# Lecture on First-principles Computations (25): Introduction to Dynamical Mean-Field Theory (DMFT)

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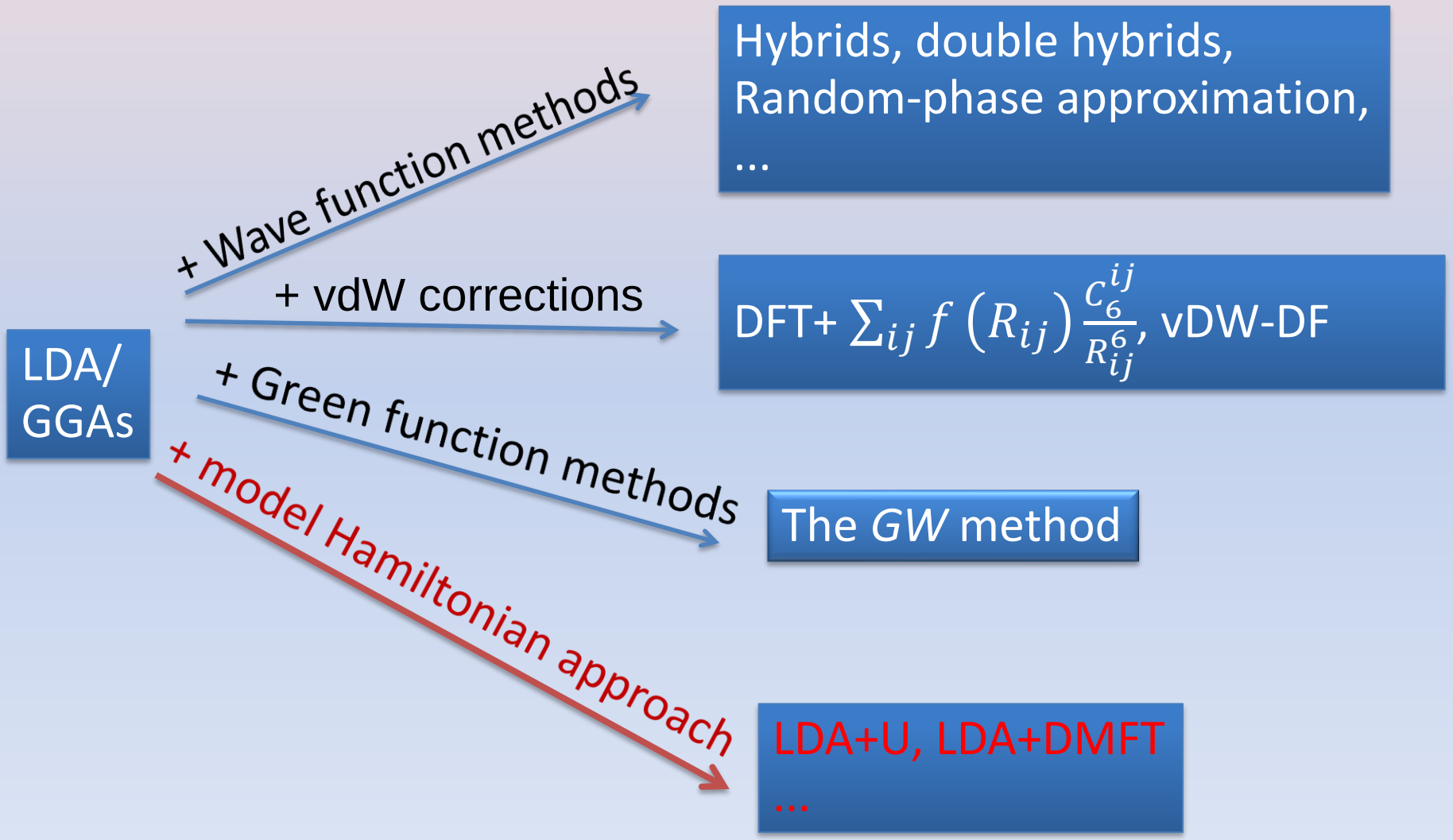
# Computational schemes beyond LDA and GGAs



# Phenomena arising from strong electron correlations

- Mott metal-insulator transition
- Kondo effect
- Heavy fermion behavior
- Itinerant ferromagnetism
- High-temperature superconductivity
- Colossal magnetoresistance
- ……

# First-principles approaches versus model Hamiltonian approach

First-principles approach
[DFT (LDA/GGAs) ]

+ Material-specific properties are accessible

- Good for weakly correlated systems, but generally fails for strongly correlated systems

+ Fast, computationally efficient software packages available

Model Hamiltonian approach
[Hubbard, Anderson, Kondo, Heisenberg, *t-J*, etc.]

- Require input model parameters

+ Good for a qualitative understanding of strongly correlated systems

- Computationally demanding, [e.g., ED, NRG, QMC, DMRG, DMFT, etc. ]

# What is mean-field theory?

- Hartree-Fock theory:

  An electron is moving in an average field provided by all other electrons.

- Weiss mean-field theory

  - For a classical spin system (e.g., the Ising model), a spin is viewed to feel an average magnetic field generated by all other spins. This leads to the Curie-Weiss law for ferromagnetism.

  - Become exact when the dimension $\mathrm{d} \to \infty$. ("Controlled approximation")

# Weiss mean-field theory for the Ising model

$$H = -\frac{J}{2}\sum_{\langle \mathbf{R_i},\mathbf{R_j}\rangle} S_i S_j - h\sum_{\mathbf{R_i}} S_i$$

$S = \pm 1; J > 0$: ferromagnetic coupling

$h$: uniform external field

Within the Weiss mean-field (MF) method:

$$H_{\mathrm{MF}} = -h_{\mathrm{MF}}\sum_i S_i$$

$$h_{\mathrm{MF}} = J\sum_{\boldsymbol{R_j}}^{(i)} \langle S_j\rangle + h = ZJ\langle S\rangle + h$$

The summation over $\boldsymbol{R}_j$ goes over the neighboring site of $i$.

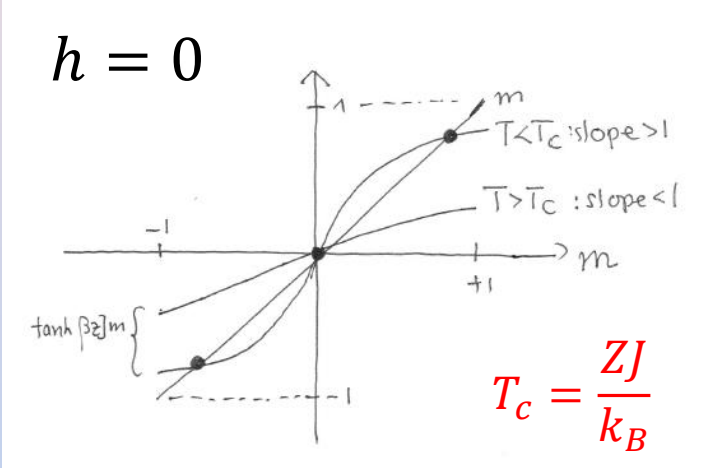
$Z$: the number of nearest neighbors
(the coordination number)

# Weiss mean-field theory for the Ising model

$$H = -\frac{J}{2}\sum_{\langle \mathbf{R_i},\mathbf{R_j}\rangle} S_i S_j - h\sum_{\mathbf{R_i}} S_i$$

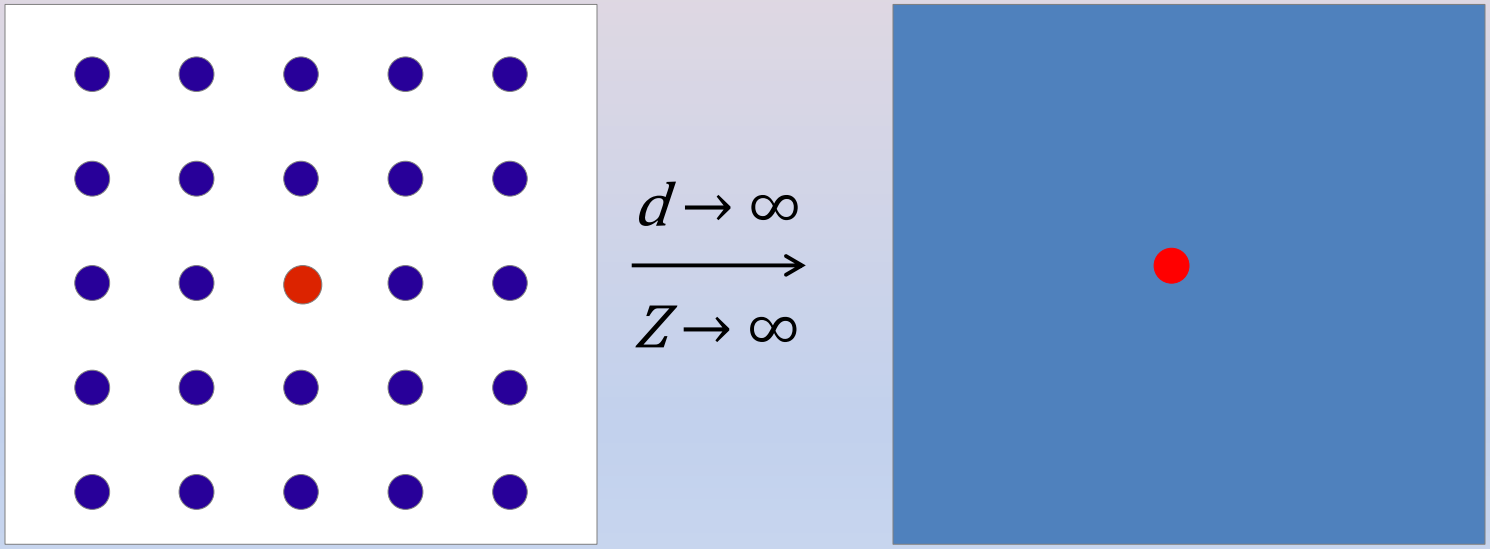
Curie-Weiss self-consistent equation:

$$\langle S\rangle = \tanh\left[\frac{ZJ\langle S\rangle + h}{k_B T}\right]$$




- A phase transition exists between the ferromagnetic state and the paramagnetic state at finite temperatures.
- The solution becomes exact when $Z \to \infty$ .
- $J$ has to properly scaled: $J = J^*/Z$ while $J^*$ is a constant.

# The $Z \to \infty$ limit




- In the $d \to \infty$ limit, for a given site *i*, the direction of an individual neighboring spin is not important; only the average value matters!

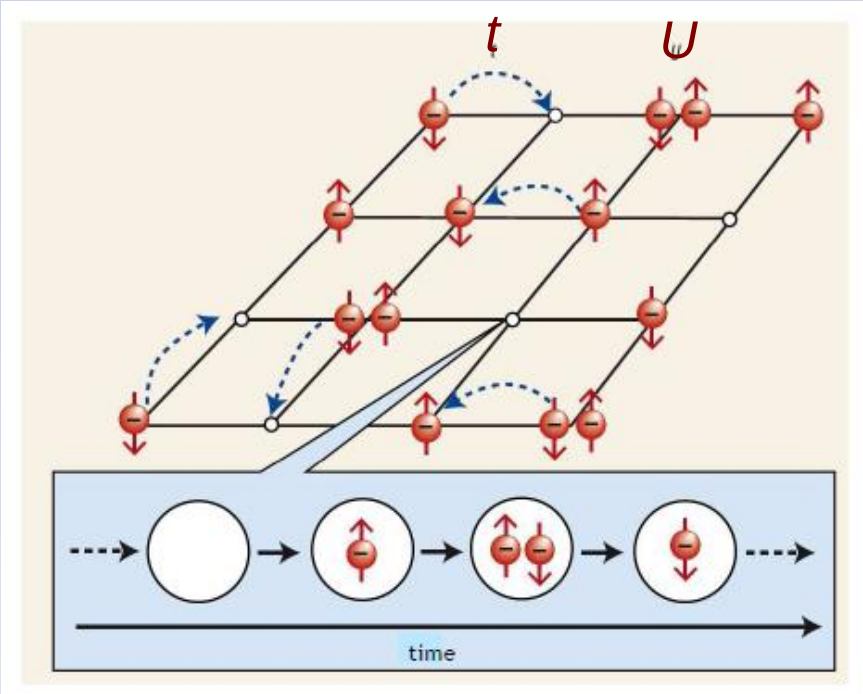
- The lattice problem reduces to a single-site problem.

Is the $d \to \infty$ also useful for the lattice models of correlated fermions?

# The minimal model for strongly correlated systems

The Hubbard model

*Hubbard (1963), Guzwiller (1963), Kanamori (1963)*




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

$$\hat{H}_0 = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}\sigma} \hat{n}_{\boldsymbol{k}\sigma}$$

For 2-dimensional cubic lattice

$$\epsilon_{\boldsymbol{k}\sigma} = -2t\left(cosk_x a + cosk_y a\right)$$

$$\hat{H}_I = U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

# Basics of the Hubbard model

- The simplest model for correlated electrons on a lattice, as the Ising model is the simplest model for spin interactions.

- Exact solution is not known except for 1D (Lieb & Wu, 1968); Many qualitative features of the model is still not fully clear.

- In the coupling regime $t \sim U$, perturbation theory does not work.

# The Hubbard model in infinite dimension

The non-interacting part:

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma}$$

For hypercubic lattice: $\epsilon_{\mathbf{k}} = -2t \sum_{i}^{d} \cos(k_i a)$

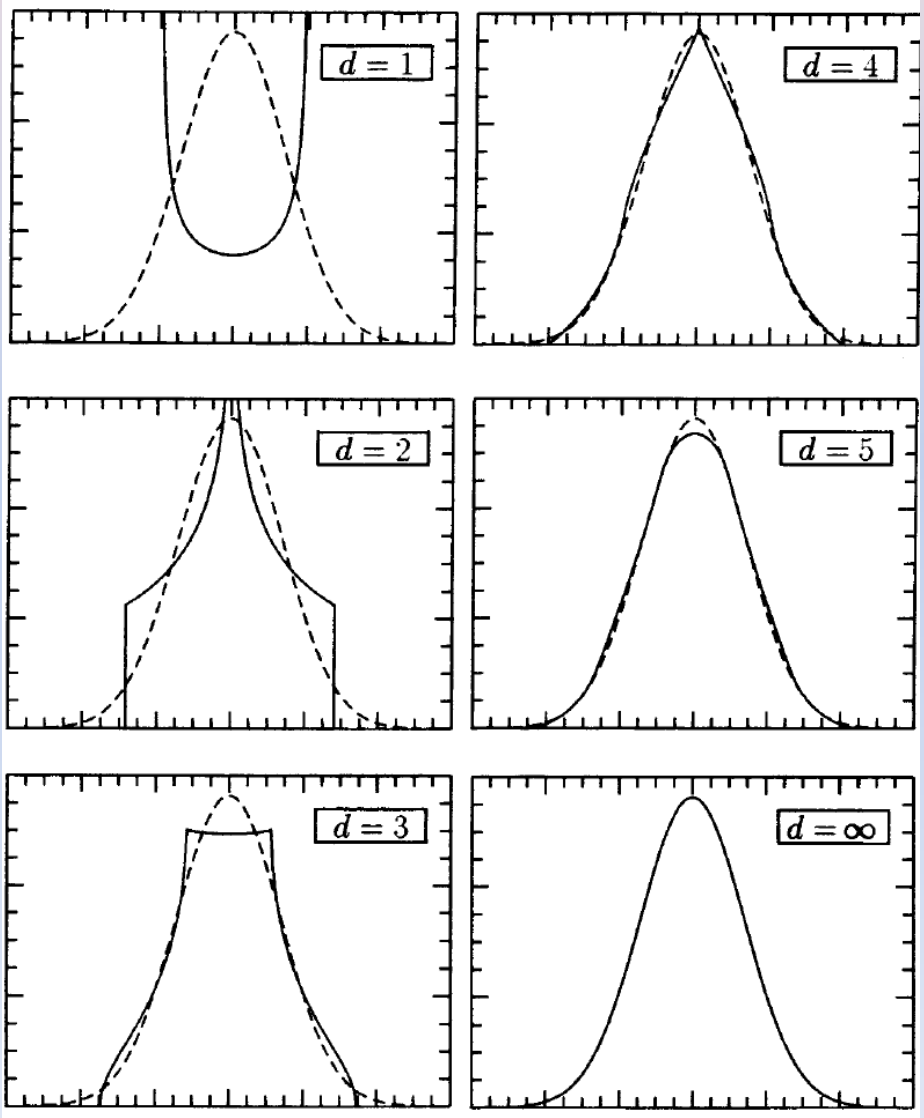
Non-interacting density of states:

$$D_0(E) = 2 \sum_{\mathbf{k}} \delta(E - \epsilon_{\mathbf{k}}) \xrightarrow{d \to \infty} \frac{1}{t\sqrt{(\pi d)}} \exp\left[ -\left( \frac{E}{2t\sqrt{(d)}} \right)^2 \right]$$

To get a non-trivial limit for $d \to \infty$, $t$ has to be scaled as:

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

# The non-interacting density of states of hypercubic lattice



# Simplification in the $d \to \infty$ limit

*Metzner & Vollhardt, Phys. Rev. Lett.* ***62****, 324 (1989).*

$$\hat{H} = -\frac{t^*}{\sqrt{d}} \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

When $d \to \infty$, $\quad G_{\langle ij \rangle, \sigma}(\omega) \sim O\left(\frac{1}{\sqrt{d}}\right)$

- The particles are however not localized:

$$\sum_j | G_{\langle ij \rangle, \sigma} |^2 \sim O(1)$$

- The proper self-energy becomes purely local:

$$\Sigma_{ij}(\omega) = \Sigma_{ii}(\omega) \delta_{ij}$$

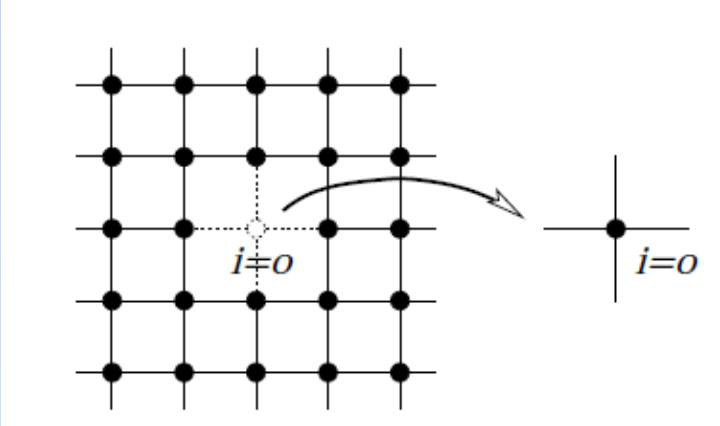
# Reduce the lattice problem to a single-site problem

The entire system can be described quantum mechanically by an action:

$$S = \int_0^\beta d\tau \left( \sum_{i\sigma} c_{i\sigma}^\dagger \partial_\tau c_{i\sigma} - t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{i\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \right)$$

$\beta = k_B T$ (here $c_{i\sigma}^\dagger, c_{i\sigma}$ are Grassmann variables.)

$$e^{-S_{eff}[c_0, c_0^\dagger]} = \int \prod_{i \neq 0, \sigma} D c_{i\sigma}^\dagger D c_{i\sigma} e^{-S[c_{i\sigma}, c_{i\sigma}^\dagger]}$$




Define the partition function:

$$\mathcal{Z}_{eff} = \int D c_{0\sigma}^\dagger D c_{0\sigma} e^{-S_{eff}[c_0, c_0^\dagger]}$$

The local propagator:

$$G_{eff} = \int D c_{0\sigma}^\dagger D c_{0\sigma} c_{0\sigma}(i\omega_n) c_{0\sigma}^\dagger(i\omega_n) e^{-S_{eff}[c_0, c_0^\dagger]}$$

# Dynamical mean-field equations

Simplification in $d \to \infty$,

$$S_{eff} = \int_0^\beta d\tau \int_0^\beta d\tau' \left( c_{0\sigma}^\dagger(\tau)\, \mathcal{G}^{-1}(\tau - \tau')\, c_{0\sigma}(\tau') \right) + U \int_0^\beta d\tau n_{0\uparrow}(\tau) n_{0\downarrow}(\tau)$$

Where the bath Green function $\mathcal{G}$ is given by,

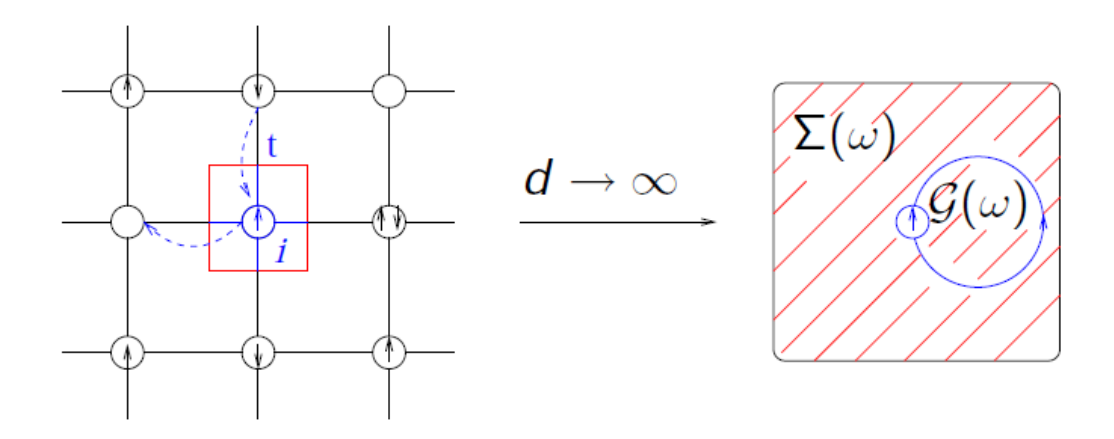
$$\mathcal{G}^{-1}(i\omega_n) = \Sigma(i\omega_n) + \left[ \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma(i\omega_n)} \right]^{-1}$$

$$= \Sigma(i\omega_n) + \left[ \sum_k G_k(i\omega_n) \right]^{-1} = \Sigma(i\omega_n) + G_{ii}^{-1}(i\omega_n)$$

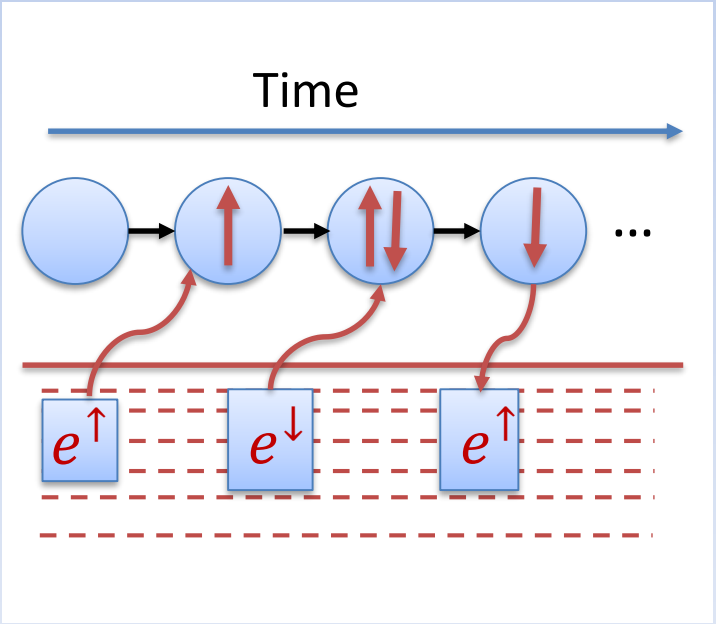
Self-consistent condition:

$$G_{eff}(i\omega_n) = G_{ii}(i\omega_n)$$

# Mean-field interpretation




- A lattice model is replaced by a quantum impurity model embedded in an effective medium, to be determined self-consistently.
- The spatial fluctuations are suppressed, but the local temporal quantum fluctuations are fully preserved.

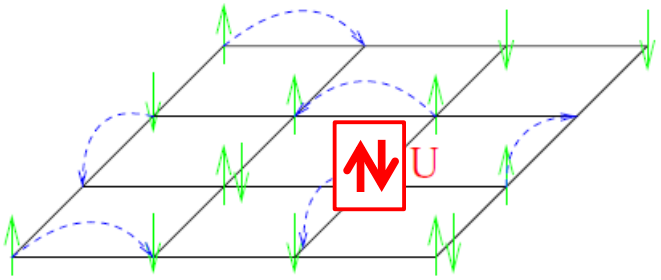


# Solving the single-site problem

Mapping the single-site problem to single-impurity Anderson model (SIAM)

*A. Georges and G. Kotliar PRB (1992)*

$$H_{\mathrm{AM}} = \sum_{l\sigma} \tilde{\epsilon}_l a^\dagger_{l\sigma} a_{l\sigma} - \mu \sum_\sigma c^\dagger_\sigma c_\sigma + U n_\uparrow n_\downarrow + \sum_{l\sigma} V_l (a^\dagger_{l\sigma} c_\sigma + c^\dagger_\sigma a_{l\sigma})$$




(magnetic impurity embedded in a normal metal (Anderson, 1961) )

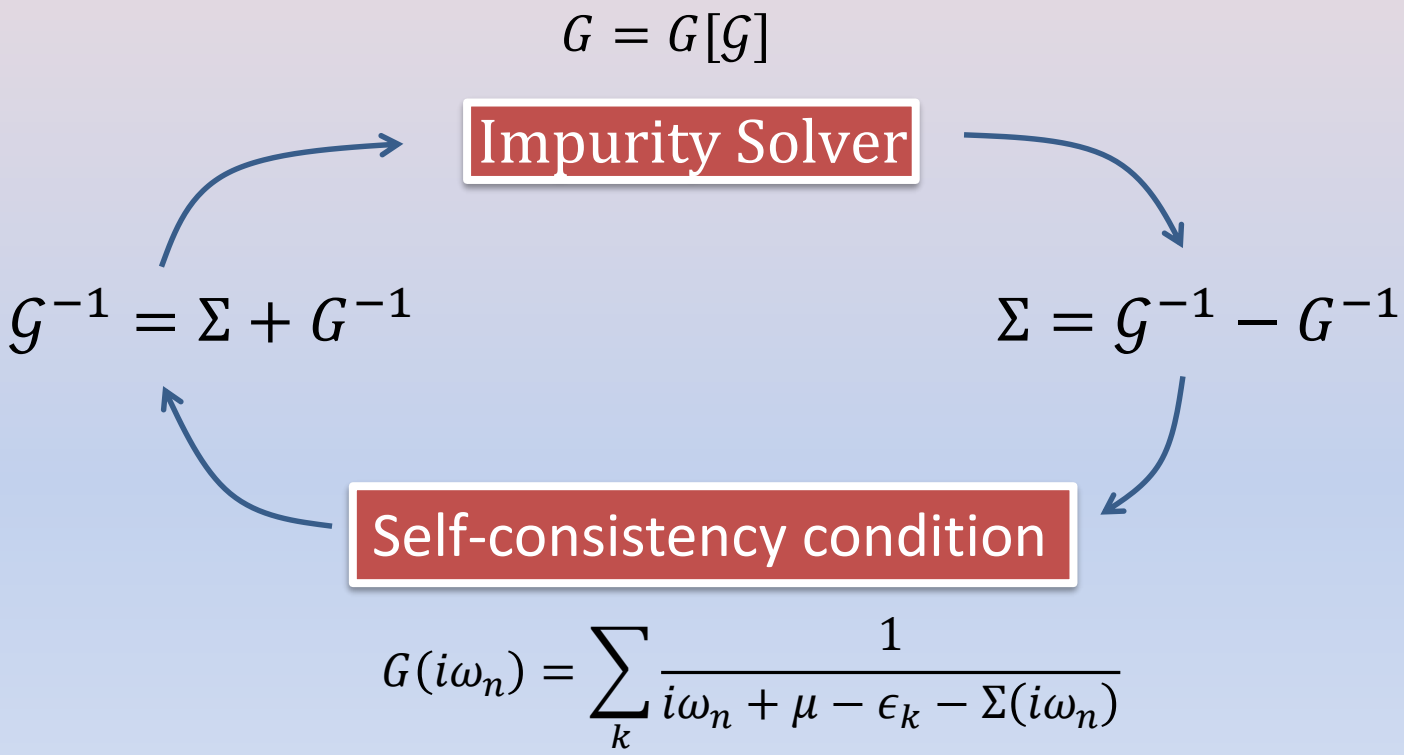
Integrating $a^\dagger_l, a_l$ out,

$$S_{\mathrm{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^\dagger_{o\sigma}(\tau) \mathcal{G}^{-1}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^\beta d\tau n_{o\uparrow}(\tau) n_{o\downarrow}(\tau)$$

with

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \int_\infty^\infty d\omega \frac{\Delta(\varepsilon)}{i\omega_n - \varepsilon}, \quad \Delta(\varepsilon) = \sum_{l\sigma} V_l^2 \delta(\varepsilon - \tilde{\epsilon}_l)$$

# Self-consistent cycle in DMFT




$D=\infty$ Hubbard model = Single-impurity Anderson model
+ self-consistent condition

# Weiss mean-field theory versus dynamical mean-field theory

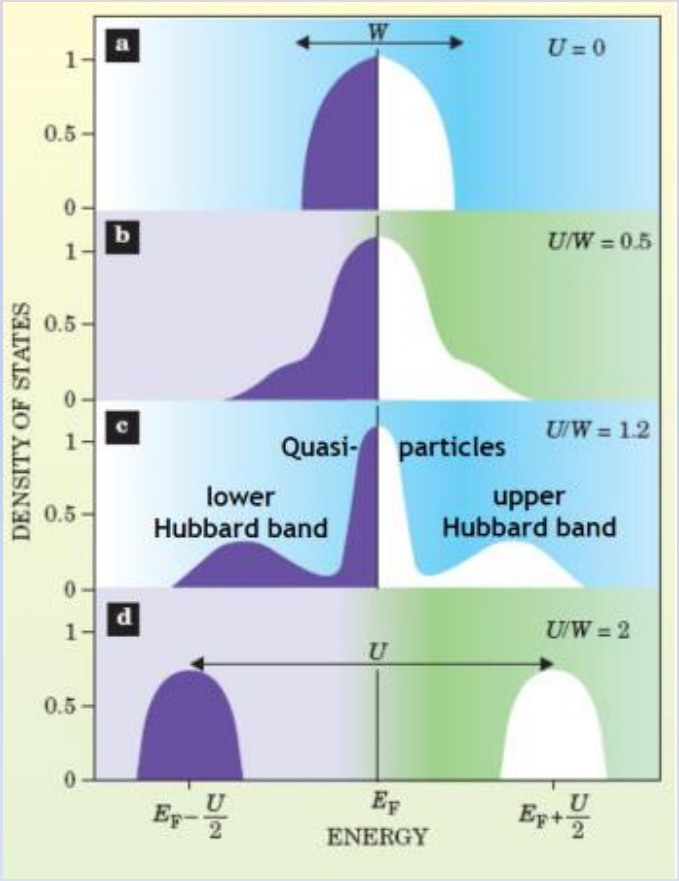
| | Classical case | Quantum case |
|---|---|---|
| Lattice Hamiltonian | Ising model | Hubbard model |
| Scaling | $J \sim 1/d$ | $t \sim 1/\sqrt{d}$ |
| Local observable | $m_i = \langle S_i \rangle$ | $G_{ii}(i\omega_n)$ |
| Single-site problem | $H_{\text{eff}} = -h_{\text{MF}} S_0$ | Anderson impurity model |
| Weiss field | $h_{\text{MF}} = ZJm + h$ | $\mathcal{G}^{-1}(\tau - \tau')$ |

# Compared to Kohn-Sham DFT

| | DFT | DMFT |
|---|---|---|
| Original system | Interacting many-electron system | Correlated lattice model |
| Reference system | Noninteracting electron gas | Anderson impurity model |
| Self-consistency Condition | $n(\boldsymbol{r}) = \sum_n^{occ} \lvert\psi_n(\boldsymbol{r})\rvert^2$ | $G_{imp} = G_{ii}$ |
| Exact limit | $E_{xc}[n]$ being exact | $d = \infty$ |

# Mott transition within the Hubbard model

*G. Kotliar & D. Vollhardt, Physics Today (2004)*



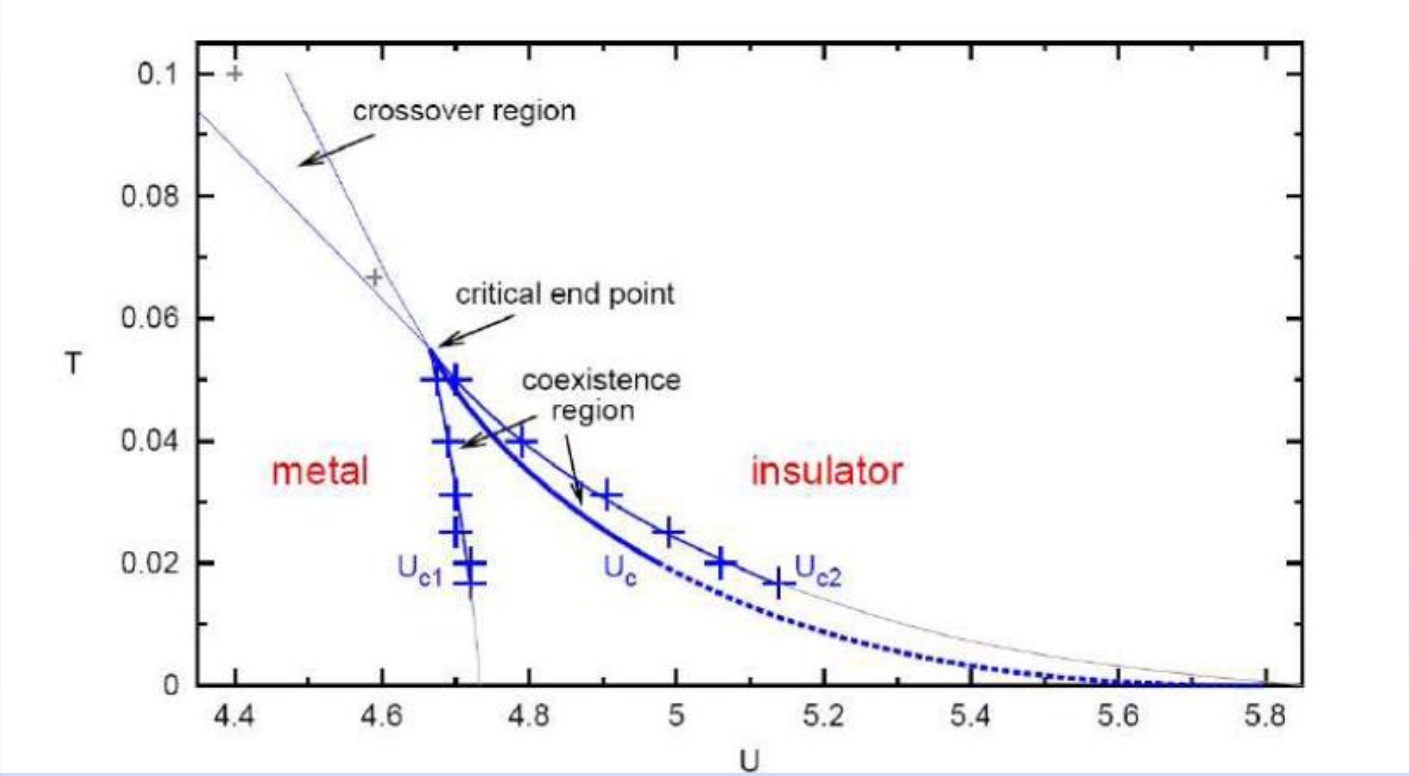

a. Free electron gas;

b. Good metals: Fermi liquid theory (and quasiparticle picture) is valid.

c. Strongly correlated metals: a characteristic three-peak structure appears (Hubbard bands + quasiparticle peak).

d. Mott insulators: quasiparticle peak vanishes, and Mott metal-insulator transition takes places.

# Phase diagram of the Hubbard model




The Mott-Hubbard transition is first-order !