Variational principles for strongly correlated Fermi systems

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outline

Basic Models and Methods:

➜ electron correlations, Hubbard model, exact diagonalization

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Variational Principles and Approximation Strategies:

➜ static mean-field theory, approximation strategies, Hartree-Fock and DFT

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➜ spectroscopy and Green's functions, properties of Green's functions

➜ S matrix, diagrams

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➜ Luttinger-Ward functional, self-energy functional

➜ reference systems and evaluation of the self-energy functional

➜ bath sites and dynamical mean-field theory, cluster extensions

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Dynamical Theory of the Mott Transition:

➜ Mott transition in infinite dimensions

➜ Mott transition in one and two dimensions

acknowledgements

thanks to:

M. Aichhorn, F.F. Assaad, E. Arrigoni, M. Balzer, R. Bulla, C. Dahnken, R. Eder, W. Hanke, A. Hewson, M. Jarrell, M. Kollar, G. Kotliar, A.I. Lichtenstein, A.J. Millis, W. Nolting, D. Senechal, A.-M.S. Tremblay, D. Vollhardt

for cooperations and many helpful discussions.

finanical support: Deutsche Forschungsgemeinschaft

SFB 668 (project A14)
SFB 668 (project B3)
FOR 1346 (project P1)
SFB 925 (project B5)

Electron Correlations

the ”standard model”

standard model of the electronic structure of a solid:

- N electrons
- kinetic energy
- external potential (ion cores)
- Coulomb interaction

$$H = H_0 + H_1$$

with

$$H_0 = \sum_{j=1}^{N} \left(\frac{\mathbf{p}_j^2}{2m} + V(\mathbf{r}_j) \right) = \sum_{j=1}^{N} H_0^{(j)}$$

$$H_1 = \frac{1}{2} \sum_{j,k}^{j \neq k} \frac{e^2}{|\mathbf{r}_j - \mathbf{r}_k|}$$

Hamiltonian: known

solution: unknown

independent particles

Hamiltonian of (effectively) independent electrons:

$$H_{\text{eff}} = \sum_{j=1}^{N} \left(\frac{\mathbf{p}_j^2}{2m} + V_{\text{eff}}(\mathbf{r}_j) \right) = \sum_{j=1}^{N} H_{0,\text{eff}}^{(j)}$$

Schrödinger's equation

$H_{\text{eff}}|\Psi\rangle = E|\Psi\rangle$

is solved by

$|\Psi\rangle = |\varphi_{\alpha_1}^{(1)}\rangle|\varphi_{\alpha_2}^{(2)}\rangle \cdots |\varphi_{\alpha_N}^{(N)}\rangle$ where $H_{0,\text{eff}}^{(j)}|\varphi_{\alpha_j}^{(j)}\rangle = \varepsilon_j|\varphi_{\alpha_j}^{(j)}\rangle$

Fermions!

$$|\Psi\rangle = \frac{1}{N!}\sum_{\mathcal{P}}(-1)^{|\mathcal{P}|}|\varphi_{\alpha_1}^{\mathcal{P}(1)}\rangle|\varphi_{\alpha_2}^{\mathcal{P}(2)}\rangle \cdots |\varphi_{\alpha_N}^{\mathcal{P}(N)}\rangle \qquad E = \sum_{j=1}^{N} \varepsilon_j$$

independent particles

- problem reduces to single-particle Schrödinger equation
- no "correlations"

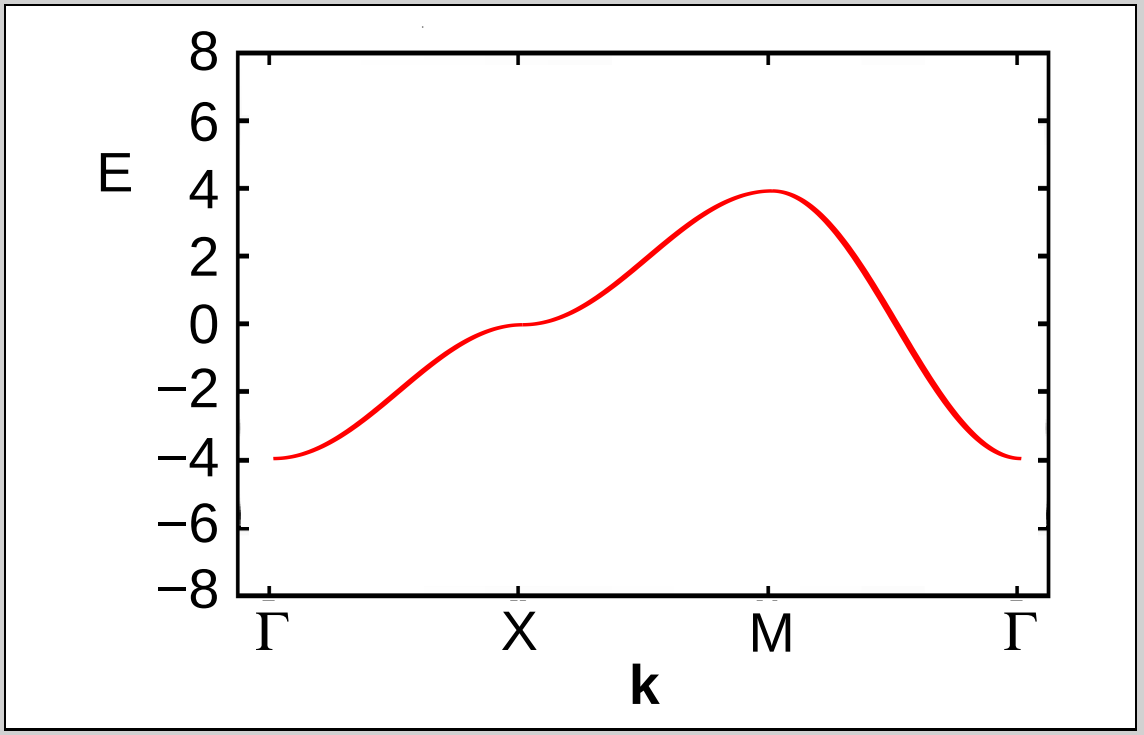
correlated band structure

one-particle energies for a solid with lattice-periodic effective potential:

$\boxed{\varepsilon_\alpha \mapsto \varepsilon_m(\mathbf{k})}$ (Bloch's theorem)

wave vector $\mathbf{k}$, band index m

single-band tight-binding model of independent electrons:



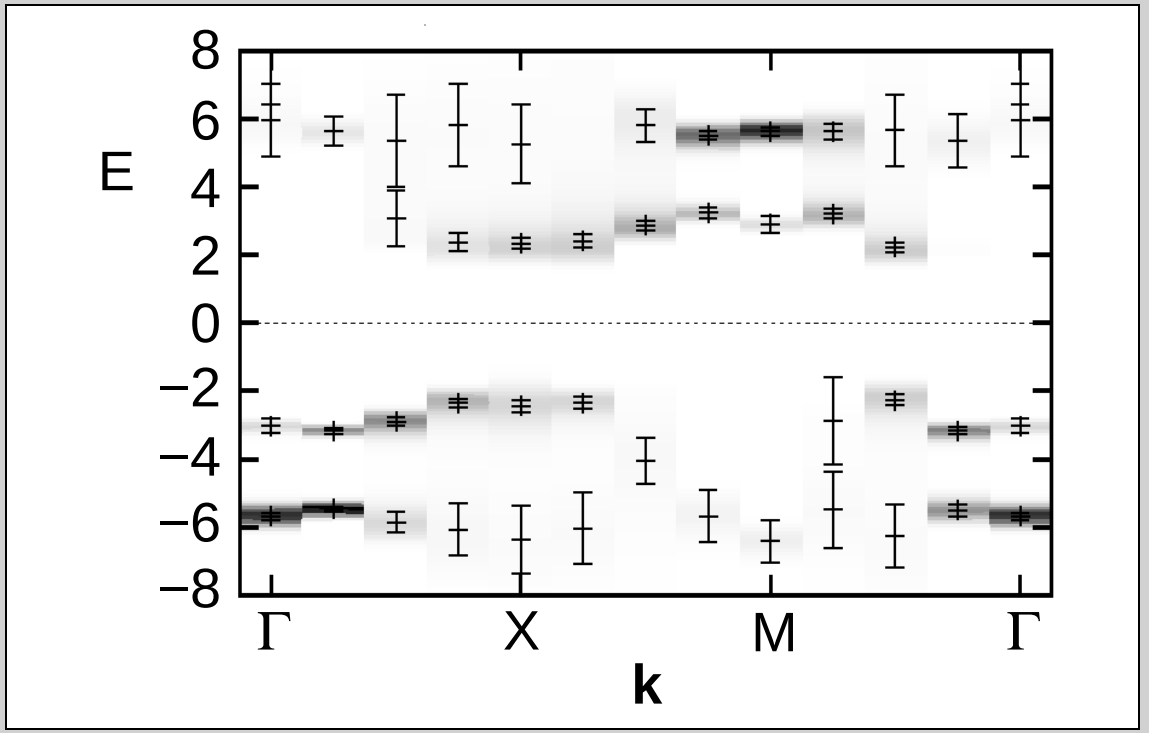
correlated band structure

one-particle energies for a solid with lattice-periodic effective potential:

$\boxed{\varepsilon_\alpha \mapsto \varepsilon_m(\mathbf{k})}$ (Bloch's theorem)

wave vector $\mathbf{k}$, band index m

with interaction:



➜ **correlation effects: there is no $V_{\mathrm{eff}}(\mathbf{r})$ producing this band structure!**

thermodynamics of independent particles

(grand canonical) partition function:

$$\boxed{Z = \text{tr}\, e^{-\beta H}} \qquad \beta = 1/T$$

independent (distinguishable) particles: $H_{\text{eff}} = \sum_{j=1}^{N} H_{0,\text{eff}}^{(j)}$

$$\boxed{Z = Z_1^N}$$

- ✧ no singularities
- ✧ no phase transitions
- ✧ no collective phenomena

independent **fermions** : ✔
independent **bosons** : BEC

➜ correlations due to statistics of particles vs. correlations due to interactions
➜ phase diagrams of Fermi systems: interaction effect

thermodynamics: correlation effects

- collective magnetism
- charge and orbital order
- superconductivity
- Mott transitions
- Kondo screening
- non-Fermi liquid behavior
- Luttinger liquid
- . . .

effect of lattice dimension

W : width of the relevant valence band

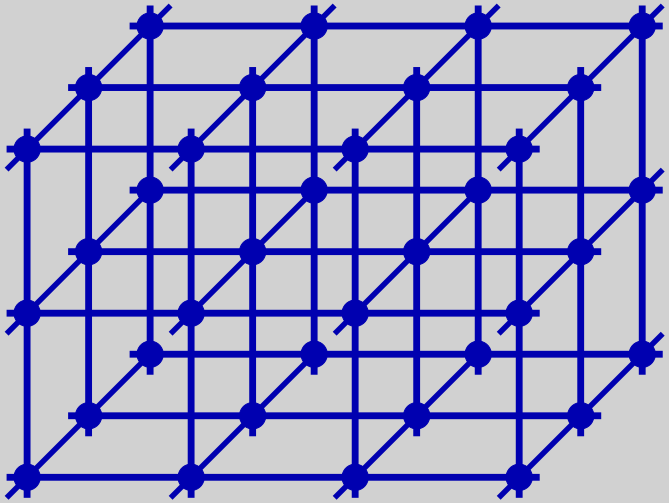
measure of the kinetic energy

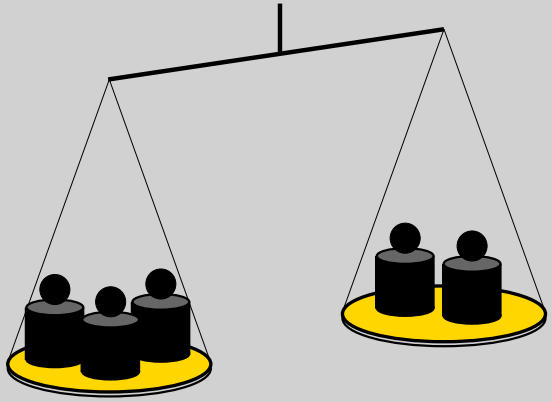
proportional to coordination number / dimension

U : strongly screened Coulomb interaction

local quantity

independent of dimension





D=3:
interaction / correlations
comparatively weak

effect of lattice dimension

W : width of the relevant valence band

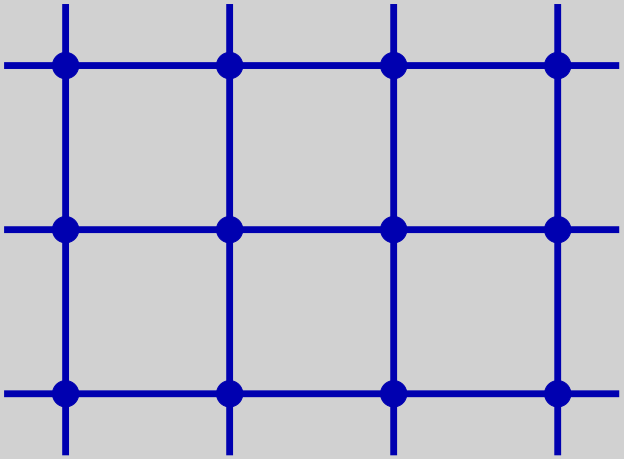
measure of the kinetic energy

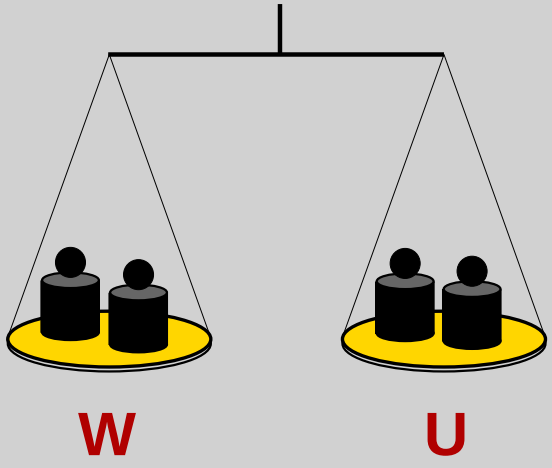
proportional to coordination number / dimension

U : strongly screened Coulomb interaction

local quantity

independent of dimension





D=2:
interaction / correlations
more important

effect of lattice dimension

W : width of the relevant valence band

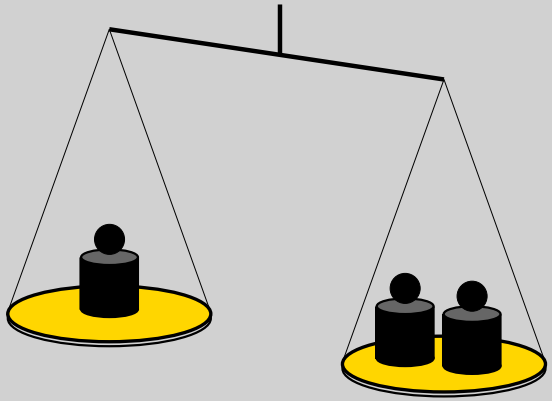
measure of the kinetic energy

proportional to coordination number / dimension

U : strongly screened Coulomb interaction

local quantity

independent of dimension



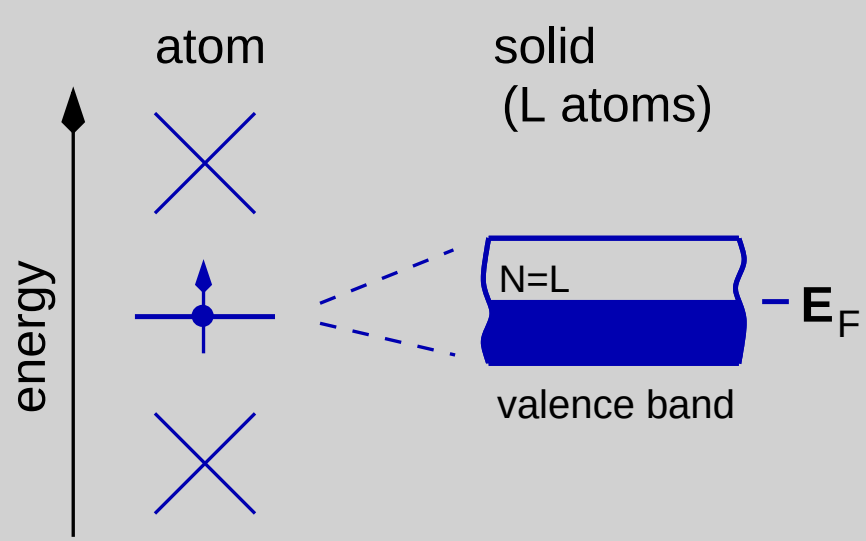
D=1:
correlations dominate
motion blocked by Pauli principle

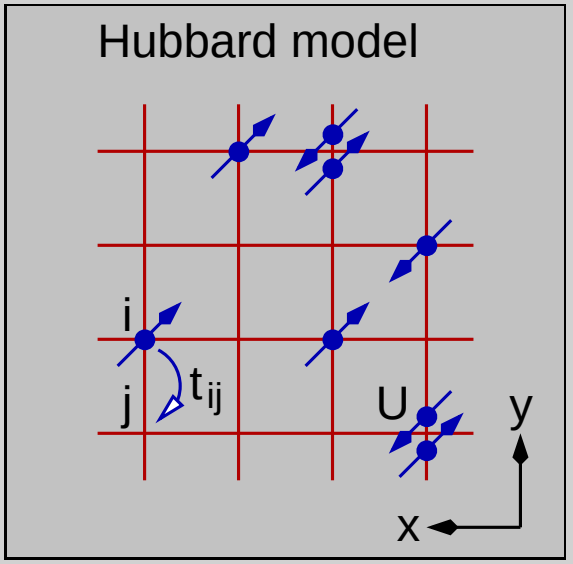
Hubbard Model

single band - local interaction

$$H = H_0 + H_1$$

$$H_0 = \sum_{j=1}^{N} \left(\frac{\mathbf{p}_j^2}{2m} + V(\mathbf{r}_j) \right) = \sum_{j=1}^{N} H_0^{(j)} \qquad H_1 = \frac{1}{2} \sum_{j,k}^{j \neq k} \frac{e^2}{|\mathbf{r}_j - \mathbf{r}_k|}$$

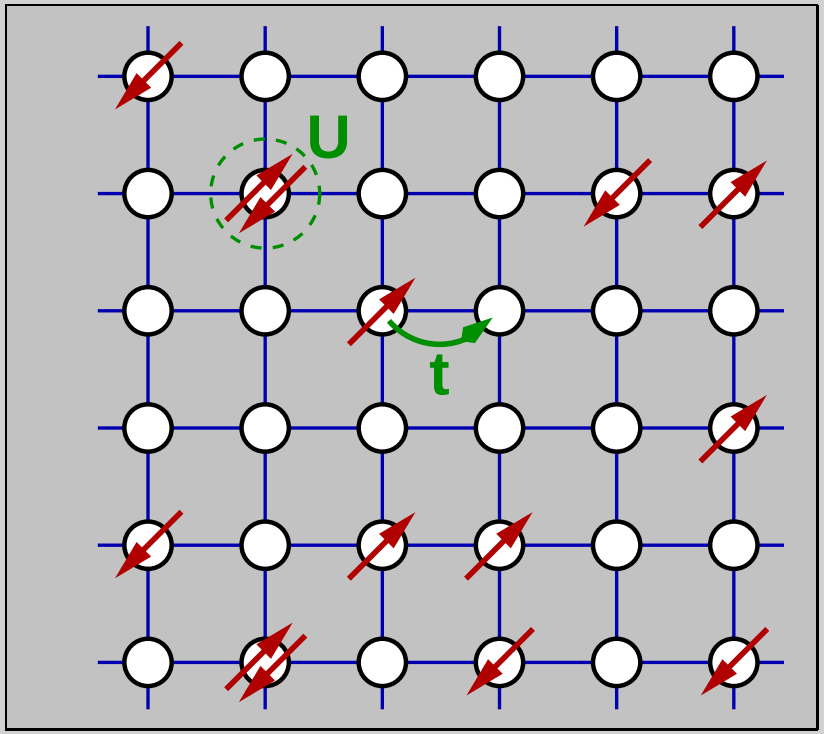




$\mathcal{H}_{\mathrm{Atom}}$ $\qquad$ $\mathcal{H} = \otimes_{i=1}^{L} \mathcal{H}_{\mathrm{Atom}}^{(i)}$ $\qquad$ $H = H_0 + H_1$

dimension: 4 $\qquad$ 4^L

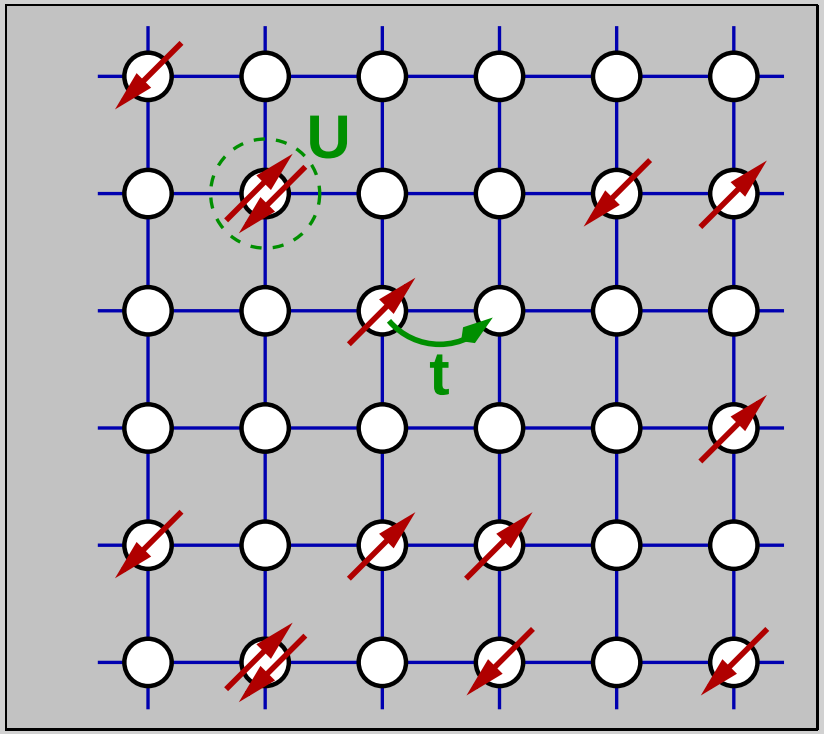
Hubbard model



$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

- i, j: lattice sites, $i = 1, ..., L$
- spin projection $\sigma = \uparrow, \downarrow$
- hopping t_{ij} ➜ tight-binding band
- Hubbard-U ➜ (screened) local Coulomb interaction
- occupation number operator $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$
- $c_{i\sigma}, c^\dagger_{i\sigma}$: annihilator, creator

Hubbard model



$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

- “kinetic” energy vs. Coulomb inteaction
- Fermi statistics
- Hilbert-space dimension: 4^L
- standard model of electronic structure in a nutshell
- collective magnetism, superconductivity, Mott transitions, Kondo effect, ...

Exact Diagonalization

exact diagonalization

simply solve the Hubbard model?

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

➜ set up Hamilton matrix:

$|m\rangle \equiv |n_1, n_2, ..., n_{2L}\rangle$

$m = 1, ..., M \qquad M = \dim \mathcal{H}$

$$H_{mm'} = \langle m|H|m'\rangle$$

➜ diagonalize Hamilton matrix numerically:

$$\mathbf{H} = \mathbf{UDU}^\dagger$$

➜ get eigenvector of lowest energy and ground state:

u_m ➜ $|E_0\rangle = \sum_m u_m |m\rangle$

➜ compute expectation value of observable A:

$$\langle E_0|A|E_0\rangle = \sum_{mm'} u^*_m u_{m'} \langle m|A|m'\rangle$$

exact diagonalization

problem :

$M \times M$ Hamilton matrix with

$$\boxed{M = 2^{2L} = 4^L = \dim \mathcal{H}}$$

$L = 6$ sites ➜ $M = 4096$

use symmetries :

e.g. conservation of total number of σ electrons:

$$\boxed{[N_\sigma, H]_- = 0} \text{ with } N_\sigma = \sum_{i=1}^{L} n_{i\sigma}$$

dimension of invariant subspace:

$$\boxed{M_{N_\uparrow, N_\downarrow} = \begin{pmatrix} L \\ N_\uparrow \end{pmatrix} \begin{pmatrix} L \\ N_\downarrow \end{pmatrix}}$$

$L = 6$ sites, $N_\uparrow = N_\downarrow = 3$ electrons (“half-filling”) ➜ $M_{N_\uparrow, N_\downarrow} = 400$

$L = 10$ sites, $N_\uparrow = N_\downarrow = 5$ electrons (“half-filling”) ➜ $M_{N_\uparrow, N_\downarrow} = 63504$

$63504 \times 63504 \times 4$Bytes ≈ 16GBytes but $N = 10 \lll 10^{23}$!

Static Mean-Field Theory

formulation of the generalized Ritz principle

Hamiltonian: $\mathbf{t}$ and $\mathbf{U}$ dependencies are made explicit

$$H_{\mathbf{t},\mathbf{U}} = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

grandcanonical density matrix:

$$\rho_{\mathbf{t},\mathbf{U}} = \frac{\exp(-\beta(H_{\mathbf{t},\mathbf{U}} - \mu N))}{\text{tr } \exp(-\beta(H_{\mathbf{t},\mathbf{U}} - \mu N))}$$

grandcanonical potential:

$$\Omega_{\mathbf{t},\mathbf{U}} = -T \ln Z_{\mathbf{t},\mathbf{U}} = -T \ln \text{ tr } \exp(-\beta(H_{\mathbf{t},\mathbf{U}} - \mu N))$$

define **density-matrix functional:**

$$\boxed{\Omega_{\mathbf{t},\mathbf{U}}[\rho] = \text{ tr } \Big(\rho(H_{\mathbf{t},\mathbf{U}} - \mu N + T \ln \rho) \Big)}$$

- T, μ fixed
- $\Omega_{\mathbf{t},\mathbf{U}}[\rho]$ real-valued functional of the operator variable ρ
- parametric dependence on $\mathbf{t}$ and $\mathbf{U}$

extremal principle:

$$\boxed{\Omega_{\mathbf{t},\mathbf{U}}[\rho] = \text{min. for } \rho = \rho_{\mathbf{t},\mathbf{U}} \text{ and } \Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t},\mathbf{U}}] = \Omega_{\mathbf{t},\mathbf{U}}}$$

proof

we have:

$$\begin{aligned}\Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t},\mathbf{U}}] &= \text{tr}\left(\rho_{\mathbf{t},\mathbf{U}}(H_{\mathbf{t},\mathbf{U}} - \mu N + T\ln\rho_{\mathbf{t},\mathbf{U}})\right)\\ &= \text{tr}\left(\rho_{\mathbf{t},\mathbf{U}}[H_{\mathbf{t},\mathbf{U}} - \mu N + T(-\beta)(H_{\mathbf{t},\mathbf{U}} - \mu N) - T\ln Z_{\mathbf{t},\mathbf{U}}]\right)\\ &= \text{tr}\,\rho_{\mathbf{t},\mathbf{U}}(-T)\ln Z_{\mathbf{t},\mathbf{U}}\\ &= \Omega_{\mathbf{t},\mathbf{U}}\end{aligned}$$

still to be shown: $\Omega_{\mathbf{t},\mathbf{U}}[\rho] \geq \Omega_{\mathbf{t},\mathbf{U}}$ for arbitrary ρ

domain of the density-matrix functional:

$$\{\rho \mid \text{tr}\,\rho = 1, \quad \rho \geq 0, \quad \rho = \rho^\dagger\}$$

general (!) ansatz:

$$\rho = \rho_{\mathbf{t}',\mathbf{U}'} = \frac{\exp(-\beta(H_{\mathbf{t}',\mathbf{U}'} - \mu N))}{\text{tr}\,\exp(-\beta(H_{\mathbf{t}',\mathbf{U}'} - \mu N))} = \frac{\exp(-\beta(H_{\mathbf{t}',\mathbf{U}'} - \mu N))}{Z_{\mathbf{t}',\mathbf{U}'}}$$

therewith:

$$\begin{aligned}\Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t}',\mathbf{U}'}] &= \text{tr}\left(\rho_{\mathbf{t}',\mathbf{U}'}(H_{\mathbf{t},\mathbf{U}} - \mu N + T\ln\rho_{\mathbf{t}',\mathbf{U}'})\right)\\ &= \text{tr}\left(\rho_{\mathbf{t}',\mathbf{U}'}(H_{\mathbf{t},\mathbf{U}} - \mu N + T(-\beta)(H_{\mathbf{t}',\mathbf{U}'} - \mu N) - T\ln Z_{\mathbf{t}',\mathbf{U}'})\right)\\ &= \text{tr}\left(\rho_{\mathbf{t}',\mathbf{U}'}(H_{\mathbf{t},\mathbf{U}} - H_{\mathbf{t}',\mathbf{U}'})\right) + \Omega_{\mathbf{t}',\mathbf{U}'}\end{aligned}$$

proof, continued

consider the following partiation:

$$H(\lambda) = H_{\mathbf{t}',\mathbf{U}'} + \lambda(H_{\mathbf{t},\mathbf{U}} - H_{\mathbf{t}',\mathbf{U}'})$$

obviously, $H(0) = H_{\mathbf{t}',\mathbf{U}'}$ and $H(1) = H_{\mathbf{t},\mathbf{U}}$
for

$$\Omega(\lambda) \equiv -T \ln \text{ tr } \exp(-\beta(H(\lambda) - \mu N))$$

we have:

$$\Omega(0) = \Omega_{\mathbf{t}',\mathbf{U}'} \text{ and } \Omega(1) = \Omega_{\mathbf{t},\mathbf{U}}$$

hence:

$$\Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t}',\mathbf{U}'}] = \Omega(0) + \left.\frac{\partial\Omega(\lambda)}{\partial\lambda}\right|_{\lambda=0}$$

on the other hand: $\Omega(\lambda)$ is concave ➜

$$\Omega(0) + \left.\frac{\partial\Omega(\lambda)}{\partial\lambda}\right|_{\lambda=0} \cdot \lambda \geq \Omega(\lambda)$$

A concave function of λ is smaller (for any λ, e.g. $\lambda = 1$) than its linear approximation in a fixed point (e.g. $\lambda = 0$).

for $\lambda = 1$ it follows:

$$\Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t}',\mathbf{U}'}] = \Omega(0) + \left.\frac{\partial\Omega(\lambda)}{\partial\lambda}\right|_{\lambda=0} \geq \Omega(1) = \Omega_{\mathbf{t},\mathbf{U}}$$

q.e.d

variational construction of mean-field theory

general scheme to contruct variational approximations:

- ✧ variational principle $\delta\Omega_{\mathbf{t},\mathbf{U}}[\rho] = 0$
- ✧ most general ansatz: $\rho = \rho_{\mathbf{t}',\mathbf{U}'}$ with $\mathbf{t}'$ and $\mathbf{U}'$ arbitrary
  ➜ exact solution $\rho = \rho_{\mathbf{t},\mathbf{U}}$
- ✧ (restricted) ansatz $\rho = \rho_\lambda$ with parameters λ:
  $$\frac{\partial}{\partial\lambda}\Omega_{\mathbf{t},\mathbf{U}}[\rho_\lambda] = 0 \text{ für } \lambda = \lambda_0$$
  yields optimal ρ_{λ_0} with
  $$\Omega_{\mathbf{t},\mathbf{U}}[\rho_{\lambda_0}] \geq \Omega_{\mathbf{t},\mathbf{U}}$$
- ✧ in practice:
  choose a reference system $H' = H'_\lambda$
  $\rho_\lambda = \exp(-\beta(H'_\lambda - \mu N))/Z_\lambda$

general Hamiltonian:

$$H = \sum_{\alpha\beta} t_{\alpha\beta} c^\dagger_\alpha c_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} c^\dagger_\alpha c^\dagger_\beta c_\gamma c_\delta$$

static mean-field theory (Hartree-Fock) :

$$H' = H_{\mathbf{t}',0} = \sum_{\alpha\beta} t'_{\alpha\beta} c^\dagger_\alpha c_\beta \quad \mathbf{t}' \text{ arbitrary}$$

variational determination of $\mathbf{t}'$

trial density matrix: $\boxed{\rho' = \frac{1}{Z'} e^{-\beta(H'-\mu N)}}$ $\qquad \langle \cdots \rangle' = \text{tr}\,(\rho' \cdots)$

conditional equation for $\mathbf{t}'$:

$$
\begin{aligned}
0 &= \frac{\partial}{\partial t'_{\mu\nu}} \Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t}'}] \\
&= \frac{\partial}{\partial t'_{\mu\nu}} \text{tr}\left(\rho_{\mathbf{t}'}(H_{\mathbf{t},\mathbf{U}} - \mu N + T \ln \rho_{\mathbf{t}'})\right) \\
&= \frac{\partial}{\partial t'_{\mu\nu}} \left(\langle H_{\mathbf{t},\mathbf{U}} - \mu N\rangle' + \text{tr}\,[\rho_{\mathbf{t}'} T(-\beta)(H' - \mu N) - \ln Z')]\right) \\
&= \frac{\partial}{\partial t'_{\mu\nu}} \left(\langle H_{\mathbf{t},\mathbf{U}} - \mu N\rangle' - \langle H' - \mu N\rangle' + \Omega_{\mathbf{t}',0}\right) \\
&= \frac{\partial}{\partial t'_{\mu\nu}} \left\langle \sum_{\alpha\beta} t_{\alpha\beta} c^\dagger_\alpha c_\beta + \frac{1}{2} \sum_{\alpha\beta\delta\gamma} U_{\alpha\beta\delta\gamma} c^\dagger_\alpha c^\dagger_\beta c_\gamma c_\delta - \sum_{\alpha\beta} t'_{\alpha\beta} c^\dagger_\alpha c_\beta \right\rangle' + \langle c^\dagger_\mu c_\nu\rangle'
\end{aligned}
$$

since $\partial \Omega_{\mathbf{t}',0}/\partial t'_{\mu\nu} = \langle c^\dagger_\mu c_\nu\rangle'$

define:

$$
K'_{\alpha\nu\mu\beta} = \frac{\partial \langle c^\dagger_\alpha c_\beta\rangle'}{\partial t'_{\mu\nu}} = \frac{1}{T}\langle c^\dagger_\alpha c_\beta\rangle' \langle c^\dagger_\mu c_\nu\rangle' - \int_0^\beta d\tau \langle c^\dagger_\alpha(\tau) c_\beta(\tau) c^\dagger_\mu c_\nu\rangle'
$$

then:

$$
0 = \sum_{\alpha\beta} t_{\alpha\beta} K'_{\alpha\nu\mu\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} \frac{\partial}{\partial t'_{\mu\nu}} \langle c^\dagger_\alpha c^\dagger_\beta c_\gamma c_\delta\rangle' - \sum_{\alpha\beta} t'_{\alpha\beta} K'_{\alpha\nu\mu\beta}
$$

variational determination of t'

H' bilinear ("free") ➜ **Wick's theorem** applies:

$$\langle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \rangle' = \langle c_\alpha^\dagger c_\delta \rangle' \langle c_\beta^\dagger c_\gamma \rangle' - \langle c_\alpha^\dagger c_\gamma \rangle' \langle c_\beta^\dagger c_\delta \rangle'$$

hence:

$$\frac{\partial}{\partial t'_{\mu\nu}} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} \langle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \rangle'$$

$$= \frac{\partial}{\partial t'_{\mu\nu}} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} \left(\langle c_\alpha^\dagger c_\delta \rangle' \langle c_\beta^\dagger c_\gamma \rangle' - \langle c_\alpha^\dagger c_\gamma \rangle' \langle c_\beta^\dagger c_\delta \rangle' \right)$$

$$= \frac{\partial}{\partial t'_{\mu\nu}} \sum_{\alpha\beta\gamma\delta} \left(U_{\alpha\beta\delta\gamma} - U_{\alpha\beta\gamma\delta} \right) \langle c_\alpha^\dagger c_\delta \rangle' \langle c_\beta^\dagger c_\gamma \rangle'$$

$$= \sum_{\alpha\beta\gamma\delta} \left(U_{\alpha\beta\delta\gamma} - U_{\alpha\beta\gamma\delta} \right) \left(\langle c_\alpha^\dagger c_\delta \rangle' K'_{\beta\nu\mu\gamma} + K'_{\alpha\nu\mu\delta} \langle c_\beta^\dagger c_\gamma \rangle' \right)$$

$$= \sum_{\alpha\beta\gamma\delta} \left(U_{\gamma\alpha\delta\beta} - U_{\gamma\alpha\beta\delta} \right) \langle c_\gamma^\dagger c_\delta \rangle' K'_{\alpha\nu\mu\beta} + \sum_{\alpha\beta\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\alpha\gamma\delta\beta} \right) K'_{\alpha\nu\mu\beta} \langle c_\gamma^\dagger c_\delta \rangle'$$

with $(\alpha\beta\gamma) \to (\gamma\alpha\beta)$ (1st term) and $(\beta\gamma\delta) \to (\gamma\delta\beta)$ (2nd term)

$$= \sum_{\alpha\beta\gamma\delta} \left((U_{\gamma\alpha\delta\beta} + U_{\alpha\gamma\beta\delta}) - (U_{\gamma\alpha\beta\delta} + U_{\alpha\gamma\delta\beta}) \right) \langle c_\gamma^\dagger c_\delta \rangle' K'_{\alpha\nu\mu\beta}$$

$$= 2 \sum_{\alpha\beta\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\gamma\alpha\beta\delta} \right) \langle c_\gamma^\dagger c_\delta \rangle' K'_{\alpha\nu\mu\beta}$$

with $U_{\alpha\beta\delta\gamma} = U_{\beta\alpha\gamma\delta}$

variational determination of t'

altogether:

$$0 = \sum_{\alpha\beta} t_{\alpha\beta} K'_{\alpha\nu\mu\beta} - \sum_{\alpha\beta} t'_{\alpha\beta} K'_{\alpha\nu\mu\beta} + \sum_{\alpha\beta\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\gamma\alpha\beta\delta}\right) \langle c^\dagger_\gamma c_\delta \rangle' K'_{\alpha\nu\mu\beta}$$

$$0 = \sum_{\alpha\beta} \left(t_{\alpha\beta} - t'_{\alpha\beta} + \sum_{\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\gamma\alpha\beta\delta}\right) \langle c^\dagger_\gamma c_\delta \rangle' \right) K'_{\alpha\nu\mu\beta}$$

assuming K be invertible:

$$\boxed{t'_{\alpha\beta} = t_{\alpha\beta} + \sum_{\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\gamma\alpha\beta\delta}\right) \langle c^\dagger_\gamma c_\delta \rangle'}$$

optimal one-particle **mean-field Hamiltonian:**

$$\boxed{H' = \sum_{\alpha\beta} \left(t_{\alpha\beta} + \Sigma^{(\mathrm{HF})}_{\alpha\beta} \right) c^\dagger_\alpha c_\beta}$$

with

$$\boxed{\Sigma^{(\mathrm{MF})}_{\alpha\beta} = \sum_{\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\gamma\alpha\beta\delta}\right) \langle c^\dagger_\gamma c_\delta \rangle'}$$ **Hartree-Fock self-energy**

self-consistent scheme required:

$$\boxed{\boldsymbol{\Sigma}^{(\mathrm{HF})} \;\rightarrow\; H' \;\rightarrow\; \langle c^\dagger_\alpha c_\beta \rangle' \;\rightarrow\; \boldsymbol{\Sigma}^{(\mathrm{HF})}}$$

Approximation Strategies

variational approach

macroscopic state: T, V, μ

Hamiltonian: $H_{\mathbf{t},\mathbf{U}} = H_{\mathrm{free}}(\mathbf{t}) + H_{\mathrm{int}}(\mathbf{U})$

thermodynamical potential: $\Omega_{\mathbf{t},\mathbf{U}} = -T \ln \mathrm{tr}\, \exp(-(H_{\mathbf{t},\mathbf{U}} - \mu N)/T)$

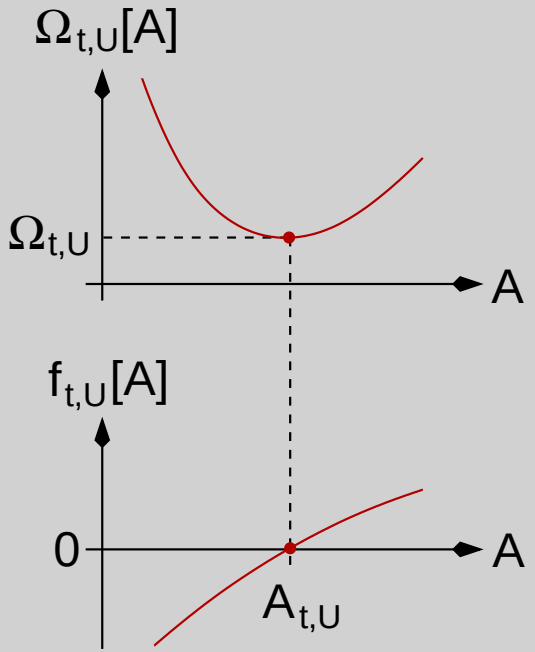
physical quantity: $\mathbf{A}_{\mathbf{t},\mathbf{U}}$

functional $\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}]$:

- $\delta\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}] = 0$ for $\mathbf{A} = \mathbf{A}_{\mathbf{t},\mathbf{U}}$
- $\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}_{\mathbf{t},\mathbf{U}}] = \Omega_{\mathbf{t},\mathbf{U}}$
- $\mathbf{A} \in \mathcal{D} = \{\mathbf{A} \mid \text{conditions}\}$, domain

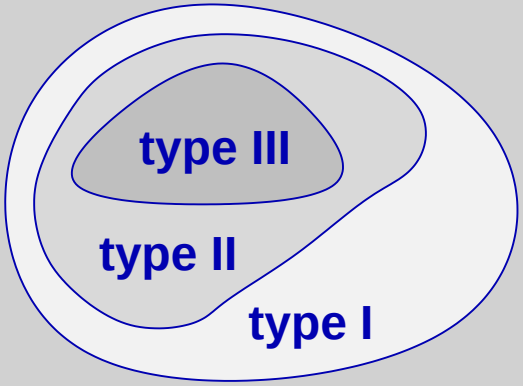
Euler equation:

$$\mathbf{f}_{\mathbf{t},\mathbf{U}}[\mathbf{A}] = 0 \text{ with } \mathbf{f}_{\mathbf{t},\mathbf{U}}[\mathbf{A}] = \frac{\delta\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}]}{\delta\mathbf{A}}$$



approximation strategies

Hamiltonian: $H_{\mathbf{t},\mathbf{U}} = H_{\text{free}}(\mathbf{t}) + H_{\text{int}}(\mathbf{U})$
grand potential: $\Omega_{\mathbf{t},\mathbf{U}} = -T \ln \operatorname{tr} \exp(-\beta(H_{\mathbf{t},\mathbf{U}} - \mu N)$
physical quantity: $\mathbf{A}_{\mathbf{t},\mathbf{U}}$



functional: $\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}]$ on domain $\mathcal{D}$
variational principle: $\delta\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}] = 0$ für $\mathbf{A} = \mathbf{A}_{\mathbf{t},\mathbf{U}}$

Euler equation: $\mathbf{f}_{\mathbf{t},\mathbf{U}}[\mathbf{A}] = \dfrac{\delta\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}]}{\delta\mathbf{A}} \stackrel{!}{=} 0$

I	simplify Euler equation $\mathbf{f}_{\mathbf{t},\mathbf{U}}[\mathbf{A}] \to \widetilde{\mathbf{f}}_{\mathbf{t},\mathbf{U}}[\mathbf{A}]$	general
II	simplify functional $\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}] \to \widetilde{\Omega}_{\mathbf{t},\mathbf{U}}[\mathbf{A}]$	thermodynamically consistent
III	restict domain $\mathcal{D} \to \widetilde{\mathcal{D}}$	thermodynamically consistent, systematic, clear concept

example: Hartree-Fock theory

Rayleigh-Ritz variational principle:

$$\Omega_{\mathbf{t},\mathbf{U}}[\rho] = \mathrm{tr}(\rho(H_{\mathbf{t},\mathbf{U}} - \mu N + T \ln \rho))$$

domain: $\rho \in \mathcal{D} = \{\rho \,|\, \text{Hermitian, positive definite, normalized}\}$

type-III: $\rho \in \widetilde{\mathcal{D}} = \{\rho \,|\, \text{Hermitian, positive definite, normalized, } \textbf{non-interacting}\} \subset \mathcal{D}$

example: Hartree-Fock theory

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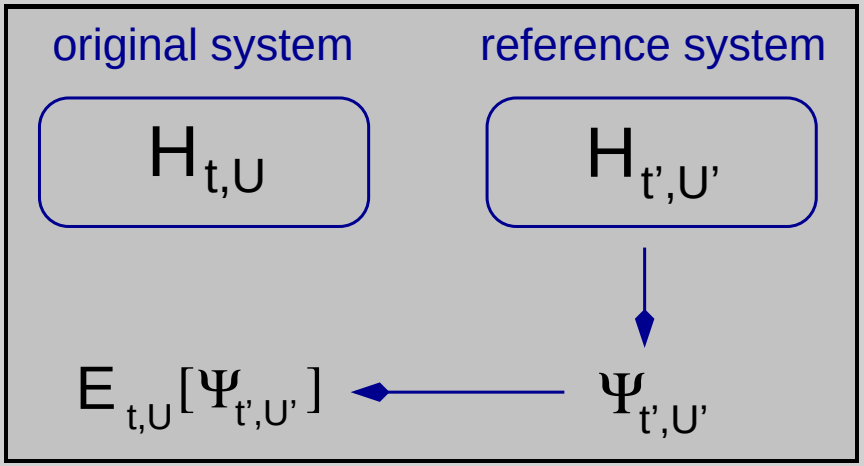

Hartree-Fock:

$\widetilde{\mathcal{D}} = \{\rho_{\mathbf{t}',\mathbf{U}'} \,|\, \mathbf{t}' \text{arbitrary}, \mathbf{U}' = 0\}$

example: Hartree-Fock theory

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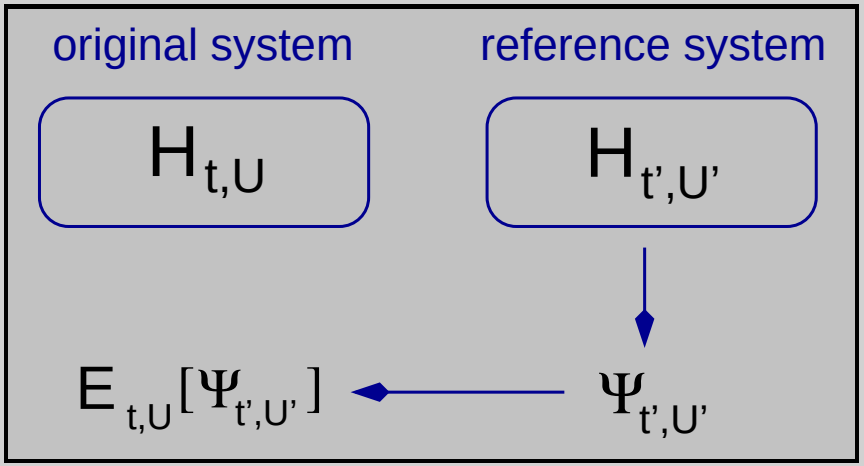

Hartree-Fock:

$\widetilde{\mathcal{D}} = \{\rho_{\mathbf{t}',\mathbf{U}'} \,|\, \mathbf{t}' \text{arbitrary}, \mathbf{U}' = 0\}$

$\Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t}',0}] = \Omega_{\mathbf{t}',0} + \mathrm{tr}(\rho_{\mathbf{t}',0}(H_0(\mathbf{t}) + H_1(\mathbf{U}) - H_0(\mathbf{t}'))$ (use Wick's theorem)

$\dfrac{\partial \Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t}',0}]}{\partial \mathbf{t}'} = 0 \;\Leftrightarrow$ **HF equations !**

➜ concept of reference system helpful for type-III approximations

example: density-functional theory

electron density $n(\mathbf{r}) = \text{tr}\,(\rho\hat{n}(\mathbf{r}))$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{n}] = \text{tr}(\mathbf{t}\,\mathbf{n}) + F_{\mathbf{U}}[\mathbf{n}]$$

Hohenberg, Kohn (1964), Kohn, Sham (1965)

potential energy

$F_{\mathbf{U}}[\mathbf{n}] = F^{(\text{kin})}[\mathbf{n}] + F^{(\text{H})}_{\mathbf{U}}[\mathbf{n}] + F^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}]$, $F^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}] =$??

existence: HK theorem

universal ($\mathbf{t}$ independent)

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existence: HK theorem

universal ($\mathbf{t}$ independent)

type-III approximation ?

$H_{\mathbf{t},\mathbf{U}}$: inhomogeneous electron "gas" (original)

$H_{\mathbf{t}^i,\mathbf{U}}$: homogeneous electron "gas" (reference)

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{n}] = \text{tr}(\mathbf{t}\,\mathbf{n}) + F_{\mathbf{U}}[\mathbf{n}]$$
$$\Omega_{\mathbf{t}^i,\mathbf{U}}[\mathbf{n}] = \text{tr}(\mathbf{t}^i\,\mathbf{n}) + F_{\mathbf{U}}[\mathbf{n}]$$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{n}] = \Omega_{\mathbf{t}^i,\mathbf{U}}[\mathbf{n}] + \text{tr}((\mathbf{t}-\mathbf{t}^i)\mathbf{n})$$

nice concept,
but poor results !

example: density-functional theory

electron density $n(\mathbf{r}) = \text{tr}\,(\rho\hat{n}(\mathbf{r}))$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{n}] = \text{tr}(\mathbf{t}\,\mathbf{n}) + F_{\mathbf{U}}[\mathbf{n}]$$

Hohenberg, Kohn (1964), Kohn, Sham (1965)

potential energy $F_{\mathbf{U}}[\mathbf{n}] = F^{(\text{kin})}[\mathbf{n}] + F^{(\text{H})}_{\mathbf{U}}[\mathbf{n}] + F^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}]$, $F^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}] =$??

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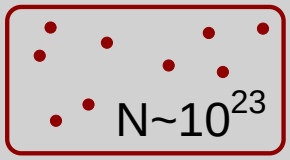
nice concept,
but poor results !

local density approximation: $F^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}] \to \widetilde{F}^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}]$

very successful, but type-II

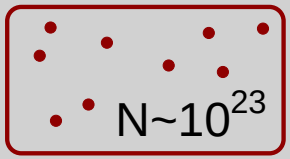
Spectroscopies and Green's Functions

Green's function, spectral density and self-energy

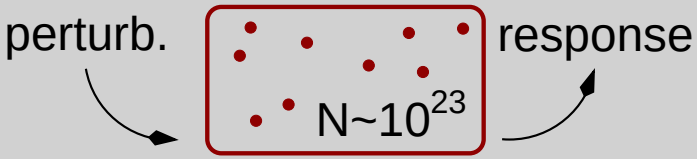


$|\Psi\rangle = ?$

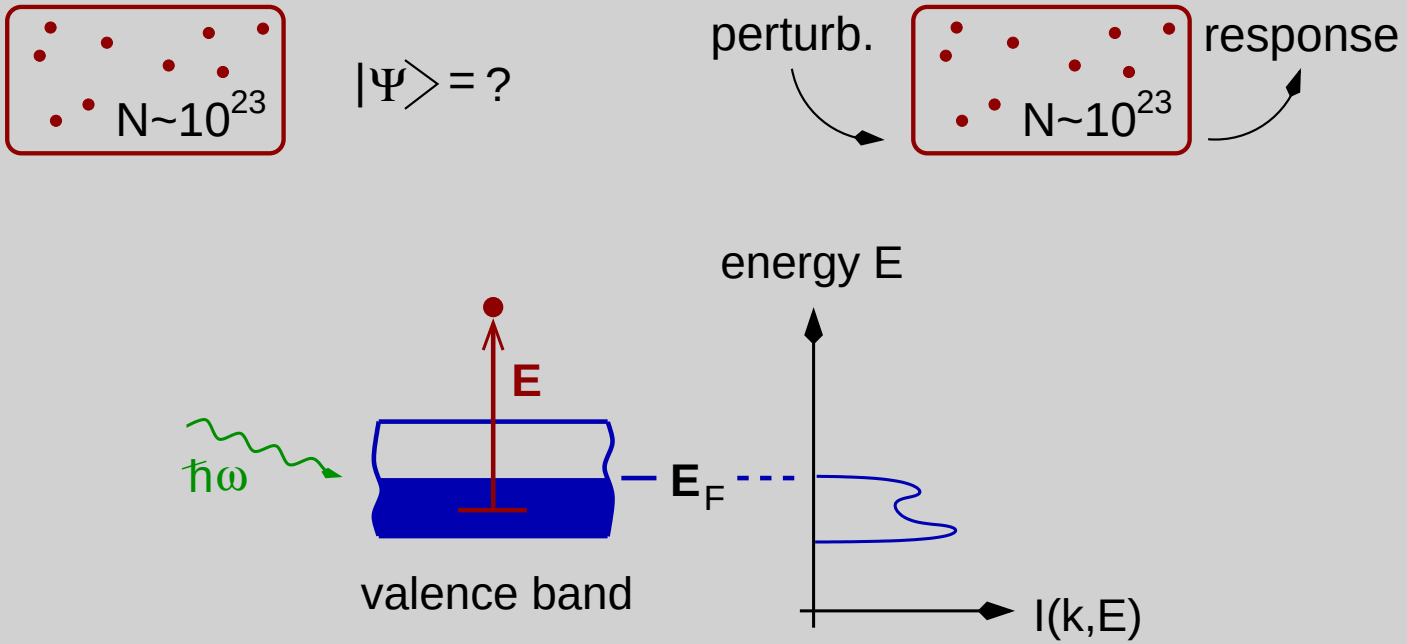
Green's function, spectral density and self-energy



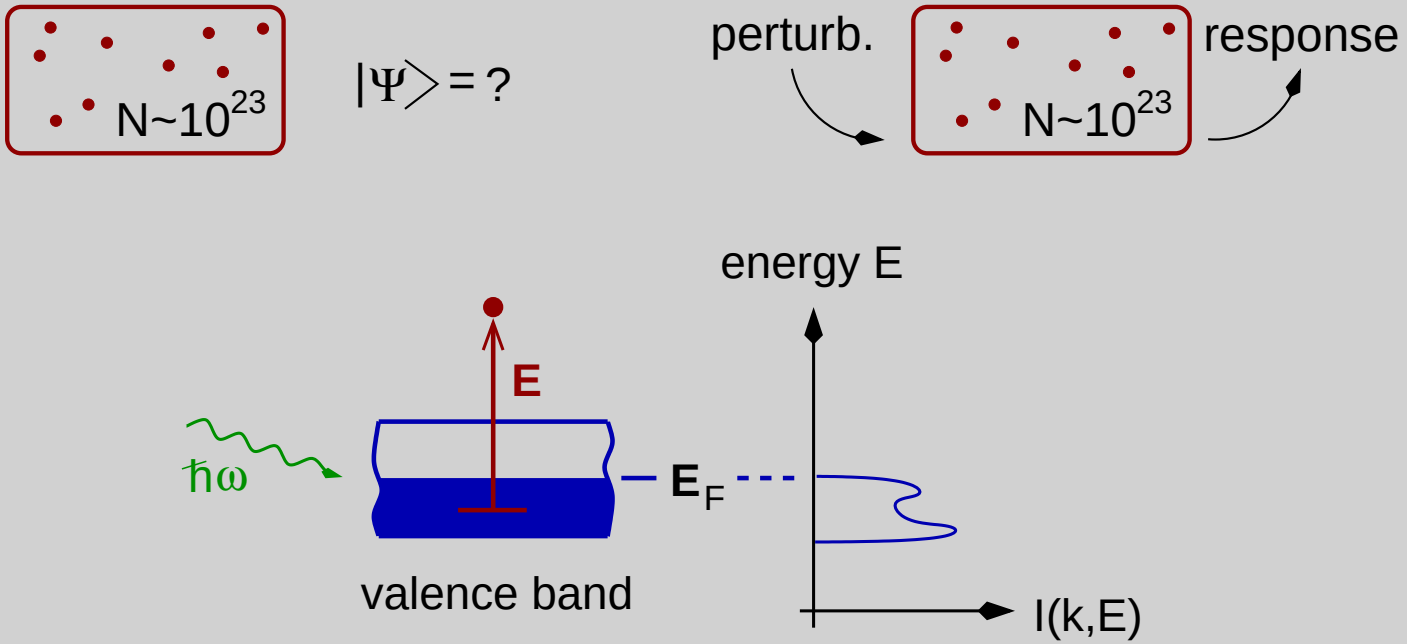
$|\Psi\rangle = ?$



Green's function, spectral density and self-energy



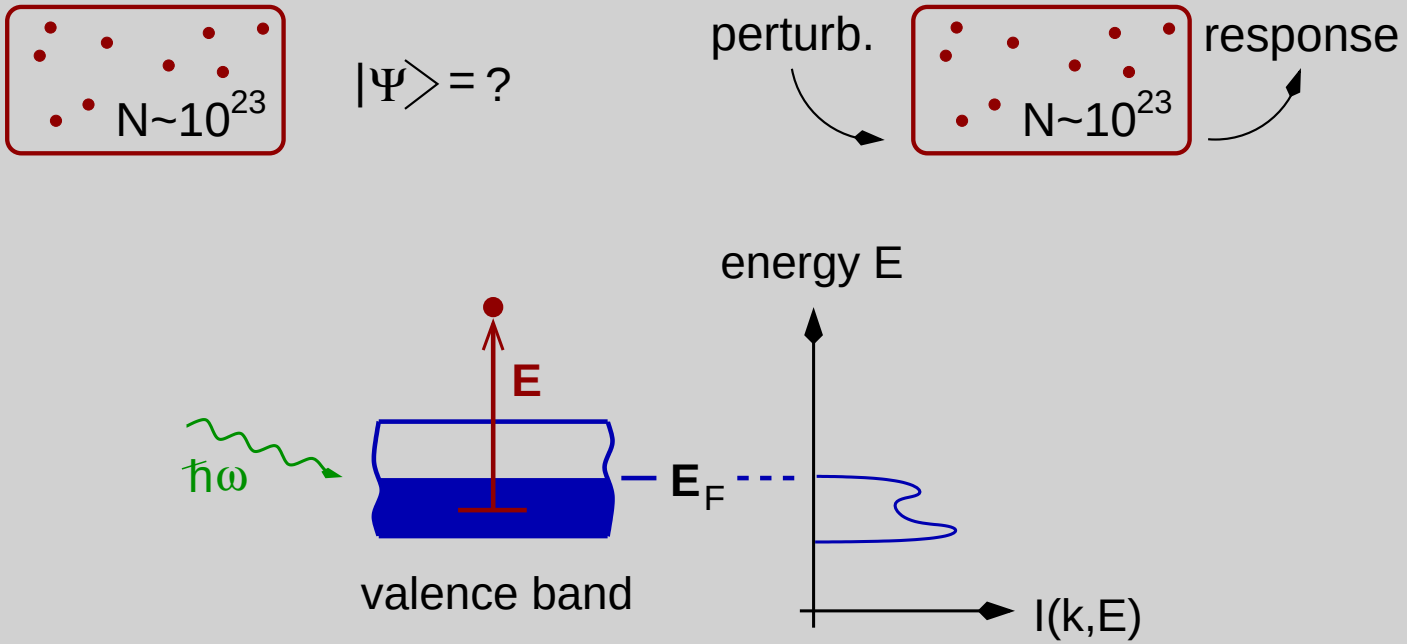
Green's function, spectral density and self-energy



$$I(\mathbf{k}, E) \propto \sum_m \left| \langle N-1, m \mid c_{\mathbf{k}} \mid N, 0 \rangle \right|^2 \delta\left(E - (E_m(N-1) - E_0(N))\right) = A(\mathbf{k}, E)$$

spectral density

Green's function, spectral density and self-energy



$$I(\mathbf{k},E) \propto \sum_m \left|\langle N-1,m \mid c_{\mathbf{k}} \mid N,0\rangle\right|^2 \delta\left(E-(E_m(N-1)-E_0(N))\right) = A(\mathbf{k},E)$$

spectral density

Green's function: $G(\mathbf{k},E) = \int dE' \, \frac{A(\mathbf{k},E')}{E-E'}$ $\qquad A(\mathbf{k},E) = -\mathrm{Im}\, G(\mathbf{k},E+i0^+)/\pi$

self-energy: $G(\mathbf{k},E) = G_0(\mathbf{k},E) + G_0(\mathbf{k},E)\Sigma(\mathbf{k},E)G(\mathbf{k},E)$ (Dyson's equation)

different spectroscopies

spectroscopies:

(weak) perturbation ➜ system's response

excitation process R ➜ cross section, intensity I

---

photoemission = removal of an electron

$R = c_\alpha$

angle- and spin-resolved: $\alpha = (\mathbf{k}, \sigma)$

inverse photoemission:

$R = c_\alpha^\dagger$

complementary spectroscopy

Auger process:

$R = c_\alpha c_\beta$

appearance-potential spectroscopy:

$R = c_\alpha^\dagger c_\beta^\dagger$

transport, Raman, neutron scattering, etc.:

$R = c_\alpha^\dagger c_\beta$

---

elementary excitation processes

one-electron excitations: $c_\alpha^\dagger, c_\alpha$

two-electron excitations: $c_\alpha c_\beta, c_\alpha^\dagger c_\beta^\dagger, c_\alpha^\dagger c_\beta$

"detailled" theory

(grandcanonical) Hamiltonian of the system:

$$\mathcal{H} = H - \mu N = \mathcal{H}_0 + H_1$$

eigenenergies, eigenstates:

$$\mathcal{H}|m\rangle = E_m|m\rangle \qquad \text{ONB:} \quad \{|m\rangle\}$$

example: photoemission

- ✧ electronic transition induced by coupling to radiation field:

$$\boxed{\mathbf{p} \to \mathbf{p} - q\mathbf{A}}$$

- ✧ neglect $\mathbf{A}^2$ term, choose Coulomb gauge, adopt dipole approximation:

$$\boxed{\mathcal{H} \to \mathcal{H} + V\ , \qquad V = \mathbf{A}_0\mathbf{p}}$$

- ✧ second quantization:

$$\boxed{V = \sum_{\beta\gamma}\langle\beta|\mathbf{A}_0\mathbf{p}|\gamma\rangle a^\dagger_\beta c_\gamma + \text{h.c.} = \sum_{\beta\gamma} M_{\beta\gamma} a^\dagger_\beta c_\gamma + \text{h.c.}}$$

where: $a \sim$ high-energy scattering states, $c \sim$ valence states

- ✧ final state within the "sudden approximation"
(no interaction between photoelectron and rest of the system):

$$\boxed{|f\rangle \approx a^\dagger_\alpha|m\rangle \qquad E_f = E_m + \varepsilon_\alpha}$$

"detailled" theory

- initial state:

$$|i\rangle = |n\rangle \qquad E_i = E_n + h\nu$$

with

$$a_\alpha |n\rangle \approx 0$$

- hence:

$$\langle f|V|i\rangle = \langle m|a_\alpha \sum_{\beta\gamma} (M_{\beta\gamma} a^\dagger_\beta c_\gamma + \text{h.c.})|n\rangle = \langle m| \sum_\gamma M_{\alpha\gamma} c_\gamma |n\rangle$$

- disregard the matrix elements:

$$\langle f|V|i\rangle = \langle m|c_\gamma|n\rangle$$

i.e.

$$R = c_\gamma$$

elementary transition operator for photoemission

one-particle Green's function and spectral density

one-particle spectral density: (cross section, intensity, experiment)

$$A_{\alpha\beta}(\omega) = \sum_{mn} \frac{e^{-\beta E_m} + e^{-\beta E_n}}{Z} \langle m|c_\alpha|n\rangle\langle n|c_\beta^\dagger|m\rangle \delta(\omega - (E_n - E_m))$$

$$A_{\alpha\beta}(t) = \frac{1}{2\pi}\langle [c_\alpha(t), c_\beta^\dagger(0)]_+\rangle$$

$$A_{\alpha\beta}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G_{\alpha\beta}^{(\mathrm{ret})}(\omega)$$

one-particle Green function:

$$G_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} dz\, \frac{A_{\alpha\beta}(z)}{\omega - z} \qquad \omega \in \mathbb{C}$$

retarded one-particle Green function:

$$G_{\alpha\beta}^{(\mathrm{ret})}(\omega) = \int_{-\infty}^{\infty} dz\, \frac{A_{\alpha\beta}(z)}{\omega + i0^+ - z}$$

$$G_{\alpha\beta}^{(\mathrm{ret})}(t) = -i\Theta(t)\langle [c_\alpha(t), c_\beta^\dagger(0)]_+\rangle$$

one-particle Matsubara function:

$$G_{\alpha\beta}(i\omega_n) = \int_{-\infty}^{\infty} dz\, \frac{A_{\alpha\beta}(z)}{i\omega_n - z}$$

$$G_{\alpha\beta}(\tau) = -\langle \mathcal{T} c_\alpha(\tau) c_\beta^\dagger(0)\rangle$$

$$i\omega_n = i(2n+1)\pi/\beta$$

S matrix

S matrix – motivation

problem: the time dependence in

$$G_{\alpha\beta}(\tau) = -\langle \mathcal{T} c_\alpha(\tau) c^\dagger_\beta(0) \rangle$$

is due to the full Hamiltonian:

$$\boxed{H = H_0 + H_1 = H_0 + V \qquad \mathcal{H} = \mathcal{H}_0 + V}$$

goal: transform all τ dependencies into **free** τ dependencies!

interaction picture:

$$\boxed{A_I(t) = e^{i\mathcal{H}_0 t} A e^{-i\mathcal{H}_0 t}}$$

modified interaction picture:

$$\boxed{A_I(\tau) = e^{\mathcal{H}_0 \tau} A e^{-\mathcal{H}_0 \tau}}$$

---

transformation from the Heisenberg to the interaction picture: mediated by S “matrix”

S matrix – definition

define:

$$\boxed{S(\tau,\tau') = e^{\mathcal{H}_0\tau} e^{-\mathcal{H}(\tau-\tau')} e^{-\mathcal{H}_0\tau'}}$$

S matrix

properties:

- $S(\tau,\tau'') = S(\tau,\tau')S(\tau',\tau'')$
- $S(\tau,\tau) = 1$
- $S(\tau,\tau')$ is not unitary
- $S(\tau,\tau')$ is the (imaginary) time evolution operator $e^{-\mathcal{H}(\tau-\tau')}$ in the (modified) interaction (Dirac) picture

we have:

$$-\frac{\partial}{\partial\tau}S(\tau,\tau') = -\frac{\partial}{\partial\tau}\left(e^{\mathcal{H}_0\tau} e^{-\mathcal{H}(\tau-\tau')} e^{-\mathcal{H}_0\tau'}\right) = e^{\mathcal{H}_0\tau}(\mathcal{H}-\mathcal{H}_0)e^{-\mathcal{H}(\tau-\tau')}e^{-\mathcal{H}_0\tau'}$$

$$= e^{\mathcal{H}_0\tau} V e^{-\mathcal{H}_0\tau} e^{\mathcal{H}_0\tau} e^{-\mathcal{H}(\tau-\tau')} e^{-\mathcal{H}_0\tau'} = V_I(\tau)S(\tau,\tau')$$

equation of motion:

$$\boxed{-\frac{\partial}{\partial\tau}S(\tau,\tau') = V_I(\tau)S(\tau,\tau')}$$

initial condition: $S(\tau,\tau) = 1$

solution of the equation of motion

if $V_I(\tau)$ **was** not operator-valued, we could solve the differential equation by:

$$S(\tau,\tau') = \exp\left(-\int_{\tau'}^{\tau} d\tau'' V_I(\tau'')\right)$$

the problem $[V_I(\tau), V_I(\tau')]_- \neq 0$ can be circumvented using the time-ordering operator:

$$\boxed{S(\tau,\tau') = \mathcal{T}\exp\left(-\int_{\tau'}^{\tau} d\tau'' V_I(\tau'')\right)}$$

explicit representation of the S matrix

- note: under $\mathcal{T}$, we have: $[V_I(\tau), V_I(\tau')]_- = 0$ (there is no sign), since

$$V_I(\tau) = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} c^\dagger_{\alpha,I}(\tau) c^\dagger_{\beta,I}(\tau) c_{\gamma,I}(\tau) c_{\delta,I}(\tau)$$

  is quartic

- note: $\mathcal{T}$ operates after expanding the exponential:

$$S(\tau,\tau') = \mathcal{T}\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_{\tau'}^{\tau} d\tau_1 \cdots \int_{\tau'}^{\tau} d\tau_k V_I(\tau_1)\cdots V_I(\tau_k)$$

preparation of the Matsubara function

from the definition, $S(\tau,\tau') = e^{\mathcal{H}_0\tau} e^{-\mathcal{H}(\tau-\tau')} e^{-\mathcal{H}_0\tau'}$, we immediately get

$$\boxed{A(\tau) = S(0,\tau) A_I(\tau) S(\tau,0)} \qquad \boxed{e^{-\beta\mathcal{H}} = e^{-\beta\mathcal{H}_0} S(\beta,0)}$$

Matsubara function for $\tau > 0$:

$$\begin{aligned}
G_{\alpha\beta}(\tau) &= -\langle \mathcal{T} c_\alpha(\tau) c^\dagger_\beta(0)\rangle \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta\mathcal{H}} c_\alpha(\tau) c^\dagger_\beta(0)\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta\mathcal{H}_0} S(\beta,0) S(0,\tau) c_{\alpha,I}(\tau) S(\tau,0) c^\dagger_{\beta,I}(0)\right) \\
&= -\frac{1}{Z}\mathrm{tr}\left(e^{-\beta\mathcal{H}_0} \mathcal{T} S(\beta,\tau) c_{\alpha,I}(\tau) S(\tau,0) c^\dagger_{\beta,I}(0)\right) \\
&= -\frac{Z_0}{Z}\frac{1}{Z_0}\mathrm{tr}\left(e^{-\beta\mathcal{H}_0} \mathcal{T} S(\beta,0) c_{\alpha,I}(\tau) c^\dagger_{\beta,I}(0)\right) \\
&= -\frac{\langle \mathcal{T} S(\beta,0) c_{\alpha,I}(\tau) c^\dagger_{\beta,I}(0)\rangle^{(0)}}{\mathrm{tr}\,(e^{-\beta\mathcal{H}_0} S(\beta,0))/Z_0}
\end{aligned}$$

$$\boxed{G_{\alpha\beta}(\tau) = -\frac{\langle \mathcal{T} S(\beta,0) c_{\alpha,I}(\tau) c^\dagger_{\beta,I}(0)\rangle^{(0)}}{\langle S(\beta,0)\rangle^{(0)}}} \qquad \boxed{S(\beta,0) = \mathcal{T}\exp\left(-\int_0^\beta d\tau V_I(\tau)\right)}$$

... ready to apply Wick's theorem

suppress the index "I" (all τ dependencies are meant as **free** τ dependencies)

$$G_{\alpha\beta}(\tau) = -\frac{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau V(\tau)\right) c_\alpha(\tau) c_\beta^\dagger(0)\right\rangle^{(0)}}{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau V(\tau)\right)\right\rangle^{(0)}}$$

free expectation values!
free (imaginary) time dependence!

Wick's theorem can be applied.

Diagrammatic Perturbation Theory

partition function

first, consider the **denomiator** in

$$G_{\alpha\beta}(\tau) = -\frac{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau V(\tau)\right) c_\alpha(\tau) c_\beta^\dagger(0)\right\rangle^{(0)}}{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau V(\tau)\right)\right\rangle^{(0)}}$$

partition function:

$$\boxed{\frac{Z}{Z_0} = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_k \, \langle \mathcal{T}(V(\tau_1)\cdots V(\tau_k))\rangle^{(0)}}$$

$$\frac{Z}{Z_0} = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^k k!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_k \sum_{\alpha_1\beta_1\gamma_1\delta_1} \cdots \sum_{\alpha_k\beta_k\gamma_k\delta_k} U_{\alpha_1\beta_1\delta_1\gamma_1} \cdots U_{\alpha_k\beta_k\delta_k\gamma_k}$$
$$\times \langle \mathcal{T}(c_{\alpha_1}^\dagger(\tau_1) c_{\beta_1}^\dagger(\tau_1) c_{\gamma_1}(\tau_1) c_{\delta_1}(\tau_1) \cdots c_{\alpha_k}^\dagger(\tau_k) c_{\beta_k}^\dagger(\tau_k) c_{\gamma_k}(\tau_k) c_{\delta_k}(\tau_k))\rangle^{(0)}$$

matrix element:

$$\boxed{\langle \mathcal{T}(\cdots)\rangle^{(0)} = \{\text{sum over all fully contracted terms}\}} \quad \text{(Wick's theorem)}$$

remember: **contraction**

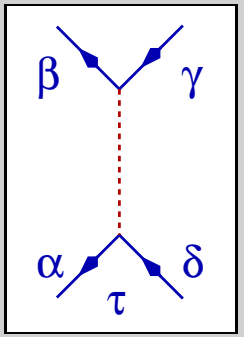
$$\boxed{\underline{c_{\alpha_i}(\tau_i) c_{\alpha_j}^\dagger(\tau_j)} = \langle \mathcal{T}(c_{\alpha_i}(\tau_i) c_{\alpha_j}^\dagger(\tau_j))\rangle^{(0)} = -G^{(0)}_{\alpha_i\alpha_j}(\tau_i - \tau_j)}$$

diagram elements

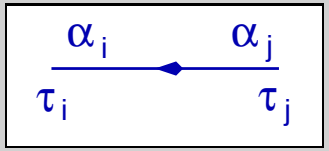
to compute the denominator, i.e. Z/Z_0

- consider the k-th term in the sum ("k-th order")
- evaluate the free expectation value using Wick's theorem for given orbital indices α_i, β_i, ... and given τ_i ($i = 1, ..., k$)
- organize the sum over all possible ways for full contractions by diagrams
- sum / integrate over all internal orbital indices and times

the building blocks of diagrams:

vertex at τ 

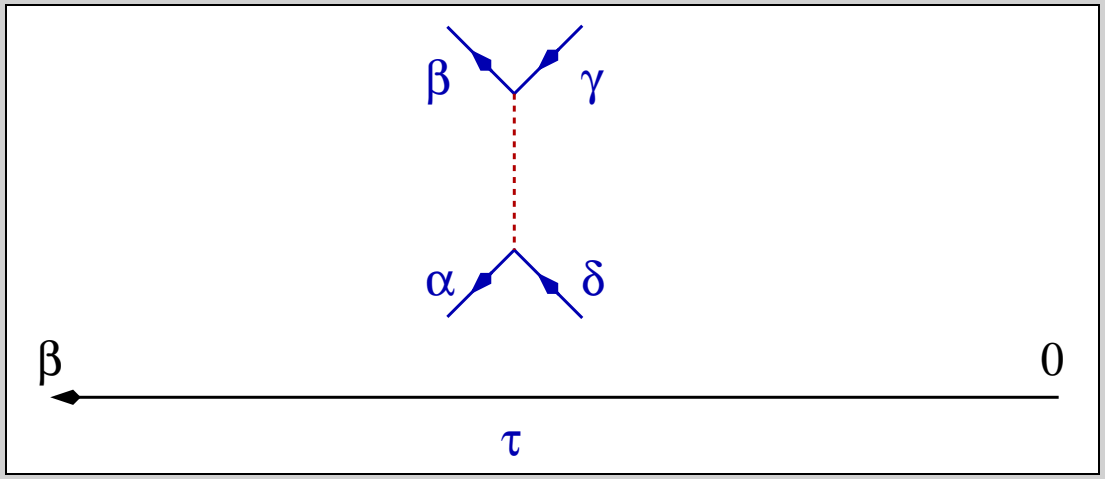
stands for $U_{\alpha_i \beta_i \delta_i \gamma_i}$

propagator 

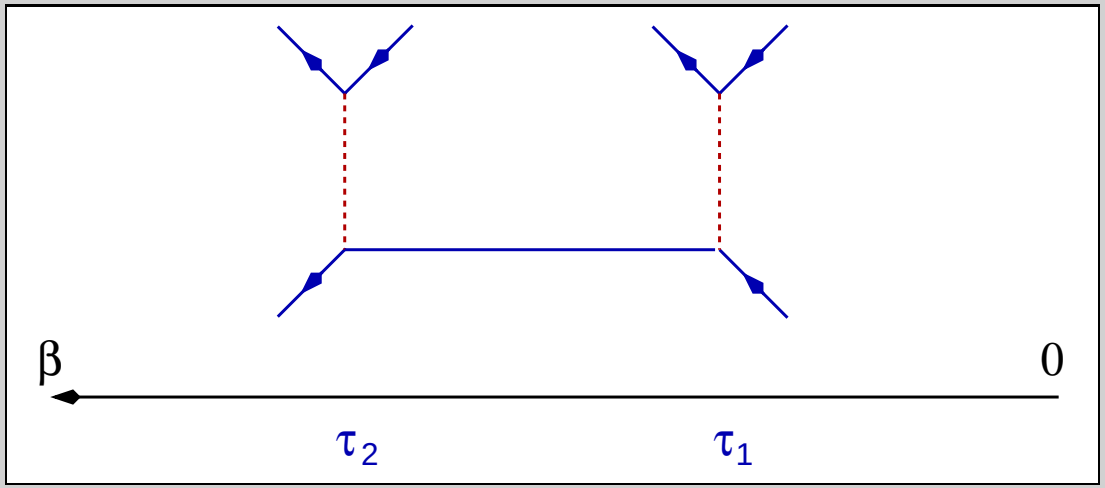
stands for a contraction, i.e. $-G^{(0)}_{\alpha_i \alpha_j}(\tau_i - \tau_j)$

building diagrams

Coulomb interaction is instanteneous ➜ place **vertex on a time axis:**



propagators connect two links at (the same or) different vertices:



full contractions

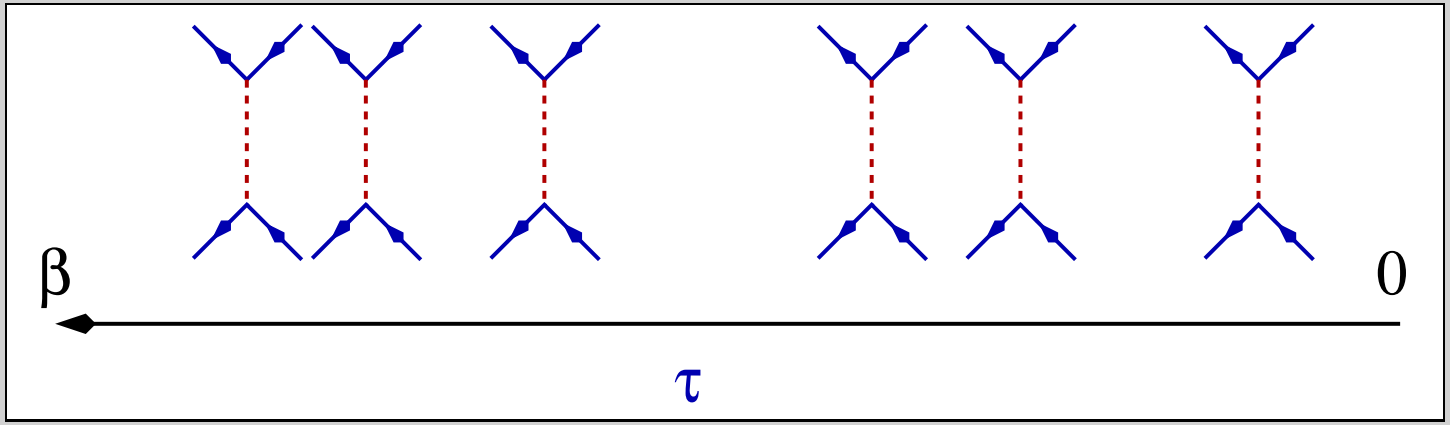
free expectation value (at k-th order):

$$\langle \mathcal{T}(c^\dagger_{\alpha_1}(\tau_1)c^\dagger_{\beta_1}(\tau_1)c_{\gamma_1}(\tau_1)c_{\delta_1}(\tau_1)\cdots c^\dagger_{\alpha_k}(\tau_k)c^\dagger_{\beta_k}(\tau_k)c_{\gamma_k}(\tau_k)c_{\delta_k}(\tau_k))\rangle^{(0)}$$

via Wick's theorem,

$$= \{\text{sum over all fully contracted terms}\}$$

represented by sum over all possible diagrams at k-th order



at the k-th order, there are $(2k)!$ different ways to connect the open links at the k vertices $(2k)!$ different possibilies for full contractions:

$(2k)!$ diagrams

all second-order diagrams

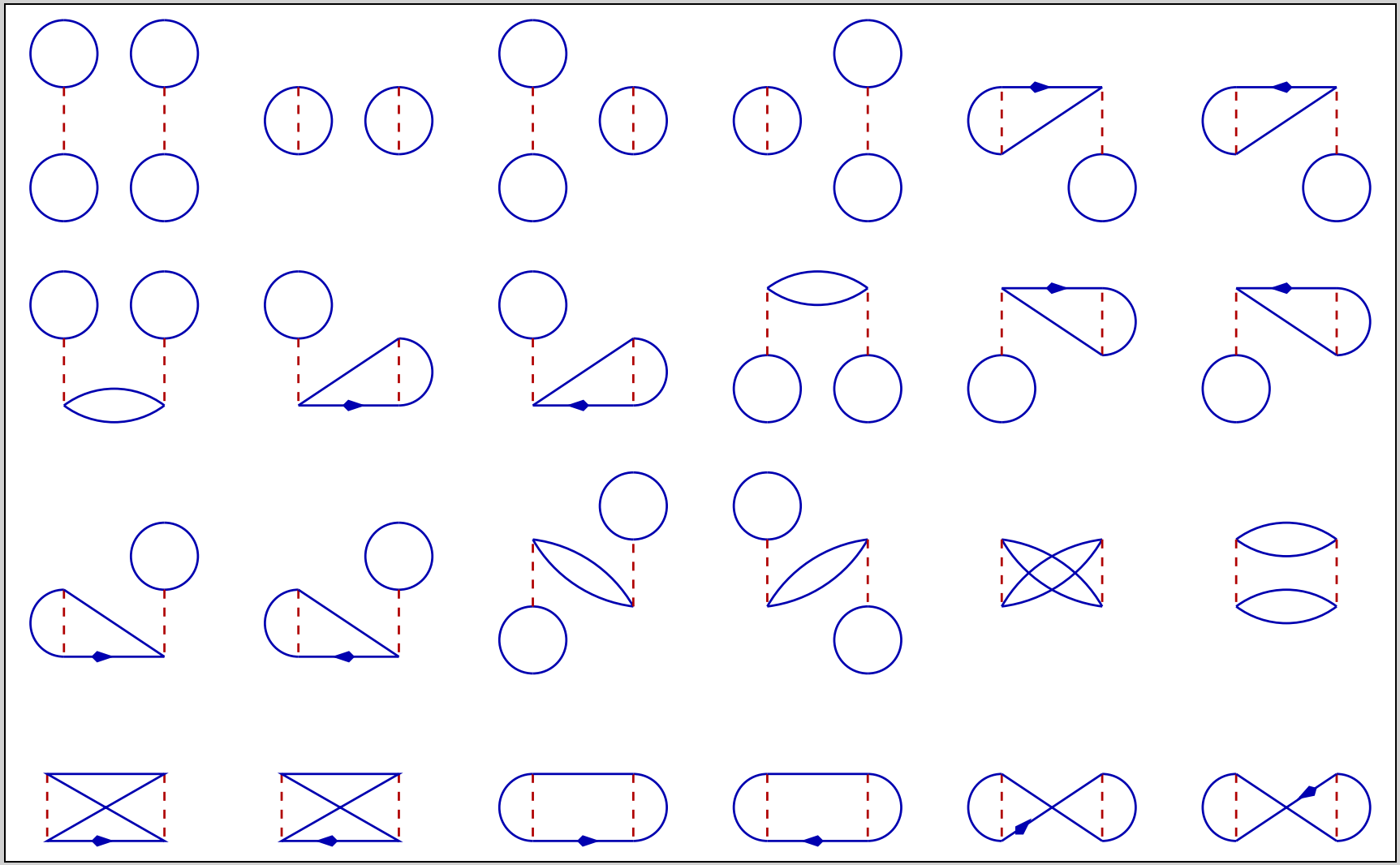
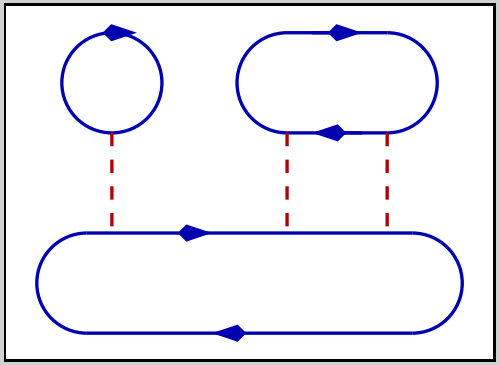


diagram rules

to compute the k-th order contribution to the denominator, i.e. to Z/Z_0,

- draw all $(2k)!$ different **diagrams** , **label** them with orbitals α_i and times τ_i vertices are fixed, propagators can be deformed
- for each **vertex** , write $U_{\alpha_i \beta_i \delta_i \gamma_i}$
- for each **propagator** , write $-G^{(0)}_{\alpha_i \alpha_j}(\tau_i - \tau_j)$
- for propagators starting and ending at the same vertex, i.e. **equal times** : $\tau_{\text{creator}} = \tau_{\text{annihilator}} + 0^+$
- **sum** over all orbital indices α_i, β_i, ...
- **integrate** over all τ_i $(i = 1, ..., k)$ from 0 to β
- multiply with the **factor** $\frac{(-1)^k}{2^k k!}$
- multiply with $(-1)^L$ with $L =$ number of fermion **loops**



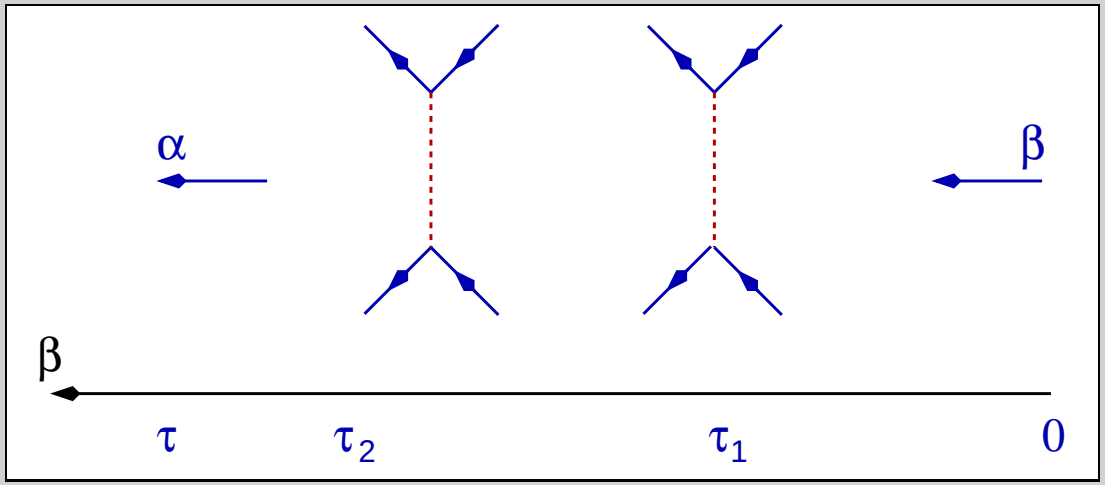
$L = 3$

diagrams for the Green's function

Green's function:

$$-G_{\alpha\beta}(\tau) = \frac{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau V(\tau)\right) c_\alpha(\tau) c_\beta^\dagger(0) \right\rangle^{(0)}}{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau V(\tau)\right) \right\rangle^{(0)}}$$

nominator:



additional fixed **external links** representing $c_\alpha(\tau)$ and $c_\beta^\dagger(0)$

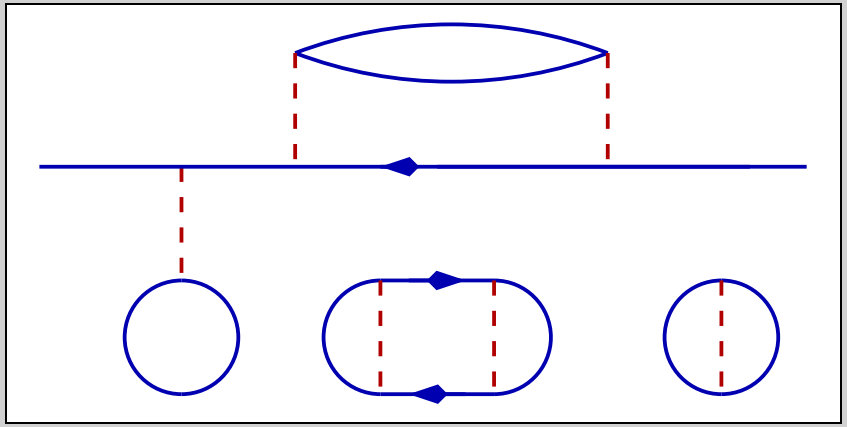
we have $2k+1$ propagators and thus

$(2k+1)!$ diagrams at the k-th order

note: **no summation / integration over external variables** , i.e. α, β and τ

connected diagrams

typical diagram contributing to the nominator:



➜ there is one part of the diagram connected to the external links

➜ there may be different disconnected parts

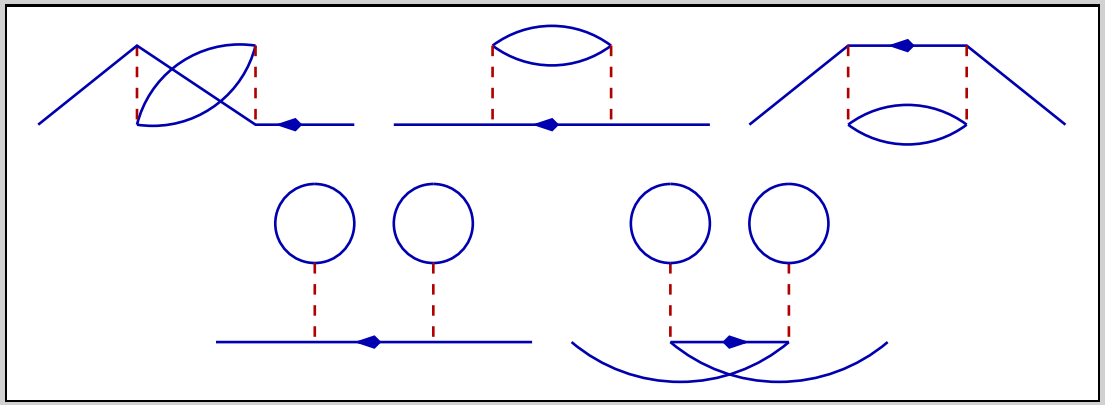
theorem:

the sum over the disconnected parts exactly cancels the denominator

- ✧ for any diagram part connected to the external links, one can add an arbitrary diagram representing Z/Z_0 (the denominator)
- ✧ its numerical value comes as a factor
- ✧ take care of combinatorics

topologically equal diagrams

consider:



the diagrams in each line are different but yield the same numerical value, since

A **flipping the vertex**

$$U_{\alpha\beta\delta\gamma} c^\dagger_\alpha c^\dagger_\beta c_\gamma c_\delta = U_{\beta\alpha\gamma\delta} c^\dagger_\beta c^\dagger_\alpha c_\delta c_\gamma$$

B **interchanging two vertices**

change of integration / summation variables $\tau_i \leftrightarrow \tau_j$ and $\alpha_i, \beta_i, ... \leftrightarrow \alpha_j, \beta_j, ...$

has no effect

$$\frac{Z}{Z_0} = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^k k!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_k \sum_{\alpha_1\beta_1\gamma_1\delta_1} \cdots \sum_{\alpha_k\beta_k\gamma_k\delta_k} U_{\alpha_1\beta_1\delta_1\gamma_1} \cdots U_{\alpha_k\beta_k\delta_k\gamma_k}$$
$$\times \langle \mathcal{T}(c^\dagger_{\alpha_1}(\tau_1) c^\dagger_{\beta_1}(\tau_1) c_{\gamma_1}(\tau_1) c_{\delta_1}(\tau_1) \cdots c^\dagger_{\alpha_k}(\tau_k) c^\dagger_{\beta_k}(\tau_k) c_{\gamma_k}(\tau_k) c_{\delta_k}(\tau_k)) \rangle^{(0)}$$

topologically equal diagrams

diagrams transforming into each other under A or B are **topologically equal**

➜ operation A generates 2^k different diagrams with the same value

➜ operation B generates $k!$ different diagrams with the same value

change the diagram rules in the following way:

– summation over topologically different diagrams only

– no additional factor $\dfrac{1}{2^k k!}$

all topologically different and connected diagrams at order $k = 0, 1, 2$:

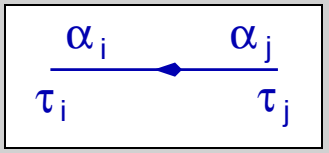
diagram rules

to compute the k-th order contribution to $-G_{\alpha\beta}(\tau)$,

- ✧ draw all topologically different **diagrams**
  label them with orbitals α_i and times τ_i
- ✧ diagrams must be connected to **external links**
  vertices and propagators can be deformed
- ✧ for each **vertex** , write $-U_{\alpha_i\beta_i\delta_i\gamma_i}$
- ✧ for each **propagator** , write $-G^{(0)}_{\alpha_i\alpha_j}(\tau_i - \tau_j)$
- ✧ for propagators starting and ending at the same vertex, i.e. **equal times** :
  $\tau_{\text{creator}} = \tau_{\text{annihilator}} + 0^+$
- ✧ **sum** over all orbital indices α_i, β_i, ...
- ✧ **integrate** over all τ_i ($i = 1, ..., k$) from 0 to β
- ✧ multiply with $(-1)^L$ with $L =$ number of fermion **loops**

frequency-dependent propagator

time-dependent propagator:



$$= -G^{(0)}_{\alpha_i\alpha_j}(\tau_i - \tau_j)$$

$$-G^{(0)}_{\alpha_i\alpha_j}(\tau_i - \tau_j) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n(\tau_i-\tau_j)}\left(-G_{\alpha_i\alpha_j}(i\omega_n)\right)$$

➜ a propagator is labelled by a single frequency

➜ sum over (internal) frequencies

attach $\frac{1}{\sqrt{\beta}}e^{-i\omega_n\tau_i}$ to vertex at which propagator ends

attach $\frac{1}{\sqrt{\beta}}e^{i\omega_n\tau_j}$ to vertex at which propagator starts

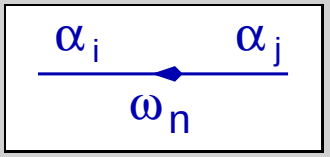
collecting factors, at each vertex we have:

$$\int_0^\beta d\tau \frac{1}{\sqrt{\beta}^4} e^{-i(\omega_1+\omega_2-\omega_3-\omega_4)\tau} = \frac{1}{\beta}\delta_{\omega_1+\omega_2,\omega_3+\omega_4}$$

energy conservation

“the sum of incoming frequencies equals the sum of outgoing frequencies”

frequency-dependent propagator:



$$= -G^{(0)}_{\alpha_i\alpha_j}(i\omega_n)$$

diagram rules for frequency-dependent Green's function

to compute the k-th order contribution to $-G_{\alpha\beta}(i\omega_n)$,

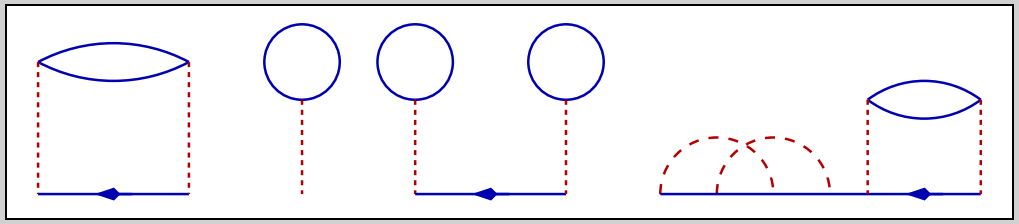
- draw all topologically different **diagrams**
  label them with orbitals α_i and frequencies ω_m
- diagrams must be connected to **external links**
  vertices and propagators can be deformed
- for each **vertex** , write $-\frac{1}{\beta}\delta_{\omega_\alpha+\omega_\beta,\omega_\gamma+\omega_\delta}U_{\alpha\beta\delta\gamma}$
- for each **propagator** , write $-G^{(0)}_{\alpha\beta}(i\omega_m)$
- for propagators starting and ending at the same vertex, **equal times** :
  factor $e^{-i\omega_m(\tau_{\rm annihilator}-\tau_{\rm creator})} = e^{i\omega_m 0^+}$
- **sum** over all internal orbital indices α, ...
- **sum** over all internal ω_m from $-\infty$ to ∞
- multiply with $(-1)^L$ with $L =$ number of fermion **loops**

Self-Energy

improper self-energy: diagrammatic definition

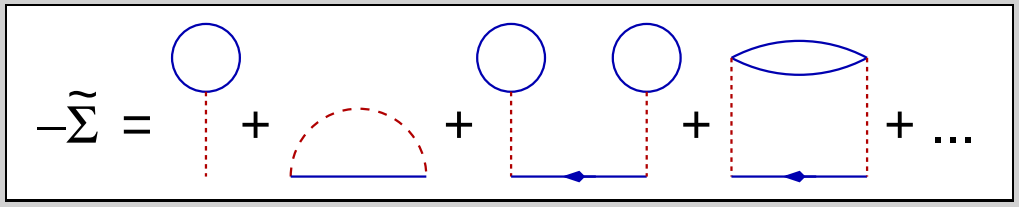
define **self-energy insertion** :

part of a diagram for the Green's function with two external links:



define **improper self-energy** :

sum of all self-energy insertions:



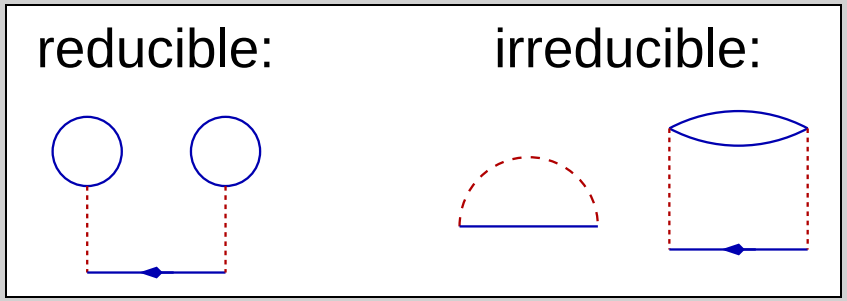
note: $-\widetilde{\Sigma}$ depends on external orbital indices and the external frequency:

$$\widetilde{\Sigma}_{\alpha\beta}(i\omega_n)$$

self-energy: definition

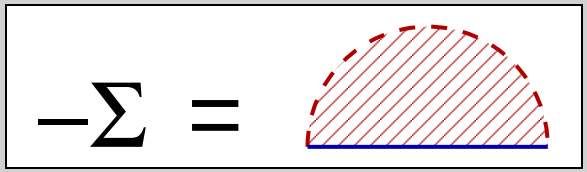
define **irreducible self-energy insertion:**

self-energy insertion that does not separate into two pieces when cutting a propagator:

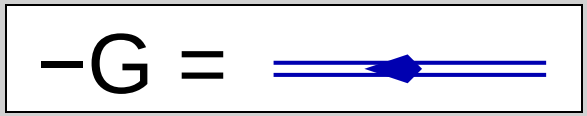


define **irreducible self-energy / proper self-energy / self-energy:**

sum of all irreducible self-energy insertions:

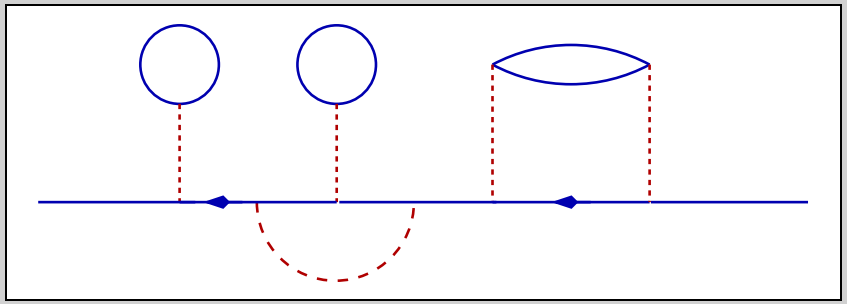


we also define the **full propagator / interacting propagator / Green's function:**



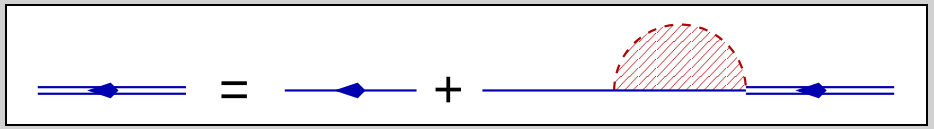
Dyson's equation, diagrammatic

consider an arbitrary diagram contributing to $-G_{\alpha\beta}(i\omega_n)$ with $k > 1$:



it necessarily starts (left) with a free propagator, followed by an irreducible self-energy insertion, and ends with a diagram contrubuting to $-G_{\alpha\beta}(i\omega_n)$

summing over all diagrams yields:



translation: $-G_{\alpha\beta}(i\omega_n) = -G^{(0)}_{\alpha\beta}(i\omega_n) + \sum_{\gamma\delta}(-G^{(0)}_{\alpha\gamma}(i\omega_n))(-\Sigma_{\gamma\delta}(i\omega_n))(-G_{\delta\beta}(i\omega_n))$

i.e.:

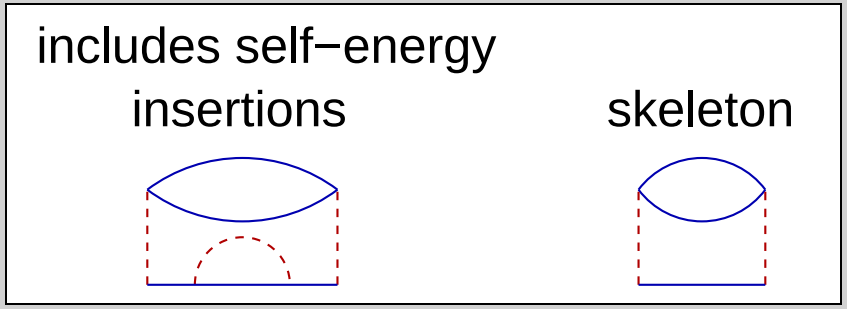
$$G_{\alpha\beta}(i\omega_n) = G^{(0)}_{\alpha\beta}(i\omega_n) + \sum_{\gamma\delta} G^{(0)}_{\alpha\gamma}(i\omega_n)\Sigma_{\gamma\delta}(i\omega_n)G_{\delta\beta}(i\omega_n)$$

Dyson's equation

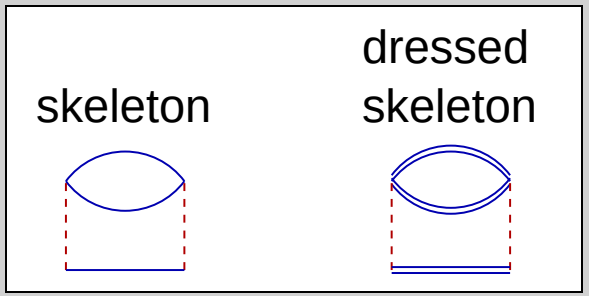
$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0\mathbf{\Sigma}\mathbf{G}$ (in matrix notation)

skeleton diagrams

a **skeleton diagram** is defined as a diagram without any self-energy insertions:



defined a **dressed skeleton** as a skeleton with free propagators replaced by full ones:

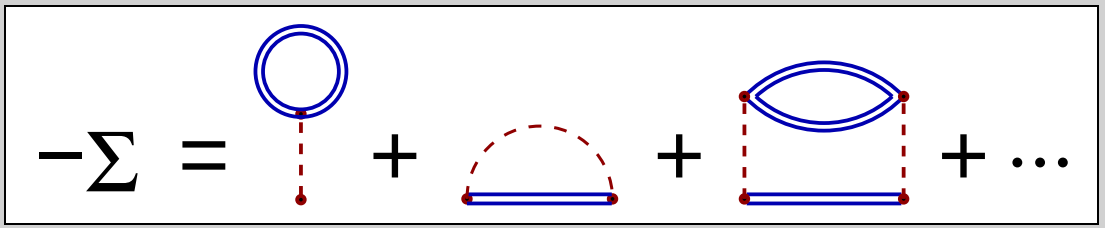


renormalization of diagrams

we have:

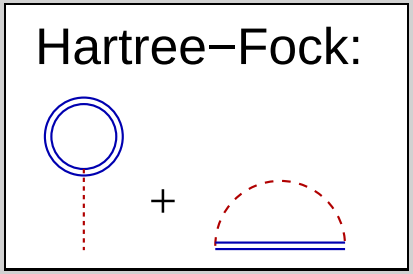
self-energy = sum over all dressed skeleton self-energy diagrams

skeleton-diagram expansion



skeleton-diagrams: first effective order

summing only the first-order diagrams:



yields the Hartree-Fock self-energy:

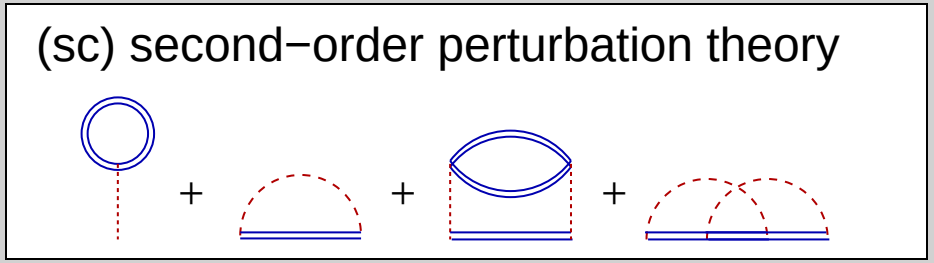
$$\Sigma^{(\mathrm{MF})}_{\alpha\beta} = \sum_{\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\gamma\alpha\beta\delta} \right) \langle c^\dagger_\gamma c_\delta \rangle'$$

Hartree-Fock self-energy

- the HF self-energy contains the full (HF) propagator
- self-consistency cycle: $\mathbf{G} \rightarrow \mathbf{\Sigma} \rightarrow \mathbf{G}$
- HF $=$ self-consistent first-order perturbation theory

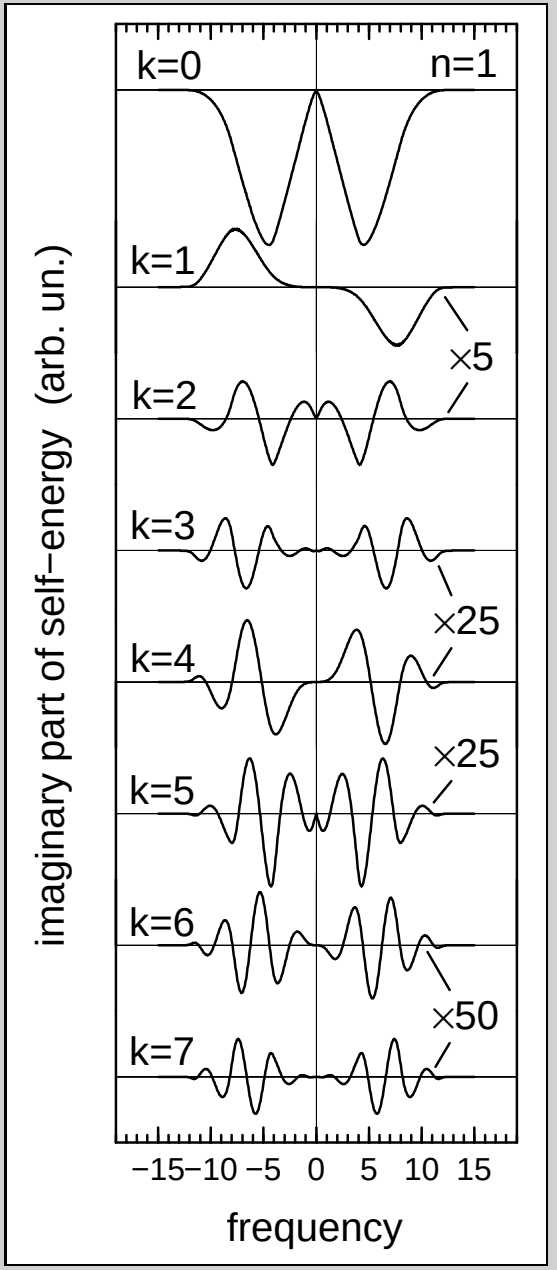
skeleton-diagrams: second effective order

summing the diagrams up to second (explicit) order:



infinitesimal retarded self-energy $\Sigma_{ij\sigma}(\omega + i0^+)$
for the Hubbard model at half-filling and $T = 0$
k labels the different shells, $\Sigma_{ij\sigma} = \Sigma_{i-j\sigma}$
$D = 2$ square lattice

discussion



summary and questions

systematic perturbation theory, leads to Green's functions

applicable to weak-coupling regime only

can we sum ALL diagrams ?

how to formulate a variational principle in terms of Green's functions ?

how to make use of such a variational principle ?

Luttinger-Ward Functional

expansion of the partition function

grand potential:

$$\Omega = -T \ln Z$$

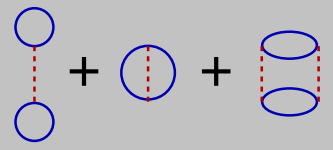
partition function:

$$Z = \mathrm{tr} e^{-\beta \mathcal{H}} = \mathrm{tr}(e^{-\beta \mathcal{H}_0} S(\beta, 0)) = Z_0 \langle S(\beta, 0) \rangle^{(0)}$$, $S(\beta, 0) = e^{\beta \mathcal{H}_0} e^{-\beta \mathcal{H}}$

from the solution of the equation of motion of the S-matrix, we have:

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \langle \mathcal{T}(V(\tau_1) \cdots V(\tau_n)) \rangle^{(0)}$$

with Wick's theorem, representation via diagrams:

$Z/Z_0 = 1 +$  $+ \cdots$

---

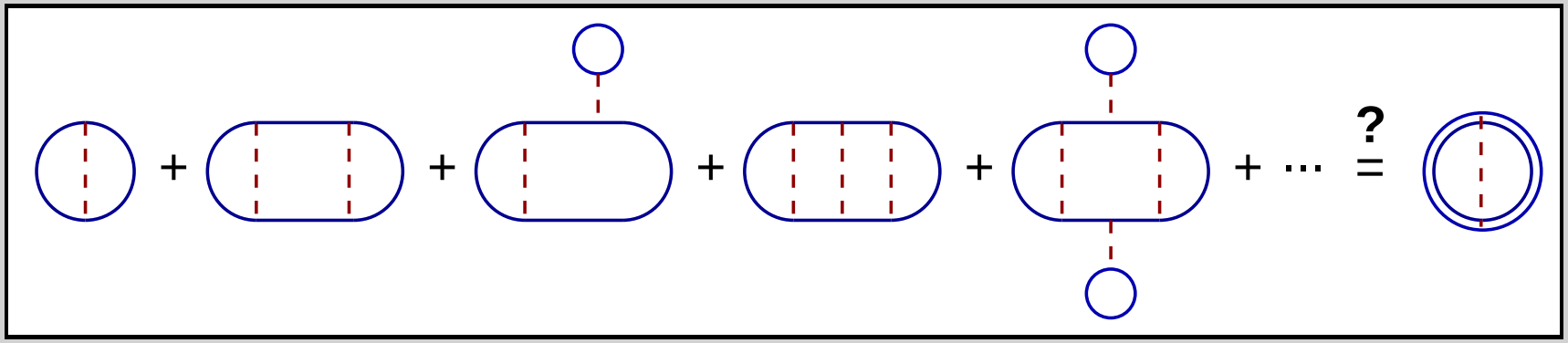
linked-cluster theorem: it is sufficient to consider connected diagrams only:

$$Z/Z_0 = \exp\left(\langle S(\beta, 0) \rangle^{(0)}_{\mathrm{conn.}} - 1 \right)$$

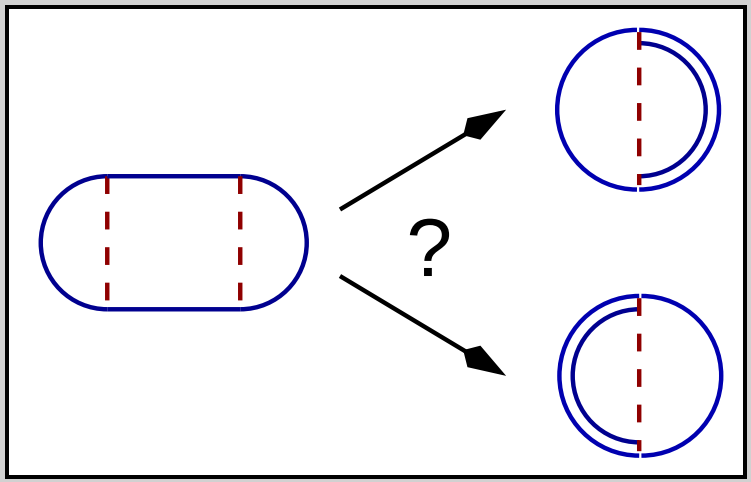
$$\Omega - \Omega_0 = -T \left(\langle S(\beta, 0) \rangle^{(0)}_{\mathrm{conn.}} - 1 \right)$$

renormalization?

partial summation of diagrams by renormalization of skeletons ?



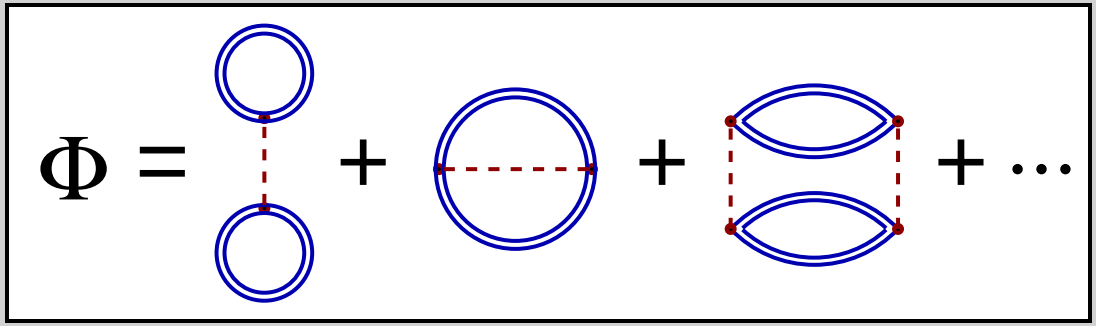
impossible because of double counting:



➜ sum of connected renormalized closed skeleton diagrams $\neq \ln Z$

Luttinger-Ward functional

define (with an additional factor $(-T)$):



Luttinger, Ward (1960)

note: $\Phi \neq -T \ln Z$

what is Φ good for ?

$$\boxed{\mathbf{\Sigma} = \frac{1}{T}\frac{\delta \Phi}{\delta \mathbf{G}}}$$ **IMPORTANT !!!**

Φ is like a potential for the self-energy !

---

proof:

note: $\boxed{\Phi = \widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]}$

– Φ is a functional of the Green's function

– the functional dependence is fixed by $\mathbf{U}$ (and independent of $\mathbf{t}$)

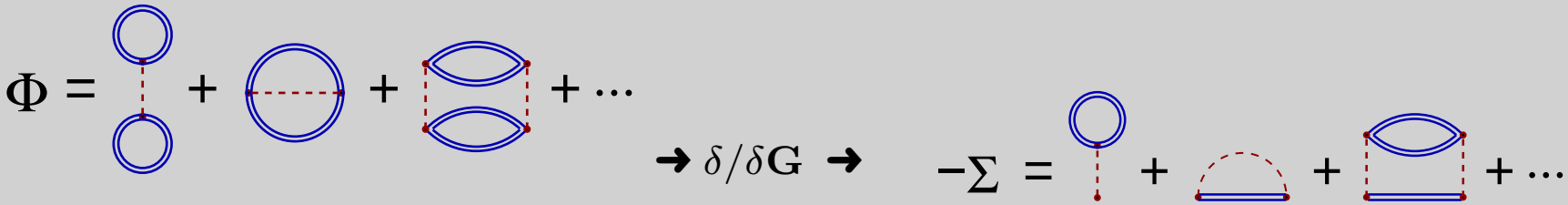
– $\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]$ is a **universal functional**

proof, continued

functional derivative $\delta/\delta\mathbf{G}$: removal of a propagator line

more precisely, we have to prove: $$\boxed{\Sigma_{\alpha\beta}(i\omega_n) = \frac{1}{T}\frac{\delta\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]}{\delta G_{\beta\alpha}(i\omega_n)}}$$

roughly:



q.e.d.

subtleties:

– the skeleton-diagram expansion yields $-\mathbf{\Sigma}$ (not $\mathbf{\Sigma}$)
– additional factor $(-T)$ in the definition of Φ
– removal of a fermion line ➜ factor (-1)
– $\delta/\delta\mathbf{G}$, but propagator is $-\mathbf{G}$ ➜ factor (-1)
– product rule: n terms in n-th order perturbation theory (treat all diagrams as different)
– $\alpha, \beta \to \beta, \alpha$: see rule for functional derivatives

we have:

$$\Sigma_{\alpha\beta}(i\omega_n) = \frac{1}{T}\frac{\delta\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]}{\delta G_{\beta\alpha}(i\omega_n)}$$

therewith, we can show that

$$\boxed{\Omega = -T\ln Z = \Phi + \mathrm{Tr}\ln\mathbf{G} - \mathrm{Tr}(\boldsymbol{\Sigma}\mathbf{G})}$$ **IMPORTANT !!!**

– here: $\mathrm{Tr}\,\mathbf{X} = T\sum_n e^{i\omega_n 0^+}\sum_\alpha X_{\alpha\alpha}(i\omega_n)$

– relation between static, thermodynamical quantity (Ω) and dynamic quantities ($\boldsymbol{\Sigma}$, $\mathbf{G}$)

– basic equation for dynamical variational principle (see below)

– double-counting correction: $\mathrm{Tr}\ln\mathbf{G} - \mathrm{Tr}(\boldsymbol{\Sigma}\mathbf{G})$

---

proof:

consider the derivative w.r.t. μ:

$$\frac{\partial}{\partial\mu}\left[\Phi + \mathrm{Tr}\ln\mathbf{G} - \mathrm{Tr}(\boldsymbol{\Sigma}\mathbf{G})\right] = (1) + (2) + (3)$$

first term:

$$\frac{\partial}{\partial\mu}(1) = \frac{\partial}{\partial\mu}\Phi = \frac{\partial}{\partial\mu}\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}] = \sum_{\alpha\beta}\sum_n \frac{\delta\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]}{\delta G_{\alpha\beta}(i\omega_n)}\frac{\partial G_{\alpha\beta}(i\omega_n)}{\partial\mu}$$

$$= \sum_{\alpha\beta} T\sum_n \Sigma_{\beta\alpha}(i\omega_n)\frac{\partial G_{\alpha\beta}(i\omega_n)}{\partial\mu} = \mathrm{Tr}\left(\boldsymbol{\Sigma}\frac{\partial\mathbf{G}}{\partial\mu}\right)$$

proof, continued

second term:

$$\frac{\partial}{\partial\mu}(2) = \frac{\partial}{\partial\mu}\mathsf{Tr}\ln\mathbf{G} = \mathsf{Tr}\left(\mathbf{G}^{-1}\frac{\partial\mathbf{G}}{\partial\mu}\right)$$

third term:

$$\frac{\partial}{\partial\mu}(3) = \frac{\partial}{\partial\mu}\mathsf{Tr}(\mathbf{\Sigma G}) = \mathsf{Tr}\left(\frac{\partial\mathbf{\Sigma}}{\partial\mu}\mathbf{G}\right) + \mathsf{Tr}\left(\mathbf{\Sigma}\frac{\partial\mathbf{G}}{\partial\mu}\right)$$

hence:

$$\boxed{\frac{\partial}{\partial\mu}\left[\Phi + \mathsf{Tr}\ln\mathbf{G} - \mathsf{Tr}(\mathbf{\Sigma G})\right] = \mathsf{Tr}\left(\mathbf{G}^{-1}\frac{\partial\mathbf{G}}{\partial\mu}\right) - \mathsf{Tr}\left(\frac{\partial\mathbf{\Sigma}}{\partial\mu}\mathbf{G}\right)}$$

$$= \mathsf{Tr}\left[\left(\mathbf{G}^{-1}\frac{\partial\mathbf{G}}{\partial\mu}\mathbf{G}^{-1} - \frac{\partial\mathbf{\Sigma}}{\partial\mu}\right)\mathbf{G}\right]$$

$$= \mathsf{Tr}\left[\frac{\partial(-\mathbf{G}^{-1} - \mathbf{\Sigma})}{\partial\mu}\mathbf{G}\right]$$

$$= -\mathsf{Tr}\left[\frac{\partial\mathbf{G}_0^{-1}}{\partial\mu}\mathbf{G}\right] \qquad \text{with Dyson's equation } \mathbf{G} = 1/(\mathbf{G}_0^{-1} - \mathbf{\Sigma})$$

$$= -\mathsf{Tr}\left[\frac{\partial(i\omega_n + \mu - \mathbf{t})}{\partial\mu}\mathbf{G}\right]$$

proof, continued

$$= -\mathrm{Tr}\,\mathbf{G}$$

$$= -\sum_\alpha T \sum_n e^{i\omega_n 0^+} G_{\alpha\alpha}(i\omega_n)$$

$$= \sum_\alpha \frac{1}{2\pi i} \oint_C d\omega\, e^{\omega 0^+} f(\omega)\, G_{\alpha\alpha}(\omega)$$

$$= \sum_\alpha \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega\, e^{\omega 0^+} f(\omega)\, G_{\alpha\alpha}(\omega + i0^+)$$

$$+ \sum_\alpha \frac{1}{2\pi i} \int_{\infty}^{-\infty} d\omega\, e^{\omega 0^+} f(\omega)\, G_{\alpha\alpha}(\omega - i0^+)$$

$$= \sum_\alpha \frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} d\omega\, e^{\omega 0^+} f(\omega)\, G_{\alpha\alpha}(\omega + i0^+)$$

$$= -\sum_\alpha \int_{-\infty}^{\infty} d\omega\, f(\omega)\, A_{\alpha\alpha}(\omega)$$

$$= -\langle N \rangle$$

$$\boxed{= \frac{\partial \Omega}{\partial \mu}}$$

proof, continued

so:

$$\boxed{\frac{\partial}{\partial \mu}\left[\Phi + \mathrm{Tr}\ln \mathbf{G} - \mathrm{Tr}(\mathbf{\Sigma G})\right] = \frac{\partial \Omega}{\partial \mu}}$$

$\mu \to -\infty$ ➜ no particles in the system ➜ setting $\mathbf{U} = 0$ is exact ➜ $\Phi, \mathbf{\Sigma} = 0$

for $\mu \to -\infty$:

$$\boxed{\mathrm{Tr}\ln \mathbf{G} = \Omega}$$ (exact representation of the non-interacting grand potential)

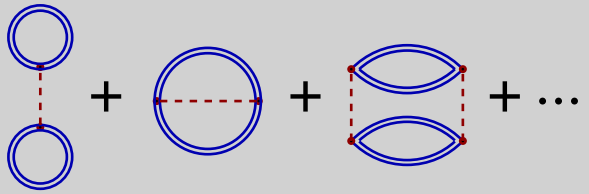
integrating over μ then yields:

$$\boxed{\Phi + \mathrm{Tr}\ln \mathbf{G} - \mathrm{Tr}(\mathbf{\Sigma G}) = \Omega}$$

q.e.d.

summary

Luttinger-Ward functional

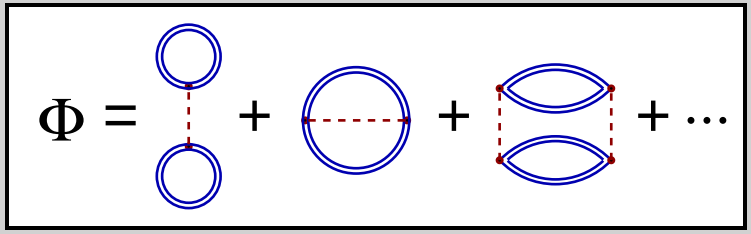
definition: $\Phi =$  $+ \cdots$

properties of the Luttinger-Ward functional:

- Φ is a functional: $\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]$
- domain of the functional: space of all Green's functions $\{\mathbf{G}_{\mathbf{t}',\mathbf{U}}\}$
- at the physical Green's function $\mathbf{G}_{\mathbf{t},\mathbf{U}}$ we have: $\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}_{\mathbf{t},\mathbf{U}}] = \Phi_{\mathbf{t},\mathbf{U}}$
- this quantity is related to the physical grand potential of the system via $\Omega_{\mathbf{t},\mathbf{U}} = \Phi_{\mathbf{t},\mathbf{U}} + \mathrm{Tr}\ln \mathbf{G}_{\mathbf{t},\mathbf{U}} - \mathrm{Tr}(\mathbf{\Sigma}_{\mathbf{t},\mathbf{U}}\mathbf{G}_{\mathbf{t},\mathbf{U}}) = \Omega$
- functional derivative: $\dfrac{1}{T}\dfrac{\delta\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]}{\delta\mathbf{G}} = \widehat{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}]$
- with a functional $\mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$ with the property $\widehat{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}_{\mathbf{t},\mathbf{U}}] = \mathbf{\Sigma}_{\mathbf{t},\mathbf{U}}$
- the functionals $\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]$ and $\widehat{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}]$ are universal
- $\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}] \equiv 0$ and $\widehat{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}] \equiv 0$ for $\mathbf{U} = 0$

conserving approximations

Luttinger-Ward functional



- defined via infinite summation of skeleton diagrams
- functional dependence unknown

conserving approximations *Baym, Kadanoff (1961)*

➜ approximate $\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}] \approx \widehat{\Phi}_{\mathbf{U}}^{(\mathrm{approx.})}[\mathbf{G}]$ by known functional $\widehat{\Phi}_{\mathbf{U}}^{(\mathrm{approx.})}[\mathbf{G}]$

➜ compute $\widehat{\mathbf{\Sigma}}_{\mathbf{U}}^{(\mathrm{approx.})}[\mathbf{G}] = \dfrac{1}{T}\dfrac{\delta\widehat{\Phi}_{\mathbf{U}}^{(\mathrm{approx.})}[\mathbf{G}]}{\delta\mathbf{G}}$

➜ solve $\mathbf{G} = \dfrac{1}{\mathbf{G}_0^{-1} - \widehat{\mathbf{\Sigma}}_{\mathbf{U}}^{(\mathrm{approx.})}[\mathbf{G}]}$ for $\mathbf{G}$ (self-consistently)

➜ evaluate $\widehat{\Omega}[\mathbf{G}] = \widehat{\Phi}[\mathbf{G}] + \mathrm{Tr}\ln\mathbf{G} - \mathrm{Tr}((\mathbf{G}_0^{-1} - \mathbf{G}^{-1})\mathbf{G})$

conserving approximations

advantages:

– thermodynamically consistent

– “conserving”: the approximation respects macrocopic conservation laws

– e.g. Luttinger’s theorem is respected (see below)

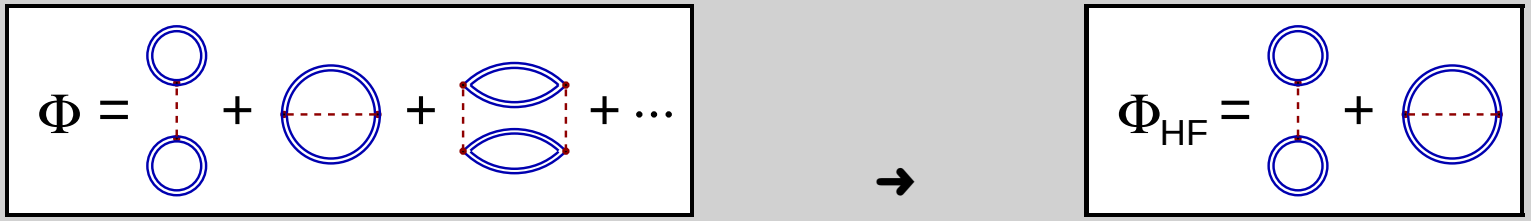
problem:

– the approximation is type-II

– approximation of a functional?

– only possibility: summation of certain clausses of diagrams

example:



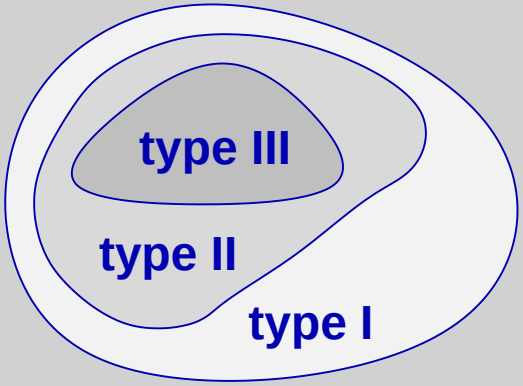
self-consistently weak-coupling perturbation theory

HF, RPA, FLEX, ...

Self-Energy Functional

approximation strategies

Hamiltonian: $H_{\mathbf{t},\mathbf{U}} = H_{\text{free}}(\mathbf{t}) + H_{\text{int}}(\mathbf{U})$
grand potential: $\Omega_{\mathbf{t},\mathbf{U}} = -T \ln \operatorname{tr} \exp(-\beta(H_{\mathbf{t},\mathbf{U}} - \mu N)$
physical quantity: $\mathbf{A}_{\mathbf{t},\mathbf{U}}$



functional: $\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}]$ on domain $\mathcal{D}$
variational principle: $\delta\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}] = 0$ für $\mathbf{A} = \mathbf{A}_{\mathbf{t},\mathbf{U}}$

Euler equation: $\mathbf{f}_{\mathbf{t},\mathbf{U}}[\mathbf{A}] = \dfrac{\delta\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}]}{\delta\mathbf{A}} \stackrel{!}{=} 0$

I	simplify Euler equation $\mathbf{f}_{\mathbf{t},\mathbf{U}}[\mathbf{A}] \to \widetilde{\mathbf{f}}_{\mathbf{t},\mathbf{U}}[\mathbf{A}]$	general
II	simplify functional $\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{A}] \to \widetilde{\Omega}_{\mathbf{t},\mathbf{U}}[\mathbf{A}]$	thermodynamically consistent
III	restict domain $\mathcal{D} \to \widetilde{\mathcal{D}}$	thermodynamically consistent, systematic, clear concept

the self-energy functional

define:

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \Phi_{\mathbf{U}}[\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}]] + \mathrm{Tr}\ln\frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}} - \mathrm{Tr}(\mathbf{\Sigma}\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}])$$

Potthoff (2003)

we have:

$$\frac{\delta}{\delta\Sigma_{\alpha\beta}(i\omega_n)}\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \mathrm{Tr}\left(\frac{\delta\Phi_{\mathbf{U}}[\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}]]}{\delta\mathbf{G}}\frac{\delta\mathbf{G}}{\delta\Sigma_{\alpha\beta}(i\omega_n)}\right) - \left(\frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}}\right)_{\beta\alpha}(i\omega_n)$$
$$-\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}]_{\beta\alpha}(i\omega_n) - \mathrm{Tr}\left(\mathbf{\Sigma}\frac{\delta\mathbf{G}}{\delta\Sigma_{\alpha\beta}(i\omega_n)}\right)$$

hence:

$$\delta\Omega_{\mathbf{t},\mathbf{U}} = 0 \Leftrightarrow \mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}] = \frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}}$$

- **exact conditional equation for self-energy**
- solution equivalent with summation of all diagrams !
- l.h.s.: $\mathbf{U}$-dependent functional of $\mathbf{\Sigma}$, functional dependence unknown
  r.h.s.: $\mathbf{t}$-dependent functional of $\mathbf{\Sigma}$, functional dependence trivial

Legendre transform

self-energy functional:

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \Phi_{\mathbf{U}}[\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}]] + \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}} - \mathrm{Tr}(\mathbf{\Sigma}\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}])$$

Legendre transformation, general:

given $f(x)$ with $y = \dfrac{df(x)}{dx} = y(x)$

define Legendre transform $g(y) = f(x(y)) - yx(y)$

we have: $\dfrac{dg(y)}{dy} = \dfrac{df(x(y))}{dx}\dfrac{dx(y)}{dy} - x(y) - y\dfrac{dx(y)}{dy} = -x(y)$

Legendre transformation of the Luttinger-Ward functional:

given $\Phi_{\mathbf{U}}[\mathbf{G}]$ with $\dfrac{1}{T}\dfrac{\delta\Phi_{\mathbf{U}}[\mathbf{G}]}{\delta\mathbf{G}} = \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$

Legendre transform: $F_{\mathbf{U}}[\mathbf{\Sigma}] = \Phi_{\mathbf{U}}[\mathbf{G}[\mathbf{\Sigma}]] - \mathrm{Tr}(\mathbf{\Sigma}\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}])$

we have: $\dfrac{1}{T}\dfrac{\delta F_{\mathbf{U}}[\mathbf{\Sigma}]}{\delta\mathbf{\Sigma}} = -\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}]$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}} + F_{\mathbf{U}}[\mathbf{\Sigma}]$$

first term: $\mathbf{t}$-dependent, trivial functional dependence

second term: $\mathbf{U}$-dependent, unknown functional dependence (“universal”)

variational approaches

$\delta\Omega[\mathbf{\Sigma}] = 0$	self-energy	**SFT**		

variational approaches

$\delta\Omega[\mathbf{\Sigma}] = 0$	self-energy	**SFT**		**dynamic**
$\delta\Omega[\mathbf{G}] = 0$	Green's function	**Luttinger Ward**		**dynamic**

variational approaches

$\delta\Omega[\mathbf{\Sigma}] = 0$	self-energy	**SFT**		**dynamic**
$\delta\Omega[\mathbf{G}] = 0$	Green's function	**Luttinger Ward**		**dynamic**
$\delta\Omega[\mathbf{n}] = 0$	electron density	**DFT**		**static**
$\delta\Omega[\rho] = 0$	density matrix	**Rayleigh Ritz**		**static**

variational approaches

$\delta\Omega[\mathbf{\Sigma}] = 0$	self-energy	**SFT**		**dynamic**
$\delta\Omega[\mathbf{G}] = 0$	Green's function	**Luttinger Ward**	**perturbation theory**	**dynamic**
$\delta\Omega[\mathbf{n}] = 0$	electron density	**DFT**	**LDA**	**static**
$\delta\Omega[\rho] = 0$	density matrix	**Rayleigh Ritz**	**Hartree-Fock, Gutzwiller, VMC, ...**	**static**

variational approaches

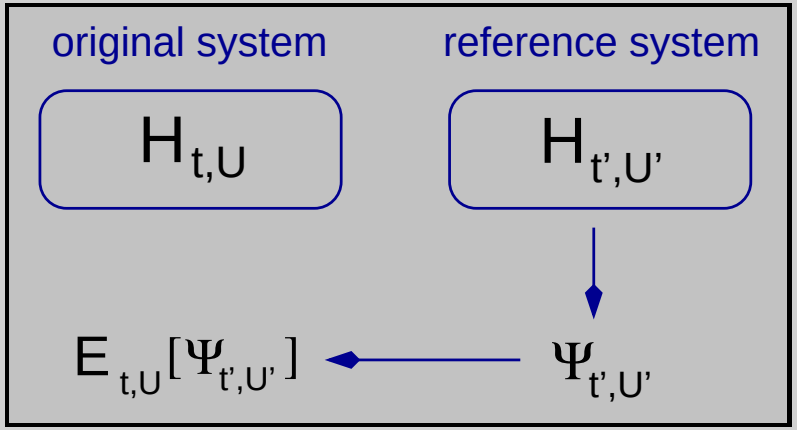
$\delta\Omega[\mathbf{\Sigma}] = 0$	self-energy	**SFT**	**new approximations?**	**dynamic**
$\delta\Omega[\mathbf{G}] = 0$	Green's function	**Luttinger Ward**	**perturbation theory**	**dynamic**
$\delta\Omega[\mathbf{n}] = 0$	electron density	**DFT**	**LDA**	**static**
$\delta\Omega[\rho] = 0$	density matrix	**Rayleigh Ritz**	**Hartree-Fock, Gutzwiller, VMC, ...**	**static**

$H = \sum_j (-\nabla_j^2/2 + v(\mathbf{r}_j)) + \frac{1}{2}\sum_{jk}{}' \frac{1}{\lvert\mathbf{r}_j - \mathbf{r}_k\rvert}$	$H = \sum_{\alpha\beta} t_{\alpha\beta}\, c_\alpha^\dagger c_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma}\, c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$
density-functional theory (DFT)	**self-energy-functional theory (SFT)**
external potential $v(\mathbf{r})$ density $n(\mathbf{r})$ ground-state densities $n = n[v]$ ground-state energy $E = E[n]$ $E[n] = \int v(\mathbf{r}) n(\mathbf{r}) + F[n]$ $\int v\, n$: explicit $F[n]$: unknown, universal (v-independent) variational principle: $\delta E[n] = 0$ exact but not explicit	hopping $\mathbf{t}$ self-energy $\Sigma_{\alpha\beta}(i\omega)$ t-representable self-energies $\mathbf{\Sigma} = \mathbf{\Sigma}[\mathbf{t}]$ grandcanonical potential $\Omega = \Omega[\mathbf{\Sigma}]$ $\Omega[\mathbf{\Sigma}] = \mathrm{Tr}\ln(\mathbf{G}_0^{-1} - \mathbf{\Sigma})^{-1} + F[\mathbf{\Sigma}]$ $\mathrm{Tr}\ln(\mathbf{G}_0^{-1} - \mathbf{\Sigma})^{-1}$: explicit $F[\mathbf{\Sigma}]$: unknown, universal ($\mathbf{t}$-independent) variational principle: $\delta\Omega[\mathbf{\Sigma}] = 0$ exact but not explicit
local-density approximation (LDA)	**different approximations**
reference system: homogeneous electron gas approximate functional F	different reference systems functional F on restricted domain

Reference System and Evaluation of the SFT

reference system

Ritz variational principle



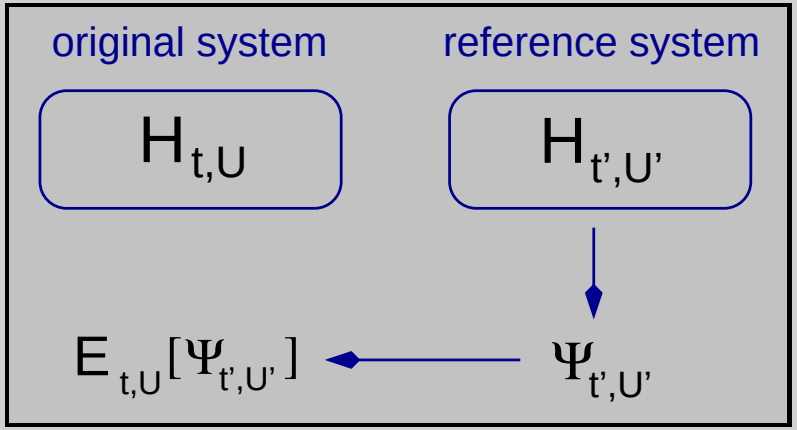
$$E_{\mathbf{t},\mathbf{U}}[|\Psi\rangle] = \langle\Psi|H_{\mathbf{t},\mathbf{U}}|\Psi\rangle$$

$$\frac{\partial E_{\mathbf{t},\mathbf{U}}[|\Psi_{\mathbf{t}',\mathbf{U}'=0}\rangle]}{\partial \mathbf{t}'} \stackrel{!}{=} 0$$

➜ **Hartree-Fock approximation**

reference system

Ritz variational principle

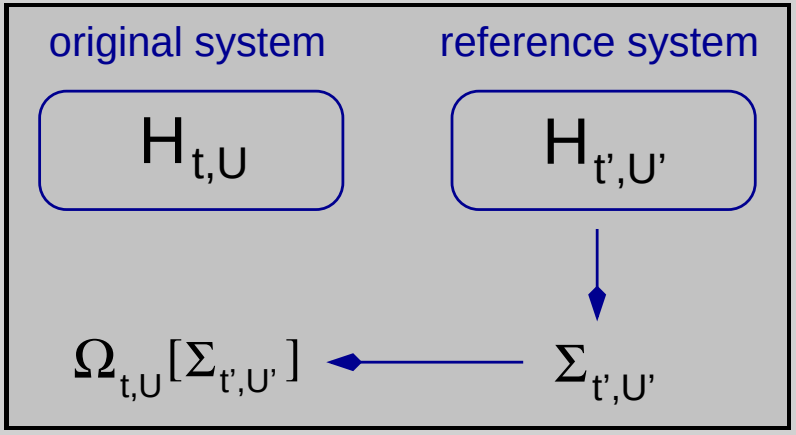


$$E_{\mathbf{t},\mathbf{U}}[|\Psi\rangle] = \langle\Psi|H_{\mathbf{t},\mathbf{U}}|\Psi\rangle$$

$$\frac{\partial E_{\mathbf{t},\mathbf{U}}[|\Psi_{\mathbf{t}',\mathbf{U}'=0}\rangle]}{\partial \mathbf{t}'} \stackrel{!}{=} 0$$

➜ **Hartree-Fock approximation**

SFT



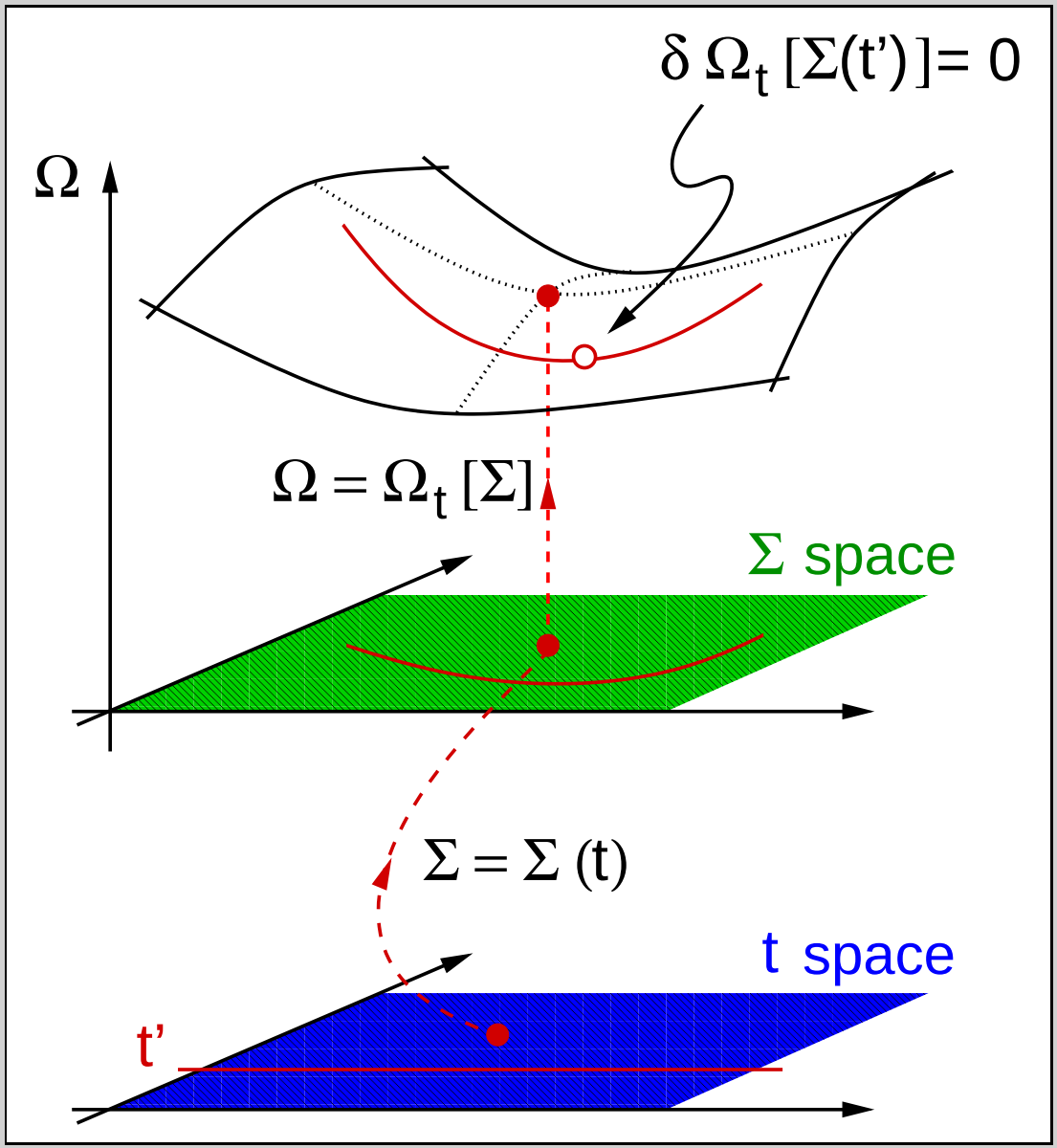
$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \textbf{?}$$

$$\frac{\partial \Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}'}]}{\partial \mathbf{t}'} \stackrel{!}{=} 0$$

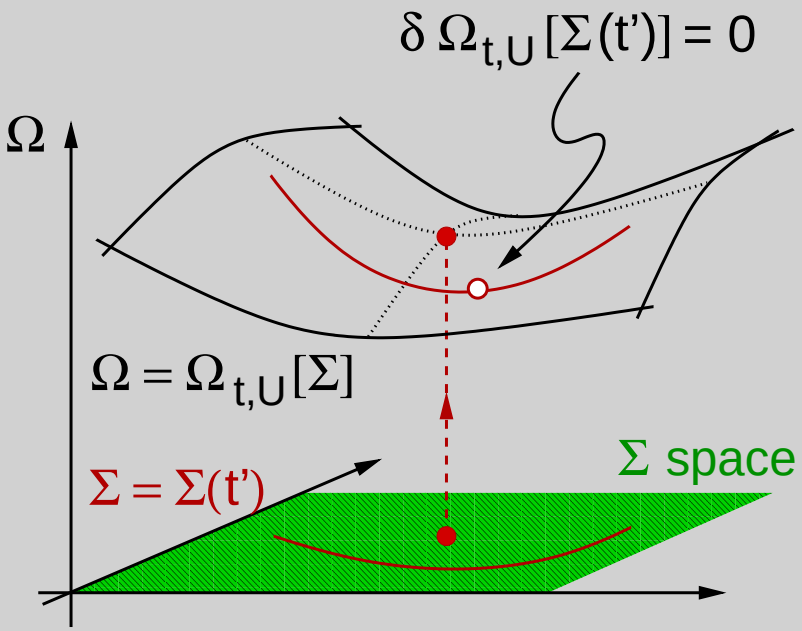
➜ **new approximations ?**

type of approximation $\Leftrightarrow$ choice of reference system

SFT



evaluation of the self-energy functional



$F_U[\mathbf{\Sigma}]$ unknown but **universal**!

original system:

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{0,\mathbf{t}} - \mathbf{\Sigma}} + F_U[\mathbf{\Sigma}]$$

reference system:

$$\Omega_{\mathbf{t}',\mathbf{U}}[\mathbf{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{0,\mathbf{t}'} - \mathbf{\Sigma}} + F_U[\mathbf{\Sigma}]$$

combination:

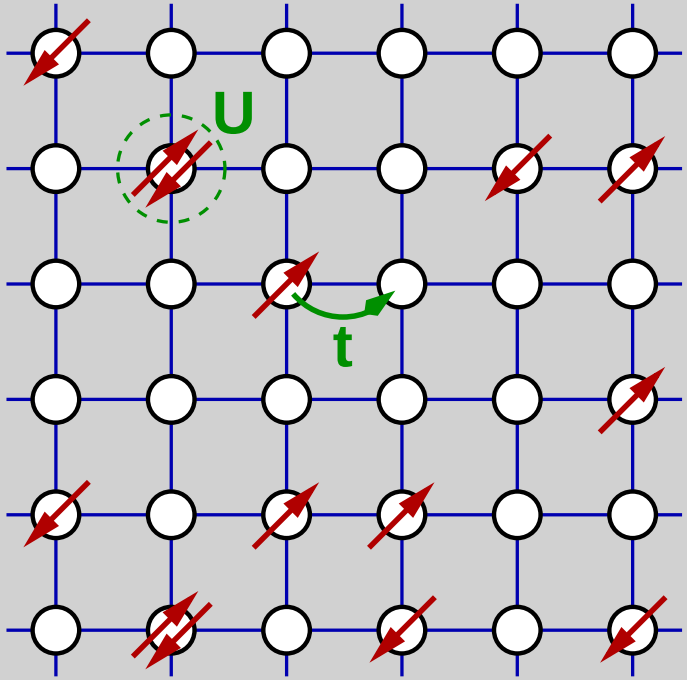
$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \Omega_{\mathbf{t}',\mathbf{U}}[\mathbf{\Sigma}] + \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{0,\mathbf{t}} - \mathbf{\Sigma}} - \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{0,\mathbf{t}'} - \mathbf{\Sigma}}$$

➜ **non-perturbative, thermodynamically consistent, systematic approximations**

Potthoff (2003)

cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:

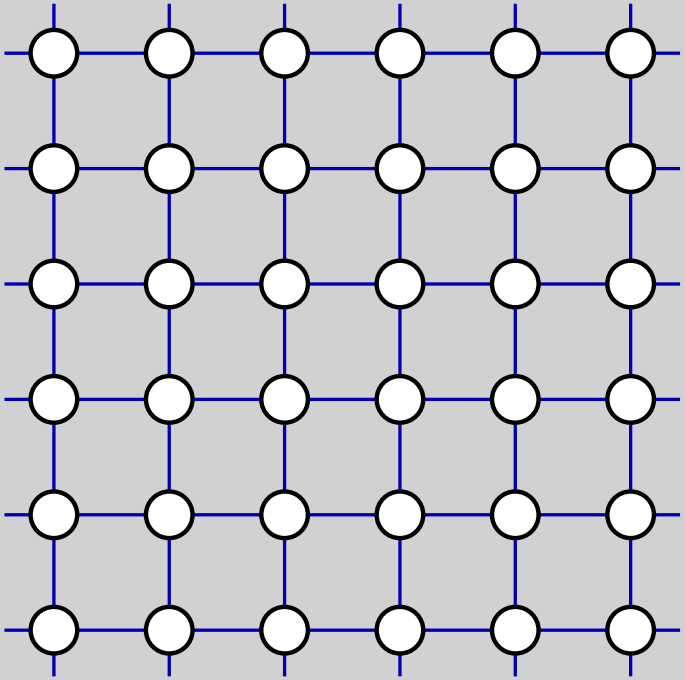


lattice model ($D = 2$) in
the thermodynamic limit

n.n. hopping: t
local interaction: U
electron density : $n = N/L$

cluster approximations

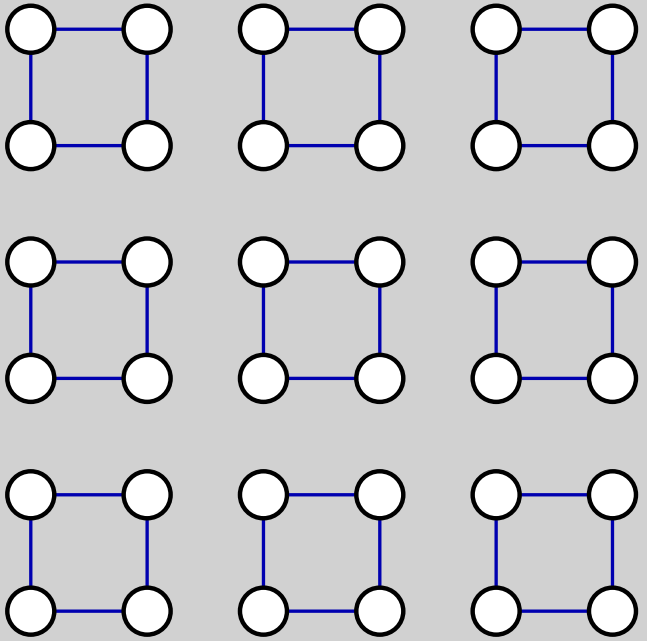
original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

n.n. hopping: t
local interaction: U
electron density : $n = N/L$

reference system, $H_{\mathbf{t}',\mathbf{U}}$:

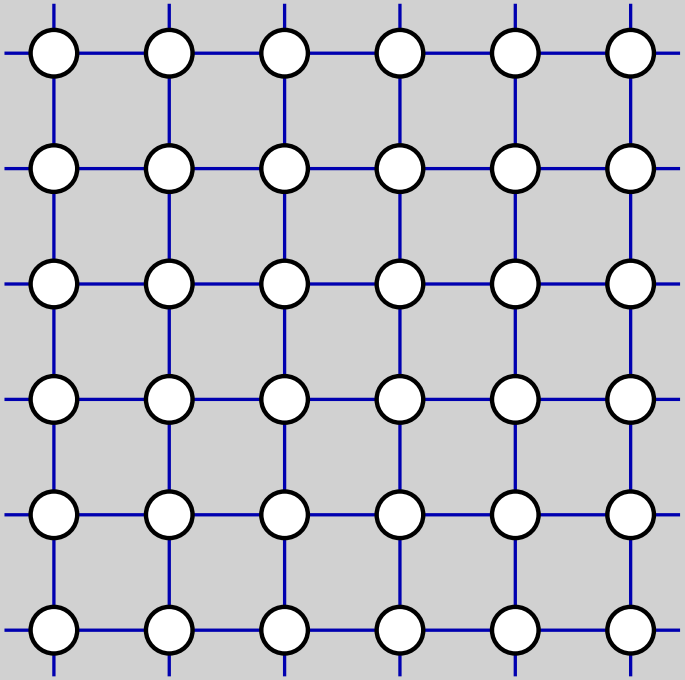


system of decoupled clusters

➜ diagonalization
➜ trial self-energy: $\mathbf{\Sigma} = \mathbf{\Sigma}(\mathbf{t}')$
➜ self-energy functional: $\Omega_{\mathbf{t}}[\mathbf{\Sigma}(\mathbf{t}')]$
stationary point: $\dfrac{\partial}{\partial \mathbf{t}'}\Omega_{\mathbf{t}}[\mathbf{\Sigma}(\mathbf{t}')] = 0$

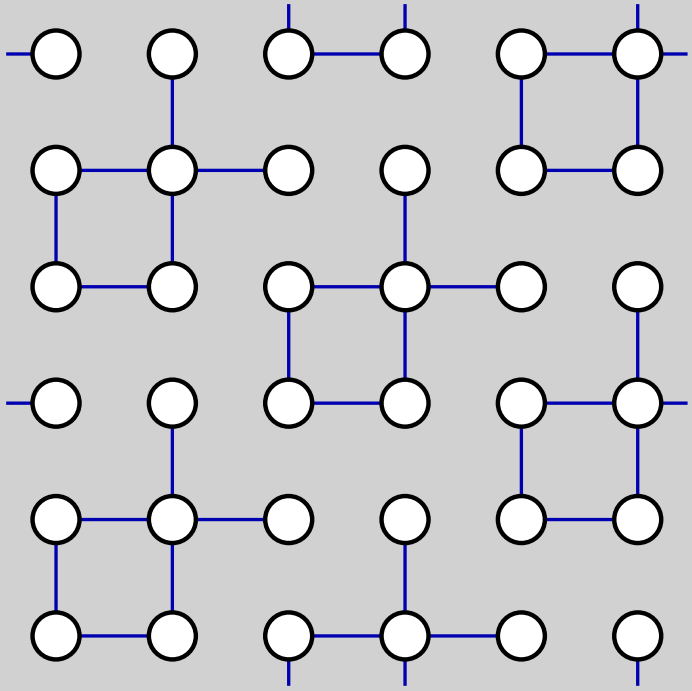
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

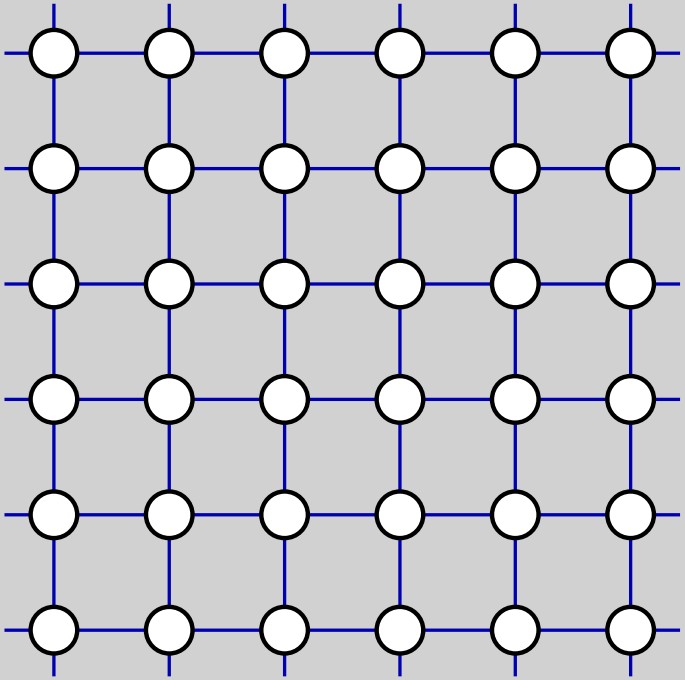
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

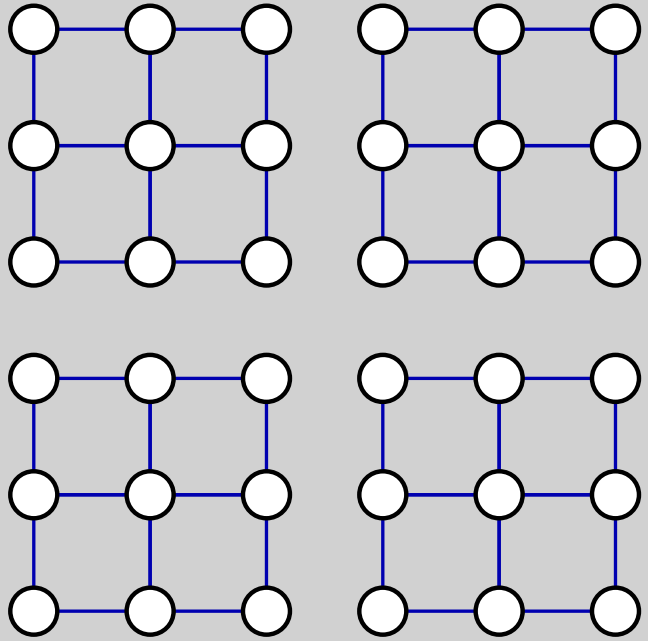
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

reference system, $H_{\mathbf{t}',\mathbf{U}}$:

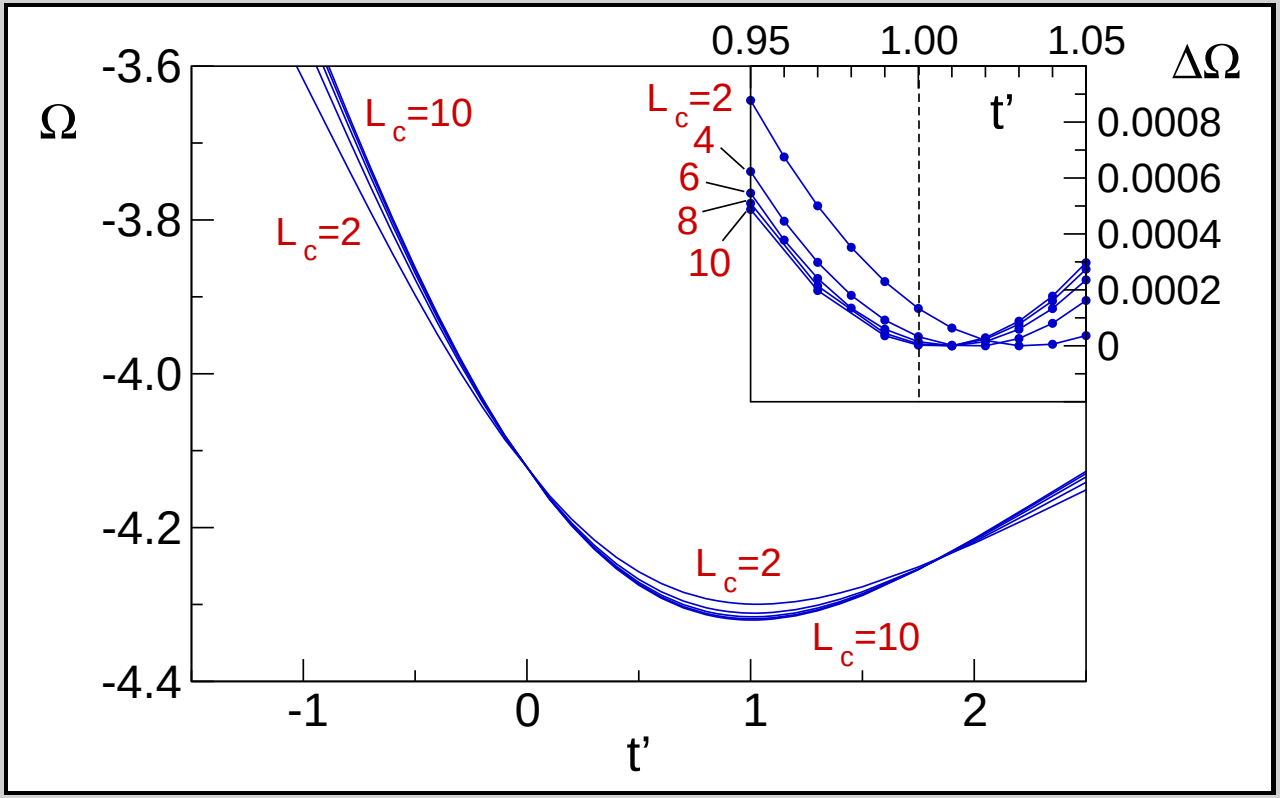


system of decoupled clusters
cluster size: L_c
$L_c \leq 2$: analytic
$L_c \leq 6$: exact diagonalization
$L_c \leq 12$: Lanczos method
$L_c \leq 100$: stochastic techniques

example: $D = 1$ Hubbard model

$T = 0$, half-filling, $U = 8$, nearest-neighbor hopping $t = 1$

variational parameter: nearest-neighbor hopping t' within the chain



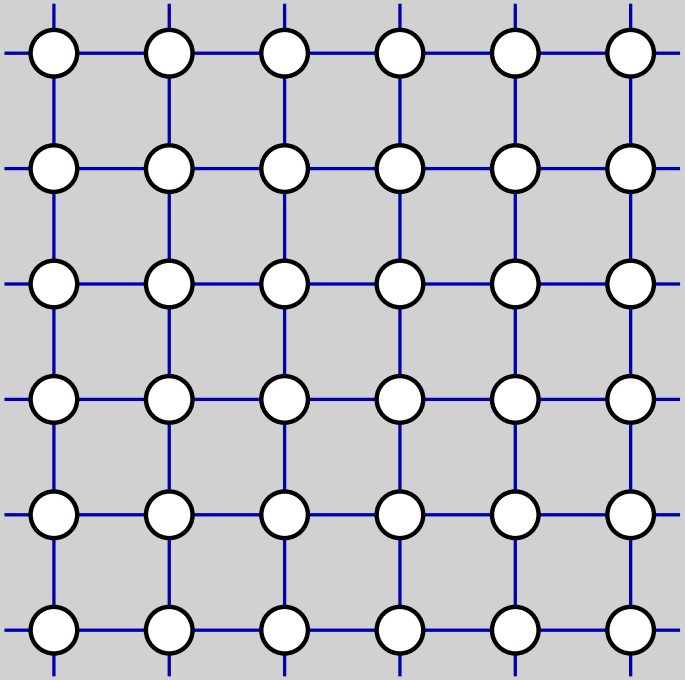
➜ $\Omega(t') \equiv \Omega[\mathbf{\Sigma}(t')]$ **stationary at** $t'_{\rm min} \neq t$

➜ $t' = 0$**: cluster size irrelevant**

➜ $t'_{\rm min} \approx t$

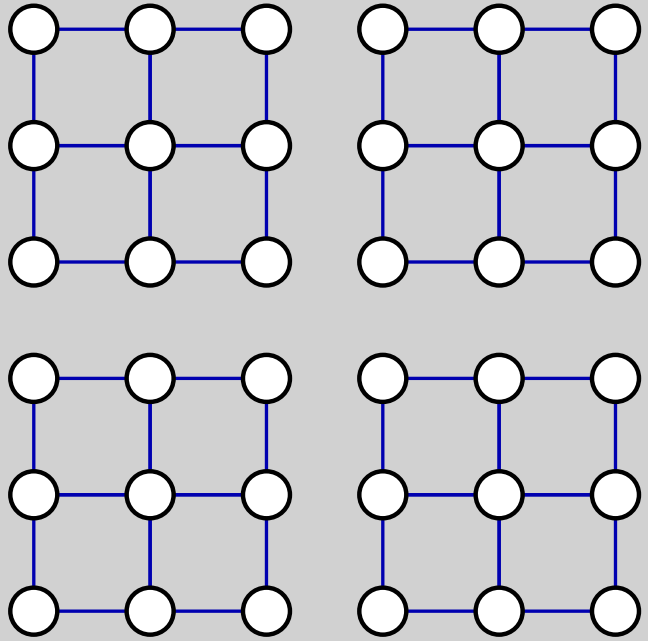
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

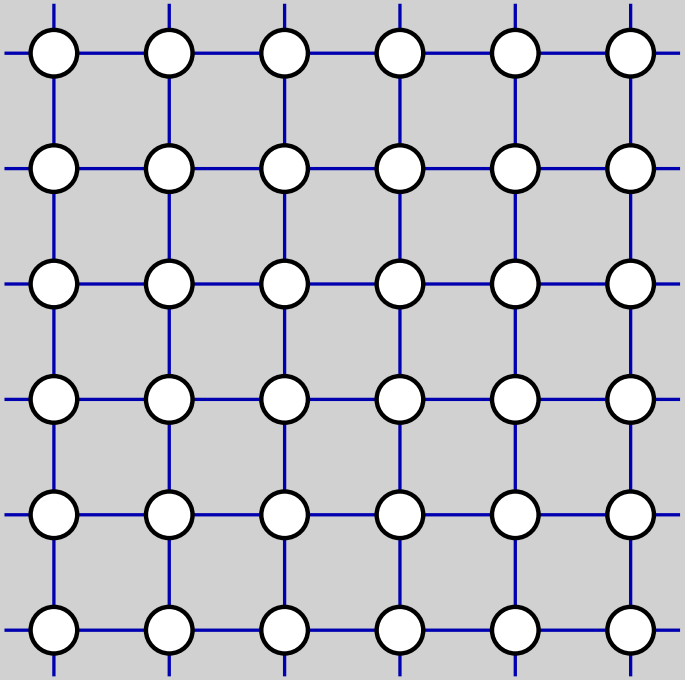
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

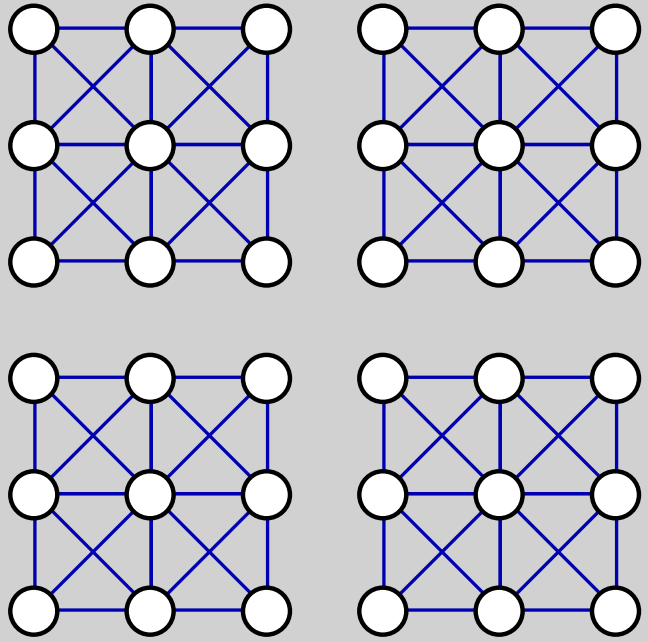
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

reference system, $H_{\mathbf{t}',\mathbf{U}}$:

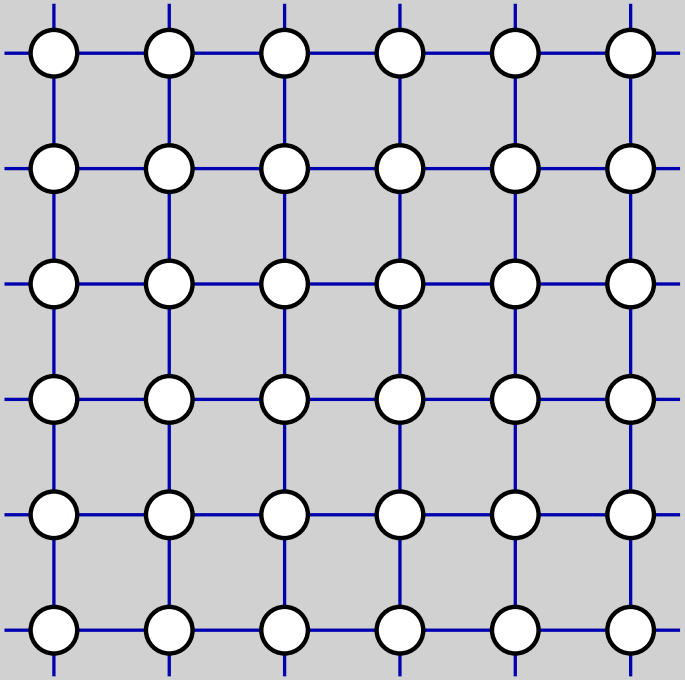


system of decoupled clusters

variational parameters:
intra-cluster hopping
partial compensation of
finite-size effects

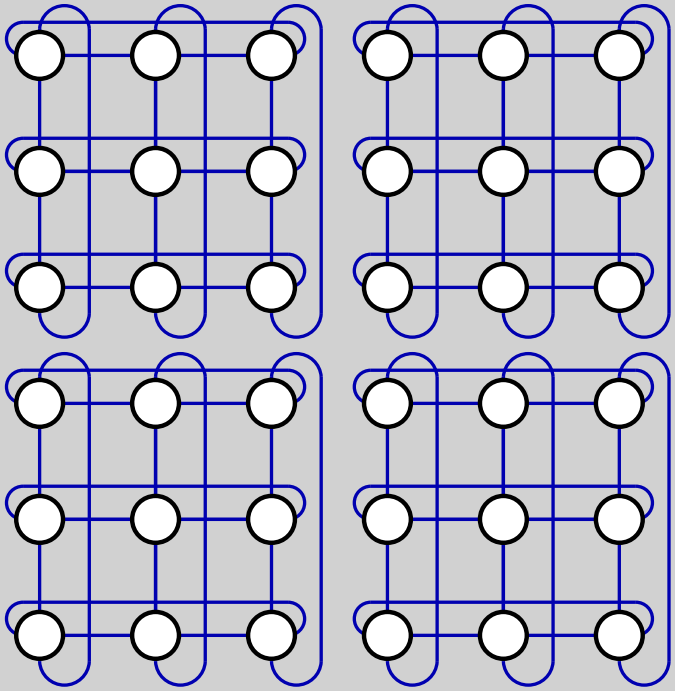
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

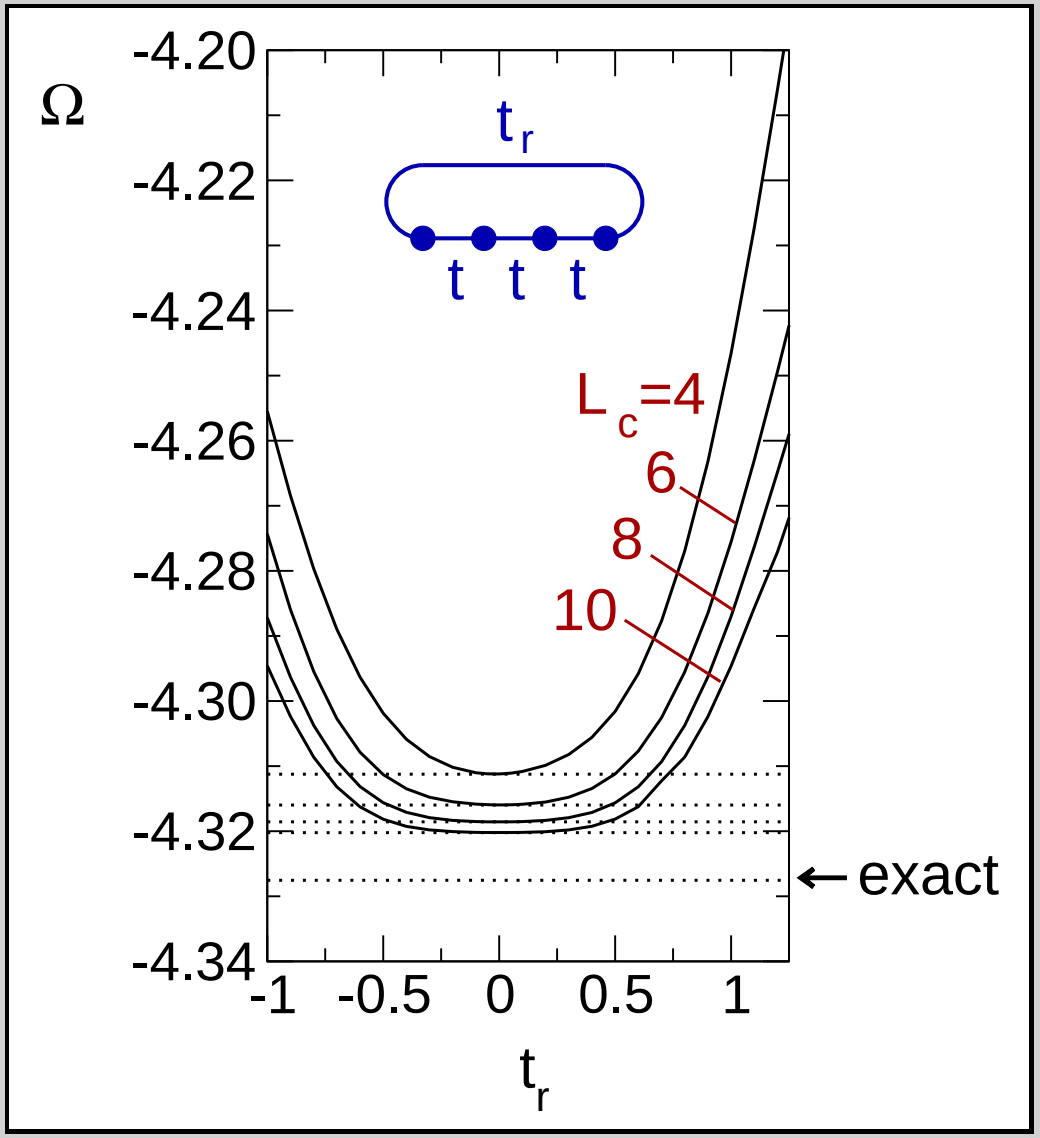
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

variational parameters:
hopping between cluster boundaries
boundary conditions

boundary conditions



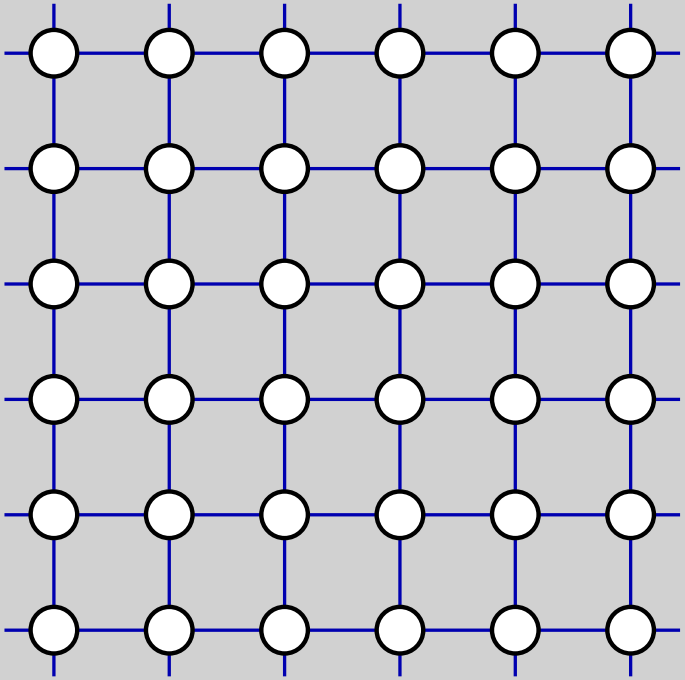
exact: *Lieb, Wu (1968)*

$D = 1$ Hubbard model
$T = 0$, half-filling, $U = 8$
$t = 1$

open or periodic b.c. ?
open boundary conditions !

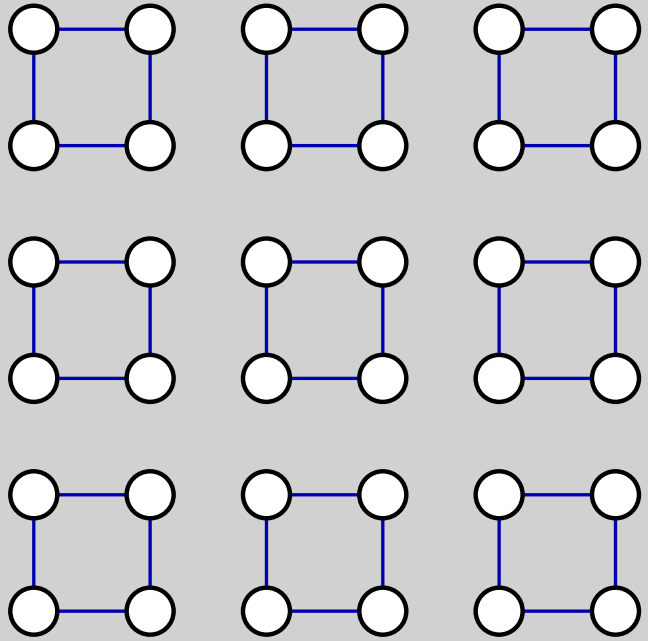
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

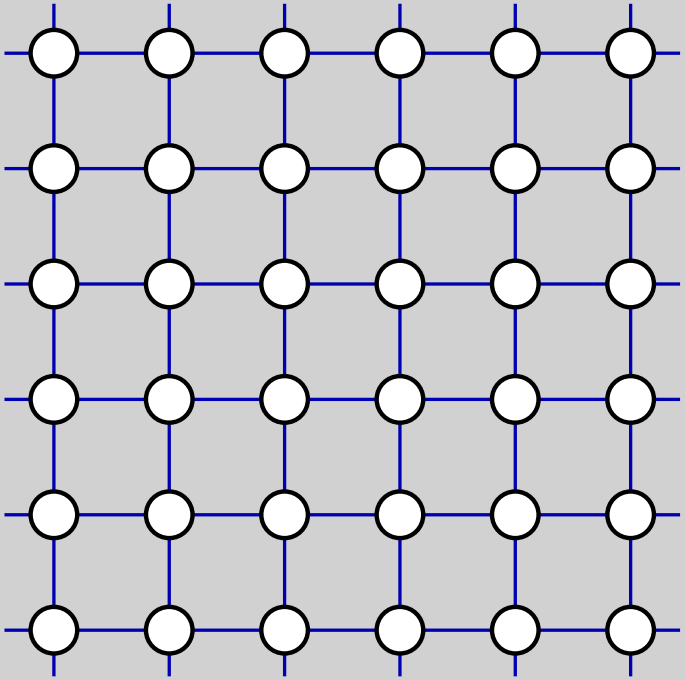
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

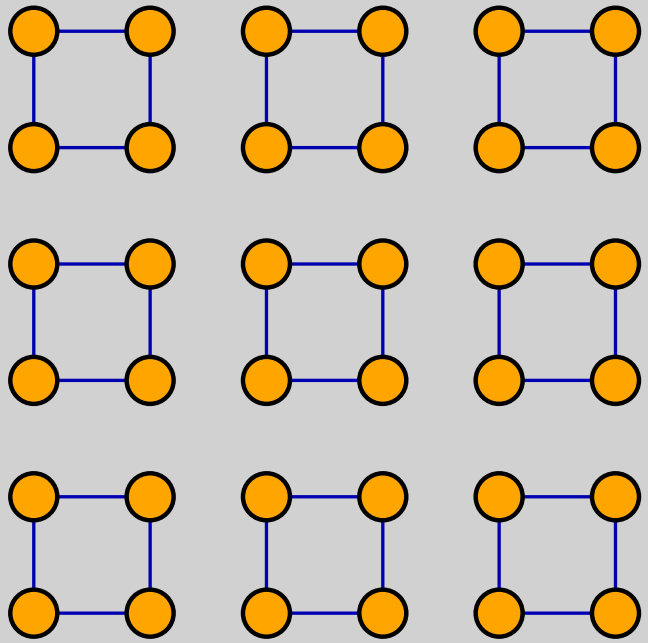
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

reference system, $H_{\mathbf{t}',\mathbf{U}}$:

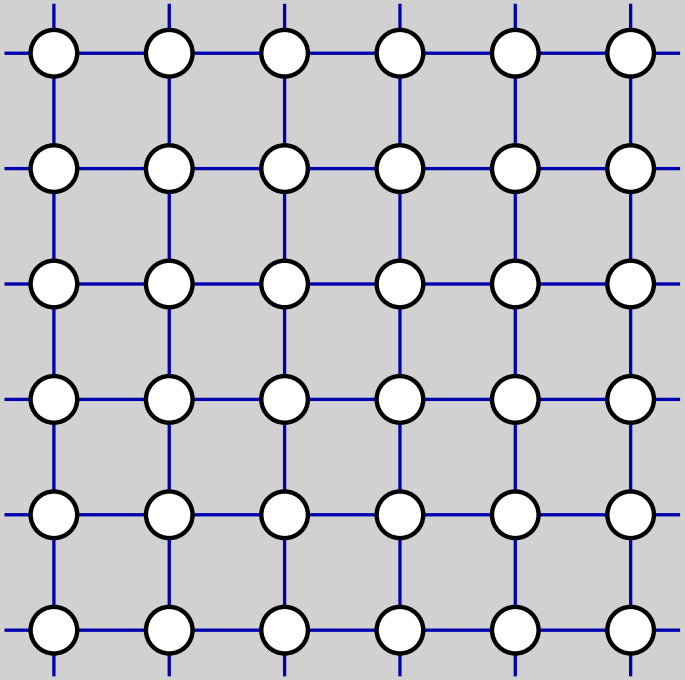


system of decoupled clusters

variational parameters:
on-site energies
thermodynamic consistency

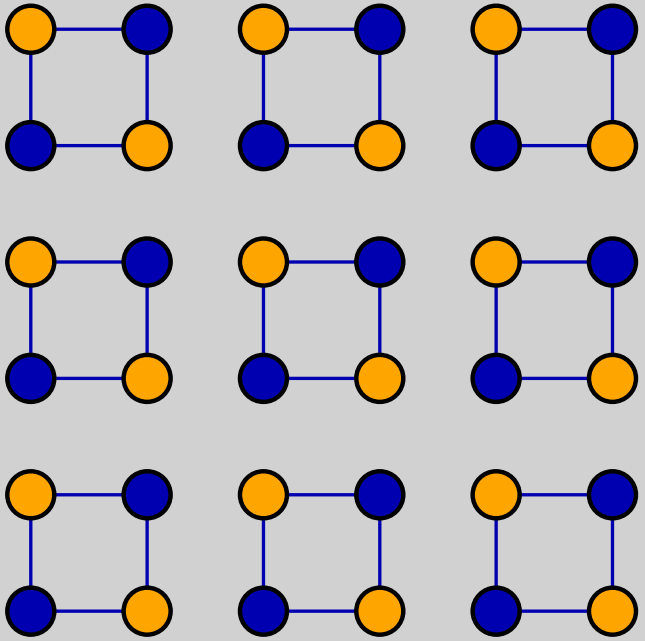
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

reference system, $H_{\mathbf{t}',\mathbf{U}}$:

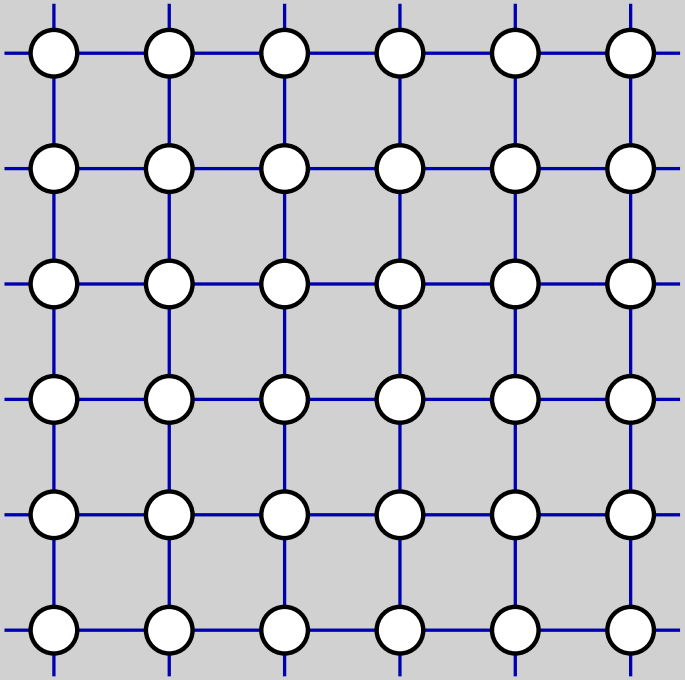


system of decoupled clusters

variational parameters:
ficticious symmetry-breaking fields
spontaneous symmetry breaking

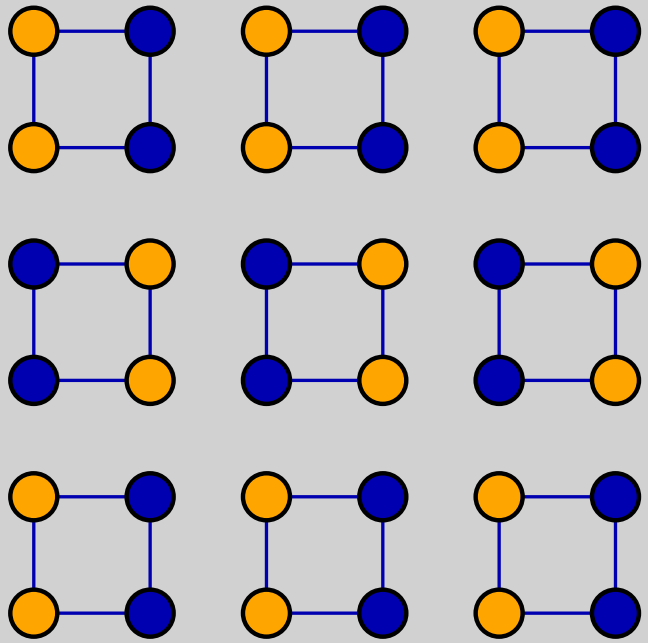
cluster approximations

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

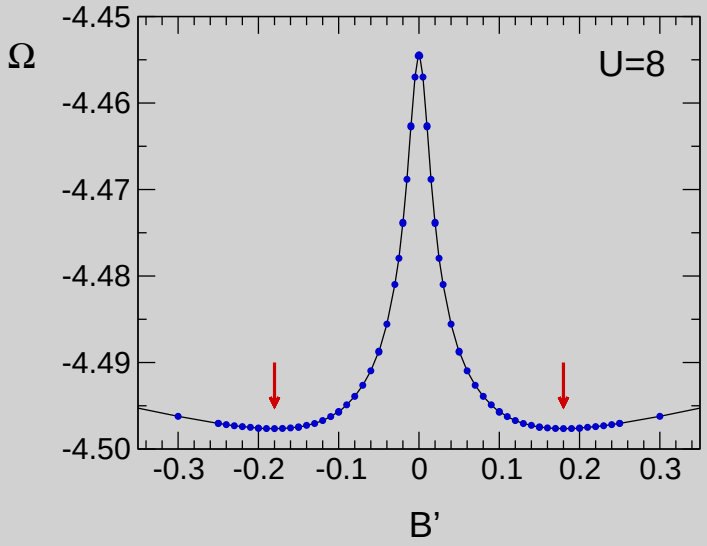
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



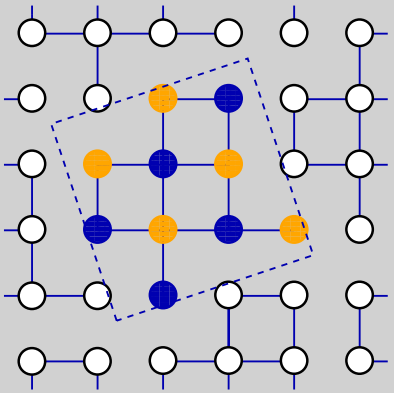
system of decoupled clusters

variational parameters:
ficticious symmetry-breaking fields
different order parameters

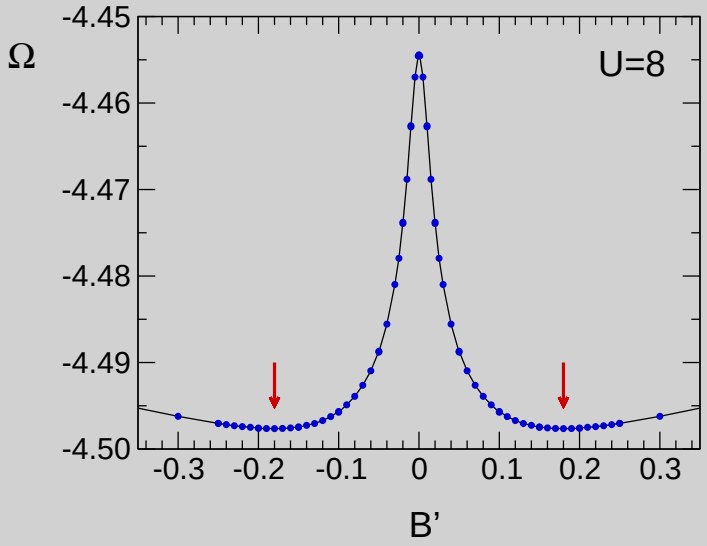
antiferromagnetism



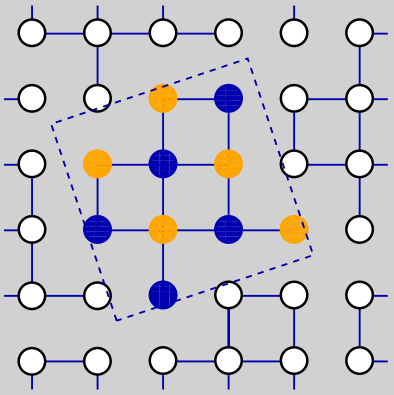
$D = 2$ Hubbard model, half-filling

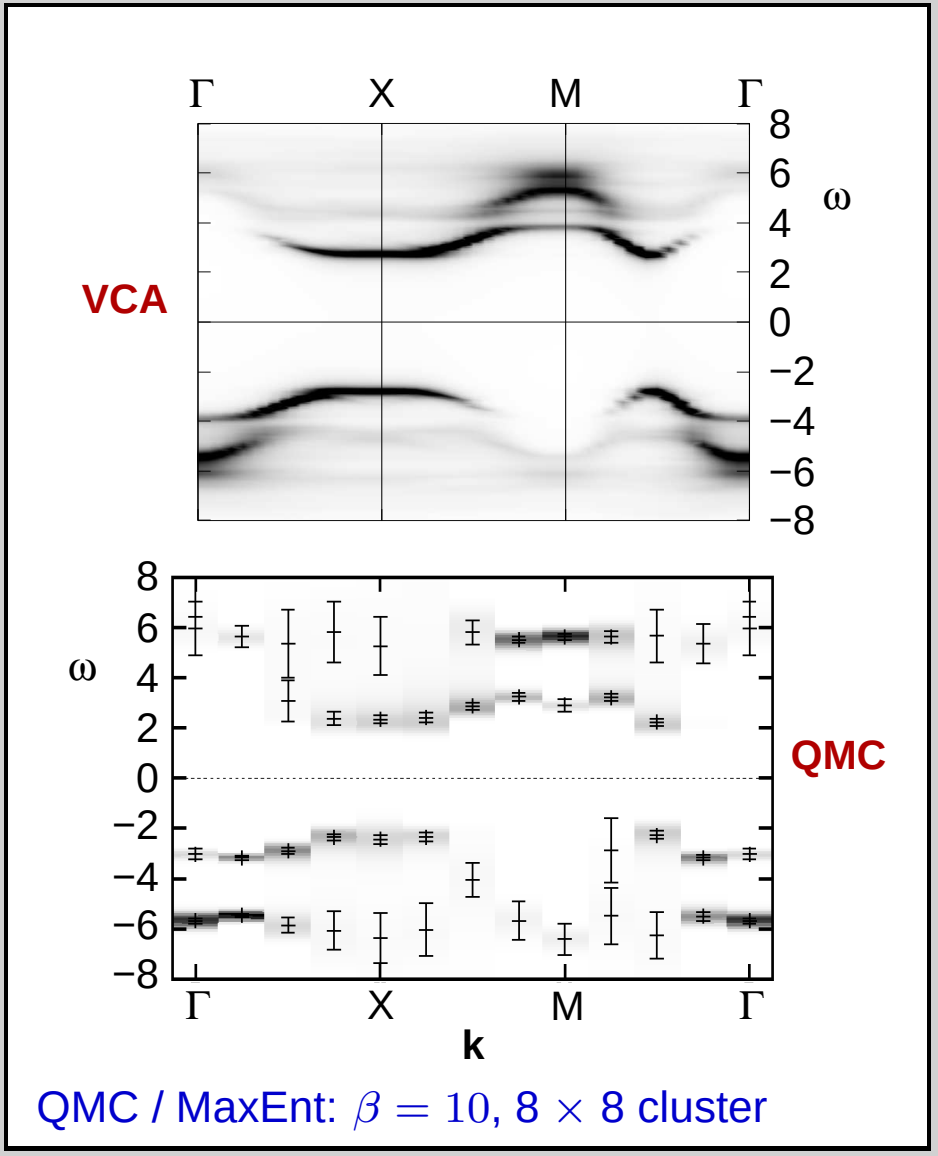


antiferromagnetism



$D = 2$ Hubbard model, half-filling

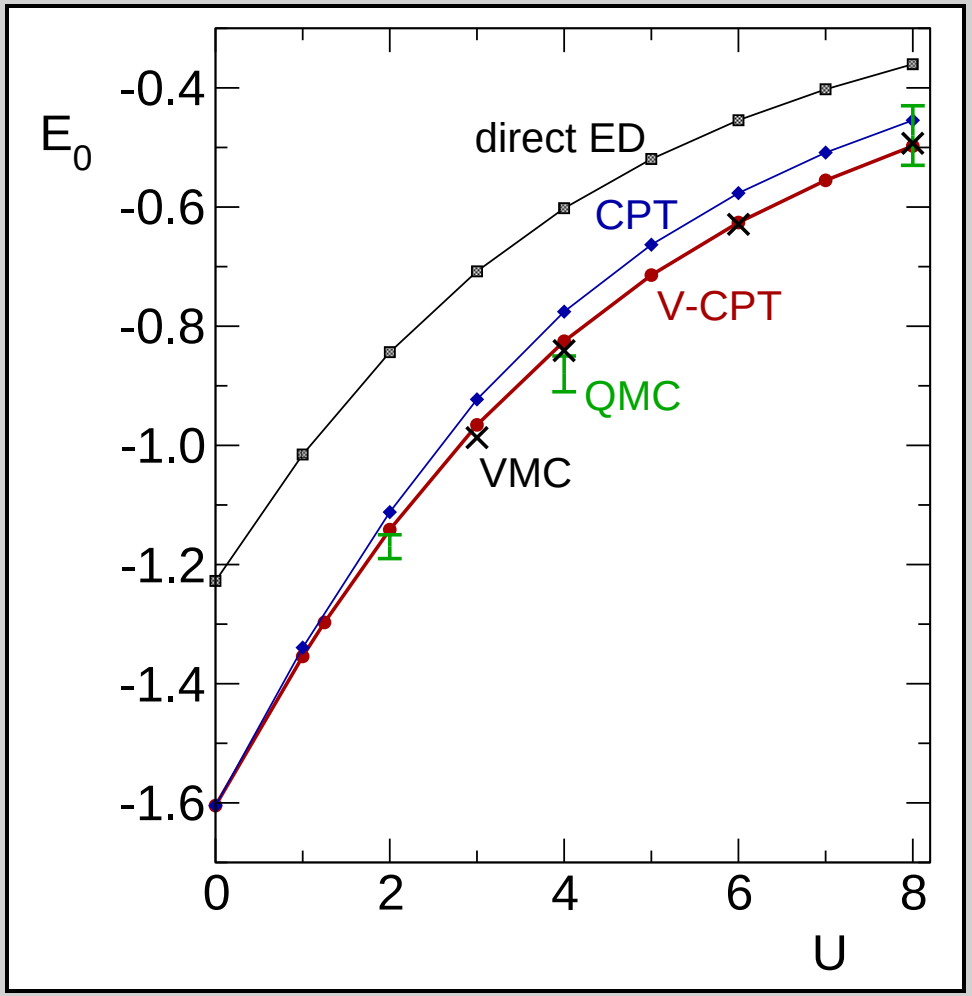




QMC / MaxEnt: $\beta = 10$, 8×8 cluster

Dahnken, Aichhorn, Hanke, Arrigoni, Potthoff (2004)

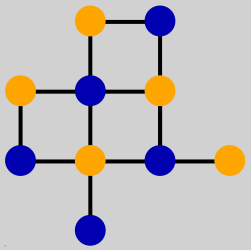
ground-state energy



Dahnken, Aichhorn, Hanke, Arrigoni, Potthoff (2004)

$D = 2$ Hubbard model
half-filling, $T = 0$
antiferromagnetic phase

$N_c = 10$, no bath sites



➜ **quantitative agreement with VMC, QMC**

symmetry-breaking fields

additional **ficticious** field / **Weiss field** : **reference system**

$$H'_{\text{fict.}} = B' \sum_{i\sigma} z_i (n_{i\uparrow} - n_{i\downarrow}) \ ,$$

AF order: staggered magnetic field ➜ $z_i = \pm 1$ for sites on sublattice 1/2

---

additional **physical** field: **original system**

$$H_{\text{phys.}} = B \sum_{i\sigma} z_i (n_{i\uparrow} - n_{i\downarrow})$$

---

in the paramagnetic state, $B = 0$:

$B'_{\text{opt}} = 0$ **no AF order**

in the paramagnetic state, $B > 0$:

$B'_{\text{opt}} > 0$ **induced AF order**

in the antiferromagnetic state, $B = 0$:

$B'_{\text{opt}} > 0$ **spontaneous AF order**

symmetry-breaking fields

SFT grand potential: $\Omega(B', B) = \Omega_B[\mathbf{\Sigma}_{B'}]$ (suppress other parameters)

stationarity condition: $\partial\Omega(B', B)/\partial B' = 0$

yields:

$$\boxed{B'_{\mathrm{opt}} = B'(B)}$$

for the SFT grand potential at the optimal Weiss field, $\Omega(B'(B), B)$, we have

$$\boxed{\frac{\partial\Omega(B'(B), B)}{\partial B'} = 0} \qquad \forall B$$

therewith:

$$\boxed{\frac{d}{dB}\frac{\partial\Omega(B'(B), B)}{\partial B'} = 0}$$

and thus:

$$\boxed{\frac{\partial^2\Omega(B'(B), B)}{\partial {B'}^2}\frac{dB'(B)}{dB} + \frac{\partial^2\Omega(B'(B), B)}{\partial B\partial B'} = 0}$$

solving for dB'/dB:

$$\boxed{\frac{dB'}{dB} = -\left[\frac{\partial^2\Omega}{\partial {B'}^2}\right]^{-1}\frac{\partial^2\Omega}{\partial B\partial B'}}$$

➜ B' is not a physical quantity (Weiss field)

➜ $B' \gg B$ for small curvature $\partial^2\Omega/\partial {B'}^2$ (flat SFT functional)

order parameter and susceptibitlity

staggered magnetization / order parameter:

$$m = \sum_{i\sigma} z_i \langle (n_{i\uparrow} - n_{i\downarrow}) \rangle = \frac{d}{dB} \Omega(B'(B), B) = \frac{\partial \Omega(B'(B), B)}{\partial B}$$

- ✧ no contribution due to the B dependence of the stationary point !

susceptibility:

$$\chi = \frac{dm}{dB} = \frac{\partial^2 \Omega(B'(B), B)}{\partial B' \partial B} \frac{dB'(B)}{dB} + \frac{\partial^2 \Omega(B'(B), B)}{\partial B^2}$$

we find:

$$\chi = \frac{\partial^2 \Omega}{\partial B^2} - \left(\frac{\partial^2 \Omega}{\partial B'^2} \right)^{-1} \left(\frac{\partial^2 \Omega}{\partial B' \partial B} \right)^2$$

- ✧ contribution to the explicit B dependence
- ✧ additional contribution to the implicit B dependence !
  i.e. the B dependence of the stationary point

order parameter and susceptibitlity

(anti-)ferromagnetic order:

- spontaneous breaking of the **SU(2)** symmetry of H (e.g. Hubbard model)
- conserved quantity: $\mathbf{S}_{\mathrm{tot}}$, total spin
- Weiss field: $\boxed{H'_{\mathrm{fict.}} = B' \sum_{i\sigma} z_i (n_{i\uparrow} - n_{i\downarrow}) \ ,}$
- order parameter: $\boxed{m = \sum_{i\sigma} z_i \langle (n_{i\uparrow} - n_{i\downarrow}) \rangle}$

---

superconductivity:

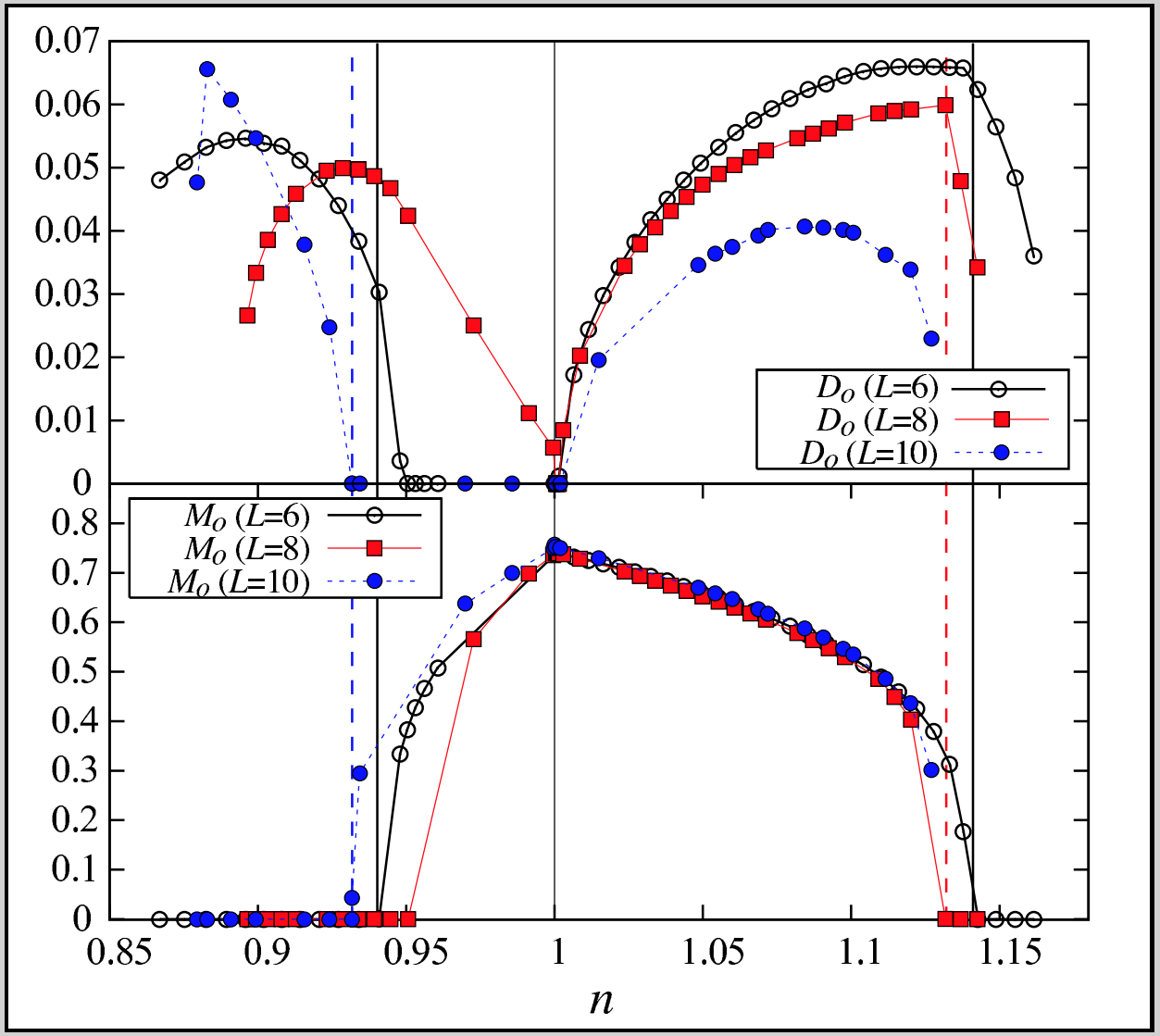
- spontaneous breaking of the **U(1)** symmetry of H
- conserved quantity: N, total particle number
- Weiss field: $\boxed{H'_{\mathrm{fict.}} = h' \sum_{ij} \frac{\eta_{ij}}{2} (c_{i\uparrow} c_{j\downarrow} + \mathrm{H.c.})}$ (d wave)

  with $\eta_{ij} = \pm 1$ for n.n. along x/y direction (2D square lattice)
- order parameter: $\boxed{\Delta = \langle c_{i\uparrow} c_{j\downarrow} \rangle}$ complex and **non-local** !

  (➜ cluster approximation)

high-temperature superconductivity

hole doping | electron doping



d-wave-superconductivity

antiferromagnetism

t-t'-t'' Hubbard model

$D = 2$

$T = 0, U = 8t$

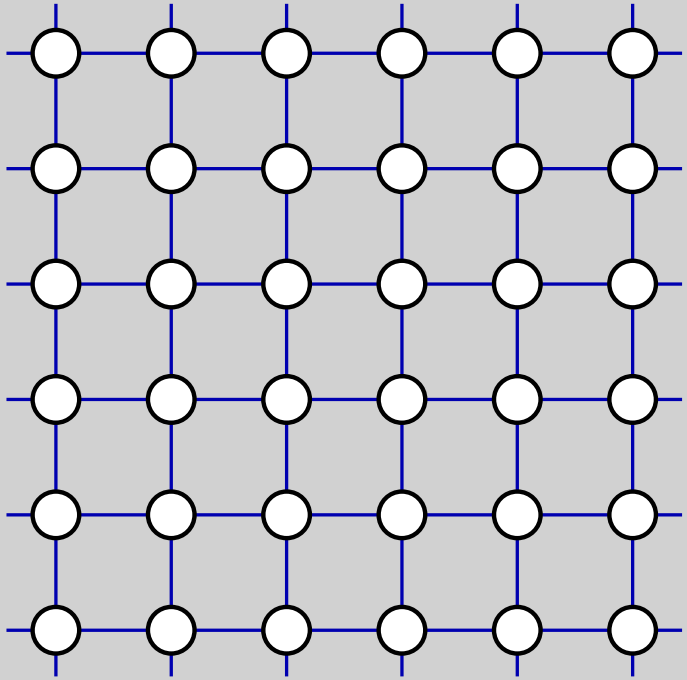
$L_c = 6, 8, 10$

Senechal, Lavertu, Marois, Tremblay (2005)

Bath Sites and Dynamical Mean-Field Theory

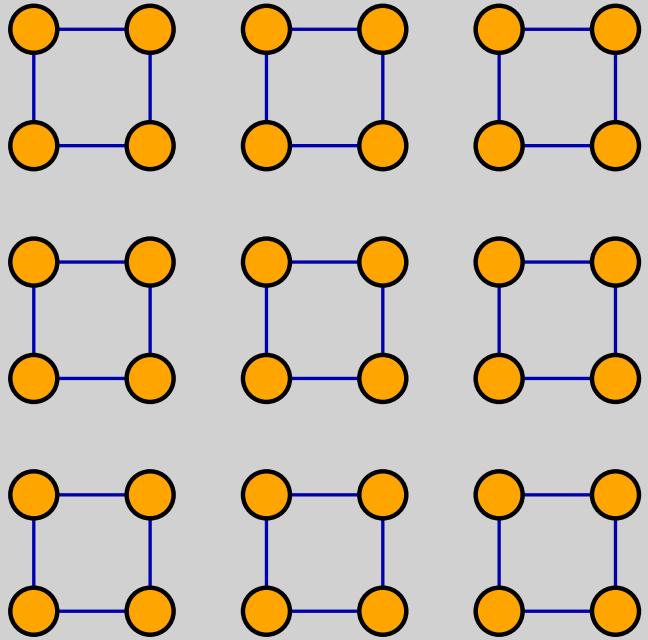
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

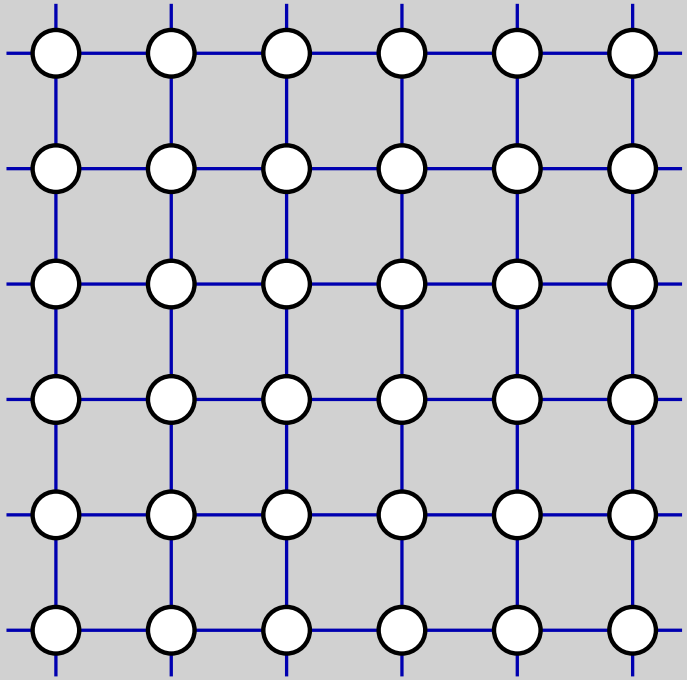
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
cluster size: $L_c = 4$
variation of on-site energies

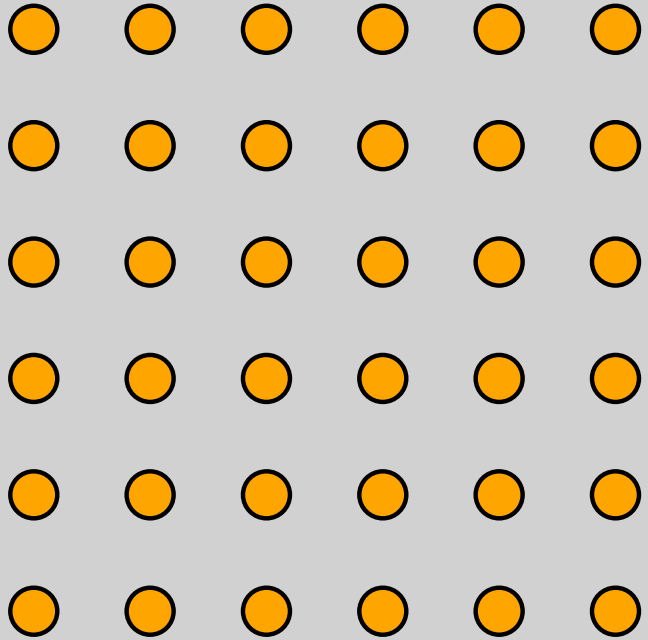
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

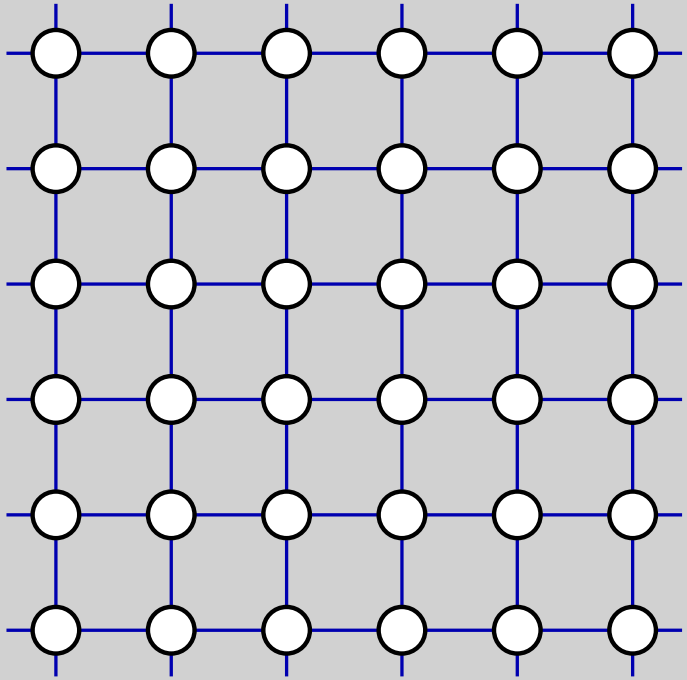
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
cluster size: $L_c = 1$
Hubbard-I-type approximation

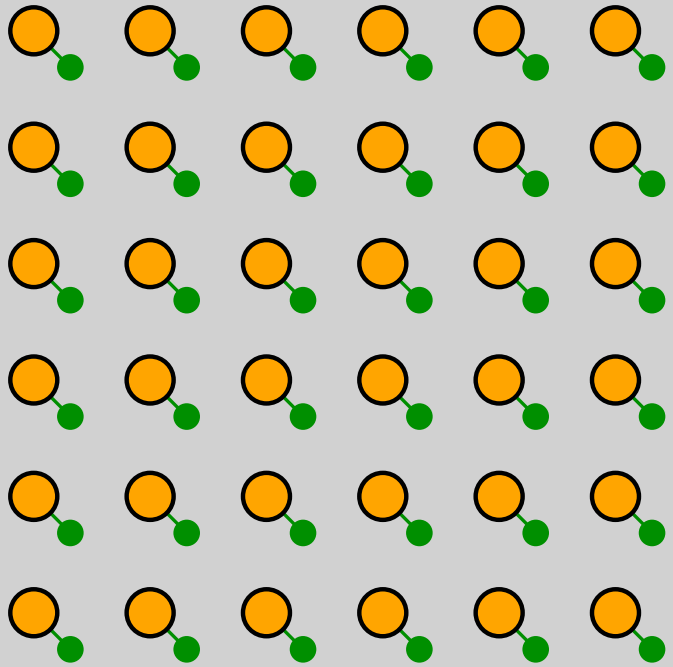
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

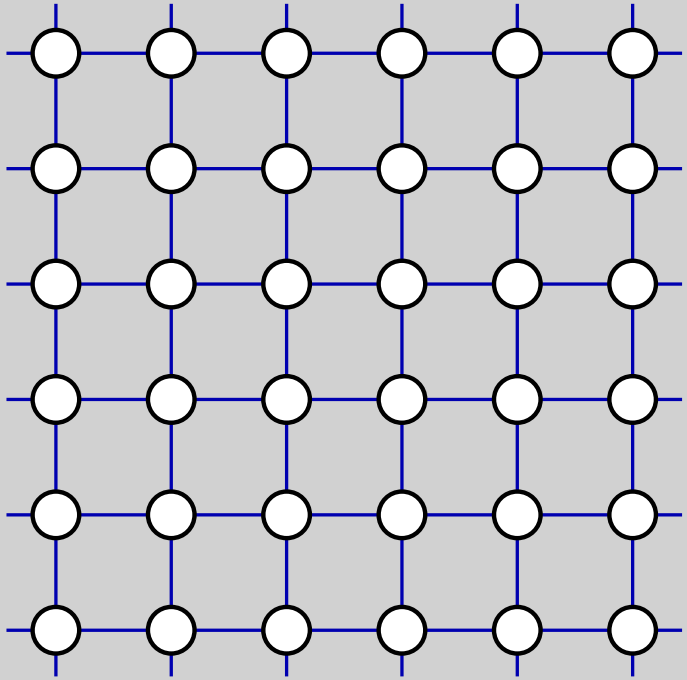
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
with additional bath sites
$L_c = 1$, $L_b = 2$
improved description of temporal
correlations

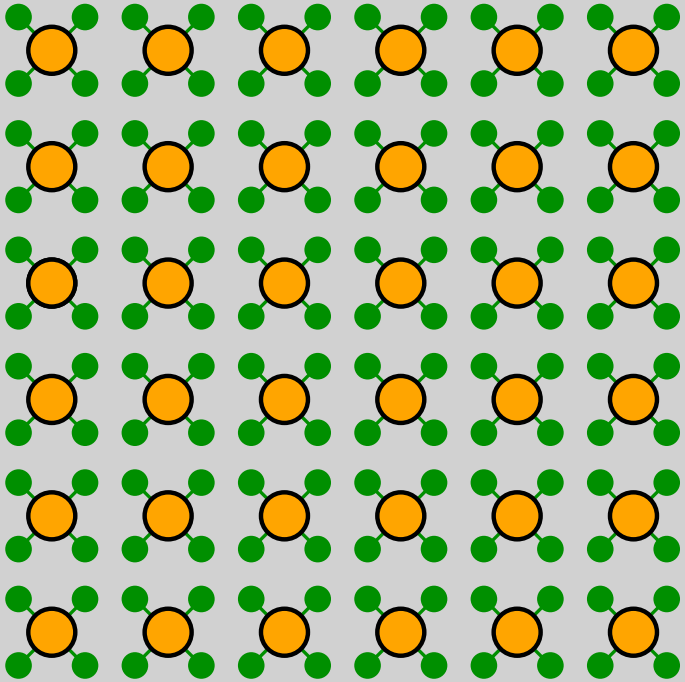
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

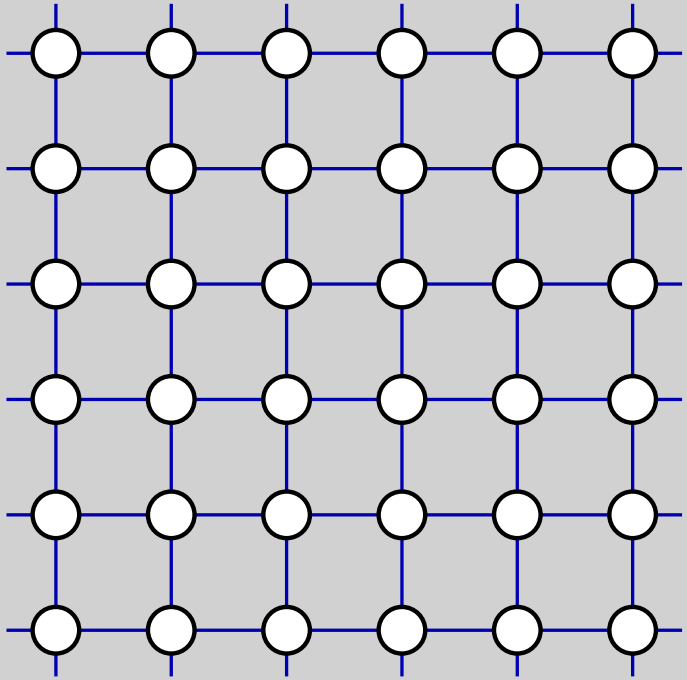
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
with additional bath sites
$L_c = 1$, $L_b = 5$
improved mean-field theory

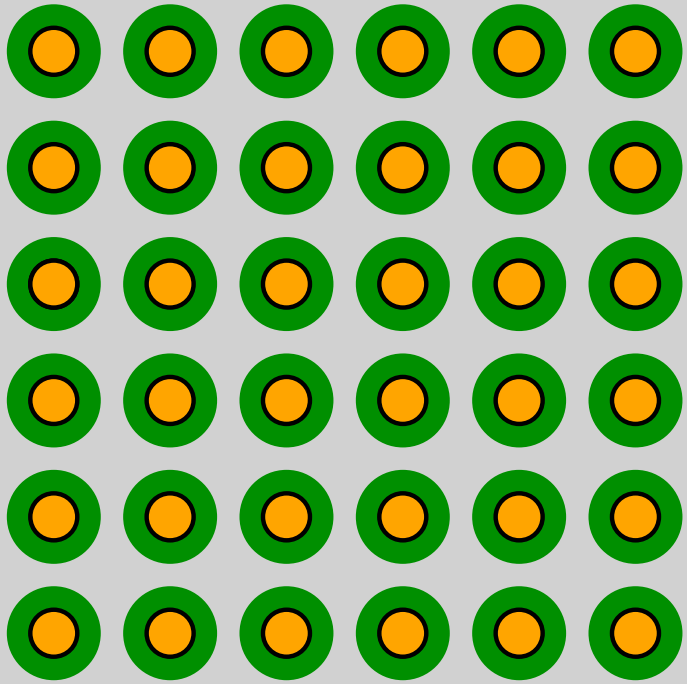
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

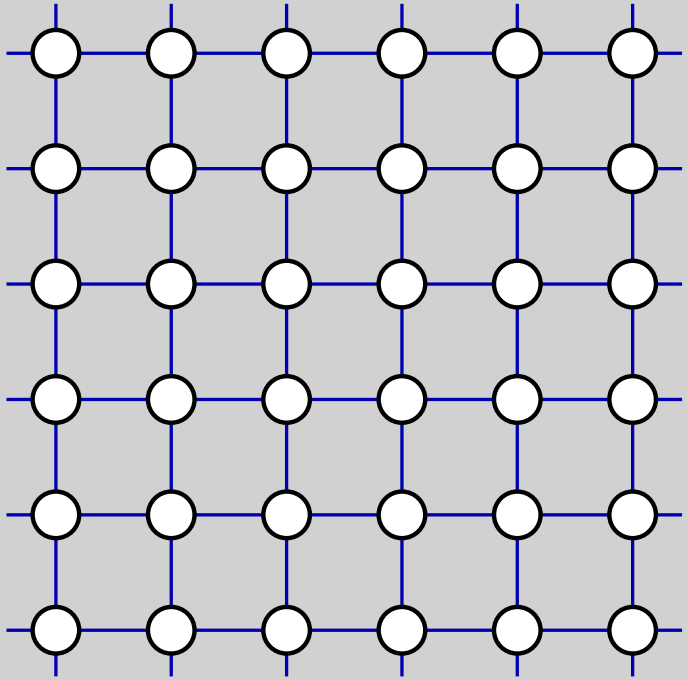
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
with additional bath sites
$L_c = 1$, $L_b = \infty$
optimum mean-field theory, DMFT
Metzner, Vollhardt (1989)
Georges, Kotliar, Jarrell (1992)

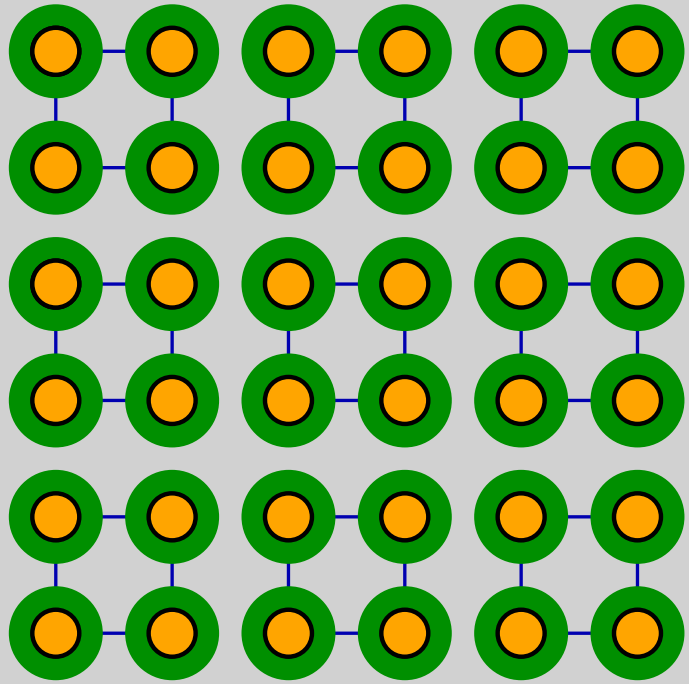
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

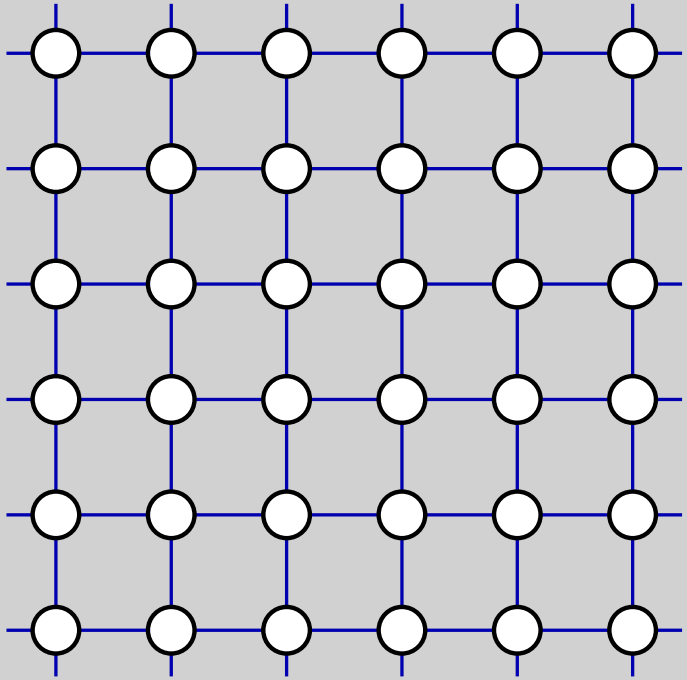
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
with additional bath sites
$L_c = 4$, $L_b = \infty$
cellular DMFT
Kotliar et al (2001)
Lichtenstein, Katsnelson (2000)

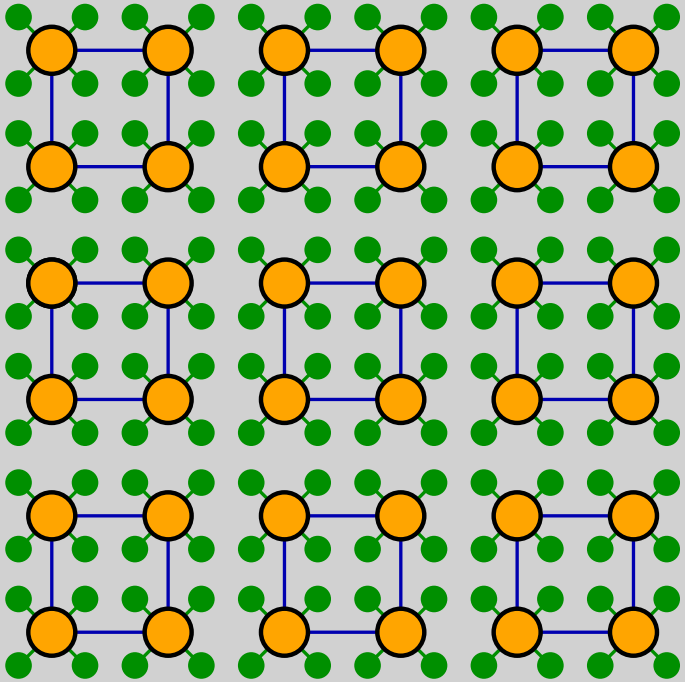
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

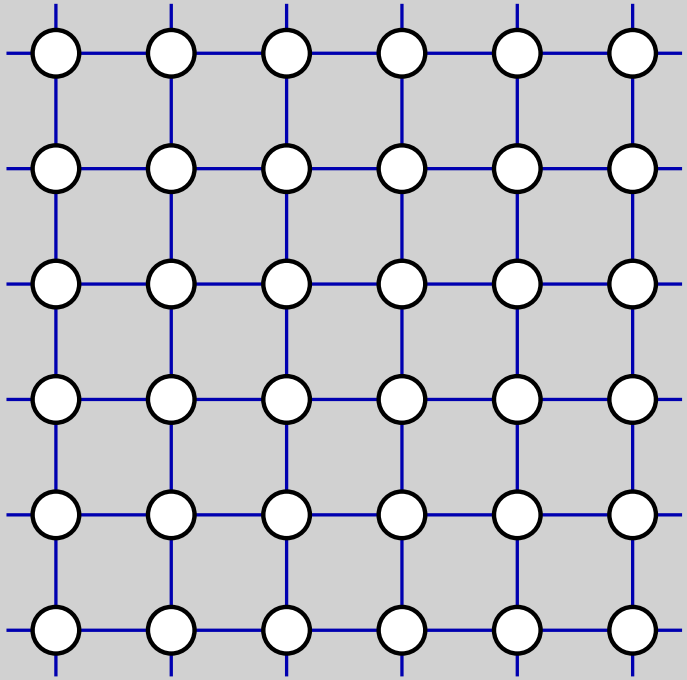
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
with additional bath sites
$L_c = 4$, $L_b = 5$
variational cluster approach (VCA)

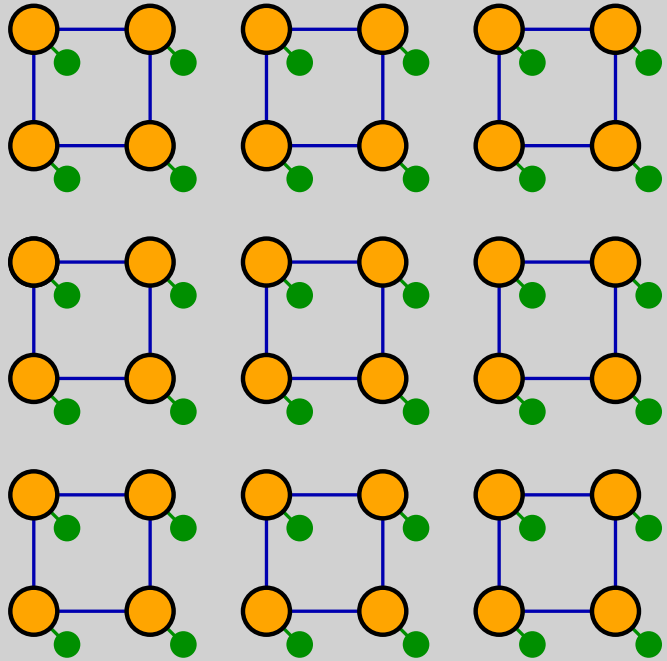
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



lattice model ($D = 2$) in
the thermodynamic limit

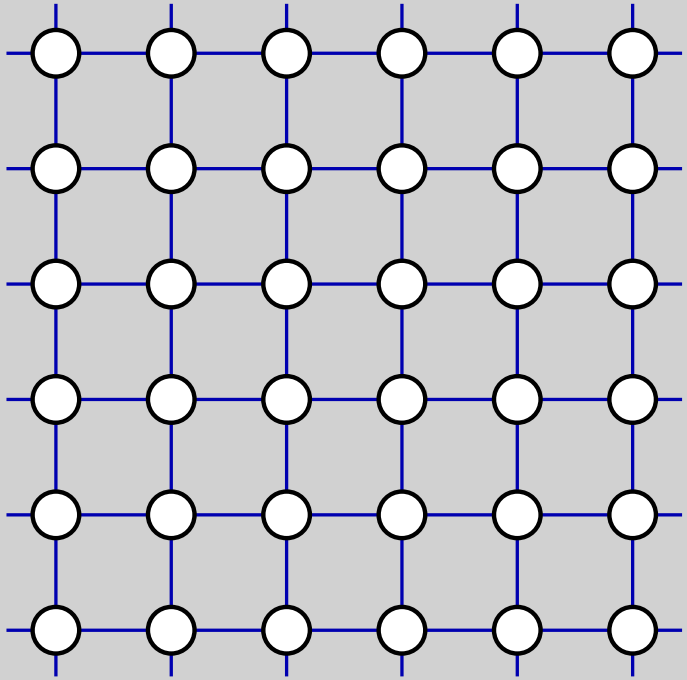
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters
with additional bath sites
$L_c = 4$, $L_b = 2$
variational cluster approach (VCA)

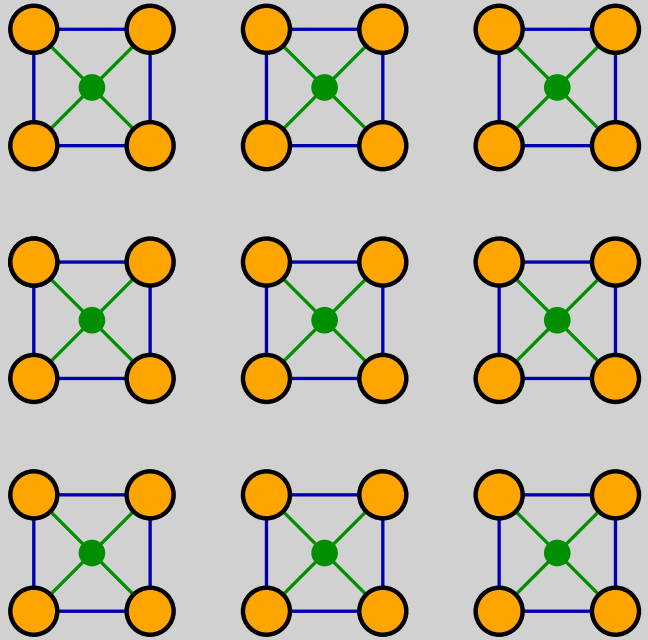
approximations using bath sites

original system, $H_{\mathbf{t},\mathbf{U}}$:



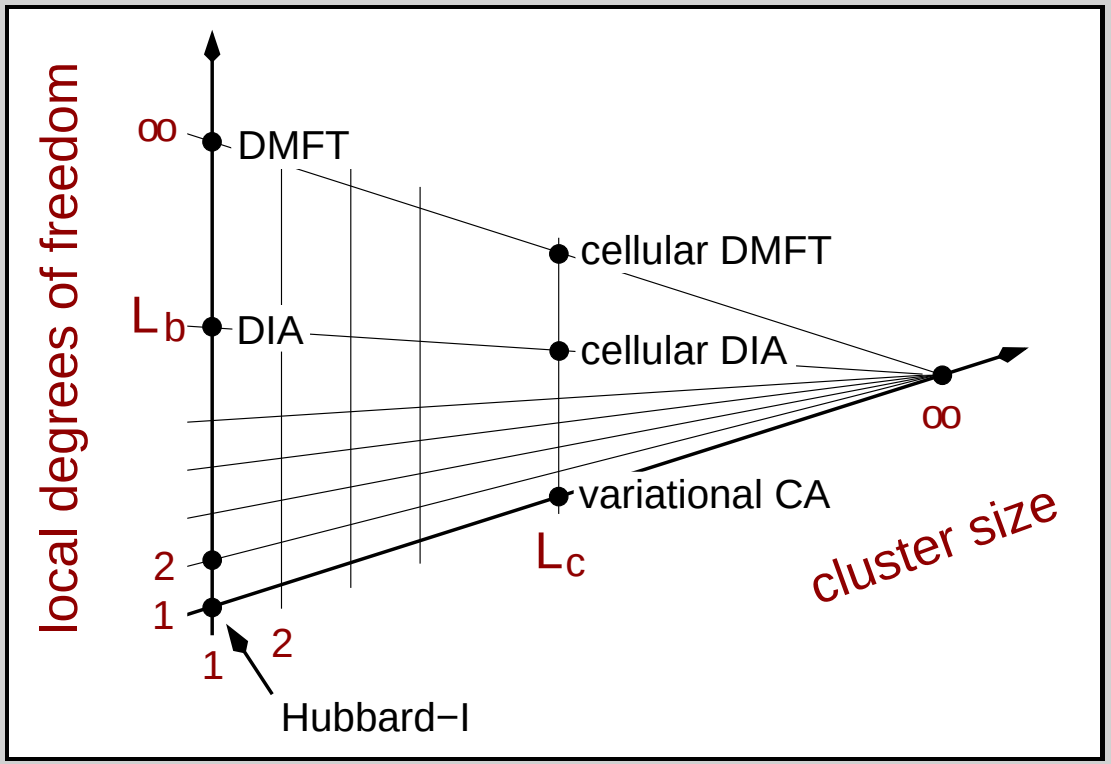
lattice model ($D = 2$) in
the thermodynamic limit

reference system, $H_{\mathbf{t}',\mathbf{U}}$:

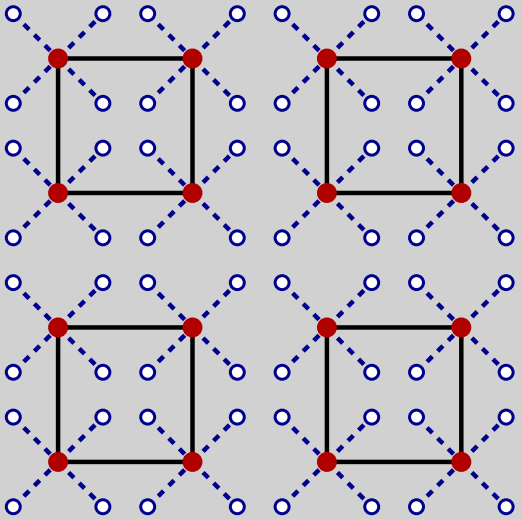


system of decoupled clusters
with additional bath sites
$L_c = 4$
variational cluster approach (VCA)

consistent approximations within SFT



$L_c = 4,\ n_s = 5$



- ➜ **DMFT** *Metzner, Vollhardt 1989, Georges, Kotliar 1992, Jarrell 1992*
- ➜ **C-DMFT** *Kotliar et al 2001, Lichtenstein, Katsnelson 2000*
- ➜ **DIA** *Potthoff 2003*
- ➜ **VCA** *Potthoff, Aichhorn, Dahnken 2003*

derivation of dynamical mean-field theory

self-energy functional:

$$\widehat{\Omega}_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \widehat{\Omega}_{\mathbf{t}',\mathbf{U}}[\mathbf{\Sigma}] + \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}} - \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t}',0} - \mathbf{\Sigma}}$$

self-energy $\mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}$ taken from the reference system inserted as a trial:

$$\widehat{\Omega}_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}] = \Omega_{\mathbf{t}',\mathbf{U}} + \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}} - \mathrm{Tr}\ln\mathbf{G}_{\mathbf{t}',\mathbf{U}}$$

stationarity condition:

$$\frac{\partial}{\partial \mathbf{t}'}\widehat{\Omega}_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}] = 0$$

first term:

$$\frac{\partial}{\partial t'_{\alpha\beta}}\Omega_{\mathbf{t}',\mathbf{U}} = \langle c^\dagger_\beta c_\alpha\rangle'$$

second term:

$$\frac{\partial}{\partial \mathbf{t}'}\mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}} = T\sum_n\sum_{\alpha\beta}\left(\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0}(i\omega_n) - \mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}(i\omega_n)}\right)_{\beta\alpha}\frac{\partial\Sigma_{\mathbf{t}',\mathbf{U},\alpha\beta}(i\omega_n)}{\partial\mathbf{t}'}$$

derivation of dynamical mean-field theory

third term:

$$\frac{\partial}{\partial \mathbf{t}'} \mathrm{Tr} \ln \mathbf{G}_{\mathbf{t}',\mathbf{U}} = \frac{\partial}{\partial \mathbf{t}'} \mathrm{Tr} \ln \frac{1}{i\omega_n + \mu - \mathbf{t}' - \mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}}$$

$$= T \sum_n e^{i\omega_n 0^+} \mathbf{G}_{\mathbf{t}',\mathbf{U}}(i\omega_n) + T \sum_n \sum_{\alpha\beta} \left(\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0}(i\omega_n) - \mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}(i\omega_n)} \right)_{\beta\alpha} \frac{\partial \Sigma_{\mathbf{t}',\mathbf{U},\alpha\beta}(i\omega_n)}{\partial \mathbf{t}'}$$

with $T \sum_n e^{i\omega_n 0^+} G_{\mathbf{t}',\mathbf{U},\alpha\beta}(i\omega_n) = \langle c^\dagger_\beta c_\alpha \rangle'$ we find the general **SFT Euler equation** :

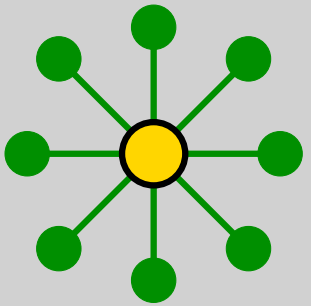
$$T \sum_n \sum_{\alpha\beta} \left(\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0}(i\omega_n) - \mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}(i\omega_n)} - \mathbf{G}_{\mathbf{t}',\mathbf{U}}(i\omega_n) \right)_{\beta\alpha} \frac{\partial \Sigma_{\mathbf{t}',\mathbf{U},\alpha\beta}(i\omega_n)}{\partial \mathbf{t}'} = 0$$

- unknowns: elements of $\mathbf{t}'$, number of equations $=$ number of unknowns
- highly non-linear system of equations, exact solution: $\mathbf{\Sigma}_{\mathbf{t},\mathbf{U}}$
- **geometrical interpretation** (for those who like this):
  Euler equation is obtained from the exact conditional equation for the "vector" $\mathbf{\Sigma}$ in the self-energy space $\mathcal{S}_\mathbf{U}$ through *projection* onto the hypersurface of $\mathbf{t}'$ representable trial self-energies $\mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}$ by taking the scalor product with vectors $\partial \Sigma_{\mathbf{t}',\mathbf{U},\alpha\beta}(i\omega_n)/\partial \mathbf{t}'$ tangential to the hypersurface

derivation of dynamical mean-field theory

test self-energy is taken from a single-impurity Anderson model (SIAM):

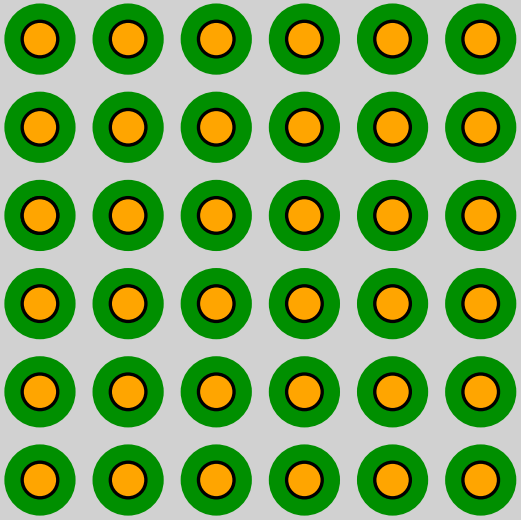
$$H_{\mathrm{SIAM}} = \sum_{\sigma} \varepsilon_{\mathrm{imp}} c_{\sigma}^{\dagger} c_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{k\sigma} \varepsilon_k a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_{k\sigma} V_k (c_{\sigma}^{\dagger} a_{k\sigma} + \mathrm{H.c.})$$



➜ actually: continuum of bath sites, $L_b \to \infty$

➜ non-zero SIAM self-energy at the impurity site only: $\Sigma_{\mathrm{imp}}(\omega)$

➜ one SIAM attached to each site of original lattice (identical replicas)



$$\Sigma_{\alpha\beta}(i\omega_n) = \Sigma_{ik,jl}(i\omega_n) = \delta_{ij} \Sigma_{i0,i0}(i\omega_n)$$

derivation of dynamical mean-field theory

Euler equation

$$T\sum_n\sum_{\alpha\beta}\left(\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0}(i\omega_n)-\mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}(i\omega_n)}-\mathbf{G}_{\mathbf{t}',\mathbf{U}}(i\omega_n)\right)_{\beta\alpha}\frac{\partial\Sigma_{\mathbf{t}',\mathbf{U},\alpha\beta}(i\omega_n)}{\partial\mathbf{t}'}=0$$

reduces to

$$T\sum_n\sum_{i\sigma}\left(\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0}(i\omega_n)-\mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}(i\omega_n)}-\mathbf{G}_{\mathbf{t}',\mathbf{U}}(i\omega_n)\right)_{ii\sigma}\frac{\partial\Sigma_{ii\sigma}(i\omega_n)}{\partial\mathbf{t}'}=0$$

sufficient for a solution the Euler equation:

$$\left(\frac{1}{\mathbf{G}_0^{-1}(\omega)-\mathbf{\Sigma}(\omega)}\right)_{ii\sigma}=\mathbf{G}'_{ii\sigma}(\omega)$$

or:

$$G_{\mathrm{loc}}(\omega)\stackrel{!}{=}\mathcal{G}(\omega)$$ **DMFT self-consistency equation**

DMFT self-consistency

lattice structure
bare dispersion $\varepsilon(\mathbf{k})$

$\Sigma(\omega)$ ← "solver" ← $H_{\mathrm{imp}} = \sum_\sigma \varepsilon_c n_\sigma + \frac{U}{2}\sum_\sigma n_\sigma n_{-\sigma} + \sum_{k\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{k\sigma} V_k c^\dagger_\sigma a_{k\sigma} + \mathrm{h.c.}$

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(\omega)}$$

$$\Delta(\omega) = \sum_k \frac{V_k^2}{\omega + \mu - \varepsilon_k}$$

$$G_{\mathrm{loc}}(\omega) = \frac{1}{L}\sum_{\mathbf{k}} G_{\mathbf{k}}(\omega)$$

$$\mathcal{G}(\omega) = \frac{1}{\omega + \mu - \varepsilon_c - \Delta(\omega) - \Sigma(\omega)}$$

$$G_{\mathrm{loc}}(\omega) \stackrel{!}{=} \mathcal{G}(\omega)$$

"self-consistency condition"

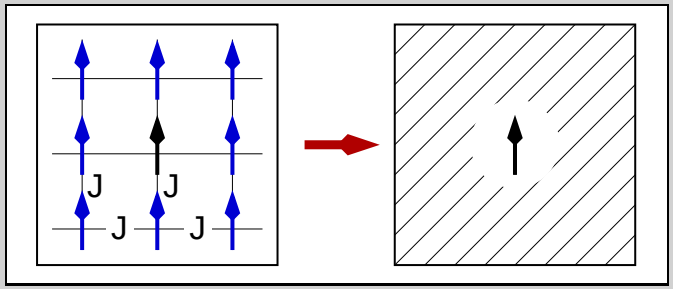
dynamical mean-field theory and $D = \infty$

Weiß molecular-field theory

magnetic phase transition

lattice spin model

$$H = -\frac{J}{2} \sum_{\langle ij \rangle} S_i S_j$$



$$H_{\rm imp} = -J \left(\sum_{\langle i \rangle} \langle S_i \rangle \right) S$$

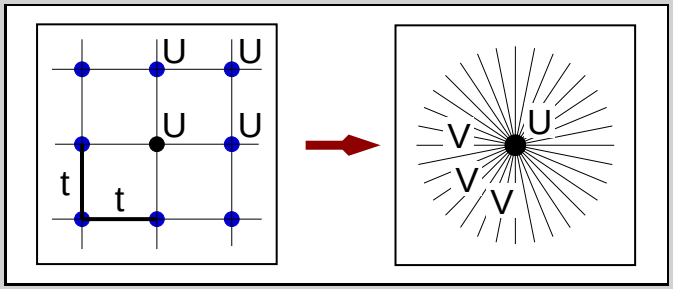
$$J \propto 1/D$$

dynamical mean-field theory

Mott transition

lattice fermion model

$$H = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$



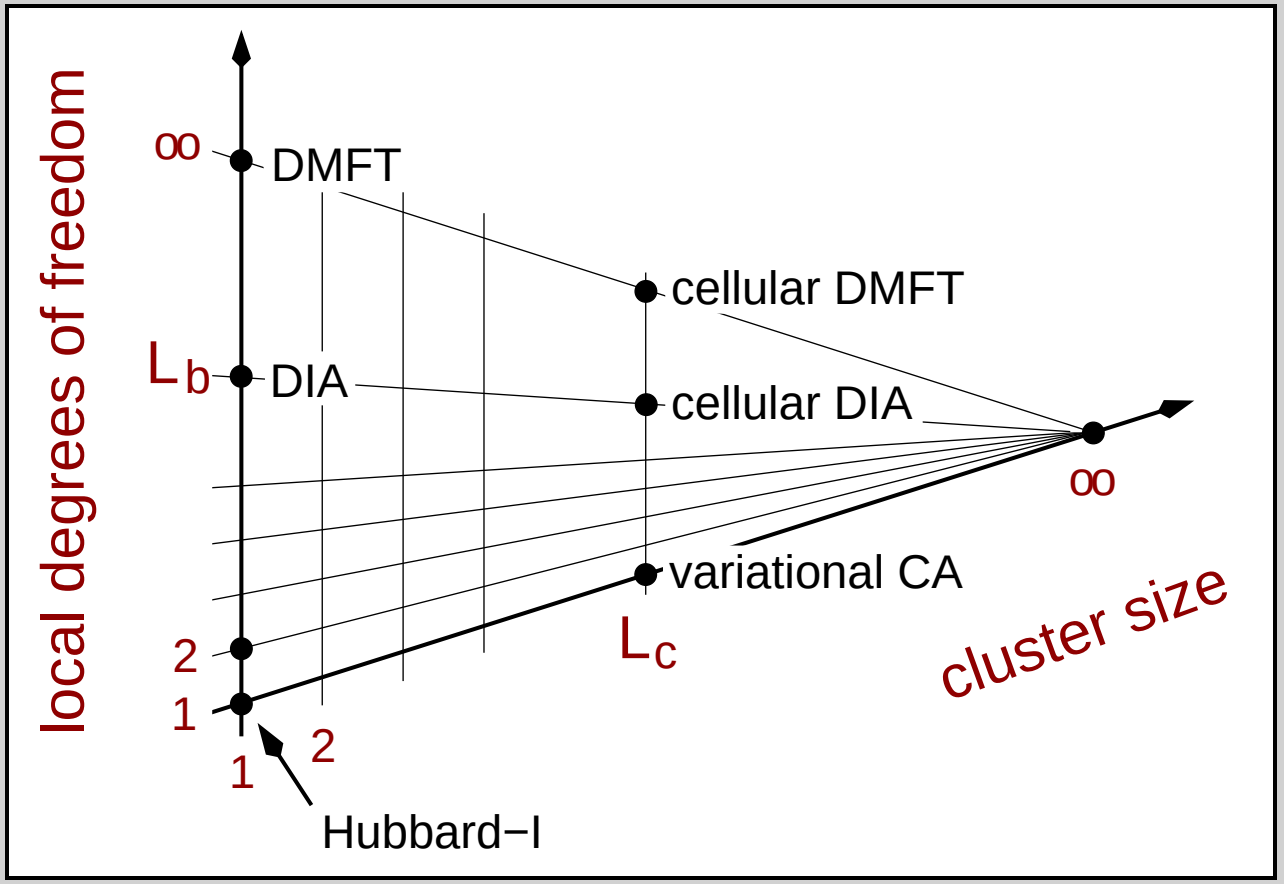
$$H_{\rm imp} = \sum_\sigma t_0 n_\sigma + \frac{U}{2} \sum_\sigma n_\sigma n_{-\sigma}$$
$$+ \sum_{k\sigma} \varepsilon_k n^{(a)}_{k\sigma} + \sum_{k\sigma} V_k c^\dagger_\sigma a_{k\sigma} + \text{h.c.}$$

$$t \propto 1/\sqrt{D}$$

Metzner, Vollhardt (1989), Georges, Kotliar (1992), Jarrell (1992)

Cluster Extensions of DMFT

classification of dynamical approximations



dynamical mean-field theory	*Metzner, Vollhardt (1989), Georges, Kotliar, Jarrell (1992)*
cellular DMFT	*Kotliar, Savrasov, Palsson (2001)*
dynamical impurity approach (DIA)	*Potthoff (2003)*
variational cluster approach	*Potthoff, Aichhorn, Dahnken (2004)*

cluster extensions of DMFT

cellular DMFT (C-DMFT)
Kotliar, Savrasov, Palsson, Biroli (2001)

dynamical cluster approximation (DCA)
Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy (1998)

periodized C-DMFT (P-C-DMFT)
Biroli, Parcollet, Kotliar (2003)

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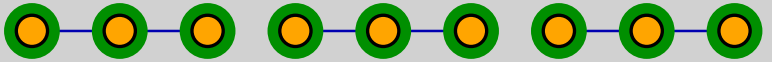
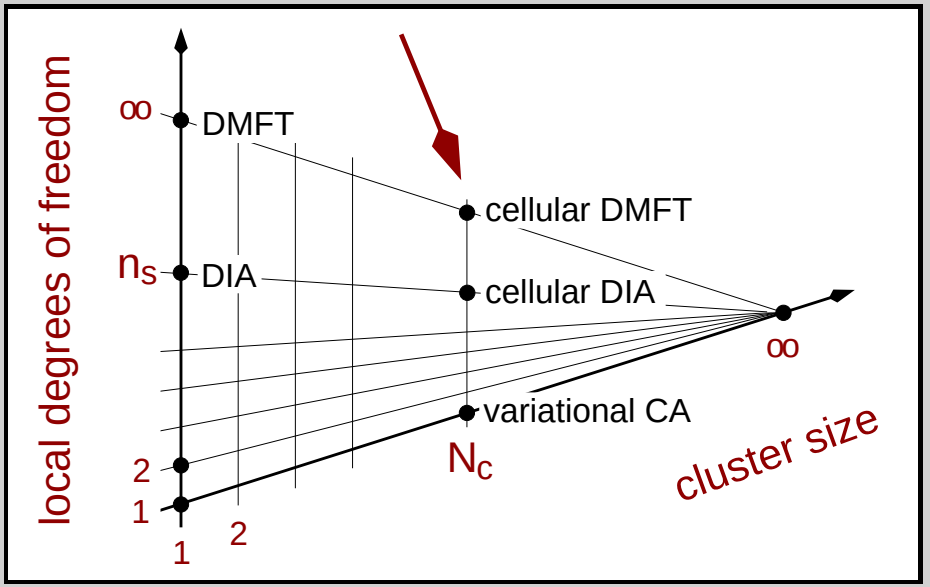
fictive impurity models
Okamoto, Millis, Monien, Fuhrmann (2003)

original system, $H_{\mathbf{t},\mathbf{U}}$:

reference system, $H_{\mathbf{t}',\mathbf{U}}$:





cluster extensions of DMFT

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original system, $H_{\mathbf{t},\mathbf{U}}$:

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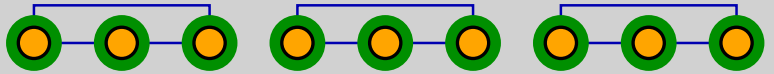

$$\frac{\partial}{\partial \mathbf{t}'}\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}(\mathbf{t}')] = 0$$

➜ open boundary conditions (see above)

there is no reference system which generates the DCA !

cluster extensions of DMFT

cellular DMFT (C-DMFT)
Kotliar, Savrasov, Palsson, Biroli (2001)

dynamical cluster approximation (DCA)
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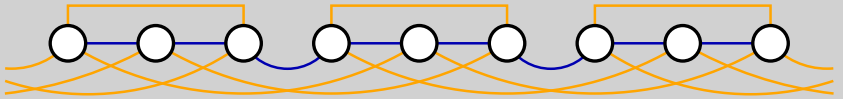
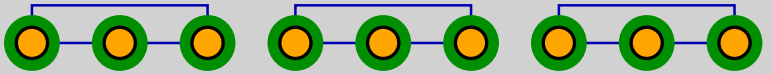
fictive impurity models
Okamoto, Millis, Monien, Fuhrmann (2003)

original system, $H_{\mathbf{t},\mathbf{U}}$:



reference system, $H_{\mathbf{t}',\mathbf{U}}$:



$$\frac{\partial}{\partial \mathbf{t}'}\Omega_{\overline{\mathbf{t}},\mathbf{U}}[\mathbf{\Sigma}(\mathbf{t}')] = 0 \qquad (\mathbf{t} \mapsto \overline{\mathbf{t}})$$

DCA self-consistency condition

$\overline{\mathbf{t}}$: invariant under superlattice translations and periodic on each cluster

➜ **systematic**
➜ **restores translational symmetry**
➜ **no implications on quality of DCA !**

cluster extensions of DMFT

cellular DMFT (C-DMFT)
Kotliar, Savrasov, Palsson, Biroli (2001)

dynamical cluster approximation (DCA)
Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy (1998)

periodized C-DMFT (P-C-DMFT)
Biroli, Parcollet, Kotliar (2003)

fictive impurity models
Okamoto, Millis, Monien, Fuhrmann (2003)

original system, $H_{\mathbf{t},\mathbf{U}}$:

reference system, $H_{\mathbf{t}',\mathbf{U}}$:

$$\frac{\partial}{\partial \mathbf{t}'}\overline{\Omega}_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}(\mathbf{t}')] = 0 \qquad (\Omega[\cdots] \mapsto \overline{\Omega}[\cdots])$$

P-C-DMFT self-consistency condition

➜ **systematic**
➜ **restores translational symmetry**

cluster extensions of DMFT

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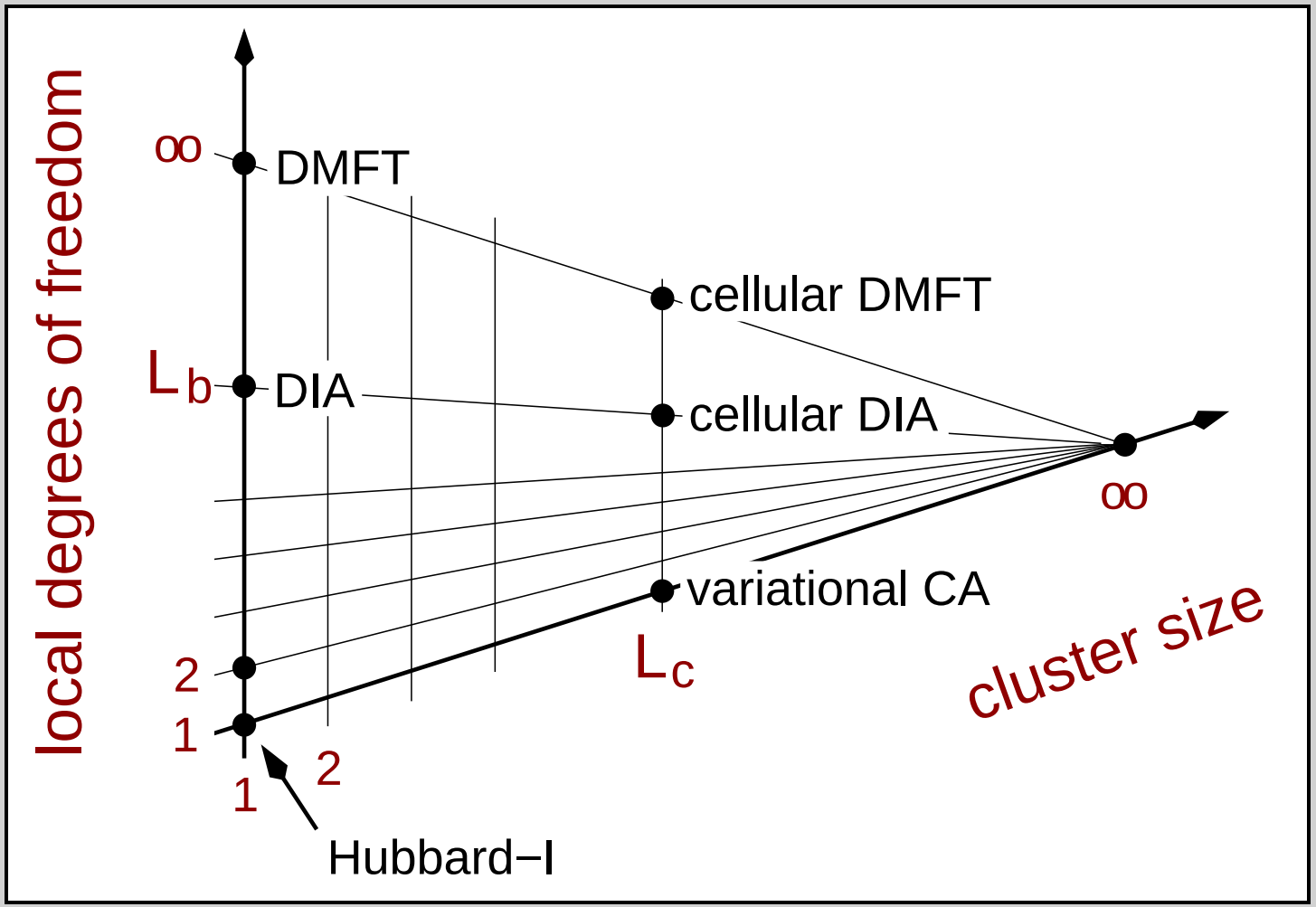
periodized C-DMFT (P-C-DMFT)
Biroli, Parcollet, Kotliar (2003)

fictive impurity models
Okamoto, Millis, Monien, Fuhrmann (2003)

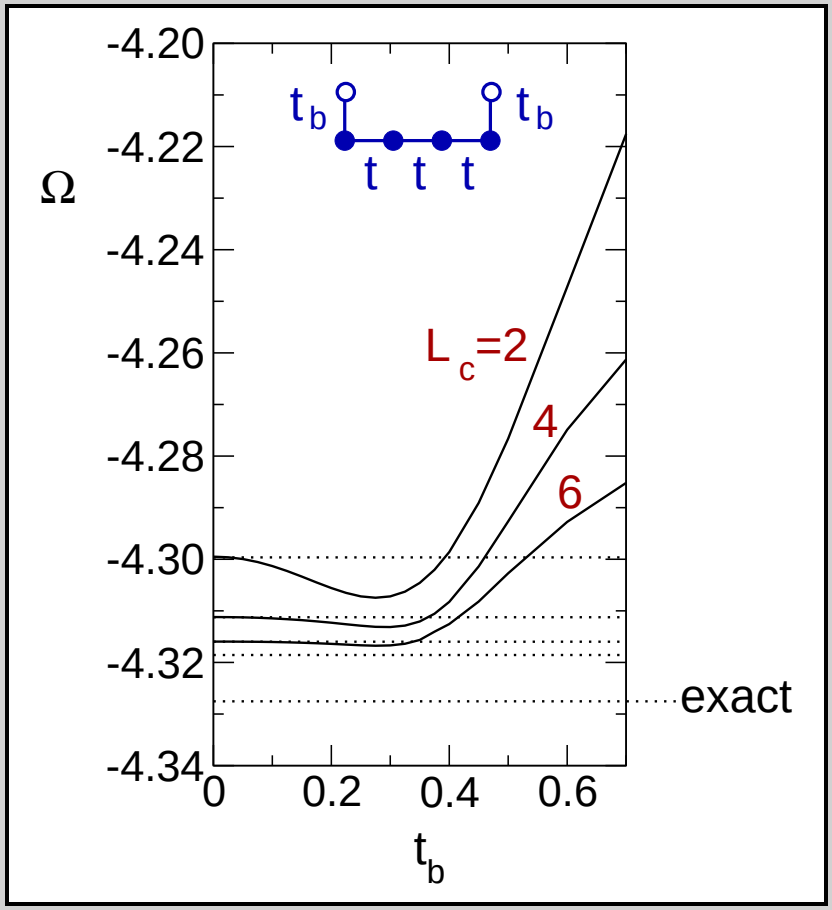
original system, $H_{\mathbf{t},\mathbf{U}}$:

reference system, $H_{\mathbf{t}',\mathbf{U}}$:
without any relation to the original system !

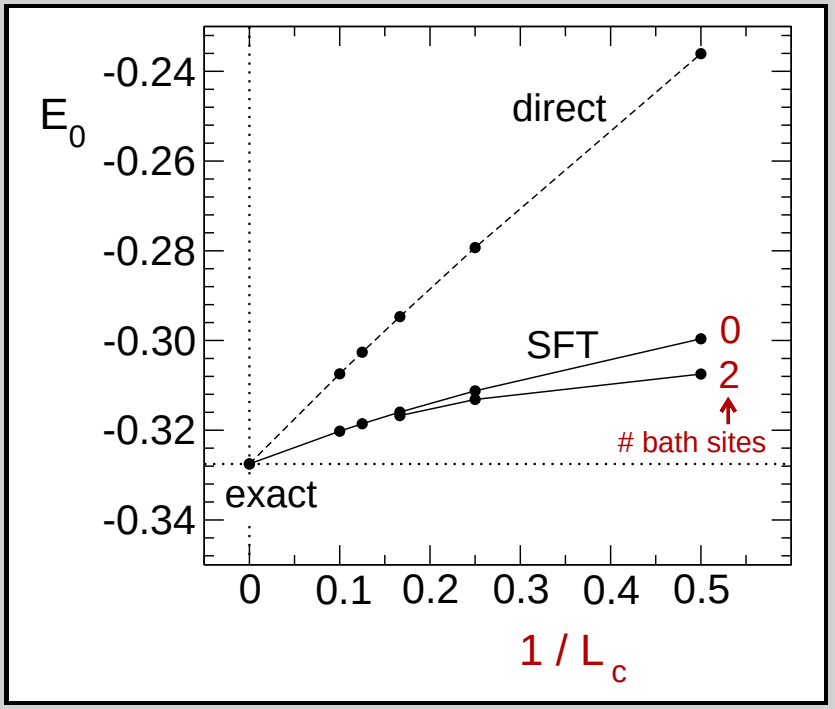
more bath sites vs. larger clusters



$D = 1$: bath sites ?



exact: *Lieb, Wu (1968)*



➜ larger cluster vs. more bath sites

➜ enhanced convergence

DMFT as Type-I,II,III Approximation

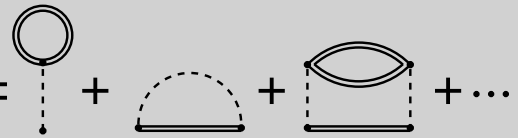
dynamical mean-field theory

information on excitations (PES,IPE) $\rightarrow$ one-particle Green's function $G_{\alpha\beta}(\omega)$

$$\mathbf{G} = \frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]}$$

Dyson's equation

free ($\mathbf{U} = 0$) Green's function

skeleton expansion $\Sigma_U[G] =$  $+\cdots$

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information on excitations (PES,IPE) $\rightarrow$ one-particle Green's function $G_{\alpha\beta}(\omega)$

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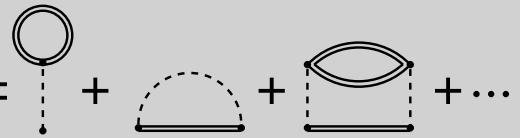
skeleton expansion $\Sigma_U[G] =$  $+ \cdots$

DMFT as type-I approximation:

$$\mathbf{G} = \frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]} \rightarrow \mathbf{G} = \frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1} - \widetilde{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}]}$$

with $\widetilde{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}]$: functional of an impurity model (vertices restricted to a single-site)

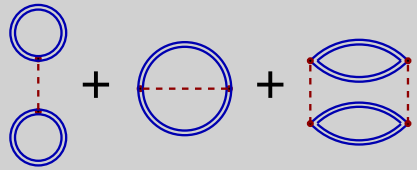
Metzner, Vollhardt (1989)
Georges, Kotliar, Jarrell (1992)

$$(\mathbf{G}_{\mathbf{t}^i,0})_{ii} = \frac{1}{(\mathbf{G}_{ii})^{-1} - (\mathbf{\Sigma})_{ii}}$$

DMFT self-consistency cycle:

$$H_{\mathbf{t}^i,\mathbf{U}} \rightarrow \mathbf{\Sigma} \rightarrow \mathbf{G} = \frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}}$$

dynamical variational principles

Luttinger-Ward functional: $\Phi =$  $+ \cdots,$ $\quad \frac{1}{T}\frac{\delta \Phi_{\mathbf{U}}[\mathbf{G}]}{\delta \mathbf{G}} = \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}] = \mathrm{Tr}\ln \mathbf{G} - \mathrm{Tr}((\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{G}^{-1})\mathbf{G}) + \Phi_{\mathbf{U}}[\mathbf{G}]$$

Luttinger, Ward (1960)

universal, extremely complicated

Euler equation $\Leftrightarrow$ Dyson's equation

$$0 = \frac{1}{T}\frac{\delta \Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}]}{\delta \mathbf{G}} = \mathbf{G}^{-1} - \mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$$

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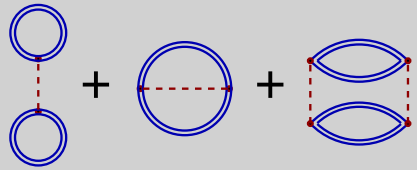
Luttinger-Ward functional: $\Phi =$  $+\cdots$, $\quad \frac{1}{T}\frac{\delta\Phi_{\mathbf{U}}[\mathbf{G}]}{\delta\mathbf{G}} = \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$

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DMFT as type-II approximation:

$\Phi_{\mathrm{U}}[\mathbf{G}] \to \widetilde{\Phi}_{\mathrm{U}}[\mathbf{G}]$ (impurity model)

➜ $\mathbf{\Sigma}_{\mathrm{U}}[\mathbf{G}] \to \widetilde{\mathbf{\Sigma}}_{\mathrm{U}}[\mathbf{G}]$

➜ Dyson's equation $\to$ DMFT s.-c. equation

conserving approximations:

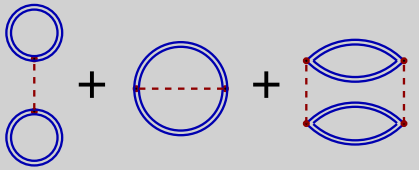
$\Phi_{\mathrm{U}}[\mathbf{G}] \to \widetilde{\Phi}_{\mathrm{U}}[\mathbf{G}]$

(certain diagram classes)

➜ **type-II**

Baym, Kadanoff (1961)

dynamical variational principles

Luttinger-Ward functional: $\Phi =$  $+\cdots$, $\quad \frac{1}{T}\frac{\delta \Phi_{\mathbf{U}}[\mathbf{G}]}{\delta \mathbf{G}} = \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}] = \mathrm{Tr}\ln \mathbf{G} - \mathrm{Tr}((\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{G}^{-1})\mathbf{G}) + \Phi_{\mathbf{U}}[\mathbf{G}]$$

Luttinger, Ward (1960)

universal, extremely complicated

Euler equation $\Leftrightarrow$ Dyson's equation

$$0 = \frac{1}{T}\frac{\delta \Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}]}{\delta \mathbf{G}} = \mathbf{G}^{-1} - \mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$$

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➜ $\mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}] \to \widetilde{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}]$

➜ Dyson's equation $\to$ DMFT s.-c. equation

conserving approximations:

$\Phi_{\mathbf{U}}[\mathbf{G}] \to \widetilde{\Phi}_{\mathbf{U}}[\mathbf{G}]$

(certain diagram classes)

➜ **type-II**

Baym, Kadanoff (1961)

type-III approximation ? choose reference system with $\mathbf{U} = \mathbf{U}^{\imath}$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}] = \mathrm{Tr}\ln \mathbf{G} - \mathrm{Tr}((\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{G}^{-1})\mathbf{G}) + \Phi_{\mathbf{U}}[\mathbf{G}]$$

$$\Omega_{\mathbf{t}^{\imath},\mathbf{U}}[\mathbf{G}] = \mathrm{Tr}\ln \mathbf{G} - \mathrm{Tr}((\mathbf{G}^{-1}_{\mathbf{t}^{\imath},0} - \mathbf{G}^{-1})\mathbf{G}) + \Phi_{\mathbf{U}}[\mathbf{G}]$$

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}] = \Omega_{\mathbf{t}^{\imath},\mathbf{U}}[\mathbf{G}] - \mathrm{Tr}(\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{G}^{-1}_{\mathbf{t}^{\imath},0})\mathbf{G} = \Omega_{\mathbf{t},\mathbf{U}}[\rho_{\mathbf{t}^{\imath},\mathbf{U}}]$$

reduces to Rayleigh-Ritz principle !

dynamical variational principles

problem:

type-III & impurity model as reference system ➜ local Green's function

dynamical variational principles

problem:

type-III & impurity model as reference system ➜ local Green's function

alternative functional:

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}] = \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]} - \mathrm{Tr}(\mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]\mathbf{G}) + \Phi_{\mathbf{U}}[\mathbf{G}]$$

Chitra, Kotliar (2001)

Euler equation $\Leftrightarrow$ Dyson's equation

DMFT as type-II approximation:

$\Phi_{\mathrm{U}}[\mathbf{G}] \to \widetilde{\Phi}_{\mathrm{U}}[\mathbf{G}]$

$\mathbf{\Sigma}_{\mathrm{U}}[\mathbf{G}] \to \widetilde{\mathbf{\Sigma}}_{\mathrm{U}}[\mathbf{G}]$

➜ DMFT self-consistency equation

type-III approximation ?

reference system:

impurity model with $\mathbf{U} = \mathbf{U}^{\imath}$

➜ $\mathbf{G}_{\mathbf{t}^{\imath},\mathbf{U}}$ is local !

dynamical variational principles

problem:

type-III & impurity model as reference system ➜ local Green's function

alternative functional:

$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}] = \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]} - \mathrm{Tr}(\mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]\mathbf{G}) + \Phi_{\mathbf{U}}[\mathbf{G}]$$

Chitra, Kotliar (2001)

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$\mathbf{\Sigma}_{\mathrm{U}}[\mathbf{G}] \rightarrow \widetilde{\mathbf{\Sigma}}_{\mathrm{U}}[\mathbf{G}]$

➜ DMFT self-consistency equation

type-III approximation ?

reference system:

impurity model with $\mathbf{U} = \mathbf{U}^{\imath}$

➜ $\mathbf{G}_{\mathbf{t}^{\imath},\mathbf{U}}$ is local !

functional of the local Green's function:

$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{G}^{(\mathrm{loc})}]$

Chitra, Kotliar (2000)

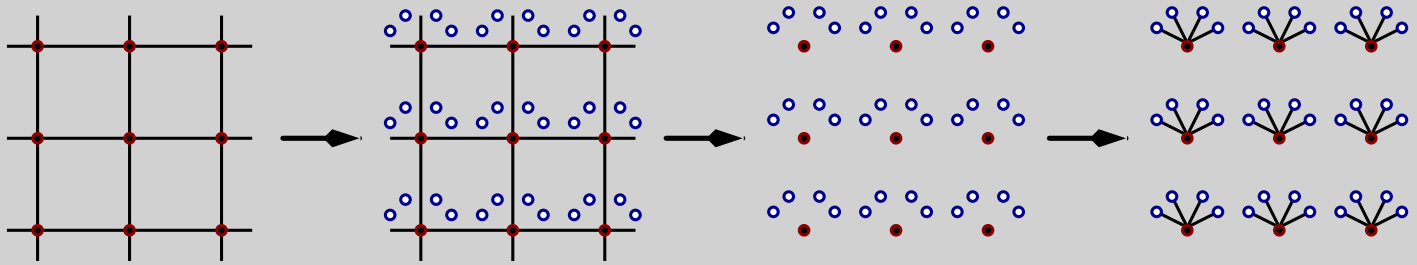
DMFT as type-II approximation

Georges (2004)

self-energy-functional approach

self-energy as the basic variable *Potthoff (2003)*

original system **reference system**



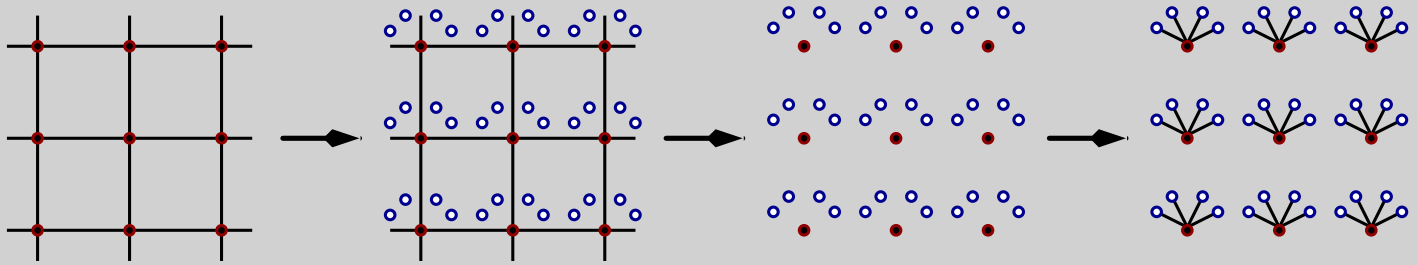
➜ Σ is local

➜ Σ is non-zero on the correlated sites only

self-energy-functional approach

self-energy as the basic variable *Potthoff (2003)*

original system **reference system**



➜ $\boldsymbol{\Sigma}$ is local

➜ $\boldsymbol{\Sigma}$ is non-zero on the correlated sites only

$$\Omega_{\mathbf{t},\mathbf{U}}[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\mathbf{G}_{\mathbf{t},0}^{-1}-\boldsymbol{\Sigma}} + F_{\mathbf{U}}[\boldsymbol{\Sigma}]$$

$F_{\mathbf{U}}[\boldsymbol{\Sigma}]$ = Legendre transform of $\Phi_{\mathbf{U}}[\mathbf{G}]$

➜ $\Omega_{\mathbf{t},\mathbf{U}}[\boldsymbol{\Sigma}_{\mathbf{t},\mathbf{U}}] = \Omega_{\mathbf{t},\mathbf{U}}$ ✔

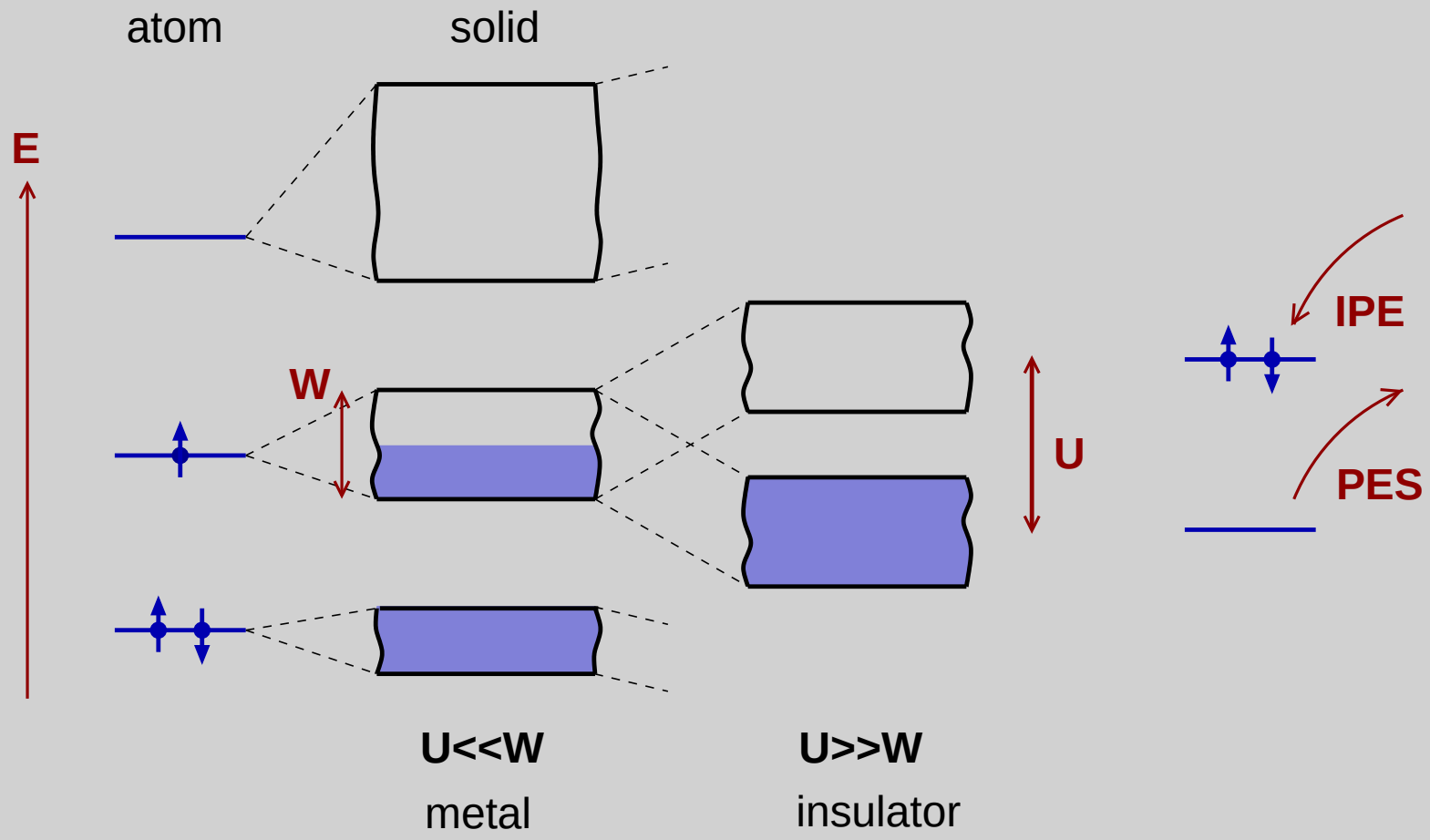
➜ Euler equation: $\dfrac{1}{\mathbf{G}_{\mathbf{t},0}^{-1}-\boldsymbol{\Sigma}} - \mathbf{G}_{\mathbf{U}}[\boldsymbol{\Sigma}] = 0 \Leftrightarrow$ Dyson's equation ✔

➜ Euler equation on $\widetilde{\mathcal{A}}$: $\dfrac{\partial}{\partial \mathbf{t}^{\imath}}\Omega_{\mathbf{t},\mathbf{U}}[\boldsymbol{\Sigma}_{\mathbf{t}^{\imath},\mathbf{U}}] = 0 \Leftrightarrow$ DMFT self-consistency equation ✔

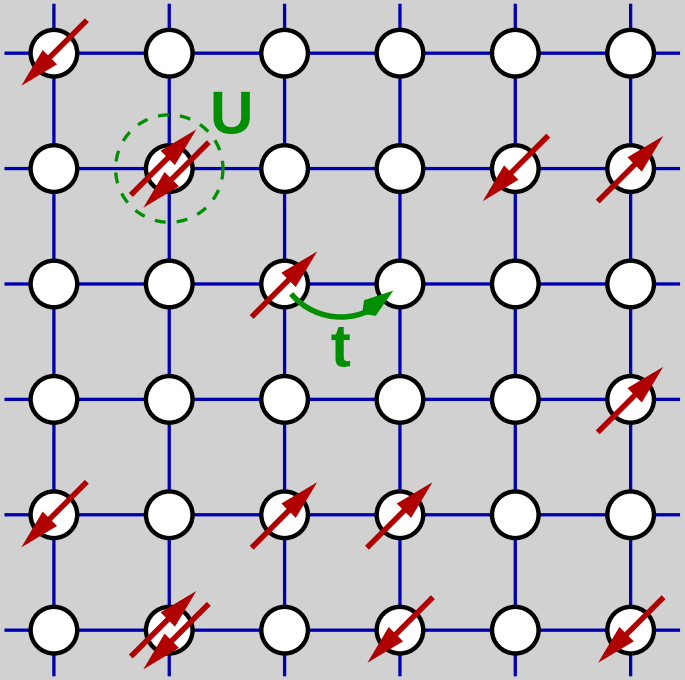
➜ **DMFT as type-III approximation**

DMFT of the Mott Transition

Mott transition



generic model



Hubbard model generic for the Mott transition

$$H = -t \sum_{ij\sigma}^{n.n.} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{\sigma} n_{i\sigma} n_{i-\sigma}$$

parameters:

— lattice structure, dimension

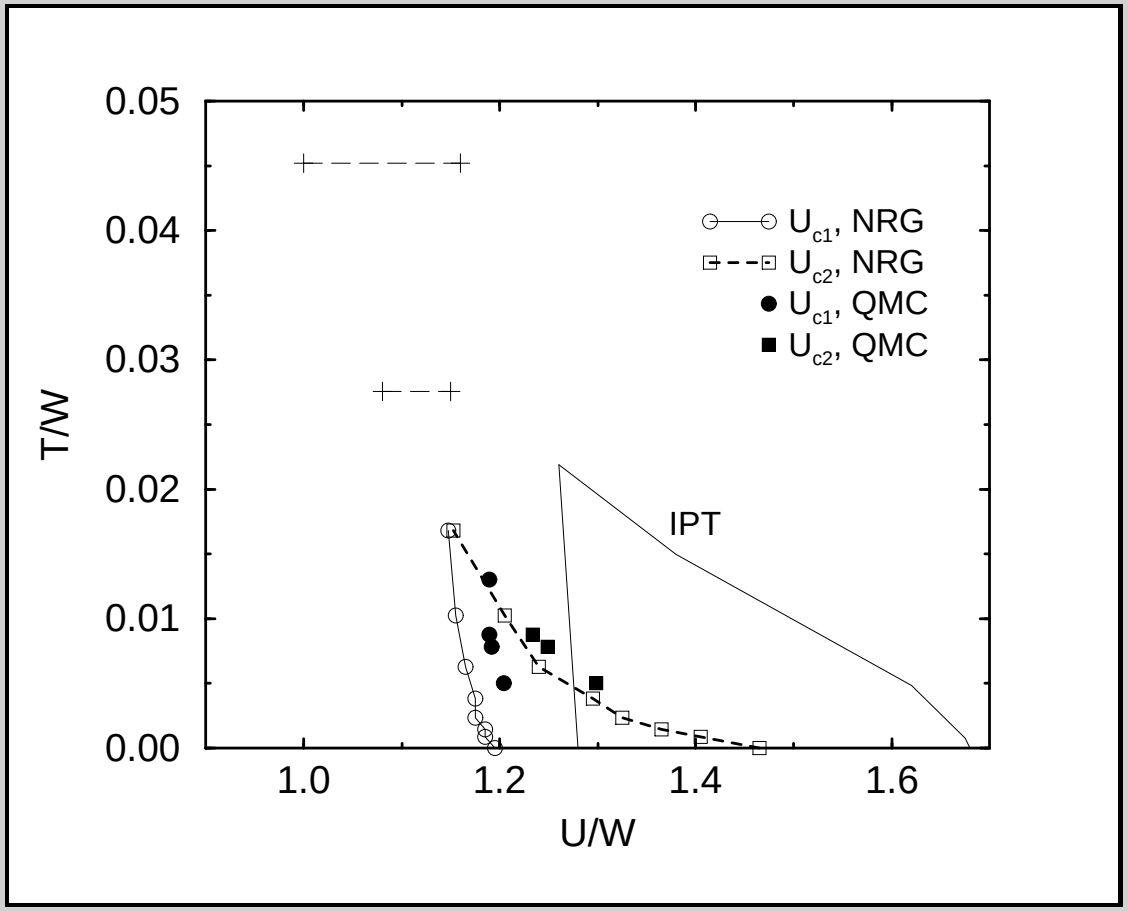
— n.n. hopping: t

— local interaction: U

— electron density : $n = N/L$

— temperature T

DMFT phase diagram



Hubbard model
half-filling
semielliptical DOS
$W = 4$

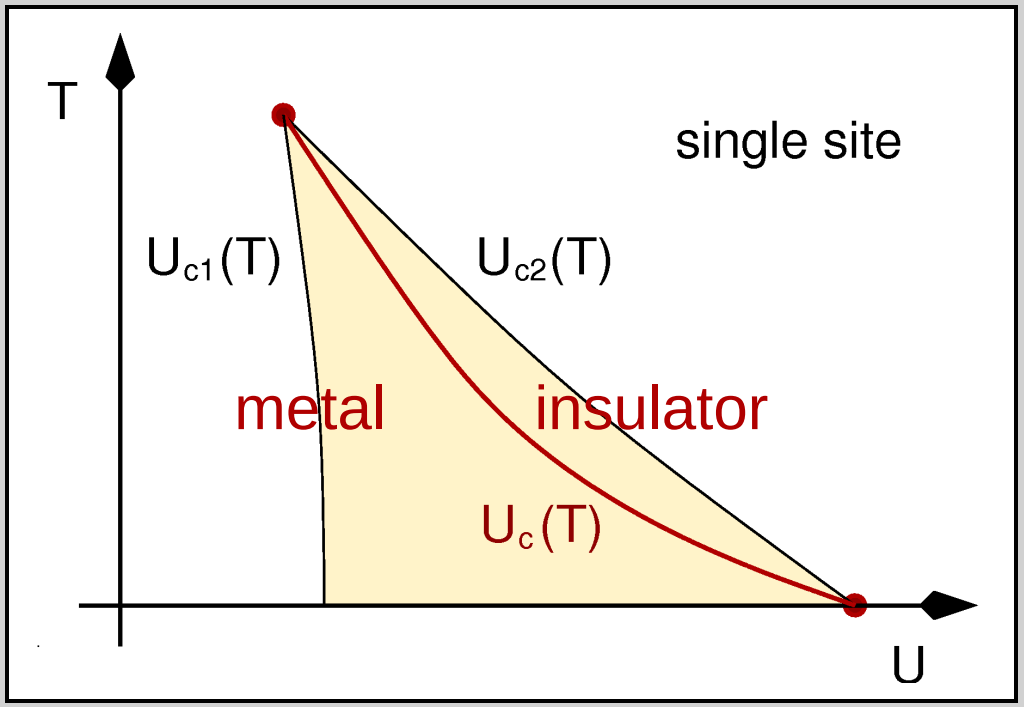
NRG
Bulla, Costi, Vollhardt (2001)

QMC
Joo, Oudovenko (2000)

$T = 0$: **continuous phase transition**
$T > 0$: **discontinuous transition**
$T > T_C$: **crossover**

Georges, Krauth, Kotliar, Rozenberg (1996)

DMFT phase diagram



$T = 0$: **continuous phase transition**

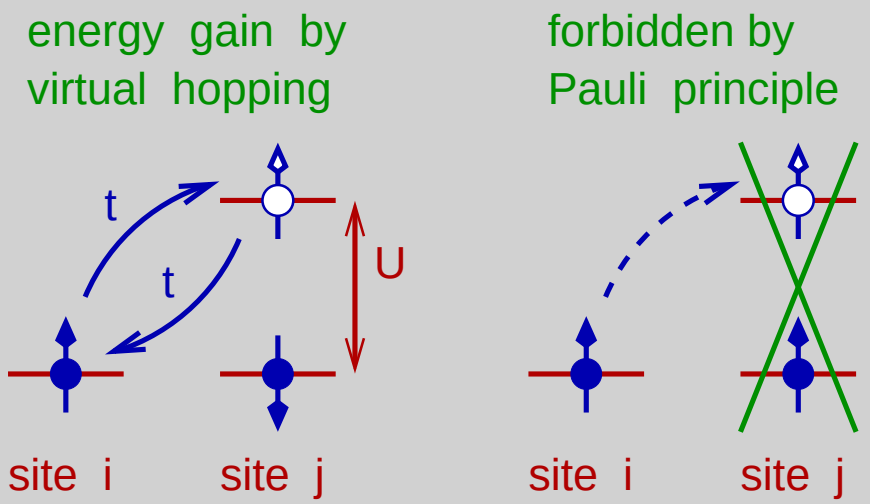
$T > 0$: **discontinuous transition**

$T > T_C$: **crossover**

Georges, Krauth, Kotliar, Rozenberg (1996)

effective Heisenberg model

Anderson's superexchange mechanism



at low energies / temperatures:

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j \qquad \text{with} \qquad J_{ij} \propto -\frac{t^2}{U}$$

antiferromagnetic Heisenberg model

magnetic correlations and entropy

Heisenberg insulator for $U \gg t$:

➜ at low energies: Heisenberg model with $J \sim -\dfrac{t^2}{U}$

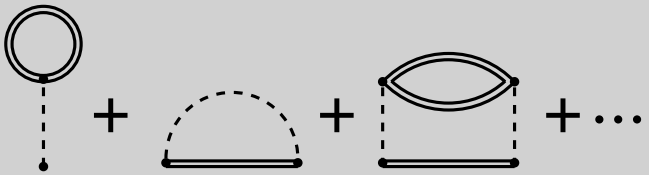
➜ long-range AF order (also for $D = \infty$, within DMFT)

Mott insulator for $U \gg t$:

➜ metastable paramagnetic state with well-formed local moment $S = 1/2$

➜ strong nearest-neighbor (AF) magnetic correlations

Mott insulator within DMFT:

$\Sigma_U[G] =$  $+ \cdots$

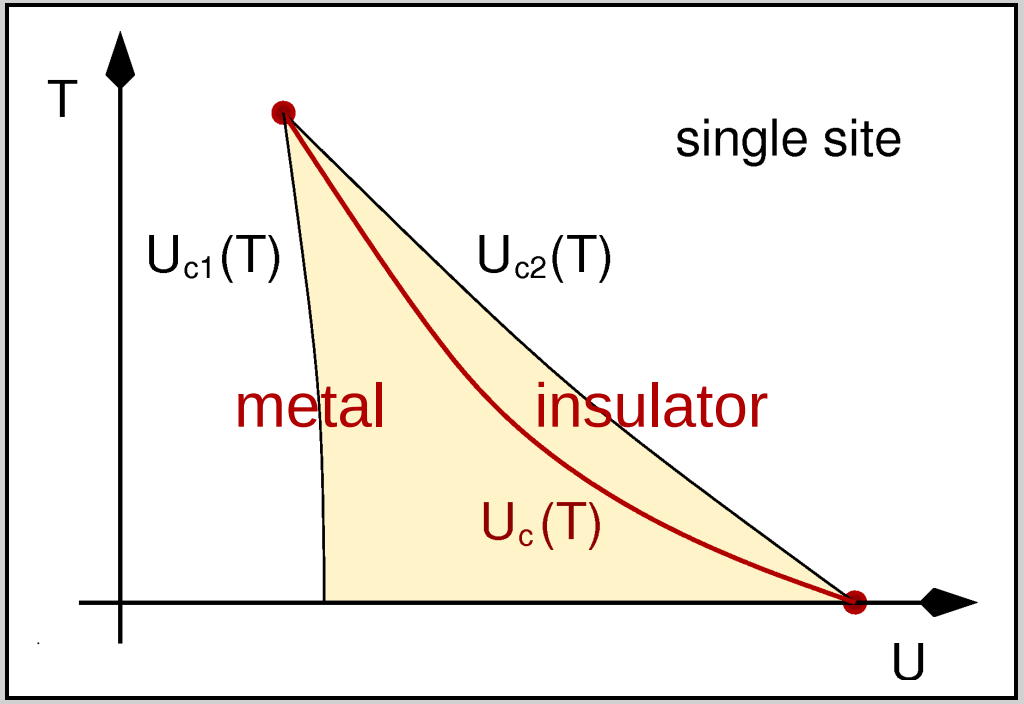
➜ no feedback of nonlocal magnetic correlations on $\mathbf{\Sigma}$

$$\Omega_{\rm DMFT} = L\Omega_{\rm imp} + \mathrm{Tr}\ln\frac{1}{\mathbf{G}_0^{-1} - \mathbf{\Sigma}} - L\mathrm{Tr}\ln G_{\rm imp}$$

➜ free energy F, entropy $S = -\dfrac{\partial F}{\partial T} \sim$ system of decoupled local moments

$$\boxed{S(T=0) = L\ \log 2} \qquad \text{(Mott insulator, DMFT)}$$

entropy problem



metal: $S(0)/L = 0$

insulator: $S(0)/L = \log 2$ (mean-field artifact)

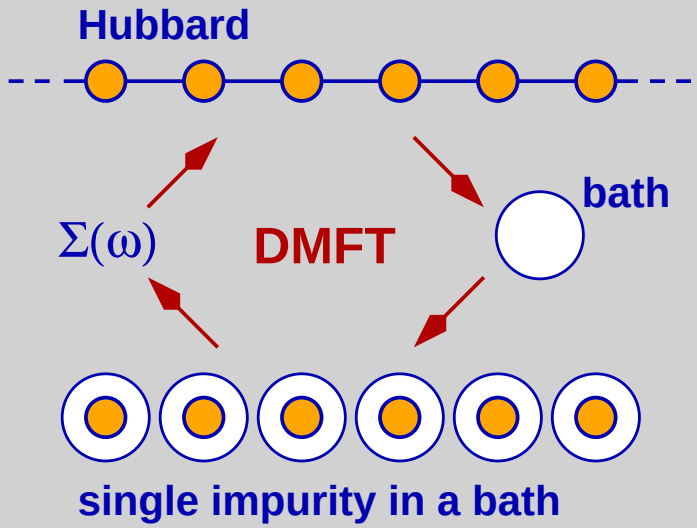
at finite T: $F_{\rm met} = E_{\rm met} - TS_{\rm met} > E_{\rm ins} - TS_{\rm ins} = F_{\rm ins}$

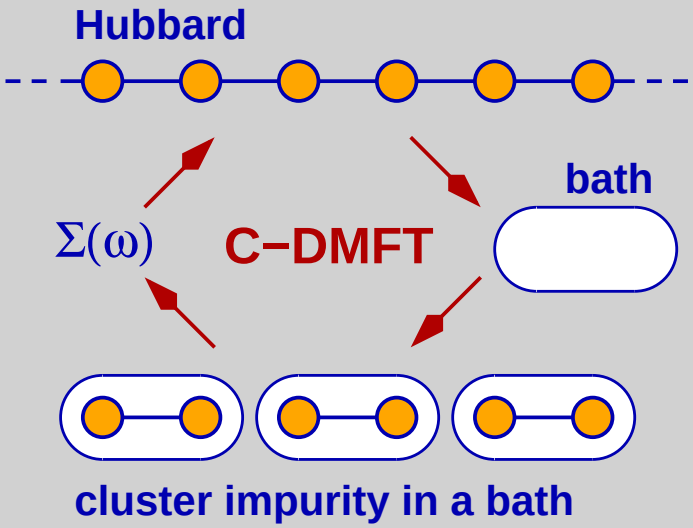
the insulator wins at higher temperatures

Q: mean-field artifact ?

Q: phase-diagram topology for $D = 2$?

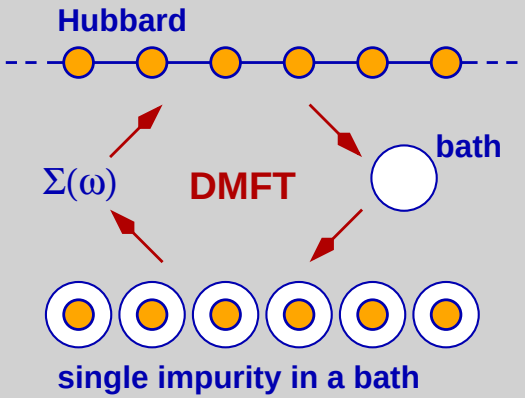
plaquette DMFT

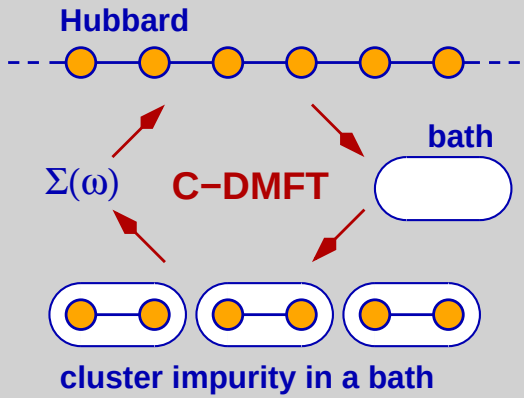




singlet formation ➜ $S(T=0)=0$

plaquette DMFT

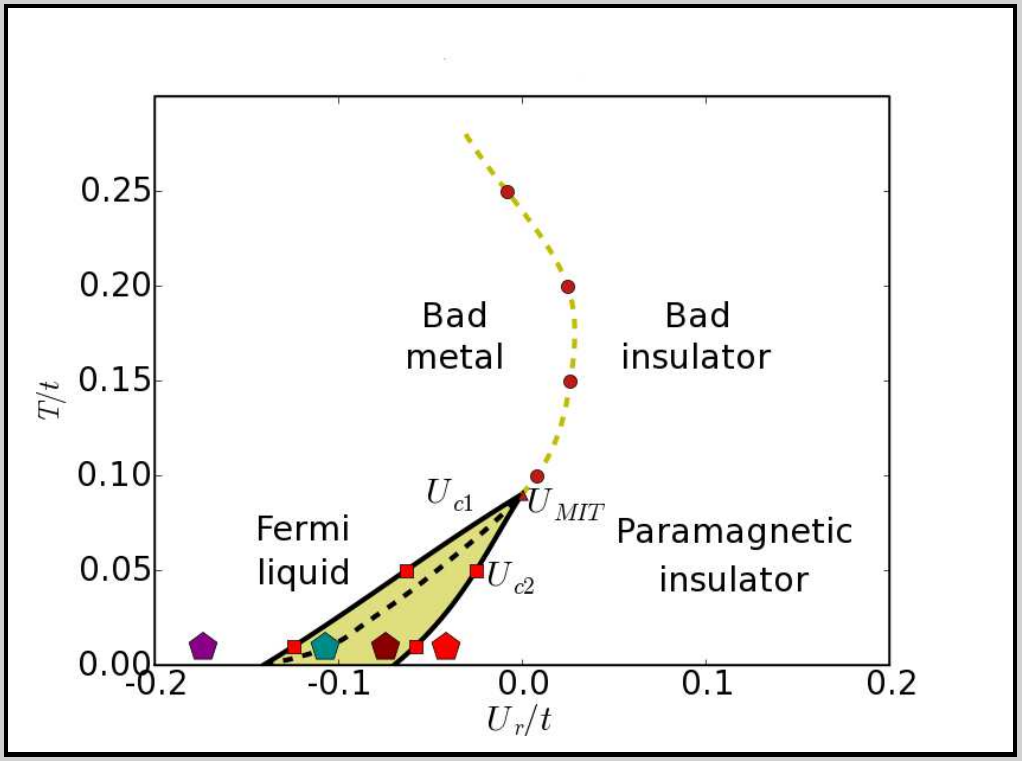




$D = 2$ square lattice:
$L_c = 4$ (plaquette)

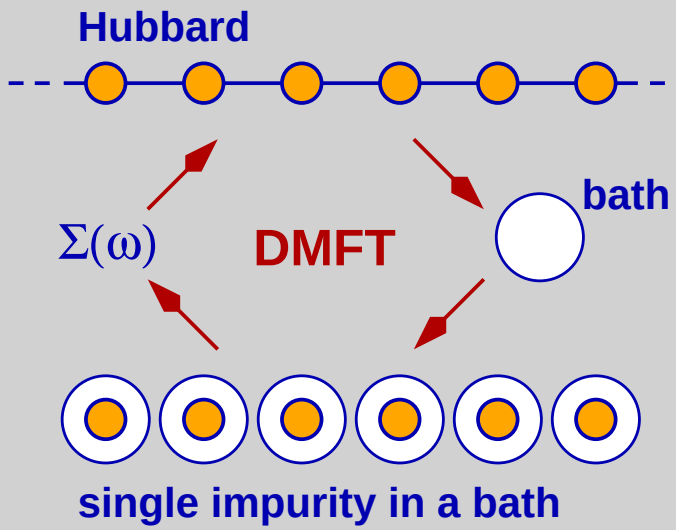
diagrammatic QMC, finite T

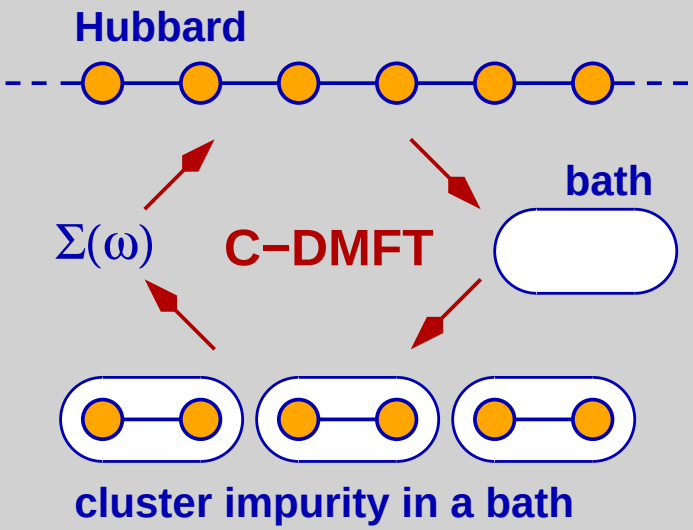
smaller U_c
coexistence (different shape)
$T > 0$: first-order transition



Park, Haule Kotliar (2008)

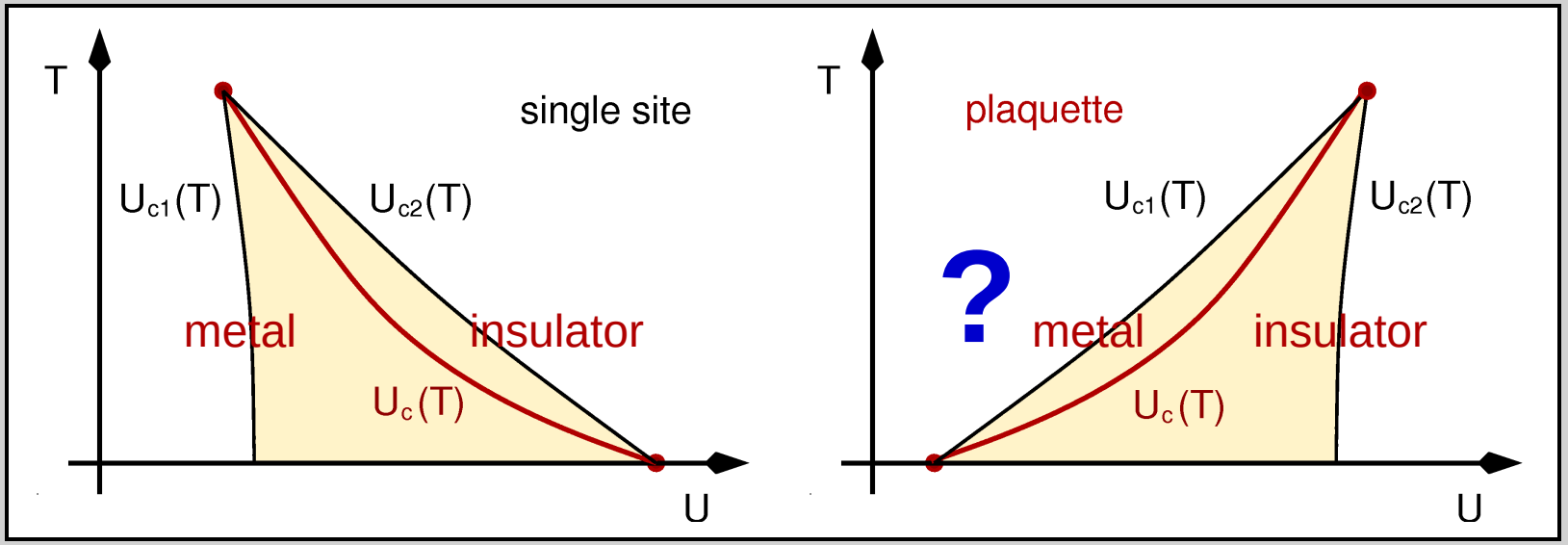
plaquette DMFT





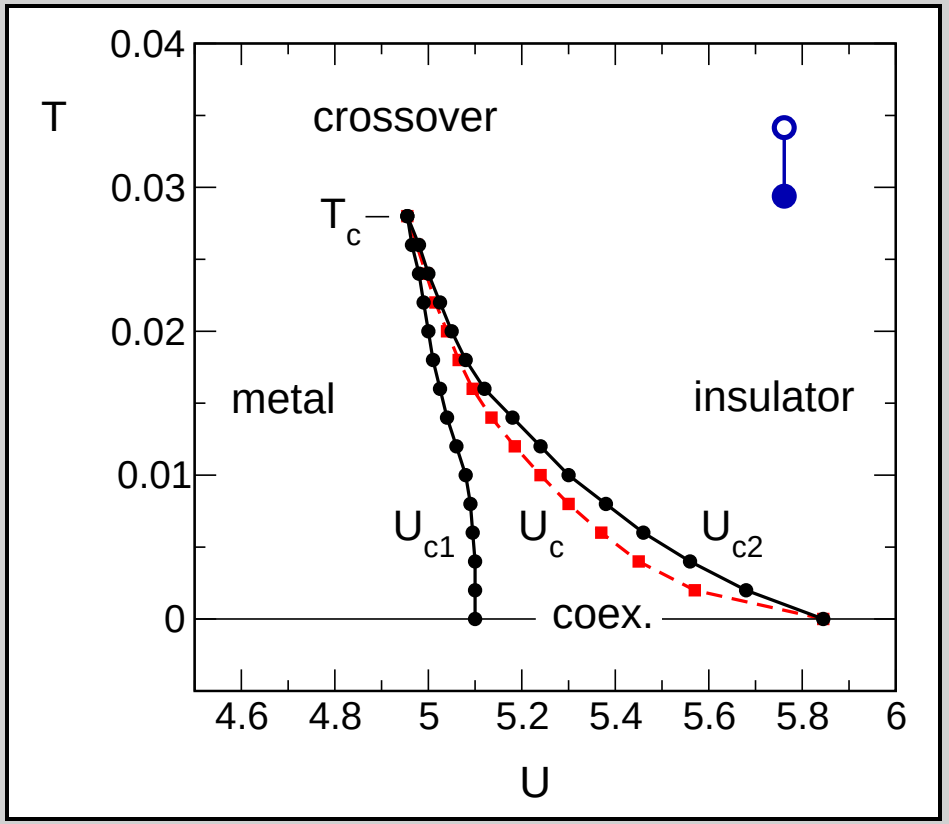
the insulator wins at higher temperatures

the metal wins at higher temperatures ?



Mott Transition within the DIA

dynamical impurity approximation (DIA)



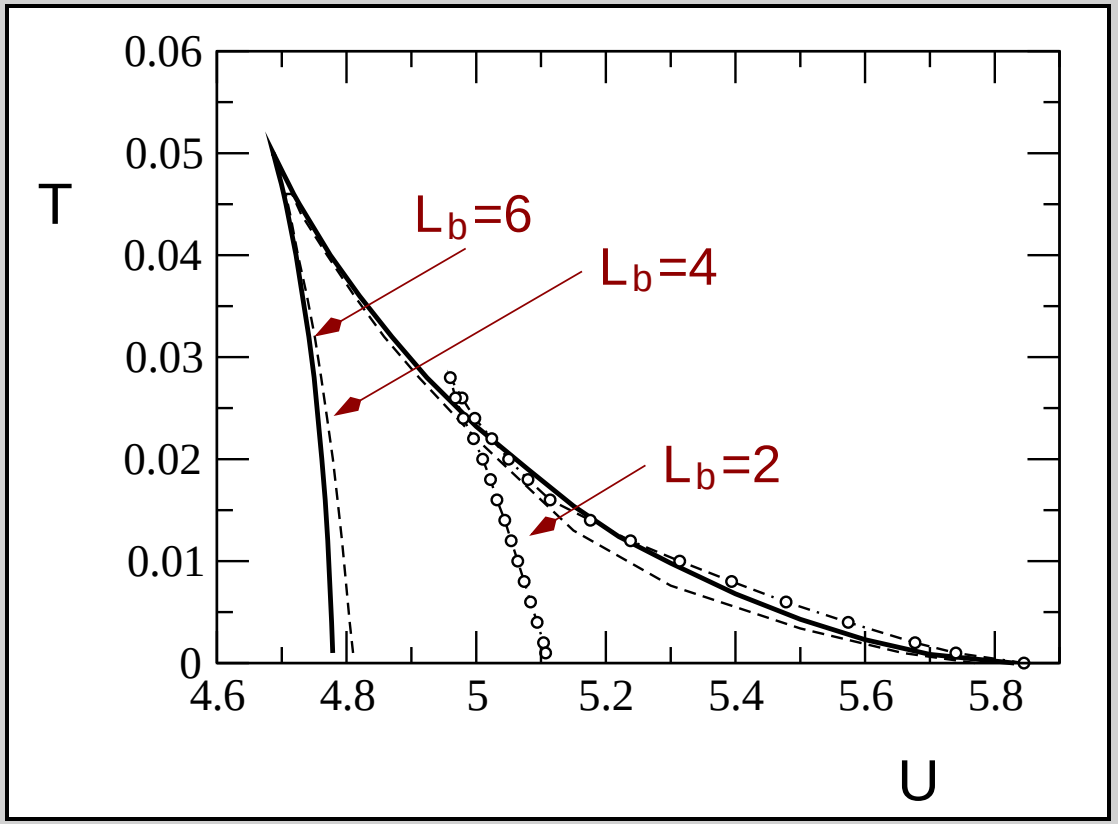
Hubbard model
half-filling
semi-elliptical DOS
$W = 4$

DIA with $n_s = 2$

➜ **qualitative agreement with full DMFT (QMC, NRG)**

Georges et al 1996, Joo, Oudovenko 2000, Bulla et al 2001

DIA - convergence to the DMFT



Hubbard model
half-filling
semi-elliptical DOS
$W = 4$

DIA with $n_s = 2$

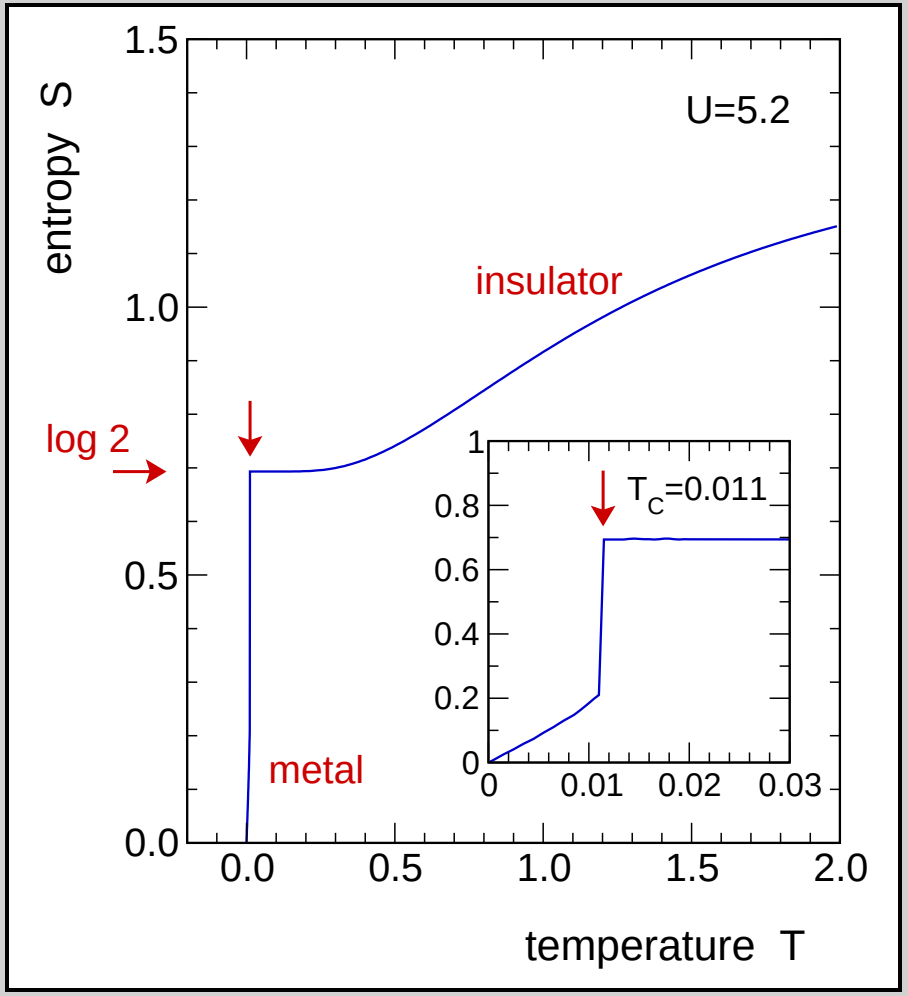
Pozgajcic 2004

➜ **quantitative agreement with full DMFT (QMC, NRG)**

Georges et al 1996, Joo, Oudovenko 2000, Bulla et al 2001

➜ **rapid convergence with increasing n_s**

entropy problem



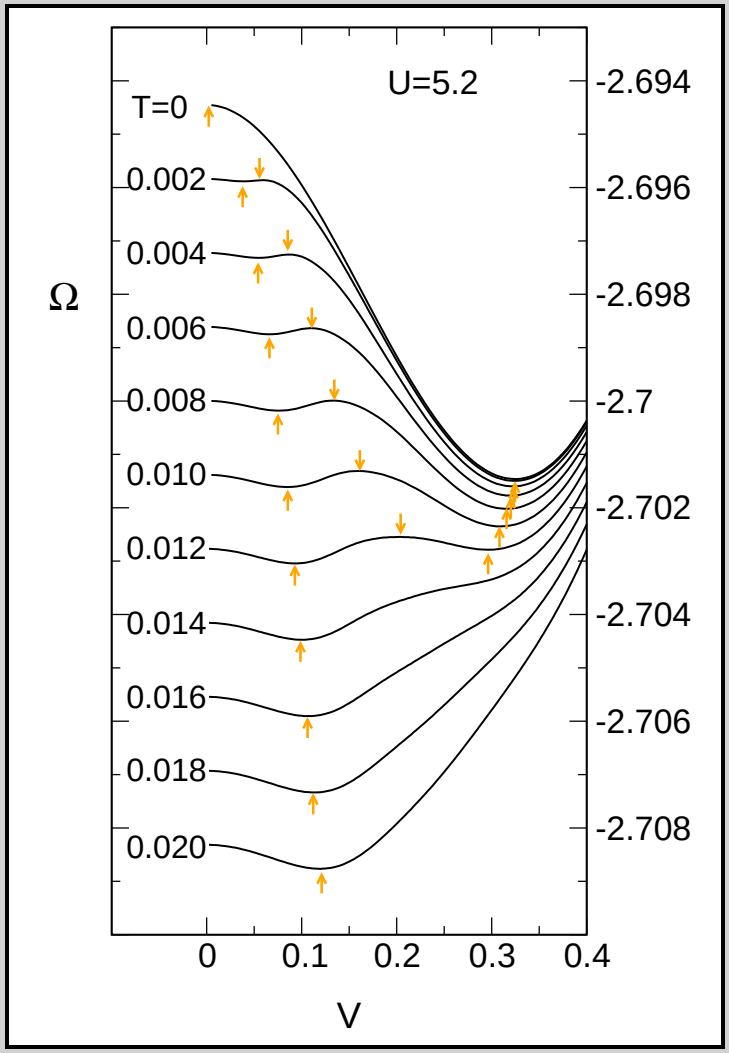
Hubbard model
half-filling
semi-elliptical DOS
$W = 4$

DIA with $n_s = 2$

➜ **Mott insulator: macroscopic ground-state degeneracy**

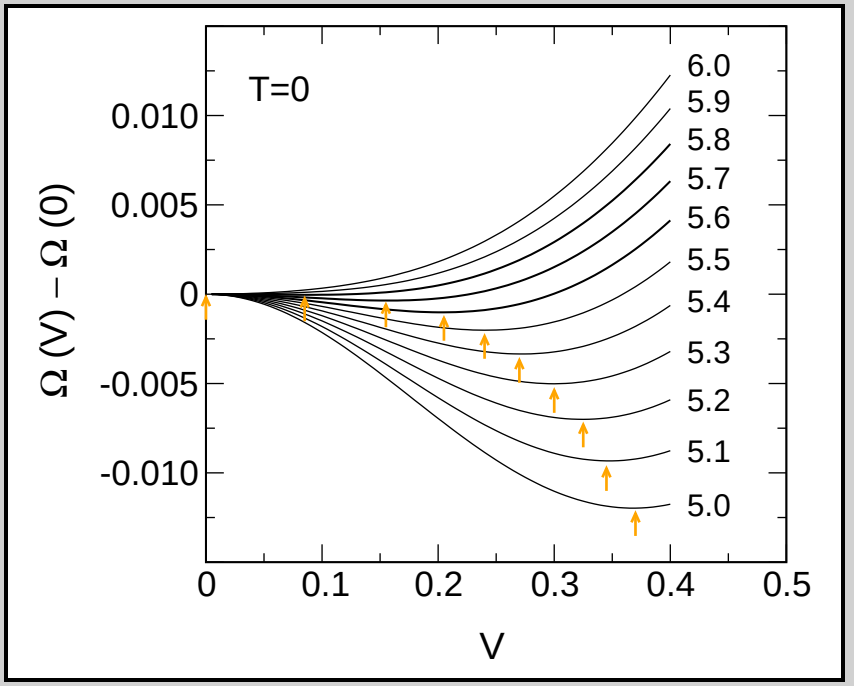
➜ **Fermi liquid: linear** $S(T) = \gamma T + \cdots$

DIA - phase transitions



$U = 5.2$, different $T > 0$: discontinuous

$T = 0$, different U: continuous

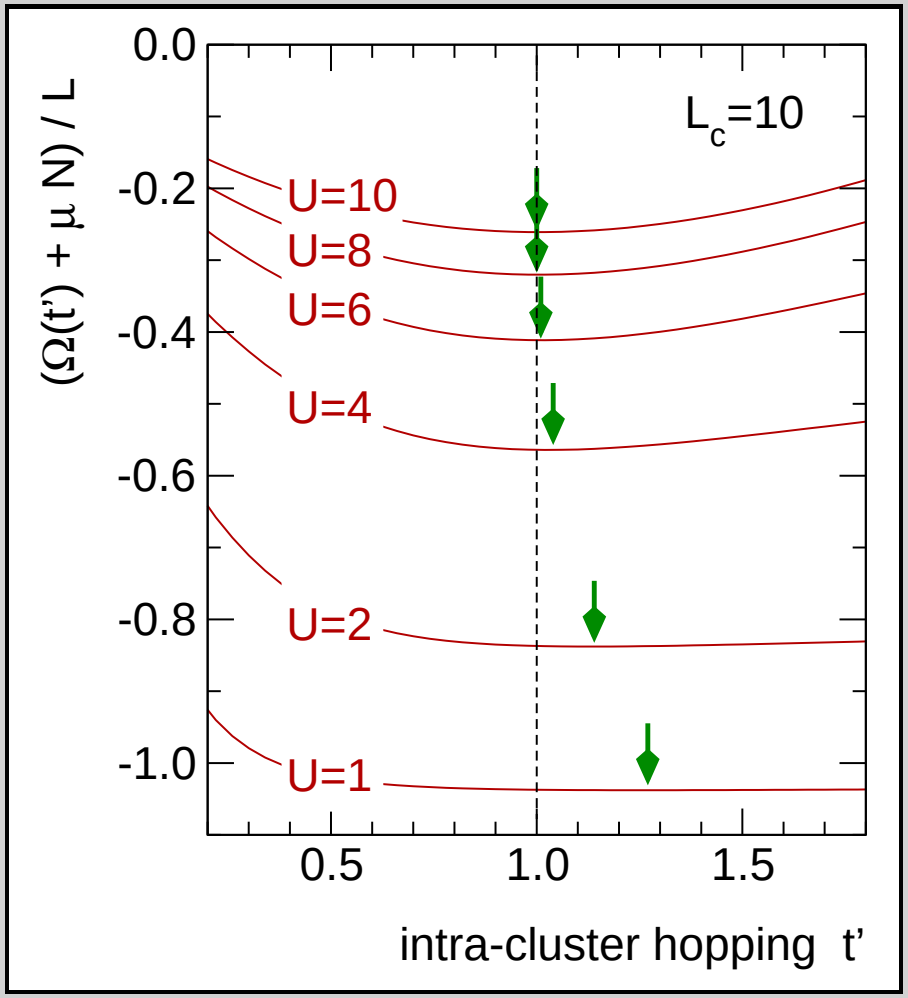


➜ **metastable states**

➜ **order of phase transitions**

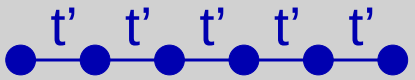
Mott Transition in $D = 1$

SFT grand potential



- $D = 1$ Hubbard model
- $L = 1000 - 2000$ sites
- energy scale:
  nearest-neighbor hopping $t = 1$
- $\mu = U/2$ (half-filling)

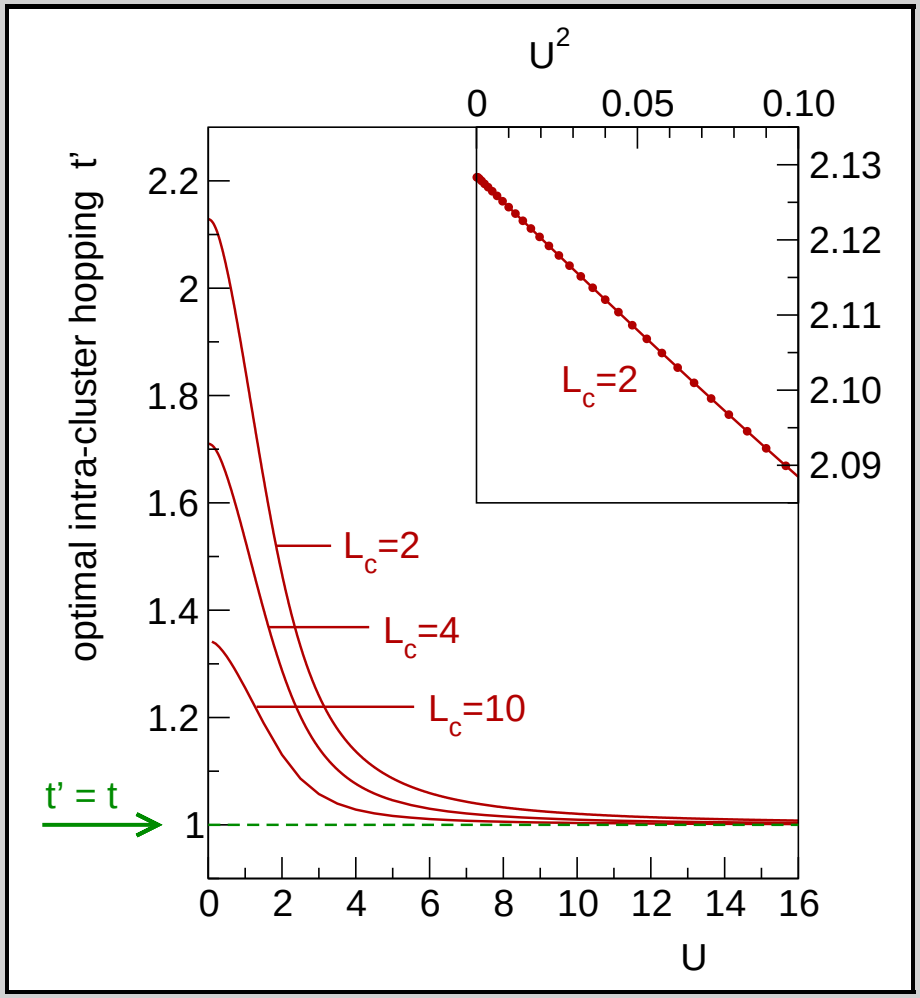
- single variational parameter:



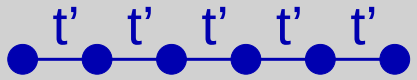
➜ **enhanced t' compensates for missing inter-cluster hopping**

➜ **for more itinerant system ($U \to 0$) stronger compensation necessary**

VCA: optimal intra-cluster hopping

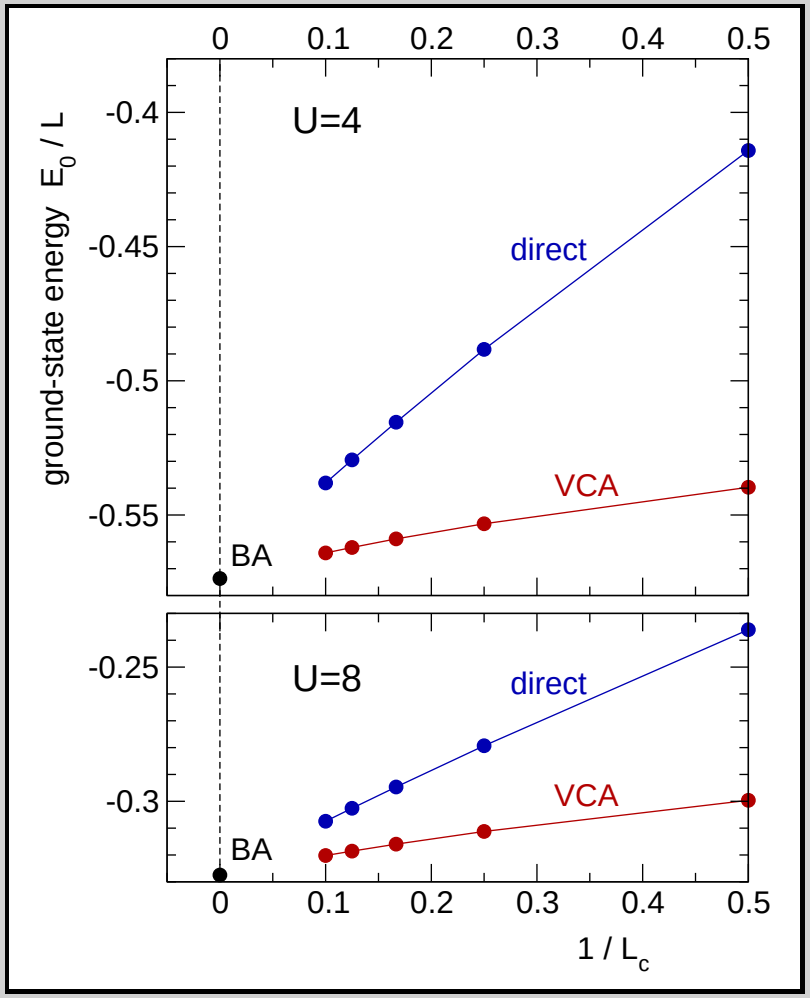


- $t = 1, \mu = U/2$
- $\Omega(t') \equiv \Omega[\mathbf{\Sigma}(t')]$

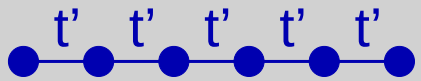


➜ **weak coupling: strong renormalization of t' vs. small self-energy**

finite-size scaling



- $t = 1$, $\mu = U/2$
- VCA vs. “direct” cluster method (isolated cluster with L_c sites)



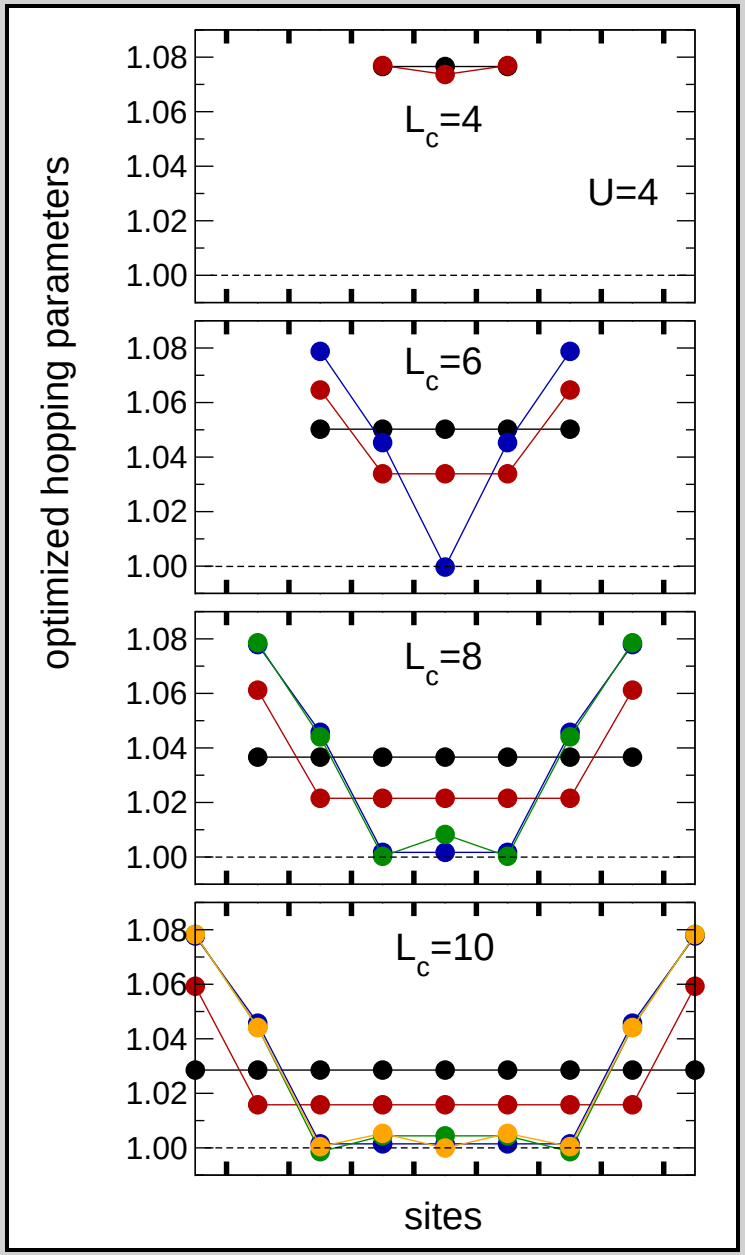
➜ **VCA: faster convergence**

➜ **no upper bounds for true ground-state energy within SFT**

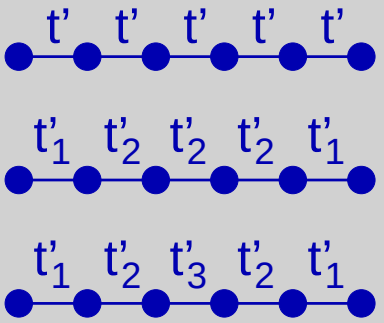
VCA: recipe for practical calculations

- set up cluster reference system (here: choose L_c, U)
  and fix the variational parameters (here: t')
- use Lanczos to get poles and weights of Green's function
  $G'_{\alpha\beta}(\omega) = \sum_m Q_{\alpha m} \frac{1}{\omega - \omega'_m} Q^\dagger_{m\beta}$
- and the cluster grand potential $\Omega' = E'_0 - \mu\langle N\rangle$
- set up $\mathbf{M} = \mathbf{\Lambda} + \mathbf{Q}^\dagger \mathbf{V} \mathbf{Q}$ with $\Lambda_{mn} = \omega'_m \delta_{mn}$ and $\mathbf{V} = \mathbf{t} - \mathbf{t}'$
- get ω_m as eigenvalues of $\mathbf{M}$ (poles of the approximate lattice Green's function)
- compute SFT grand potential for $T = 0$:
  $\Omega(t') \equiv \Omega[\mathbf{\Sigma}(\mathbf{t}')] = \Omega' + \sum_m \omega_m \Theta(-\omega_m) - \sum_m \omega'_m \Theta(-\omega'_m)\ .$
- redo these steps for different cluster parameters

more variational parameters



- $t = 1, \mu = U/2$
- $U = 4$
- several hopping paramters optimized simultaneously



➜ **variation of optimal t_i' less that 10%**

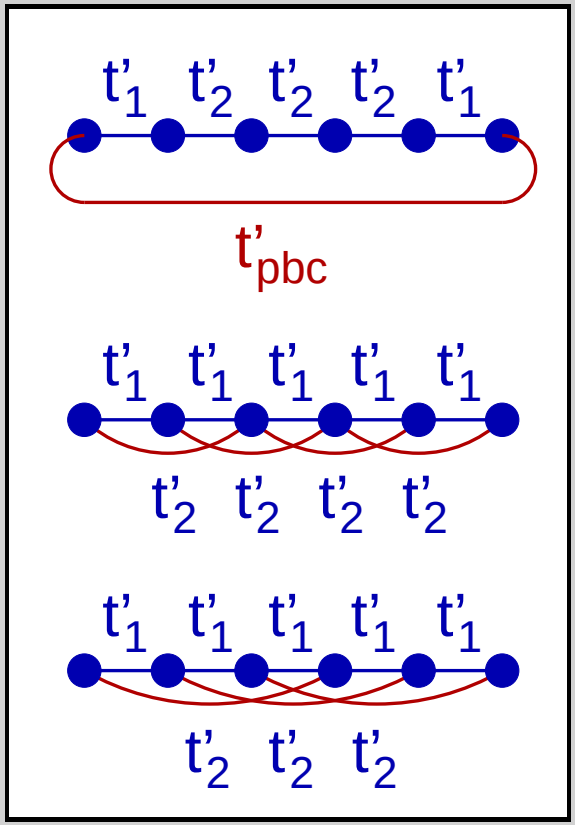
➜ **significant effects at chain edges**

➜ **third hopping parameter bulk-like**

➜ **Friedel oscillations**

➜ **almost no effect on E_0 and Δ**

more variational parameters



additional hopping linking chain edges
(boundary conditions)

second-neareast-neighbor hopping
(magnetic frustration)

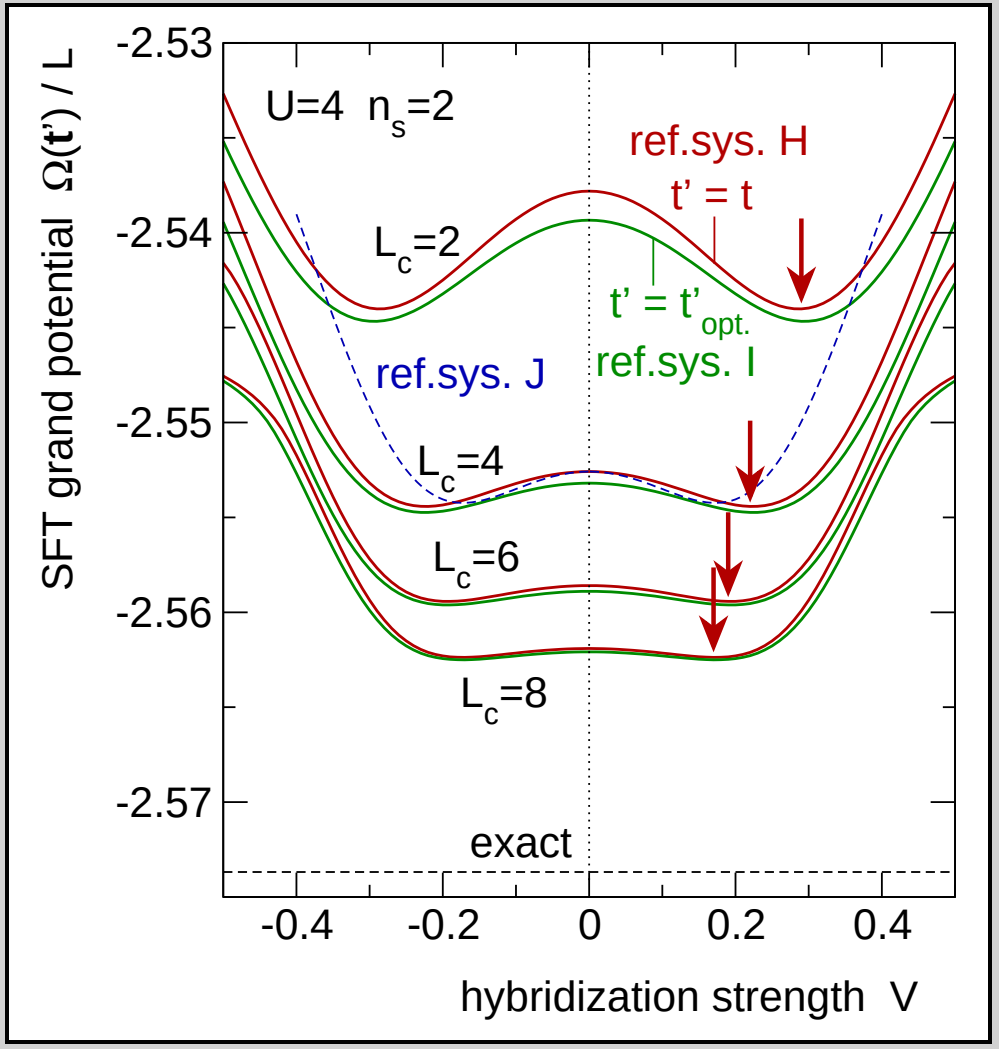
third-neareast-neighbor hopping

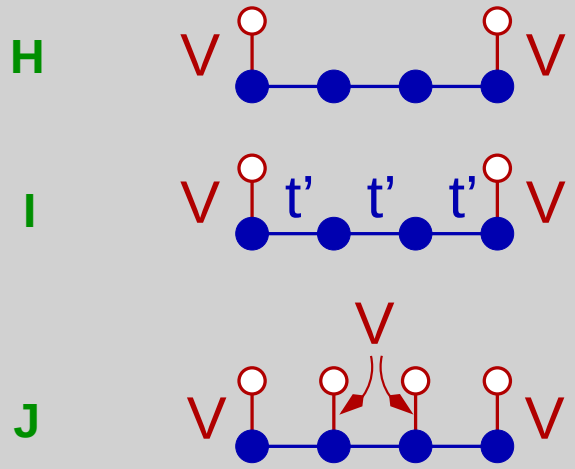
➜ **hopping parameters not present in original system: almost vanishing**

➜ **optimal $t_{\mathrm{pbc}} = 0$, no periodic (but open) boundary conditions**

➜ **optimal hopping $= 0$, if incompatible with particle-hole symmetry**

bath sites



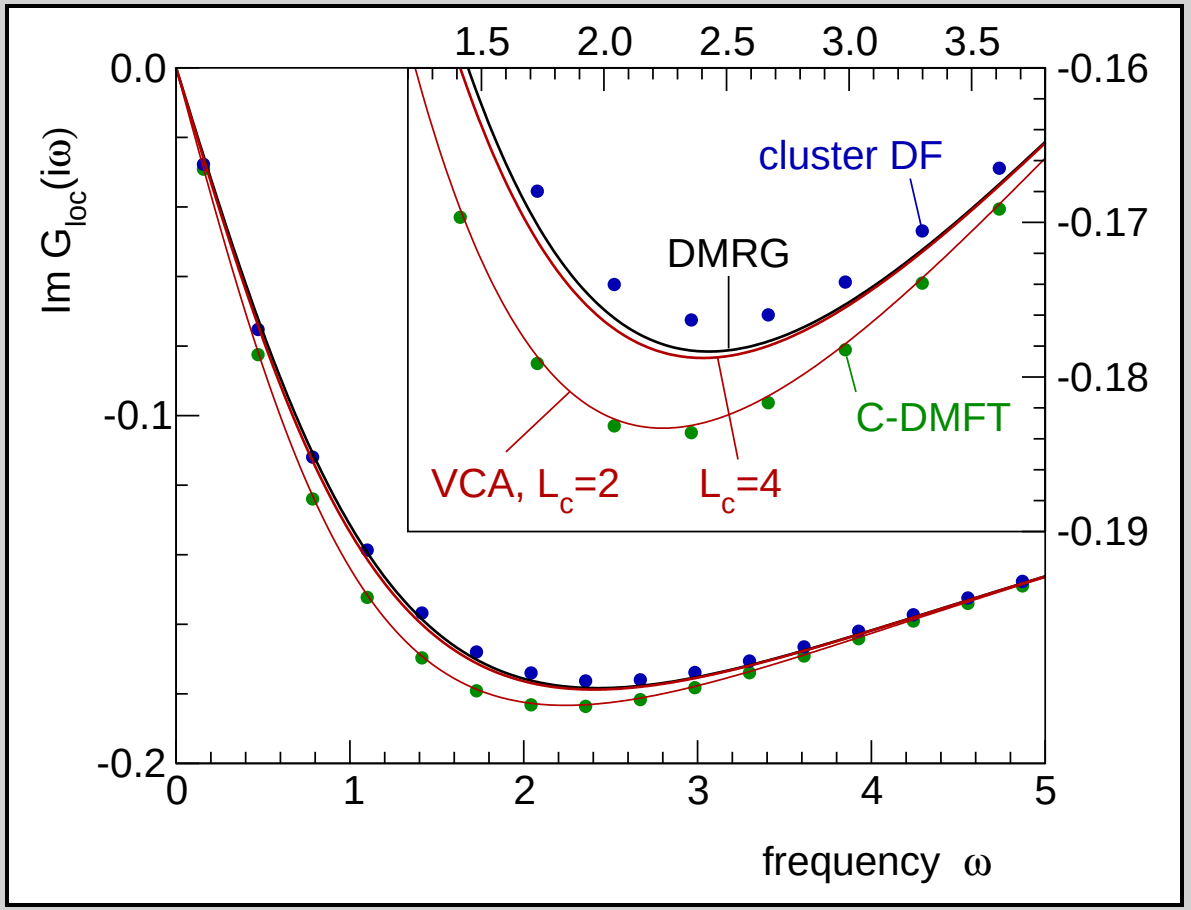


➜ **I vs. H: optimization of bath sites more effective than hopping**

➜ **J vs. H, I: bath sites at chain center ineffective**

➜ **different L_c: larger clusters more effective than optimization**

local Matsubara Green's function



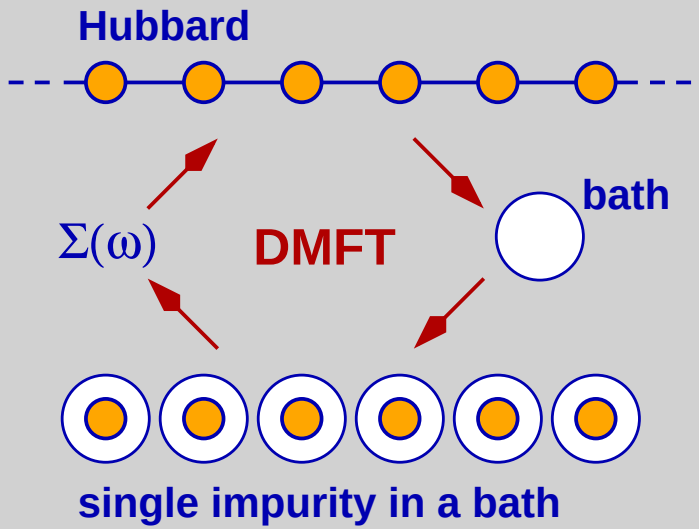
- $t = 1$, $\mu = U/2$, $U = 6$
- VCA with $n_s = 3$
- C-DMFT with $n_s = \infty$ ($\beta = 20$)
- cluster DF for $L_c = 2$ ($\beta = 20$)
- (dynamical) DMRG: numerically exact

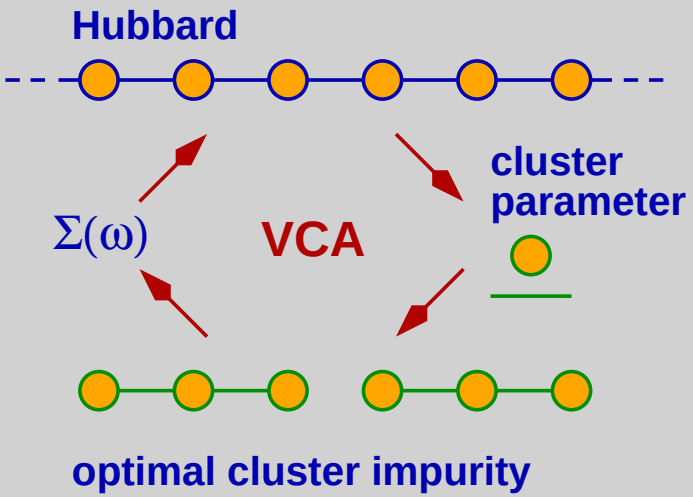
➜ **VCA comparable to C-DMFT**

DMRG, C-DMFT, cluster DF: *Hafermann et al. 2007*

Mott Transition in $D = 2$

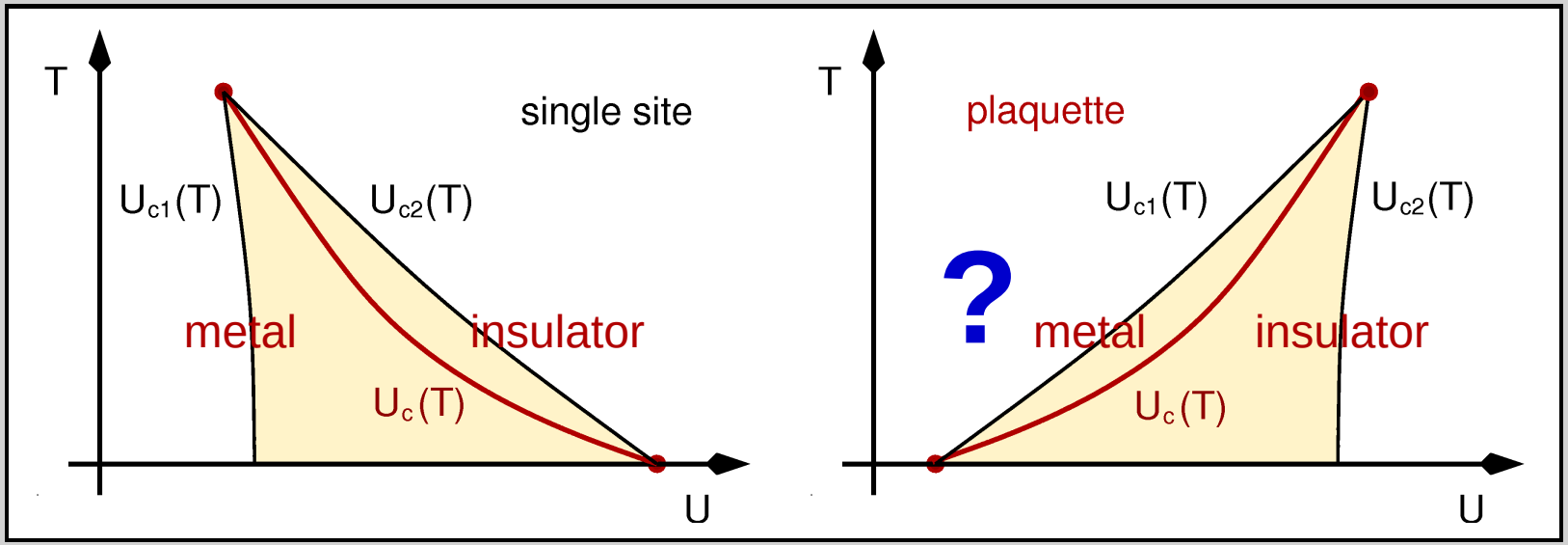
plaquette VCA





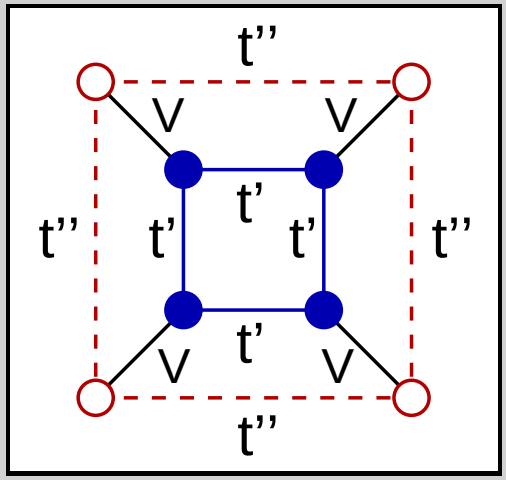
the insulator wins at higher temperatures

the metal wins at higher temperatures ?



parameter optimization

reference system
for plaquette VCA

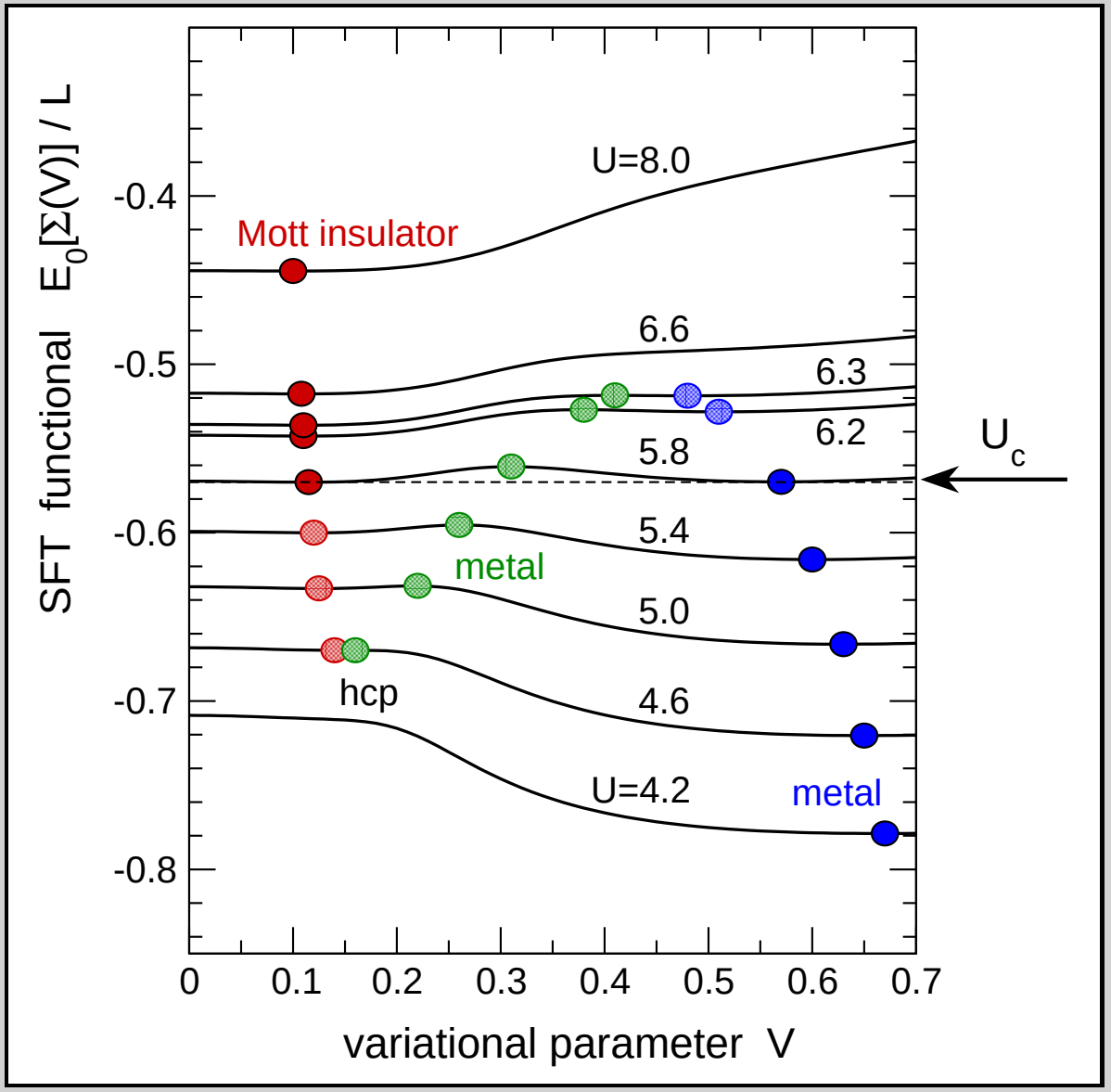


- on-site energies at correlated sites: $\varepsilon_c = 0$ (particle-hole symmetry)
- on-site energies at bath sites: $\varepsilon_b = U/2 = \mu$ (particle-hole symmetry)
- t'': optimal value small, $|t''_{\rm opt}| < t/25$ (t'' irrelevant for $L_b \to \infty$)
- t': optimal value $t'_{\rm opt} = t + \Delta t'_{\rm opt}$ with $\Delta t'_{\rm opt} < t/10$ ($t' = t$ for $L_b \to \infty$)
- setting $t' = t$ and $t'' = 0$ ➜ change of $V_{\rm opt} < 1\%$, Ω essentially unchanged

➜ **one-dimensional optimization of V sufficient**

- critical interaction:
  $U_c = 5.79$ with V, t', t'' optimized simultaneously (downhill simplex)
  $U_c = 5.79$ with V optimized only
- DIA ($n_s = 2$): $U_c = 11.3$
  DMFT: $U_c = 11$ *Zhang, Imada 2007*, $U_c = 12$ *Gull et al. 2008*

SFT functional



$D = 2$, $n = 1$, $T = 0$

VCA, $L_c = 4$, $L_b = 4$

physical states:
$\Omega(V) = \min, \max$

small $V_{\rm opt}$: insulator

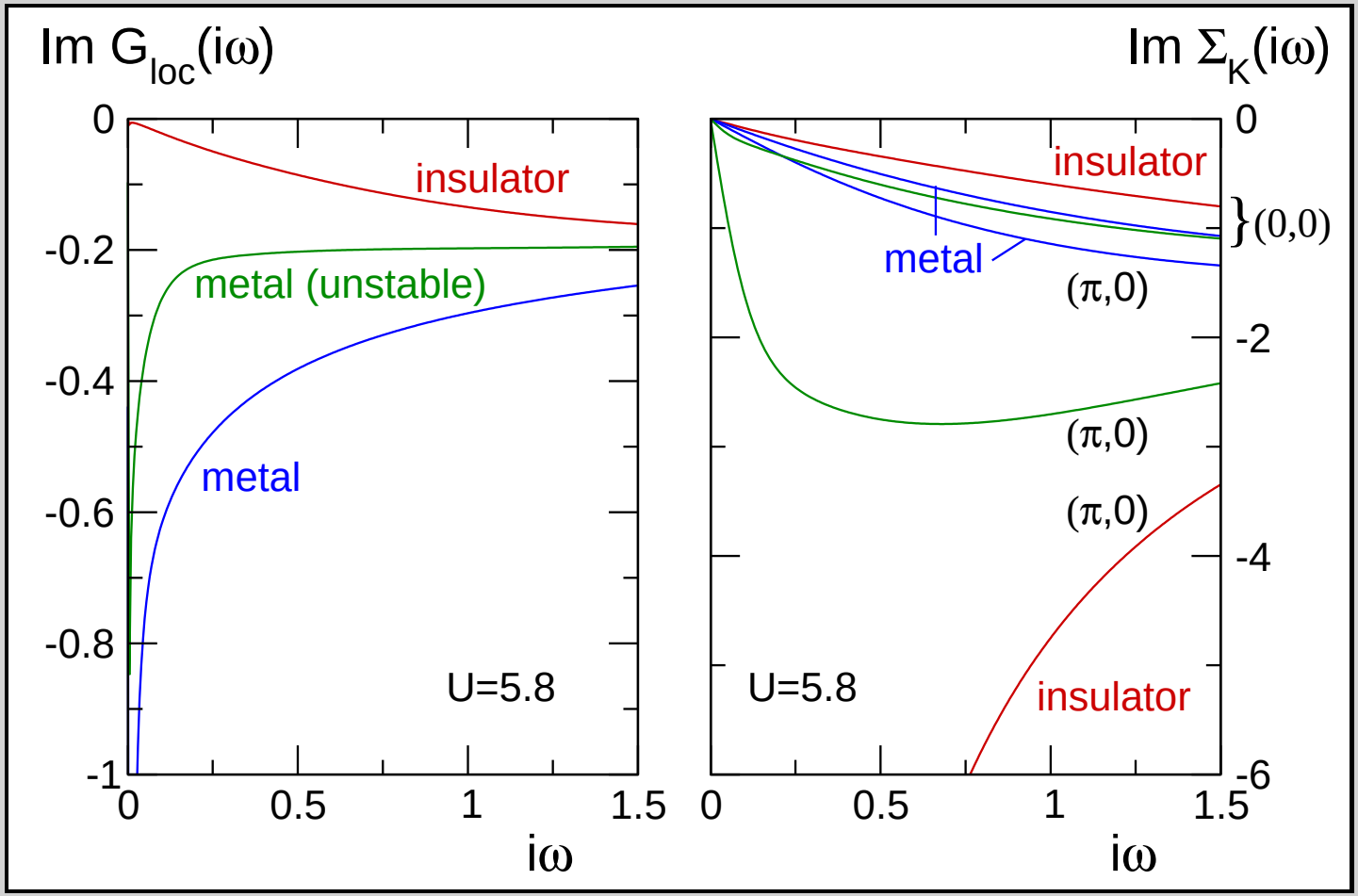
large $V_{\rm opt}$: metal

coexistence:
$4.6 \approx U_{c1} < U_{c2} \approx 6.35$

first-order transition
at $U_c = 5.79$ ($T = 0$)

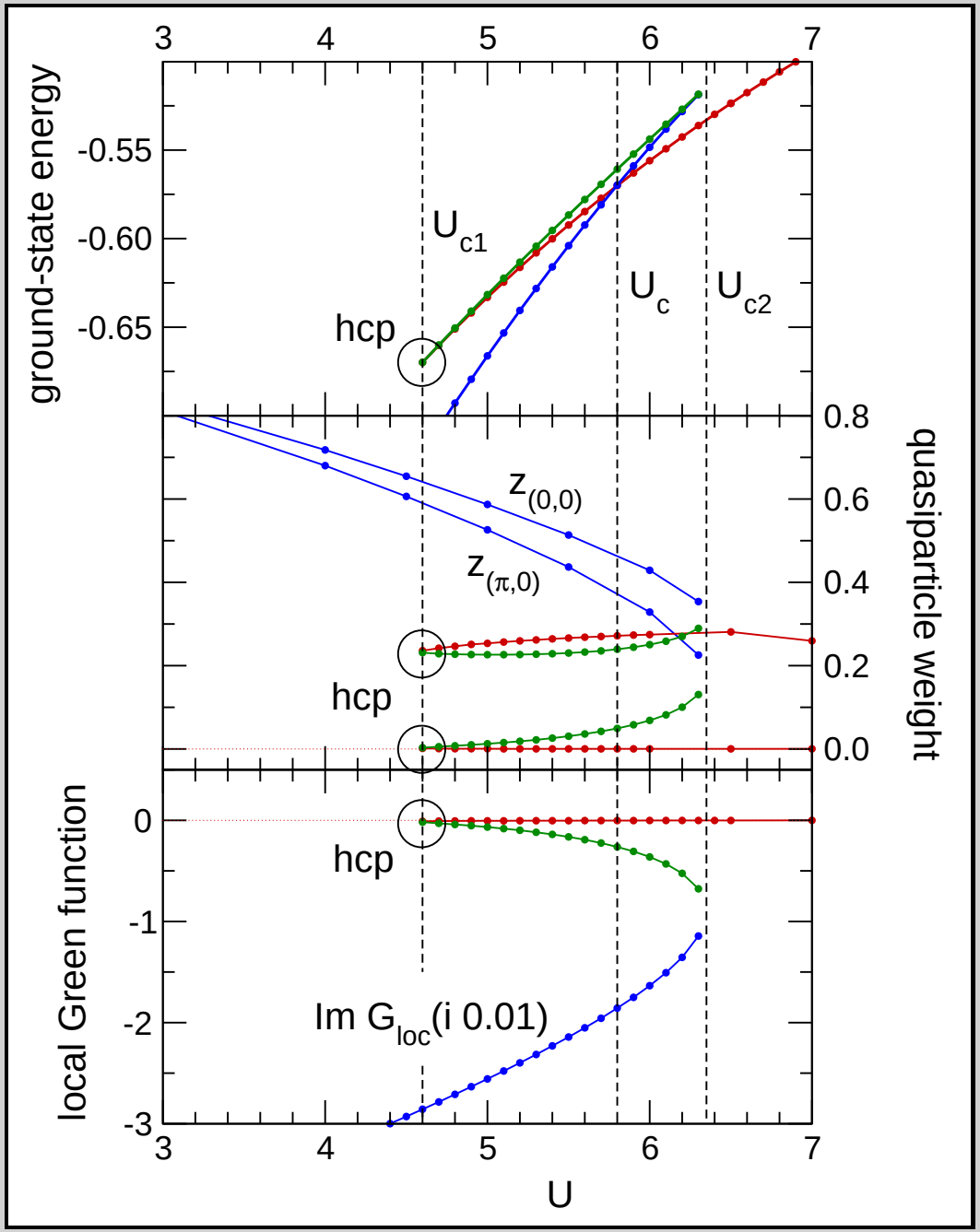
hidden critical point

$G_{\mathrm{loc}}(i\omega)$ and $\Sigma_K(i\omega)$ at $U = 5.8$



➜ **third, metastable solution is metallic**

physical quantities in the coexistence range



hidden critical point scenario