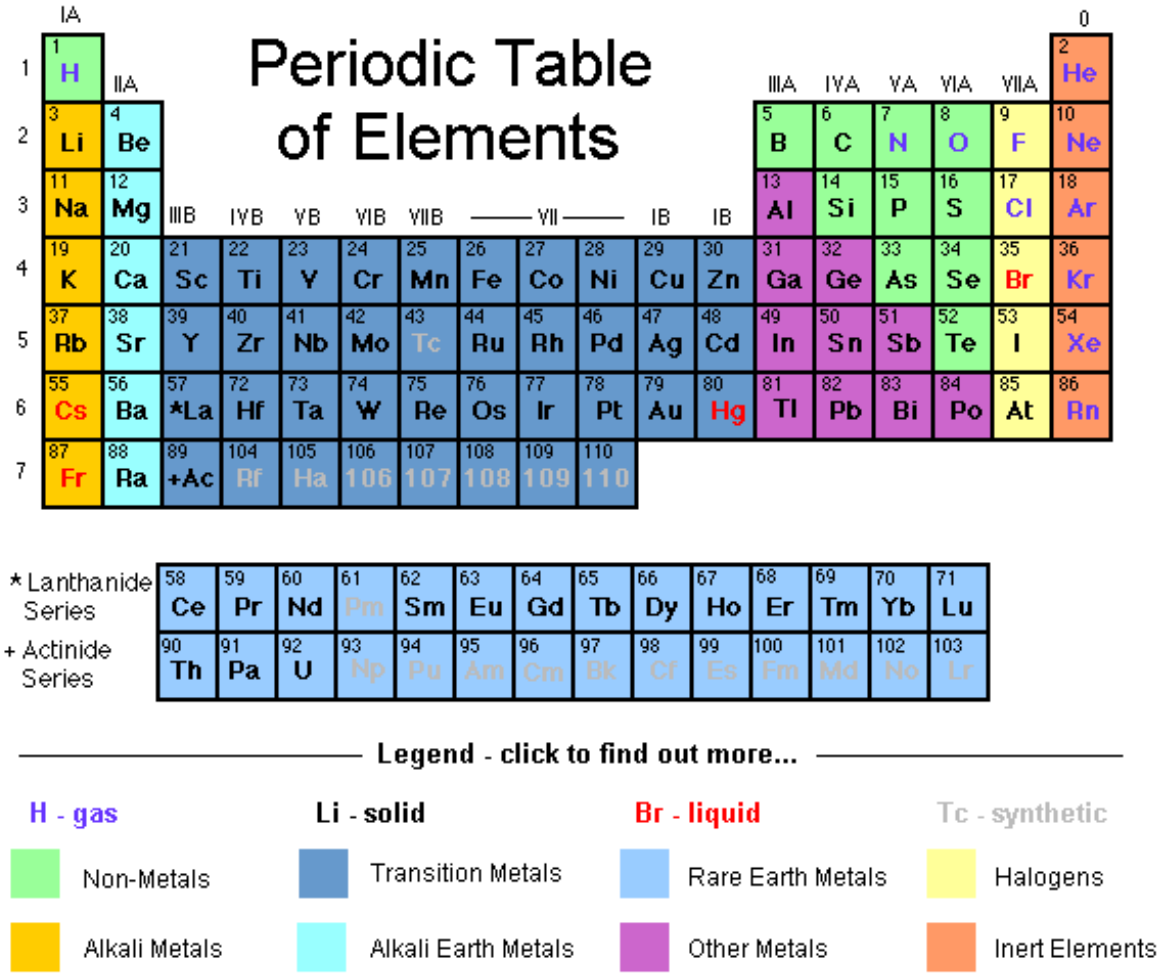




$LaCuO_4$ Mott (correlated) insulator predicted to be a metal

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

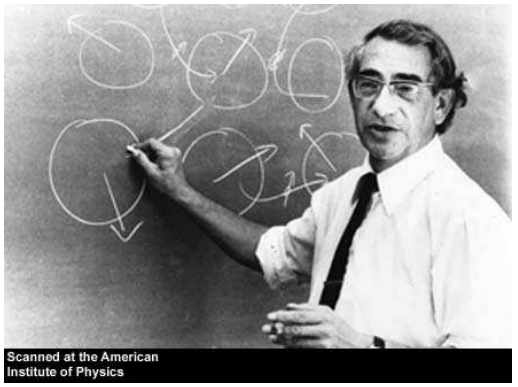
Correlated electrons



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

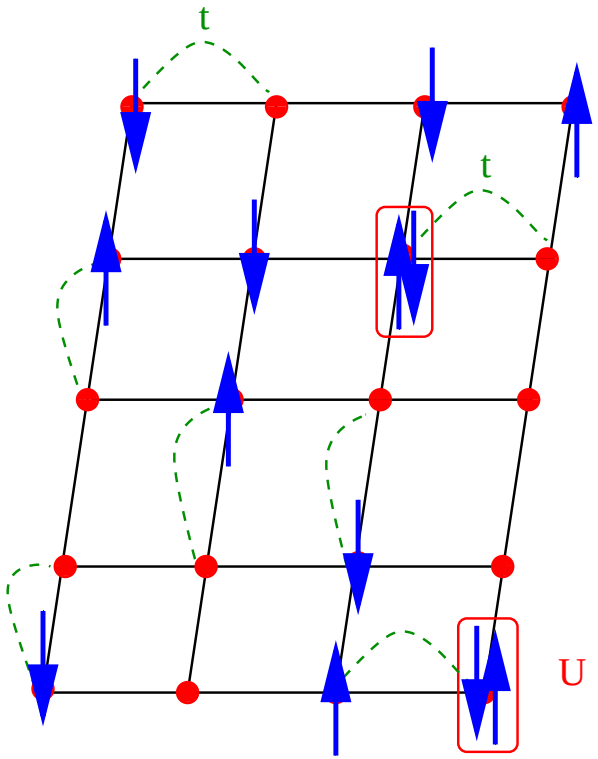
Correlated fermions on lattices

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

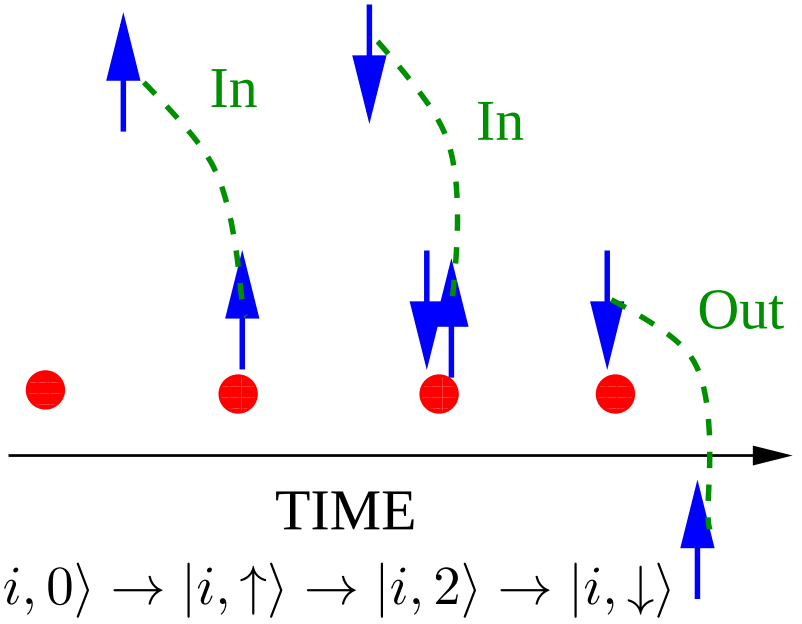


fermionic Hubbard model

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



Local Hubbard physics



The Holy Grail for correlated electrons

Fact: Hubbard model is not solved for arbitrary cases

Find the best comprehensive approximation

- valid for all values of parameters t, U, $n = N_e/N_L$, T
- thermodynamically consistent
- conserving
- possessing a small expansion (control) parameter and exact in some limit
- flexible to be applied to different systems and material specific calculations

What we need for Hubbard model

We need propagator (one-particle Green function)

$$G_{ij\sigma}(t) = -i\langle T_t c_{i\sigma}(t) c^\dagger_{j\sigma}(0)\rangle \underbrace{\longrightarrow}_{F.T.} G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\mathbf{k},\omega)}$$

At finite temperatures $t \to -i\tau$

$$G_{ij\sigma}(\tau) = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{j\sigma}(0)\rangle = -\frac{1}{Z}\int D[c^*, c] c_{i\sigma}(\tau) c^*_{j\sigma}(0) e^{-S[c^*,c]}$$

with the action (Lagrangian)

$$S[c^*, c] = -\int_0^{\beta=1/T} d\tau \sum_{i\sigma} c^*_{i\sigma}(\tau)(\partial_\tau - \mu) c_{i\sigma}(\tau) - H[c^*, c]$$

Later two-particle Green functions

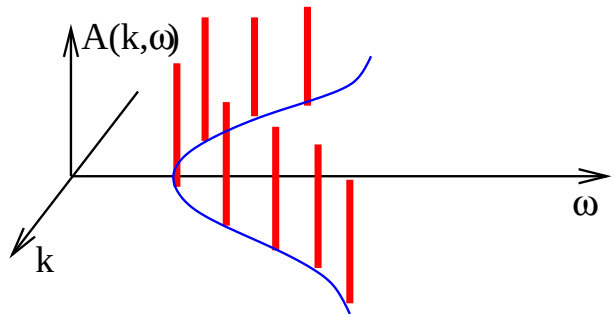
All what we know about Hubbard model

Solved in $U = 0$ limit (non-interacting limit)

$$G_\sigma(\mathbf{k}, \omega) = \frac{1}{\omega + \mu - \epsilon_\mathbf{k}}$$

Dispersion relation

$$\epsilon_\mathbf{k} = \sum_{j(i)} t_{ij} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}$$

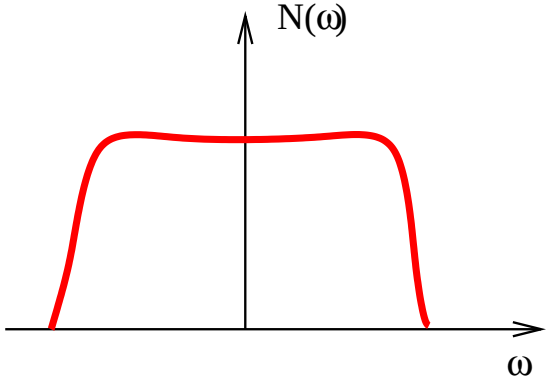


Spectral function - one-particle excitations

$$A_\sigma(\mathbf{k}, \omega) \equiv -\frac{1}{\pi} \mathrm{Im} G(\mathbf{k}, \omega) = \delta(\omega + \mu - \epsilon_\mathbf{k})$$

Density of states (DOS) - thermodynamics

$$N_\sigma(\omega) \equiv \sum_\mathbf{k} A(\mathbf{k}, \omega) = \sum_\mathbf{k} \delta(\omega + \mu - \epsilon_\mathbf{k})$$



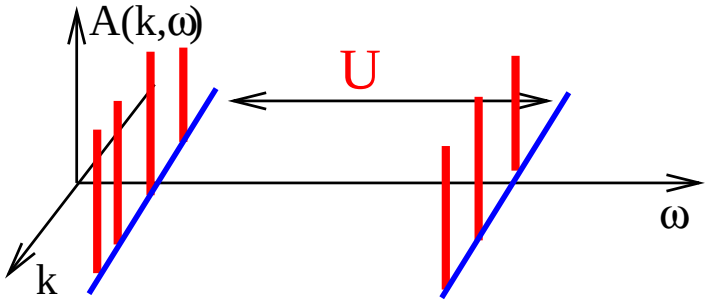
All what we know about Hubbard model

Solved in $t = 0$ limit (atomic limit)

$$G_\sigma(\mathbf{k},\omega) = \frac{1-n_{-\sigma}}{\omega+\mu} + \frac{n_{-\sigma}}{\omega+\mu-U} = \frac{1}{\omega+\mu-\Sigma_\sigma(\omega)}$$

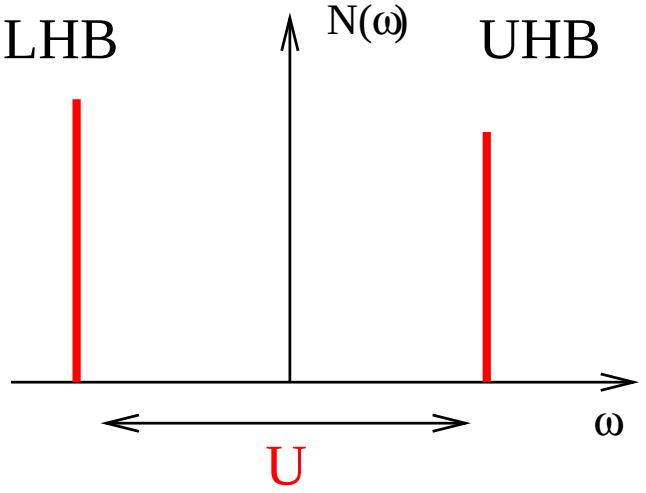
Real self-energy

$$\Sigma_\sigma(\omega) = n_\sigma U + \frac{n_{-\sigma}(1-n_{-\sigma})U^2}{\omega+\mu-(1-n_{-\sigma})U}$$



Spectral function

$$A_\sigma(\mathbf{k},\omega) = (1-n_{-\sigma})\delta(\omega+\mu) + n_{-\sigma}\delta(\omega+\mu-U)$$



Green function and self-energy are local,
i.e. $\mathbf{k}$ independent

Static mean-field for exchange Hamiltonian

Replace many-body Hamiltonian by one-body Hamiltonian with external (molecular or Weiss) field

$$Z = e^{-\beta F} = Tr_{\mathbf{S}_i} e^{-\beta H_{exch}} = Tr_{\mathbf{S}_i} e^{-\beta H_{MF}}$$

where

$$H_{MF} = \sum_i \mathbf{B}_{MF} \cdot \mathbf{S}_i + E_{shift}$$

Make mean-field (decoupling) approximation and determine $\mathbf{B}_{MF}$

$$\mathbf{B}_{MF} = \sum_{j(i)} J_{ij} \langle \mathbf{S}_j \rangle_{H_{MF}}$$

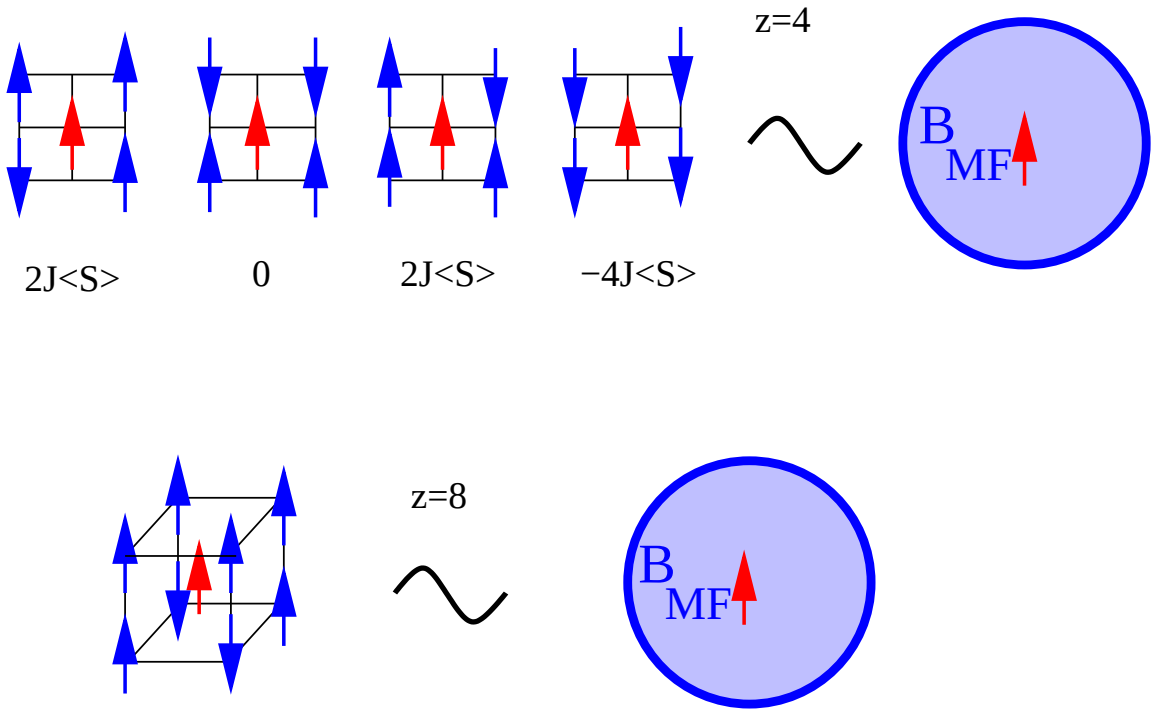
where $\langle \mathbf{S}_j \rangle = \langle S^z \rangle_{H_{MF}}$ is found self-consistently

$$\langle S^z \rangle_{H_{MF}} = \tanh\left(\beta J \langle S^z \rangle_{H_{MF}}\right)$$

Static mean-field – principal approximation

Spin-spin correlations are neglected

$$\langle [\mathbf{S}_i - \langle \mathbf{S}_i \rangle] \cdot [\mathbf{S}_j - \langle \mathbf{S}_j \rangle] \rangle = 0 \Longrightarrow \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle$$



Quality of mean-field approximation improves when z is large

Static mean-field – exact when $z \to \infty$

$$\langle [\mathbf{S}_i - \langle \mathbf{S}_i \rangle] \cdot [\mathbf{S}_j - \langle \mathbf{S}_j \rangle] \rangle \to_{z\to\infty} 0 \Longrightarrow \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \to_{z\to\infty} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle$$

No spatial correlations in $z \to \infty$ limit

Rescaling for nearest neighbor (nn) exchange coupling

$$J \to \frac{J^*}{z}, \quad J^* = \text{const}$$

then

$$\mathbf{B}_{MF} = \sum_{j=1}^{z} J \langle \mathbf{S} \rangle_{H_{MF}} = \frac{J^*}{z} \sum_{j=1}^{z} \langle \mathbf{S} \rangle_{H_{MF}} = J^* \langle \mathbf{S} \rangle_{H_{MF}}$$

is bounded when $z \to \infty$

Static mean-field theory is exact and nontrivial when $z \to \infty$;
there exists a small (expansion) parameter $1/z$

Dynamical mean-field theory – heuristic approach

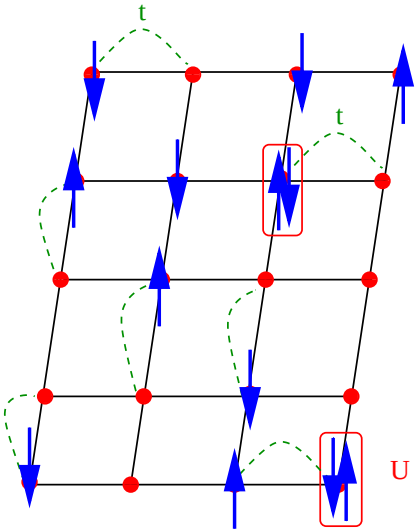
Find a comprehensive mean-field theory for Hubbard model

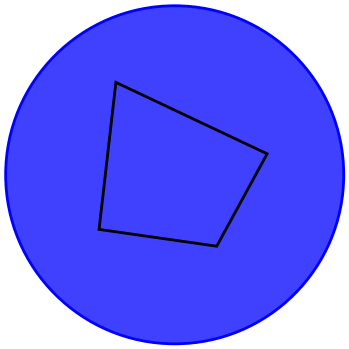
Exact free energy

$$F = -\frac{1}{\beta}\ln\int D[c^*,c]e^{-S[c^*,c]} = \frac{1}{\beta}\mathrm{Tr}\ln G_\sigma(\mathbf{k},\omega_n) = -\frac{1}{\beta}\mathrm{Tr}\ln[i\omega_n+\mu-\epsilon_{\mathbf{k}}-\Sigma_\sigma(\mathbf{k},\omega_n)]$$

Approximation $\Sigma_\sigma(\mathbf{k},\omega_n) = \Sigma_\sigma(\omega_n)$ - local approximation keeping full dynamics

$$F_{med}[\Sigma] = -\frac{1}{\beta}\mathrm{Tr}\ln[i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\omega_n)]$$





$\Sigma(\omega)$

Dynamical mean-field theory – heuristic approach

Need a prescription to determine $\Sigma_\sigma(\omega_n)$

"Remove" a single site in the effective medium and replace it by the actual, bare interaction

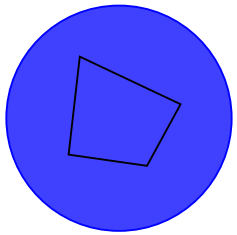
$$F = F_{med}[\Sigma] - F_i[\Sigma] + F_i^{bare}$$

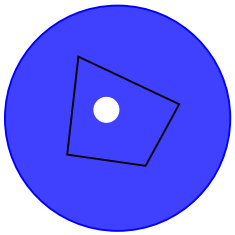
Local Green function ($i = j$ and index omitted)

$$G_\sigma(i\omega_n) = \sum_{\mathbf{k}} G_\sigma(\mathbf{k}, \omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\omega_n)} = G^0_\sigma(i\omega + \mu - \Sigma_\sigma(\omega_n))$$

and

$$F_i[\Sigma] = -\frac{1}{\beta} \mathrm{Tr} \ln[G^0_\sigma(i\omega + \mu - \Sigma_\sigma(\omega_n))]^{-1}$$





Dynamical mean-field theory – heuristic approach

Actual bare interaction

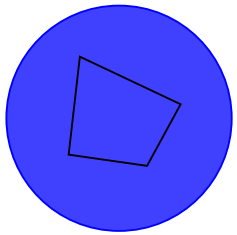
$$F_i^{bare}[\mathcal{G}] = -\frac{1}{\beta}\ln\int D[c^*,c]e^{-S_{loc}^{bare}[c^*,c]}$$

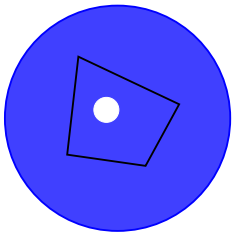
where

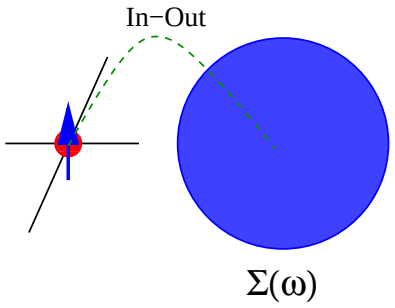
$$S_{loc}^{bare} = \sum_\sigma \int d\tau d\tau' c_\sigma^*(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + U\int d\tau n_\uparrow(\tau)n_\downarrow(\tau)$$

and the local-Dyson equation defines

$$\mathcal{G}_\sigma^{-1}(\omega_n) = G_\sigma^{-1}(\omega_n) + \Sigma_\sigma(\omega_n)$$







Dynamical mean-field theory – heuristic approach

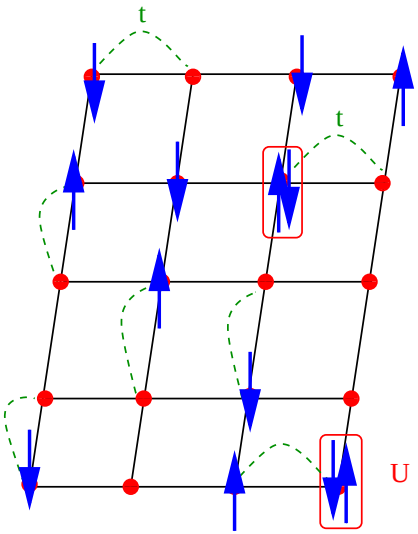
to close the set of equations use stationary condition

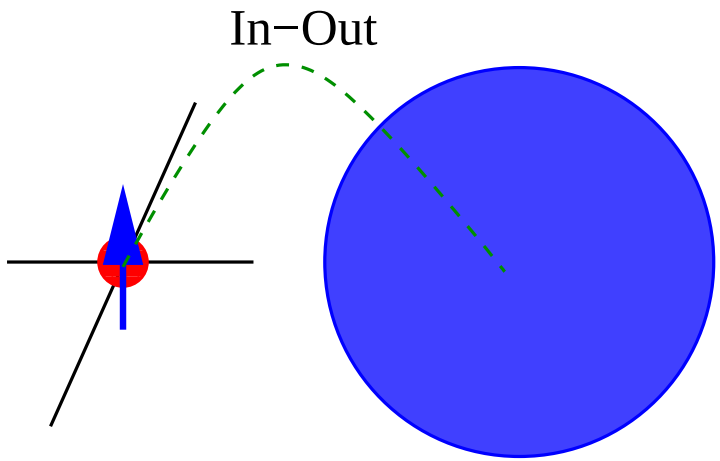
$$\frac{\delta F[\Sigma, \mathcal{G}^{-1}]}{\delta \mathcal{G}^{-1}} = 0$$

hence

$$G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c_\sigma^*(0) \rangle_{S_{loc}^{bare}}$$

and all three local but dynamical variables G, $\mathcal{G}$, and Σ are determined





Summary – DMFT - full glory

Local Green function

$$G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c_\sigma^*(0) \rangle_{S_{loc}^{bare}}$$

where

$$S_{loc}^{bare} = \sum_\sigma \int d\tau d\tau' c_\sigma^*(\tau) \mathcal{G}_\sigma^{-1}(\tau - \tau') c_\sigma(\tau') + U \int d\tau n_\uparrow(\tau) n_\downarrow(\tau)$$

Weiss (mean-field) function and self-energy

$$\mathcal{G}_\sigma^{-1}(\omega_n) = G_\sigma^{-1}(\omega_n) + \Sigma_\sigma(\omega_n)$$

Local Green function and lattice system self-consistency

$$G_\sigma(i\omega_n) = \sum_{\mathbf{k}} G_\sigma(\mathbf{k}, \omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_\sigma(\omega_n)} = G_\sigma^0(i\omega + \mu - \Sigma_\sigma(\omega_n))$$

DMFT – what is neglected, what is kept

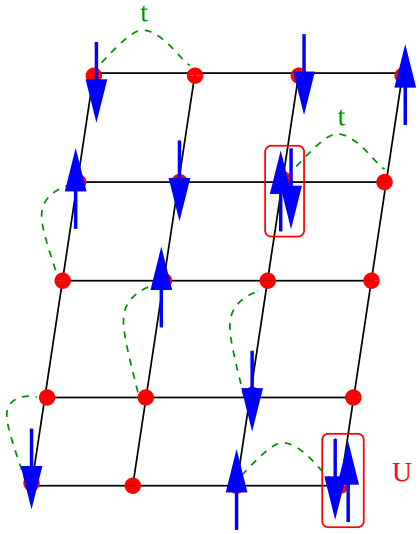
Spatial correlations are neglected (LRO is OK)

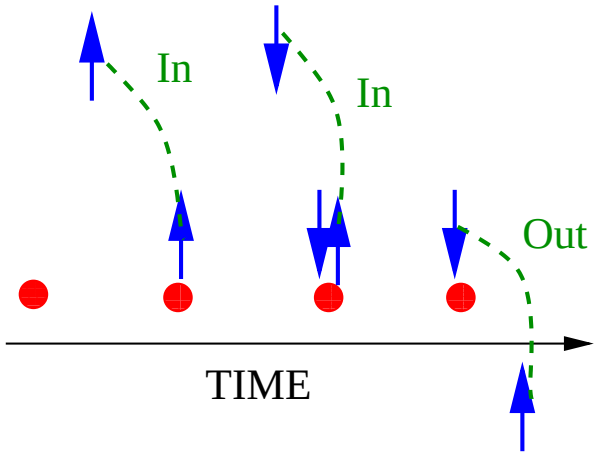
$$\langle [n_{i\sigma}(\tau) - \langle n_{i\sigma}(\tau)\rangle][n_{j\sigma'}(\tau') - \langle n_{j\sigma'}(\tau')\rangle]\rangle_{S_{loc}} = 0$$

Local temporal correlations are kept exactly

$$\langle [n_{i\sigma}(\tau) - \langle n_{i\sigma}(\tau)\rangle][n_{i\sigma'}(\tau') - \langle n_{i\sigma'}(\tau')\rangle]\rangle_{S_{loc}} = \text{“exact”}$$

Local dynamical Hubbard physics described well





DMFT – conserving theory

any reliable approximation should be conserving, i.e. all microscopic conservation laws should be preserved by an approximate theory

Φ-derivable theory (Baym, Kadanoff - 1962)

$$\Omega[\Sigma] = \Phi[\Sigma] - \mathrm{Tr}(\Sigma G) - \mathrm{Tr}(G_0^{-1} - \Sigma)$$

where

$$\Sigma = \frac{\delta \Phi}{\delta \Sigma}$$

is conserving because vertices

$$\Lambda = \frac{\delta^2 \Phi}{\delta \Sigma \delta \Sigma}$$

are approximated in the same way

dynamical mean-field theory is a conserving approximation due to construction

DMFT – consistent and comprehensive

DMFT is thermodynamically consistent, e.g.

$$n = -\frac{1}{\beta}\frac{\partial F}{\partial \mu} = -\frac{1}{\beta}\sum_{n\sigma} G_\sigma(\omega_n)$$

DMFT is valid for any value of the microscopic parameters,
no expansion wrt U, t, β, n or $1/n$

DMFT is comprehensive theory for correlated electrons

DMFT – flexibility; LDA+DMFT

Multi-band systems (Anisimov et al. 97; ... Nekrasov et al. 00, ...)

$$H = H_{LDA} + H_{int} - H^{U}_{LDA} = H^{0}_{LDA} + H_{int}$$

direct and exchange interaction

$$H_{int} = \frac{1}{2} \sum_{i=i_d, l=l_d} \sum_{m\sigma, m'\sigma'} U^{\sigma\sigma'}_{mm'} \, n_{ilm\sigma} n_{ilm'\sigma'}$$

$$-\frac{1}{2} \sum_{i=i_d, l=l_d} \sum_{m\sigma, m'} J_{mm'} \, c^{\dagger}_{ilm\sigma} c^{\dagger}_{ilm'-\sigma} c_{ilm'\sigma} c_{ilm-\sigma}$$

kinetic part, determined from DFT-LDA calculation (material specific)

$$H^{0}_{LDA} = \sum_{ilm, jl'm', \sigma} t^{0}_{ilm, jl'm'} c^{\dagger}_{ilm\sigma} c_{jl'm'\sigma}$$

LDA+DMFT - state of the art for realistic approach to correlated electron systems

DMFT scheme

S_{loc} - local interactions U or J from a model **TB** or a microscopic **LDA** Hamiltonian

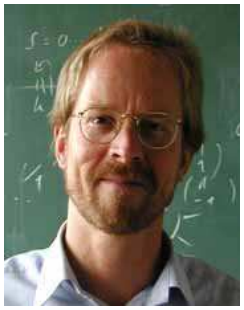
D. Vollhardt

$$\hat{G} = -\langle T\hat{C}(\tau)\hat{C}^*(0)\rangle_{S_{loc}}$$

DMFT

$$\hat{\mathcal{G}}^{-1} = \hat{G}^{-1} + \hat{\Sigma} \qquad \hat{\Sigma} \qquad \hat{\Sigma} = \hat{\mathcal{G}}^{-1} - \hat{G}^{-1}$$

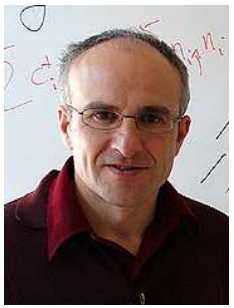
$$\hat{G} = \sum[(\omega + \mu)\hat{1} - \hat{H}^0 - \hat{\Sigma}]^{-1}$$



W. Metzner

G. Kotliar

A. Georges



$\hat{H}^0$ is a model **TB** or a microscopic **LDA** Hamiltonian

DMFT – flexibility; disordered systems

Correlated electrons with local disorder

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

where ϵ_i is random (on-site) local energy with fixed probability distribution function (PDF) $P(\epsilon_i)$

In self-averaged systems, physical quantities are given by arithmetic average

$$G(\omega)_{av} = -\int d\epsilon_i P(\epsilon_i) \langle c(\omega) c^*(\omega) \rangle_{S_{loc}(\epsilon_i)} \equiv \langle \langle c(\omega) c^*(\omega) \rangle_{S_{loc}(\epsilon_i)} \rangle_{dis}$$

In non-self-averaged systems, physical quantities are given by typical ones - geometric average $O_{geom} = \exp[\langle \ln O \rangle]$

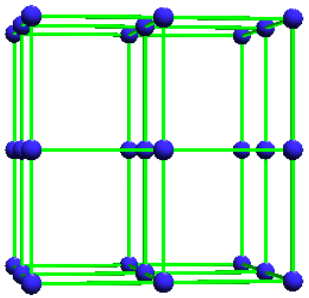
$$-\mathrm{Im} G(\omega)_{typ} = e^{\langle \ln[-\mathrm{Im} \langle c(\omega) c^*(\omega) \rangle_{S_{loc}(\epsilon_i)}] \rangle_{dis}}$$

DMFT – $d \to \infty$ limit, small parameter O$(1/z)$

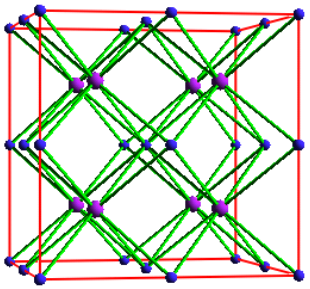
Idea: spatial correlations are absent when number of neighbors is large (infinite)

Crystal lattices in $d = 3$:

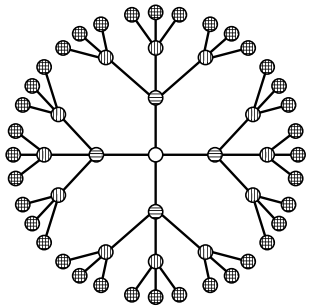
simple cubic (sc) - $z = 6$
body center cubic (bcc) - $z = 8$
face centered cubic (fcc) - $z = 12$

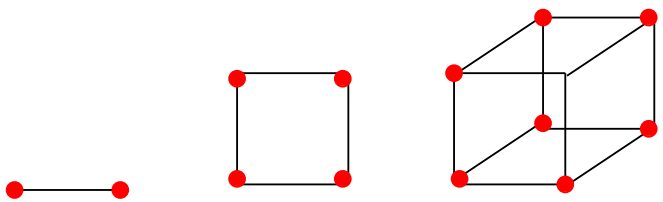


Hypercubic lattice in d-dimension - $z = 2d$

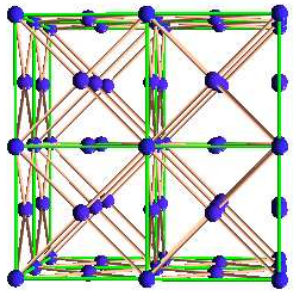


Bethe (Caley) tree - $z = K + 1$





d=1 d=2 d=3



Simple $d \to \infty$ limit

Kinetic energy

$$H_0 = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

NN hopping:

$$t_{ij} = t(\mathbf{R}_i - \mathbf{R}_j) = \begin{cases} -t & \text{if} \quad \mathbf{R}_i - \mathbf{R}_j = \pm \mathbf{e}_n \\ 0 & \text{otherwise} \end{cases}$$

Bare dispersion

$$\epsilon_{\mathbf{k}} = -2t \sum_{i=1}^{d} \cos k_i$$

Density of states

$$N_d(\epsilon) \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}) \to_{d\to\infty} \frac{1}{2t\sqrt{\pi d}} e^{-\left(\frac{\epsilon}{2t\sqrt{d}}\right)^2}$$

arbitrary broad and featureless in $d \to \infty$ limit

Non-trivial $d \to \infty$ limit

Non-trivial DOS is obtained when hopping is rescaled

$$t \to \frac{t^*}{\sqrt{2d}}, \qquad t^* = \text{const}$$

$$N_\infty(\epsilon) = \frac{1}{\sqrt{2\pi}t^*} e^{-\left(\frac{\epsilon}{2t^*}\right)^2}$$

(Metzner, Vollhardt, 1989)

In general

$$t_{ij} \to \frac{t^*_{ij}}{\sqrt{d||\mathbf{R}_i - \mathbf{R}_j||}}$$

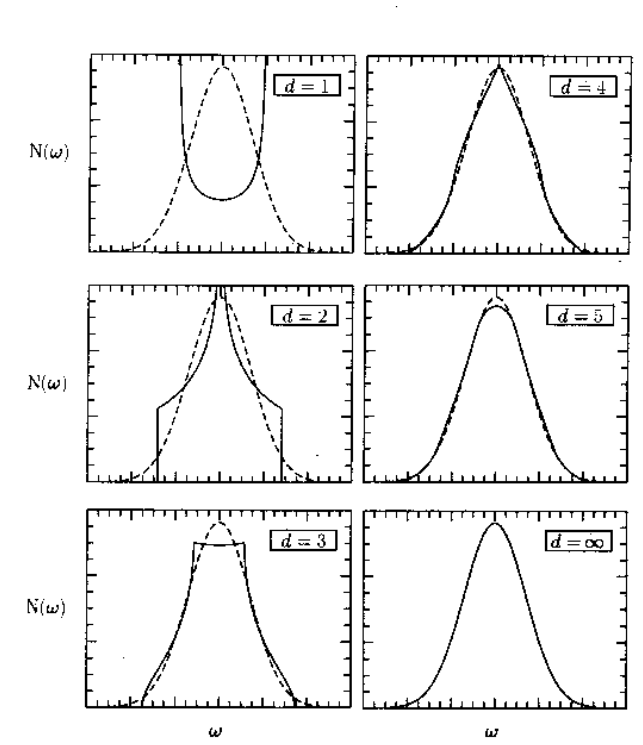
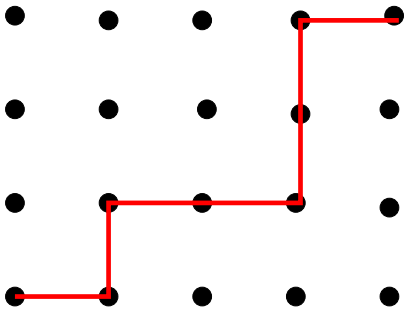


Fig. 1.2 Tight-binding density of states in $d = 1, 2, 3, 4, 5$ as compared with t for $d = \infty$.



$||\mathbf{R}_i - \mathbf{R}_j||$ - taxi cab (Manhattan, New York) distance

Non-trivial $d \to \infty$ limit

Non-trivial (asymptotic) theory is well defined such that the energy density is generically finite and non-zero

$$\frac{1}{N_L} E_{kin} = \frac{1}{N_L} \sum_{ij\sigma} t_{ij} \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle = \frac{1}{N_L} \sum_{i\sigma} \underbrace{\sum_{j(i)}}_{O(d^{||\mathbf{R}_i - \mathbf{R}_j||})} t_{ij} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} G_{ij\sigma}(\omega) \sim O(1)$$

Fact, since G_{ij} is probability amplitude for hopping,

$$G_{ij} \sim O(d^{-\frac{||\mathbf{R}_i - \mathbf{R}_j||}{2}})$$

with rescaling

$$t_{ij} \to \frac{t^*_{ij}}{\sqrt{d^{||\mathbf{R}_i - \mathbf{R}_j||}}}$$

sum $\sum_{j(i)}$ is compensated and energy is finite (Metzner, Vollhardt, 1989)

$d \to \infty$ limit – Feynman diagrams simplification

One proves, term by term, that skeleton expansion for the self-energy $\Sigma_{ij}[G]$ has only local contributions

$$\Sigma_{ij\sigma}(\omega_n) \to_{d\to\infty} \Sigma_{ii\sigma}(\omega_n)\delta_{ij}$$

Fourier transform is $\mathbf{k}$-independent

$$\Sigma_{\sigma}(\mathbf{k},\omega_n) \to_{d\to\infty} \Sigma_{\sigma}(\omega_n)$$

DMFT is an exact theory in infinite dimension (coordination number) and small control parameter is $1/d$ $(1/z)$

(Metzner, Vollhardt, 1989)

ansatz in heuristic derivation is then exact (Janis, Vollhrdt, 1992)

$$F = F_{med}[\Sigma] = -\frac{1}{\beta}\mathrm{Tr}\ln[i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\sigma}(\omega_n)]$$

DMFT in practice

The hardest part of DMFT is to solve local, many-body problem

$$G_\sigma(\tau) = -\langle T_\tau c_\sigma(\tau) c^*_\sigma(0) \rangle_{S^{bare}_{loc}}$$

where

$$S^{bare}_{loc} = \sum_\sigma \int d\tau d\tau' c^*_\sigma(\tau) \mathcal{G}^{-1}_\sigma(\tau - \tau') c_\sigma(\tau') + U \int d\tau n_\uparrow(\tau) n_\downarrow(\tau)$$

it is usually mapped onto the Single Impurity Anderson Model
(Kotliar, Georges, 1992; Jarrell, 1992)

$$H_{SIAM} = \epsilon_d \sum_\sigma n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} d^\dagger_\sigma c_{\mathbf{k}\sigma} + H.c. + \sum_{\mathbf{k}\sigma} \epsilon^{aux}_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

DMFT solvers in practice

- Analytical approaches (approximate, but fast)
  - (IPT) Iterative perturbation expansion
  - (NCA) Non-crossing approximation
  - (LMA) Local moment approach
  - (LDMFT) Linear DMFT
  - (Hubbard I or III) Strong coupling approach

- Numerical approaches (formally exact, but expensive)
  - (HF-QMC) Quantum Monte Carlo - Trotter decomposition, large T, limited U
  - (CT-QMC) Quantum Monte Carlo - continuum time, perturbative character
  - (PQMC) Projected quantum Monte Carlo - only ground state
  - (ED) Exact diagonalization - small system, discrete spectrum
  - (NRG) Numerical renormalization group - logarithmic broadening
  - (DMRG) Dynamical matrix renormalization group

Find the best solver to you physical problem

DMFT – long-range orders and susceptibilities

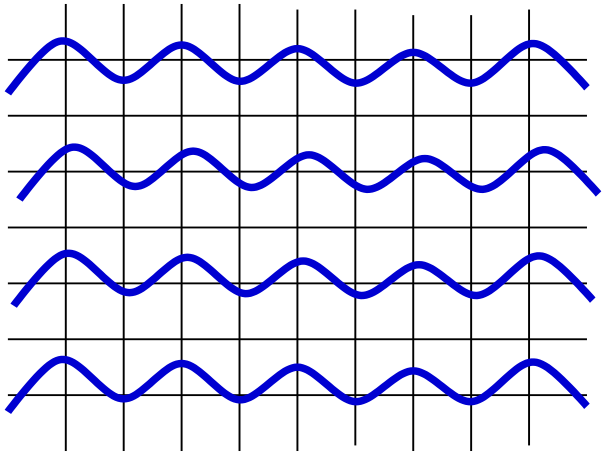
Broken symmetry phases (infinite-long range orders) are described by generalized local problem and self-consistency condition

e.g., for AF we need to sites (A or B) which are coupled be opposite spins

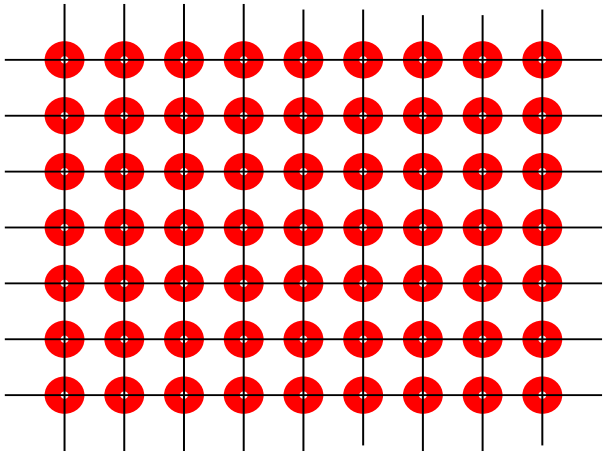
Susceptibilities (two-particle correlation functions) are determined by the corresponding local quantities and non-interacting lattice parts

$$\hat{\chi}_{\mathbf{q}}^{-1} = \hat{\chi}_{loc}^{-1} + \hat{\chi}_{0,\mathbf{q}}^{-1} - \hat{\chi}_{0,loc}^{-1}$$

Eg. 1 - MIT at half-filling

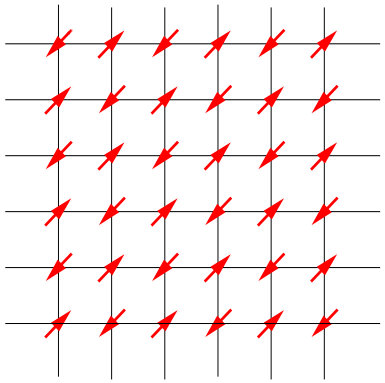


$U \ll |t_{ij}|$, $\Delta \mathbf{p} = 0$



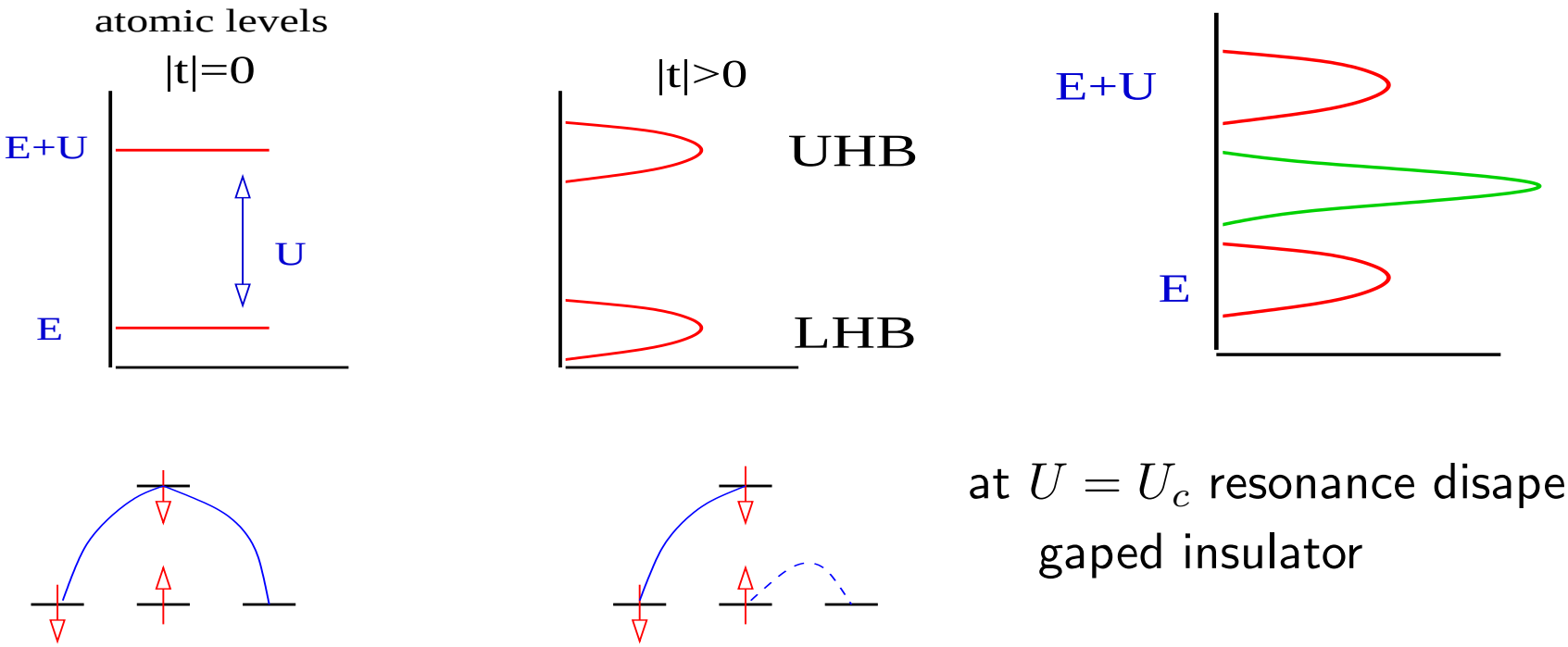
$U \gg |t_{ij}|$, $\Delta \mathbf{r} = 0$

Antiferromagnetic Mott insulator



typical intermediate coupling problem $U_c \approx |t_{ij}|$

Eg. 1 - MIT at half-filling



spin flip on central site

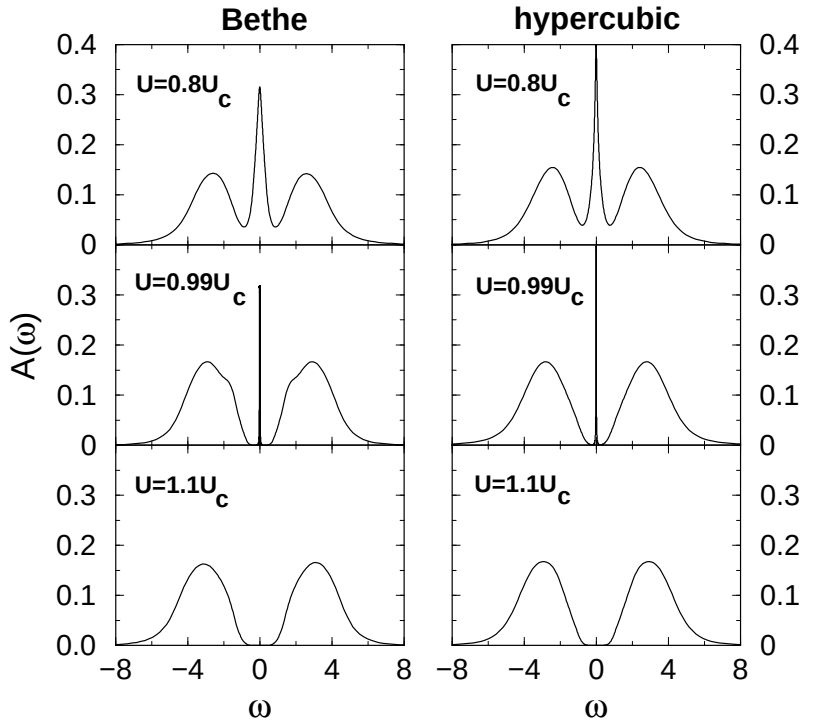
at $U = U_c$ resonance disapears

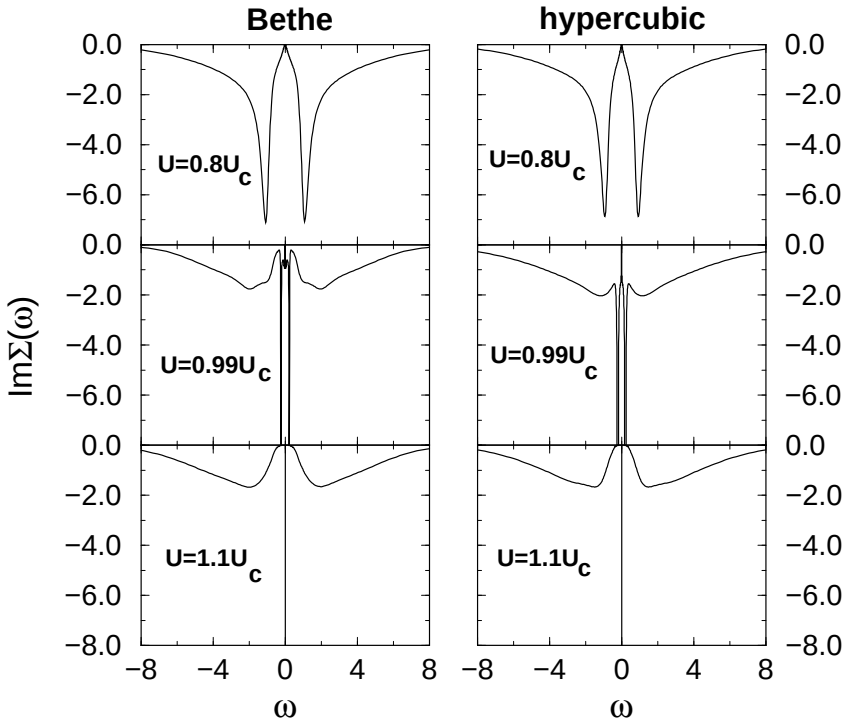
gaped insulator

dynamical processes with spin-flips inject states into correlation gap giving a quasiparticle resonance

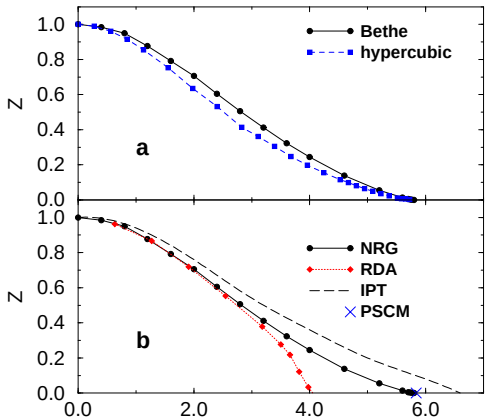
Eg. 1 - MIT at half-filling at $T = 0$ according to DMFT

Kotliar et al. 92-96, Bulla, 99





$$G(k,\omega) \sim \frac{Z}{\omega - \tilde{\epsilon}_k - i\alpha\ \omega^2} + G_{inc}$$



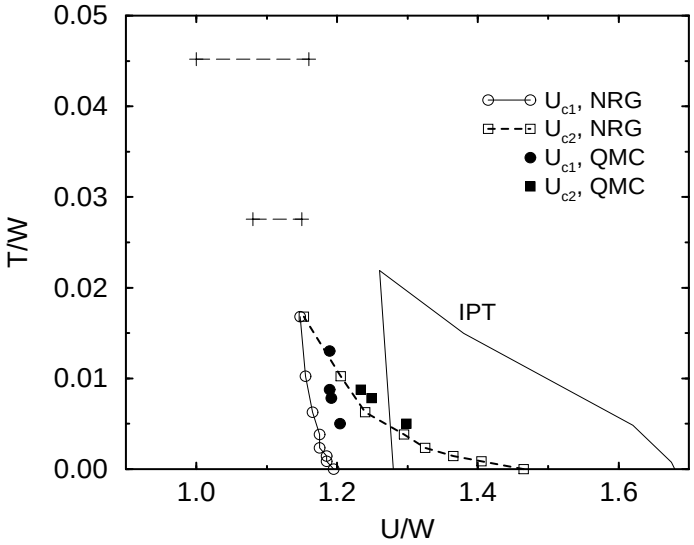
Luttinger pinning $A(0) = N_0(0)$

Fermi liquid

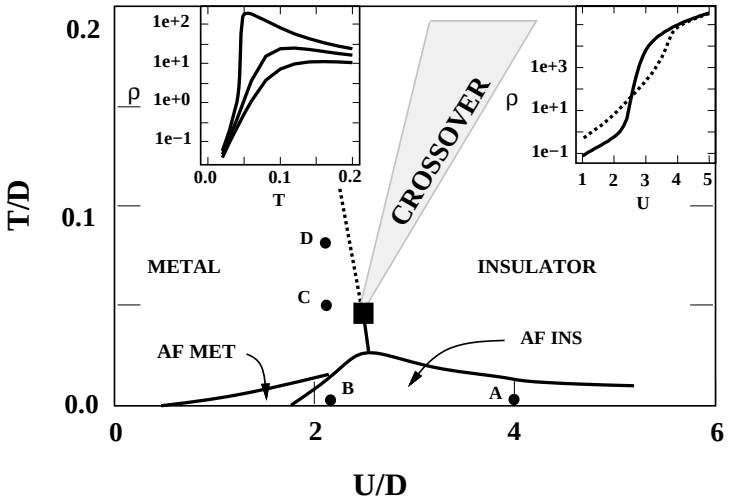
Muller-Hartmann 1989

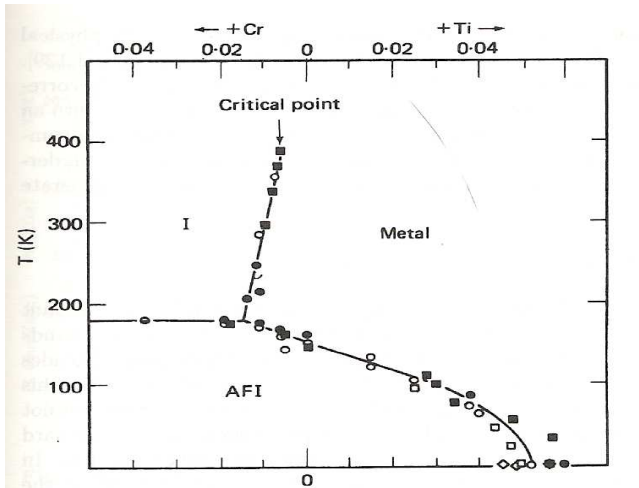
Eg. 1 - MIT at half-filling at $T > 0$ according to DMFT

Kotliar et al. 92-96, Bulla et al. 01, also Spalek 87

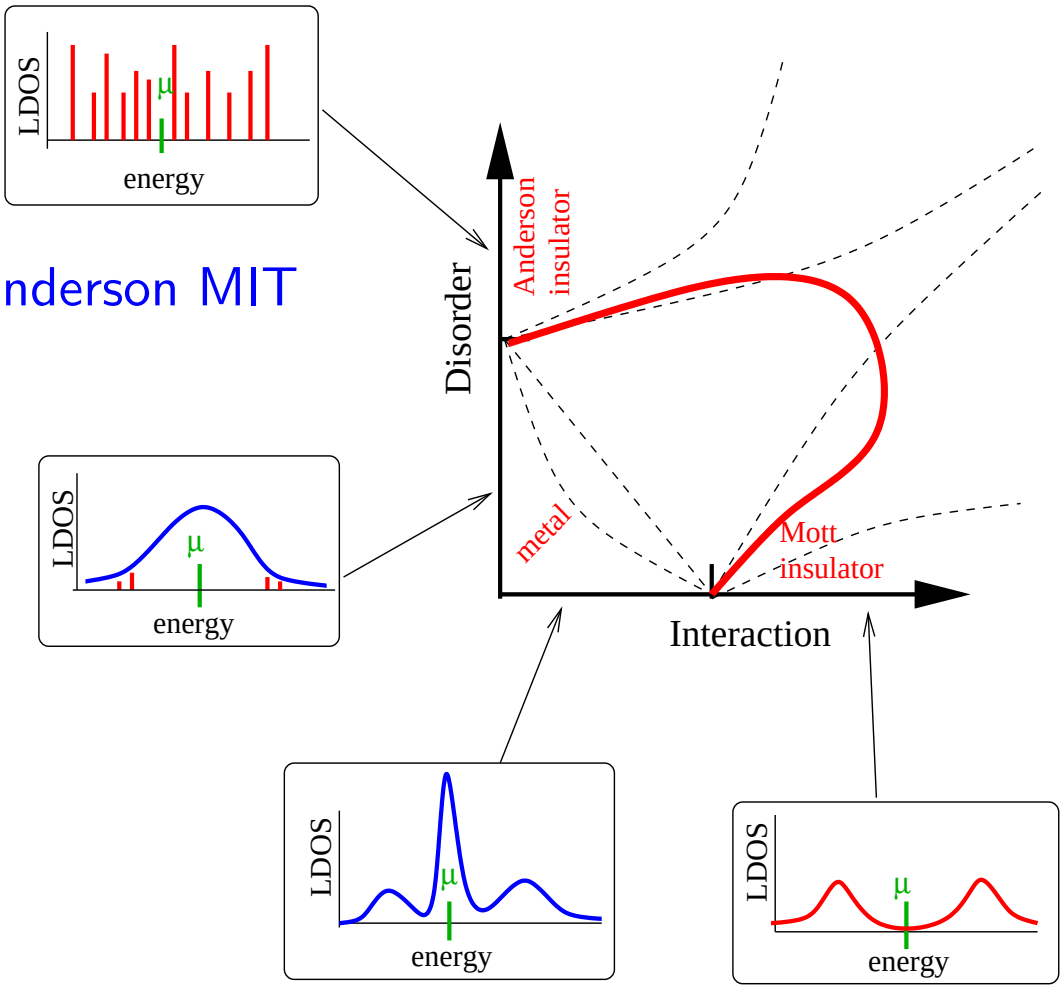


1^{st}-order transition





Eg. 2 - Mott-Anderson MIT



Two insulators are continously connected

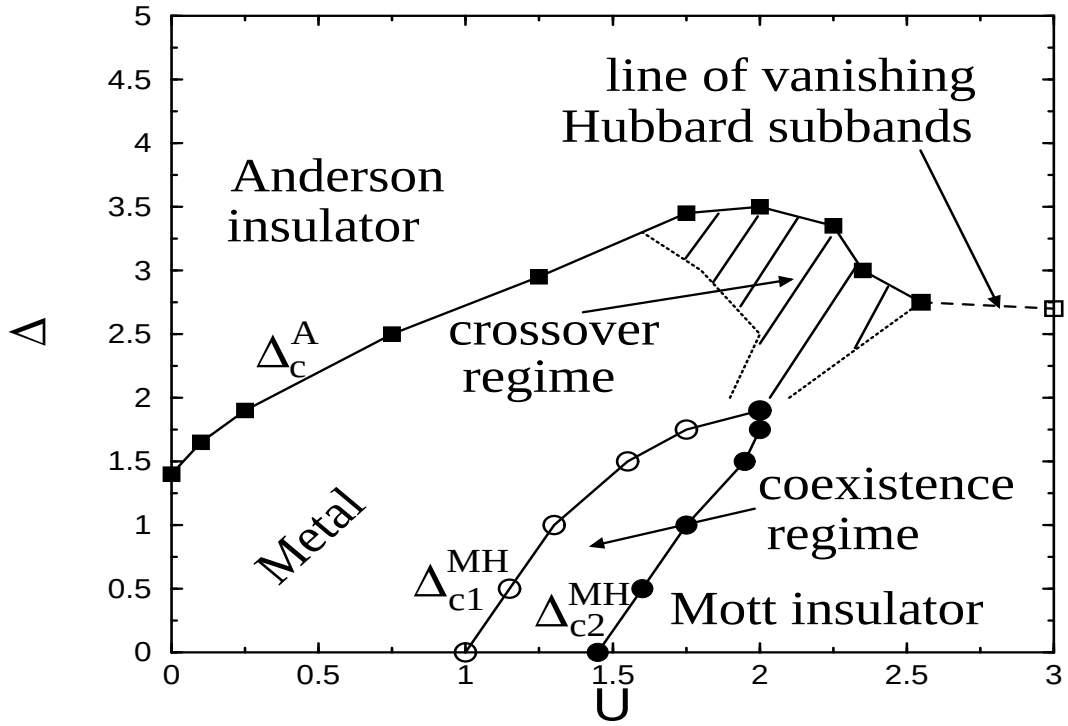
BUT

Interaction and disorder compete with each other stabilizing the metallic phase against the occurring one of the insulators

Eg. 2 - Phase diagram for disordered Hubbard model

$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4}G(\omega)$$

$T = 0$, $n = 1$, $W = 2D = 1$, NRG solver, KB, W. Hofstetter, D. Vollhardt (2005)



U - interaction, Δ - disorder

Summary – DMFT - flexibility

- Local temporal correlations exact
- Spatial correlations neglected
- Conserving and thermodynamically consistent
- Comprehensive mean-field theory
- LDA+DMFT
- DMFT for disordered electrons