Variational principles for strongly correlated Fermi systems

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outline

Basic Models and Methods:

- electron correlations, example: magnetism, Hubbard model
- second quantization, exact diagonalization

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Variational Wave Functions:

- Ritz principle, Hartree-Fock, Gutzwiller, variation of matrix-product states
- generalized Ritz principle, variation of density matrices, Wick's theorem

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- 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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- ➜ Mott transition in infinite dimensions
- ➜ Mott transition in one and two dimensions

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The Luttinger Sum Rule:

- ➜ examples, proof, relation to self-energy-functional theory

acknowledgements

thanks to:

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I Basic Models and Methods

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:

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

Schrödinger's equation

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

is solved by

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

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"

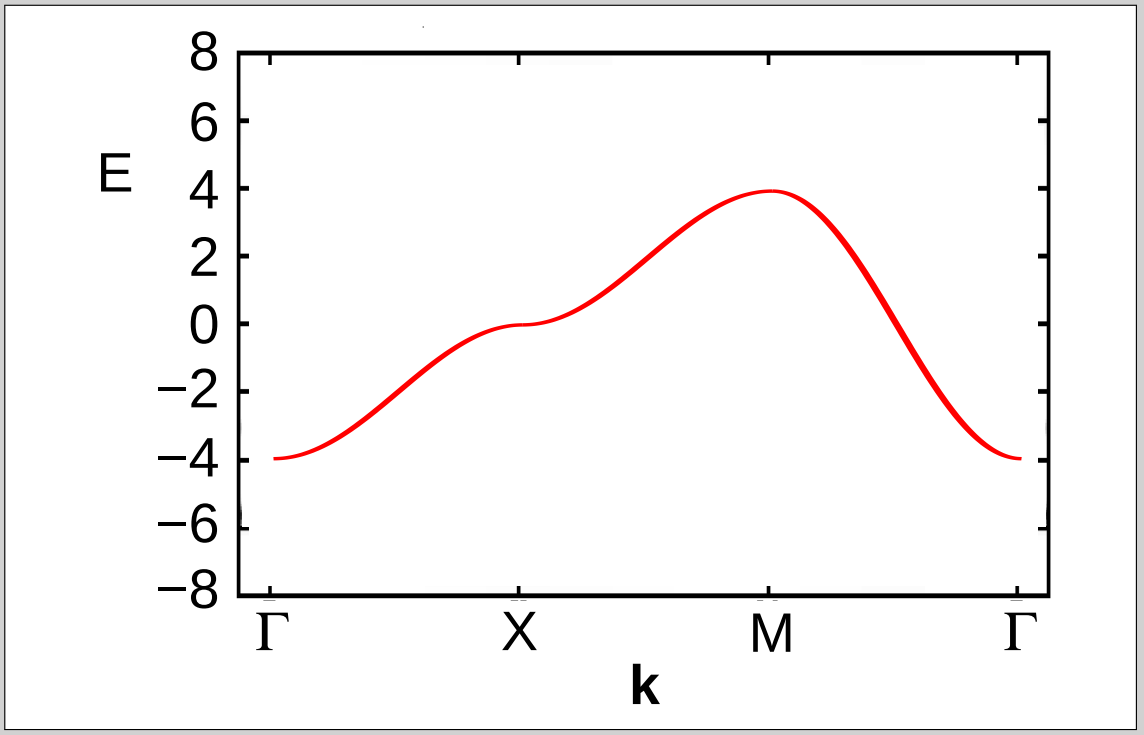
correlated band structure

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:



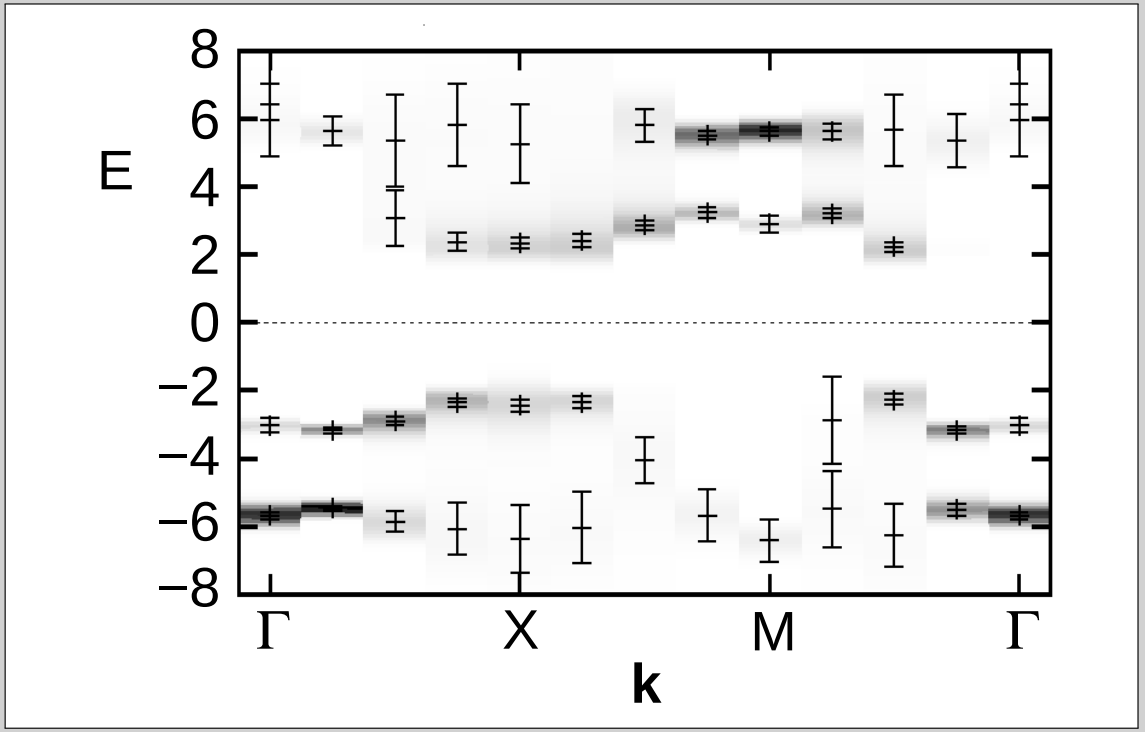
correlated band structure

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 $V_{\text{eff}}(\mathbf{r})$ 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

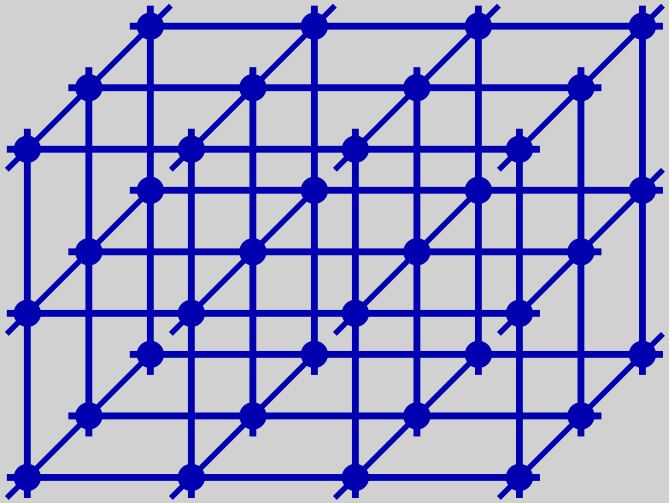
measure of the kinetic energy

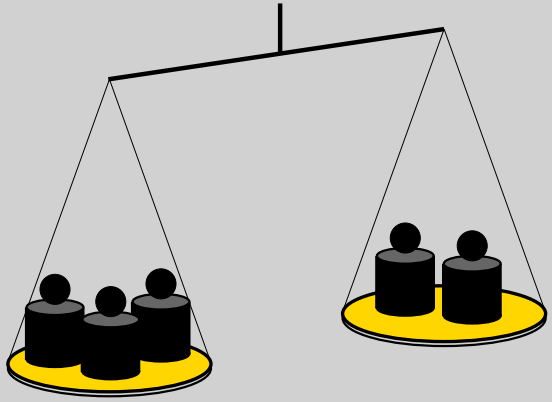
proportional to coordination number / dimension

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

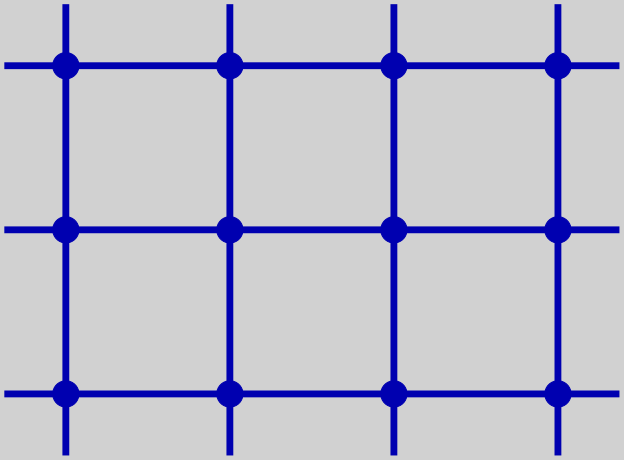
measure of the kinetic energy

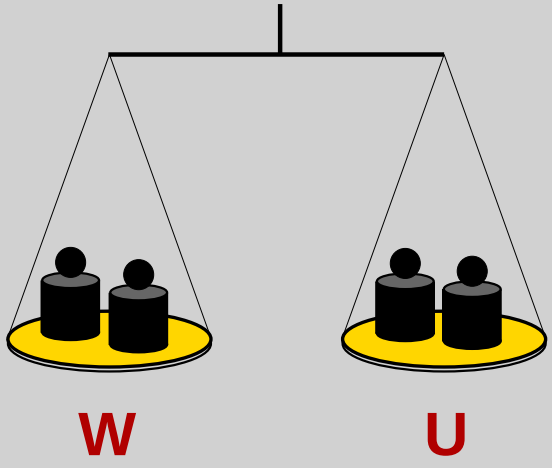
proportional to coordination number / dimension

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

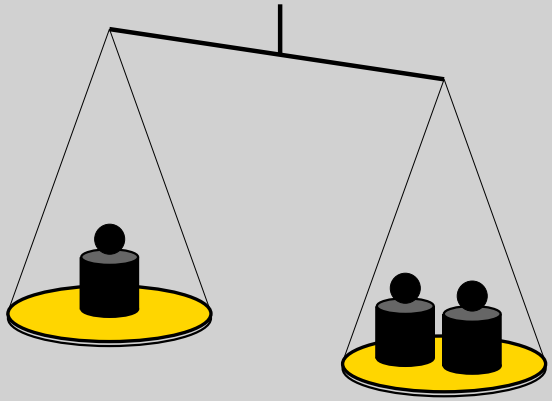
measure of the kinetic energy

proportional to coordination number / dimension

U : strongly screened Coulomb interaction

local quantity

independent of dimension



D=1:
correlations dominate
motion blocked by Pauli principle

Example: Collective Magnetism

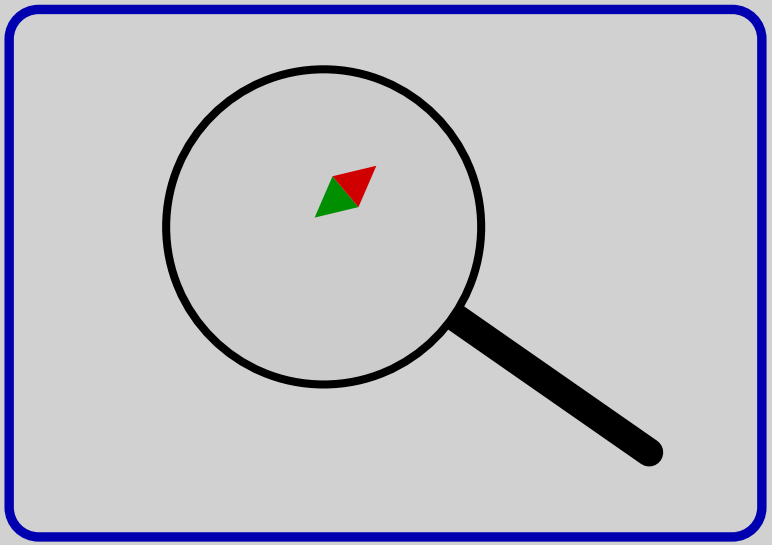
sketch: collective magnetism

magnetic material
example: magnetite (Fe_2O_3), Fe, Gd

➜ permanent magnetization

task:
development and application of quantum-statistical methods for an understanding of the collective order of magnetic moments within a non-perturbative, thermodynamically consistent picture of the electronic structure of Coulomb-interacting many-electron systems in low dimensions

sketch: collective magnetism



microscopic cause?
necessary:
elementary magnetic moments

➜ permanent moments

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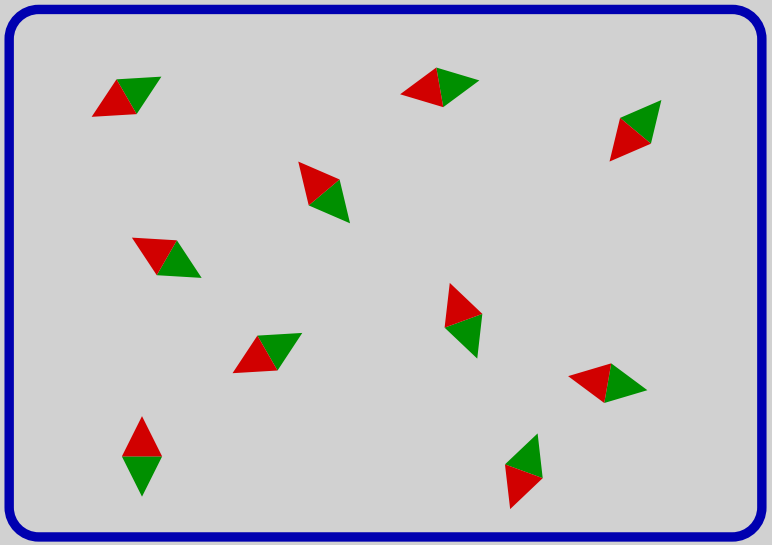

directions distributed randomly
total moment: $\sum_i \mathbf{m}_i = 0$
vanishing magnetization

➜ paramagnetism

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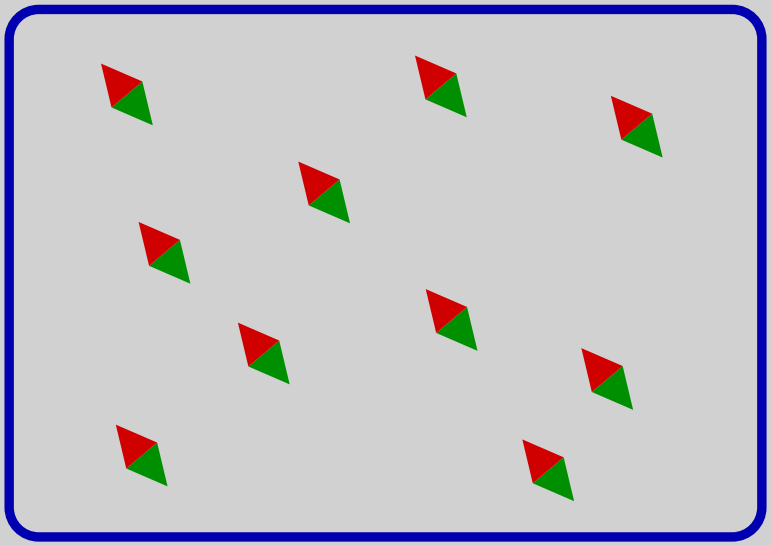

non-vanishing
magnetization requires:

➜ collective ordering of moments

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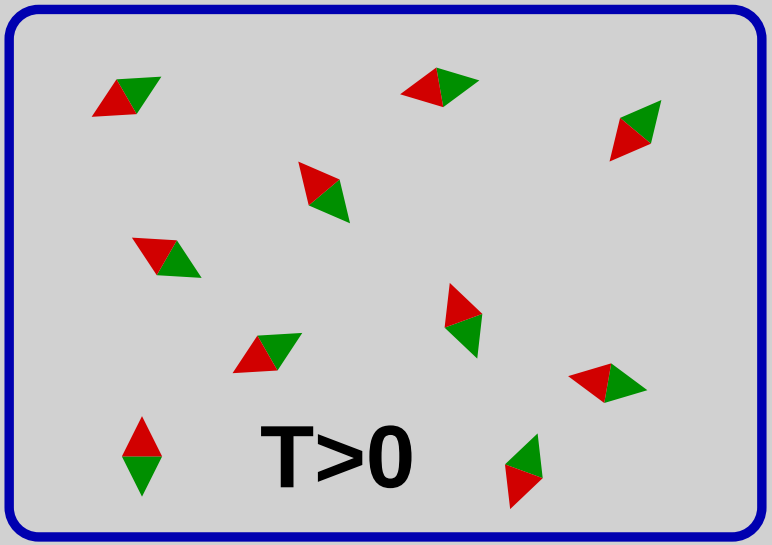

thermal fluctuations destroy magnetic order

➜ stability of order?

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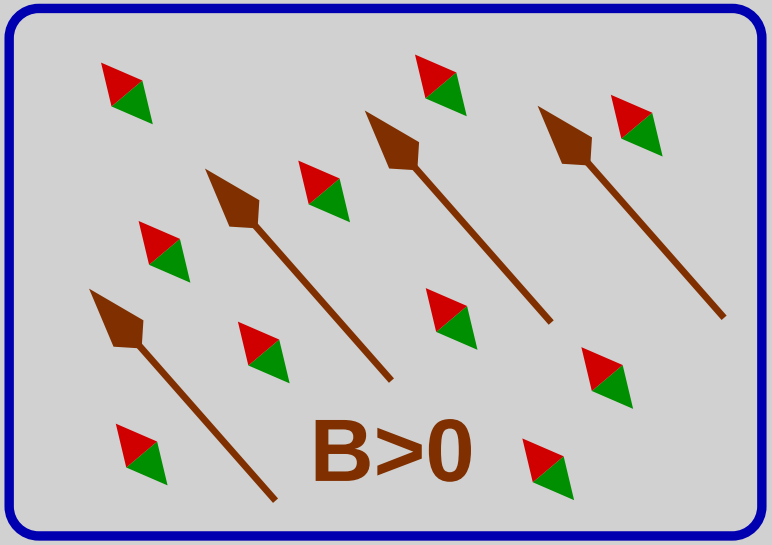

external magnetic field

$H \to H - \sum_i \mathbf{m}_i \mathbf{B}$

➜ induced magnetic order

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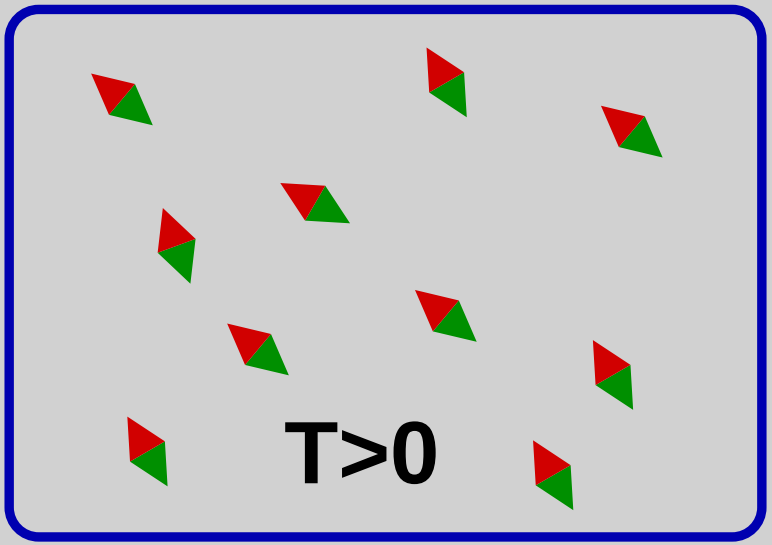

collective, non-induced order

$\sum_i \mathbf{m}_i \neq 0$ **für** $T > 0$

$\sum_i \mathbf{m}_i = 0$ **für** $T \to \infty$

➜ spontaneous order

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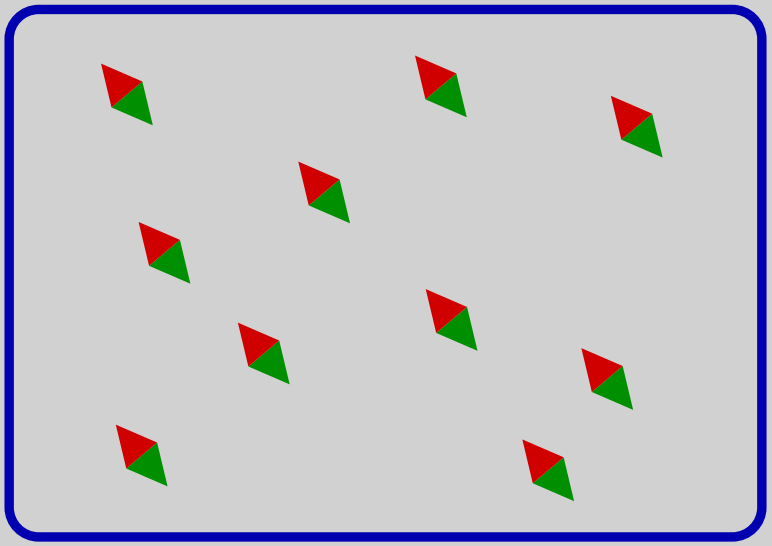
sketch: collective magnetism



direction of magnetization?

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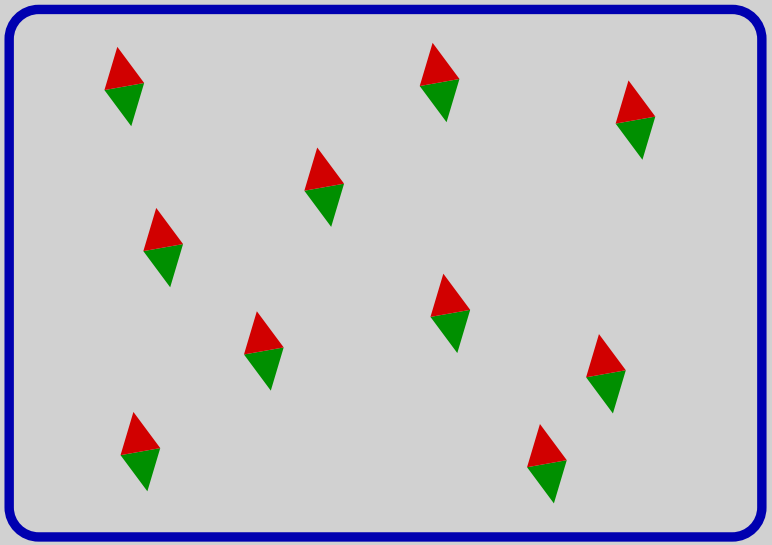

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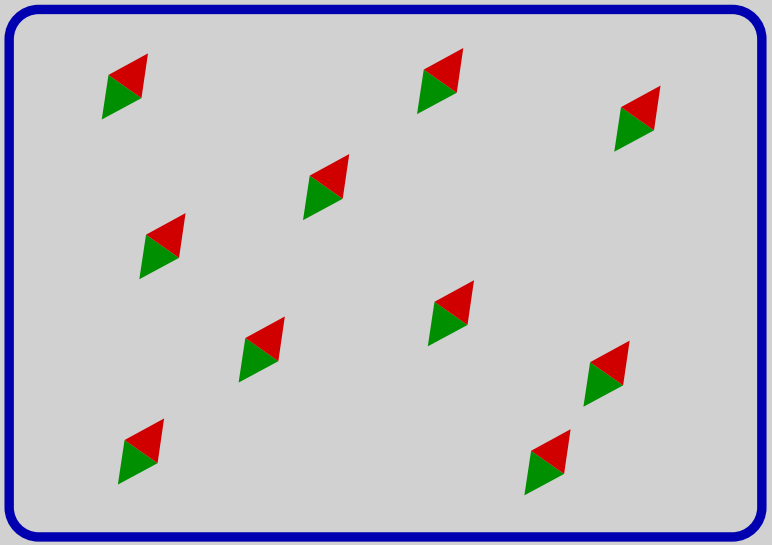

H: **magnetically isotropic**

$|\Psi\rangle$: **lower symmetry**

➜ **spontaneous symmetry breaking**

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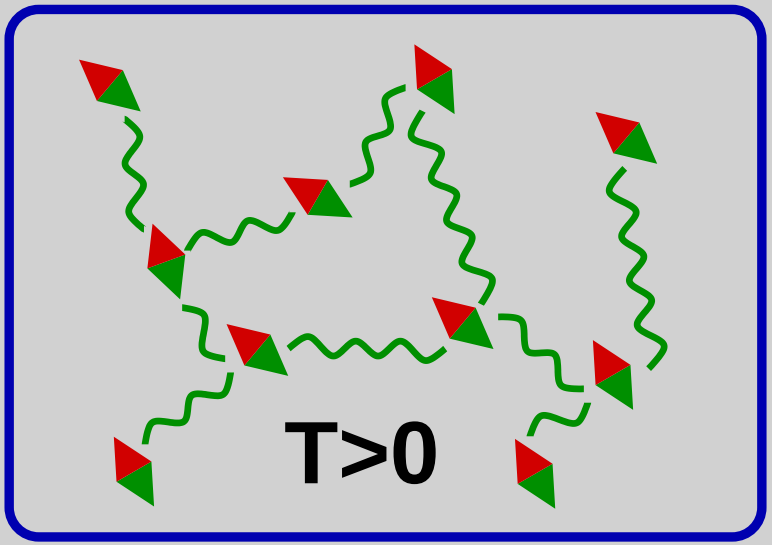

spontaneous collective order requires:

➜ interaction

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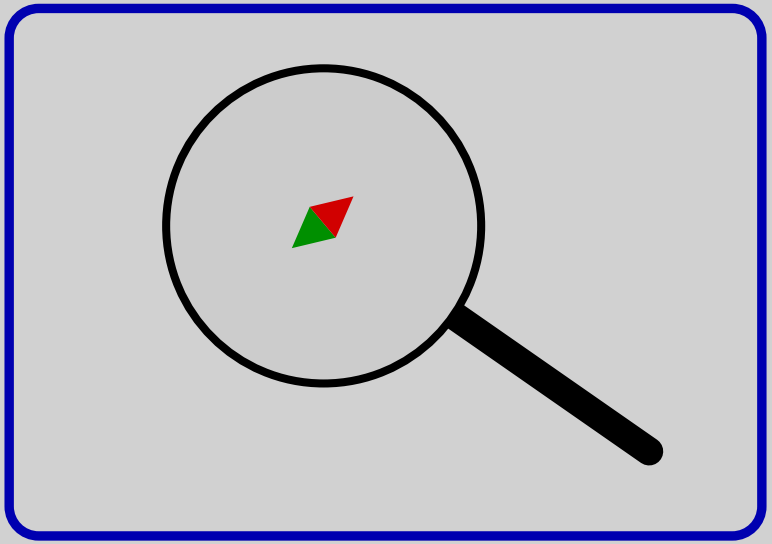

➜ **cause of magnetic moments?**

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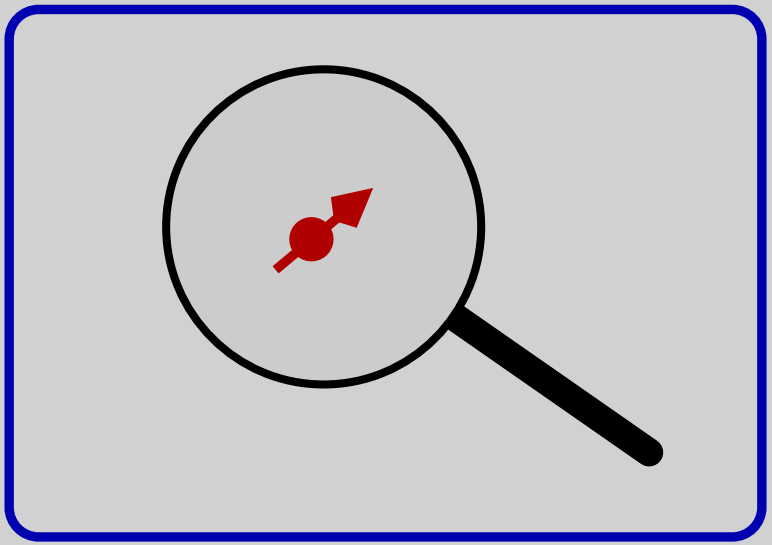

angular momentum ➜ magnetic moment

orbital momentum ➜ orbital moment
spin ➜ spin moment

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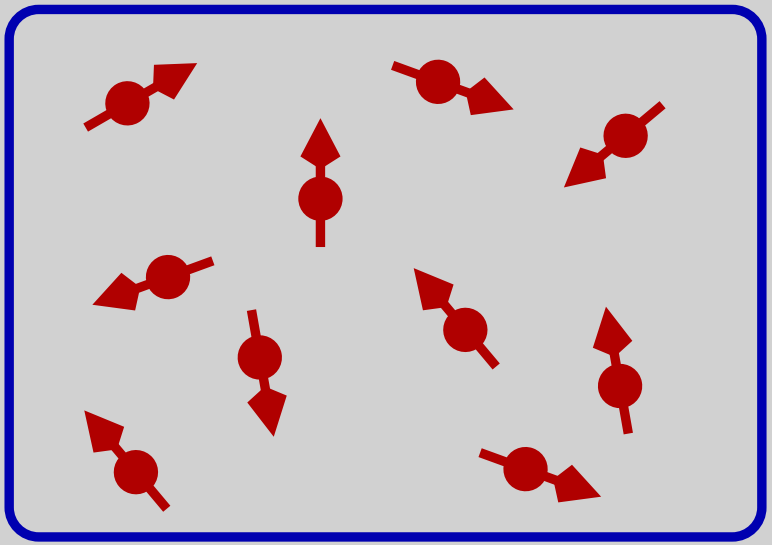

➜ **spin moments**

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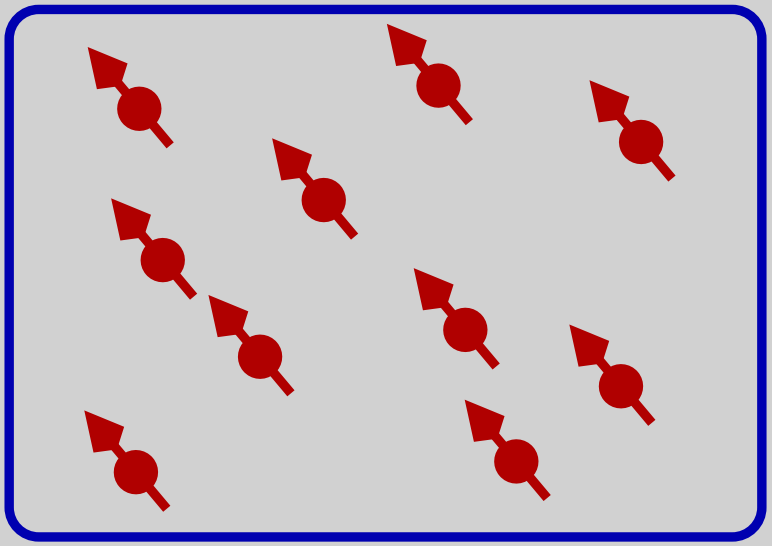
sketch: collective magnetism



collective spontaneous order

➜ interaction ?

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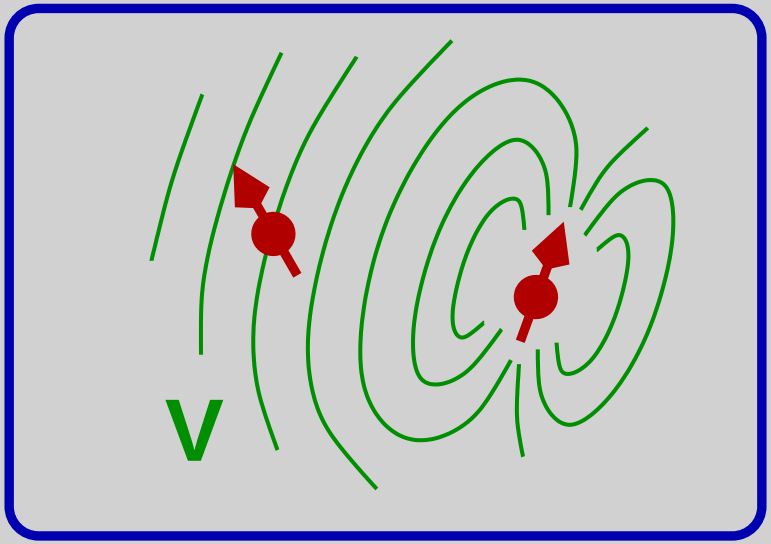

energy of a magnetic moment at $\mathbf{r}_i$ in the dipole field of all other moments:

$$\frac{\mu_0}{4\pi} \sum_{j \neq i} \frac{r_{ij}^2 \mathbf{m}_i \mathbf{m}_j - 3(\mathbf{m}_i \mathbf{m}_j)(\mathbf{m}_j \mathbf{r}_{ij})}{r_{ij}^5}$$

estimate: $\sim 10^{-4}$ **eV,** 1 **T,** 1 **K**

➜ **dipole interaction too weak**

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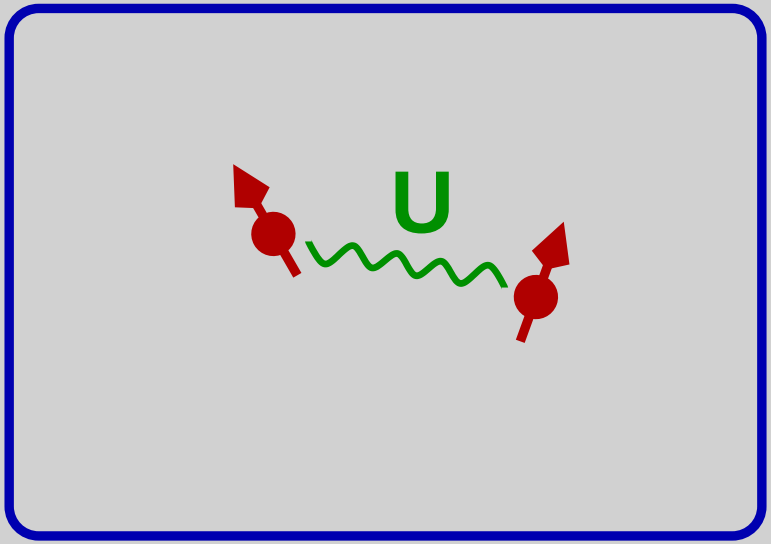

strong coupling via Coulomb-interaction U

$\mathrm{U} \sim \mathrm{W}$

W: kinetic energy (band width)

➜ strong Coulomb interaction

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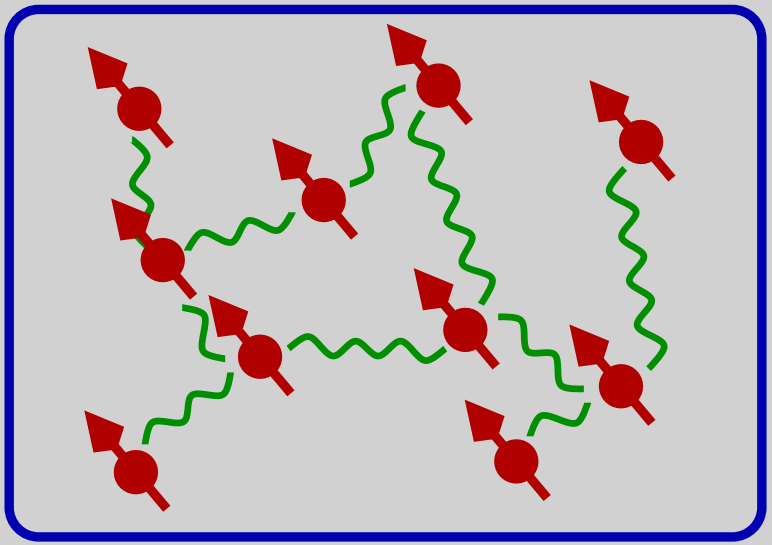
sketch: collective magnetism



Coulomb interaction as
cause of collective magnetism

Bohr-van Leeuwen theorem
“magnetism cannot be explained within classical statistics”

➜ quantum statistics

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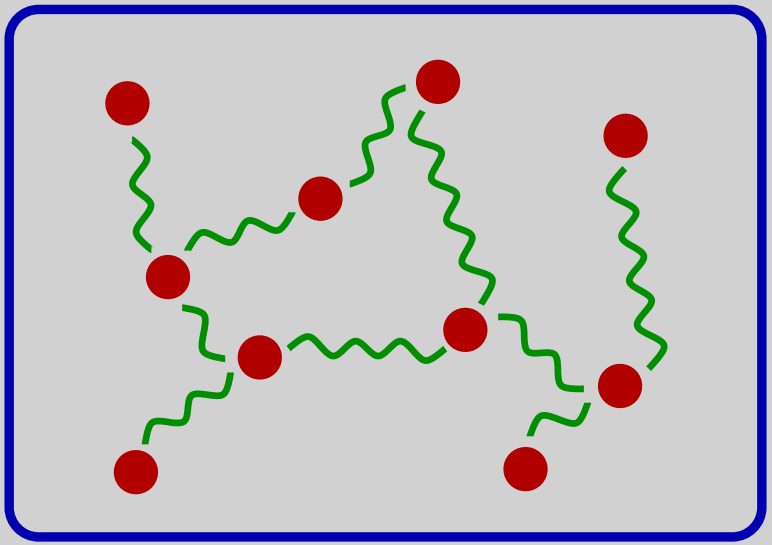
sketch: collective magnetism



quanten mechanical system of strongly interacting Fermions
$\sim 10^{23}$ coupled degrees of freedom

➜ central problem of theoretical physics

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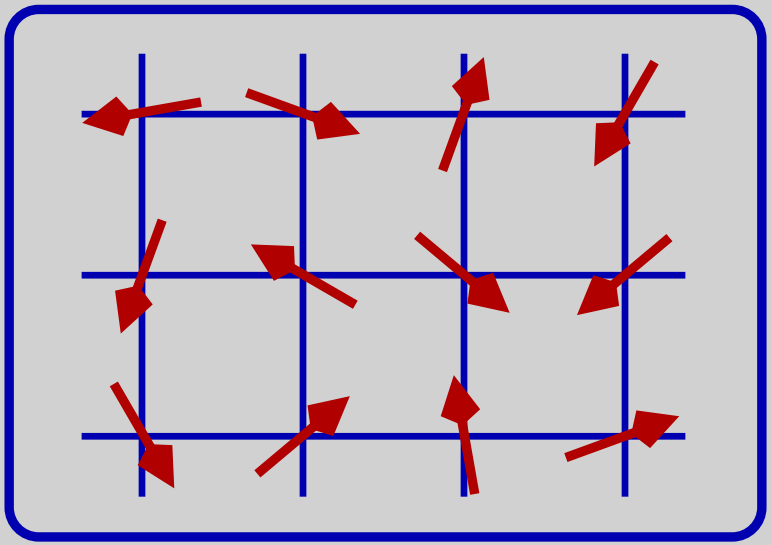
sketch: collective magnetism

quantum mechanics:
Fermions are indistinguishable !

➜ observable: spin density

task:
development and application of quantum-statistical methods for an understanding of the collective order of magnetic moments within a non-perturbative, thermodynamically consistent picture of the electronic structure of Coulomb-interacting many-electron systems in low dimensions

sketch: collective magnetism

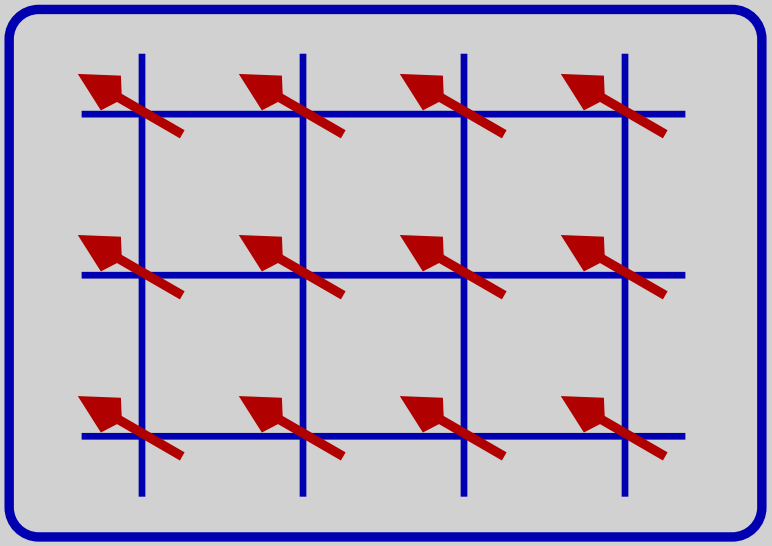


solid: translational symmetry
magnetic moment at
a lattice site

➜ local magnetic moment

task:
development and application of quantum-statistical methods for an understanding of the collective order of magnetic moments within a non-perturbative, thermodynamically consistent picture of the electronic structure of Coulomb-interacting many-electron systems in low dimensions

sketch: collective magnetism

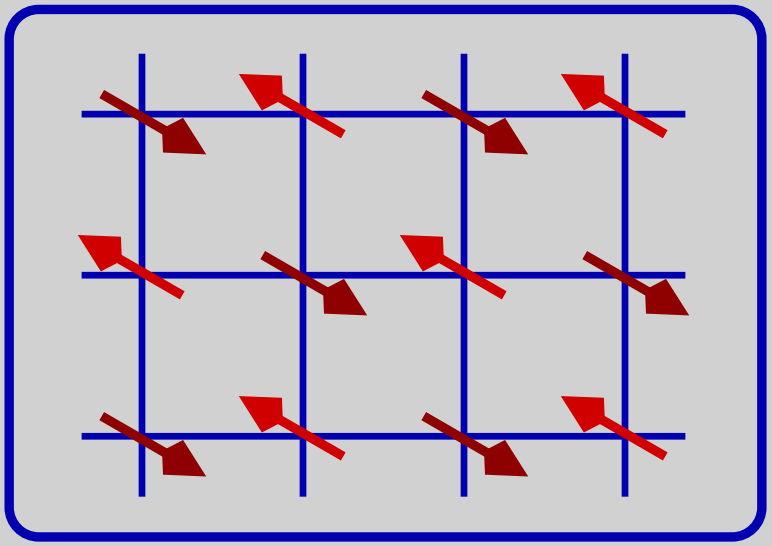


collective magnetism:
spontaneous order of local moments

➜ ferromagnetism

task:
development and application of quantum-statistical methods for an understanding of the collective order of magnetic moments within a non-perturbative, thermodynamically consistent picture of the electronic structure of Coulomb-interacting many-electron systems in low dimensions

sketch: collective magnetism



➜ **antiferromagnetism**

task:

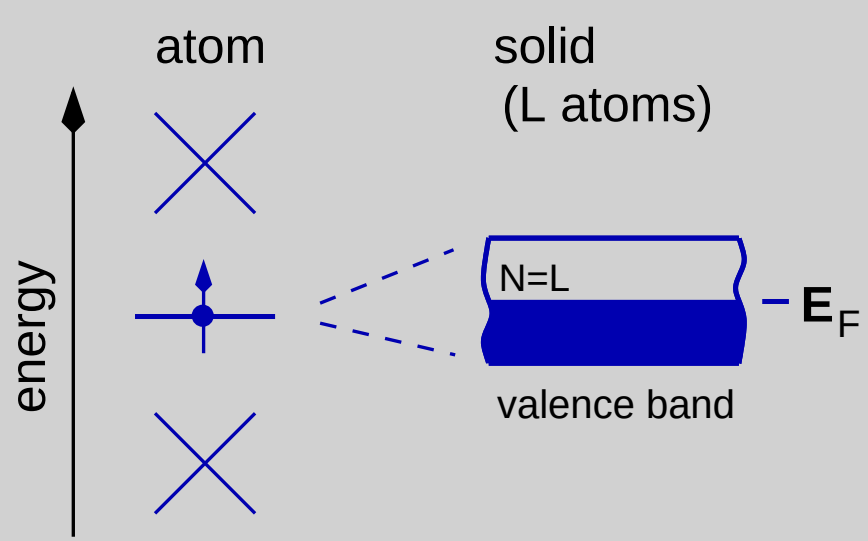
development and application of quantum-statistical methods for an understanding of the collective order of magnetic moments within a non-perturbative, thermodynamically consistent picture of the electronic structure of Coulomb-interacting many-electron systems in low dimensions

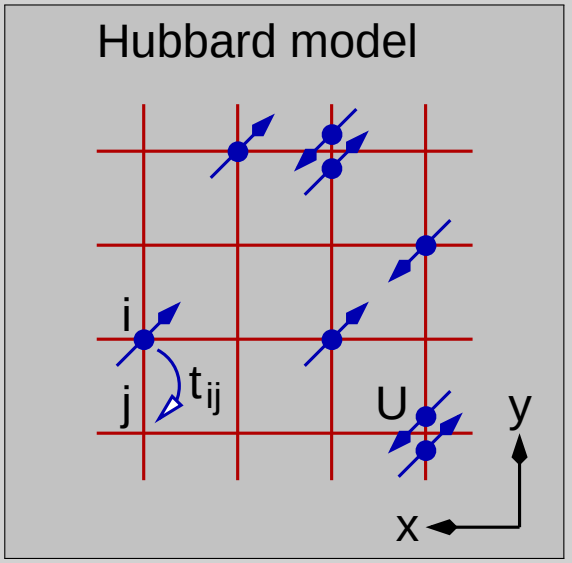
Hubbard Model

single band - local interaction

$$H = H_0 + H_1$$

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

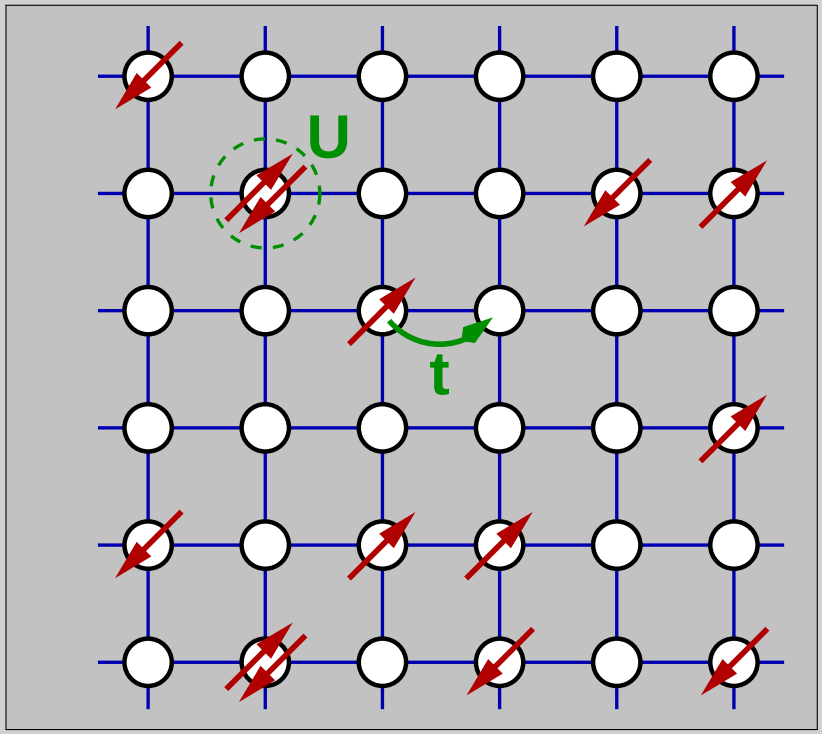




$\mathcal{H}_{\rm Atom}$ $\qquad$ $\mathcal{H} = \otimes_{i=1}^{L} \mathcal{H}_{\rm Atom}^{(i)}$ $\qquad$ $H = H_0 + H_1$

dimension: $\quad 4 \qquad\qquad 4^L$

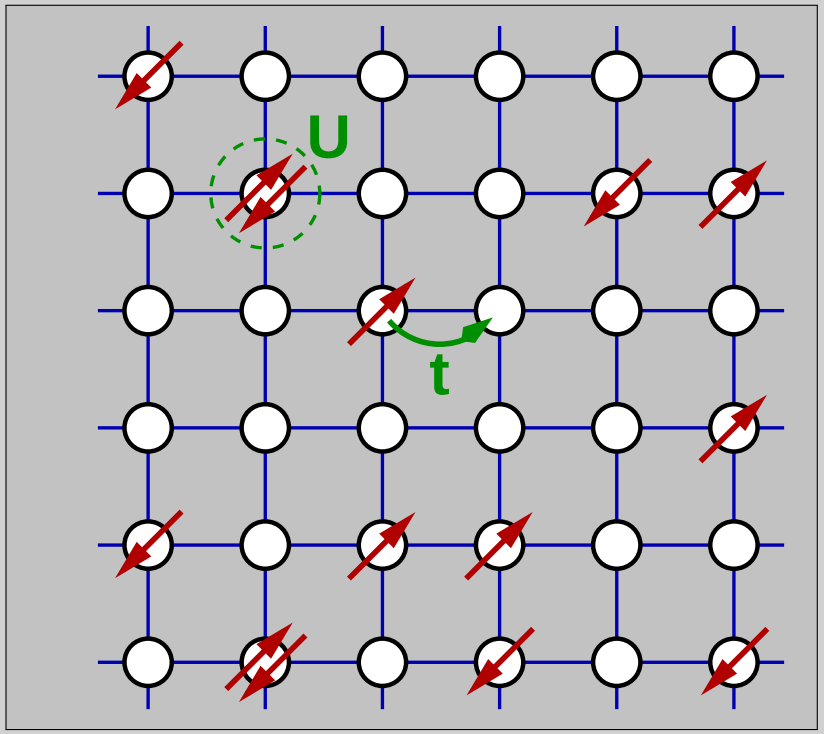
Hubbard model



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

- 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, ...

language of second quantization

one-particle orbitals:

$$\boxed{|\alpha\rangle = |i,\sigma\rangle}$$

orthonormal basis on one-particle Hilbert space $\mathcal{H}_1$:

$$\boxed{\langle\alpha|\beta\rangle = \delta_{\alpha\beta}}$$

electron vacuum:

$$\boxed{|0\rangle}$$

one electron

using creator:

$$\boxed{|\alpha\rangle = c^\dagger_\alpha|0\rangle}$$

---

two-electron basis state:

$$\boxed{\text{const.}\left(|\alpha^{(1)}\rangle|\beta^{(2)}\rangle - |\alpha^{(2)}\rangle|\beta^{(1)}\rangle\right)}$$

occupation-number respresentation:

$$\boxed{|n_1 = 0, n_2 = 0, ..., n_\alpha = 1, ..., n_\beta = 1, ...\rangle}$$

using creators:

$$\boxed{c^\dagger_\alpha c^\dagger_\beta|0\rangle = -c^\dagger_\beta c^\dagger_\alpha|0\rangle}$$

two electrons

if $\alpha = \beta$:

$$\boxed{\left(c^\dagger_\alpha\right)^2|0\rangle = 0}$$

language of second quantization

anti-commutation relation:

$$[c_\alpha^\dagger, c_\beta^\dagger]_+ = 0$$

annihilator:

$$c_\alpha \equiv \left(c_\alpha^\dagger\right)^\dagger$$

anticommutator relations

anti-commutation relations:

$$[c_\alpha, c_\beta]_+ = 0 \qquad [c_\alpha, c_\beta^\dagger]_+ = \delta_{\alpha\beta}$$

N-electron basis state:

$$\text{const.} \sum_{\mathcal{P}} (-1)^{|\mathcal{P}|} |\alpha_1^{\mathcal{P}(1)}\rangle |\alpha_2^{\mathcal{P}(2)}\rangle \cdots |\alpha_N^{\mathcal{P}(N)}\rangle$$

occupation-number representation:

$$|n_1, n_2, n_3, ..., n_\alpha, ...\rangle$$

N electrons

orthornormal basis of N-electron Hilbert space $\mathcal{H}_N$:

$$\langle ..., n_\alpha, ... | ..., n'_\alpha, ... \rangle = \cdots \delta_{n_\alpha, n'_\alpha}$$

$$\sum_{n_1, n_2, ..., n_\alpha, ...} |..., n_\alpha, ...\rangle\langle ..., n_\alpha, ...| = \mathbf{1}$$

language of second quantization

creator, annihilator:

$$c_\alpha^\dagger |..., n_\alpha, ...\rangle = (-1)^{\sum_{\beta=1}^{\alpha-1}} |..., n_\alpha + 1, ...\rangle$$

$$c_\alpha |..., n_\alpha, ...\rangle = (-1)^{\sum_{\beta=1}^{\alpha-1}} |..., n_\alpha - 1, ...\rangle$$

note:

$$n_\alpha = 0, 1$$

second-quantized form of N-electron states:

$$|n_1, n_2, ..., n_\alpha, ...\rangle = \left(c_1^\dagger\right)^{n_1} \left(c_2^\dagger\right)^{n_2} \cdots \left(c_\alpha^\dagger\right)^{n_\alpha} \cdots |0\rangle$$

---

one-particle operator:

$$A = \sum_{j=1}^{N} A^{(j)}$$

one-particle operator on $\mathcal{H}_1$:

$$A = \sum_{\alpha\beta} |\alpha\rangle\langle\alpha|A^{(1)}|\beta\rangle\langle\beta|$$

one-particle operator on $\mathcal{H}_N$:

$$A = \sum_{\alpha\beta} \langle\alpha|A^{(1)}|\beta\rangle c_\alpha^\dagger c_\beta$$

one-particle operators

language of second quantization

occupation-number operator and total particle number operator:

$$n_\alpha = c_\alpha^\dagger c_\alpha \qquad N = \sum_\alpha n_\alpha$$

examples

non-interacting Hamiltonian:

$$H_0 = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta$$

---

two-particle operator:

$$A = \frac{1}{2} \sum_{i,j}^{i \neq j} A^{(i,j)}$$

two-particle operator on $\mathcal{H}_N$:

two-particle operators

$$A = \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | A^{(1,2)} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

---

double occupancy ($\alpha = (i, \sigma)$):

$$d_i = n_{i\sigma} n_{i-\sigma}$$

Hubbard interaction:

examples

$$H_U = \frac{U}{2} \sum_{i\sigma} d_i = \frac{U}{2} \sum_{i\sigma} c_{i\sigma}^\dagger c_{i-\sigma}^\dagger c_{i-\sigma} c_{i\sigma}$$

language of second quantization

SUMMARY

anticommutation relations:

$$[c_\alpha, c_\beta]_+ = [c_\alpha^\dagger, c_\beta^\dagger]_+ = 0 \qquad [c_\alpha, c_\beta^\dagger]_+ = \delta_{\alpha\beta}$$

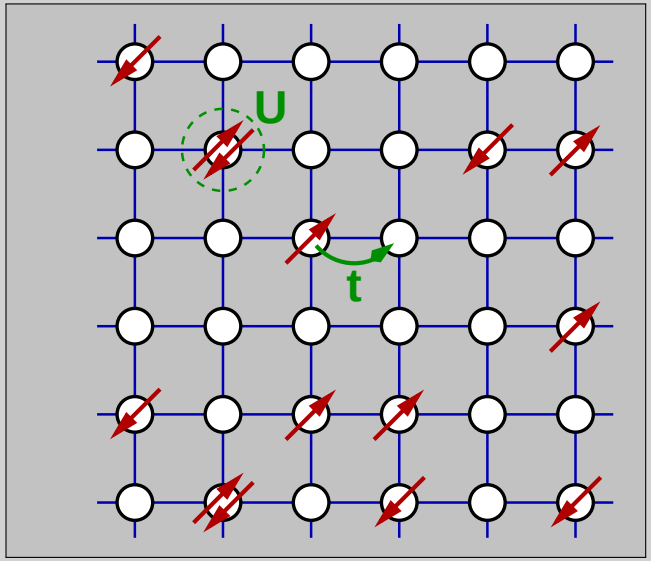
basis states:

$$|n_1, n_2, ..., n_\alpha, ...\rangle = \left(c_1^\dagger\right)^{n_1} \left(c_2^\dagger\right)^{n_2} \cdots \left(c_\alpha^\dagger\right)^{n_\alpha} \cdots |0\rangle$$

general Hamiltonian:

$$H = H_0 + H_1 = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$

$t_{\alpha\beta}, U_{\alpha\beta\delta\gamma}$: hopping and Coulomb matrix elements



Hubbard model

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

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 $N = 10 \lll 10^{23}$!

Lanczos method

don't store full Hamilton-matrix!

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

➜ consider (arbitrary) start vector $\mathbf{u}_0$

n-th Krylov space of $\mathbf{u}_0$ (with dimension n):

$$\mathcal{K}_n = \text{span}\left\{\mathbf{u}_0, \mathbf{H}\mathbf{u}_0, ..., \mathbf{H}^{n-1}\mathbf{u}_0\right\}$$

➜ construct orthogonal (not normalized) basis of $\mathcal{K}_n$:

$$\{\mathbf{u}_0, \mathbf{u}_1, ..., \mathbf{u}_{n-1}\}$$

start:

$$\mathbf{u}_{-1} = 0, \quad \mathbf{b}_0 = 0$$

interative construction for $i = 0, ..., n-1$: **needs MVM's only!**

$$a_i = \frac{\mathbf{u}_i^\dagger \mathbf{H}\mathbf{u}_i}{\mathbf{u}_i^\dagger \mathbf{u}_i}$$

$$b_i^2 = \frac{\mathbf{u}_i^\dagger \mathbf{u}_i}{\mathbf{u}_{i-1}^\dagger \mathbf{u}_{i-1}}$$

$$\mathbf{u}_{i+1} = \mathbf{H}\mathbf{u}_i - a_i \mathbf{u}_i - b_i^2 \mathbf{u}_{i-1}$$

store 3 vectors at the same time only!

we have $\mathbf{u}_i \in \mathcal{K}_n$ and $\mathbf{u}_i^\dagger \mathbf{u}_j \propto \delta_{ij}$

Lanczos method

➜ normalization:

$$\mathbf{v}_i = \frac{\mathbf{u}_i}{\sqrt{\mathbf{u}_i^\dagger \mathbf{u}_i}}$$

orthonormal basis of n-th Krylov space of u_0:

$$\boxed{\{\mathbf{v}_0, \mathbf{v}_1, ..., \mathbf{v}_{n-1}\}}$$

define

$$T_{ij} = \mathbf{v}_i^\dagger H \mathbf{v}_j$$

then

$$\mathbf{T} = \begin{pmatrix} a_0 & b_1 & & & \\ b_1 & a_1 & b_2 & & \\ & b_2 & a_2 & \cdots & \\ & & \cdots & \cdots & b_{n-1} \\ & & & b_{n-1} & a_{n-1} \end{pmatrix}$$

$n \times n$ **matrix only**

$\mathbf{V} \equiv (\mathbf{v}_0, \mathbf{v}_1, ..., \mathbf{v}_{n-1})$

$\mathbf{T} = \mathbf{V}^\dagger \mathbf{H} \mathbf{V}$

$\mathbf{T}$ is the Hamilton matrix in the subspace $\mathcal{K}_n$!

Lanczos method

➜ solve **small** $n \times n$ eigenvalue problem $\mathbf{T} = \mathbf{QDQ}^\dagger$

since $\mathbf{T}$ is the Hamilton matrix in the subspace $\mathcal{K}_n$ this would be exact if:

$\boxed{\mathbf{H}\mathcal{K}_n \subset \mathcal{K}_n}$ ($\mathcal{K}_n$ is an invariant subspace)

---

excellent approximation for $n = \mathcal{O}(100)$:

let $|u_0\rangle = \sum_m c_m |E_m\rangle$

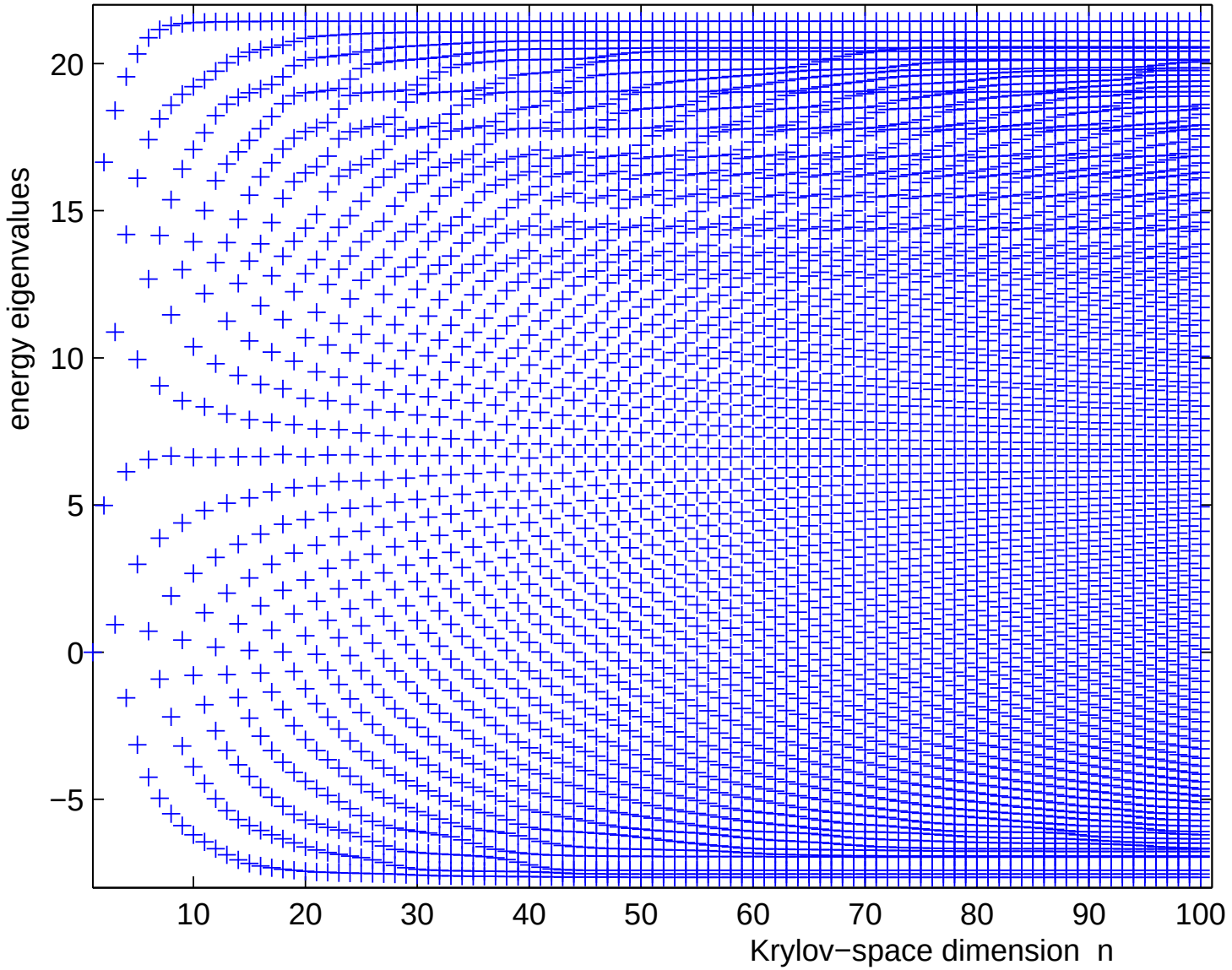
then $H^{n-1}|u_0\rangle = \sum_m c_m E_m^{n-1}|E_m\rangle \in \mathcal{K}_n$

but $H^n|u_0\rangle \to |E_0\rangle$ for $n \to \infty$

- Lanczos method limited by need to store $\mathbf{u}_i$
- $N = L = 10$ sites easily accessible
- $N = L = 20$ using symmetries and supercomputers
- ... but not much more!

Lanczos method

Lanczos for the $L = 10$ Hubbard chain, pbc, $N = 8$, $U = 4t$



Lanczos method

Lanczos can easily keep any supercomputer busy

16.447 TFlops and 159-Billion-dimensional Exact-diagonalization for Trapped Fermion-Hubbard Model on the Earth Simulator

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ABSTRACT

In order to study a possibility of superfluidity in trapped atomic Fermi gases loaded on optical lattices, we implement an exact diagonalization code for the trapped Hubbard model on the Earth Simulator. Comparing two diagonalization algorithms, we find that the performance of the preconditioned conjugate gradient (PCG) method is 1.5 times superior to the conventional Lanczos one since the PCG method can conceal the communication overhead much more efficiently. Consequently, the PCG method shows 16.447 TFlops (50.2% of the peak) on 512 nodes. On the other hand, we succeed in solving a 159-billion-dimensional matrix by using the conventional Lanczos method. To our knowledge, this dimension is a world-record. Numerical results reveal that an unconventional type of superfluidity specific to the confined system develops under repulsive interaction.

wave created due to two laser interference [8] in the atomic Fermi gas.

The Hubbard model is one of the most intensively-studied models by computers because it owns very rich physics although the model expression is quite simple [7]. The Hamiltonian of the Hubbard model with a trap potential [6, 9] is given as

$$H = -t \sum_{i,j,\sigma} (a^{\dagger}_{j\sigma} a_{i\sigma} + H.C.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \left(\frac{2}{N}\right)^2 V \sum_{i,\sigma} n_{i\sigma} \left(i - \frac{N}{2}\right)^2, \quad (1)$$

where t, U, and V are the hopping parameter from i-th to j-th sites (normally j is the nearest neighbor site of i), the repulsive energy for on-site double occupation of two

Lanczos method

... invented in 1950

Journal of Research of the National Bureau of Standards Vol. 45, No. 4, October 1950 Research Paper 2133

An Iteration Method for the Solution of the Eigenvalue Problem of Linear Differential and Integral Operators[1]

By Cornelius Lanczos

The present investigation designs a systematic method for finding the latent roots and the principal axes of a matrix, without reducing the order of the matrix. It is characterized by a wide field of applicability and great accuracy, since the accumulation of rounding errors is avoided, through the process of "minimized iterations". Moreover, the method leads to a well convergent successive approximation procedure by which the solution of integral equations of the Fredholm type and the solution of the eigenvalue problem of linear differential and integral operators may be accomplished.

I. Introduction

The eigenvalue problem of linear operators is of central importance for all vibration problems of physics and engineering. The vibrations of elastic structures, the flutter problems of aerodynamics, the stability problem of electric networks, the atomic and molecular vibrations of particle physics, are all diverse aspects of the same fundamental problem, viz., the principal axis problem of quadratic forms.

In view of the central importance of the eigen-

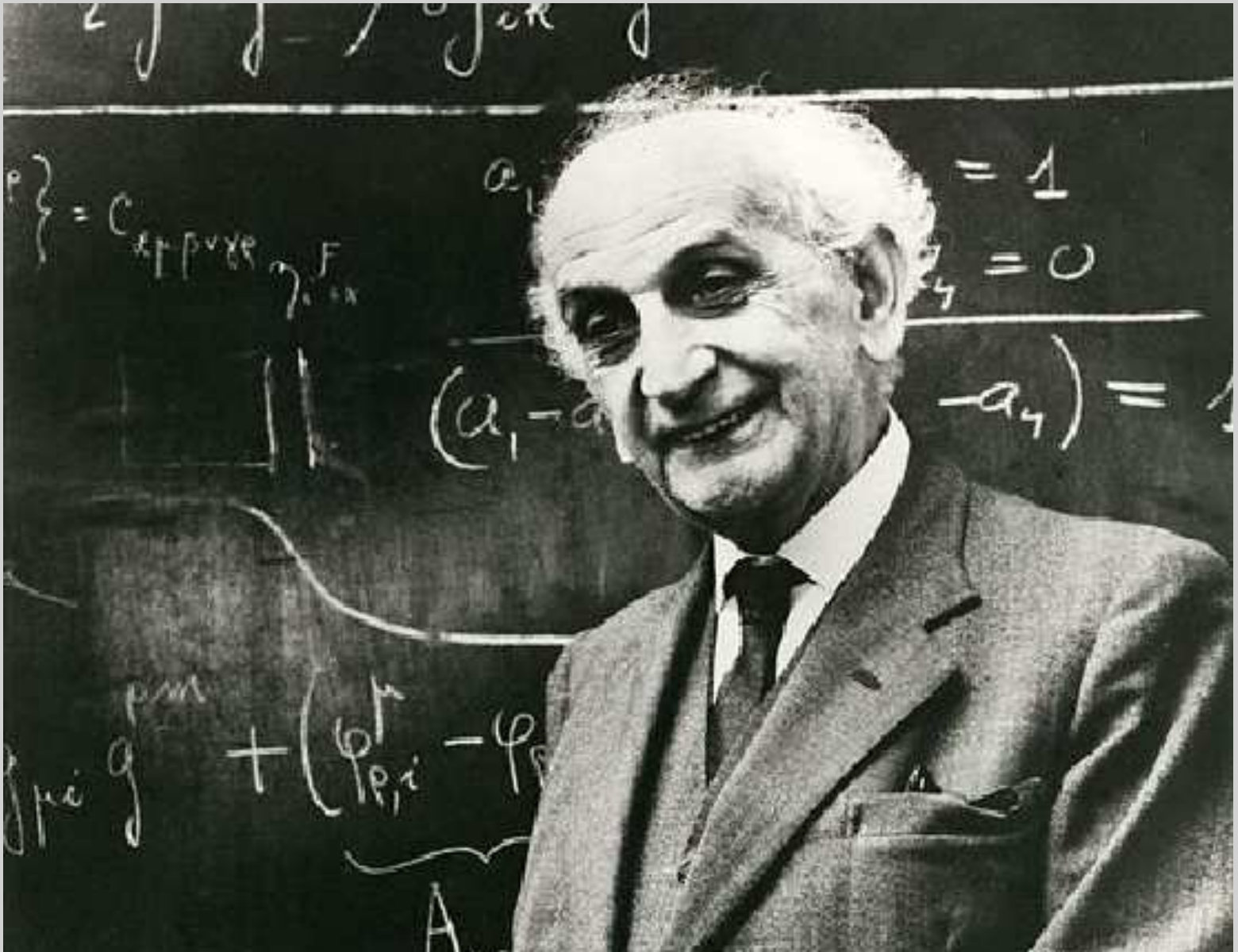
The present investigation, although starting out along classical lines, proceeds nevertheless in a different direction. The advantages of the method here developed [4] can be summarized as follows:

1. The iterations are used in the most economical fashion, obtaining an arbitrary number of eigenvalues and eigensolutions by one single set of iterations, without reducing the order of the matrix.

2. The rapid accumulation of fatal rounding errors, common to all iteration processes if applied

Lanczos method

... by Cornelius Lanczos



II Variational Wave Functions

Variational Principle

minimal energy

"Any system always tries to minimize its total energy"- why?

1) thermodynamics: total (internal) energy is a thermodynamical potential
   $E = E(S, V, N)$ =min. for fixed S, V, N (gas)
2) quantum mechanics: Ritz principle
   $E = E[|\Psi\rangle]$ =min.

The energy functional must be specified!

(trivial) example:

$$E = E(x) = \frac{1}{2}ax^2 + bx \qquad (a > 0)$$

$E(x)$ is at a minimum for

$$0 = \frac{dE(x_0)}{dx} = ax_0 + b$$

the "physical" x is:

$$x_0 = -\frac{b}{a}$$

the physical energy is:

$$E_0 = E(x_0) = \frac{1}{2}ax_0^2 + bx_0 = -\frac{1}{2}\frac{b^2}{a} = \frac{1}{2}bx_0$$

consider now:

$$E = \widetilde{E}(x) = \frac{1}{2}bx$$

we have $E_0 = \widetilde{E}(x_0)$ but $\widetilde{E}(x)$ is not a minimum at x_0

Ritz functional

$$E = E[|\Psi\rangle] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

$E[|\Psi\rangle]$ is minimal at the ground state $|\Psi_0\rangle$:

$$\langle\Psi|H|\Psi\rangle = \sum_m \langle\Psi|H|m\rangle\langle m|\Psi\rangle = \sum_m E_m |\langle m|\Psi\rangle|^2 \geq E_0 \sum_m |\langle m|\Psi\rangle|^2 = E_0 \langle\Psi|\Psi\rangle$$

domain of the functional: entire Hilbert space

$$\mathcal{D} = \{|\Psi\rangle \,|\, |\Psi\rangle \in \mathcal{H}\}$$

choose ONB $\{|m\rangle\}$, we have $|\Psi\rangle = \sum_m c_m |m\rangle$

$$\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\sum_{mm'} c_m^* c_{m'} \langle m|H|m'\rangle}{\sum_m c_m^* c_m}$$

➜ find minimum of a function of a function with $M = \dim \mathcal{H}$ variables!

➜ minimization of quadratic form $\Leftrightarrow \mathbf{Hc} = E_0 \mathbf{c}$ (full eigenvalue problem)

variational approximations

construct **approximations** by restricting the domain

$E[|\Psi\rangle] =$ min. on subspace $\mathcal{D}' \subset \mathcal{D} = \mathcal{H}$

a domain can be specified by **variational parameters** :

$\mathcal{D}' = \{|\Psi(\lambda_1, ..., \lambda_n)\rangle \mid \lambda_i \in \mathbb{R}\} \subset \mathcal{D}$

the Ritz functional becomes a function: $\lambda = (\lambda_1, ..., \lambda_n)$

$E(\lambda) \equiv E[|\Psi(\lambda)\rangle]$

find minimum:

$\frac{\partial E(\lambda)}{\partial \lambda_i} = 0$ for $\lambda = \lambda_0$ n (non-linear) equations for n unknowns λ_0

get approximate ground state and ground-state energy:

$|\Psi_0\rangle = |\Psi(\lambda_0)\rangle \qquad E_0 = E(\lambda_0)$

upper bound property :

$E_0 \geq E_{0,\mathrm{exact}}$

Hartree-Fock Approximation

Hartree-Fock: main idea

Hubbard model:

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

restricted domain:

$\mathcal{D}' = \{$ independent-electron wave functions $\}$

maybe justfified for weakly interacting systems, i.e. $U \to 0$

independent electrons: Slater determinants

$$|\Psi\rangle = |n_1, n_2, ..., n_\alpha, ...\rangle = \left(c^\dagger_1\right)^{n_1} \left(c^\dagger_2\right)^{n_2} \cdots \left(c^\dagger_\alpha\right)^{n_\alpha} \cdots |0\rangle$$

$n_\alpha = 0, 1$ electrons in (one-particle) state $|\alpha\rangle$

variational freedom: one-particle states

$|\alpha\rangle \to |\alpha'\rangle = \sum_\alpha U_{\alpha\alpha'} |\alpha\rangle$

variational parameters:

$U_{\alpha\alpha'}$

elegant evaluation:

Hartree-Fock: main idea

Hubbard model:

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

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$n_\alpha = 0, 1$ electrons in (one-particle) state $|\alpha\rangle$

variational freedom: one-particle states

$|\alpha\rangle \to |\alpha'\rangle = \sum_\alpha U_{\alpha\alpha'} |\alpha\rangle$

variational parameters:

$U_{\alpha\alpha'}$

elegant evaluation: **below**

Gutzwiller Wave Function

suppressing double occupancies

Hubbard model:

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

non-interacting case:

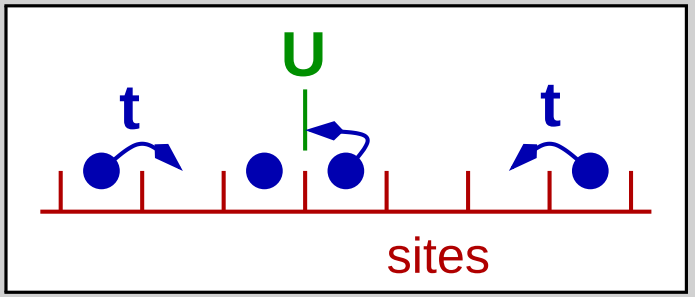
$$H_0 = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}$$

diagonalization:

$$H_0 = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \qquad (\mathbf{t} = \mathbf{U}\varepsilon\mathbf{U}^\dagger)$$

ground state:

$$|FS\rangle = \prod_{\mathbf{k}}^{\varepsilon(\mathbf{k}) \le \varepsilon_F} c^\dagger_{\mathbf{k}} |0\rangle$$



what happens for large U ?

➜ **suppression of double occupancies**

variational wave function

Gutzwiller wave function:

$$|\Psi\rangle = \prod_i [1-(1-g)n_{i\uparrow}n_{i\downarrow}]\,|FS\rangle = g^{\sum_i n_{i\uparrow}n_{i\downarrow}}\,|FS\rangle$$

variational parameter: g

$g = 1$: $|\Psi\rangle = |FS\rangle$ ➜ $U = 0$

$g = 0$: $|\Psi\rangle = |$doubly occupied sites projected out$\rangle$ ➜ $U = \infty$

note: $[1-(1-g)n_{i\uparrow}n_{i\downarrow}]^2 = 1-(1-g)n_{i\uparrow}n_{i\downarrow}$

todo:

- ✧ calculate $\langle\Psi|\Psi\rangle$
- ✧ calculate $\langle\Psi|H|\Psi\rangle$
- ✧ minimize $E[|\Psi(g)\rangle]$ w.r.t. g

$$\langle\Psi|\Psi\rangle = \prod_{\mathbf{k}}^{\varepsilon(\mathbf{k})\le\varepsilon_F} \langle 0|c_{\mathbf{k}} \prod_i [1-(1-g)n_{i\uparrow}n_{i\downarrow}] \prod_j [1-(1-g)n_{j\uparrow}n_{j\downarrow}] \prod_{\mathbf{p}}^{\varepsilon(\mathbf{p})\le\varepsilon_F} c^\dagger_{\mathbf{p}}|0\rangle$$

cannot be done analytically

variational Monte Carlo

way out: do the high-dimensional sums using Monte-Carlo summation:

$$E(g) = \frac{\langle \Psi(g)|H|\Psi(g)\rangle}{\langle \Psi(g)|\Psi(g)\rangle}$$

using the occupation-number basis $|n\rangle = |n_1, n_2, ...\rangle$, we can write:

$$E = \frac{\langle \Psi|H|\Psi\rangle}{\langle \Psi|\Psi\rangle} = \sum_n \frac{\langle \Psi|n\rangle\langle n|H|\Psi\rangle}{\langle \Psi|\Psi\rangle} = \sum_n \frac{\langle \Psi|n\rangle\langle n|\Psi\rangle}{\langle \Psi|\Psi\rangle} \frac{\langle n|H|\Psi\rangle}{\langle n|\Psi\rangle}$$

$$\boxed{E = \sum_n P(n) \frac{\langle n|H|\Psi\rangle}{\langle n|\Psi\rangle}}$$

with probability:

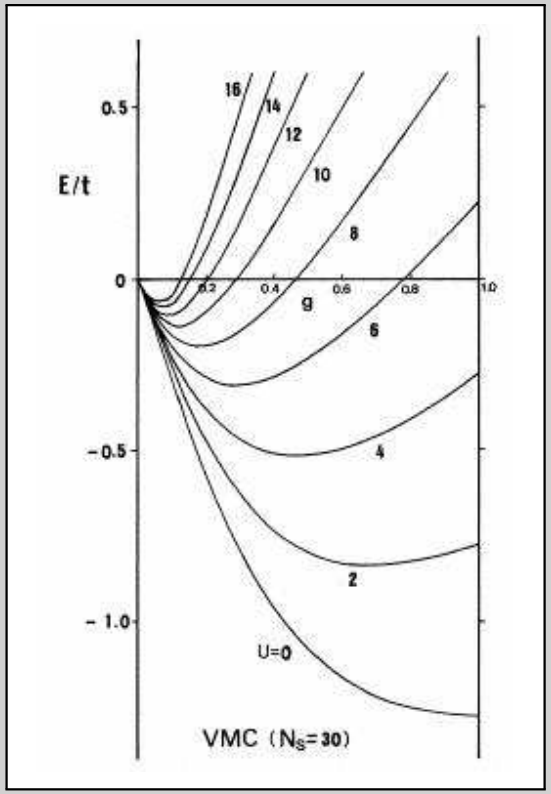
$$\boxed{P(n) = \frac{\langle \Psi|n\rangle\langle n|\Psi\rangle}{\langle \Psi|\Psi\rangle}} \qquad \sum_n P(n) = 1$$

Monte-Carlo walk in the configurations space: $n_1 \rightarrow n_2 \rightarrow \cdots$ (e.g. Metropolis)

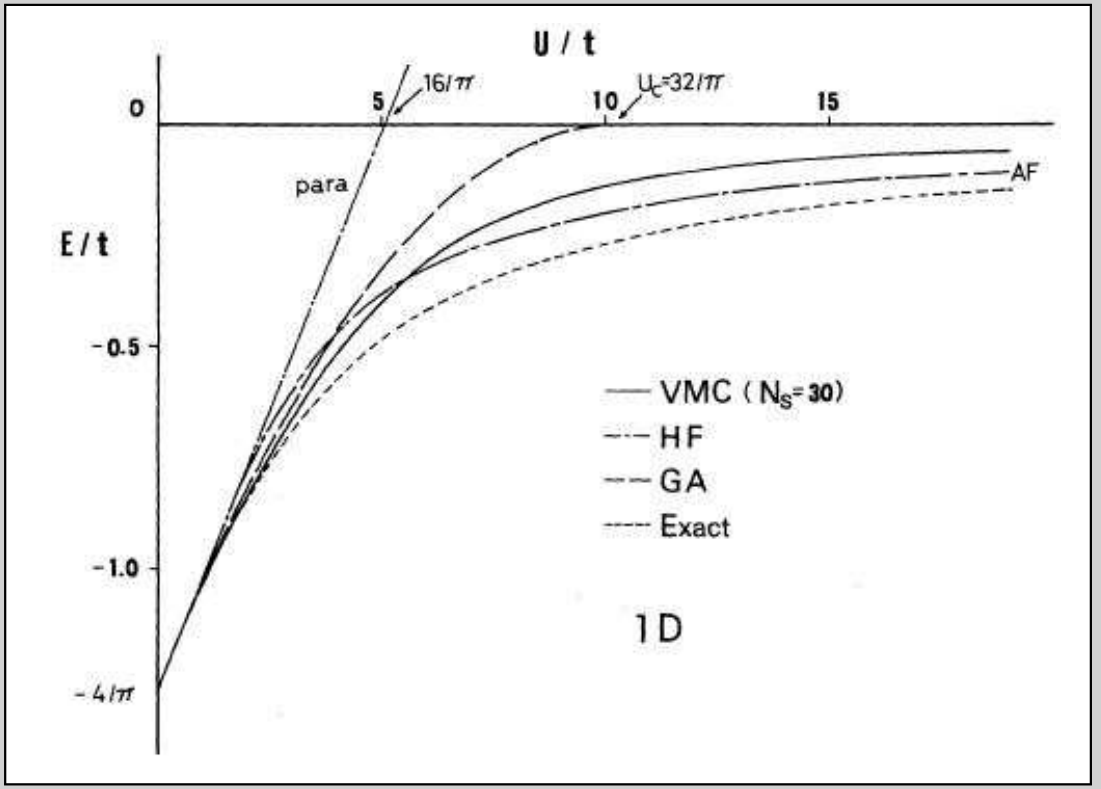
$$\boxed{E = \frac{1}{M} \sum_{i=1}^{M} \frac{\langle n_i|H|\Psi\rangle}{\langle n_i|\Psi\rangle}}$$ **VMC**

variational Monte Carlo

$E(g)$



$E_{\mathrm{opt.}}(U)$



Yokoyama, Shiba (1986)

- approximate evaluation of the Ritz principle (Gutzwiller approximation)
- numerically exact evaluation of the Ritz principle (VMC) with high computational effort
- approximate test wave function !

VMPS

matrix-product states

one-dimensional Hubbard model:

$$H = -t \sum_{i=1}^{L-1} \sum_{\sigma} c_{i\sigma}^{\dagger} c_{i+1\sigma} + \text{H.c.} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

Hilbert space:

$$\mathcal{H} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_L$$

local Hilbert space at site q:

$$\mathcal{H}_q = \text{span}\{|n_q\rangle\} \qquad n_q = 1, \ldots d_q \qquad d_q = \dim \mathcal{H}_q$$

local basis for Hubbard model: $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ $(d_q = 4)$

representation of general state:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} a^{n_1,\ldots,n_L} |n_1\rangle \ldots |n_L\rangle$$ (high dimensional: d^L terms for $d_q = d$)

product ansatz:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} a^{n_1} \ldots a^{n_L} |n_1\rangle \ldots |n_L\rangle$$

matrix-product state:

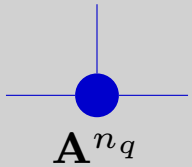
$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \text{tr}\, (\mathbf{A}^{n_1} \ldots \mathbf{A}^{n_L}) |n_1\rangle \ldots |n_L\rangle$$

graphical representation

MPS:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \text{tr}\ \left(\mathbf{A}^{n_1}\ldots\mathbf{A}^{n_L}\right)|n_1\rangle\ldots|n_L\rangle$$

an $\mathbf{A}$ matrix:

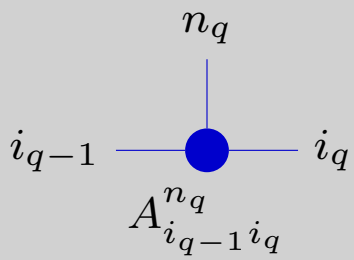


graphical representation

MPS:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \text{tr}\ (\mathbf{A}^{n_1} \ldots \mathbf{A}^{n_L})\, |n_1\rangle \ldots |n_L\rangle$$

an $\mathbf{A}$ matrix:



graphical representation

MPS:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \text{tr}\ \left(\mathbf{A}^{n_1}\ldots\mathbf{A}^{n_L}\right)|n_1\rangle\ldots|n_L\rangle$$

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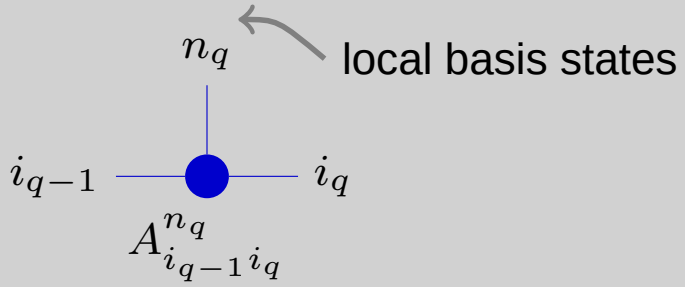
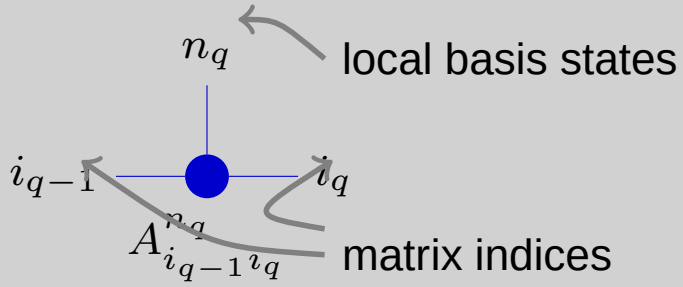


graphical representation

MPS:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \text{tr}\ \left(\mathbf{A}^{n_1}\ldots\mathbf{A}^{n_L}\right)|n_1\rangle\ldots|n_L\rangle$$

an $\mathbf{A}$ matrix:



graphical representation

MPS:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \text{tr}\ (\mathbf{A}^{n_1} \ldots \mathbf{A}^{n_L})\, |n_1\rangle \ldots |n_L\rangle$$

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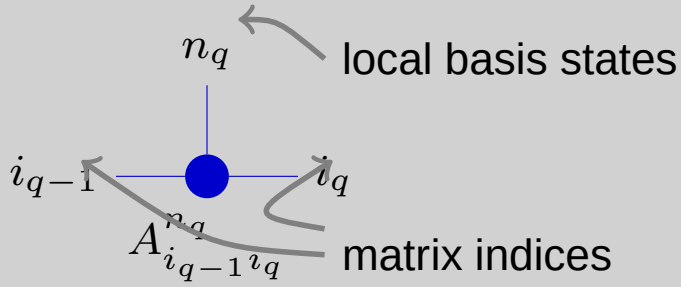
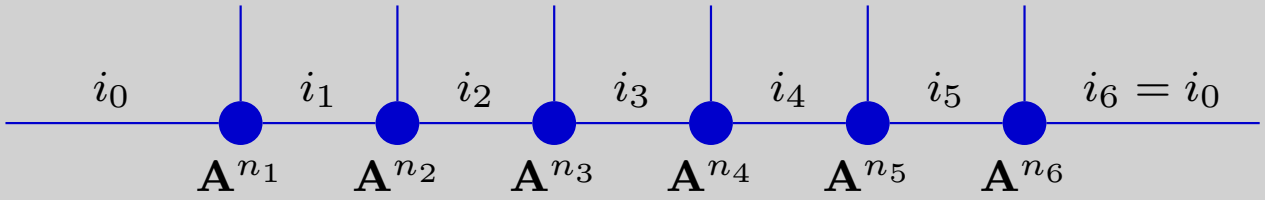


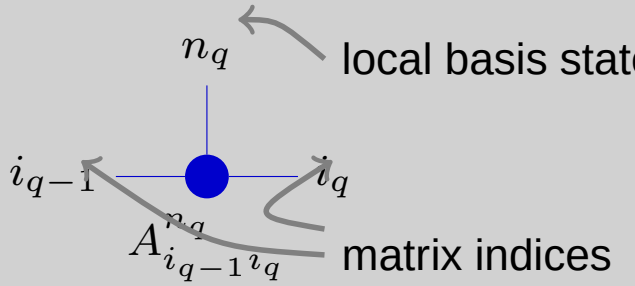
an MPS for six sites:



open boundary conditions

local orthogonalization

MPS:



$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \mathbf{A}^{n_1} \ldots \mathbf{A}^{n_L} |n_1\rangle \ldots |n_L\rangle$$

useful:

locally orthogonal MPS ($\mathbf{A}^{n_q} = \mathbf{L}^{n_q}$ or $\mathbf{A}^{n_q} = \mathbf{R}^{n_q}$)

$$\sum_{n_q} \mathbf{L}^{n_q\dagger}\mathbf{L}^{n_q} = \mathbf{1}, \qquad \sum_{n_q} \mathbf{R}^{n_q}\mathbf{R}^{n_q\dagger} = \mathbf{1}$$

graphical:

SVD

q-th step of **left orthogonalization:**

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \mathbf{L}^{n_1} \ldots \mathbf{L}^{n_{q-1}} \mathbf{A}^{n_q} \ldots \mathbf{A}^{n_L} |n_1\rangle \ldots |n_L\rangle$$

block up matrix $\mathbf{A}^{n_q}$:

$$A^{n_q}_{i_{q-1},i_q} = \widetilde{A}_{(i_{q-1}n_q),i_q}$$

SVD:

$$\widetilde{\mathbf{A}} = \mathbf{U}\mathbf{D}\mathbf{V}^\dagger \qquad \text{with } \mathbf{D} \text{ diagonal, } \mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger\mathbf{U} = \mathbf{1},\ \mathbf{V}\mathbf{V}^\dagger = \mathbf{V}^\dagger\mathbf{V} = \mathbf{1}$$

block down matrix $\mathbf{U}$:

$$L^{n_q}_{i_{q-1},i_q} = U_{(i_{q-1}n_q),i_q} \qquad \overline{\mathbf{A}}^{n_{q+1}} \equiv \mathbf{D}\mathbf{V}^\dagger \mathbf{A}^{n_{q+1}}$$

new representation of the MPS (ready for $q+1$-st step):

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \mathbf{L}^{n_1} \ldots \mathbf{L}^{n_{q-1}} \mathbf{L}^{n_q} \overline{\mathbf{A}}^{n_{q+1}} \ldots \mathbf{A}^{n_L} |n_1\rangle \ldots |n_L\rangle$$

right orthogonalization : analogous

standard representation of an MPS:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \mathbf{L}^{n_1} \ldots \mathbf{L}^{n_{q-1}} \mathbf{C}^{n_q} \mathbf{R}^{n_{q+1}} \ldots \mathbf{R}^{n_L} |n_1\rangle \ldots |n_L\rangle$$

normalization

reminder: $$E = E[|\Psi\rangle] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

MPS with 6 sites:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_6} \mathbf{L}^{n_1}\mathbf{L}^{n_2}\mathbf{L}^{n_3}\mathbf{C}^{n_4}\mathbf{R}^{n_5}\mathbf{R}^{n_6}|n_1\rangle\ldots|n_6\rangle$$

calculate norm:

normalization

reminder: $$E = E[|\Psi\rangle] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

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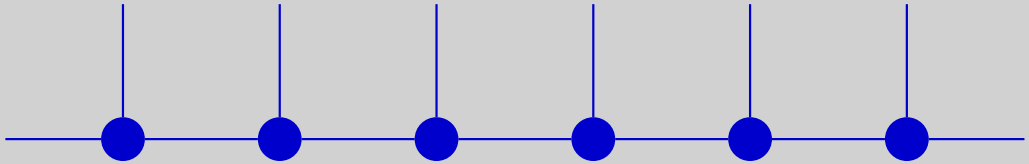
calculate norm:



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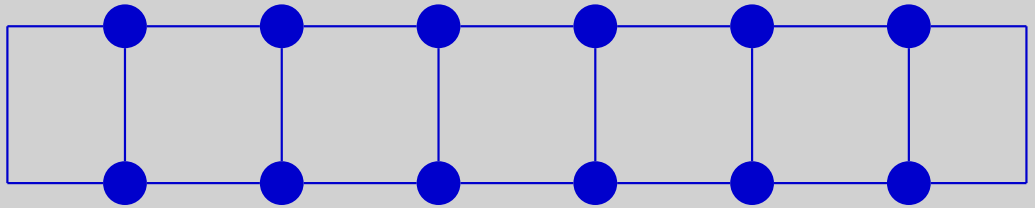
calculate norm:

$\langle\Psi|\Psi\rangle =$



normalization

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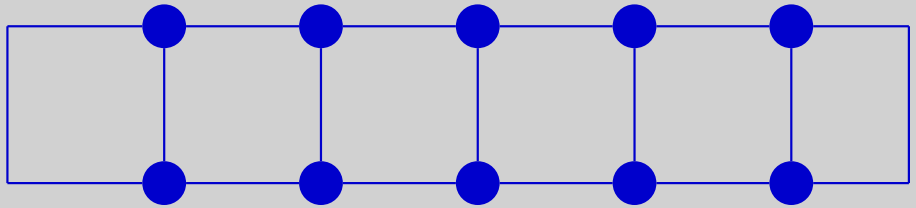

normalization

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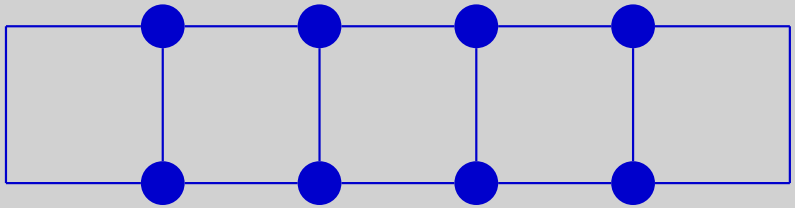

normalization

reminder: $$E = E[|\Psi\rangle] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

MPS with 6 sites:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_6} \mathbf{L}^{n_1}\mathbf{L}^{n_2}\mathbf{L}^{n_3}\mathbf{C}^{n_4}\mathbf{R}^{n_5}\mathbf{R}^{n_6}|n_1\rangle\ldots|n_6\rangle$$

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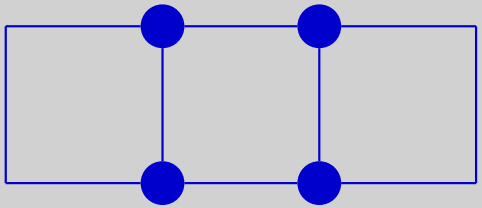

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calculate norm:

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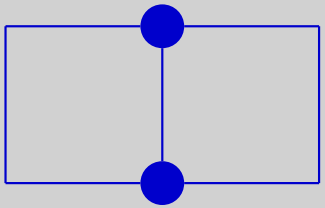


normalization

reminder: $$E = E[|\Psi\rangle] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

MPS with 6 sites:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_6} \mathbf{L}^{n_1}\mathbf{L}^{n_2}\mathbf{L}^{n_3}\mathbf{C}^{n_4}\mathbf{R}^{n_5}\mathbf{R}^{n_6}|n_1\rangle\ldots|n_6\rangle$$

calculate norm:

$$\langle\Psi|\Psi\rangle = \sum_{n_4} \mathrm{Tr}(\mathbf{C}^{n_4\dagger}\mathbf{C}^{n_4})$$

normalization

reminder: $$\boxed{E = E[|\Psi\rangle] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}}$$

MPS with 6 sites:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_6} \mathbf{L}^{n_1}\mathbf{L}^{n_2}\mathbf{L}^{n_3}\mathbf{C}^{n_4}\mathbf{R}^{n_5}\mathbf{R}^{n_6}|n_1\rangle\ldots|n_6\rangle$$

calculate norm:

$$\langle\Psi|\Psi\rangle = \sum_{n_4} \mathrm{Tr}(\mathbf{C}^{n_4\dagger}\mathbf{C}^{n_4})$$

---

compare with:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} a^{n_1,\ldots,n_L}|n_1\rangle\ldots|n_L\rangle$$

norm:

$$\langle\Psi|\Psi\rangle = \sum_{n_1,\ldots,n_L} a^{n_1,\ldots,n_L}\langle n_1|\ldots\langle n_L| \sum_{n'_1,\ldots,n'_L} a^{n'_1,\ldots,n'_L}|n'_1\rangle\ldots|n'_L\rangle$$

$$\langle\Psi|\Psi\rangle = \sum_{n_1,\ldots,n_L} |a^{n_1,\ldots,n_L}|^2 \text{ (cannot be computed!)}$$

matrix-product operators

operator X: $X|\Psi\rangle$? $\langle\Psi|X|\Psi\rangle$? e.g.: $\langle\Psi|H|\Psi\rangle$

MPO

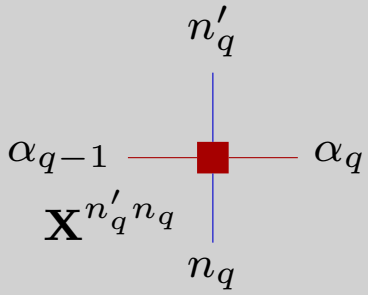
$$X = \sum_{n_1,\ldots,n_L} \sum_{n'_1,\ldots n'_L} \mathbf{X}^{n'_1 n_1} \ldots \mathbf{X}^{n'_L n_L} |n'_1\rangle\langle n_1| \ldots |n'_L\rangle\langle n_L|$$

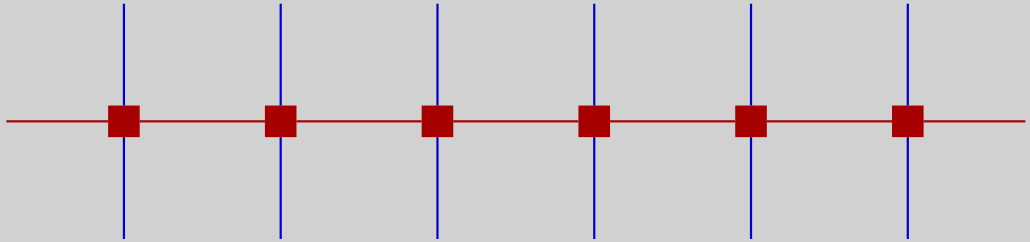
example: Ising model $H = -J \sum_i S^z_i S^z_{i+1}$ (local basis: $m \in \{\uparrow, \downarrow\}$)

$$\mathbf{X}^{m'_q m_q} = \delta_{m'_q m_q} \begin{pmatrix} 1 & 0 & 0 \\ m_q & 0 & 0 \\ 0 & -J m_q & 1 \end{pmatrix}$$

exact representation!

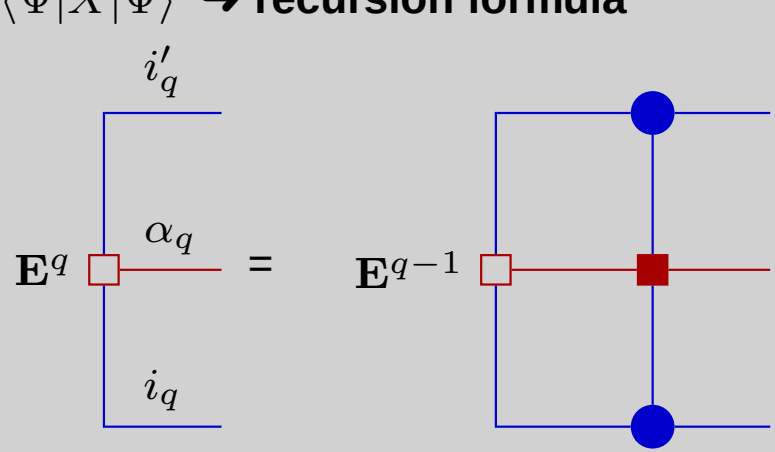
graphical:

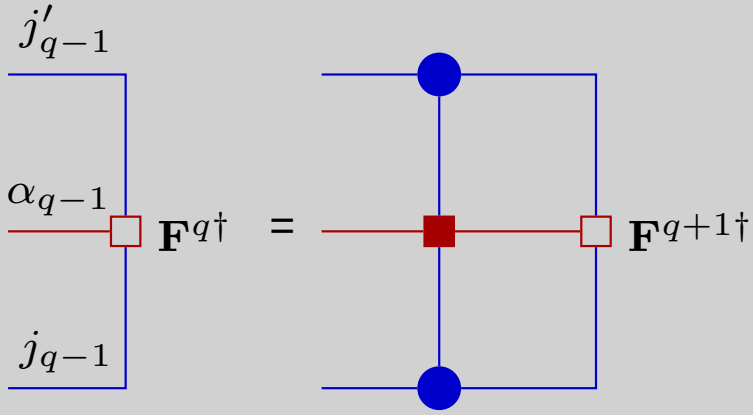




expectation values

$\langle\Psi|X|\Psi\rangle$ ➜ **recursion formula**

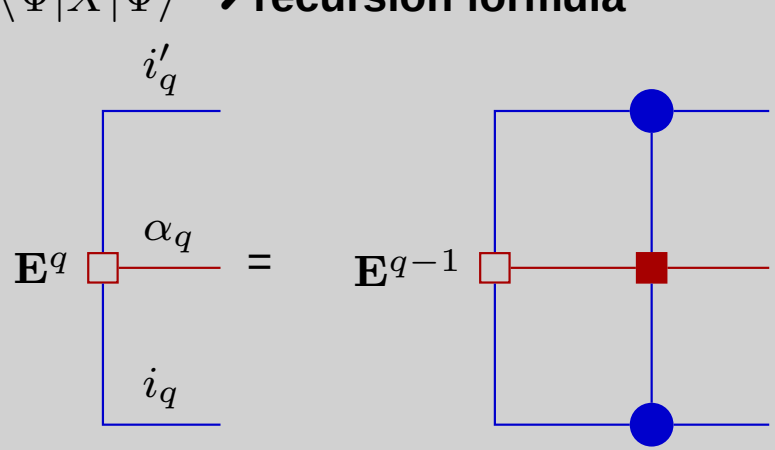


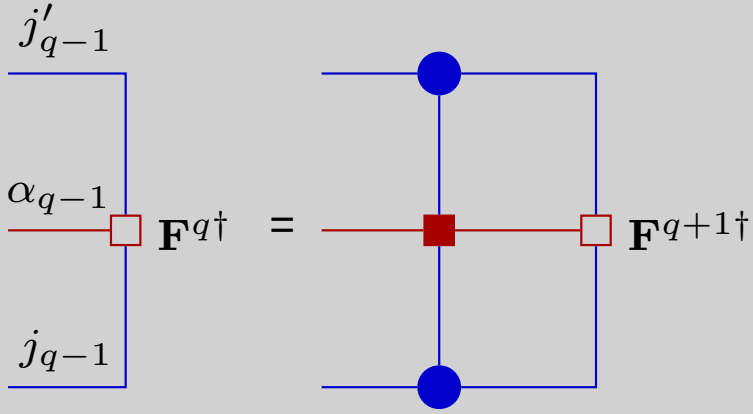


expectation value $\langle\Psi|X|\Psi\rangle =$

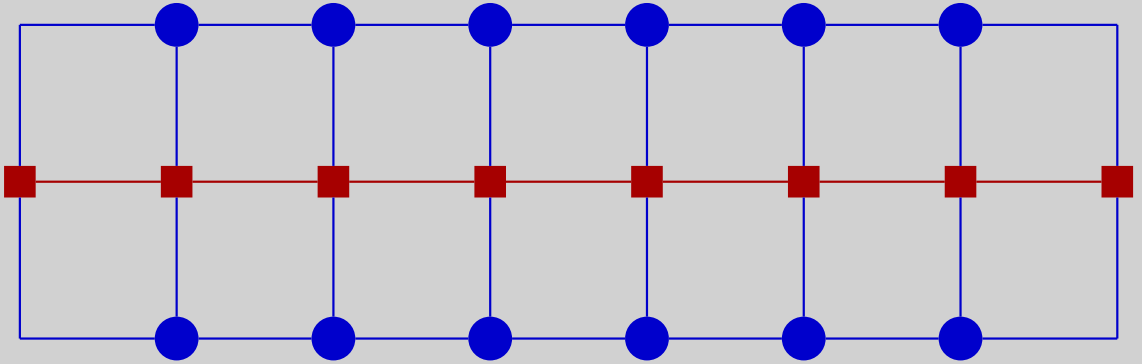
expectation values

$\langle\Psi|X|\Psi\rangle$ ➜ **recursion formula**



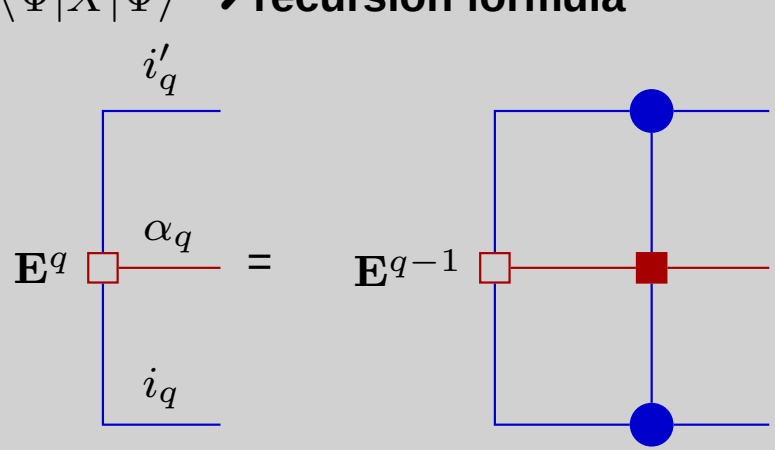


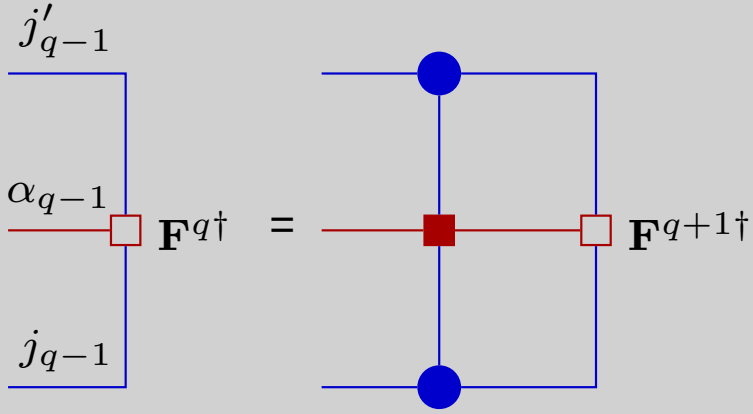
expectation value $\langle\Psi|X|\Psi\rangle =$



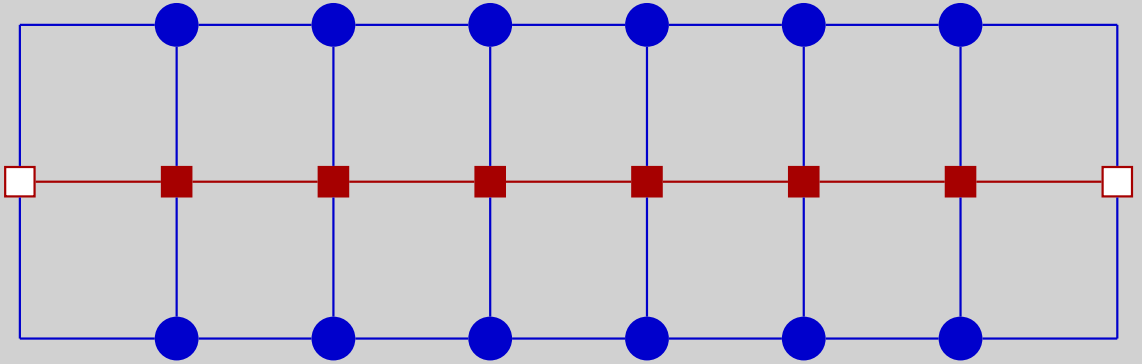
expectation values

$\langle\Psi|X|\Psi\rangle$ ➜ **recursion formula**



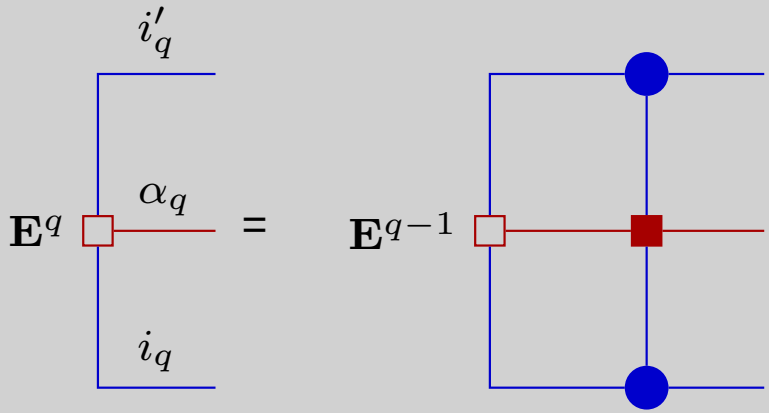


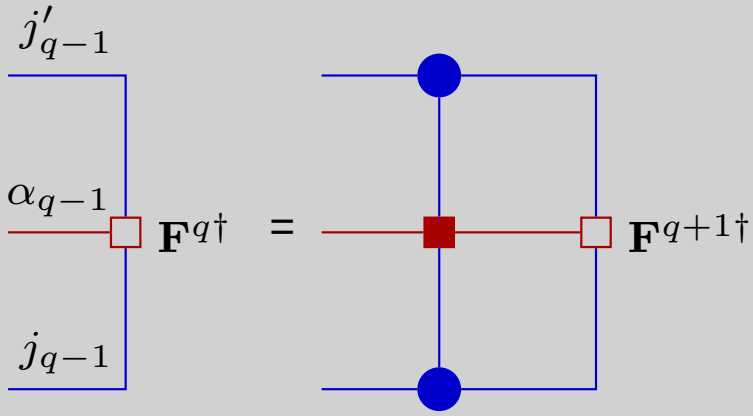
expectation value $\langle\Psi|X|\Psi\rangle =$



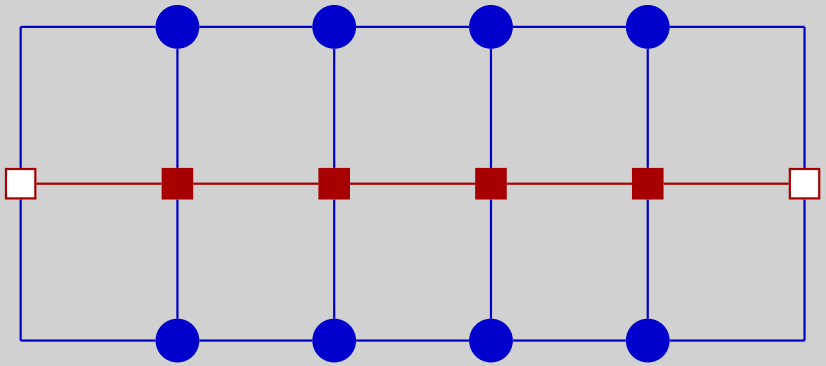
expectation values

$\langle\Psi|X|\Psi\rangle$ ➜ **recursion formula**



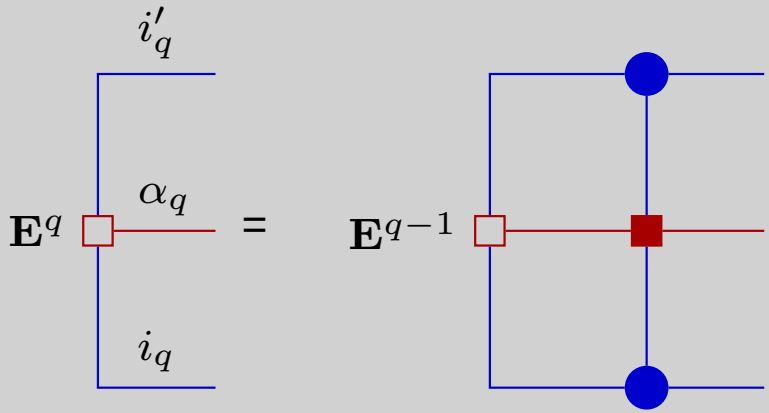


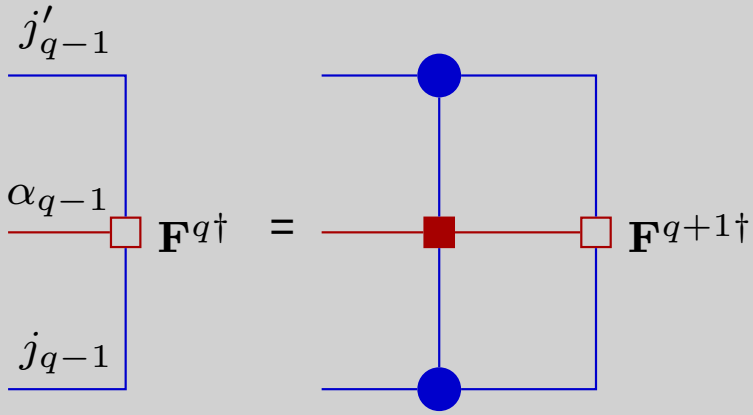
expectation value $\langle\Psi|X|\Psi\rangle =$



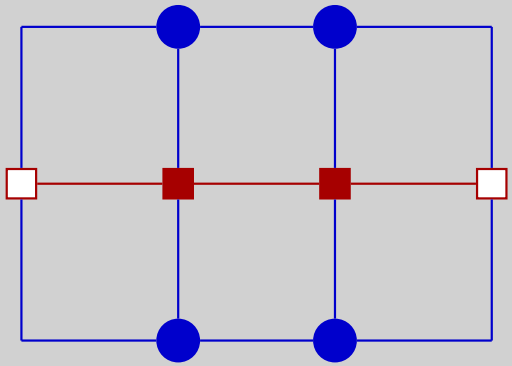
expectation values

$\langle\Psi|X|\Psi\rangle$ ➜ **recursion formula**



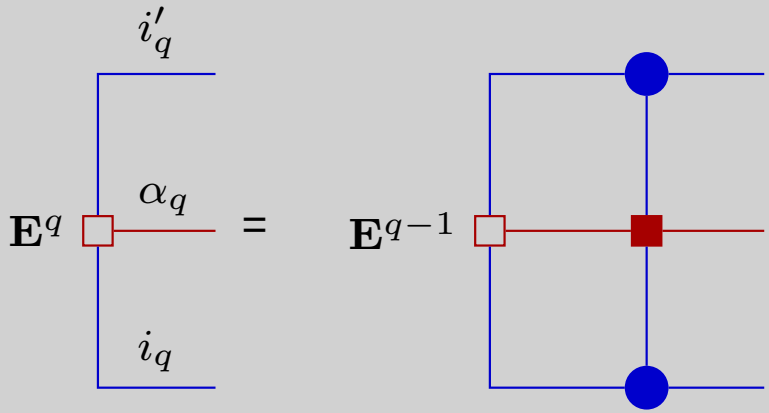


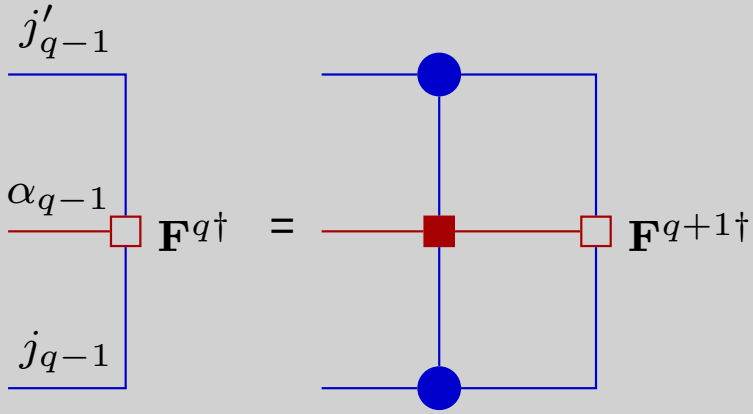
expectation value $\langle\Psi|X|\Psi\rangle =$



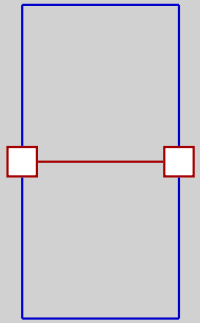
expectation values

$\langle\Psi|X|\Psi\rangle$ ➜ **recursion formula**

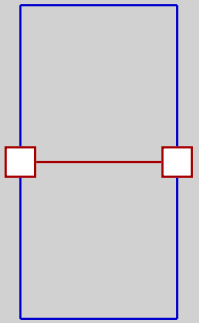




expectation value $\langle\Psi|X|\Psi\rangle =$



expectation values



need $\mathbf{E}$ and $\mathbf{F}^\dagger$ of two adjacent sites only for global expectation value

$$\langle\Psi|X|\Psi\rangle = \sum_{\alpha_q} \mathrm{Tr}\left(\mathbf{E}^q_{\alpha_q}\mathbf{F}^{q+1\dagger}_{\alpha_q}\right)$$

where

$$\mathbf{E}^p_{\alpha_p} = \sum_{n_p n'_p}\sum_{\alpha_{p-1}} X^{n'_p n_p}_{\alpha_{p-1}\alpha_p}\mathbf{A}^{n'_p\dagger}\mathbf{E}^{p-1}_{\alpha_{p-1}}\mathbf{A}^{n_p}$$

$$\mathbf{F}^{p\dagger}_{\alpha_{p-1}} = \sum_{n_p n'_p}\sum_{\alpha_p} X^{n'_p n_p}_{\alpha_{p-1}\alpha_p}\mathbf{A}^{n_p}\mathbf{F}^{p+1\dagger}_{\alpha_p}\mathbf{A}^{n'_p\dagger}$$

or:

$$\langle\Psi|X|\Psi\rangle = \mathrm{tr}\left(\sum_{n_q n'_q}\sum_{\alpha_q,\alpha_{q-1}} X^{n'_q n_q}_{\alpha_{q-1}\alpha_q}\mathbf{A}^{n'_q\dagger}\mathbf{E}^{q-1}_{\alpha_{q-1}}\mathbf{A}^{n_q}\mathbf{F}^{q+1\dagger}_{\alpha_q}\right)$$

local optimization

insert trial MPS

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \mathbf{L}^{n_1} \ldots \mathbf{L}^{n_{q-1}} \mathbf{C}^{n_q} \mathbf{R}^{n_{q+1}} \ldots \mathbf{R}^{n_L} |n_1\rangle \ldots |n_L\rangle$$

into Ritz energy functional:

$$E[|\Psi\rangle] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

we have:

$$\langle\Psi|\Psi\rangle = \sum_{n_q} \mathrm{Tr}(\mathbf{C}^{n_q\dagger}\mathbf{C}^{n_q})$$

and

$$\langle\Psi|H|\Psi\rangle = \mathrm{tr}\left(\sum_{n_q n_q'} \sum_{\alpha_q,\alpha_{q-1}} H^{n_q' n_q}_{\alpha_{q-1}\alpha_q} \mathbf{C}^{n_q'\dagger} \mathbf{E}^{q-1}_{\alpha_{q-1}} \mathbf{C}^{n_q} \mathbf{F}^{q+1\dagger}_{\alpha_q}\right)$$

minimization with respect to $\mathbf{C}^{n_q}$ only equivalent with:

$\boxed{\mathbf{KC} = E\,\mathbf{SC}}$ generalized eigenvalue problem ➜ Lanczos

where

$$K_{i'j'n_q',ijn_q} = \sum_{\alpha_q,\alpha_{q-1}} E^{q-1}_{\alpha_{q-1};i'i} H^{n_q' n_q}_{\alpha_{q-1}\alpha_q} F^{q+1*}_{\alpha_q;j'j}$$ effective Hamiltonian

$$S_{i'j'n_q',ijn_q} = E^{q-1}_{i'i} \delta_{n_q' n_q} F^{q+1*}_{j'j}$$

sweep algorithm

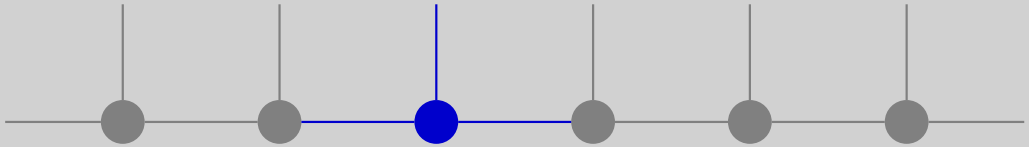
local optimization

sweep algorithm

local optimization

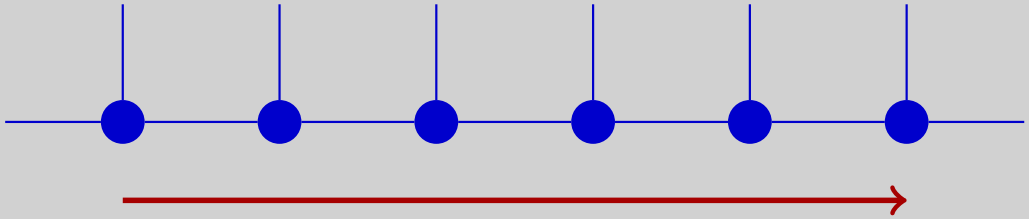
sweep algorithm

local optimization



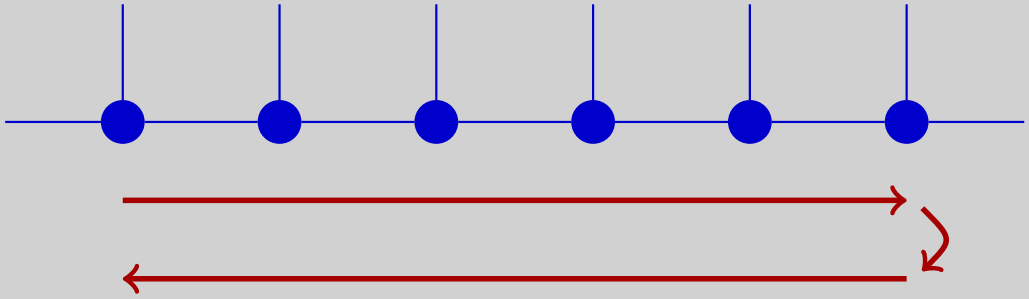
sweep algorithm

local optimization



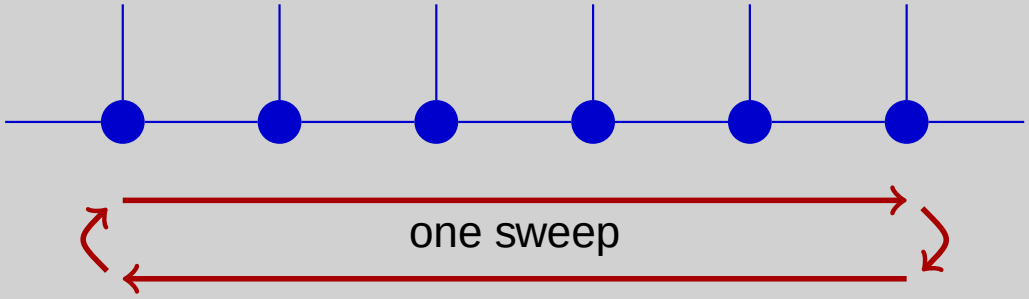
sweep algorithm

local optimization



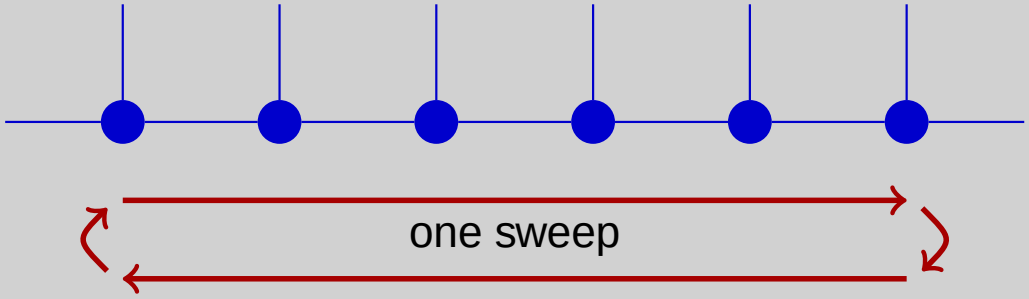
sweep algorithm

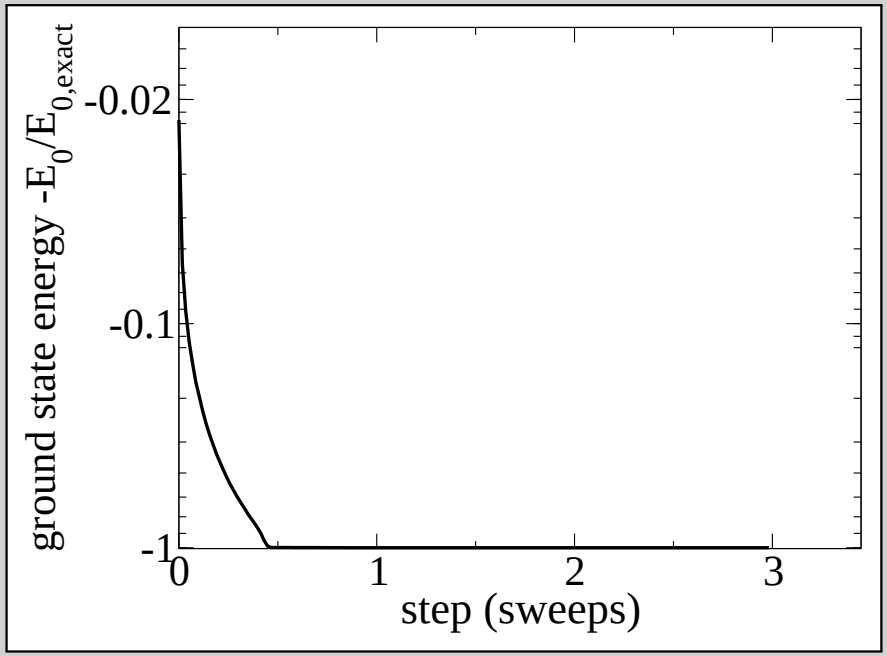
local optimization



sweep algorithm

local optimization

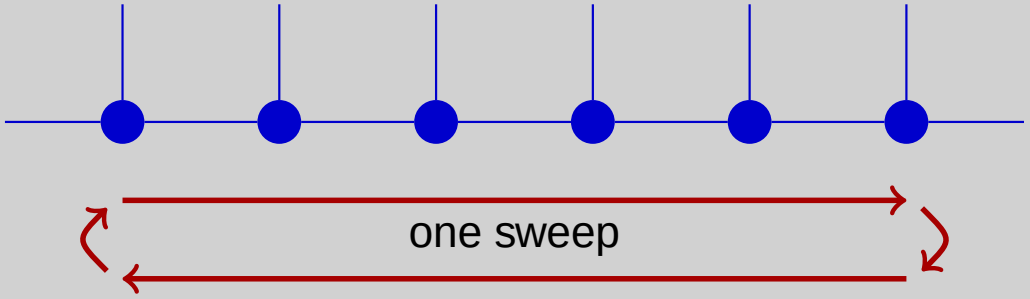


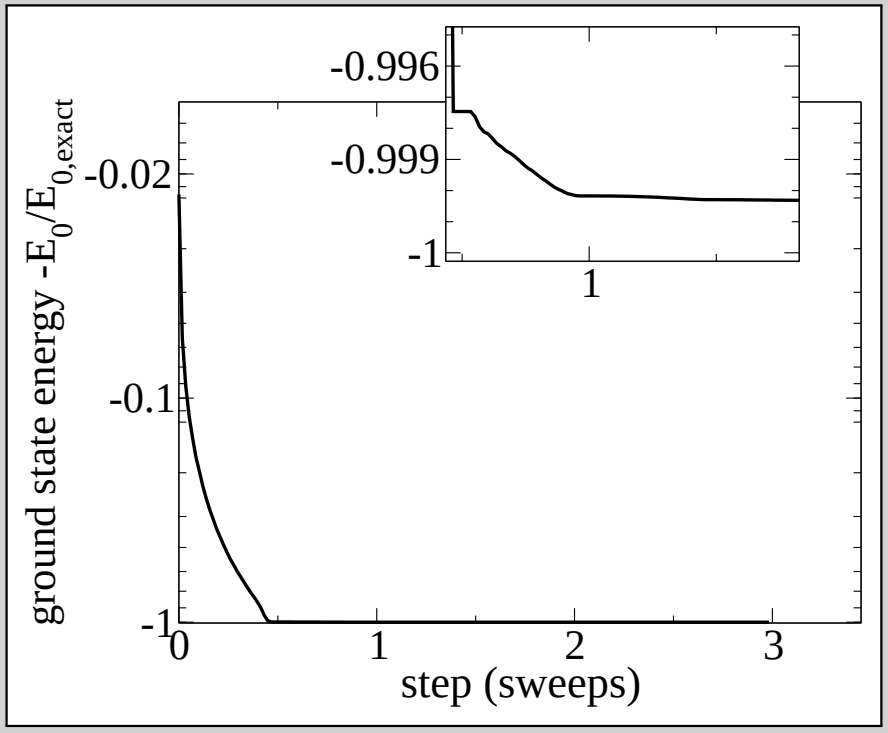


$L = 30, U = 0, t = -0.1$

sweep algorithm

local optimization

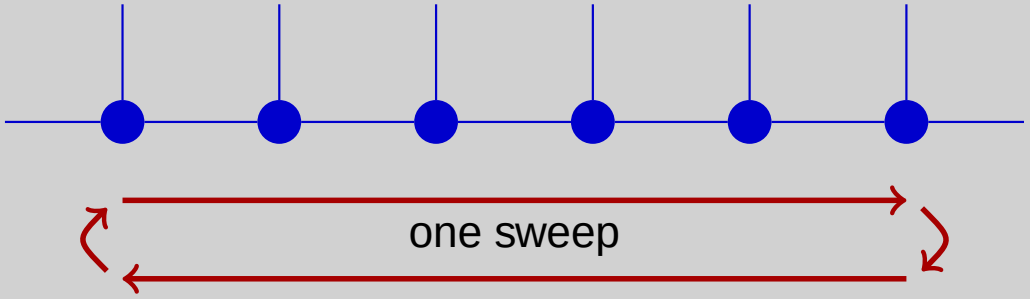


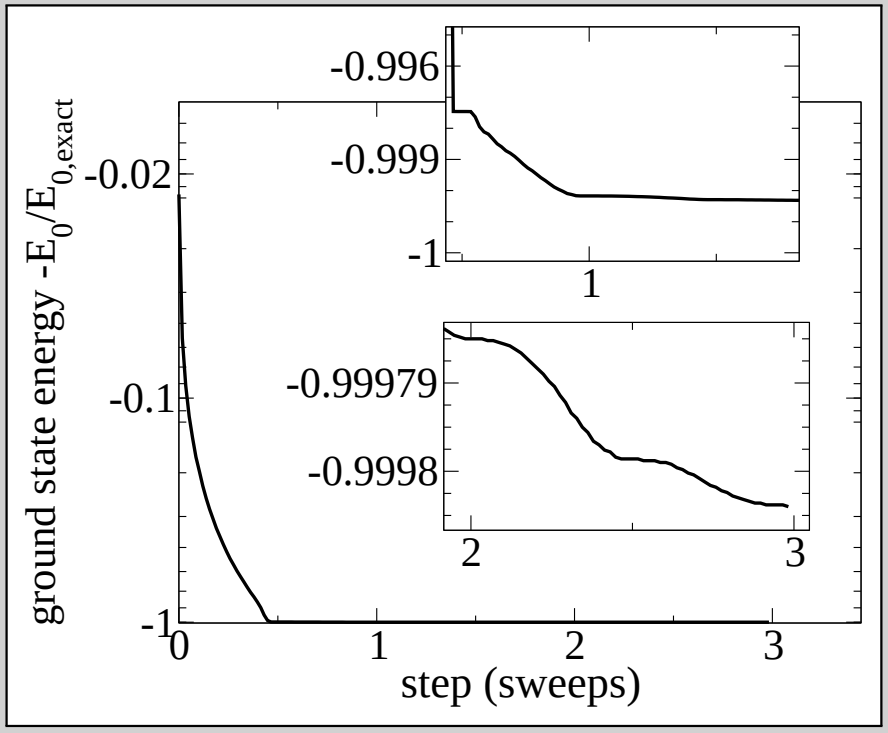


$L = 30, U = 0, t = -0.1$

sweep algorithm

local optimization

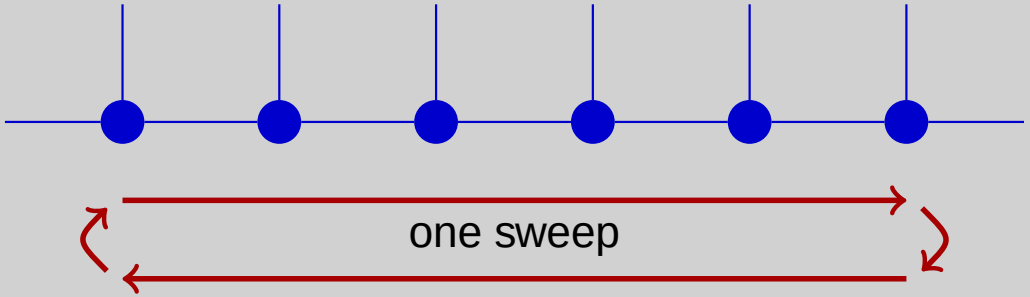


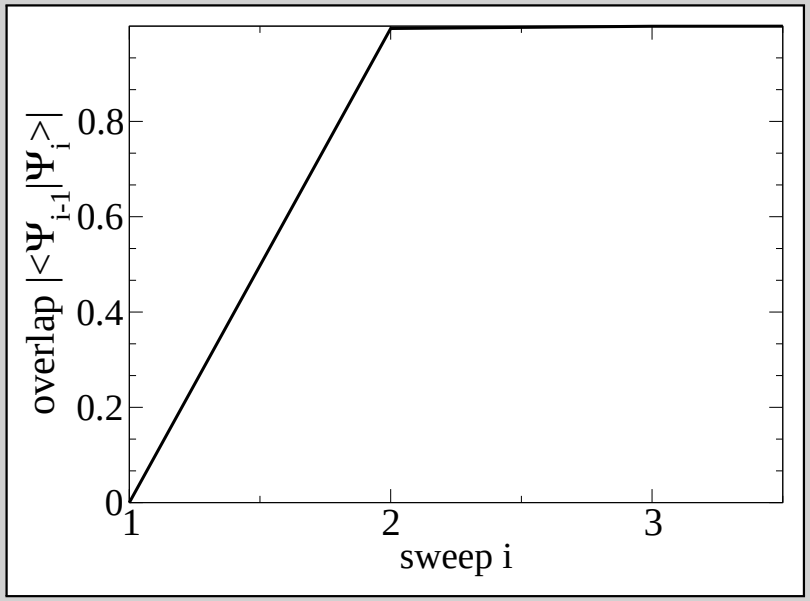


$L = 30, U = 0, t = -0.1$

sweep algorithm

local optimization

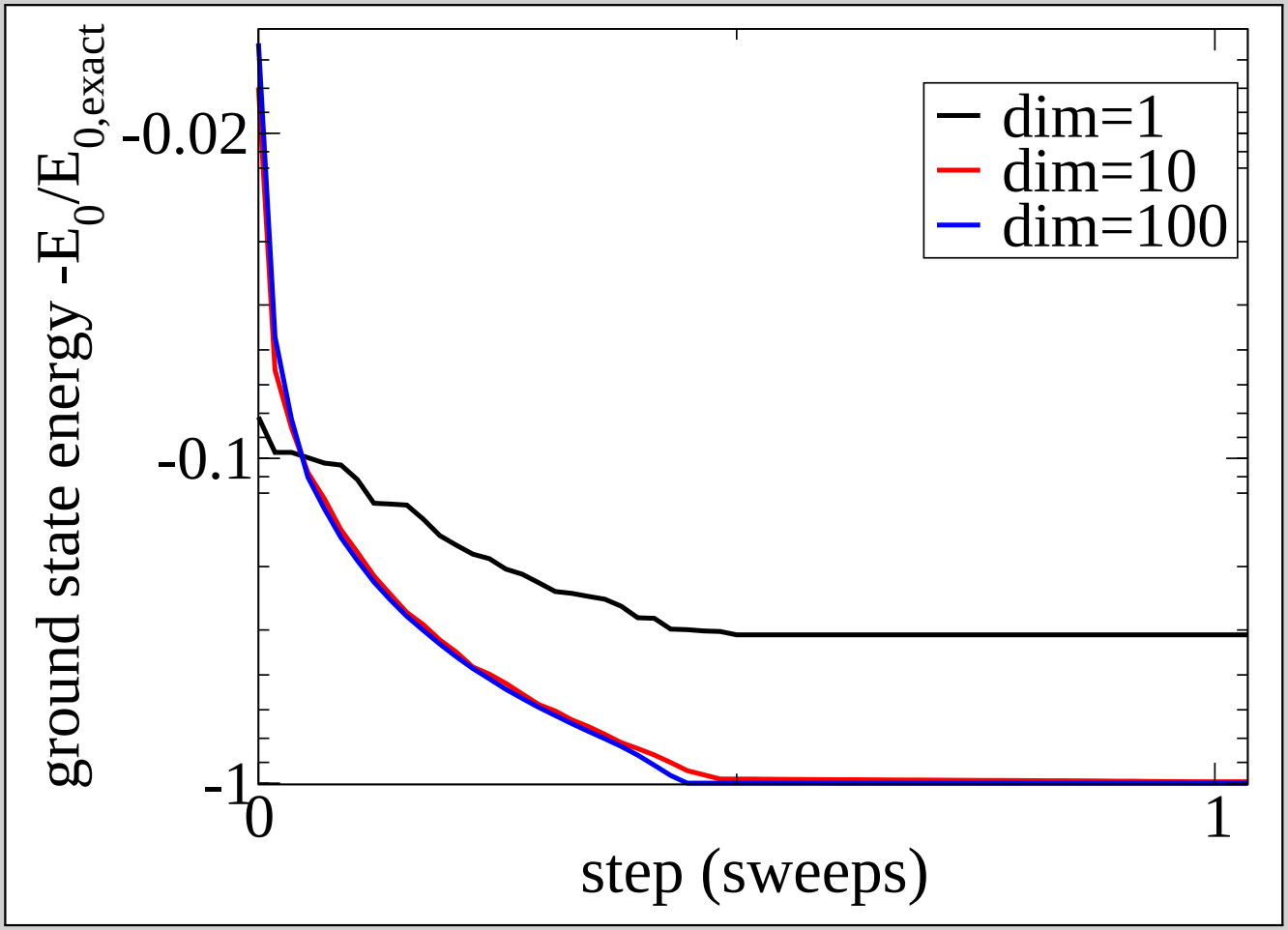




$L = 30, U = 0, t = -0.1$

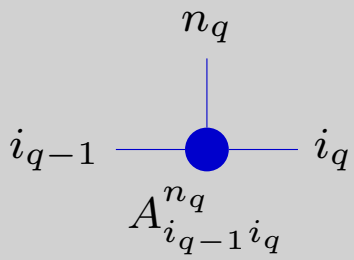
A matrix dimensions

$L = 30, U = 0, t = -0.1$



performance

MPS:



$n_q = 1, ..., d$, d: **local Hilbert space dimension**
$i_q = 1, ..., m$, m: A **matrix dimension**

largest array: MPS ➜

storage:	$L \cdot d \cdot m^2$

most time-consuming: $\mathbf{KC}$ within Lanczos ➜

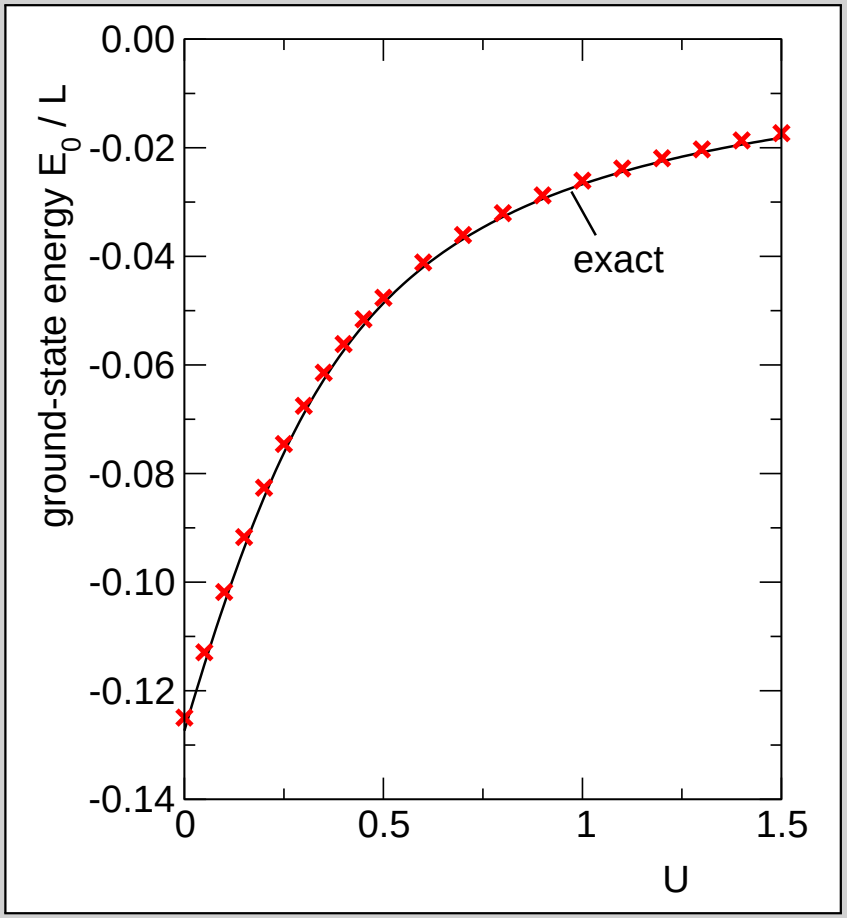
CPU time:	$L \cdot dm^2 \cdot dm^2$

$\mathbf{KC}$: "sparse" (use $K = EHF^\dagger$) ➜

CPU time:	$L \cdot d^2 \cdot m^3$

system size

$L = 30, t = -0.1$



VMPS and DMRG

MPS:

$$|\Psi\rangle = \sum_{n_1,\ldots,n_L} \mathbf{L}^{n_1} \ldots \mathbf{L}^{n_{q-1}} \mathbf{C}^{n_q} \mathbf{R}^{n_{q+1}} \ldots \mathbf{R}^{n_L} |n_1\rangle \ldots |n_L\rangle$$

define:

$$|j_{p-1}\rangle = \sum_{n_p j_p} R^{n_p}_{j_{p-1} j_p} |n_p\rangle |j_p\rangle \qquad p > q,\ n_p = 1, ..., d_p,\ j_p = 1, ..., m_p$$

$$|i_p\rangle = \sum_{i_{p-1} n_p} L^{n_p}_{i_{p-1} i_p} |i_{p-1}\rangle |n_p\rangle \qquad p < q,\ n_p = 1, ..., d_p,\ i_p = 1, ..., m_p$$

blocking	add one site	$\|i_{p-1}\rangle \rightarrow \|i_{p-1}\rangle\|n_p\rangle$
decimation	reduce Hilbert space	$\|i_{p-1}\rangle\|n_p\rangle \rightarrow \|i_p\rangle$

variational wave functions

conclusion:

- application of the Ritz principle for correlated trial wave functions:
  can be as complicated as the full many-body problem
- is simple for simple (uncorrelated) trial wave functions only
- can be done almost exactly in one dimension:
  VMPS (DMRG), NRG

Grand Potential and Derivatives

grandcanonical ensemble

Hamiltonian:

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

grandcanonical partition function and grandcanonical potential:

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

$$\boxed{\Omega = -T \ln Z = \Omega(T, V, \mu, \{t_{\alpha\beta}\}, \{U_{\alpha\beta\gamma\delta}\})}$$

---

expectation value of observable A:

$$\boxed{\langle A \rangle = \frac{1}{Z} \text{tr}\, A e^{-\beta\mathcal{H}}}$$

can be obtained from grand potential:

consider partition: $\boxed{H = H_0 + \lambda A}$ physical H at $\lambda = 1$

we have:

$$\boxed{\frac{\partial \Omega}{\partial \lambda} = \langle A \rangle}$$

motivation: **thermodynamical consistency**

derive all (approximate!) quantities from explicit (approximate) thermodynamical potential

grandcanonical expectation value

$$\boxed{\frac{\partial \Omega}{\partial \lambda} = \langle A \rangle}$$

proof:

$$\frac{\partial \Omega}{\partial \lambda} = -T \frac{\partial}{\partial \lambda} \ln Z = -T \frac{1}{Z} \,\mathrm{tr}\, \frac{\partial}{\partial \lambda} e^{-\beta(H_0 + \lambda A - \mu N)}$$

and:

$$\mathrm{tr}\, \frac{\partial}{\partial \lambda} e^{-\beta(H_0 + \lambda A - \mu N)} = \mathrm{tr} \sum_{k=0}^{\infty} \frac{1}{k!} (-\beta)^k \frac{\partial}{\partial \lambda} (H_0 + \lambda A - \mu N)^k$$

$$= \mathrm{tr} \sum_{k=0}^{\infty} \frac{1}{k!} (-\beta)^k \sum_{r=1}^{k} \mathcal{H}^{k-r} A \mathcal{H}^{r-1} \qquad (\mathcal{H} = H_0 + \lambda A - \mu N = H - \mu N)$$

$$= \mathrm{tr} \sum_{k=0}^{\infty} \frac{1}{k!} (-\beta)^k k \mathcal{H}^{k-1} A$$

$$= \mathrm{tr} \sum_{k=0}^{\infty} \frac{1}{(k-1)!} (-\beta)^{k-1} \mathcal{H}^{k-1} (-\beta A)$$

$$= -\beta \,\mathrm{tr}\, A e^{-\beta \mathcal{H}}$$

hence::

$$\frac{\partial \Omega}{\partial \lambda} = -T \frac{1}{Z} \left(-\beta \,\mathrm{tr}\, A e^{-\beta \mathcal{H}} \right) = \frac{1}{Z} \,\mathrm{tr}\, A e^{-\beta \mathcal{H}} = \langle A \rangle$$

second derivative

$$\frac{\partial^2 \Omega}{\partial \lambda^2} = ?$$

problem:

cyclic invariace of the trace does not help in expressions like $\mathcal{H} \cdots \mathcal{H} A \mathcal{H} \cdots \mathcal{H} A \mathcal{H} \cdots \mathcal{H}$

we have:

$$\begin{aligned} \frac{\partial^2 \Omega}{\partial \lambda^2} &= \frac{\partial}{\partial \lambda} \left(\frac{1}{Z} \text{ tr } \left(A e^{-\beta(H_0 + \lambda A - \mu N)} \right) \right) \\ &= -\frac{1}{Z^2} \frac{\partial Z}{\partial \lambda} \text{ tr } A e^{-\beta \mathcal{H}} + \frac{1}{Z} \text{ tr } A \frac{\partial}{\partial \lambda} e^{-\beta(H_0 + \lambda A - \mu N)} \end{aligned}$$

and with

$$\frac{\partial Z}{\partial \lambda} = -\frac{1}{T} \text{ tr } A e^{-\beta \mathcal{H}}$$

we get:

$$\frac{\partial^2 \Omega}{\partial \lambda^2} = \beta \langle A \rangle^2 + \frac{1}{Z} \text{ tr } A \frac{\partial}{\partial \lambda} e^{-\beta(H_0 + \lambda A - \mu N)}$$

use **Trotter decomposition** :

$$\exp\left(\frac{1}{m}(A+B)\right) = \exp\left(\frac{1}{m}A\right) \exp\left(\frac{1}{m}B\right) + \mathcal{O}\left(\frac{1}{m^2}\right)$$

second derivative

it follows:

$$\text{tr}\, A\frac{\partial}{\partial\lambda}e^{-\beta\mathcal{H}} = \text{tr}\, A\frac{\partial}{\partial\lambda}\lim_{m\to\infty}\left(e^{-\frac{\beta}{m}\lambda A}e^{-\frac{\beta}{m}(H_0-\mu N)}\right)^m$$

carry out partial derivative:

$$\text{tr}\, A\frac{\partial}{\partial\lambda}e^{-\beta\mathcal{H}} = \lim_{m\to\infty}\text{tr}\, A\sum_{r=1}^{m}X^{m-r}\frac{\partial X}{\partial\lambda}X^{r-1}$$

consider:

$$\frac{\partial X}{\partial\lambda} = \frac{\partial}{\partial\lambda}\left(e^{-\frac{\beta}{m}\lambda A}e^{-\frac{\beta}{m}(H_0-\mu N)}\right) = \frac{\partial}{\partial\lambda}\left(e^{-\frac{\beta}{m}\lambda A}\right)e^{-\frac{\beta}{m}(H_0-\mu N)} = -\frac{\beta}{m}AX$$

therewith:

$$\text{tr}\, A\frac{\partial}{\partial\lambda}e^{-\beta\mathcal{H}} = \lim_{m\to\infty}\text{tr}\, A\sum_{r=1}^{m}X^{m-r}\left(-\frac{\beta}{m}A\right)XX^{r-1}$$

$$= -\,\text{tr}\lim_{m\to\infty}\sum_{r=1}^{m}\frac{\beta}{m}AX^{m-r}AX^{r}$$

---

continuum limit $m\to\infty$:

$$\tau = r\frac{\beta}{m}\in[0,\beta] \qquad d\tau = \frac{\beta}{m}$$

$$X^r = e^{-r\frac{\beta}{m}\mathcal{H}} = e^{-\mathcal{H}\tau} \qquad X^m = e^{-\beta\mathcal{H}} \qquad X^{m-r} = e^{-\beta\mathcal{H}}e^{\mathcal{H}\tau}$$

second derivative

in the limit:

$$\begin{aligned}
&\text{tr}\, A\frac{\partial}{\partial\lambda}e^{-\beta\mathcal{H}} = -\,\text{tr}\int_0^\beta d\tau A e^{-\beta\mathcal{H}}e^{\mathcal{H}\tau}Ae^{-\mathcal{H}\tau}\\
&= -\int_0^\beta d\tau\,\text{tr}\, e^{-\beta\mathcal{H}}e^{\mathcal{H}\tau}Ae^{-\mathcal{H}\tau}A\\
&= -Z\int_0^\beta d\tau\langle A(\tau)A(0)\rangle
\end{aligned}$$

here we have defined

modified Heisenberg representation

$$\boxed{A(\tau) = e^{\mathcal{H}\tau}Ae^{-\mathcal{H}\tau}} \qquad (\mathcal{H} = H - \mu N)$$

- ✧ note the missing i
- ✧ **imaginary time** τ

collecting the results:

$$\boxed{\frac{\partial^2\Omega}{\partial\lambda^2} = \beta\langle A\rangle^2 - \int_0^\beta d\tau\langle A(\tau)A(0)\rangle = \frac{\partial\langle A\rangle}{\partial\lambda}}$$

second derivative

more general:

let $\boxed{H = H_0 + \lambda_A A + \lambda_B B}$ ➜ $\Omega = \Omega(\lambda_A, \lambda_B)$

then:

$$\frac{\partial \Omega}{\partial \lambda_A} = \langle A \rangle \qquad \frac{\partial \Omega}{\partial \lambda_B} = \langle B \rangle$$

and:

$$\boxed{\frac{\partial^2 \Omega}{\partial \lambda_B \partial \lambda_A} = \frac{\partial \langle A \rangle}{\partial \lambda_B} = \beta \langle B \rangle \langle A \rangle - \int_0^\beta d\tau \langle B(\tau) A(0) \rangle = \frac{\partial \langle B \rangle}{\partial \lambda_A} = \frac{\partial^2 \Omega}{\partial \lambda_A \partial \lambda_B}}$$

$(\partial \langle A \rangle / \partial \lambda_B) d\lambda_B$: change of expectation value of A due to small perturbation $\lambda_B \rightarrow \lambda_B + d\lambda_B$

➜ classical mechanics: response quantities are correlation functions

➜ quantum mechanics: time-depdendent correlation functions

Generalized Ritz Prinziple

grand potential is concave

if $[A,\mathcal{H}]_- = 0$ then $A(\tau) = A(0) = A$ and

$$\frac{\partial^2\Omega}{\partial\lambda^2} = \beta\langle A\rangle^2 - \beta\langle A^2\rangle = -\beta\langle(A-\langle A\rangle)^2\rangle \leq 0$$

this is also true in general (if $[A,\mathcal{H}]_- \neq 0$):

$$\boxed{\frac{\partial^2\Omega}{\partial\lambda^2} \leq 0}$$ ➜ Ω is a concave function λ!

---

proof: write $\Delta A = A - \langle A\rangle$, then (with $A = A^\dagger$):

$$\frac{\partial^2\Omega}{\partial\lambda^2} = -\int_0^\beta d\tau\langle(A-\langle A\rangle)(\tau)(A-\langle A\rangle)(0)\rangle$$

$$= -\int_0^\beta d\tau \frac{1}{Z}\,\text{tr}\,\left(e^{-\beta\mathcal{H}}\Delta A(\tau)\Delta A(0)\right)$$

$$= -\int_0^\beta d\tau \frac{1}{Z}\,\text{tr}\,\left(e^{-\beta\mathcal{H}}e^{\mathcal{H}\tau}\Delta A e^{-\mathcal{H}\tau}\Delta A\right)$$

$$= -\int_0^\beta d\tau \frac{1}{Z}\,\text{tr}\,\left(e^{-\beta\mathcal{H}}e^{\mathcal{H}\tau/2}\Delta A e^{-\mathcal{H}\tau/2}e^{-\mathcal{H}\tau/2}\Delta A e^{\mathcal{H}\tau/2}\right)$$

$$= -\int_0^\beta d\tau \frac{1}{Z}\,\text{tr}\,\left(e^{-\beta\mathcal{H}}\Delta A(\tau/2)\Delta A(\tau/2)^\dagger\right)$$

$$= -\int_0^\beta d\tau \frac{1}{Z}\sum_{mn} e^{-\beta\mathcal{E}_m}\langle m|\Delta A(\tau/2)|n\rangle\langle n|\Delta A(\tau/2)^\dagger|m\rangle$$

$$= -\int_0^\beta d\tau \frac{1}{Z}\sum_{mn} e^{-\beta\mathcal{E}_m}|\langle m|\Delta A(\tau/2)|n\rangle|^2 \leq 0$$ where $\mathcal{H}|m\rangle = \mathcal{E}_m|m\rangle$

formulation of the generalized Ritz principle

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

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

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:

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

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

Wick's Theorem

free one-particle correlation functions

- ✧ important for static mean-field theory
- ✧ essential for diagrammatic perturbation theory

one-particle ("free") Hamiltonian:

$$H_0 = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta$$

diagonalize hopping matrix:

$$\mathbf{t} = \mathbf{U}\varepsilon\mathbf{U}^\dagger$$

yields:

$$H_0 = \sum_k \varepsilon(k) c_k^\dagger c_k$$

free Fermi gas

diagonal correlation function:

$$\langle c_k^\dagger c_k \rangle^{(0)} = \frac{1}{e^{\beta(\varepsilon(k)-\mu)}+1}$$

Fermi function

back-transformation:

$$\langle c_\alpha^\dagger c_\beta \rangle^{(0)} = \sum_k U_{\alpha,k} \frac{1}{e^{\beta(\varepsilon(k)-\mu)}+1} U_{k,\beta}^*$$

$$\langle c_\beta c_\alpha^\dagger \rangle^{(0)} = \sum_k U_{\beta,k} \frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}} U_{k,\alpha}^*$$

(using $[c_\alpha, c_\beta^\dagger]_+ = \delta_{\alpha\beta}$)

free time dependence

(modified) Heisenberg **free** (imaginary) time dependence:

$$\boxed{c_\alpha(\tau) = e^{\mathcal{H}_0\tau} c_\alpha e^{-\mathcal{H}_0\tau}} \qquad \mathcal{H}_0 = H_0 - \mu N = \sum_{\alpha\beta}(t_{\alpha\beta} - \mu\delta_{\alpha\beta}) c^\dagger_\alpha c_\beta$$

using Baker-Campbell-Hausdorff formula / Hadamard-Lemma:

$$c_\alpha(\tau) = e^{-\tau \mathcal{L}_{\mathcal{H}_0}} c_\alpha$$

with

$$\mathcal{L}_{\mathcal{H}_0} c_\alpha \equiv [c_\alpha, \mathcal{H}_0]_- = \sum_\beta (t_{\alpha\beta} - \mu\delta_{\alpha\beta}) c_\beta$$

hence:

$$c_\alpha(\tau) = \sum_k \frac{1}{k!}(-\tau)^k \mathcal{L}^k_{\mathcal{H}_0} c_\alpha = \sum_k \frac{1}{k!}(-\tau)^k \sum_\beta (\mathbf{t} - \mu\mathbf{1})^k_{\alpha\beta} c_\beta$$

and:

$$\boxed{c_\alpha(\tau) = \sum_\beta \left(e^{-(\mathbf{t}-\mu\mathbf{1})\tau} \right)_{\alpha\beta} c_\beta}$$

$$\boxed{c^\dagger_\alpha(\tau) = e^{\mathcal{H}_0\tau} c^\dagger_\alpha e^{-\mathcal{H}_0\tau} = \sum_\beta \left(e^{+(\mathbf{t}-\mu\mathbf{1})\tau} \right)_{\alpha\beta} c^\dagger_\beta}$$

simple, exponential time dependence

free time-dependent one-particle correlation function

collecting:

$$\langle c_\gamma c_\beta^\dagger \rangle^{(0)} = \sum_k U_{\gamma,k} \frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}} U_{k,\beta}^*$$

$$c_\alpha(\tau) = e^{\mathcal{H}_0 \tau} c_\alpha e^{-\mathcal{H}_0 \tau} = \sum_\gamma \left(e^{-(\mathbf{t}-\mu\mathbf{1})\tau} \right)_{\alpha\gamma} c_\gamma$$

free time-dependent one-particle correlation function:

$$\langle c_\alpha(\tau) c_\beta^\dagger(0) \rangle^{(0)} = \sum_\gamma \left(e^{-(\mathbf{t}-\mu\mathbf{1})\tau} \right)_{\alpha\gamma} \langle c_\gamma c_\beta^\dagger \rangle^{(0)}$$

thus:

$$\langle c_\alpha(\tau) c_\beta^\dagger(0) \rangle^{(0)} = \sum_{\gamma,k} \left(e^{-(\mathbf{t}-\mu\mathbf{1})\tau} \right)_{\alpha\gamma} U_{\gamma,k} \frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}} U_{k,\beta}^*$$

and:

$$\langle c_\alpha(\tau) c_\beta^\dagger(0) \rangle^{(0)} = \left(\frac{e^{-(\mathbf{t}-\mu\mathbf{1})\tau}}{1+e^{-\beta(\mathbf{t}-\mu\mathbf{1})}} \right)_{\alpha\beta}$$

(and analogous expressions for $\langle c_\alpha(0) c_\beta^\dagger(\tau) \rangle^{(0)}$, $\langle c_\alpha^\dagger(\tau) c_\beta(0) \rangle^{(0)}$, ...)

more?

free time-dependent N-particle correlation functions

definie **time ordering** for creators/annihilators $d = c^\dagger / c$:

$$\mathcal{T}(d_1(\tau_1)d_2(\tau_2)) = \Theta(\tau_1 - \tau_2)d_1(\tau_1)d_2(\tau_2) - \Theta(\tau_2 - \tau_1)d_2(\tau_2)d_1(\tau_1)$$

remember:

earlier operators operate earlier

equal times: creator is "later", i.e.

$$\tau_{\text{creator}} = \tau_{\text{annihilator}} + 0^+$$

define **contraction** :

$$\underline{d_\alpha(\tau_\alpha)d_\beta(\tau_\beta)} = \langle \mathcal{T}(d_\alpha(\tau_\alpha)d_\beta(\tau_\beta))\rangle^{(0)}$$

$$= \Theta(\tau_\alpha - \tau_\beta)\langle d_\alpha(\tau_\alpha)d_\beta(\tau_\beta)\rangle^{(0)} - \Theta(\tau_\beta - \tau_\alpha)\langle d_\beta(\tau_\beta)d_\alpha(\tau_\alpha)\rangle^{(0)}$$

free one-particle Green function :

$$-\underline{c_\alpha(\tau)c^\dagger_\beta(\tau')} = -\langle \mathcal{T}(c_\alpha(\tau)c^\dagger_\beta(\tau'))\rangle^{(0)} \equiv G_{\alpha\beta}(\tau,\tau') = G_{\alpha\beta}(\tau - \tau')$$

note: **free** expectation value and **free** time dependence

free time-dependent N-particle correlation functions

Wick's theorem:

$$\langle \mathcal{T}(d_{\alpha_1}(\tau_1)\cdots d_{\alpha_s}(\tau_s)\rangle^{(0)} = \{\text{sum over all fully contracted terms}\}$$

note: **free** expectation value and **free** time dependence

➜ reduces free N-particle correlation functions to free one-particle correlation functions
➜ essential for diagrammatic perturbations theory
➜ apply to construct static mean-field theory

example:

$$\begin{aligned}
\langle n_\alpha n_\beta\rangle^{(0)} &= \langle c_\alpha^\dagger c_\alpha c_\beta^\dagger c_\beta\rangle^{(0)} = \langle c_\alpha^\dagger(\delta_{\alpha\beta} - c_\beta^\dagger c_\alpha)c_\beta\rangle^{(0)} = \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} - \langle c_\alpha^\dagger c_\beta^\dagger c_\alpha c_\beta\rangle^{(0)} \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} - \langle \mathcal{T}(c_\alpha^\dagger c_\beta^\dagger c_\alpha c_\beta)\rangle^{(0)} \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} - (-\underline{c_\alpha^\dagger c_\alpha}\ \underline{c_\beta^\dagger c_\beta} + \underline{c_\alpha^\dagger c_\beta}\ \underline{c_\beta^\dagger c_\alpha}) \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} + \langle \mathcal{T}(c_\alpha^\dagger c_\alpha)\rangle^{(0)}\langle \mathcal{T}(c_\beta^\dagger c_\beta)\rangle^{(0)} - \langle \mathcal{T}(c_\alpha^\dagger c_\beta)\rangle^{(0)}\langle \mathcal{T}(c_\beta^\dagger c_\alpha)\rangle^{(0)} \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} + \langle c_\alpha^\dagger c_\alpha\rangle^{(0)}\langle c_\beta^\dagger c_\beta\rangle^{(0)} - \langle c_\alpha^\dagger c_\beta\rangle^{(0)}\langle c_\beta^\dagger c_\alpha\rangle^{(0)}
\end{aligned}$$

proof of Wick's theorem

free time-dependent N-particle correlation functions

Wick's theorem:

$$\langle \mathcal{T}(d_{\alpha_1}(\tau_1)\cdots d_{\alpha_s}(\tau_s)\rangle^{(0)} = \{\text{sum over all fully contracted terms}\}$$

note: **free** expectation value and **free** time dependence

➜ reduces free N-particle correlation functions to free one-particle correlation functions
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example:

$$\begin{aligned}
\langle n_\alpha n_\beta\rangle^{(0)} &= \langle c_\alpha^\dagger c_\alpha c_\beta^\dagger c_\beta\rangle^{(0)} = \langle c_\alpha^\dagger(\delta_{\alpha\beta} - c_\beta^\dagger c_\alpha)c_\beta\rangle^{(0)} = \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} - \langle c_\alpha^\dagger c_\beta^\dagger c_\alpha c_\beta\rangle^{(0)} \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} - \langle \mathcal{T}(c_\alpha^\dagger c_\beta^\dagger c_\alpha c_\beta)\rangle^{(0)} \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} - (-\underline{c_\alpha^\dagger c_\alpha}\ \underline{c_\beta^\dagger c_\beta} + \underline{c_\alpha^\dagger c_\beta}\ \underline{c_\beta^\dagger c_\alpha}) \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} + \langle \mathcal{T}(c_\alpha^\dagger c_\alpha)\rangle^{(0)}\langle \mathcal{T}(c_\beta^\dagger c_\beta)\rangle^{(0)} - \langle \mathcal{T}(c_\alpha^\dagger c_\beta)\rangle^{(0)}\langle \mathcal{T}(c_\beta^\dagger c_\alpha)\rangle^{(0)} \\
&= \delta_{\alpha\beta}\langle c_\alpha^\dagger c_\beta\rangle^{(0)} + \langle c_\alpha^\dagger c_\alpha\rangle^{(0)}\langle c_\beta^\dagger c_\beta\rangle^{(0)} - \langle c_\alpha^\dagger c_\beta\rangle^{(0)}\langle c_\beta^\dagger c_\alpha\rangle^{(0)}
\end{aligned}$$

proof of Wick's theorem ... see problems!

III Variational Principles and Approximation Strategies

Static Mean-Field Theory

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:

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

hence:

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

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

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

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

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

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

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

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

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 as invertible:

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

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

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

with

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

Hartree-Fock self-energy

self-consistent scheme required:

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

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

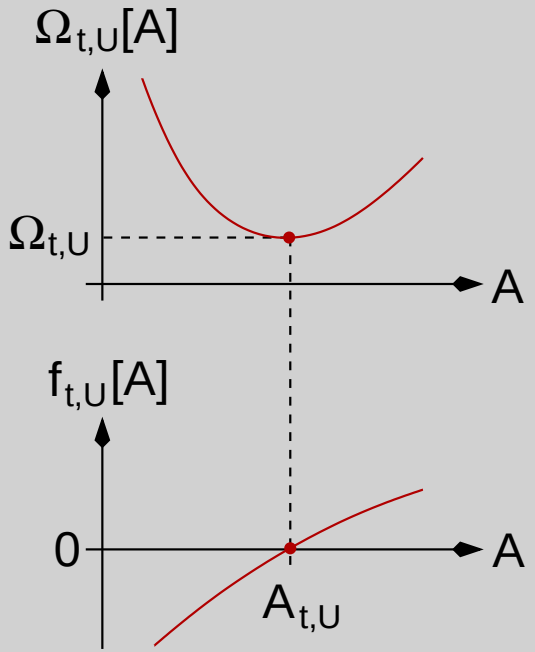
physical quantity: $\mathbf{A}_{\mathbf{t},\mathbf{U}}$

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

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

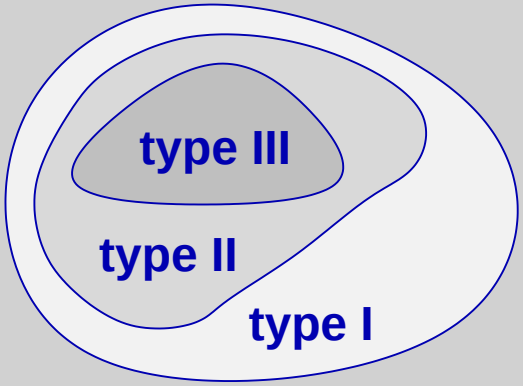
Euler equation:

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



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

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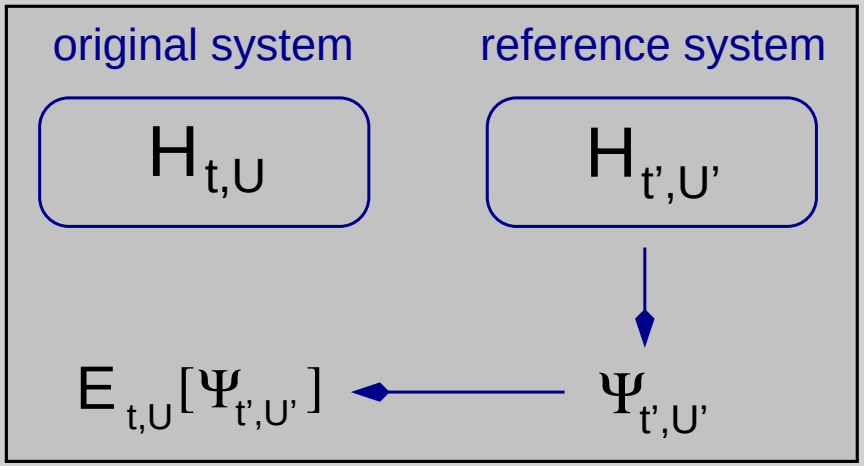

Hartree-Fock:

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

example: Hartree-Fock theory

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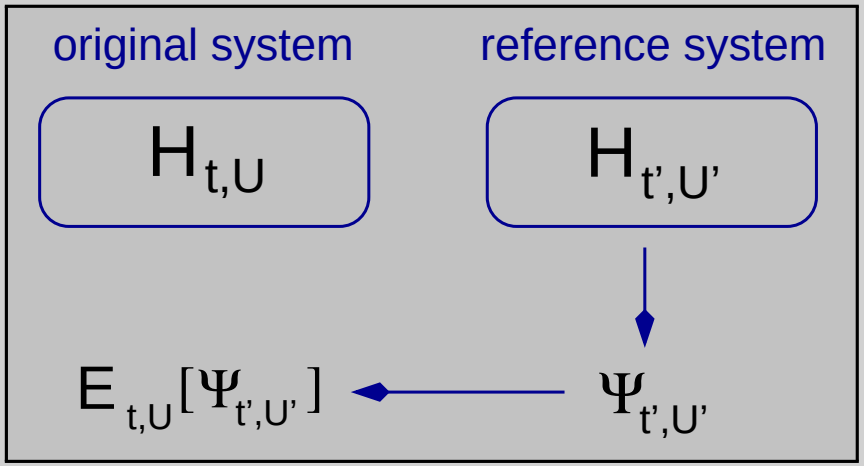

Hartree-Fock:

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

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

Density-Functional Theory

example: density-functional theory

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

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

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)

example: density-functional theory

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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 !

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nice concept,
but poor results !

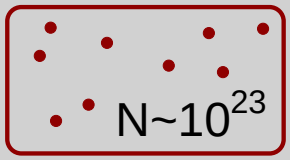
local density approximation: $F^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}] \to \widetilde{F}^{(\text{xc})}_{\mathbf{U}}[\mathbf{n}]$

very successful, but type-II

IV Green's Functions and Perturbation Theory

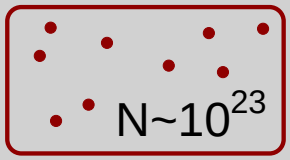
Motivation: Spectroscopies

Green's function, spectral density and self-energy



$|\Psi\rangle = ?$

Green's function, spectral density and self-energy



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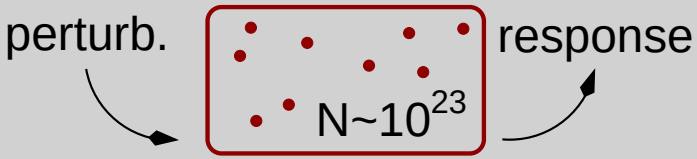
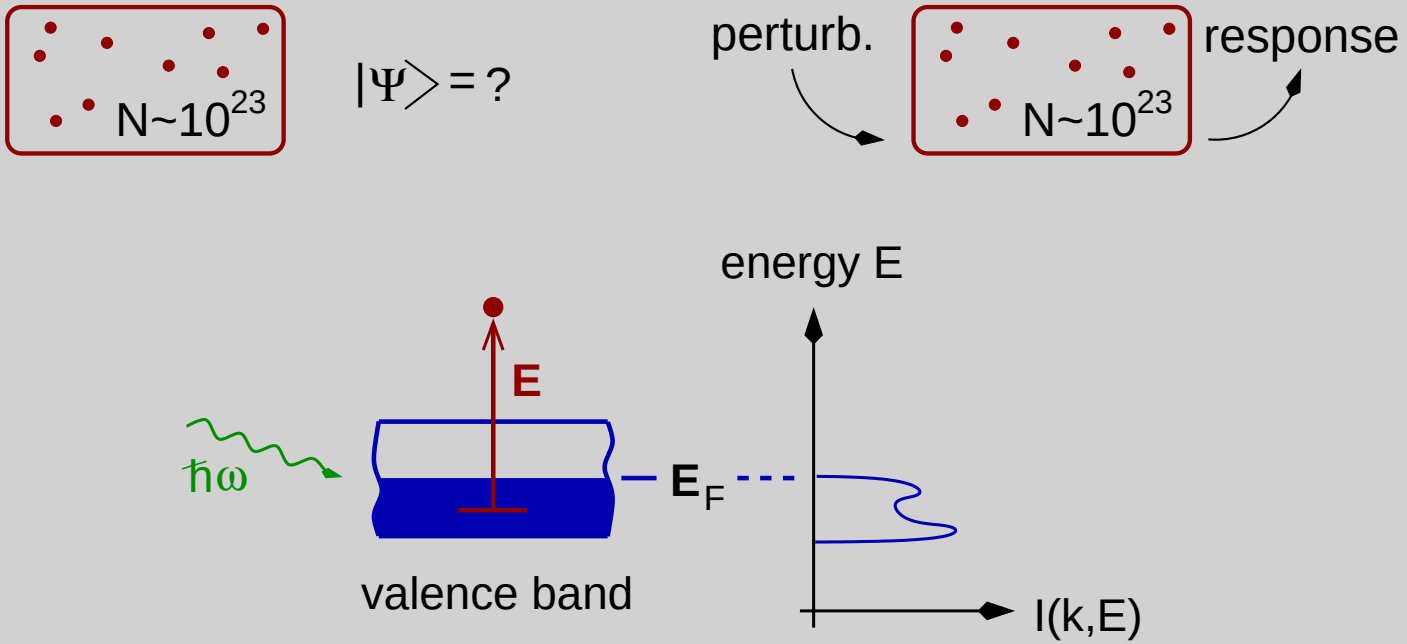
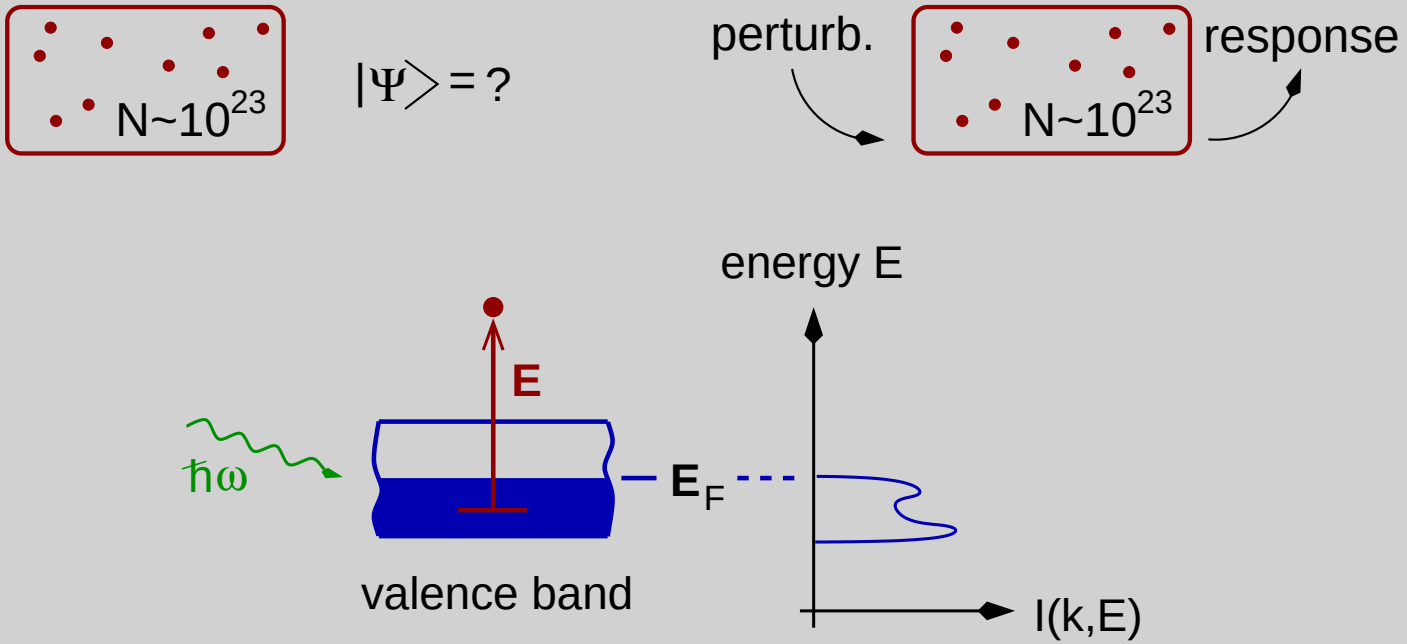


Green's function, spectral density and self-energy



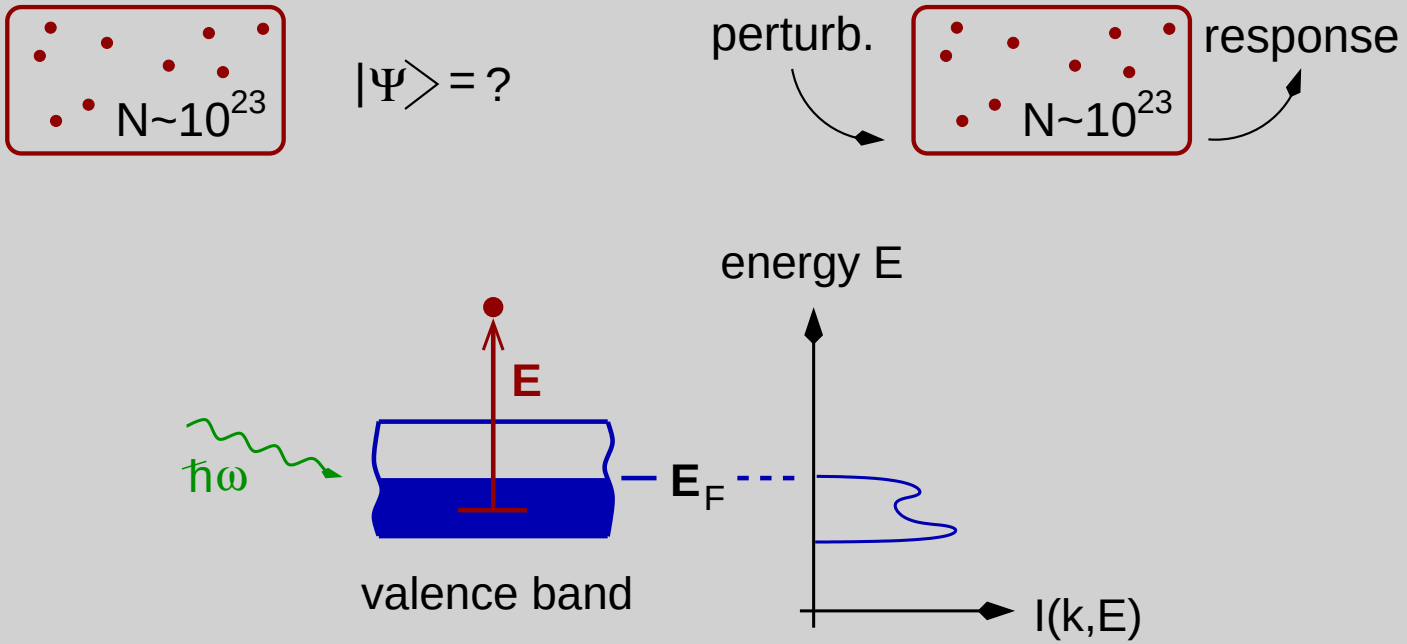
Green's function, spectral density and self-energy



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

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)

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:

$R = c^\dagger_\alpha$

complementary spectroscopy

Auger process:

$R = c_\alpha c_\beta$

appearance-potential spectroscopy:

$R = c^\dagger_\alpha c^\dagger_\beta$

transport, Raman, neutron scattering, etc.:

$R = c^\dagger_\alpha c_\beta$

---

elementary excitation processes

one-electron excitations: $c^\dagger_\alpha, c_\alpha$

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

"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

calculation of the intensity / cross section

zero temperature, $T = 0$:

system is in its ground state $|0\rangle$

probability for transition $|0\rangle \longrightarrow |m\rangle$

$$\boxed{|\langle m|R|0\rangle|^2}$$ (first-order perturbation theory in R)

excitation energy:

$$\boxed{\omega = E_m - E_0}$$

intensity $\sim$ spectral density of transitions with excitation energies between ω and $\omega + d\omega$:

$$\boxed{I_R(\omega) = \sum_m |\langle m|R|0\rangle|^2 \delta(\omega - (E_m - E_0))}$$

(including $\omega = 0$, $E_m = E_{m'}$)

---

finite temperature, $T \geq 0$:

with probability

$$\boxed{p_n = \frac{1}{Z} e^{-\beta E_n}}$$

the system is in the state $|n\rangle$ initially ➜

$$\boxed{I_R(\omega) = \frac{1}{Z} \sum_{mn} e^{-\beta E_n} |\langle m|R|n\rangle|^2 \delta(\omega - (E_m - E_n))}$$

($\omega < 0$ possible)

complementary spectroscopy

analogously for $R^\dagger$:

$$I_{R^\dagger}(\omega) = \frac{1}{Z}\sum_{mn} e^{-\beta E_n} |\langle m|R^\dagger|n\rangle|^2 \delta(\omega - (E_m - E_n))$$
$$= \frac{1}{Z}\sum_{mn} e^{-\beta E_n} |\langle n|R|m\rangle|^2 \delta(\omega - (E_m - E_n))$$
$$= \frac{1}{Z}\sum_{mn} e^{-\beta E_m} |\langle m|R|n\rangle|^2 \delta(\omega - (E_n - E_m)) \; (m \leftrightarrow n)$$
$$= e^{\beta\omega}\frac{1}{Z}\sum_{mn} e^{-\beta E_n} |\langle m|R|n\rangle|^2 \delta(-\omega - (E_m - E_n))$$

we have: $\boxed{I_{R^\dagger}(\omega) = e^{\beta\omega} I_R(-\omega)}$ and: $\boxed{I_R(\omega) = e^{\beta\omega} I_{R^\dagger}(-\omega)}$

---

discussion for $R = c_\alpha$ (photoemission), $R^\dagger = c_\alpha^\dagger$ (inverse PE)

- $I_{R^\dagger}(\omega)$ for $\omega > 0$: “normal” IPE spectrum
- $I_{R^\dagger}(-\omega)$ for $\omega > 0$ exponentially suppressed but can be measured
- multiplication with exponential yields “normal” PE spectrum
  $I_R(\omega) = e^{\beta\omega} I_{R^\dagger}(-\omega)$
- but: error bars are also enhanced exponentially

spectral density

(Lehmann representation of the) spectral density:

$$S(\omega) = \sum_{mn} \frac{e^{-\beta E_m} - \overline{\varepsilon}\, e^{-\beta E_n}}{Z} \langle m|R|n\rangle\langle n|R^\dagger|m\rangle \delta(\omega - (E_n - E_m))$$

$\overline{\varepsilon} = +1$: commutator spectral density

$\overline{\varepsilon} = -1$: anticommutator spectral density

choose (for fermions): $\boxed{\overline{\varepsilon} = (-1)^k}$ with k: number of creators/annihilators in R

we have:

$$S(\omega) = I_{R^\dagger}(\omega) - \overline{\varepsilon}\, e^{-\beta\omega} I_{R^\dagger}(\omega) = (1 - \overline{\varepsilon}\, e^{-\beta\omega}) I_{R^\dagger}(\omega)$$

and:

$$\boxed{I_{R^\dagger}(\omega) = \frac{e^{\beta\omega}}{e^{\beta\omega} - \overline{\varepsilon}} S(\omega)}$$

$$\boxed{I_R(-\omega) = \frac{1}{e^{\beta\omega} - \overline{\varepsilon}} S(\omega)}$$

and:

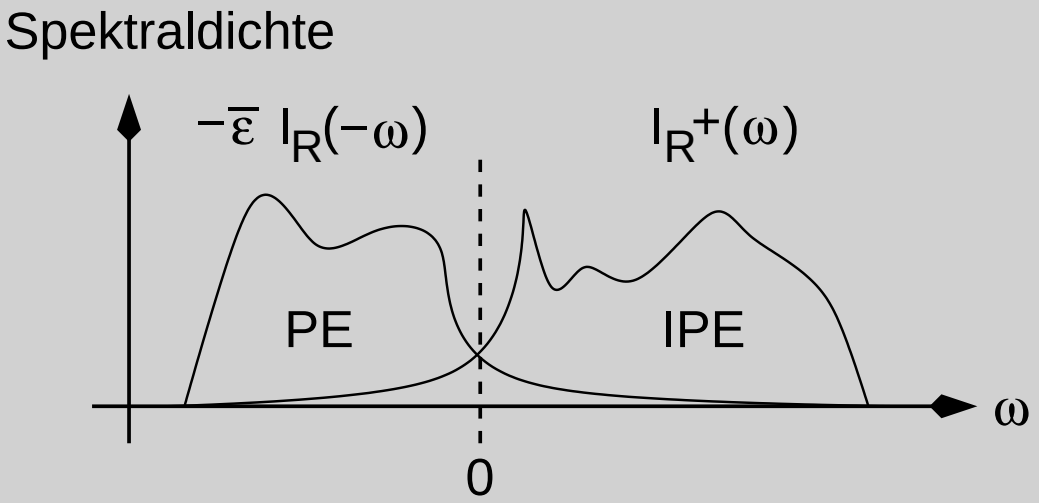
$$\boxed{S(\omega) = I_{R^\dagger}(\omega) - \overline{\varepsilon}\, I_R(-\omega)}$$

comprises spectroscopy and its inverse

one-particle spectral density

(inverse) photoemission: $R = c_\alpha$

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



Fourier transformation:

$$X(\omega) = \int \exp(i\omega t) X(t) dt \qquad X(t) = \frac{1}{2\pi} \int \exp(-i\omega t) X(\omega) d\omega$$

we have:

$$A_{\alpha\beta}(\omega) = \sum_{mn} \frac{e^{-\beta E_m} + e^{-\beta E_n})}{Z} \langle m|c_\alpha|n\rangle\langle n|c_\beta^\dagger|m\rangle \frac{1}{2\pi} \int e^{i(\omega - (E_n - E_m))t} dt$$

one-particle spectral density

➜ **time-dependent** correlation function

$$
\begin{aligned}
A_{\alpha\beta}(t) &= \frac{1}{2\pi}\sum_{mn}\frac{e^{-\beta E_m}+e^{-\beta E_n}}{Z}\langle m|c_\alpha|n\rangle\langle n|c_\beta^\dagger|m\rangle e^{-iE_n t}e^{iE_m t} \\
&= \frac{1}{2\pi}\sum_{mn}\frac{e^{-\beta E_m}+e^{-\beta E_n}}{Z}\langle m|e^{i\mathcal{H}t}c_\alpha e^{-i\mathcal{H}t}|n\rangle\langle n|c_\beta^\dagger|m\rangle \\
&= \frac{1}{2\pi}\frac{1}{Z}\sum_{mn}\left(e^{-\beta E_m}\langle m|c_\alpha(t)|n\rangle\langle n|c_\beta^\dagger|m\rangle + e^{-\beta E_n}\langle m|c_\alpha(t)|n\rangle\langle n|c_\beta^\dagger|m\rangle\right) \\
&= \frac{1}{2\pi}\left(\langle c_\alpha(t)c_\beta^\dagger(0)\rangle + \langle c_\beta^\dagger(0)c_\alpha(t)\rangle\right)
\end{aligned}
$$

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

with: $A(t) = \exp(i\mathcal{H}t)A\exp(-i\mathcal{H}t)$ (grandcanonical Heisenberg representation)

---

example: **Fermi-Gas** $\mathcal{H} = \sum_\alpha(\varepsilon_\alpha - \mu)c_\alpha^\dagger c_\alpha$

$$\boxed{A_{\alpha\beta}(\omega) = \delta_{\alpha\beta}\int dt\; e^{i\omega t}A_{\alpha\beta}(t) = \delta_{\alpha\beta}\int dt\, e^{i\omega t}\frac{1}{2\pi}e^{-i(\varepsilon_\alpha-\mu)t} = \delta_{\alpha\beta}\delta(\omega-(\varepsilon_\alpha-\mu)}$$

interaction effects: damping, satellites, weight transfer, ...

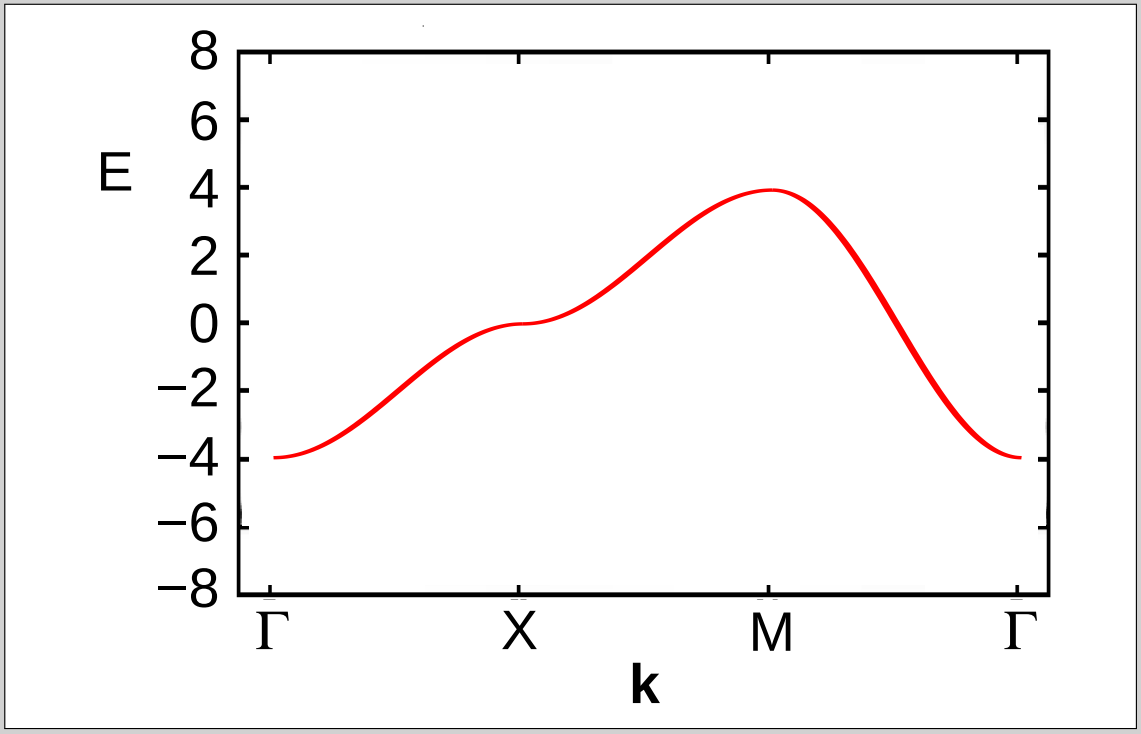
correlated band structure

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:

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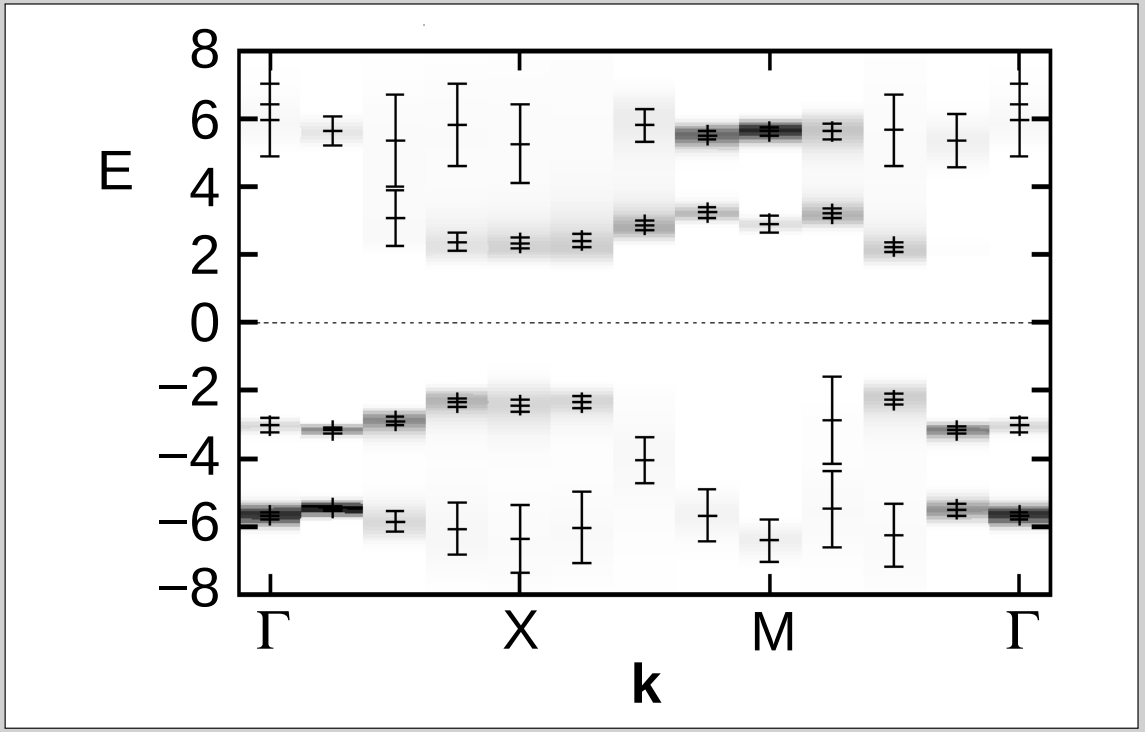
wave vector $\mathbf{k}$, band index m

with interaction:



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

Green's Function

spectral respresentation

define:

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

special cases:

retarded Green's function

$$\boxed{G^{(\mathrm{ret})}_{\alpha\beta}(\omega) = G_{\alpha\beta}(\omega + i0^+)} \qquad (\omega \text{ real})$$

advanced Green's function

$$\boxed{G^{(\mathrm{av})}_{\alpha\beta}(\omega) = G_{\alpha\beta}(\omega - i0^+)} \qquad (\omega \text{ real})$$

thermal Green's function, Matsubara function

$$\boxed{G^{(\mathrm{M})}_{\alpha\beta}(\omega_n) = G_{\alpha\beta}(i\omega_n)}$$

with

$$\boxed{\omega_n = (2n+1)\pi T \qquad n \in \mathbb{Z}} \qquad \text{(fermions)}$$

(for bosons: $\omega_n = 2n)\pi T \qquad n \in \mathbb{Z}$)

properties of the Green's function

inserting the Lehmann representation for the spectral density:

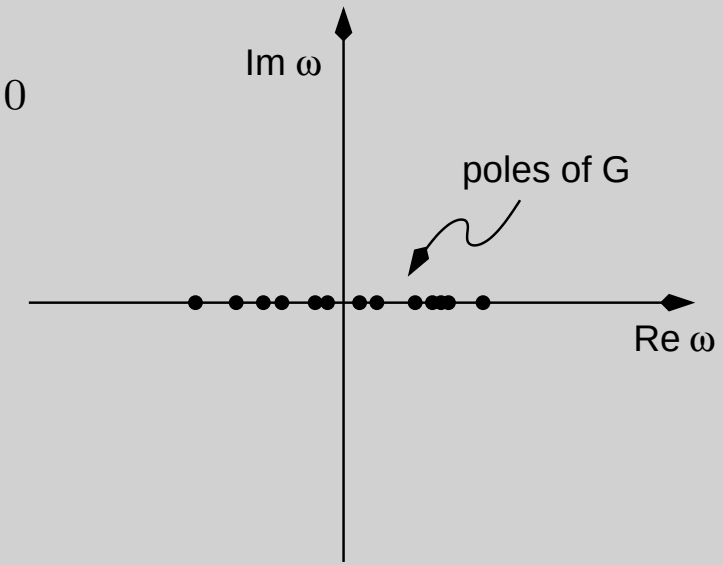
$$A_{\alpha\beta}(\omega) = \frac{1}{Z}\sum_{mn}(e^{-\beta E_m} + e^{-\beta E_n})\langle m|c_\alpha|n\rangle\langle n|c_\beta^\dagger|m\rangle\delta(\omega - (E_n - E_m))$$

we find:

$$\boxed{G_{\alpha\beta}(\omega) = \frac{1}{Z}\sum_{mn}(e^{-\beta E_m} + e^{-\beta E_n})\langle m|c_\alpha|n\rangle\langle n|c_\beta^\dagger|m\rangle\frac{1}{\omega - (E_n - E_m)}}$$

- $G_{\alpha\beta}(\omega)$ is analytical in $\mathbb{C} \setminus \mathbb{R}$
- $G_{\alpha\beta}(\omega)$ has first-order poles at the excitation energies $\omega = E_n - E_m \in \mathbb{R}$
- residues (for $\alpha = \beta$):

  $$a_{nm} = \frac{1}{Z}(e^{-\beta E_m} + e^{-\beta E_n})|\langle m|c_\alpha|n\rangle|^2 \geq 0$$



➜ complex analysis

retarded Green's function

with Dirac's identity

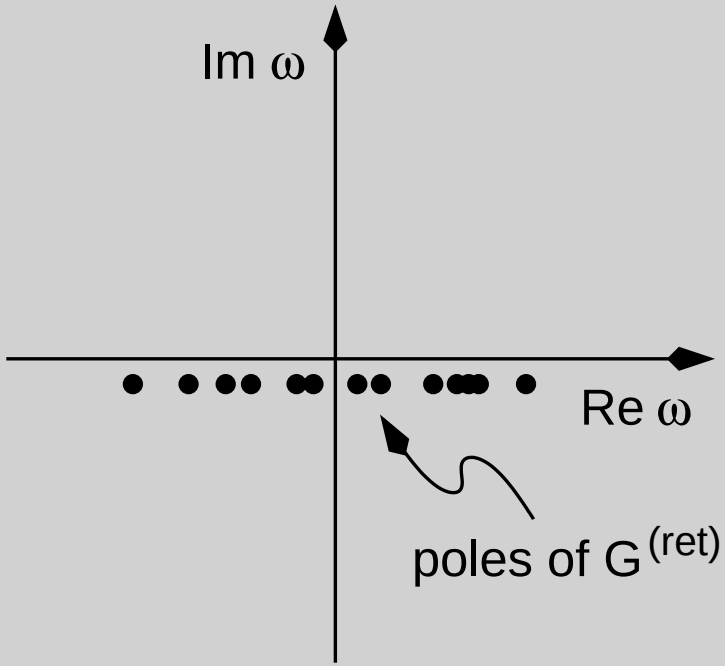
$$\boxed{\frac{1}{x+i0^+} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)}$$

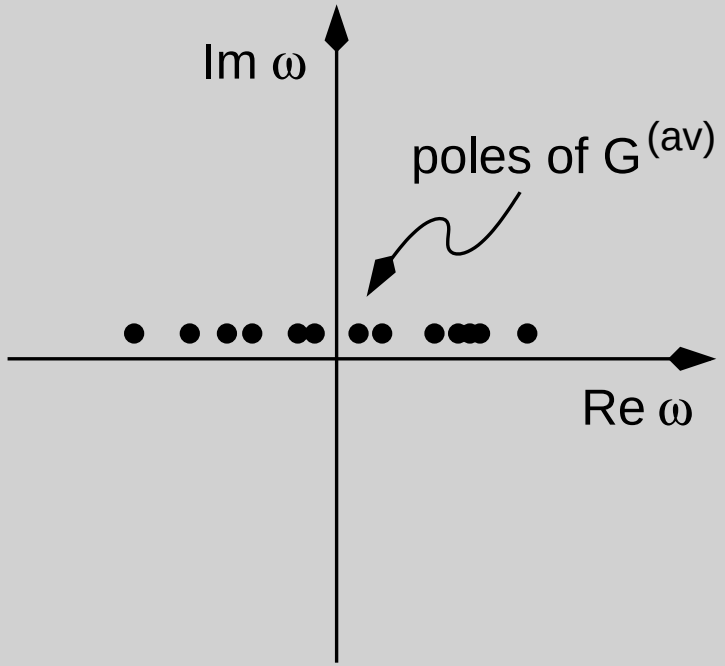
we have:

$$-\frac{1}{\pi}\mathrm{Im}\, G_{\alpha\beta}(\omega+i0^+) = -\frac{1}{\pi}\mathrm{Im}\int dz \frac{A_{\alpha\beta}(z)}{\omega+i0^+-z}$$

hence:

$$\boxed{-\frac{1}{\pi}\mathrm{Im}\, G_{\alpha\beta}(\omega+i0^+) = A_{\alpha\beta}(\omega)}$$





Kramers-Kronig relations

$G^{(\mathrm{ret})}_{\alpha\beta}(\omega)$ analytical for $\mathrm{Im}\,\omega \geq 0$ ➜ $0 = \oint_{\mathcal{C}} d\omega \, \dfrac{G^{(\mathrm{ret})}_{\alpha\beta}(\omega)}{\omega' - \omega - i0^+}$ (ω' real)

(poles of $G^{(\mathrm{ret})}_{\alpha\beta}(\omega)$ below real axis, another pole at $\omega = \omega' - i0^+$)

with $G^{(\mathrm{ret})}_{\alpha\beta}(\omega) \to \dfrac{1}{\omega}$ for $\omega \to \infty$:

$$0 = \int_{-\infty}^{\infty} d\omega \, \frac{G^{(\mathrm{ret})}_{\alpha\beta}(\omega)}{\omega' - \omega - i0^+}$$

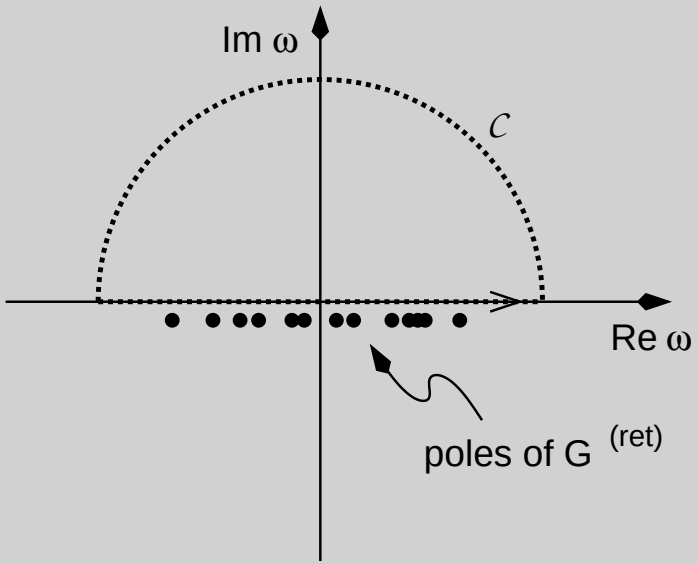
with Dirac identity:

$$0 = \mathcal{P}\int d\omega \, \frac{G^{(\mathrm{ret})}_{\alpha\beta}(\omega)}{\omega' - \omega} + i\pi G^{(\mathrm{ret})}_{\alpha\beta}(\omega')$$

hence:

$$G^{(\mathrm{ret})}_{\alpha\beta}(\omega) = \frac{i}{\pi}\mathcal{P}\int d\omega' \, \frac{G^{(\mathrm{ret})}_{\alpha\beta}(\omega')}{\omega - \omega'} \quad (\omega \text{ reell})$$

and:



$$\mathrm{Re}\,G^{(\mathrm{ret})}_{\alpha\beta}(\omega) = -\frac{1}{\pi}\mathcal{P}\int d\omega' \, \frac{\mathrm{Im}\,G^{(\mathrm{ret})}_{\alpha\beta}(\omega')}{\omega - \omega'} \qquad \mathrm{Im}\,G^{(\mathrm{ret})}_{\alpha\beta}(\omega) = \frac{1}{\pi}\mathcal{P}\int d\omega' \, \frac{\mathrm{Re}\,G^{(\mathrm{ret})}_{\alpha\beta}(\omega')}{\omega - \omega'}$$

time-dependent retarded Green's function

Fourier transformation:

$$G(\omega) = \int dt\, e^{i\omega t} G(t) \qquad G(t) = \frac{1}{2\pi} \int d\omega\, e^{-i\omega t} G(\omega)$$

ω is real ! ➜ Fourier transformation for $G^{(\mathrm{ret/av})}_{\alpha\beta}(\omega)$ only

using the identiy:

$$\boxed{\frac{1}{2\pi} \int d\omega\, e^{-i\omega t} \frac{1}{\omega - \omega' + i0^+} = -i\Theta(t) e^{-i\omega' t}}$$

we find:

$$\begin{aligned} G^{(\mathrm{ret})}_{\alpha\beta}(t) &= \frac{1}{2\pi} \int d\omega\, e^{-i\omega t} G^{(\mathrm{ret})}_{\alpha\beta}(\omega) \\ &= \frac{1}{2\pi} \int d\omega\, e^{-i\omega t} \int d\omega' \frac{A_{\alpha\beta}(\omega')}{\omega + i0^+ - \omega'} \\ &= \int d\omega' A_{\alpha\beta}(\omega')(-i)\Theta(t) e^{-i\omega' t} \\ &= (-i)\Theta(t) 2\pi\, A_{\alpha\beta}(t) = -i\Theta(t) \langle [c_\alpha(t), c^\dagger_\beta(0)]_+ \rangle \end{aligned}$$

the time dependence is homogeneous:

$$\boxed{G^{(\mathrm{ret})}_{\alpha\beta}(t - t') = -i\Theta(t - t') \langle [c_\alpha(t), c^\dagger_\beta(t')]_+ \rangle}$$

analogously:

$$\boxed{G^{(\mathrm{av})}_{\alpha\beta}(t - t') = i\Theta(t' - t) \langle [c_\alpha(t), c^\dagger_\beta(t')]_+ \rangle}$$

free Green's function

example: **non-interacting system**

$$\mathcal{H} = \sum_{\alpha} (\varepsilon_\alpha - \mu) c^\dagger_\alpha c_\alpha$$

free spectral density: $A^{(0)}_{\alpha\beta}(\omega) = \delta_{\alpha\beta}\delta(\omega - (\varepsilon_\alpha - \mu)$

using the definition of the Green's function:

$$G^{(0)}_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} dz \, \frac{A^{(0)}_{\alpha\beta}(z)}{\omega - z} = \delta_{\alpha\beta} \frac{1}{\omega - (\varepsilon_\alpha - \mu)}$$

more general:

$$\mathcal{H} = \sum_{\alpha\beta} (t_{\alpha\beta} - \mu\delta_{\alpha\beta}) c^\dagger_\alpha c_\beta$$

non-interacting Green's function

$$G^{(0)}_{\alpha\beta}(\omega) = \left(\frac{1}{(\omega + \mu)\mathbf{1} - \mathbf{t}} \right)_{\alpha\beta}$$

(matrix notation)

$$\mathbf{G}^{(0)}(\omega) = \frac{1}{\omega + \mu - \mathbf{t}}$$

remember:

- $\omega \notin \mathbb{R}$!
- $\omega = z + i0^+$ ➜ retarded Green's function (z real)
- $\omega = z - i0^+$ ➜ advanced Green's function
- $\omega = i(2n+1)\pi T$ ➜ Matsubara Green's function (n integer)

self-energy

non-interacting Green's function: $\mathbf{G}^{(0)}(\omega)$

interacting Green's function: $\mathbf{G}(\omega)$

define **self-energy:** $\boxed{\mathbf{\Sigma}(\omega) = \mathbf{G}^{(0)}(\omega)^{-1} - \mathbf{G}^{-1}(\omega)}$

again:

- $\omega \notin \mathbb{R}$!
- $\omega = z + i0^+$ ➜ retarded self-energy (z real)
- $\omega = z - i0^+$ ➜ advanced self-energy
- $\omega = i(2n+1)\pi T$ ➜ Matsubara self-energy (n integer)

we have:

$$\boxed{\mathbf{G}(\omega) = \mathbf{G}^{(0)}(\omega) + \mathbf{G}^{(0)}(\omega)\mathbf{\Sigma}(\omega)\mathbf{G}(\omega)}$$ **Dyson's equation**

and

$$\boxed{\mathbf{G}(\omega) = \mathbf{G}^{(0)}(\omega) + \mathbf{G}^{(0)}(\omega)\mathbf{\Sigma}(\omega)\mathbf{G}^{(0)}(\omega) + \mathbf{G}^{(0)}(\omega)\mathbf{\Sigma}(\omega)\mathbf{G}^{(0)}(\omega)\mathbf{\Sigma}(\omega)\mathbf{G}^{(0)}(\omega) + \cdots}$$

and

$$\boxed{\mathbf{G}(\omega) = \frac{1}{\mathbf{G}^{(0)}(\omega)^{-1} - \mathbf{\Sigma}(\omega)}}$$ and $$\boxed{\mathbf{G}(\omega) = \frac{1}{\omega + \mu - \mathbf{t} - \mathbf{\Sigma}(\omega)}}$$

Matsubara Green's function

plan

Green's functions

↓

Matsubara functions

↓

perturbation theory

↓

formal summation, functionals

↓

dynamical variational principle

homogeneity

assume Hamiltonian to be **time independent**, $H \neq H(t)$ (Schrödinger picture)

thermodynamical **expectation value** of an observable A:

$$\boxed{\langle A \rangle = \frac{1}{Z} \mathrm{tr}(e^{-\beta \mathcal{H}} A)} \qquad (\mathcal{H} \equiv H - \mu N)$$

time evolution of A in (grandcanonical) Heisenberg picture:

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

time-dependent correlation function:

$$\begin{aligned} \langle A(t)B(t') \rangle &= \frac{1}{Z} \mathrm{tr}(e^{-\beta \mathcal{H}} e^{i\mathcal{H}t} A e^{-i\mathcal{H}t} e^{i\mathcal{H}t'} B e^{-i\mathcal{H}t'}) \\ &= \frac{1}{Z} \mathrm{tr}(e^{-\beta \mathcal{H}} e^{i\mathcal{H}(t-t')} A e^{-i\mathcal{H}(t-t')} B) \end{aligned}$$

correlation functions are homogeneous in time:

$$\boxed{\langle A(t)B(t') \rangle = \langle A(t-t')B(0) \rangle}$$

Wick rotation

consider **imaginary time** $t = -i\tau$ with $\tau \in \mathbb{R}$

unified description of **time evolution** and **thermal averages**

$$e^{-i\mathcal{H}t} = e^{-\beta\mathcal{H}} \quad \text{for} \quad t = i\tau \quad \text{and} \quad \tau = \beta$$

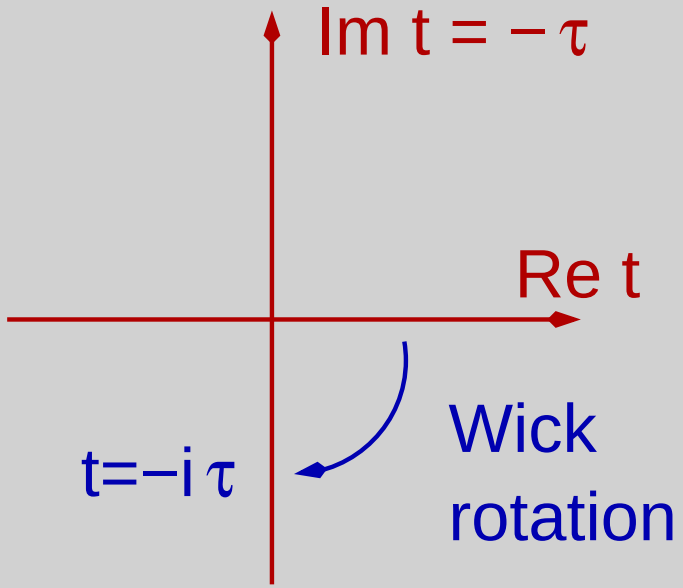
(time evolution operator $=$ statistical operator)

imaginary time evolution:

$$A(t) = e^{i\mathcal{H}t} A e^{-i\mathcal{H}t} = e^{\mathcal{H}\tau} A e^{-\mathcal{H}\tau}$$

modified Heisenberg picture

define: $A(\tau) = e^{\mathcal{H}\tau} A e^{-\mathcal{H}\tau}$



modified Heisenberg picture

imaginary time evolution: $A(\tau) = e^{\mathcal{H}\tau} A e^{-\mathcal{H}\tau}$

annihilator: $c_\alpha(\tau) = e^{\mathcal{H}\tau} c_\alpha e^{-\mathcal{H}\tau}$

creator: $c_\alpha^\dagger(\tau) = e^{\mathcal{H}\tau} c_\alpha^\dagger e^{-\mathcal{H}\tau}$ note: $\boxed{c^\dagger(\tau) \neq c(\tau)^\dagger}$

equation of motion?

$$\frac{d}{d\tau} A(\tau) = \frac{d}{d\tau}(e^{\mathcal{H}\tau} A e^{-\mathcal{H}\tau}) = e^{\mathcal{H}\tau}(\mathcal{H}A - A\mathcal{H})e^{-\mathcal{H}\tau} = \mathcal{H}A(\tau) - A(\tau)\mathcal{H}$$

$$\rightarrow \boxed{-\frac{d}{d\tau} A(\tau) = [A(\tau), \mathcal{H}]_-} \qquad \textbf{Bloch equation}$$

---

free system: $\mathcal{H}_0 = H_0 - \mu N = \sum_k (\varepsilon(k) - \mu) c_k^\dagger c_k$:

we have: $[c_k, \mathcal{H}_0]_- = (\varepsilon(k) - \mu) c_k$ and $[c_k(\tau), \mathcal{H}_0]_- = (\varepsilon(k) - \mu) c_k(\tau)$

$$\boxed{c_k(\tau) = e^{-(\varepsilon(k)-\mu)\tau} c_k} \qquad \boxed{c_k^\dagger(\tau) = e^{(\varepsilon(k)-\mu)\tau} c_k^\dagger}$$

free imaginary time dependence

Matsubara function – motivation

motivation:

$H = H_0 + \lambda_A A + \lambda_B B \;\rightarrow\; \Omega = \Omega(\lambda_A, \lambda_B)$

then

$$\frac{\partial \Omega}{\partial \lambda_A} = \langle A \rangle \qquad \frac{\partial \Omega}{\partial \lambda_B} = \langle B \rangle$$

and:

$$\boxed{\frac{\partial^2 \Omega}{\partial \lambda_B \partial \lambda_A} = \frac{\partial \langle A \rangle}{\partial \lambda_B} = \beta \langle B \rangle \langle A \rangle - \int_0^\beta d\tau \langle B(\tau) A(0) \rangle = \frac{\partial \langle B \rangle}{\partial \lambda_A} = \frac{\partial^2 \Omega}{\partial \lambda_A \partial \lambda_B}}$$

with

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

linear response $\leftrightarrow$ imaginary time-dependent correlation functions

Matsubara function – definition

define:

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

one-particle Matsubara function

- ✧ homogeneous in time
- ✧ $\tau \in [-\beta, \beta]$
- ✧ $\mathcal{T}$: (imaginary) time-ordering operator
  (prepare for application of Wick's theorem)
- ✧ sign: convention

---

two-particle Matsubara function

$$G_{\alpha\beta\gamma\delta}(\tau) = \langle \mathcal{T} c_\alpha(\tau_\alpha) c_\beta(\tau_\beta) c^\dagger_\gamma(\tau_\gamma) c^\dagger_\delta(\tau_\delta) \rangle$$

N-particle Matsubara function

analogous

free Matsubara function

non-interacting Hamiltonian: $\boxed{\mathcal{H}_0 = \sum_k (\varepsilon(k) - \mu) c_k^\dagger c_k}$

free one-particle Matsubara function:

$$G_k^{(0)}(\tau) = -\langle \mathcal{T} c_k(\tau) c_k^\dagger(0) \rangle^{(0)}$$

$$= -\Theta(\tau) \langle c_k(\tau) c_k^\dagger(0) \rangle^{(0)} + \Theta(-\tau) \langle c_k^\dagger(0) c_k(\tau) \rangle^{(0)}$$

$$= -\Theta(\tau) e^{-(\varepsilon(k)-\mu)\tau} \langle c_k c_k^\dagger \rangle^{(0)} + \Theta(-\tau) e^{-(\varepsilon(k)-\mu)\tau} \langle c_k^\dagger c_k \rangle^{(0)}$$

$$= -e^{-(\varepsilon(k)-\mu)\tau} \left(\Theta(\tau)(1 - \langle c_k^\dagger c_k \rangle^{(0)}) - \Theta(-\tau) \langle c_k^\dagger c_k \rangle^{(0)} \right)$$

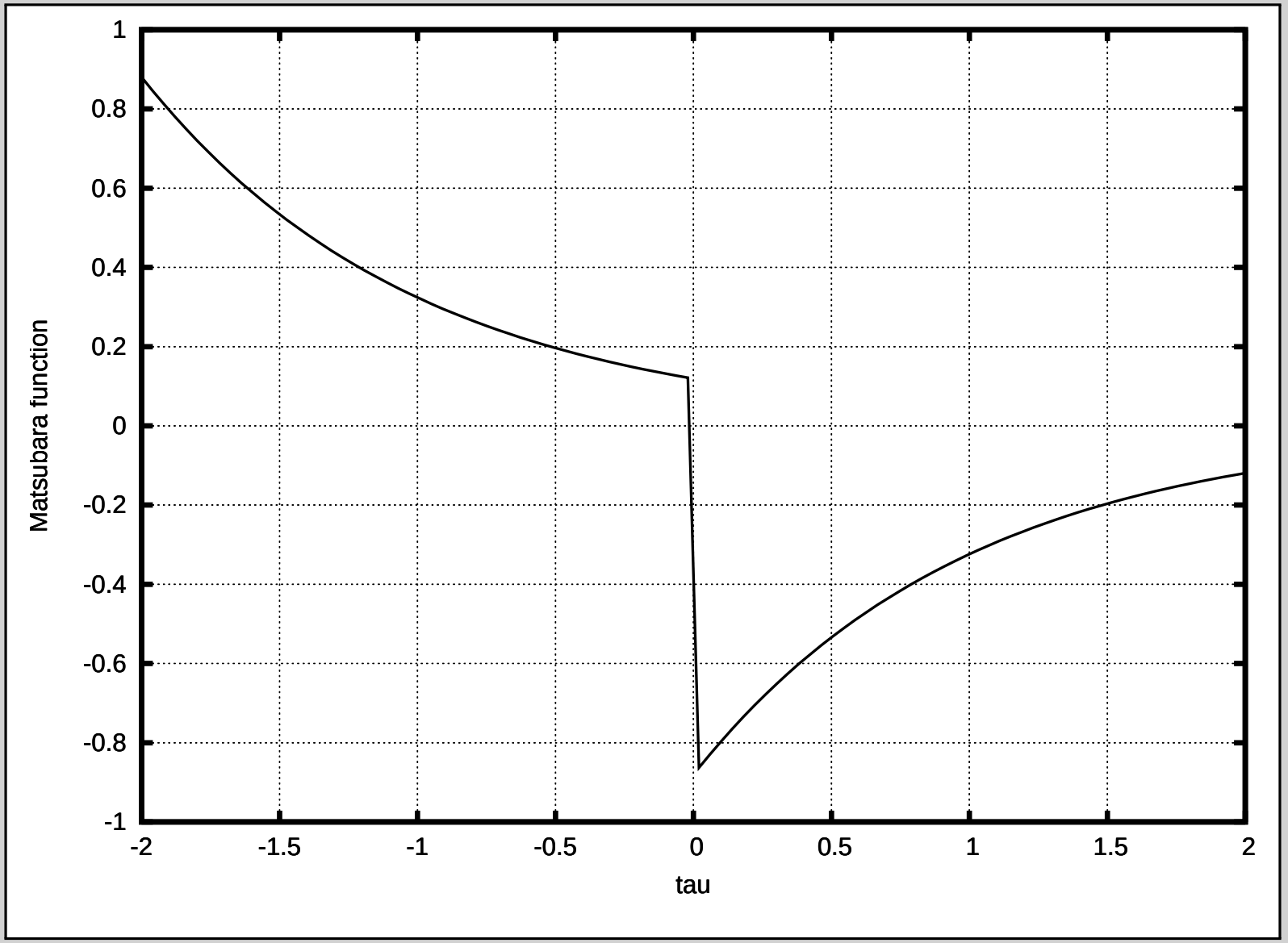
and with

$$\langle c_k^\dagger c_k \rangle^{(0)} = \frac{1}{e^{\beta(\varepsilon(k)-\mu)} + 1} \qquad \text{(Fermi function)}$$

we get:

$$\boxed{G_k^{(0)}(\tau) = -e^{-(\varepsilon(k)-\mu)\tau} \left(\Theta(\tau) \frac{1}{1 + e^{-\beta(\varepsilon(k)-\mu)}}) - \Theta(-\tau) \frac{1}{e^{\beta(\varepsilon(k)-\mu)} + 1} \right)}$$

Matsubara function – properties



$\varepsilon(k) - \mu = +1 \qquad \beta = 2$

Matsubara function – properties

$$\boxed{G_k^{(0)}(\tau) = -e^{-(\varepsilon(k)-\mu)\tau}\left(\Theta(\tau)\frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}}) - \Theta(-\tau)\frac{1}{e^{\beta(\varepsilon(k)-\mu)}+1}\right)}$$

jump of $G_k^{(0)}(\tau)$ at $\tau = 0$: $\quad G_k^{(0)}(0^+) - G_k^{(0)}(0^-) = -\langle c_k c_k^\dagger\rangle^{(0)} - \langle c_k^\dagger c_k\rangle^{(0)} = -1$

general:

$$\boxed{G_{\alpha\beta}(0^+) - G_{\alpha\beta}(0^-) = -\delta_{\alpha\beta}}$$ **jump at $\tau = 0$**

Matsubara function at $\tau < 0$:

$$G_k^{(0)}(\tau) = \frac{e^{-(\varepsilon(k)-\mu)\tau}}{e^{\beta(\varepsilon(k)-\mu)}+1} = \frac{e^{-(\varepsilon(k)-\mu)(\tau+\beta)}}{1+e^{-\beta(\varepsilon(k)-\mu)}} = -G_k^{(0)}(\tau+\beta)$$

general:

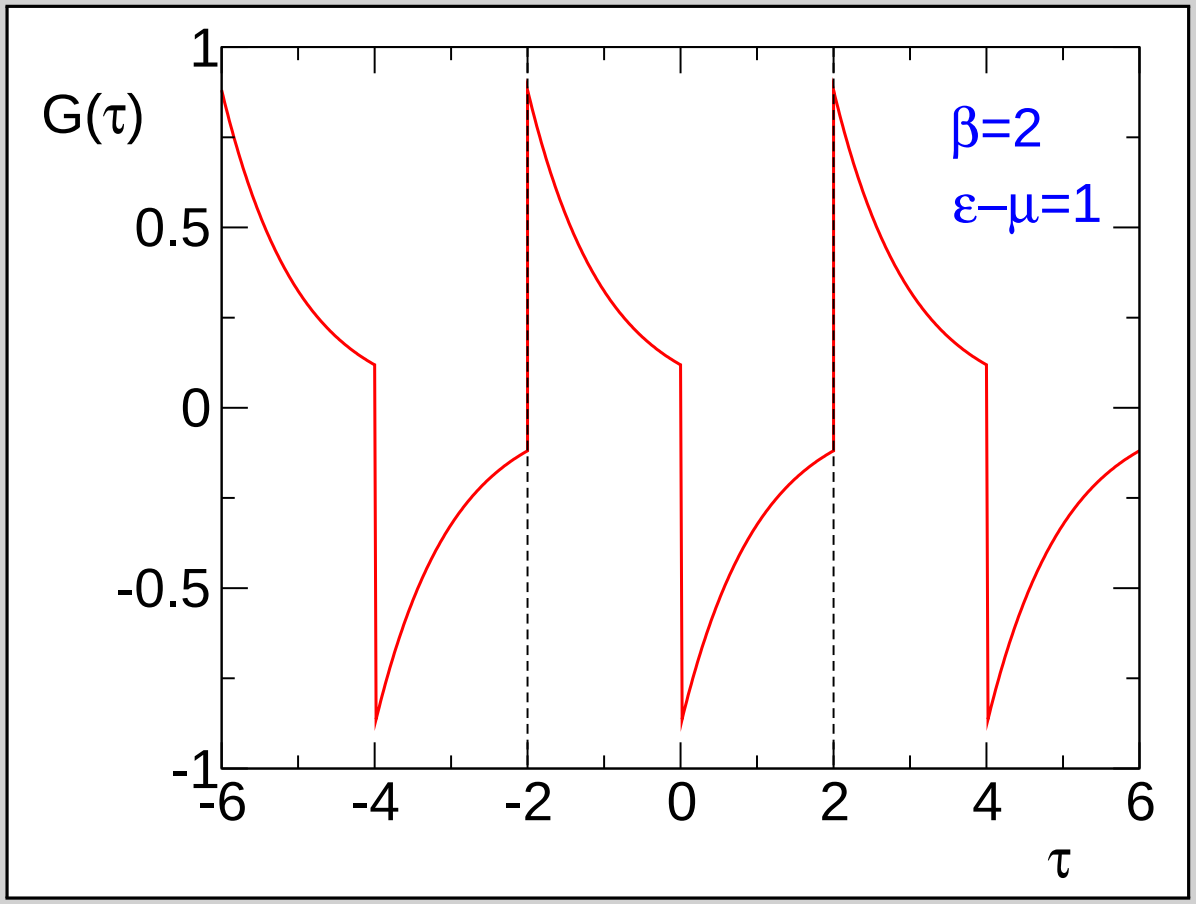
$$\boxed{G_{\alpha\beta}(\tau) = -G_{\alpha\beta}(\tau+\beta)}$$ for $\tau < 0$ **negative imaginary time**

$G_k^{(0)}(\tau)$ diverges for $\tau \to +\infty$ if $\varepsilon(k) - \mu < 0$ and diverges for $\tau \to -\infty$ if $\varepsilon(k) - \mu > 0$!

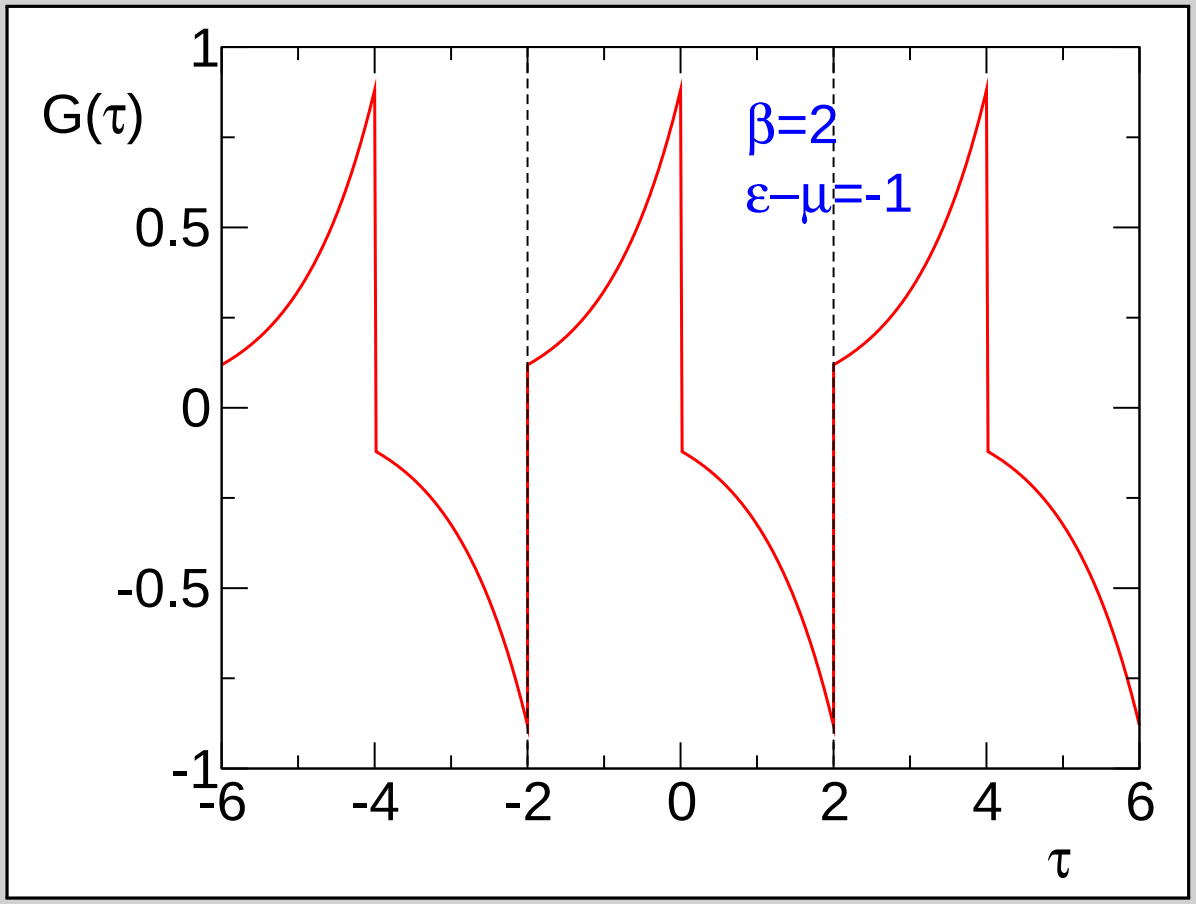
$$\boxed{\tau \in [-\beta, \beta]}$$ **(original) domain**

$$\boxed{G_{\alpha\beta}(\tau \pm 2\beta) \stackrel{!}{=} G_{\alpha\beta}(\tau)}$$ **periodic continuation to $\tau \in \mathbb{R}$**

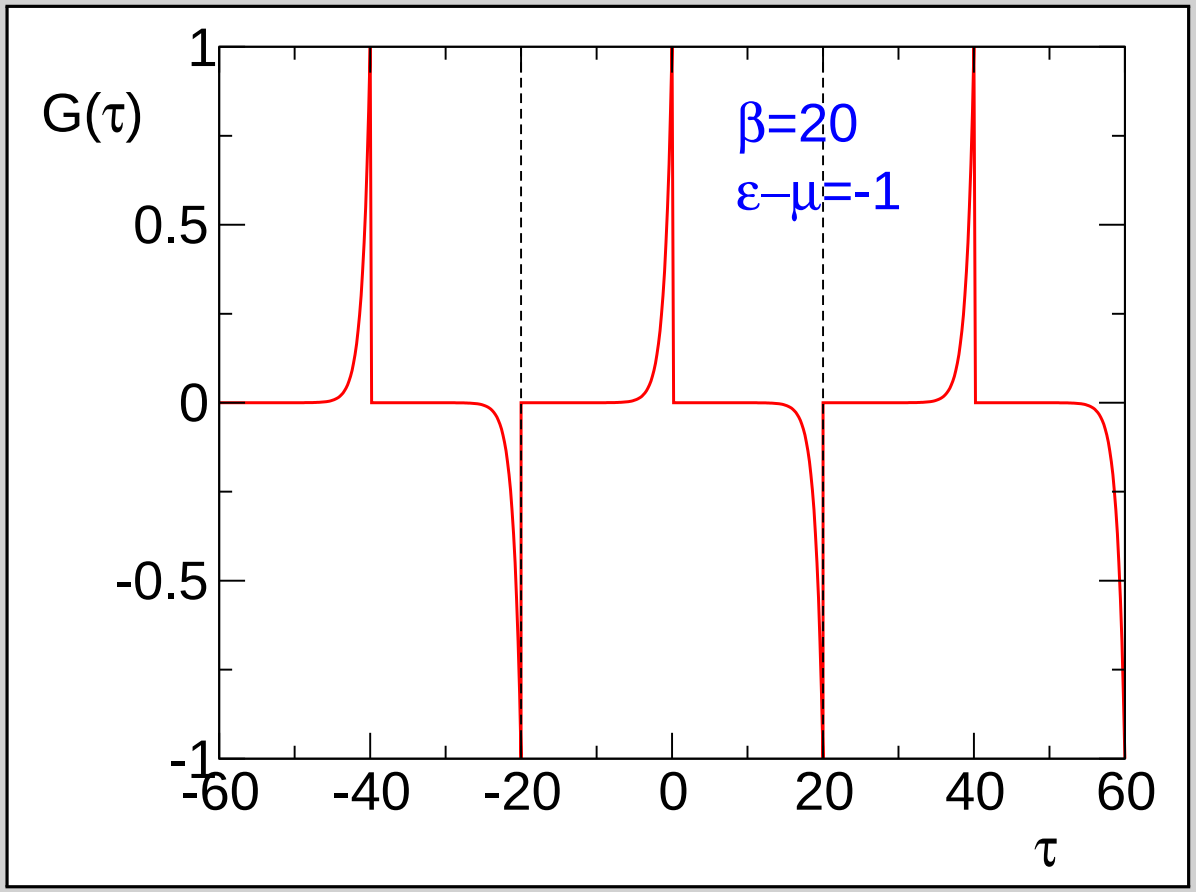
Matsubara function – periodicity



Matsubara function – periodicity



Matsubara function – periodicity



Matsubara function – discrete Fourier transform

orthonormal basis of periodic functions with period $T = 2\beta$:

$$\boxed{\frac{1}{\sqrt{2\beta}}\, e^{-im\pi\,\tau/\beta}} \qquad m = ..., -1, 0, 1, ...$$

we have:

$$\boxed{G_{\alpha\beta}(\tau) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} a_{\alpha\beta}^{(m)}\, e^{-im\pi\,\tau/\beta}}$$

where $a_{\alpha\beta}^{(m)} = \frac{1}{2}\int_{-\beta}^{\beta} d\tau\, G_{\alpha\beta}(\tau)\, e^{im\pi\,\tau/\beta} = \frac{1}{2}\int_{0}^{\beta} d\tau\,(\cdots) + \frac{1}{2}\int_{-\beta}^{0} d\tau\,(\cdots)$

using $G_{\alpha\beta}(\tau) = -G_{\alpha\beta}(\tau+\beta)$ for $\tau < 0$ and $e^{im\pi\,\tau/\beta} = e^{im\pi\,(\tau+\beta)/\beta} e^{-im\pi}$, we find:

$$\boxed{a_{\alpha\beta}^{(m)} = \frac{1}{2}\int_{0}^{\beta} d\tau\,(\cdots) - e^{-im\pi}\frac{1}{2}\int_{-\beta}^{0} d\tau\,(\cdots) = \frac{1}{2}(1 - e^{-im\pi})\int_{0}^{\beta} d\tau\, G_{\alpha\beta}(\tau)\, e^{im\pi\,\tau/\beta}}$$

non-zero Fourier coefficients $G_{\alpha\beta}(i\omega_n) \equiv a_{\alpha\beta}^{(m)}$ for **odd** $m = 2n+1$ with $n \in \mathbb{Z}$ only

➜ $\boxed{G_{\alpha\beta}(i\omega_n)}$ **frequency-dependent Matsubara function**

Matsubara function – Matsubara frequencies

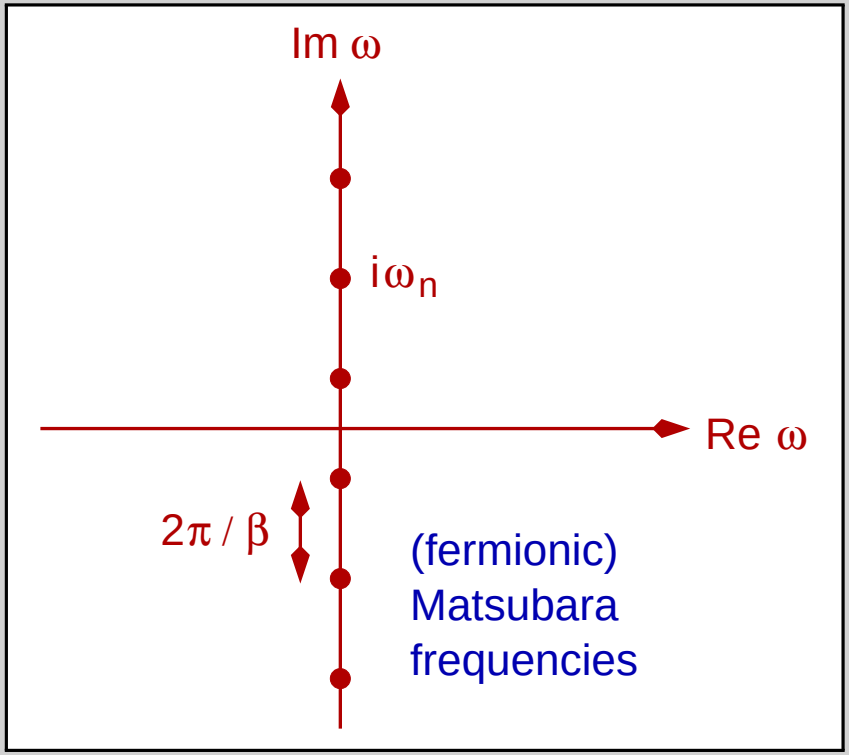
hence:

$$G_{\alpha\beta}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} G_{\alpha\beta}(i\omega_n)\, e^{-i\omega_n \tau}$$

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

and

$$G_{\alpha\beta}(i\omega_n) = \int_0^\beta d\tau\, G_{\alpha\beta}(\tau)\, e^{i\omega_n \tau}$$



free Matsubara function

with $$G_k^{(0)}(\tau) = -e^{-(\varepsilon(k)-\mu)\tau}\left(\Theta(\tau)\frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}}) - \Theta(-\tau)\frac{1}{e^{\beta(\varepsilon(k)-\mu)}+1}\right)$$

we find:

$$G_k^{(0)}(i\omega_n) = \int_0^\beta d\tau\, G_k(\tau)\, e^{i\omega_n\tau} = -\int_0^\beta d\tau\, e^{-(\varepsilon(k)-\mu)\tau}\frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}}\, e^{i\omega_n\tau}$$

$$= -\frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}}\int_0^\beta d\tau\, e^{[i\omega_n-(\varepsilon(k)-\mu)]\tau}$$

$$= -\frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}}\frac{1}{i\omega_n-(\varepsilon(k)-\mu)}e^{[i\omega_n-(\varepsilon(k)-\mu)]\tau}\Big|_0^\beta$$

$$= -\frac{1}{1+e^{-\beta(\varepsilon(k)-\mu)}}\frac{1}{i\omega_n-(\varepsilon(k)-\mu)}\left(e^{i\beta\omega_n}e^{-\beta(\varepsilon(k)-\mu)}-1\right) \qquad e^{i\beta\omega_n} = -1$$

$$G_k^{(0)}(i\omega_n) = \frac{1}{i\omega_n-(\varepsilon(k)-\mu)} = \frac{1}{\omega-(\varepsilon(k)-\mu)}\Big|_{\omega=i\omega_n} = G_k^{(0)}(\omega)\Big|_{\omega=i\omega_n}$$

Matsubara function = Green function evaluated at the Matsubara frequencies

summary

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

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

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

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

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:

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

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

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:

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

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

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**

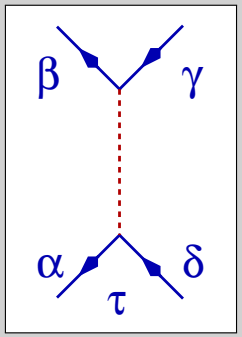
$$\boxed{\underline{c_{\alpha_i}(\tau_i) c_{\alpha_j}^\dagger(\tau_j)} = \langle \mathcal{T}(c_{\alpha_i}(\tau_i) c_{\alpha_j}^\dagger(\tau_j))\rangle^{(0)} = -G^{(0)}_{\alpha_i\alpha_j}(\tau_i - \tau_j)}$$

diagram elements

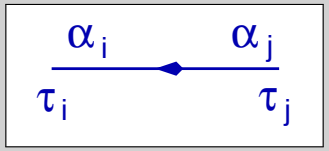
to compute the denominator, i.e. Z/Z_0

- 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 

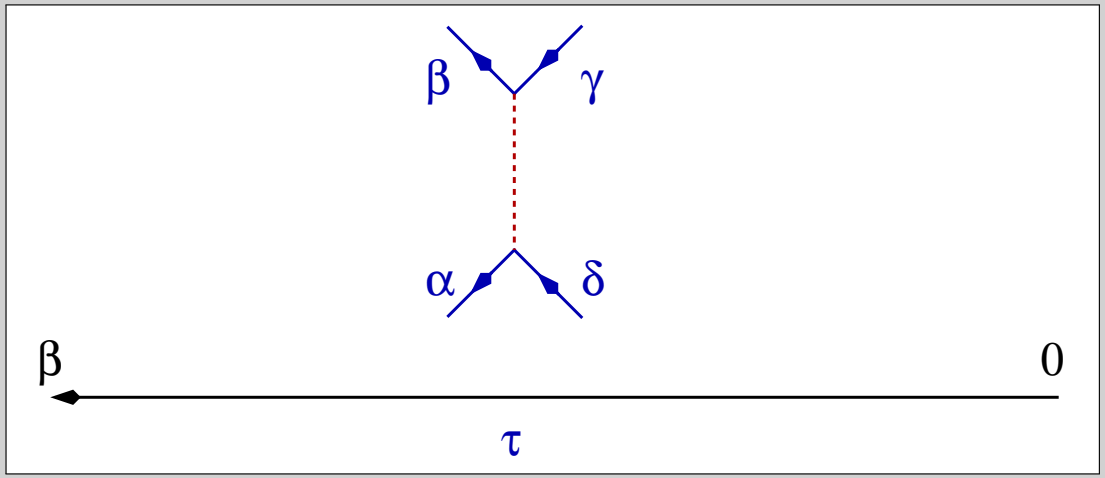
stands for $U_{\alpha_i \beta_i \delta_i \gamma_i}$

propagator 

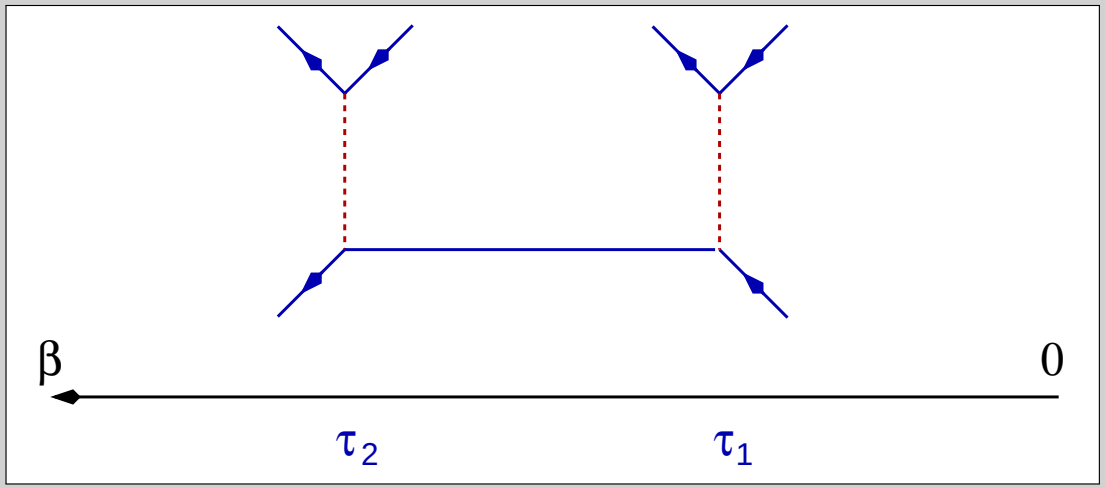
stands for a contraction, i.e. $-G^{(0)}_{\alpha_i \alpha_j}(\tau_i - \tau_j)$

building diagrams

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



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



full contractions

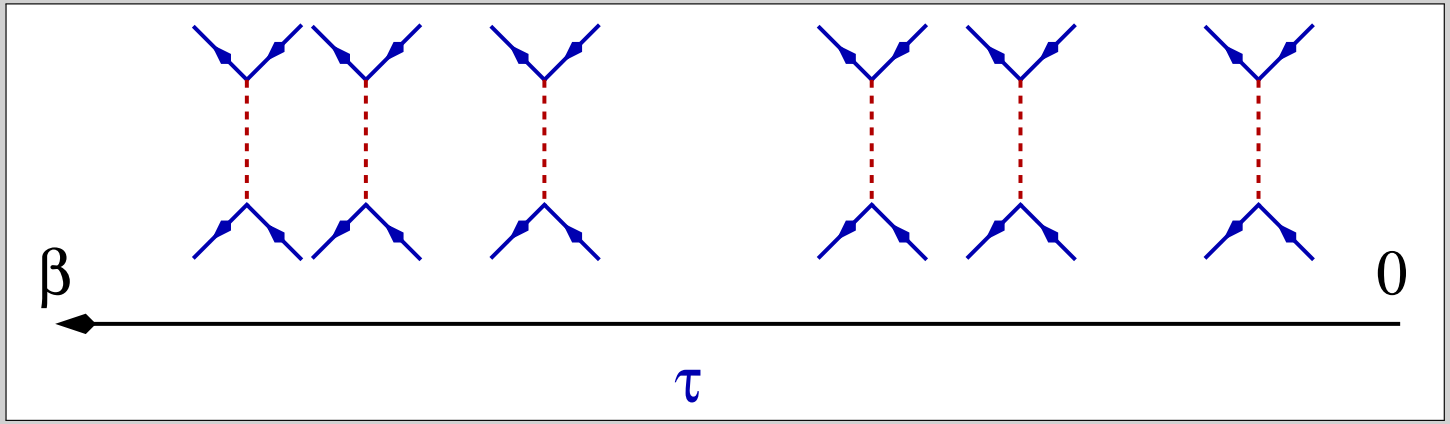
free expectation value (at k-th order):

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

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

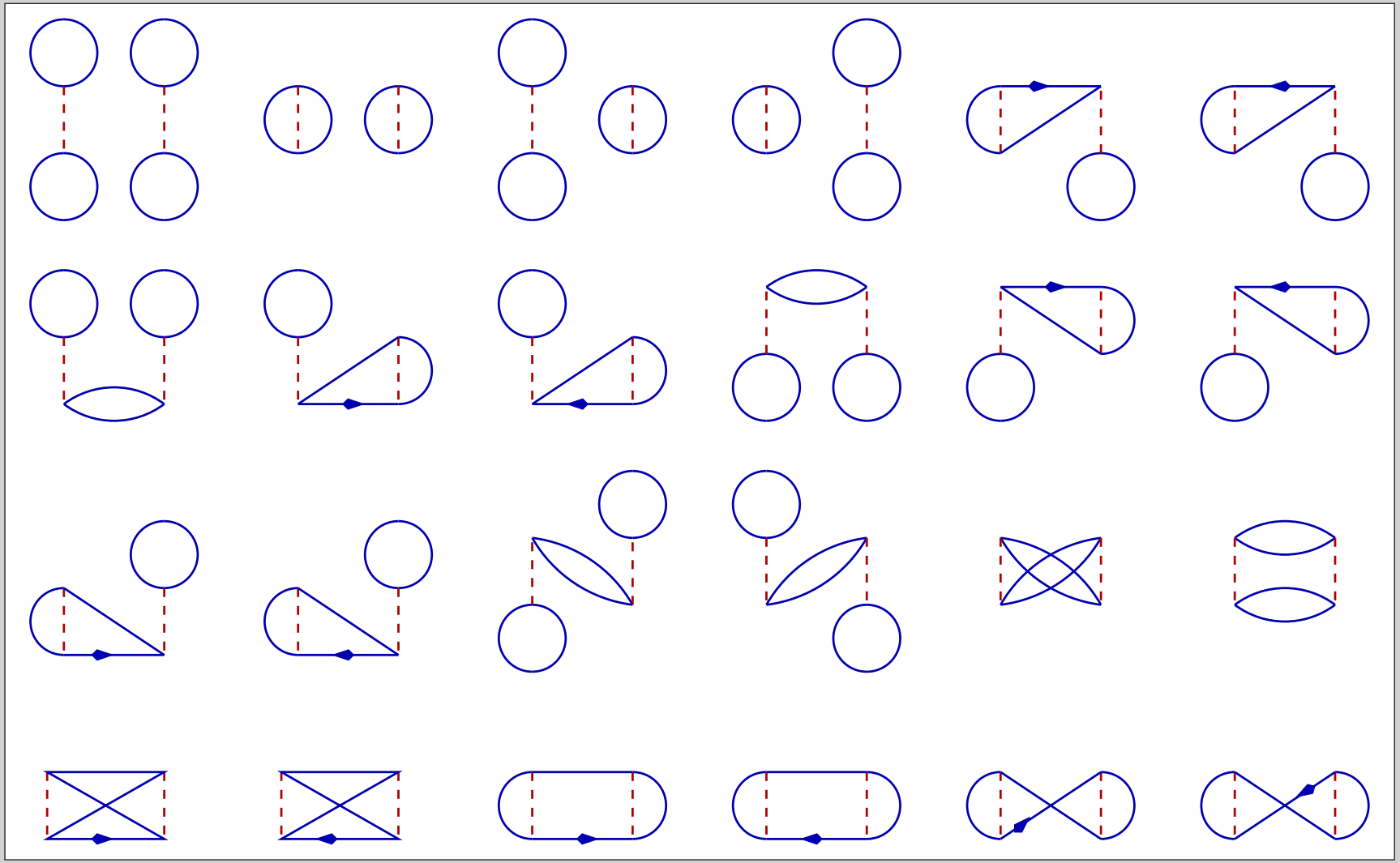
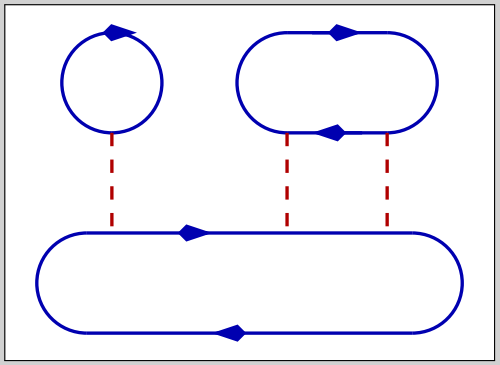


diagram rules

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**



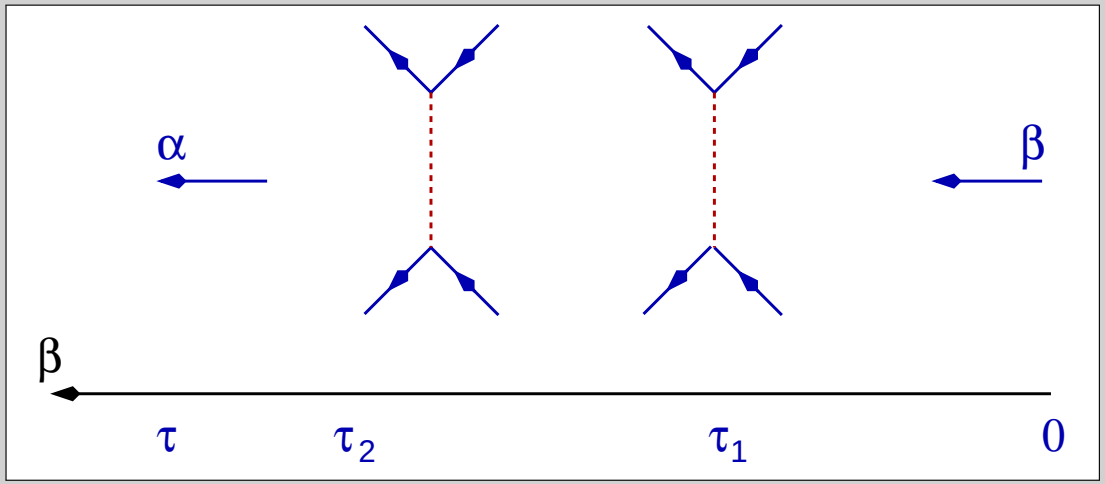
$L = 3$

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 $c_\beta^\dagger(0)$

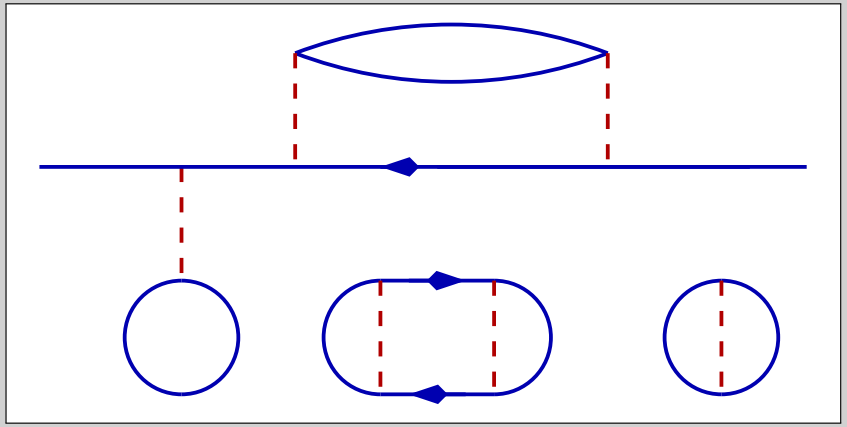
we have $2k+1$ propagators and thus

$(2k+1)!$ 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

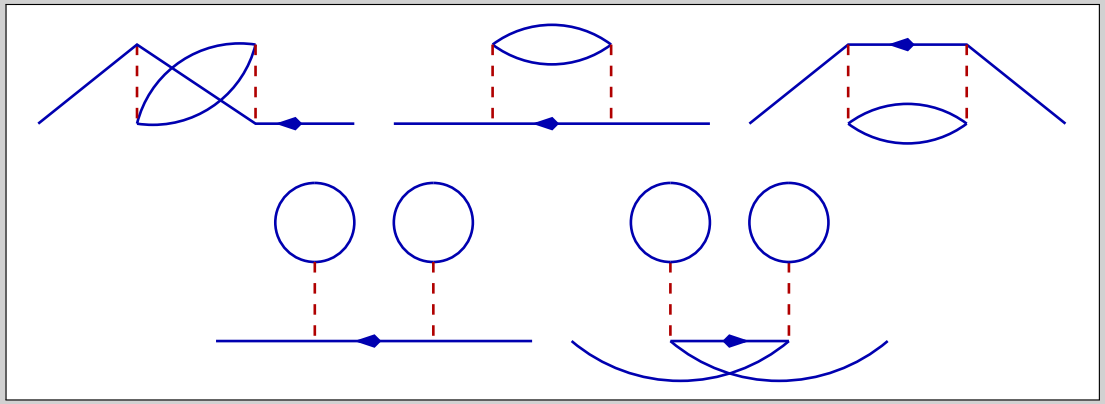
theorem:

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 $\dfrac{1}{2^k k!}$

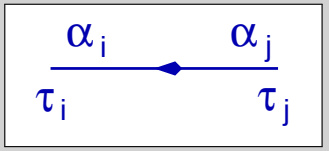
all topologically different and connected diagrams at order $k = 0, 1, 2$:

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** :
  $\tau_{\rm creator} = \tau_{\rm annihilator} + 0^+$
- ✧ **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

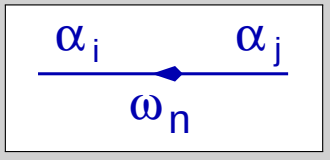
attach $\frac{1}{\sqrt{\beta}}e^{i\omega_n\tau_j}$ to vertex at which propagator starts

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 $-G_{\alpha\beta}(i\omega_n)$,

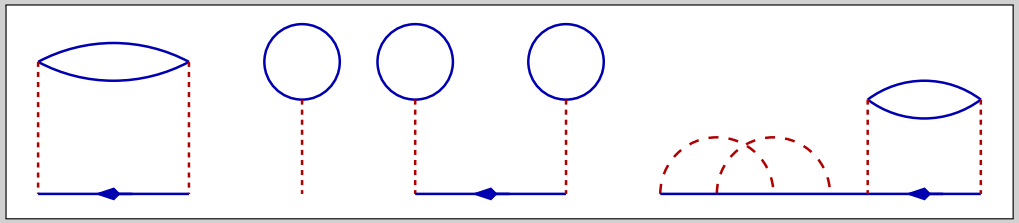
- ✧ draw all topologically different **diagrams**
  label them with orbitals α_i and frequencies ω_m
- ✧ diagrams must be connected to **external links**
  vertices and propagators can be deformed
- ✧ for each **vertex** , write $-\frac{1}{\beta}\delta_{\omega_\alpha+\omega_\beta,\omega_\gamma+\omega_\delta}U_{\alpha\beta\delta\gamma}$
- ✧ 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

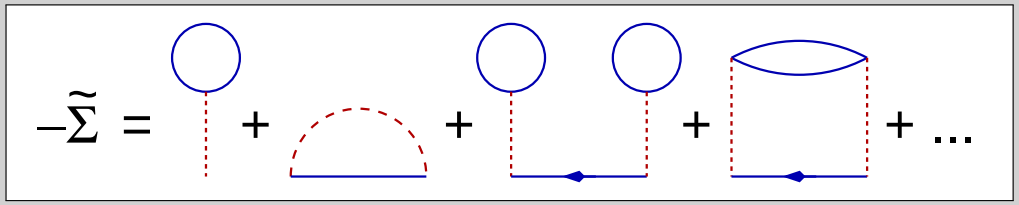
define **self-energy insertion** :

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



define **improper self-energy** :

sum of all self-energy insertions:



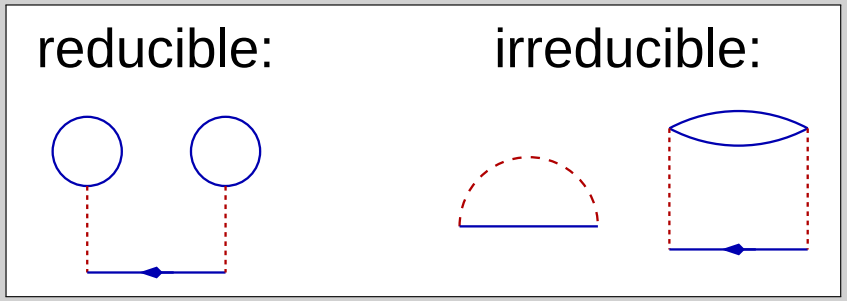
note: $-\widetilde{\Sigma}$ depends on external orbital indices and the external frequency:

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

self-energy: definition

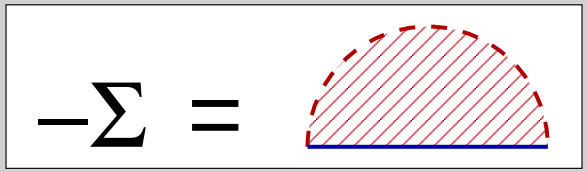
define **irreducible self-energy insertion:**

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

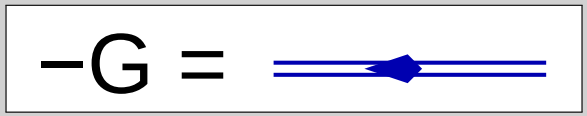


define **irreducible self-energy / proper self-energy / self-energy:**

sum of all irreducible self-energy insertions:

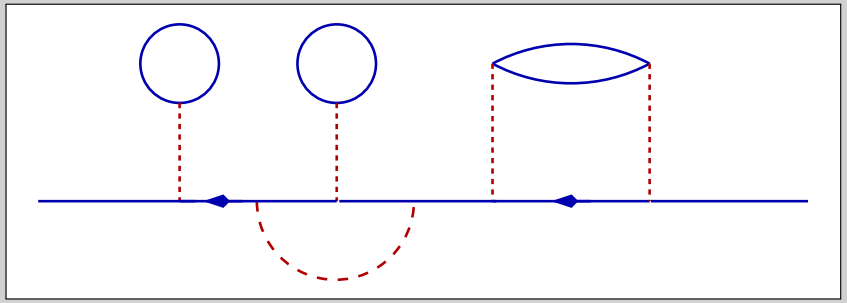


we also define the **full propagator / interacting propagator / Green's function:**



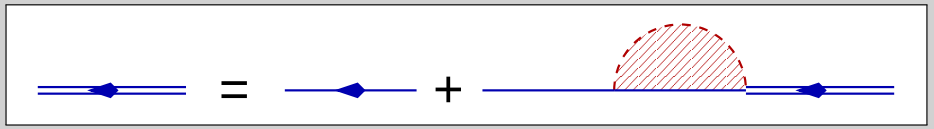
Dyson's equation, diagrammatic

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.:

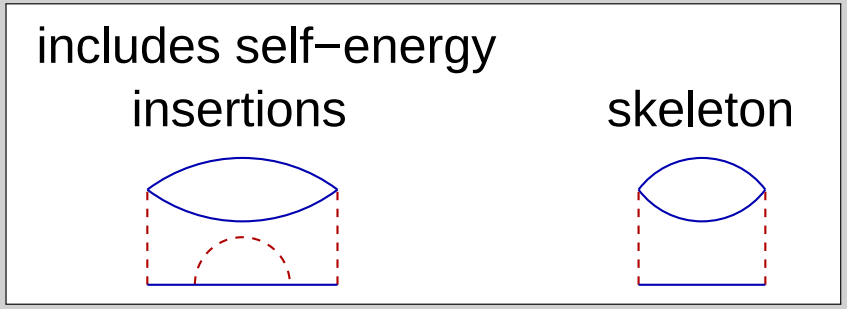
$$G_{\alpha\beta}(i\omega_n) = G^{(0)}_{\alpha\beta}(i\omega_n) + \sum_{\gamma\delta} G^{(0)}_{\alpha\gamma}(i\omega_n)\Sigma_{\gamma\delta}(i\omega_n)G_{\delta\beta}(i\omega_n)$$

Dyson's equation

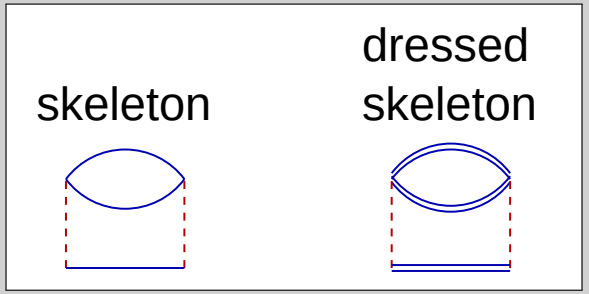
$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0\mathbf{\Sigma}\mathbf{G}$ (in matrix notation)

skeleton diagrams

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



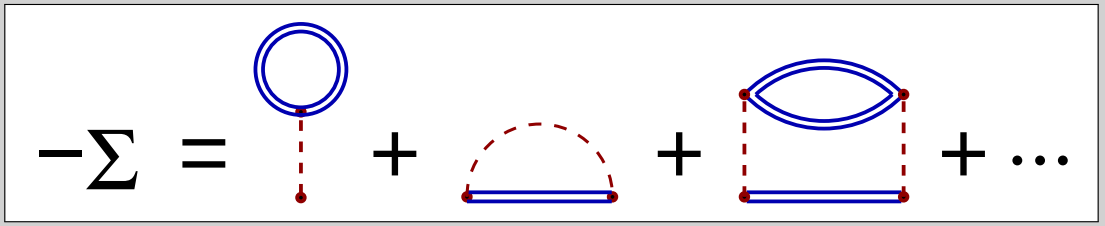
defined a **dressed skeleton** as a skeleton with free propagators replaced by full ones:



renormalization of diagrams

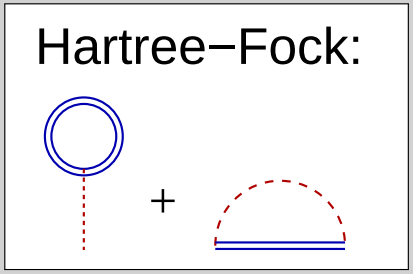
we have: self-energy = sum over all dressed skeleton self-energy diagrams

skeleton-diagram expansion



skeleton-diagrams: first effective order

summing only the first-order diagrams:



yields the Hartree-Fock self-energy:

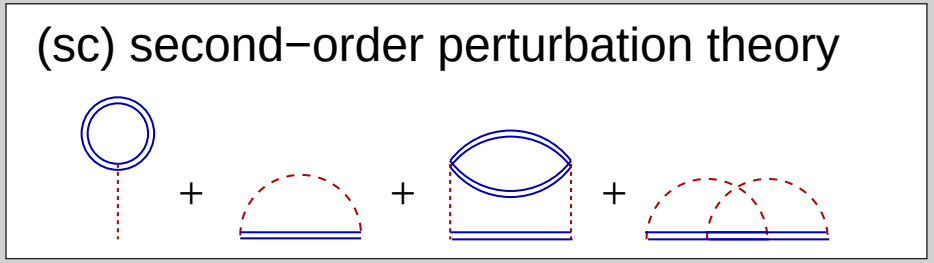
$$\Sigma^{(\mathrm{MF})}_{\alpha\beta} = \sum_{\gamma\delta} \left(U_{\alpha\gamma\beta\delta} - U_{\gamma\alpha\beta\delta} \right) \langle c^\dagger_\gamma c_\delta \rangle'$$

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

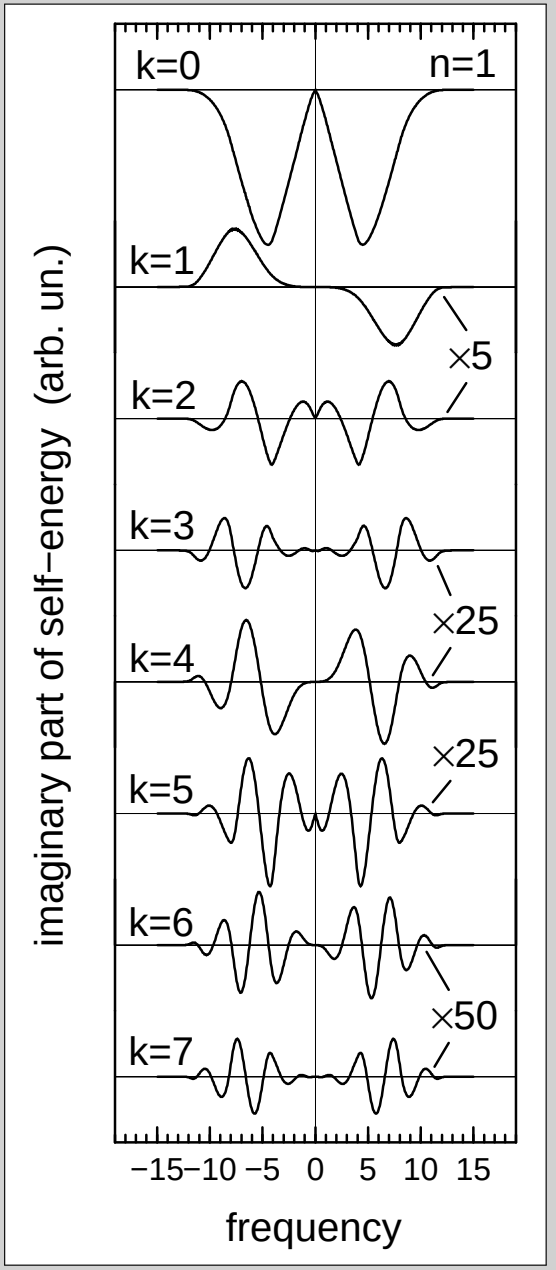
skeleton-diagrams: second effective order

summing the diagrams up to second (explicit) order:



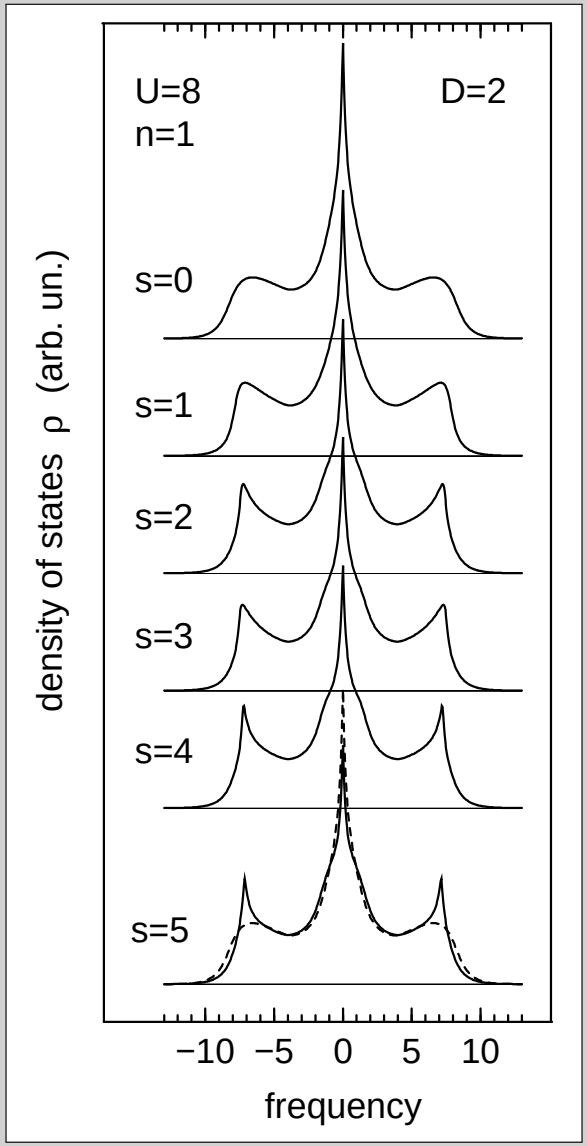
infinitesimal retarded self-energy $\Sigma_{ij\sigma}(\omega + i0^+)$
for the Hubbard model at half-filling and $T = 0$
k labels the different shells, $\Sigma_{ij\sigma} = \Sigma_{i-j\sigma}$
$D = 2$ square lattice

discussion



skeleton-diagrams: second effective order

density of states at $U = 8t$:



summary and a question

systematic perturbation theory

applicable to weak-coupling regime only

can we sum ALL diagrams ?

V Dynamical Variational Principle

Luttinger-Ward Functional

expansion of the partition function

grand potential:

$$\boxed{\Omega = -T \ln Z}$$

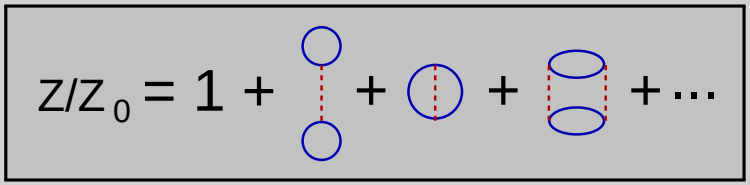
partition function:

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

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

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

with Wick's theorem, representation via diagrams:



n-th order: closed diagrams with n vertices and $2n$ propagators

– vertex ➜ $T\delta_{\text{energy conservation}} U_{\alpha\beta\gamma\delta}$

– propagator ➜ $-G_{\alpha\beta}(i\omega_n)$ (start and end at same vertex: $e^{i\omega_n 0^+}$ additionally)

– sums / integrals over $\alpha, \beta, \ldots$ and $\omega_n, \ldots$

– factor $\dfrac{(-1)^n}{2^n n!}(-1)^S$, for S fermion loops

linked-cluster theorem

it is sufficient to consider connected diagrams only:

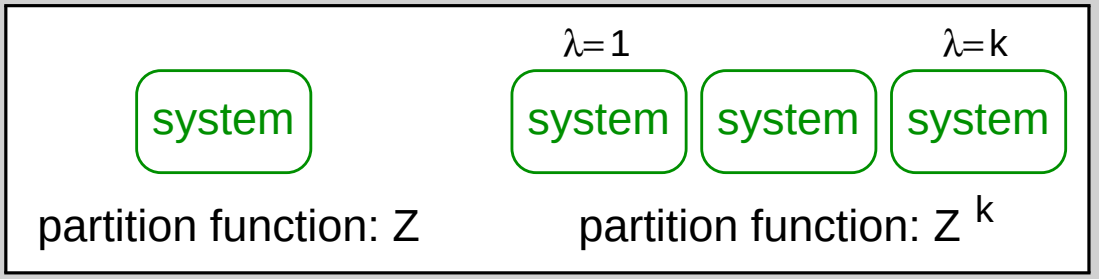
$$Z/Z_0 = \exp\left(\langle S(\beta,0)\rangle^{(0)}_{\text{conn.}} - 1\right)$$

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

---

proof:

consider k replicas of the system:



we have: $Z^k = e^{k \ln Z} = 1 + k \ln Z + \frac{1}{2} k^2 (\ln Z)^2 + \cdots$

hence: $$\ln Z = \lim_{k \to 0} \frac{d}{dk} Z^k$$

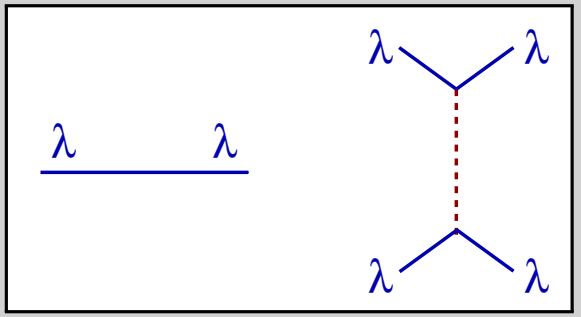
compute Z^k by perturbation theory applied to the k-fold replicated system

extract the term proportional to k ➜ $\ln Z$

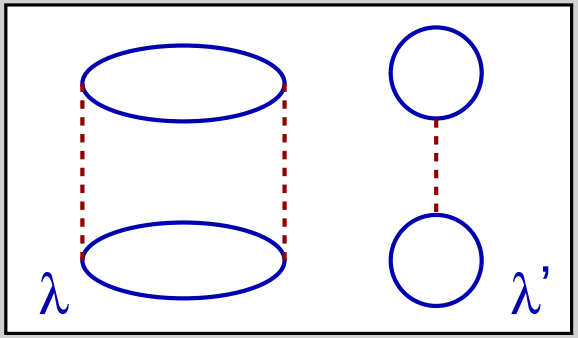
linked-cluster theorem, proof

compute Z^k by perturbation theory applied to the k-fold replicated system

➜ same diagrams, but:
– propagators carry index λ
– summation of $\lambda = 1, ..., k$
– propagators and vertices diagonal w.r.t λ



connected part of a diagram carries single index λ:



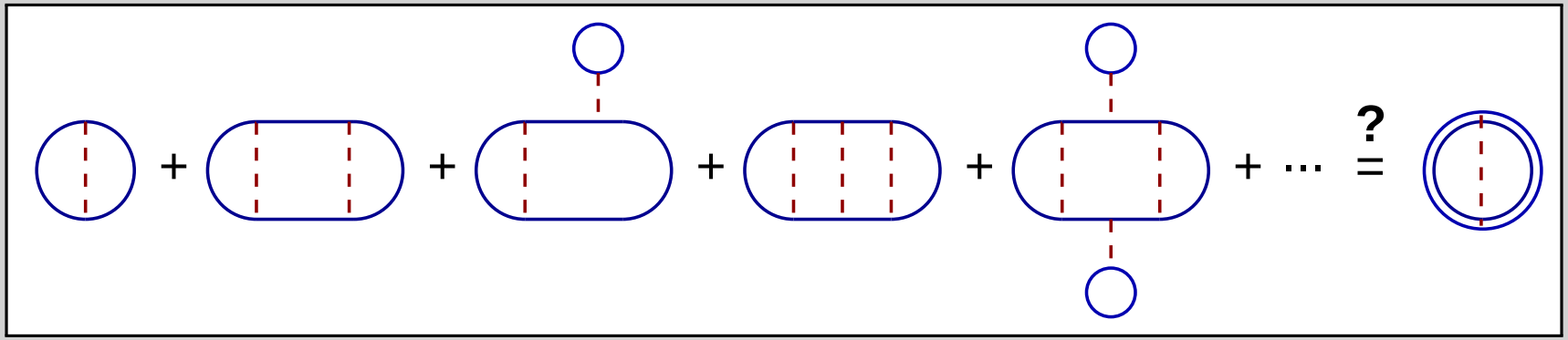
$$\sum_{\lambda} = k \,, \qquad \sum_{\lambda'} = k \qquad \text{➜ } k^2$$

➜ summation yields k^r if the diagram consists of r connected parts
➜ diagrams $\propto k$ consist of one connected part only
➜ summation of connected diagrams yields $\ln Z$

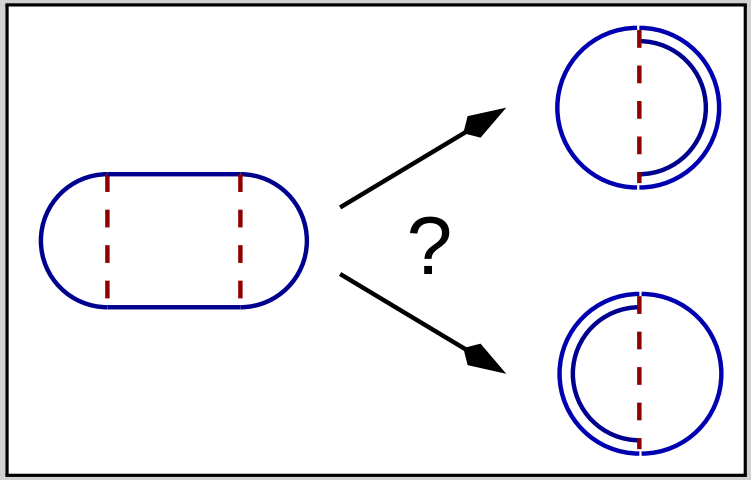
q.e.d.

renormalization?

partial summation of diagrams by renormalization of skeletons ?



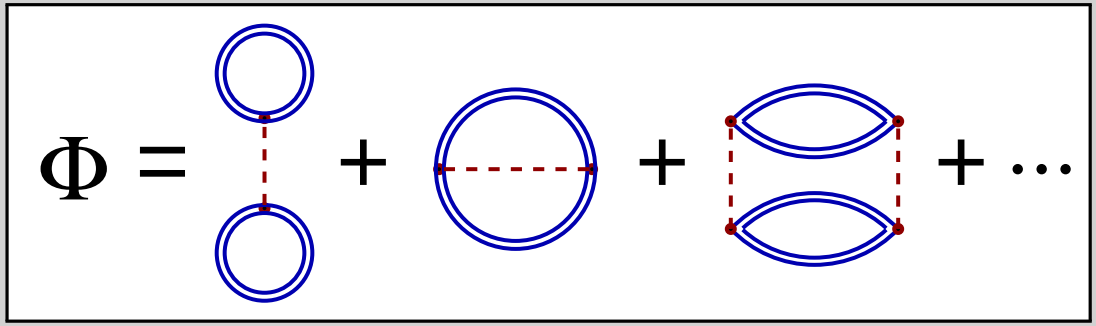
impossible because of double counting:



➜ 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 ?

$$\boldsymbol{\Sigma} = \frac{1}{T}\frac{\delta \Phi}{\delta \mathbf{G}}$$

IMPORTANT !!!

Φ is like a potential for the self-energy !

---

proof:

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

– Φ is a functional of the Green's function

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

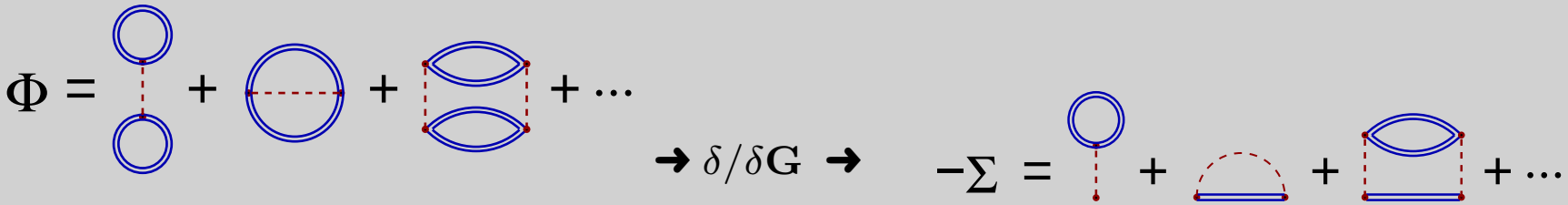
– $\widehat{\Phi}_{\mathbf{U}}[\mathbf{G}]$ is a **universal functional**

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

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

– basic equation for dynamical variational principle (see below)

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

---

proof:

consider the derivative w.r.t. μ:

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

first term:

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

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

proof, continued

second term:

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

third term:

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

hence:

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

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

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

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

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

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:

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

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

for $\mu \to -\infty$:

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

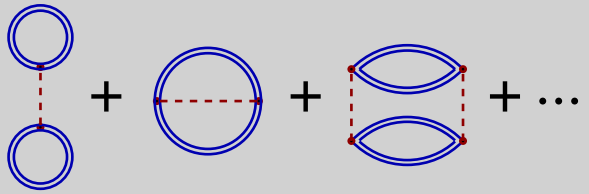
integrating over μ then yields:

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

q.e.d.

summary

Luttinger-Ward functional

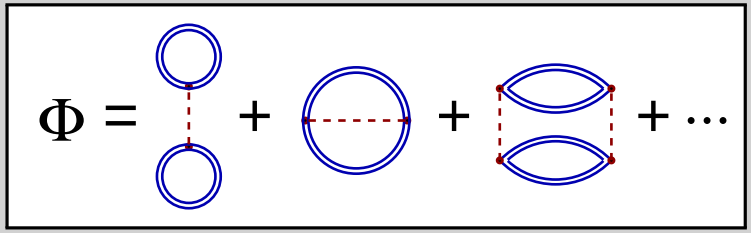
definition: $\Phi =$  $+ \cdots$

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)

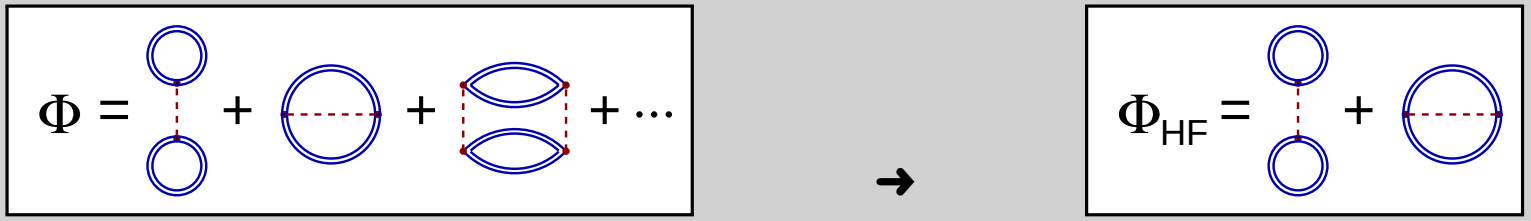
➜ evaluate $\widehat{\Omega}[\mathbf{G}] = \widehat{\Phi}[\mathbf{G}] + \mathrm{Tr}\ln\mathbf{G} - \mathrm{Tr}((\mathbf{G}_0^{-1} - \mathbf{G}^{-1})\mathbf{G})$

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:



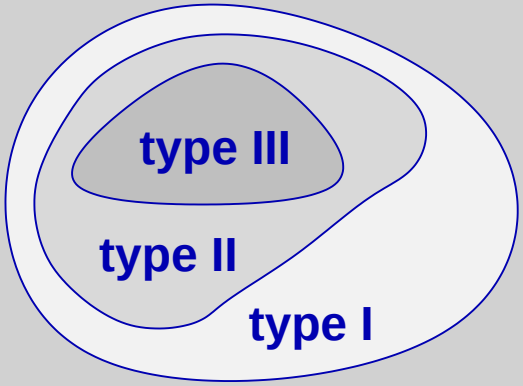
self-consistently weak-coupling perturbation theory

HF, RPA, FLEX, ...

Self-Energy Functional

approximation strategies

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

functionals of dynamic quantities

wanted: $\boxed{\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}]}$ with $\dfrac{\delta\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}]}{\delta\mathbf{\Sigma}} = 0 \Leftrightarrow \mathbf{\Sigma} = \mathbf{\Sigma}_{\mathbf{t},\mathbf{U}}$

elements: $\Phi_{\mathbf{U}}[\mathbf{G}]$, $\mathbf{\Sigma}$, $\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}]$ (inverse of $\mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$), $\dfrac{1}{\mathbf{G}^{-1}_{\mathbf{t},0} - \mathbf{\Sigma}}$

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

candidates :

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

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

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

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

functionals of dynamic quantities

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

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

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

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

functionals of dynamic quantities

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

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

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

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(4) works and includes unknown but **universal** functionals !

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

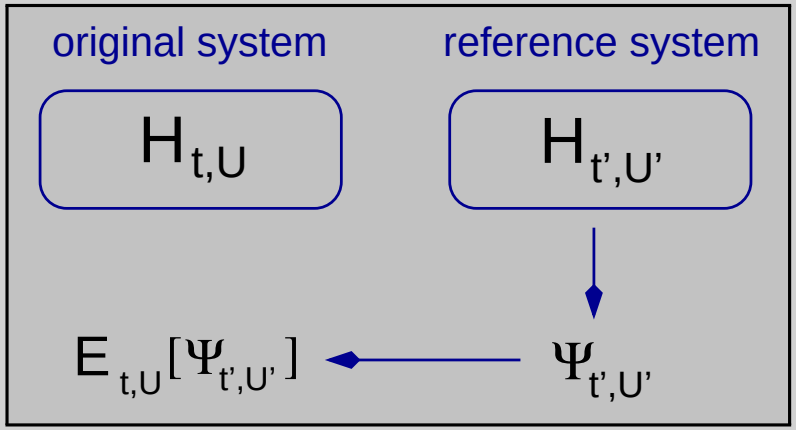
$\delta\Omega[\mathbf{\Sigma}] = 0$	self-energy	**SFT**	**new approximations?**	**dynamic**
$\delta\Omega[\mathbf{G}] = 0$	Green's function	**Luttinger Ward**	**perturbation theory**	**dynamic**
$\delta\Omega[\mathbf{n}] = 0$	electron density	**DFT**	**LDA**	**static**
$\delta\Omega[\rho] = 0$	density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



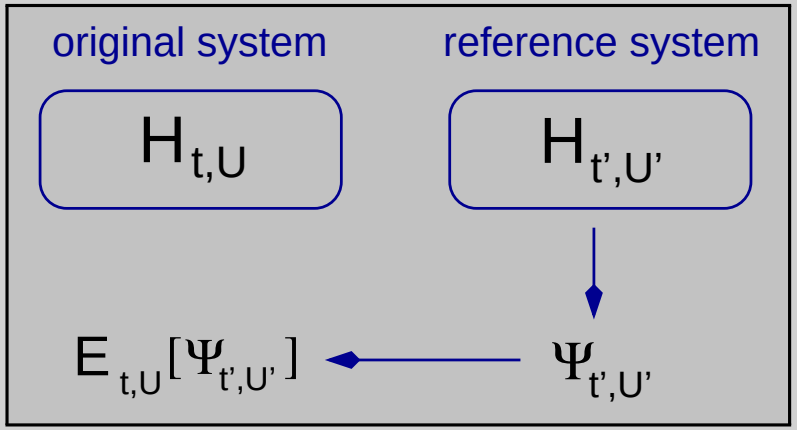
$$E_{\mathbf{t},\mathbf{U}}[|\Psi\rangle] = \langle\Psi|H_{\mathbf{t},\mathbf{U}}|\Psi\rangle$$

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

➜ **Hartree-Fock approximation**

reference system

Ritz variational principle

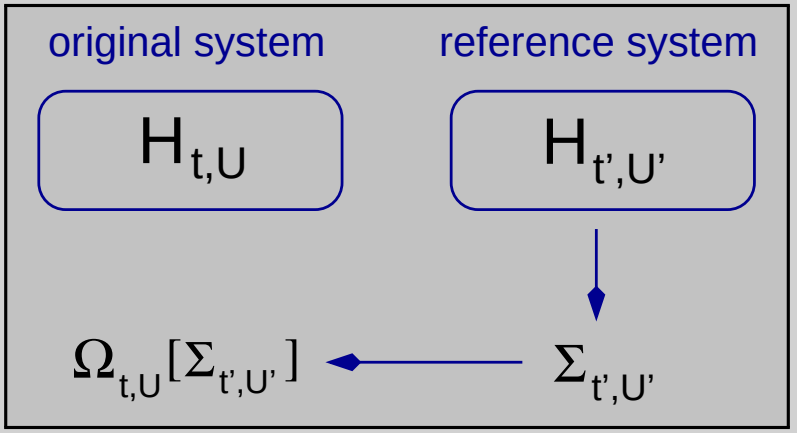


$$E_{\mathbf{t},\mathbf{U}}[|\Psi\rangle] = \langle\Psi|H_{\mathbf{t},\mathbf{U}}|\Psi\rangle$$

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

➜ **Hartree-Fock approximation**

SFT



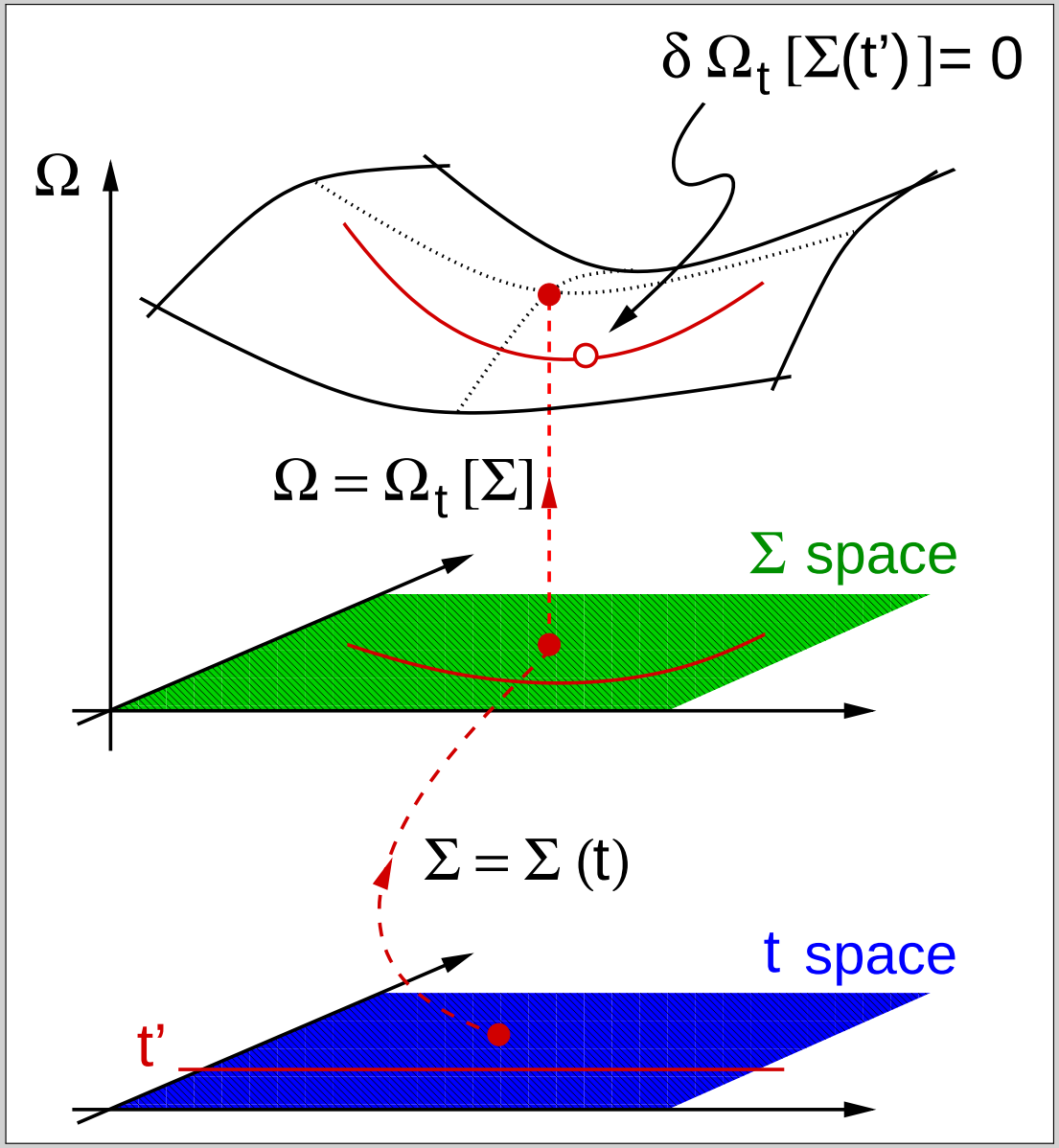
$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \textbf{?}$$

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

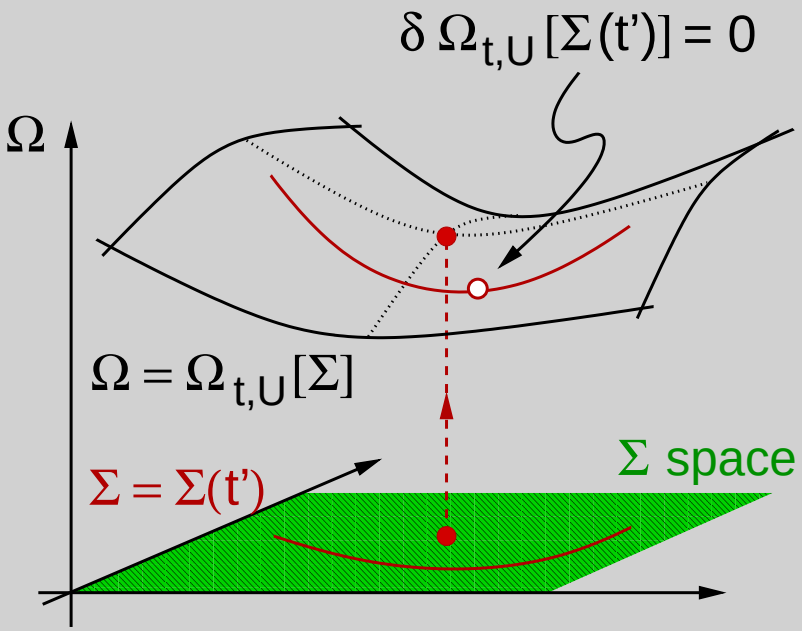
➜ **new approximations ?**

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:

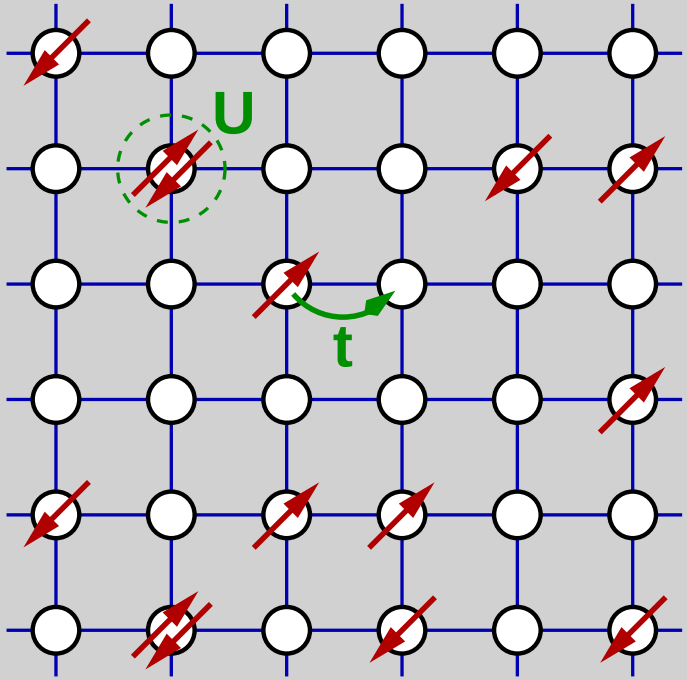
$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \Omega_{\mathbf{t}',\mathbf{U}}[\mathbf{\Sigma}] + \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{0,\mathbf{t}} - \mathbf{\Sigma}} - \mathrm{Tr}\ln\frac{1}{\mathbf{G}^{-1}_{0,\mathbf{t}'} - \mathbf{\Sigma}}$$

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

Potthoff (2003)

cluster approximations

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

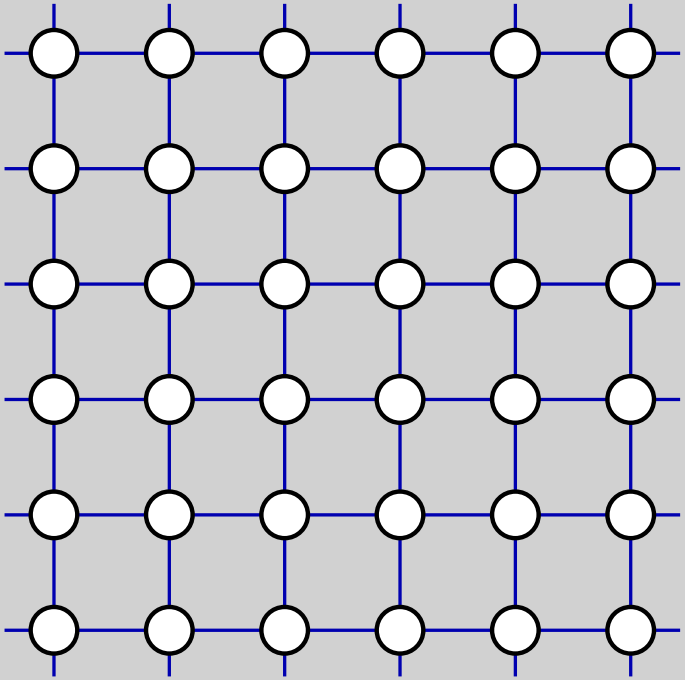


lattice model ($D = 2$) in
the thermodynamic limit

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

cluster approximations

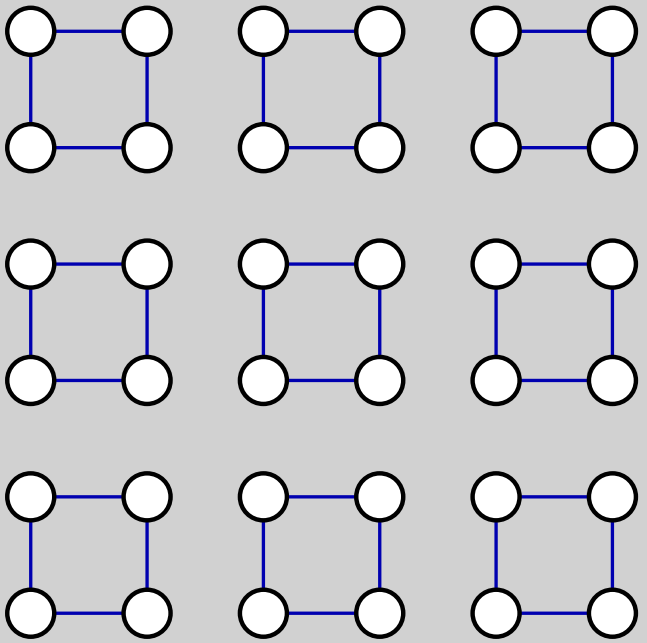
original system, $H_{\mathbf{t},\mathbf{U}}$:



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

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

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

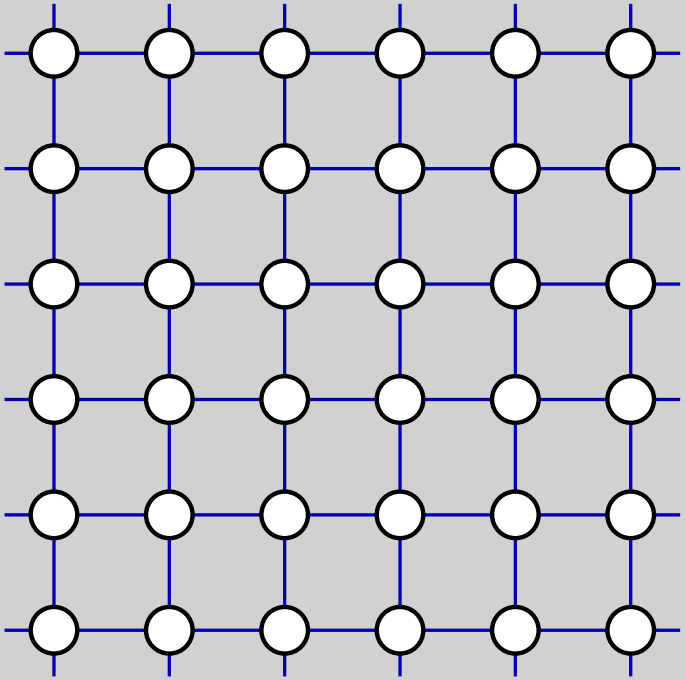


system of decoupled clusters

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

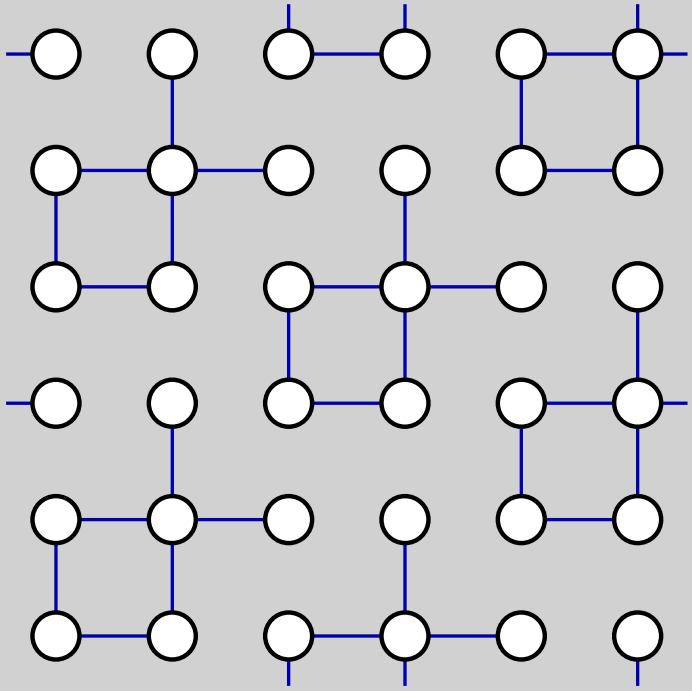
cluster approximations

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



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

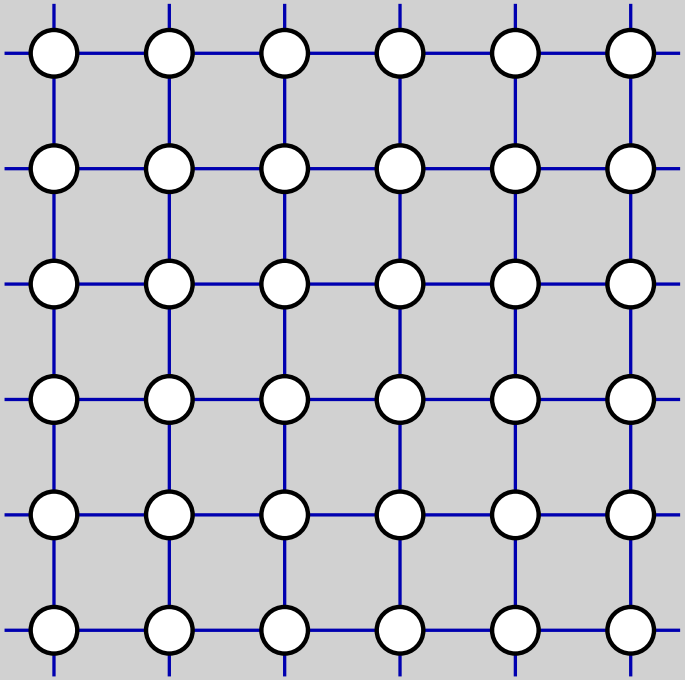
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

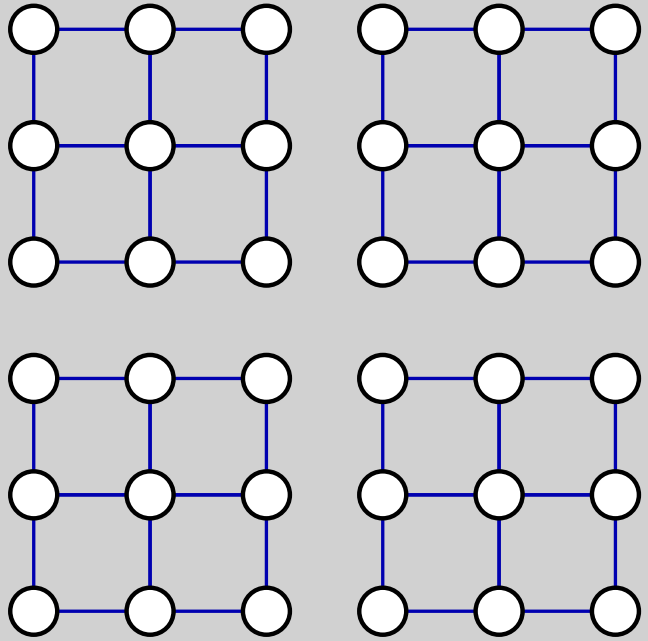
cluster approximations

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



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

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

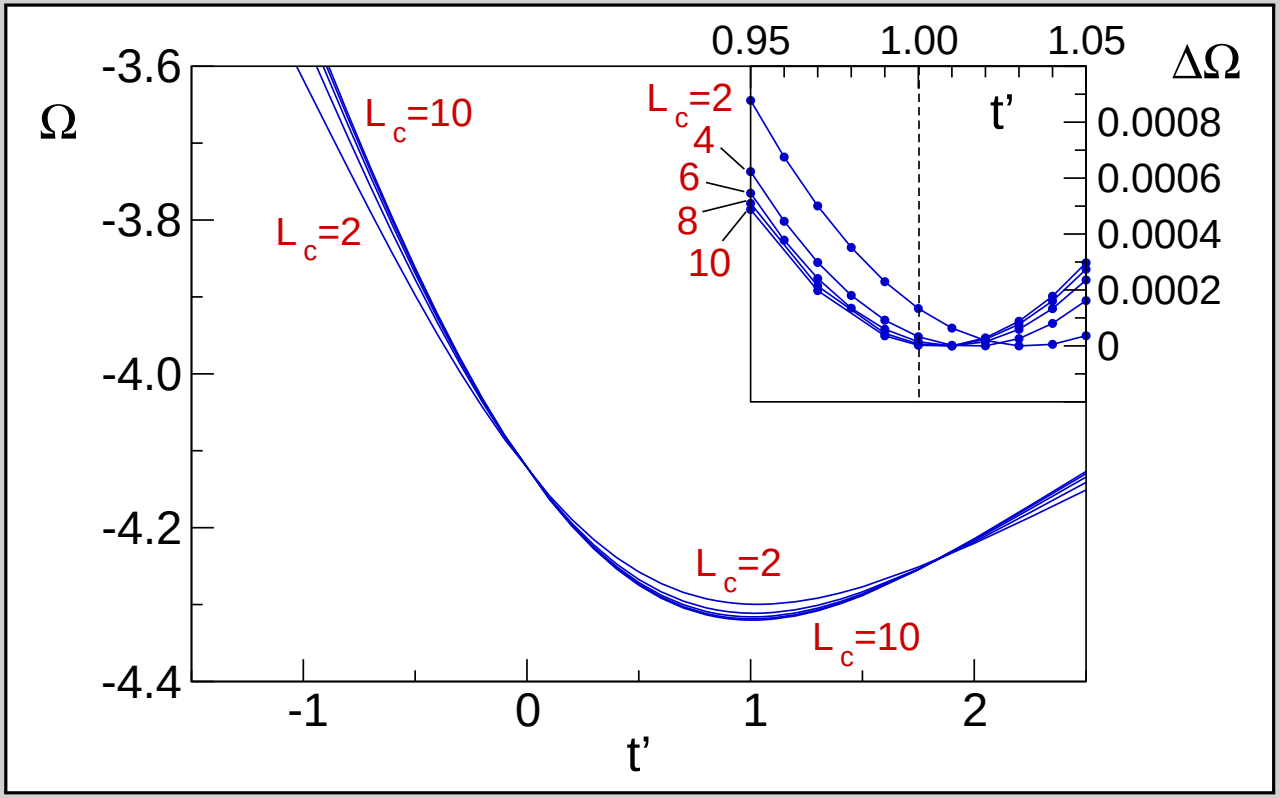


system of decoupled clusters
cluster size: L_c
$L_c \leq 2$: analytic
$L_c \leq 6$: exact diagonalization
$L_c \leq 12$: Lanczos method
$L_c \leq 100$: stochastic techniques

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



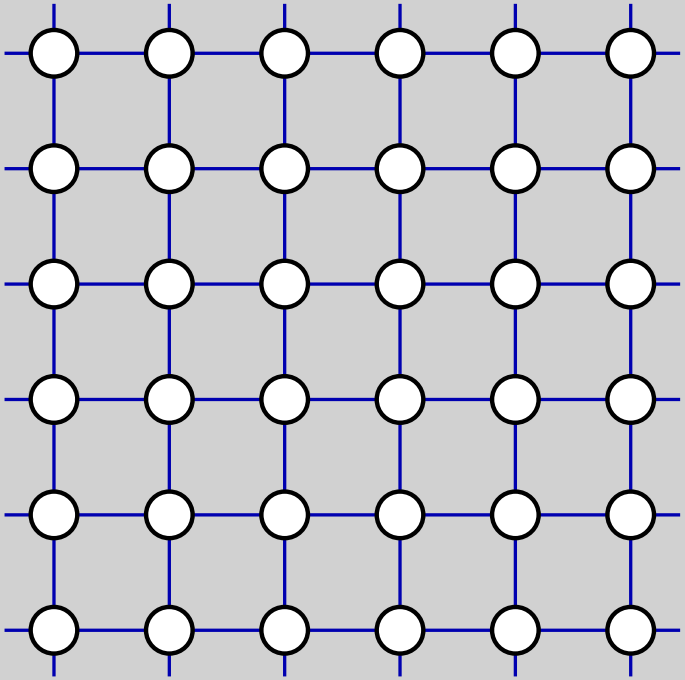
➜ $\Omega(t') \equiv \Omega[\mathbf{\Sigma}(t')]$ **stationary at** $t'_{\rm min} \neq t$

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

➜ $t'_{\rm min} \approx t$

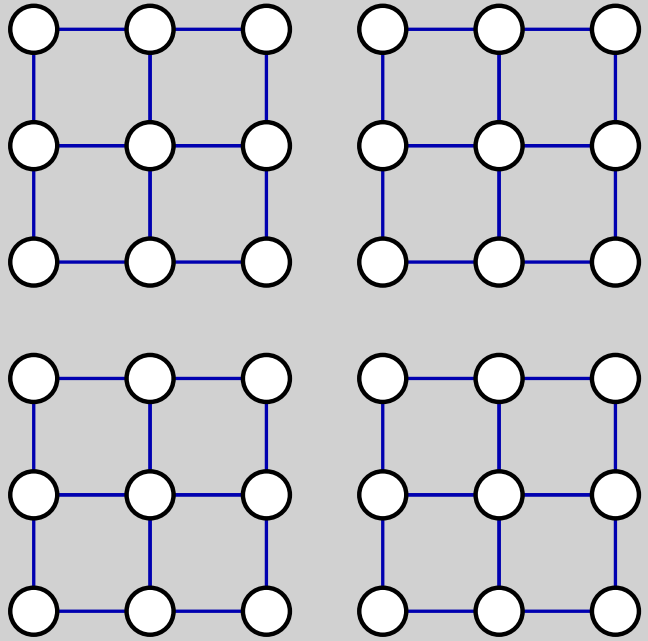
cluster approximations

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



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

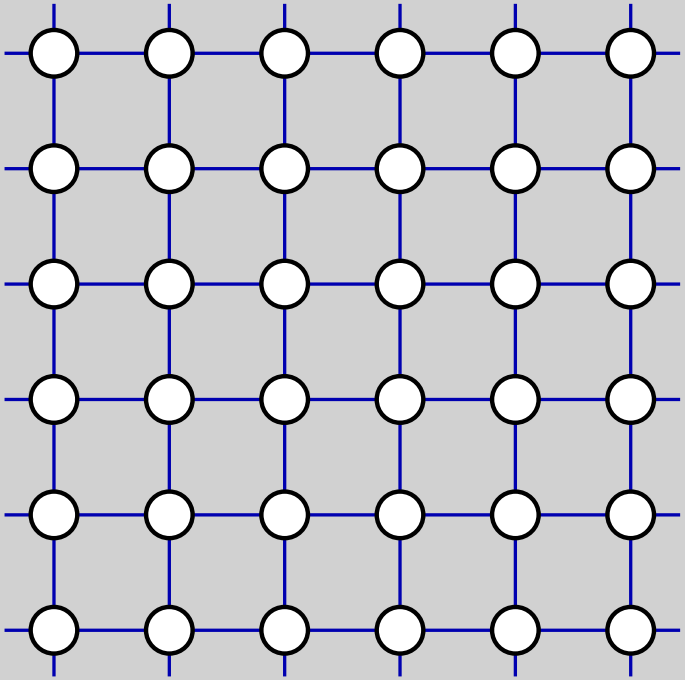
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

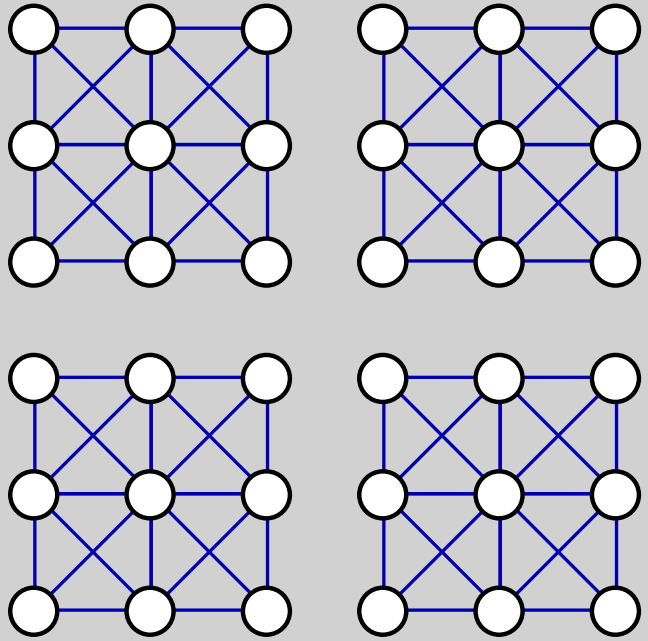
cluster approximations

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



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

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

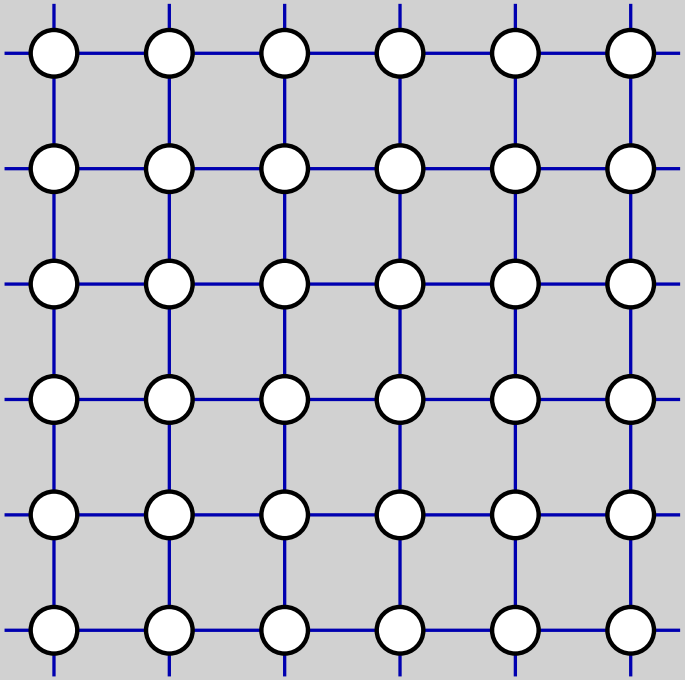


system of decoupled clusters

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

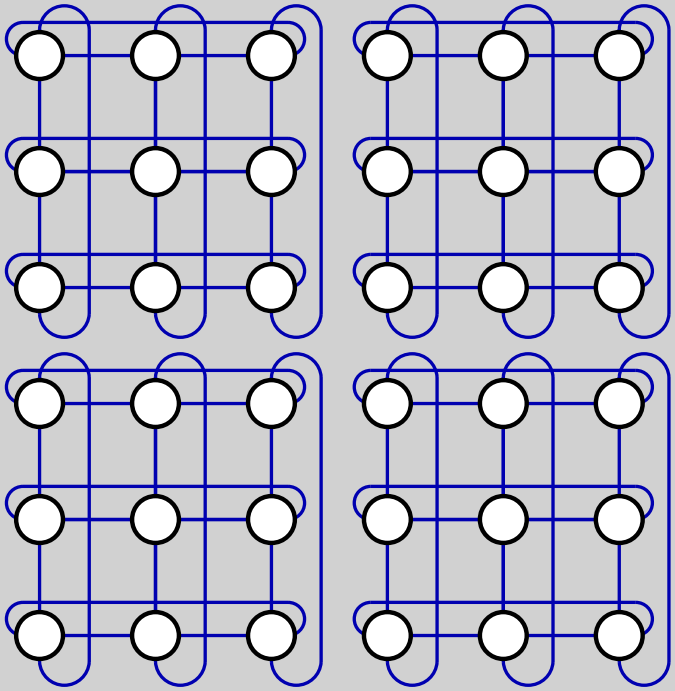
cluster approximations

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



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

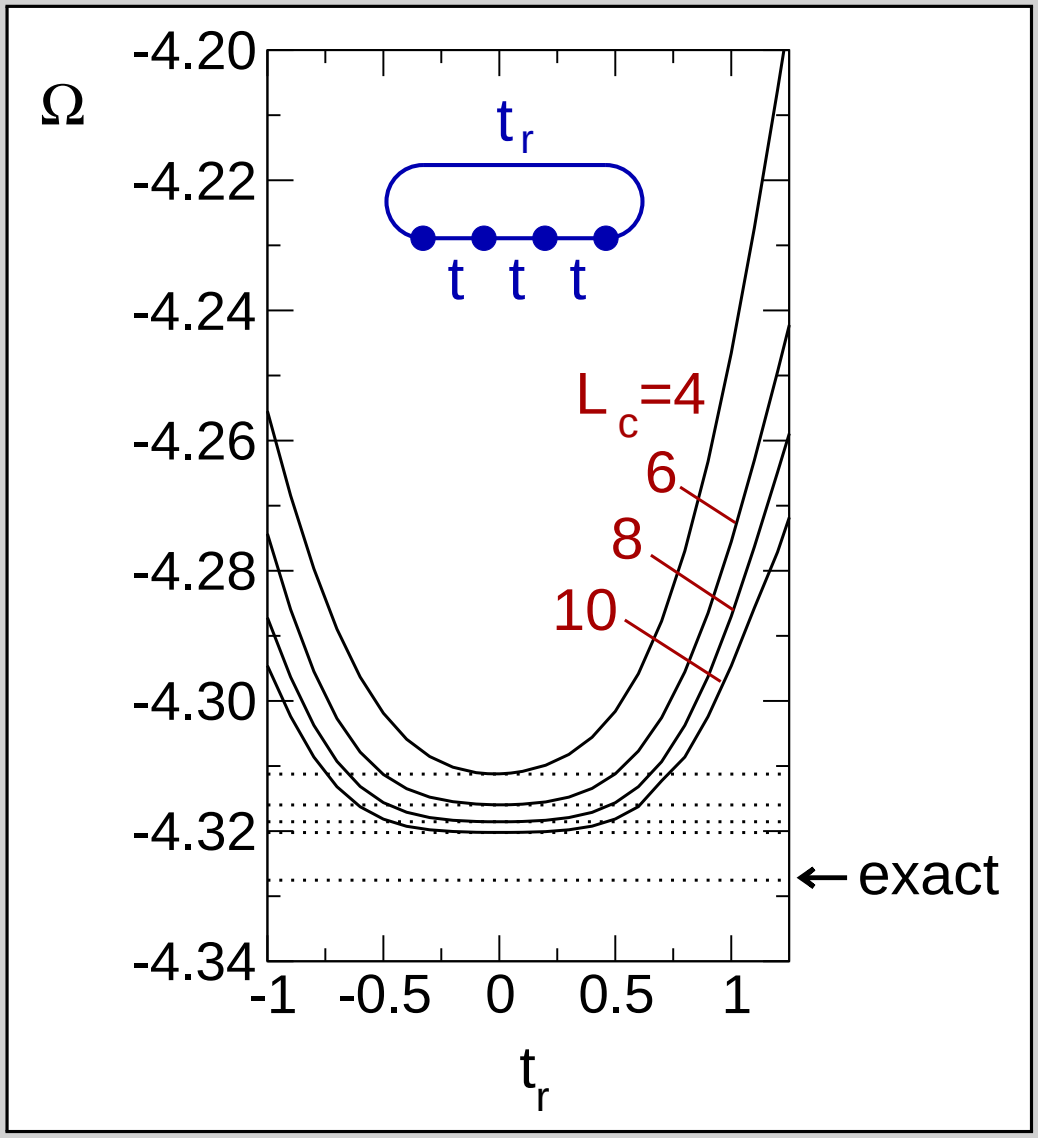
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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, $U = 8$

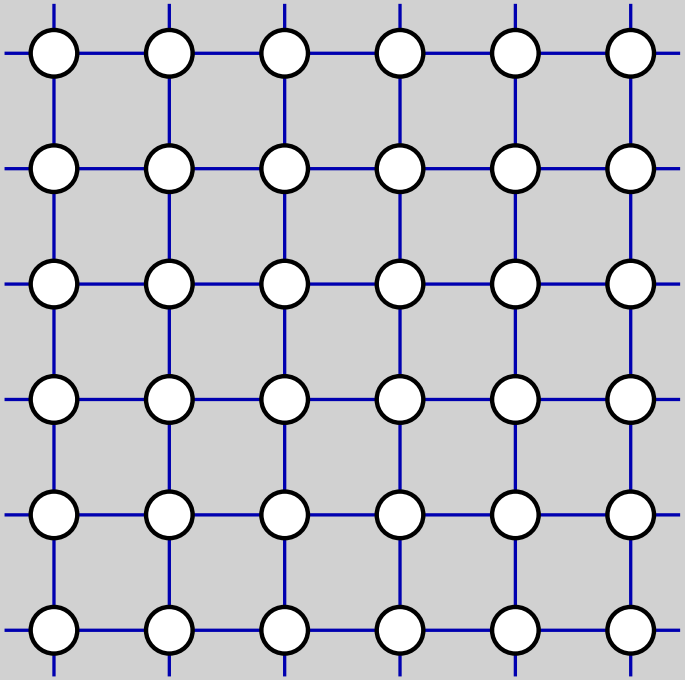
$t = 1$

open or periodic b.c. ?

open boundary conditions !

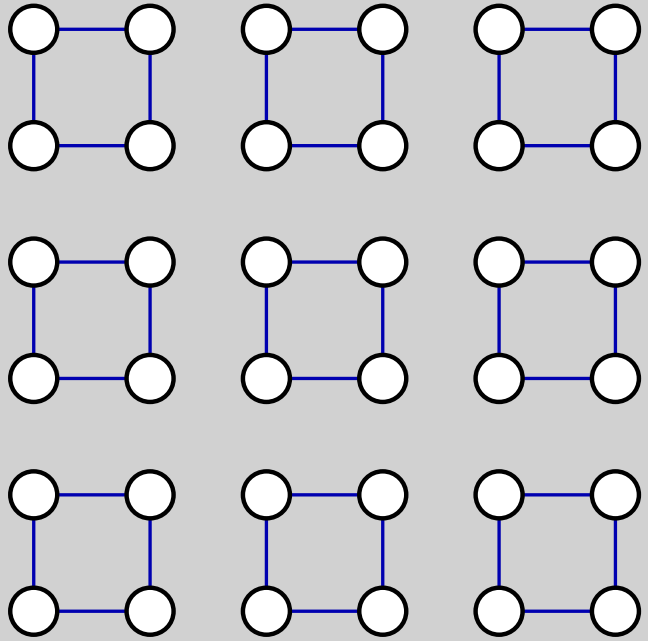
cluster approximations

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



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

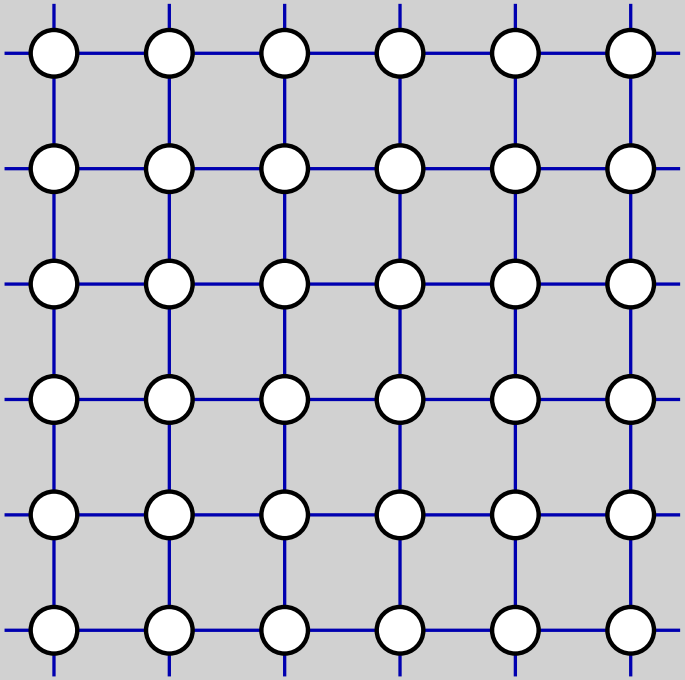
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

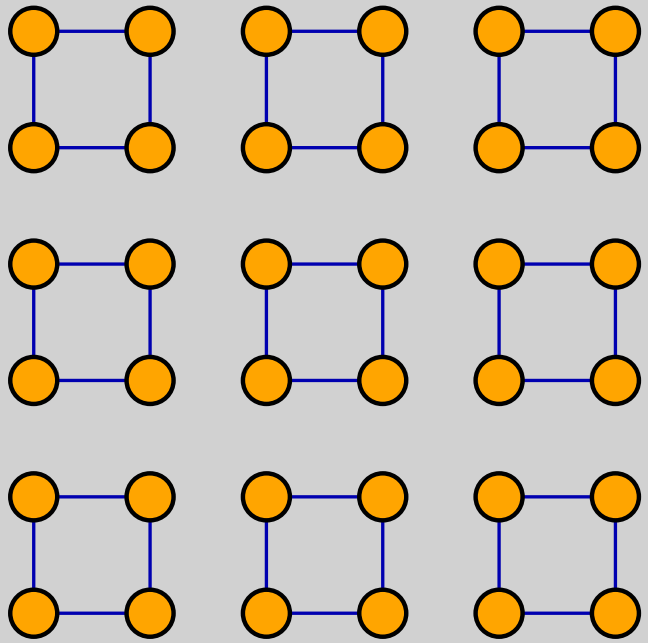
cluster approximations

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



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

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

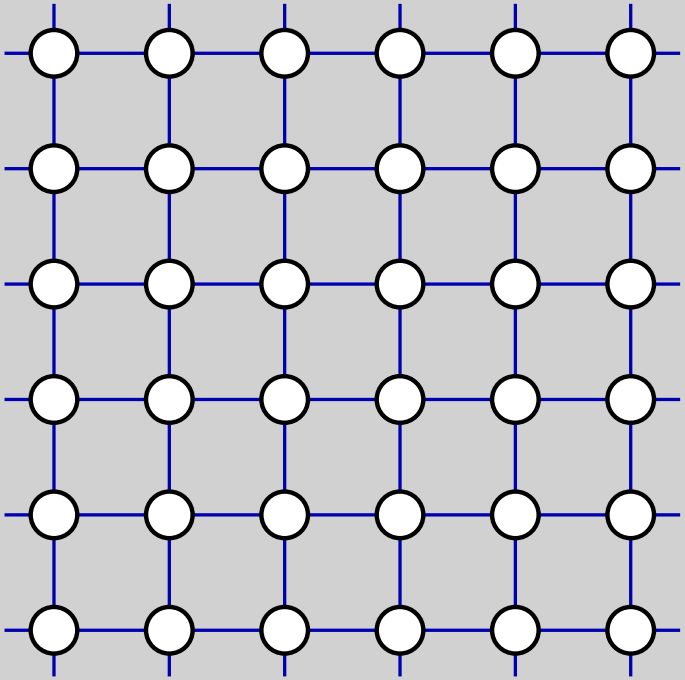


system of decoupled clusters

variational parameters:
on-site energies
thermodynamic consistency

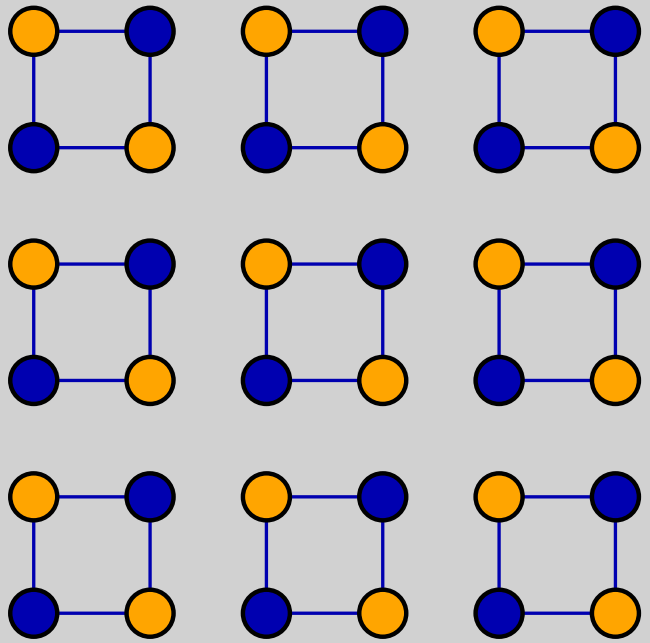
cluster approximations

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



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

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

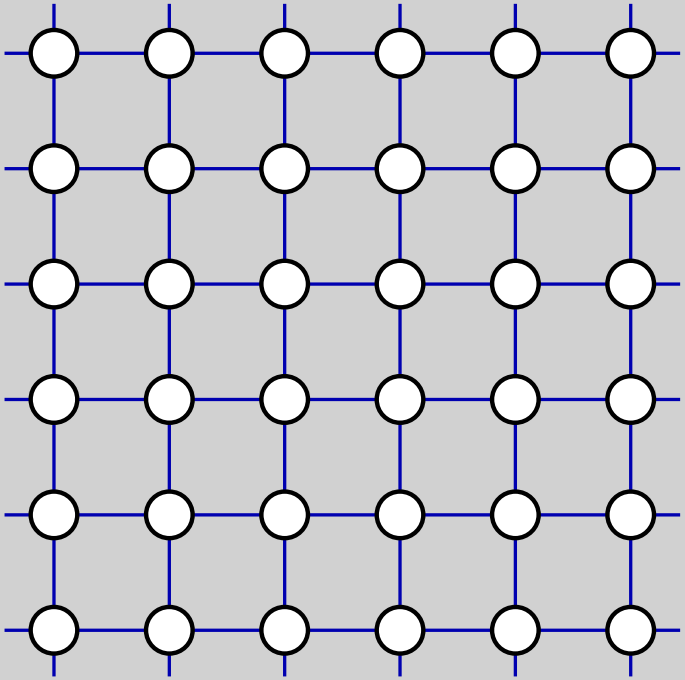


system of decoupled clusters

variational parameters:
ficticious symmetry-breaking fields
spontaneous symmetry breaking

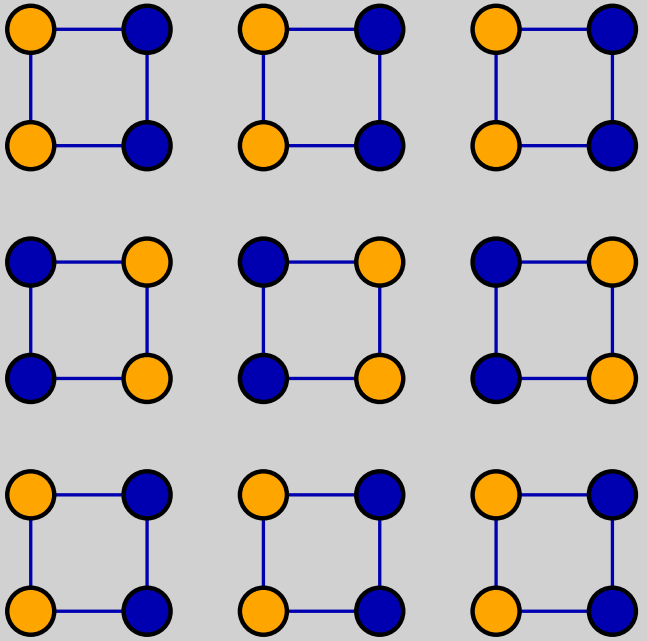
cluster approximations

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



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

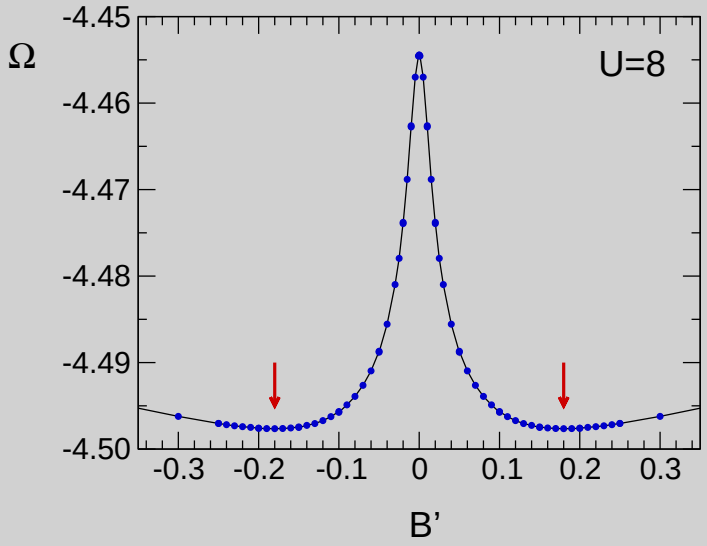
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



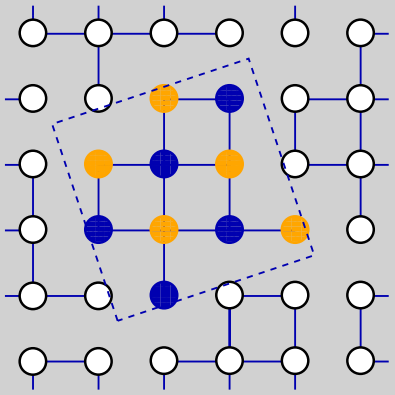
system of decoupled clusters

variational parameters:
ficticious symmetry-breaking fields
different order parameters

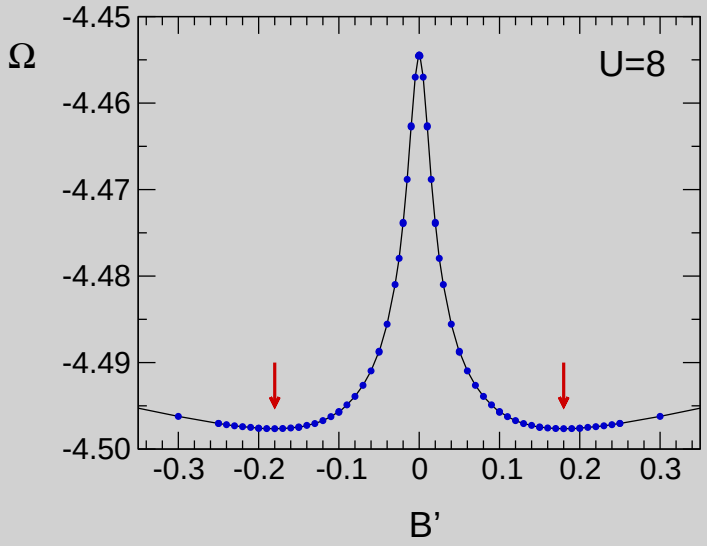
antiferromagnetism



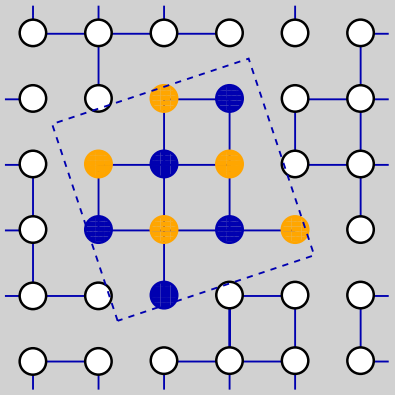
$D = 2$ Hubbard model, half-filling

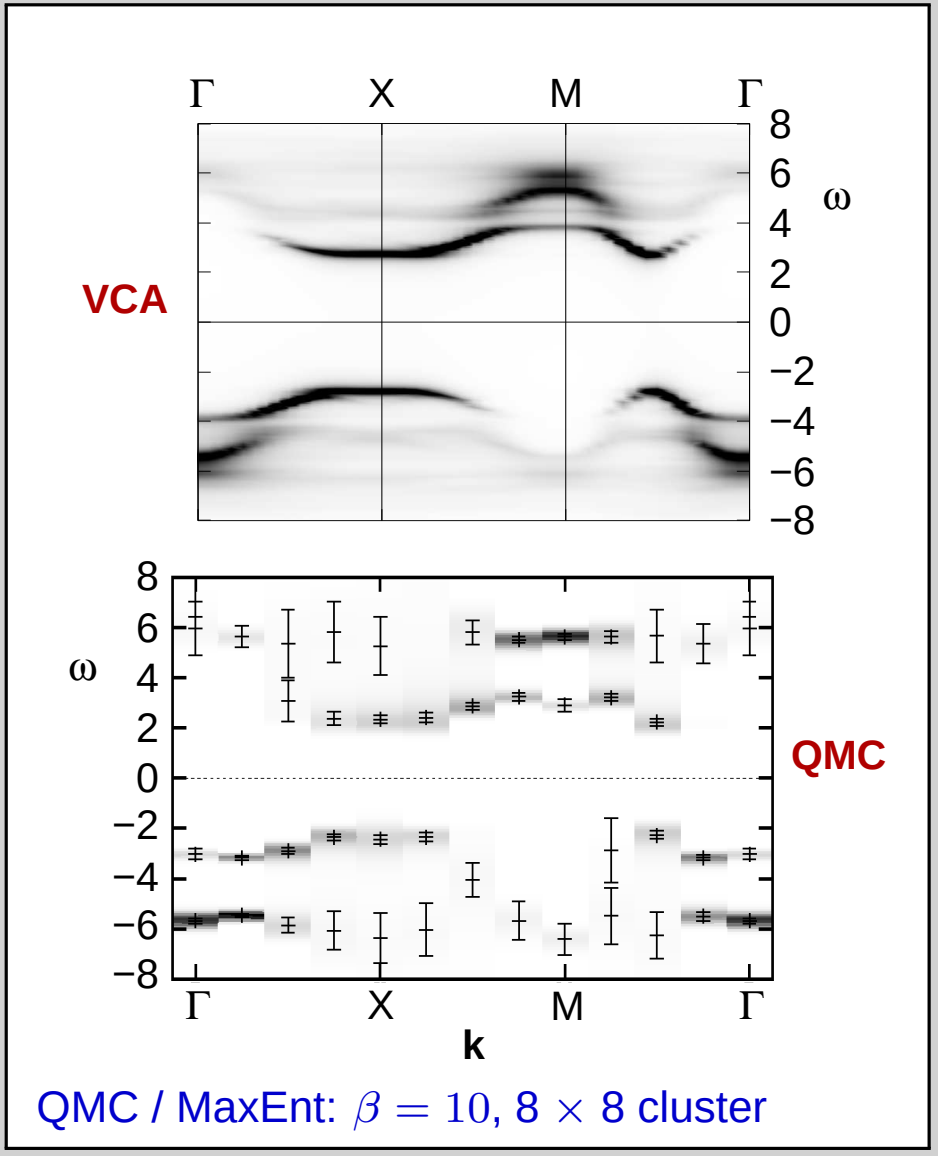


antiferromagnetism



$D = 2$ Hubbard model, half-filling

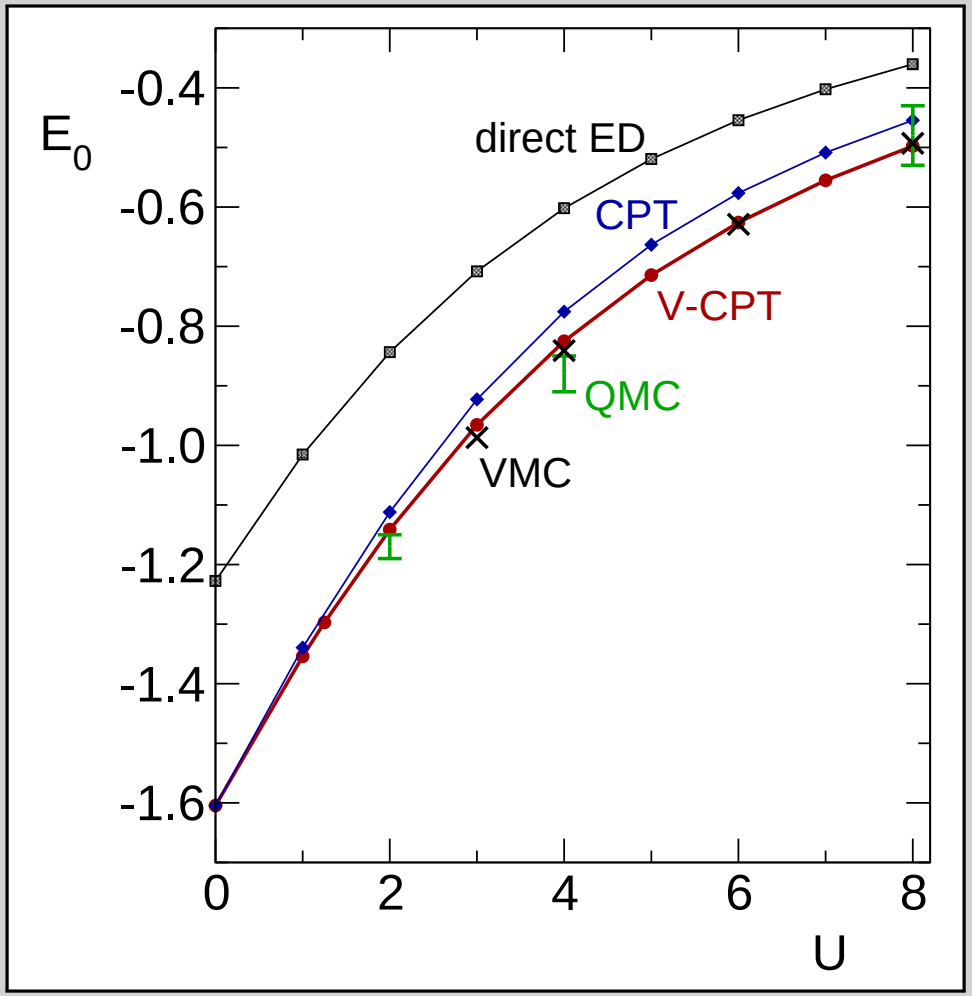




QMC / MaxEnt: $\beta = 10$, 8×8 cluster

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

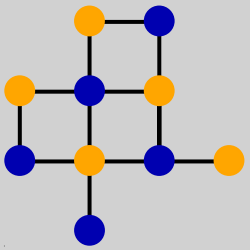
ground-state energy



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:

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

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: $\mathbf{S}_{\rm tot}$, total spin
- Weiss field: $\boxed{H'_{\rm fict.} = B' \sum_{i\sigma} z_i (n_{i\uparrow} - n_{i\downarrow}) \ ,}$
- order parameter: $\boxed{m = \sum_{i\sigma} z_i \langle (n_{i\uparrow} - n_{i\downarrow}) \rangle}$

---

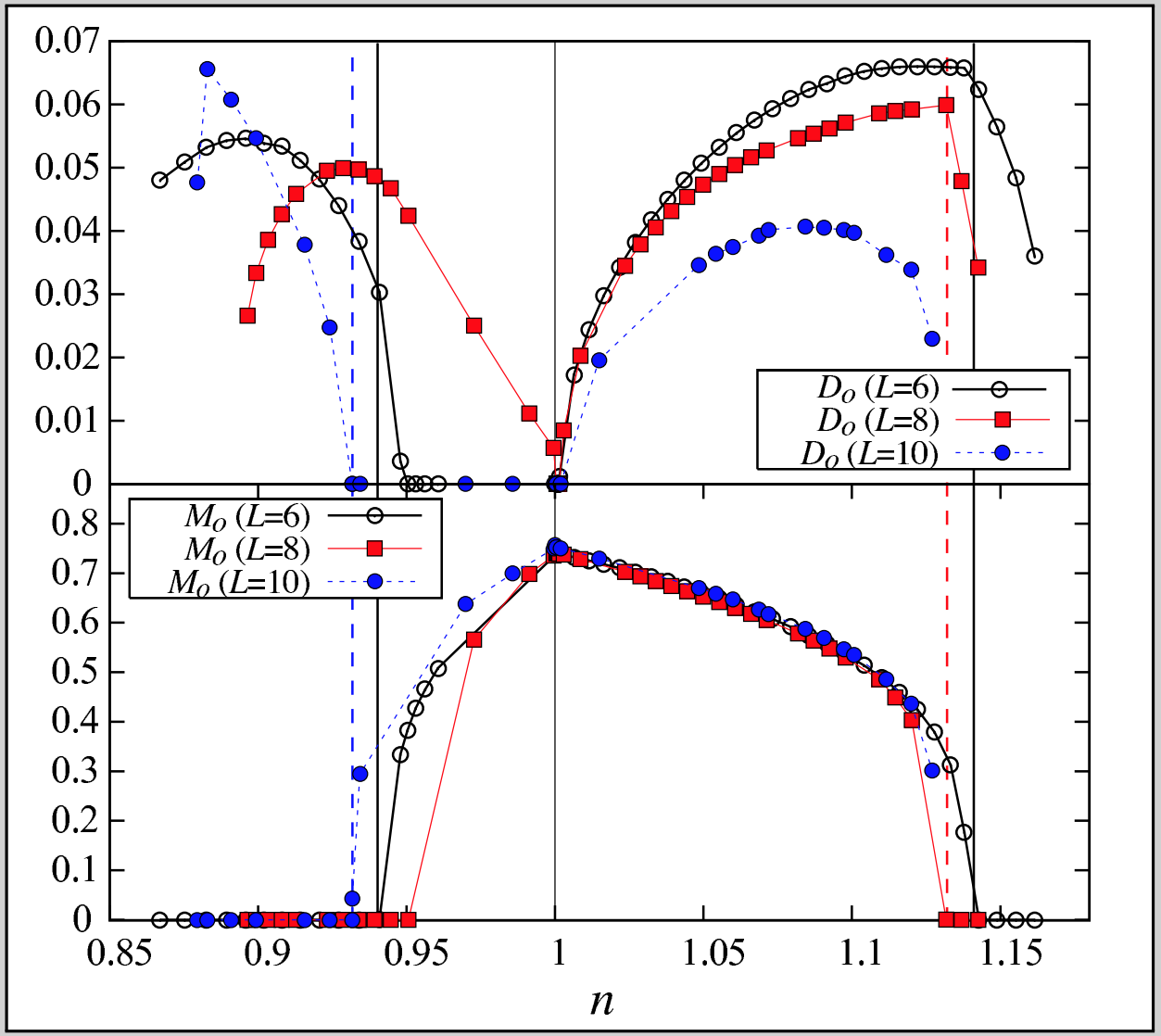
superconductivity:

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



d-wave-superconductivity

antiferromagnetism

t-t'-t'' Hubbard model

$D = 2$

$T = 0, U = 8t$

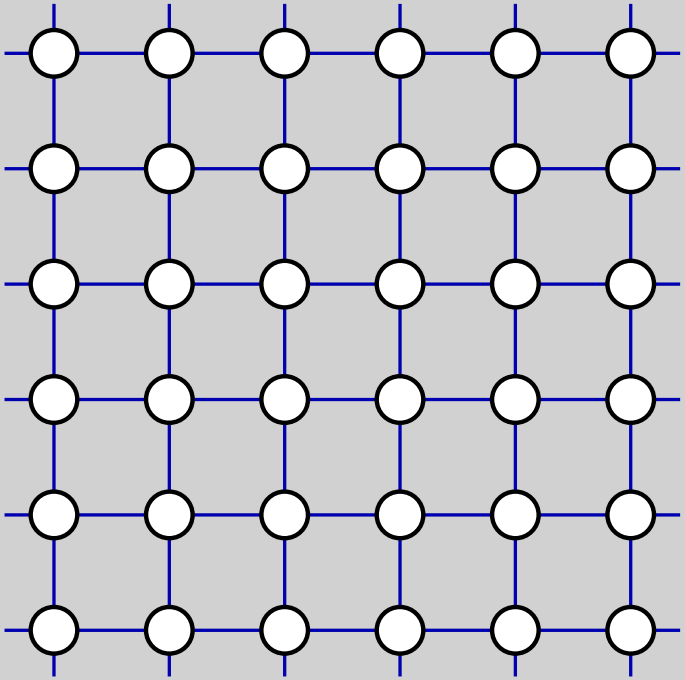
$L_c = 6, 8, 10$

Senechal, Lavertu, Marois, Tremblay (2005)

Bath Sites and Dynamical Mean-Field Theory

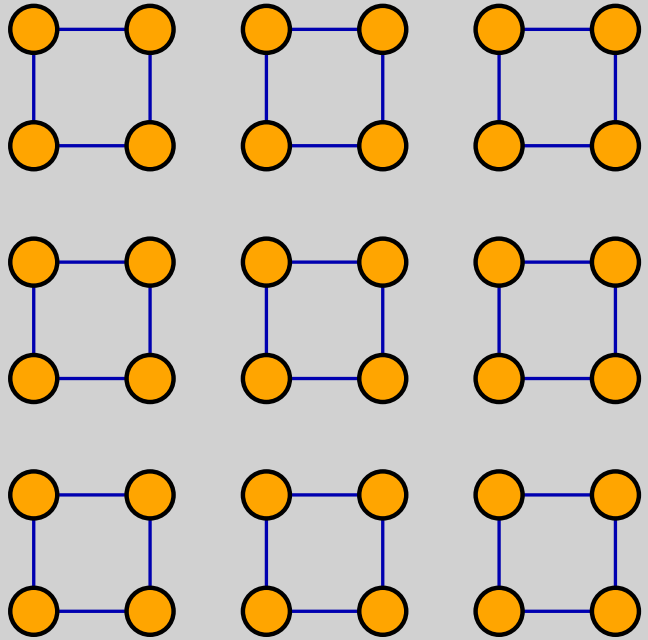
approximations using bath sites

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



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

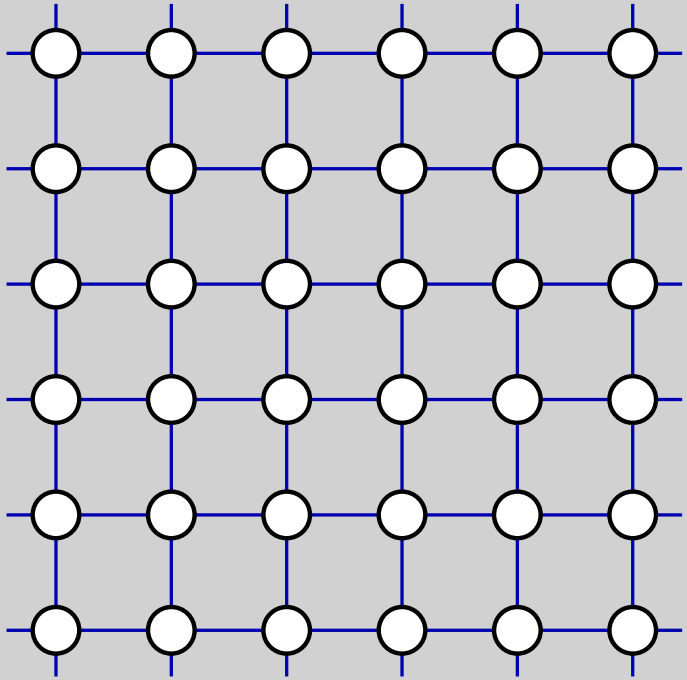
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

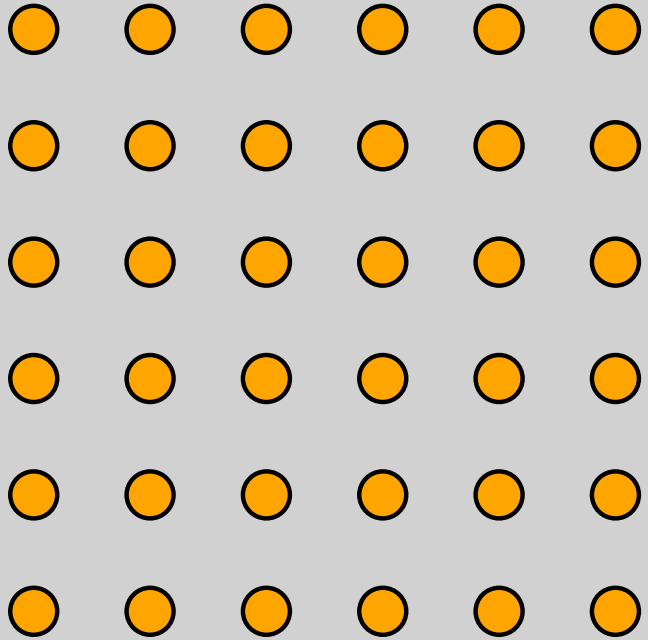
approximations using bath sites

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



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

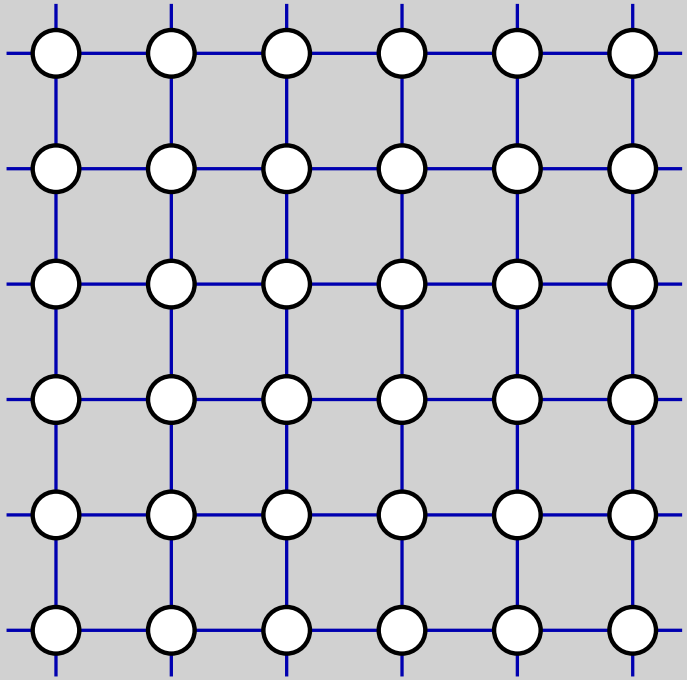
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

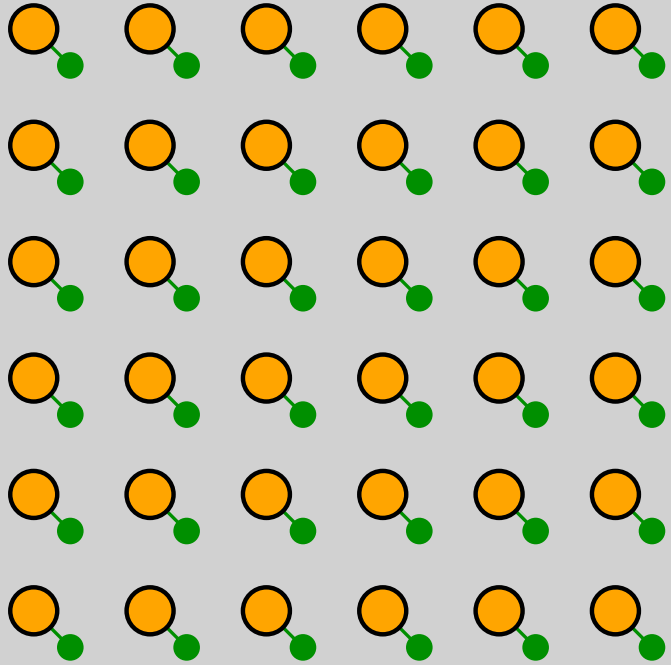
approximations using bath sites

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



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

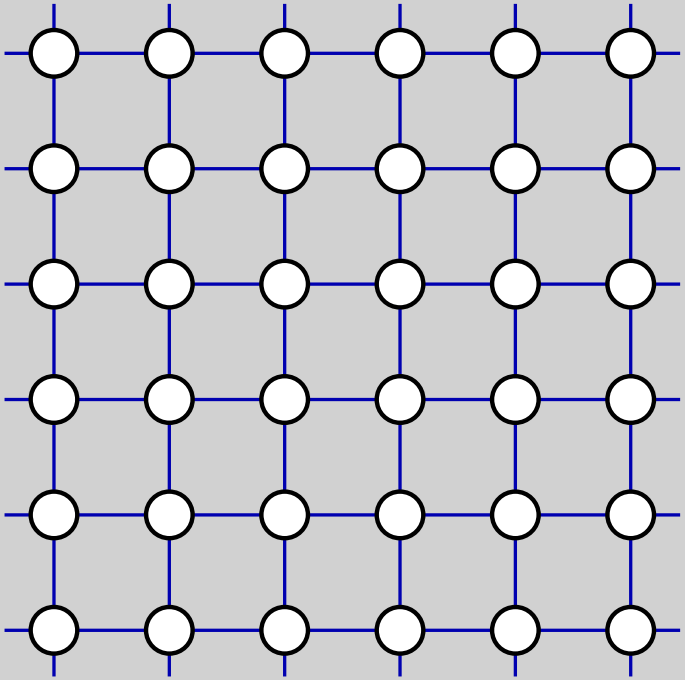
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

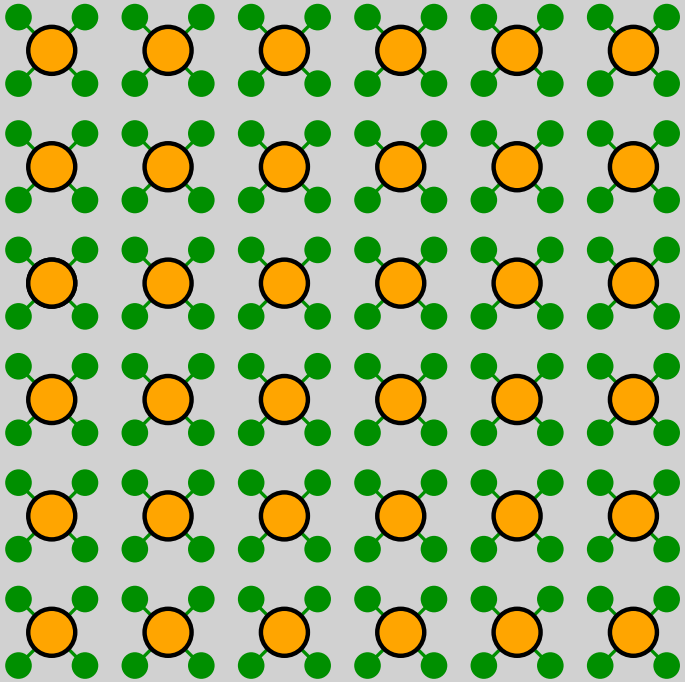
approximations using bath sites

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



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

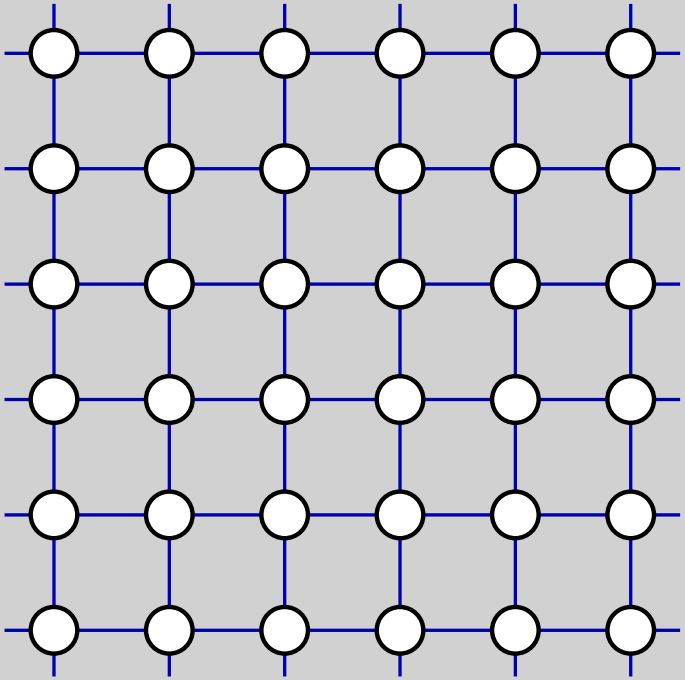
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

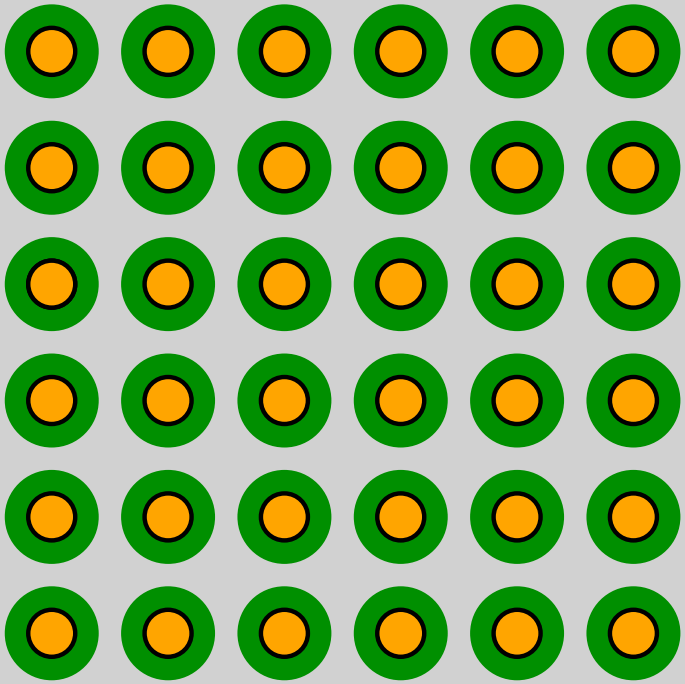
approximations using bath sites

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



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

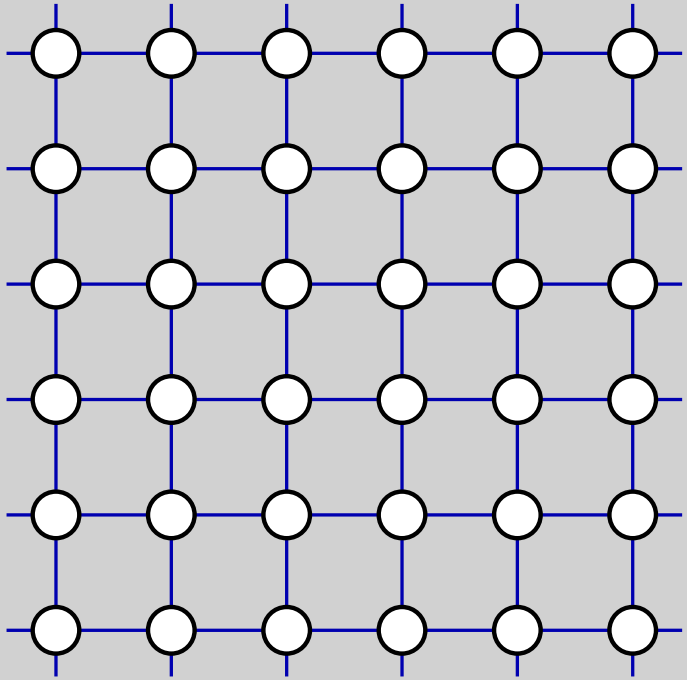
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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)

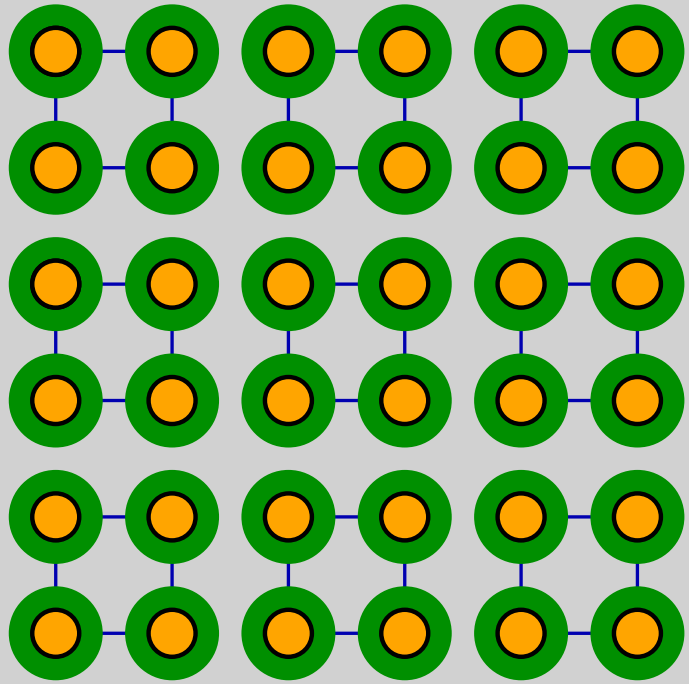
approximations using bath sites

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



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

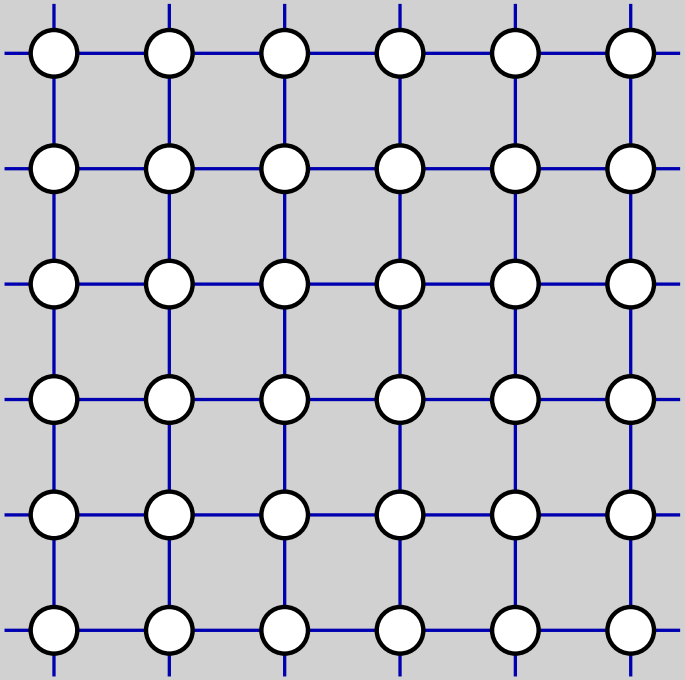
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

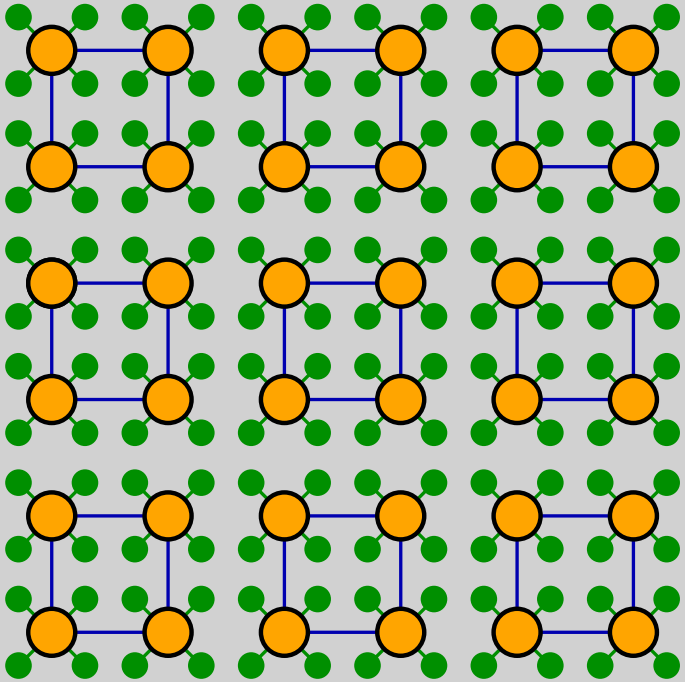
approximations using bath sites

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



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

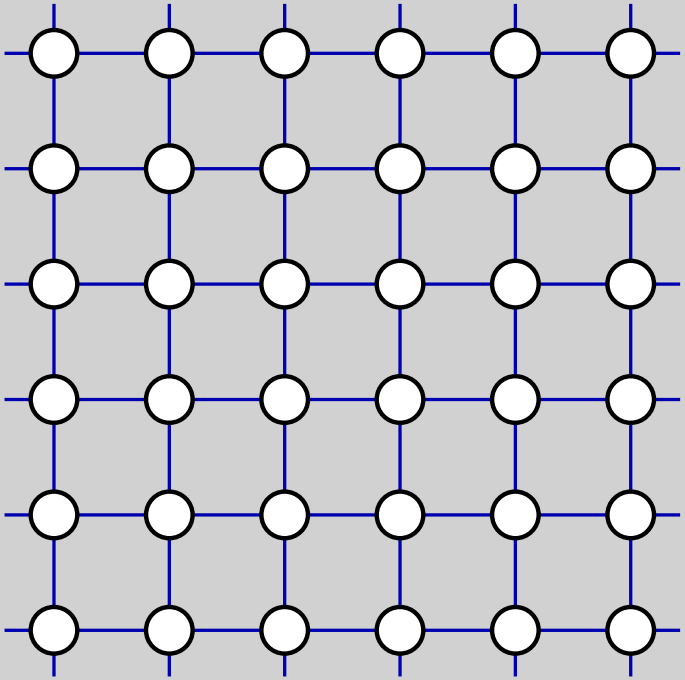
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

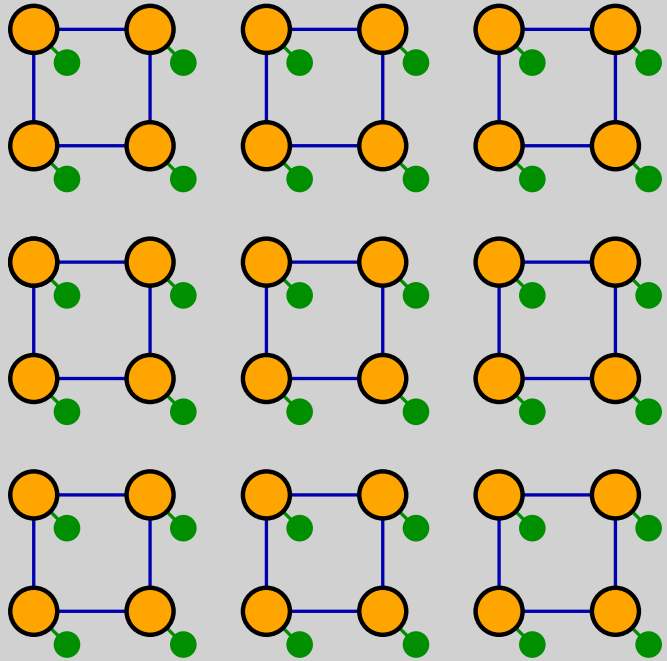
approximations using bath sites

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



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

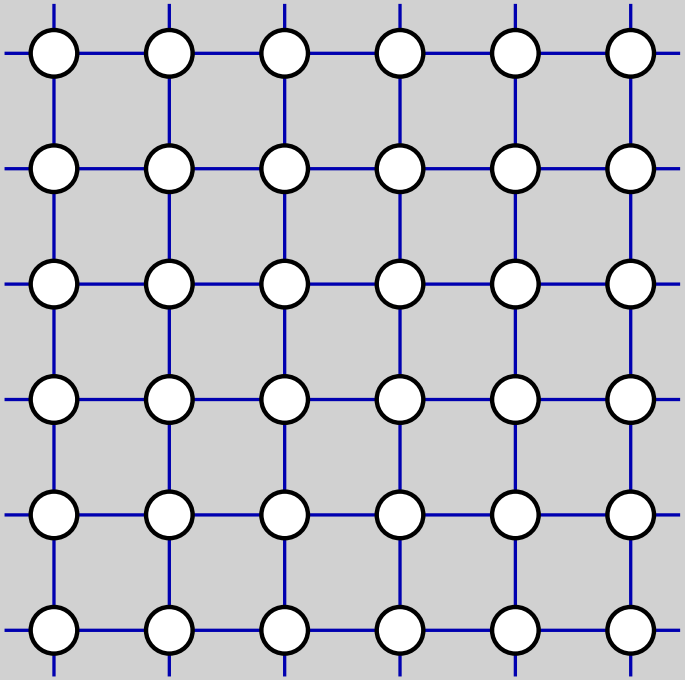
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

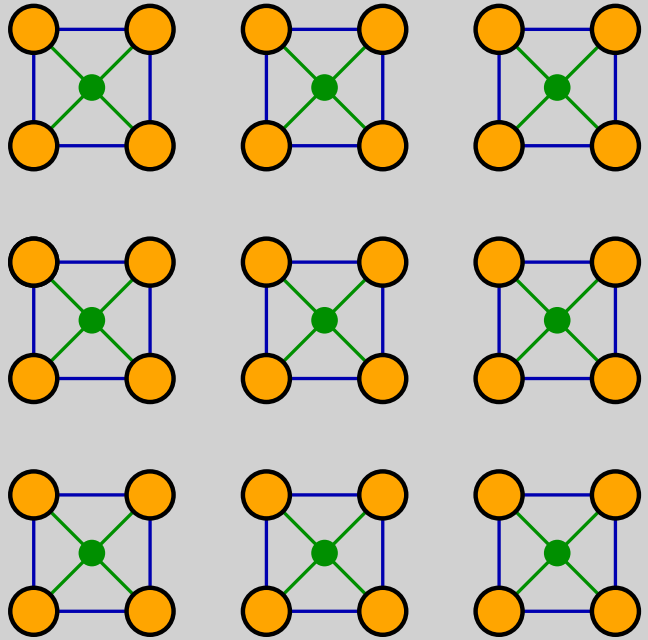
approximations using bath sites

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



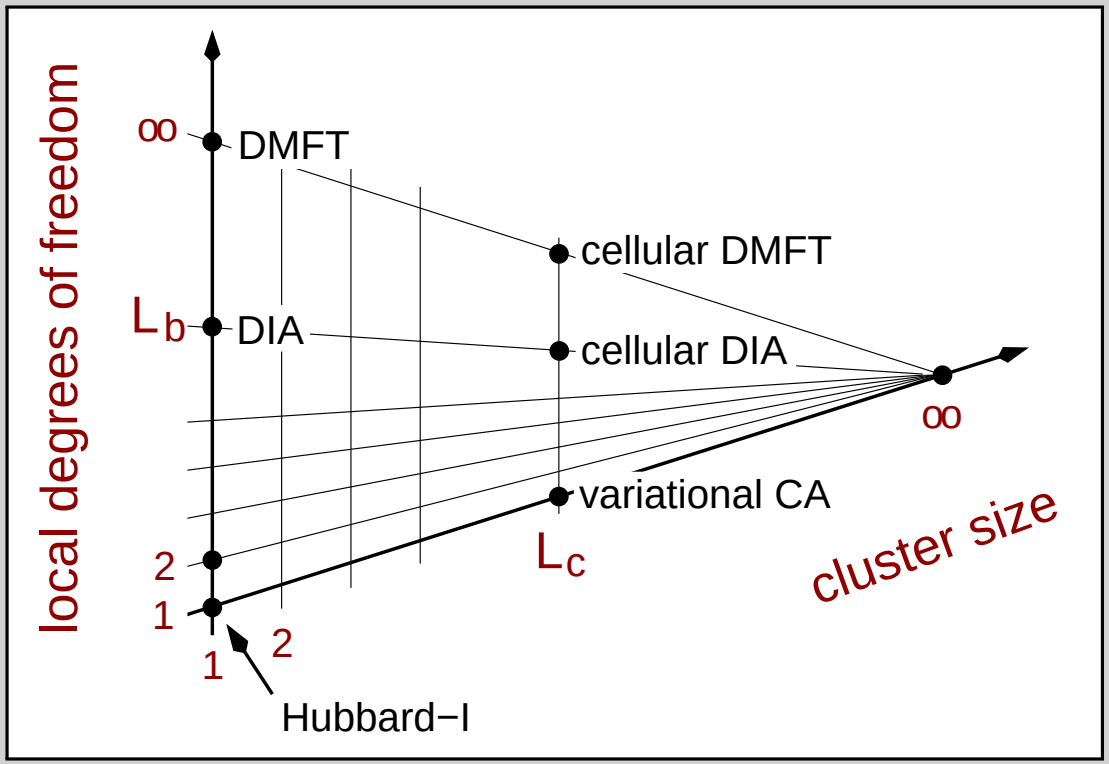
lattice model ($D = 2$) in
the thermodynamic limit

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

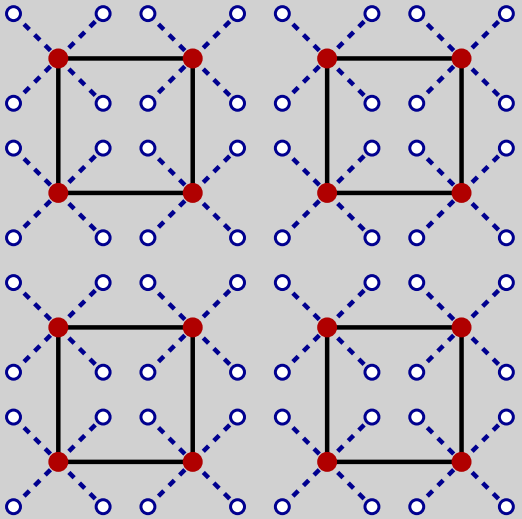


system of decoupled clusters
with additional bath sites
$L_c = 4$
variational cluster approach (VCA)

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:

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

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

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

stationarity condition:

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

first term:

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

second term:

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

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** :

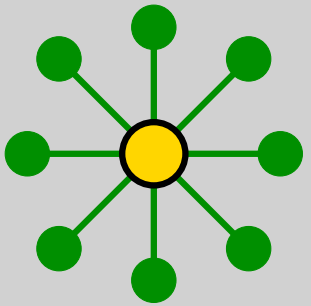
$$T \sum_n \sum_{\alpha\beta} \left(\frac{1}{\mathbf{G}^{-1}_{\mathbf{t},0}(i\omega_n) - \mathbf{\Sigma}_{\mathbf{t}',\mathbf{U}}(i\omega_n)} - \mathbf{G}_{\mathbf{t}',\mathbf{U}}(i\omega_n) \right)_{\beta\alpha} \frac{\partial \Sigma_{\mathbf{t}',\mathbf{U},\alpha\beta}(i\omega_n)}{\partial \mathbf{t}'}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

- 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):

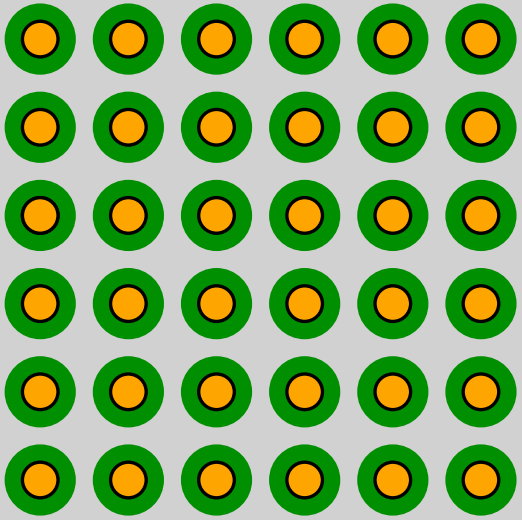
$$H_{\rm SIAM} = \sum_\sigma \varepsilon_{\rm imp} c^\dagger_\sigma c_\sigma + U n_\uparrow n_\downarrow + \sum_{k\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \sum_{k\sigma} V_k (c^\dagger_\sigma a_{k\sigma} + \text{H.c.})$$



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

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

➜ 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:

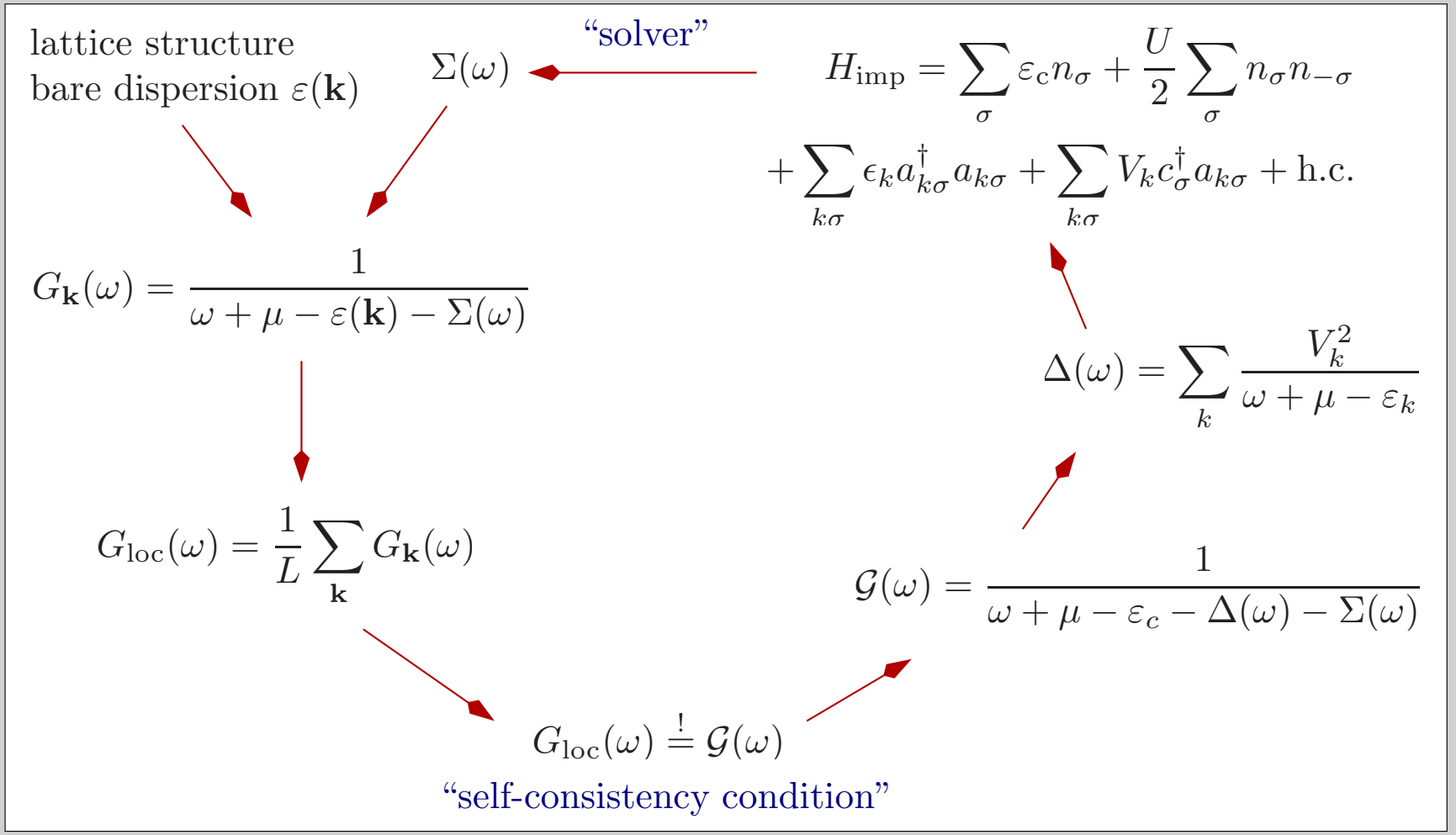
$$\left(\frac{1}{\mathbf{G}_0^{-1}(\omega)-\mathbf{\Sigma}(\omega)}\right)_{ii\sigma}=\mathbf{G}'_{ii\sigma}(\omega)$$

or:

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

DMFT self-consistency equation

DMFT self-consistency



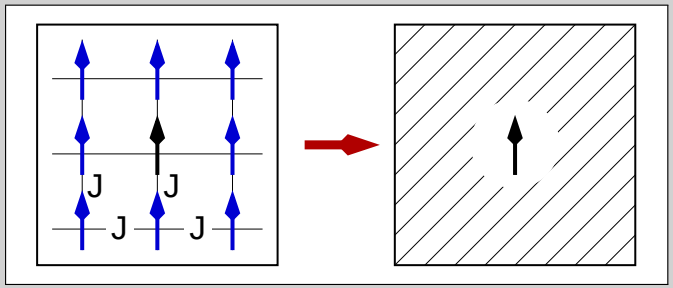
dynamical mean-field theory and $D = \infty$

Weiß molecular-field theory

magnetic phase transition

lattice spin model

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



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

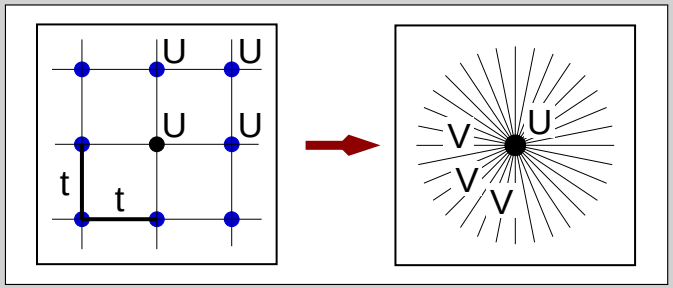
$$J \propto 1/D$$

dynamical mean-field theory

Mott transition

lattice fermion model

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



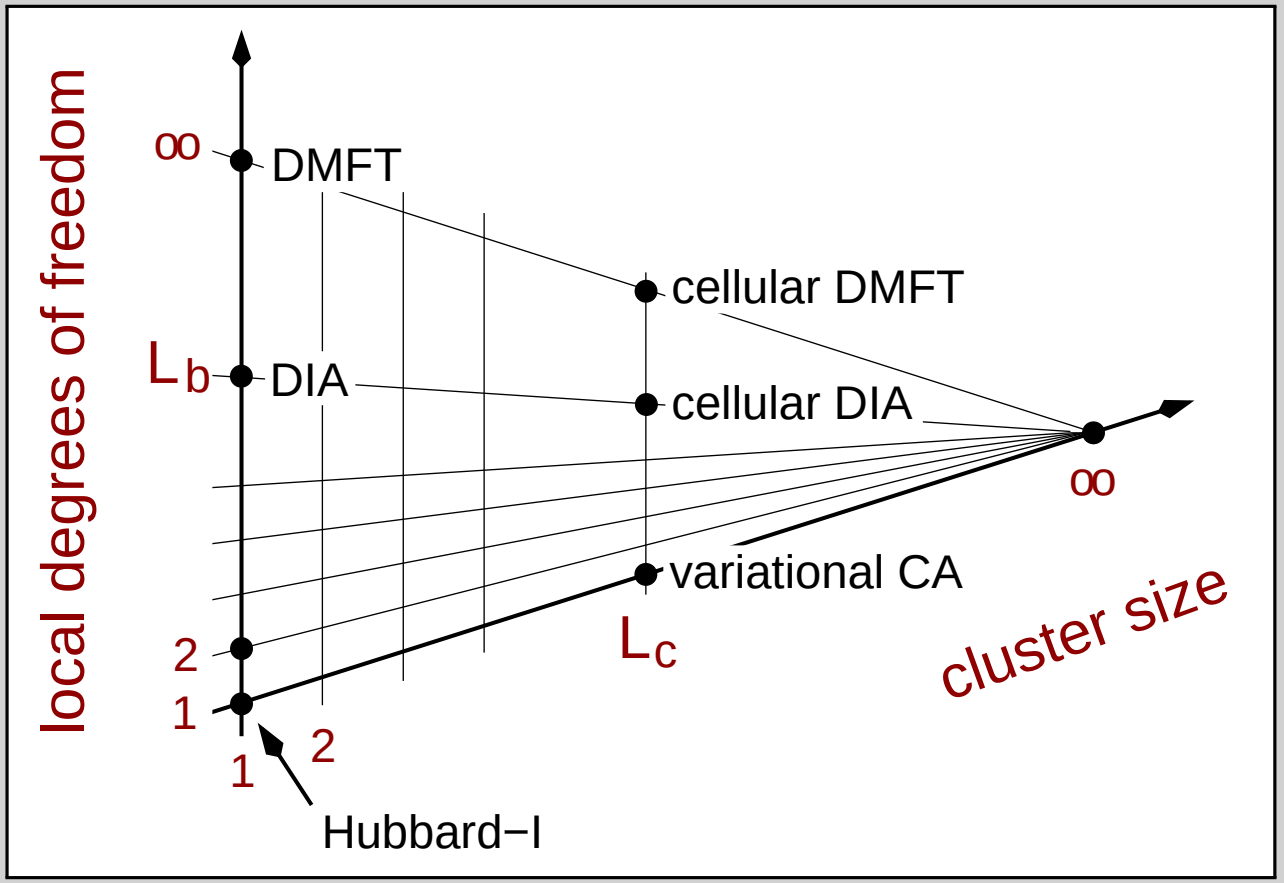
$$H_{\rm imp} = \sum_\sigma t_0 n_\sigma + \frac{U}{2} \sum_\sigma n_\sigma n_{-\sigma}$$
$$+ \sum_{k\sigma} \varepsilon_k n^{(a)}_{k\sigma} + \sum_{k\sigma} V_k c^\dagger_\sigma a_{k\sigma} + \text{h.c.}$$

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

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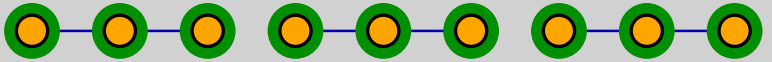
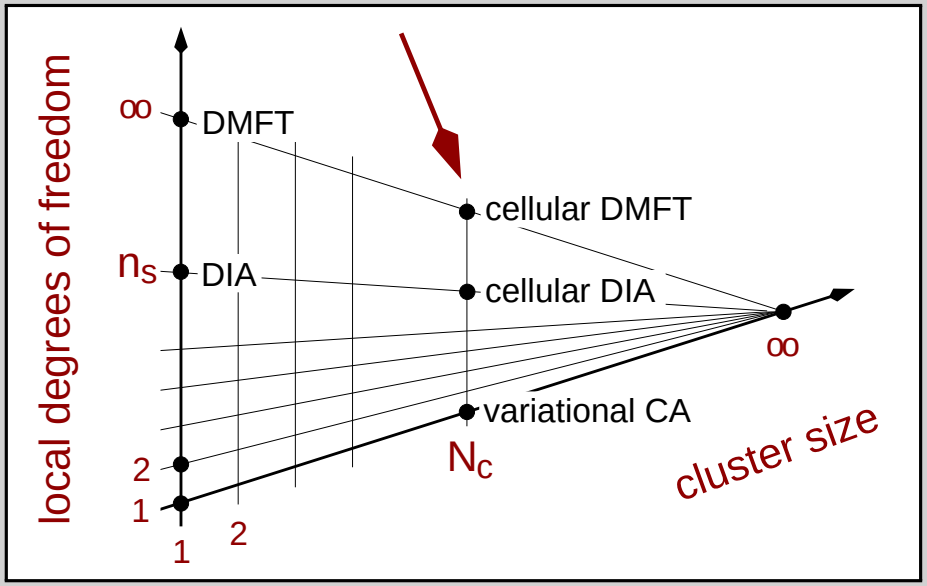
original system, $H_{\mathbf{t},\mathbf{U}}$:

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





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Okamoto, Millis, Monien, Fuhrmann (2003)

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

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

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

➜ open boundary conditions (see above)

there is no reference system which generates the DCA !

cluster extensions of DMFT

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Kotliar, Savrasov, Palsson, Biroli (2001)

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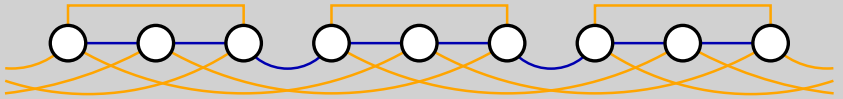
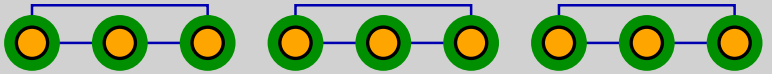
original system, $H_{\mathbf{t},\mathbf{U}}$:



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



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

DCA self-consistency condition

$\bar{\mathbf{t}}$: 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)
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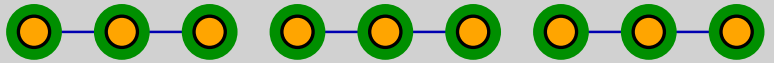
periodized C-DMFT (P-C-DMFT)
Biroli, Parcollet, Kotliar (2003)

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

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

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



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

P-C-DMFT self-consistency condition

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

cluster extensions of DMFT

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

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

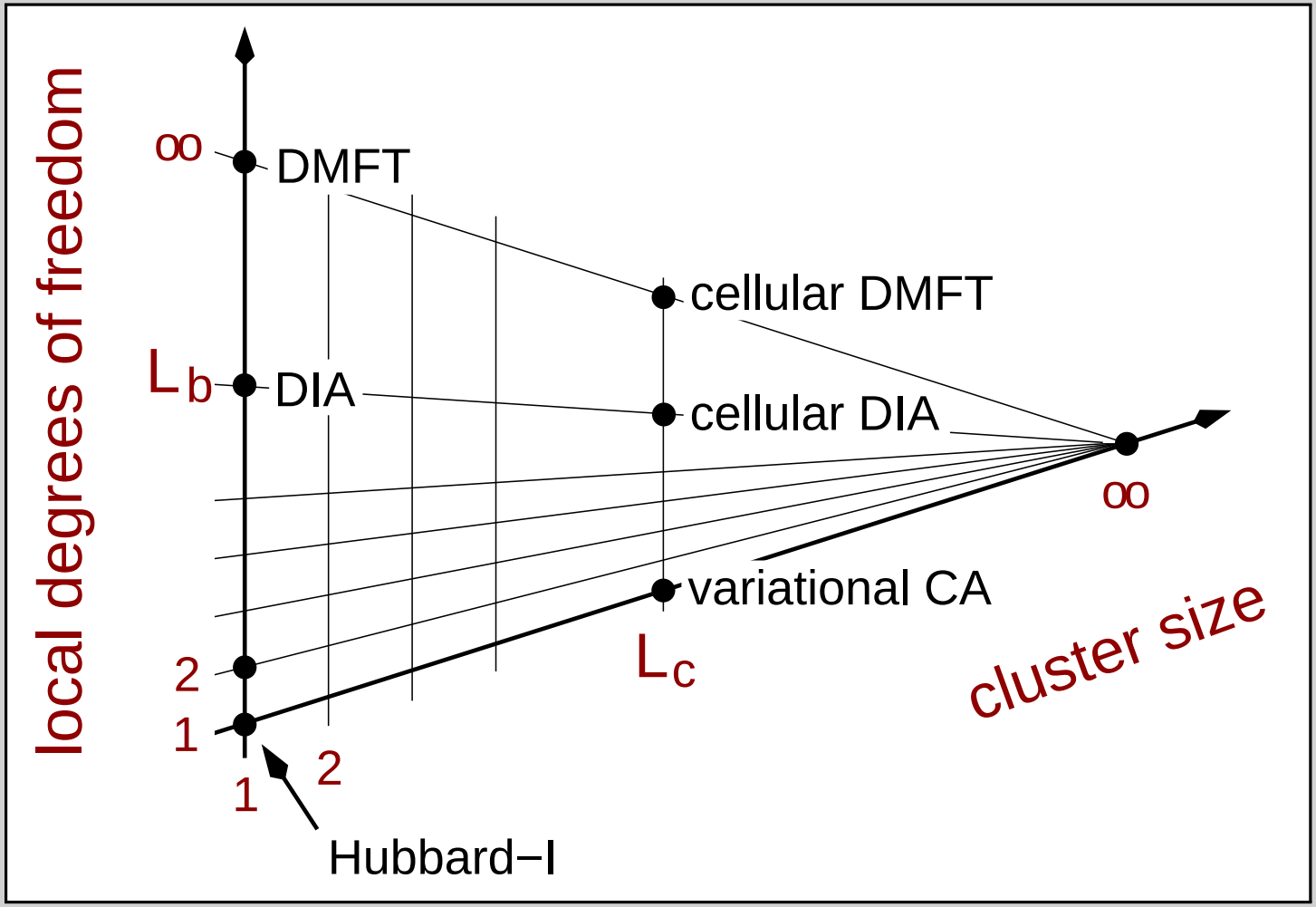
periodized C-DMFT (P-C-DMFT)
Biroli, Parcollet, Kotliar (2003)

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

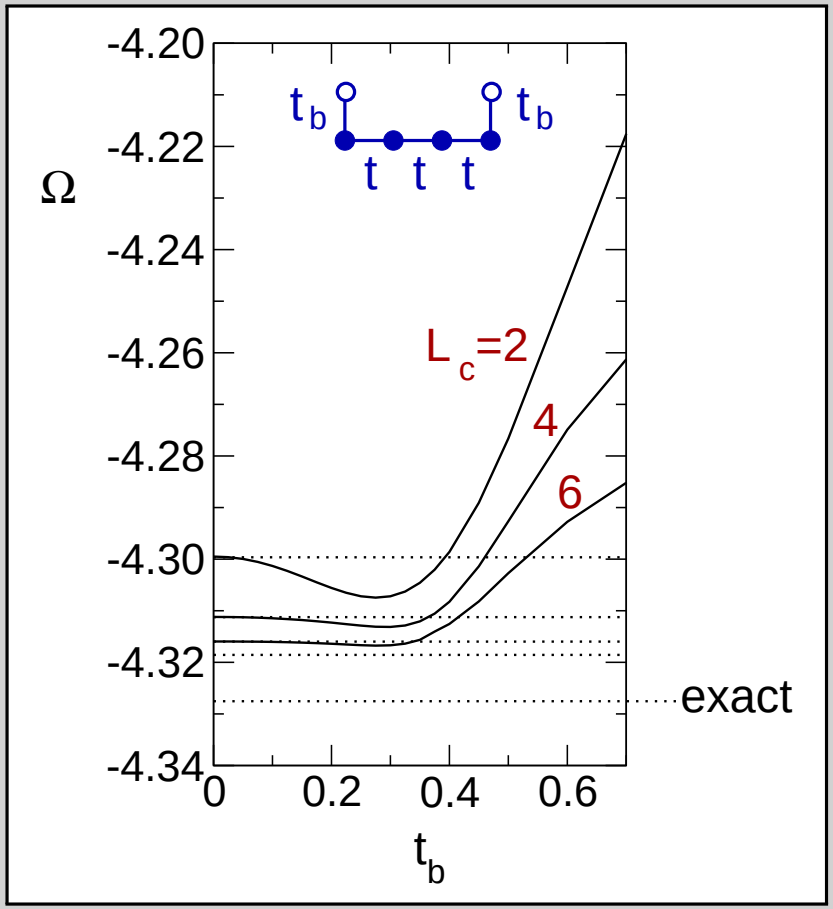
original system, $H_{\mathbf{t},\mathbf{U}}$:

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

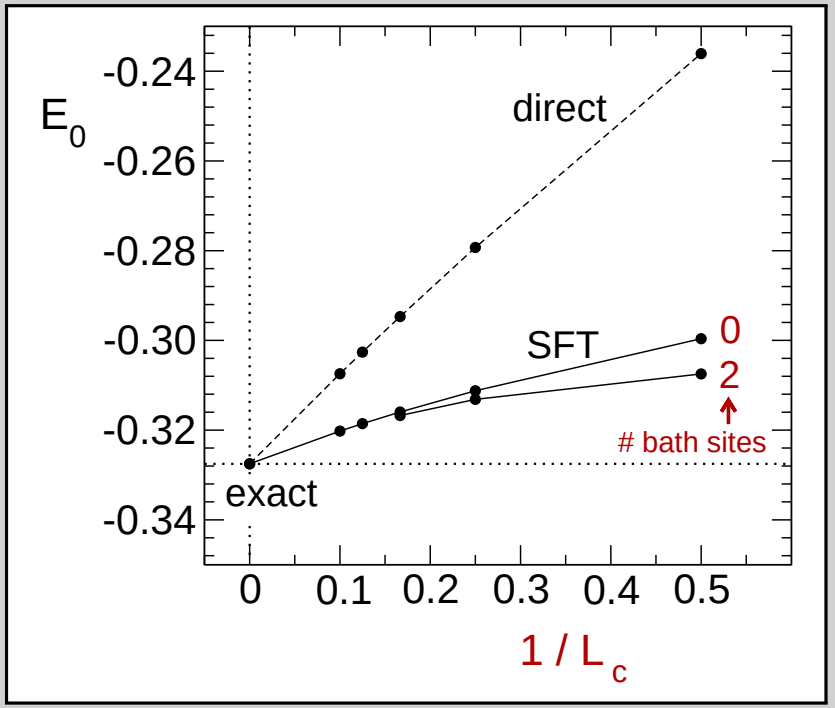
more bath sites vs. larger clusters



$D = 1$: bath sites ?



exact: *Lieb, Wu (1968)*



➜ larger cluster vs. more bath sites

➜ enhanced convergence

DMFT as Type-I,II,III Approximation

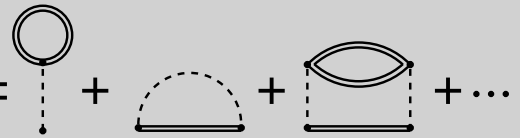
dynamical mean-field theory

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 $\Sigma_U[G] =$ 

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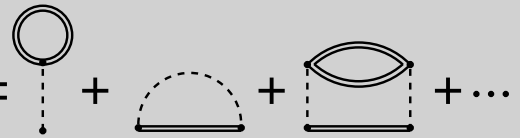
skeleton expansion $\Sigma_U[G] =$  $+ \cdots$

DMFT as type-I approximation:

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

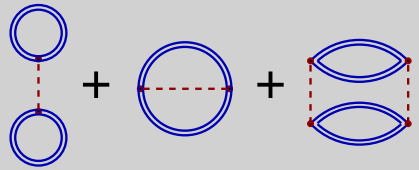
with $\widetilde{\mathbf{\Sigma}}_{\mathbf{U}}[\mathbf{G}]$: functional of an impurity model (vertices restricted to a single-site)

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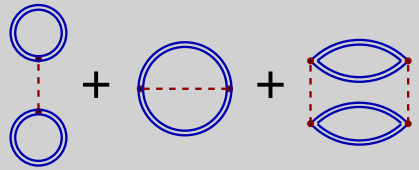
Luttinger-Ward functional: $\Phi =$  $+ \cdots,$ $\quad \frac{1}{T}\frac{\delta \Phi_{\mathbf{U}}[\mathbf{G}]}{\delta \mathbf{G}} = \mathbf{\Sigma}_{\mathbf{U}}[\mathbf{G}]$

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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:

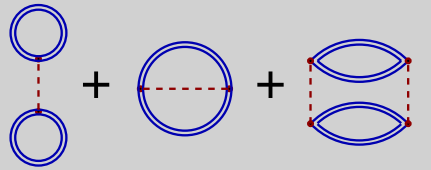
$\Phi_{\mathrm{U}}[\mathbf{G}] \to \widetilde{\Phi}_{\mathrm{U}}[\mathbf{G}]$

(certain diagram classes)

➜ **type-II**

Baym, Kadanoff (1961)

dynamical variational principles

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

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Luttinger, Ward (1960)

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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(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

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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 !

dynamical variational principles

problem:

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

alternative functional:

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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)

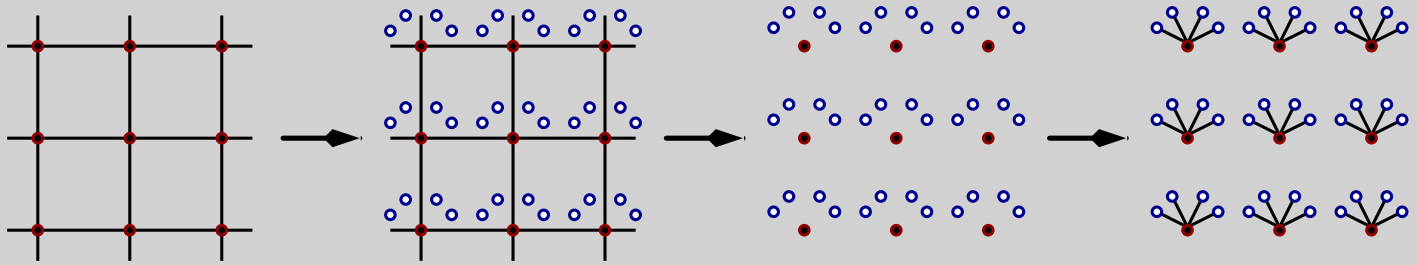
DMFT as type-II approximation

Georges (2004)

self-energy-functional approach

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

original system **reference system**



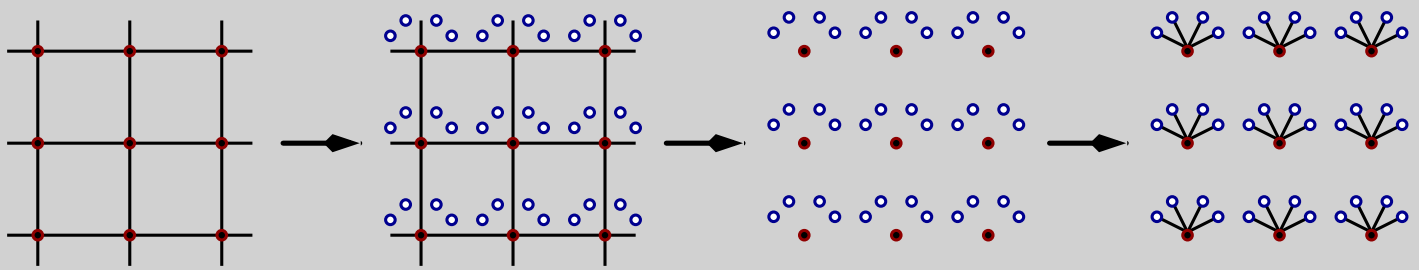
➜ Σ is local

➜ 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 ✔

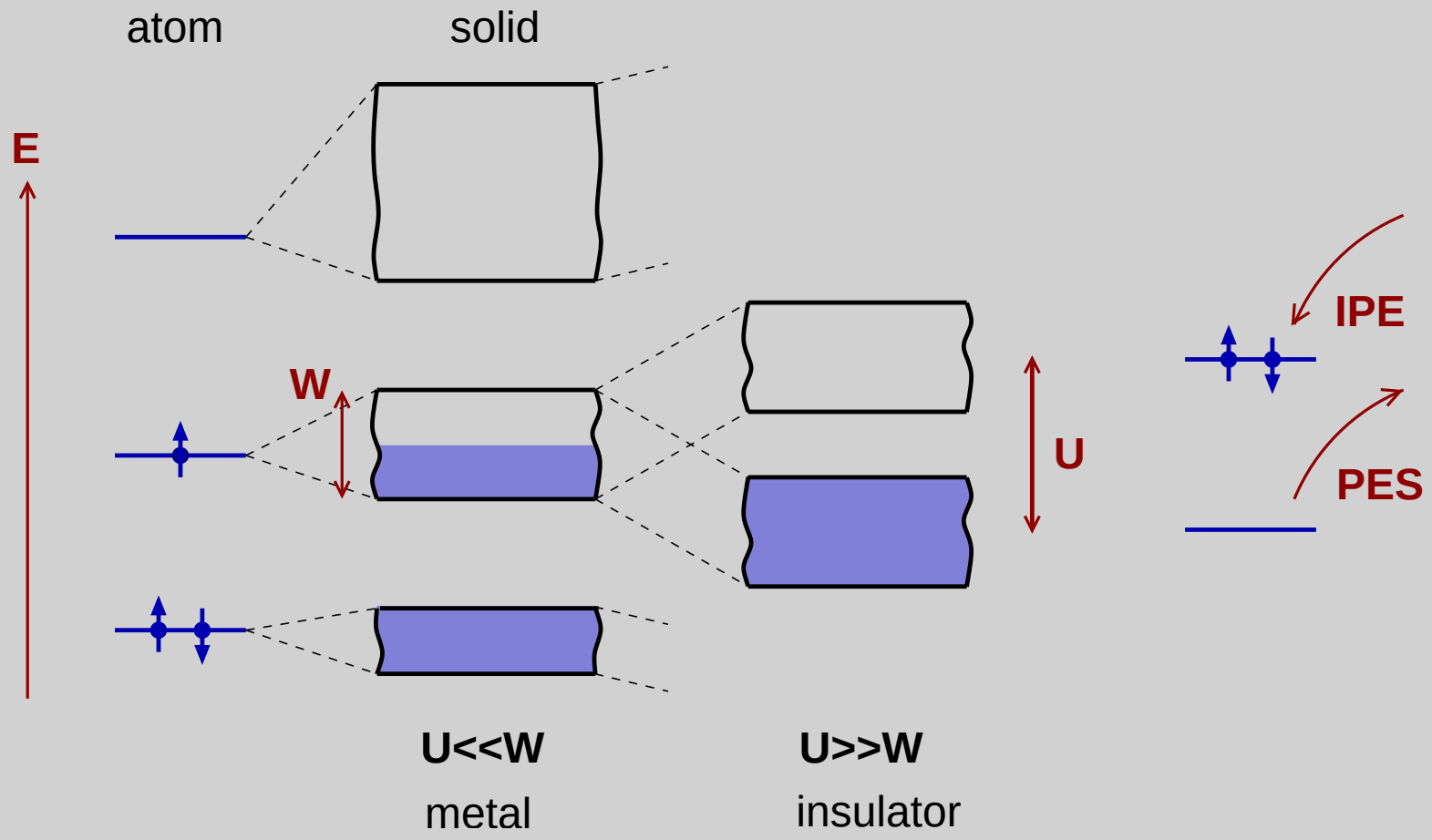
➜ Euler equation on $\widetilde{\mathcal{A}}$: $\dfrac{\partial}{\partial \mathbf{t}^{\imath}}\Omega_{\mathbf{t},\mathbf{U}}[\boldsymbol{\Sigma}_{\mathbf{t}^{\imath},\mathbf{U}}] = 0 \;\Leftrightarrow$ DMFT self-consistency equation ✔

➜ DMFT as type-III approximation

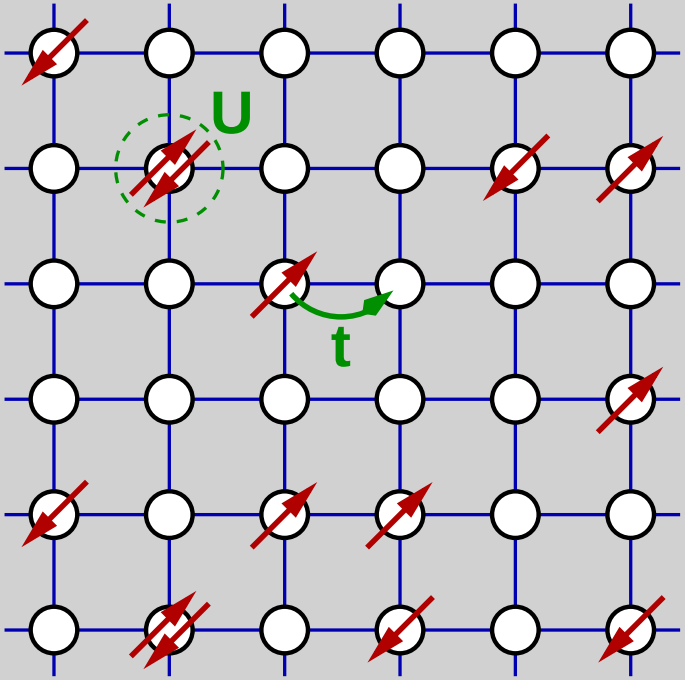
VI Dynamical Theory of the Mott Transition

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

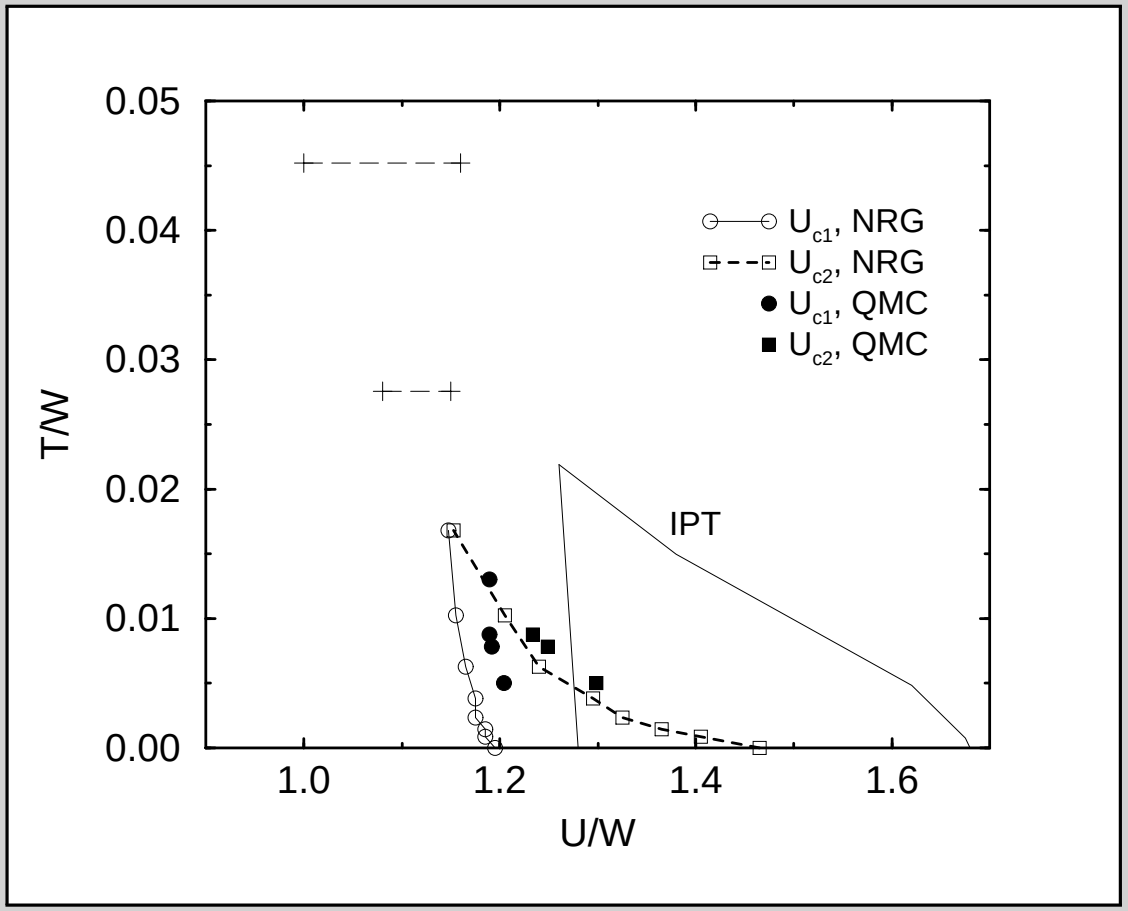
— n.n. hopping: t

— local interaction: U

— electron density : $n = N/L$

— temperature T

DMFT phase diagram



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

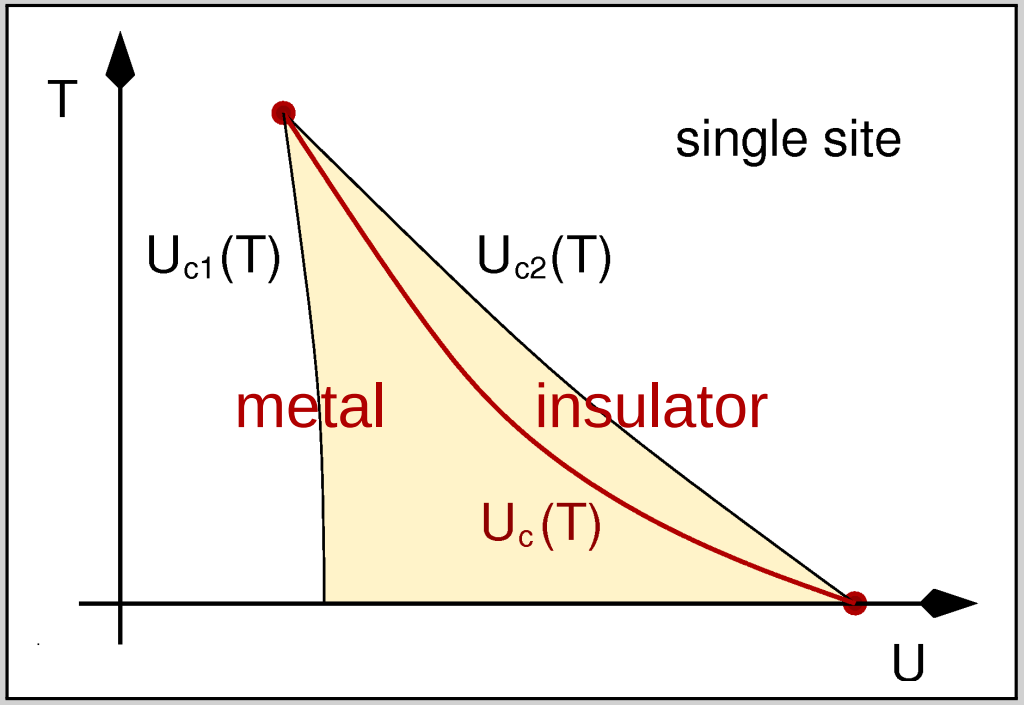
NRG
Bulla, Costi, Vollhardt (2001)

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**

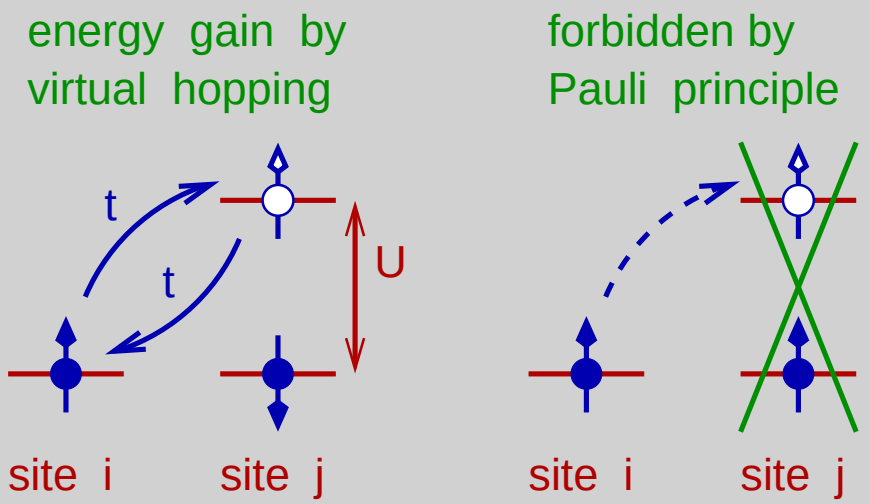
$T > 0$: **discontinuous transition**

$T > T_C$: **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 $J \sim -\dfrac{t^2}{U}$

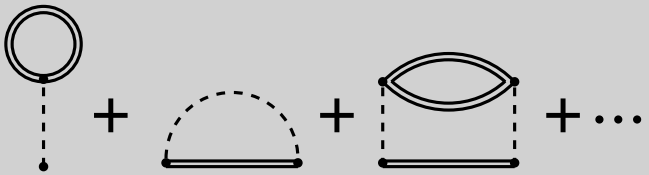
➜ long-range AF order (also for $D = \infty$, within DMFT)

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:

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

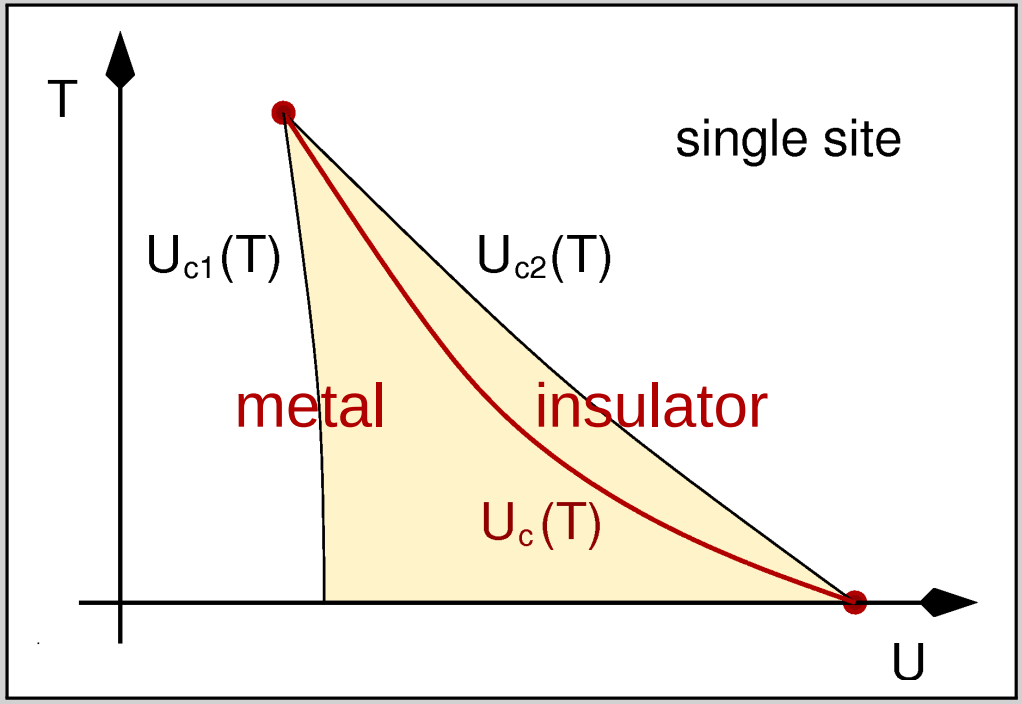
➜ no feedback of nonlocal magnetic correlations on $\mathbf{\Sigma}$

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

➜ 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)

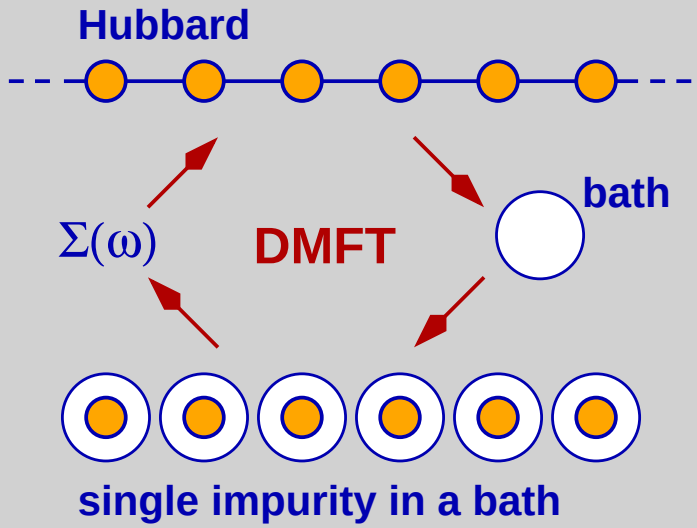
at finite T: $F_{\rm met} = E_{\rm met} - TS_{\rm met} > E_{\rm ins} - TS_{\rm ins} = F_{\rm ins}$

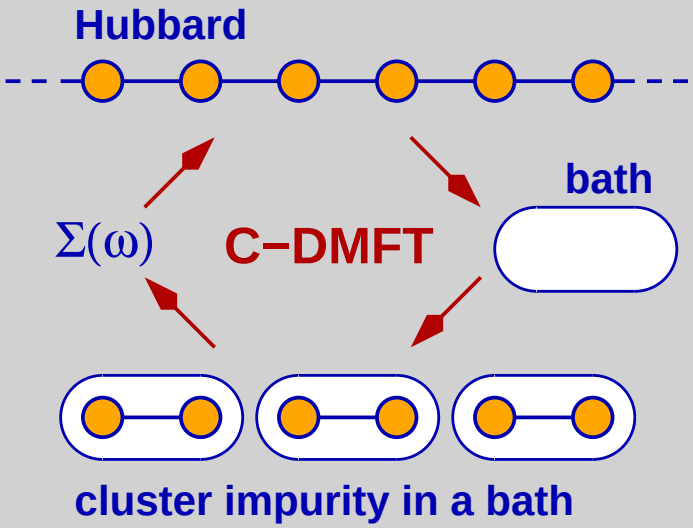
the insulator wins at higher temperatures

Q: mean-field artifact ?

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

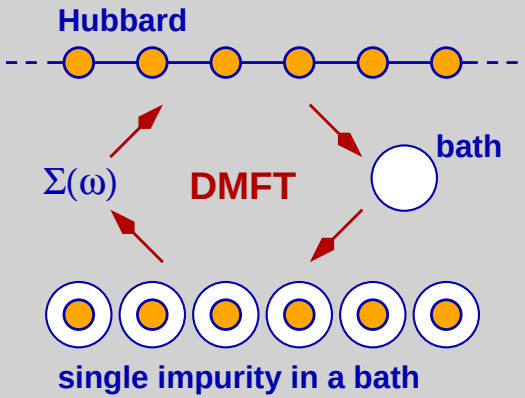
plaquette DMFT

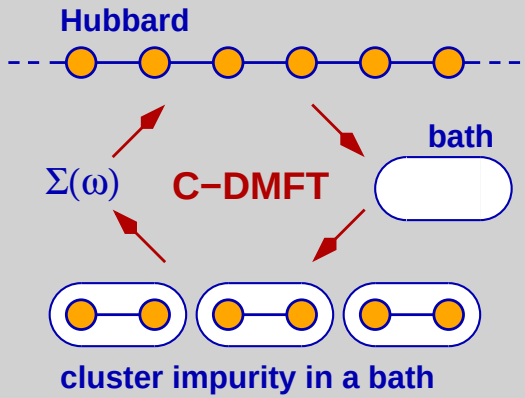




singlet formation ➜ $S(T=0)=0$

plaquette DMFT

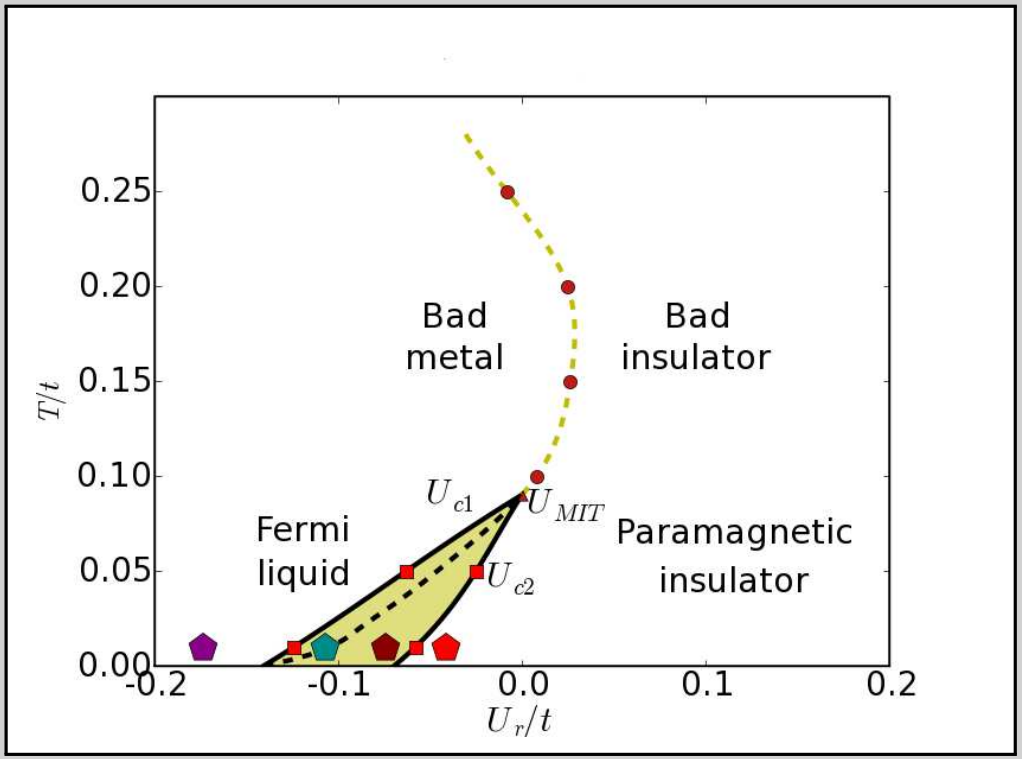




$D = 2$ square lattice:
$L_c = 4$ (plaquette)

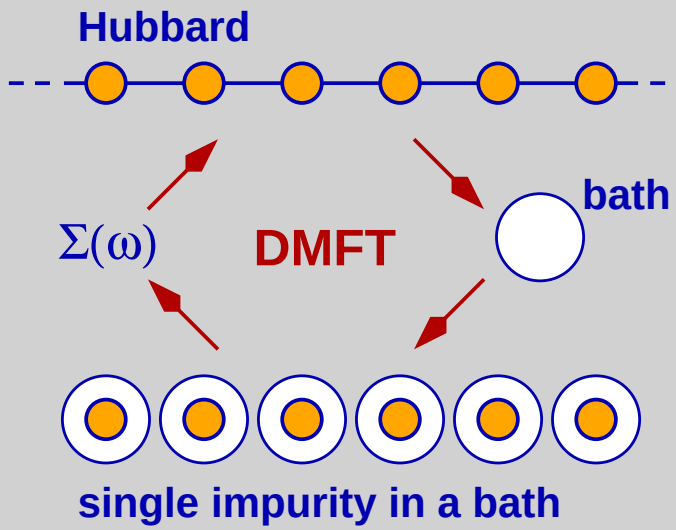
diagrammatic QMC, finite T

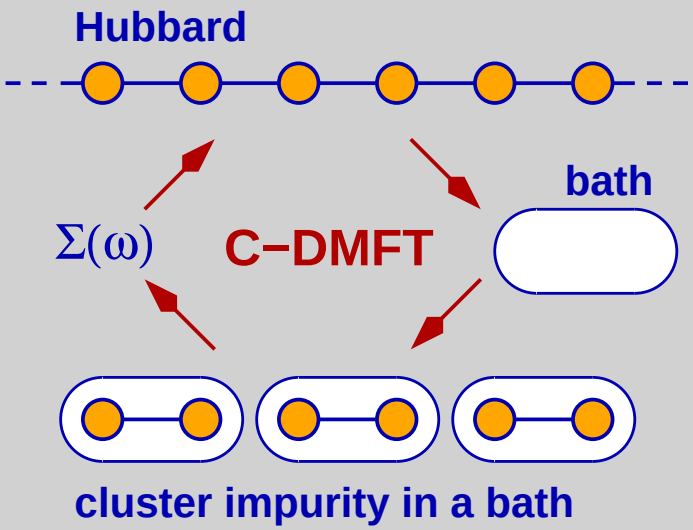
smaller U_c
coexistence (different shape)
$T > 0$: first-order transition



Park, Haule Kotliar (2008)

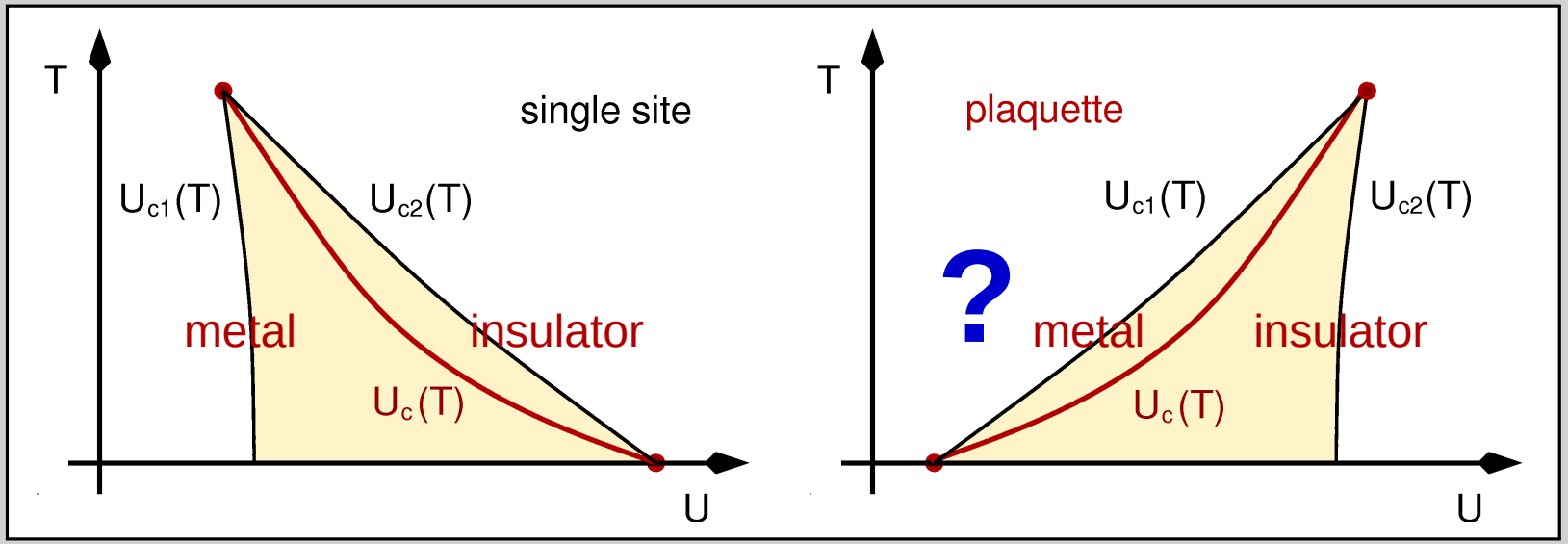
plaquette DMFT





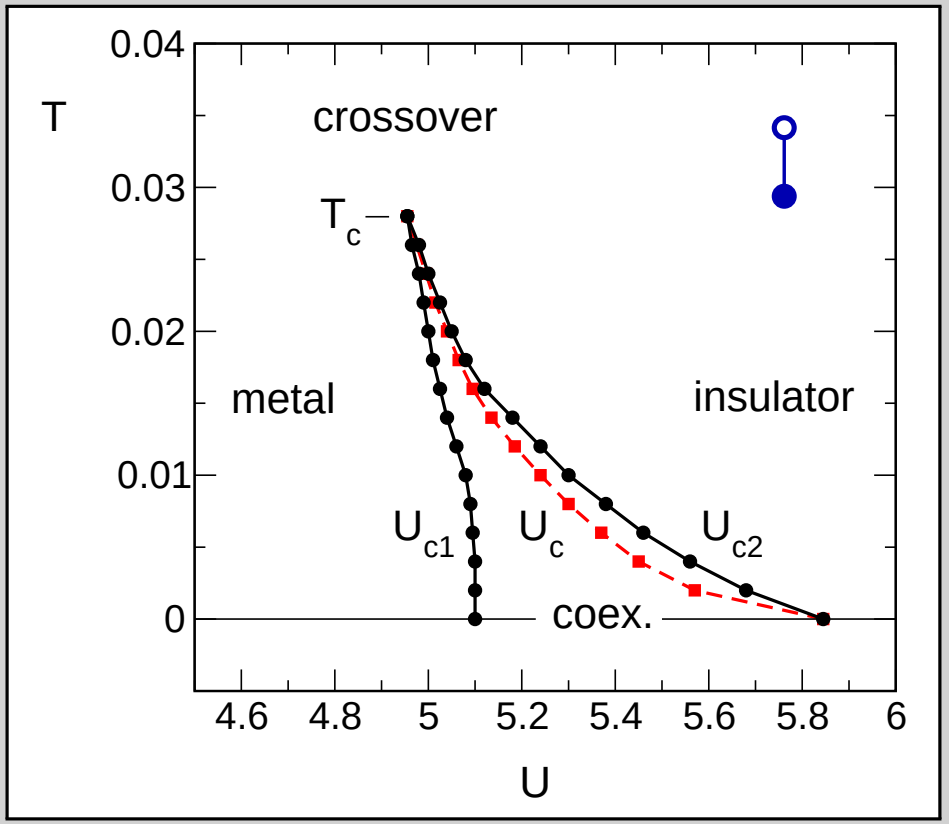
the insulator wins at higher temperatures

the metal wins at higher temperatures ?



Mott Transition within the DIA

dynamical impurity approximation (DIA)



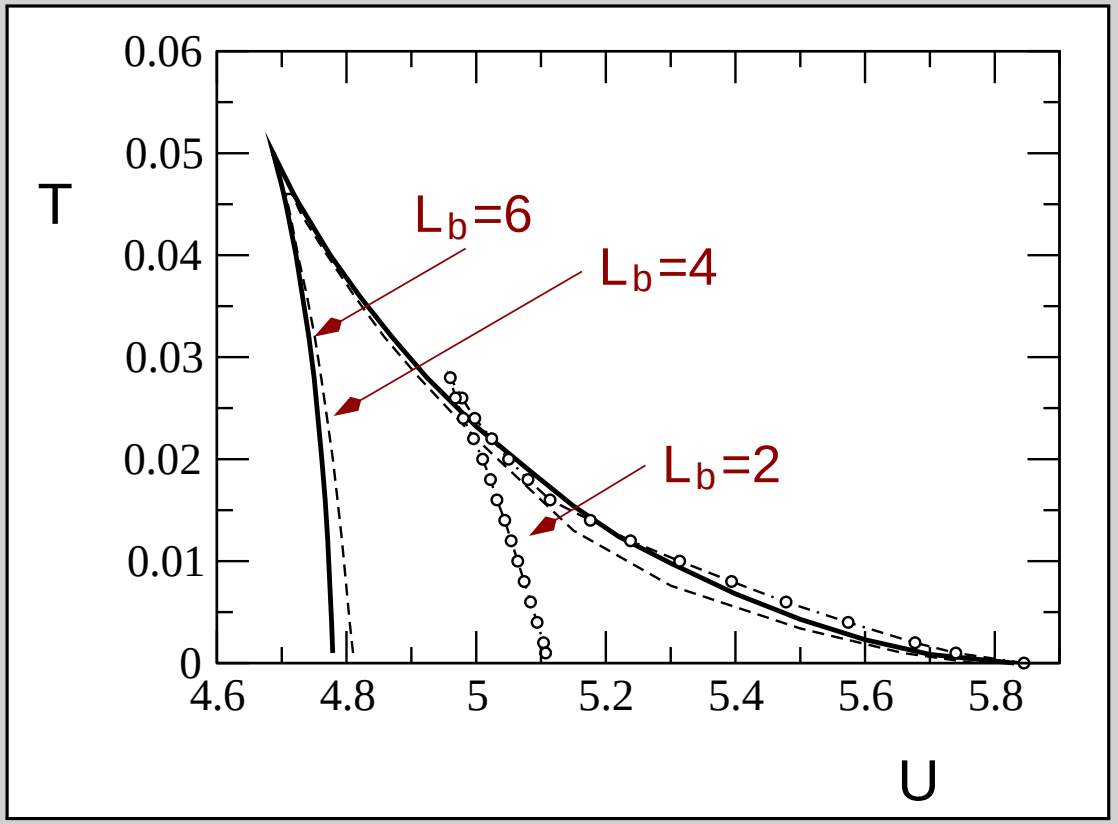
Hubbard model
half-filling
semi-elliptical DOS
$W = 4$

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 $n_s = 2$

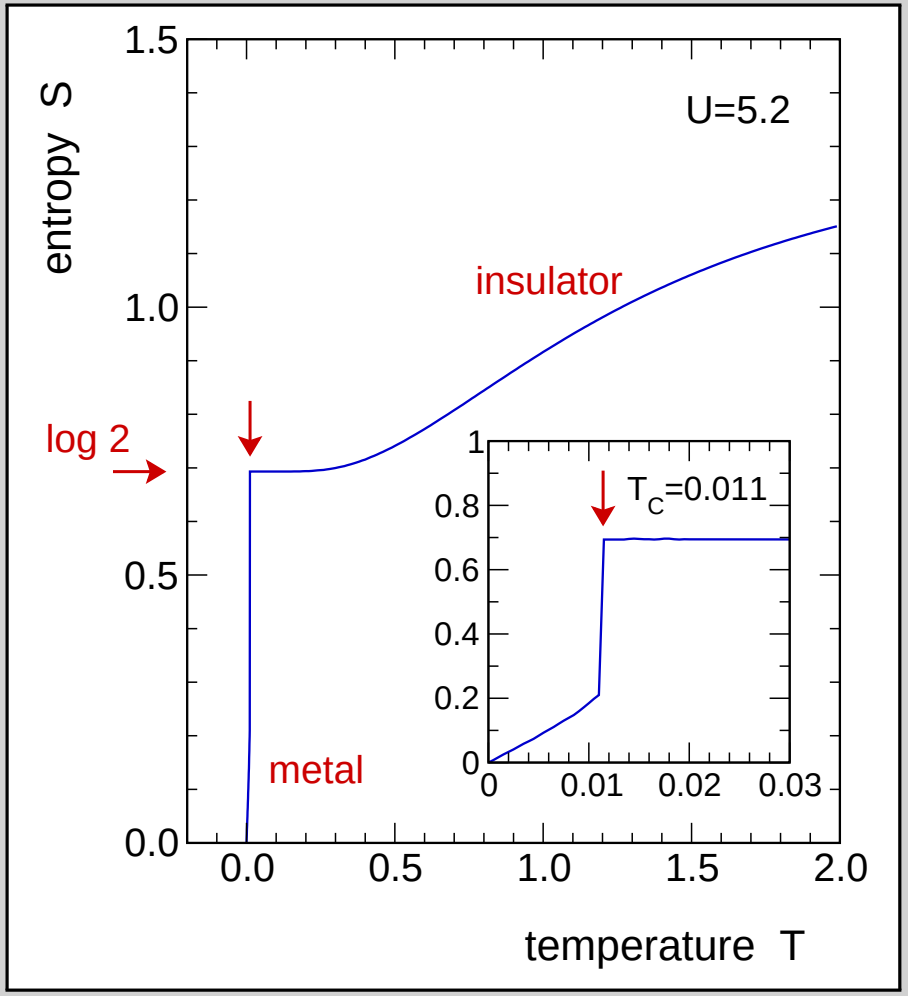
Pozgajcic 2004

➜ **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



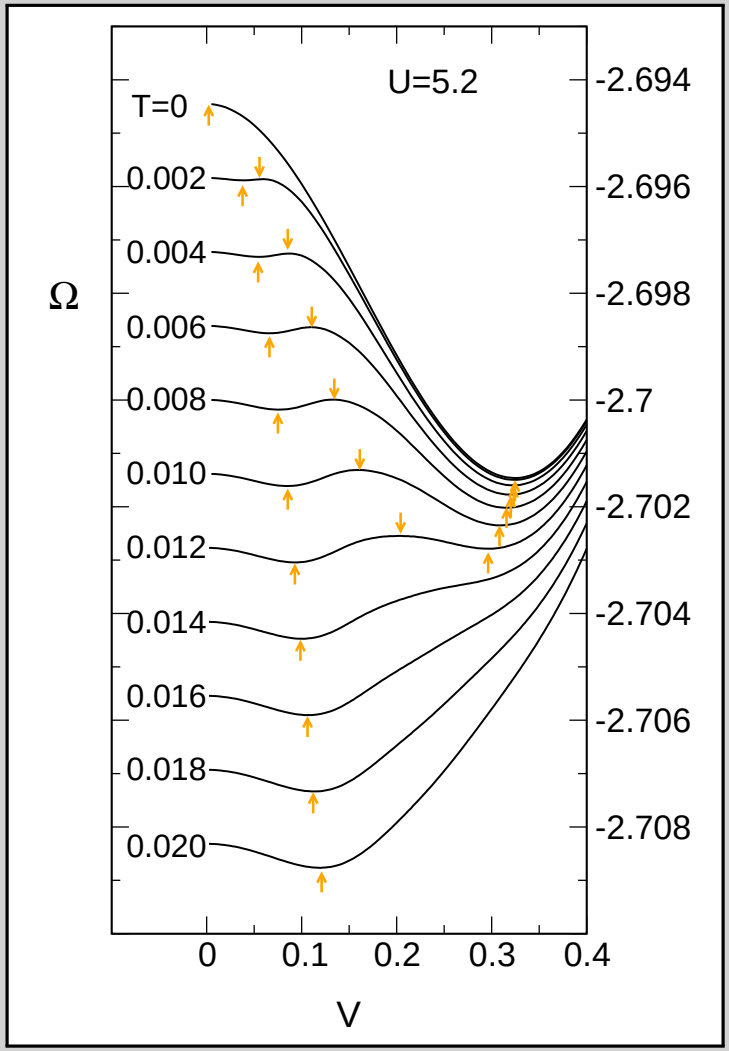
Hubbard model
half-filling
semi-elliptical DOS
$W = 4$

DIA with $n_s = 2$

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

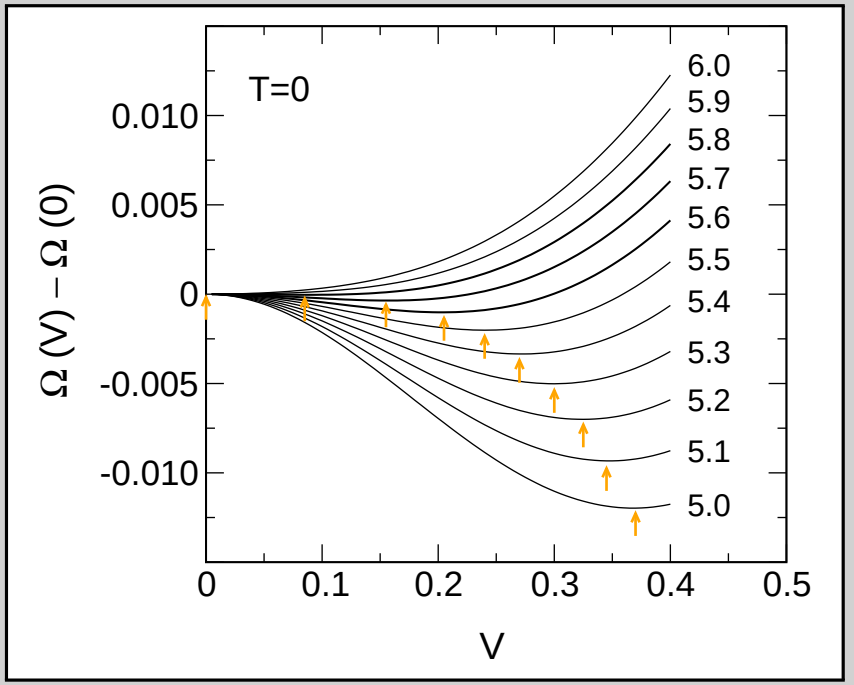
➜ **Fermi liquid: linear** $S(T) = \gamma T + \cdots$

DIA - phase transitions



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

$T = 0$, different U: continuous

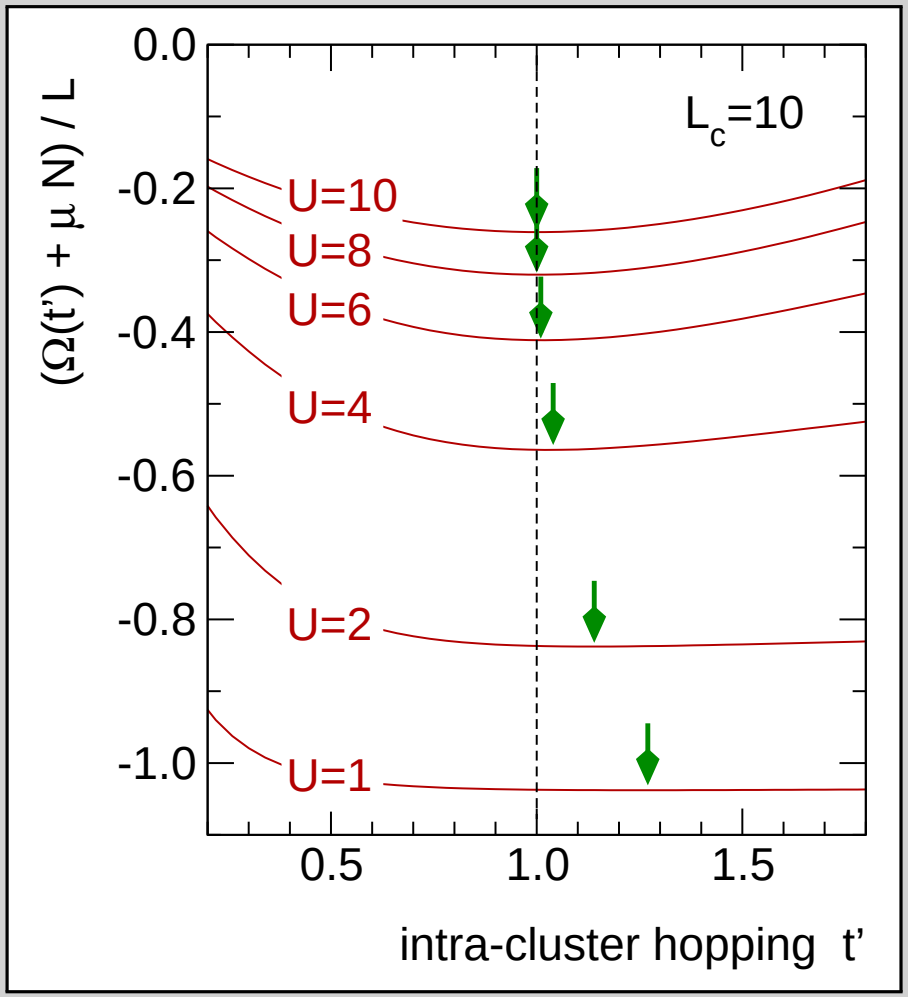


➜ **metastable states**

➜ **order of phase transitions**

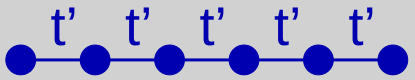
Mott Transition in $D = 1$

SFT grand potential



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

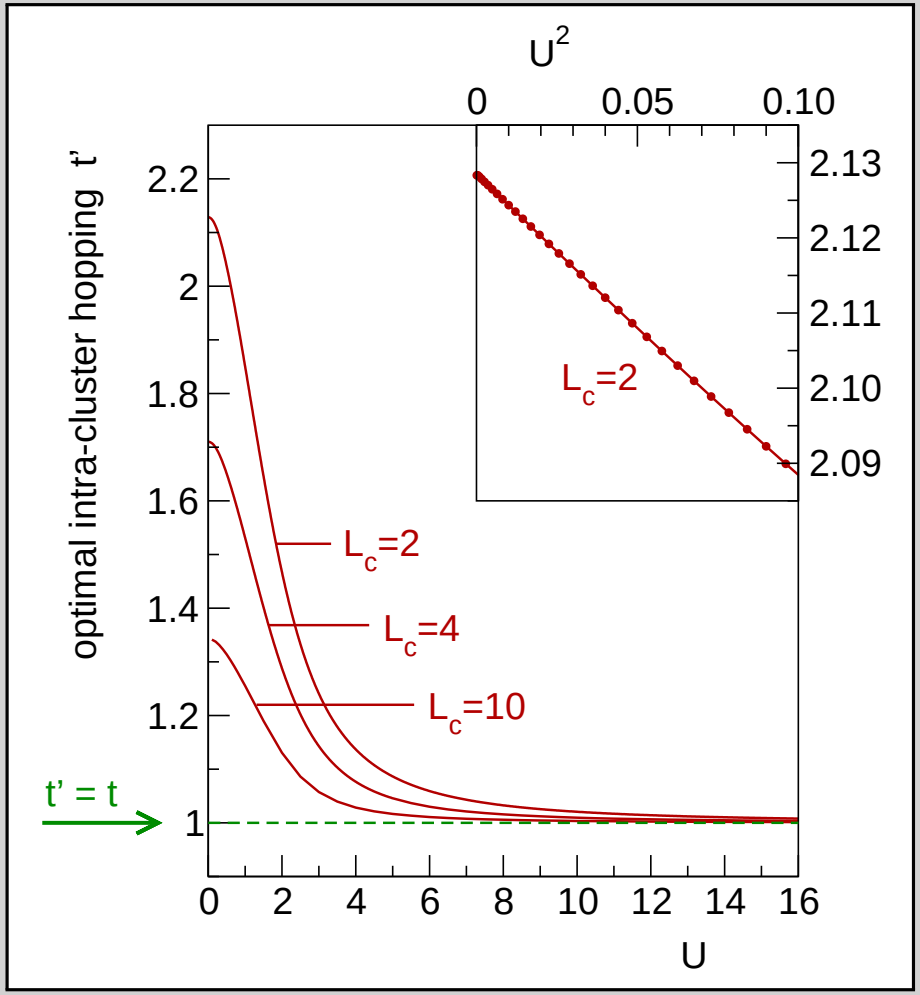
- single variational parameter:



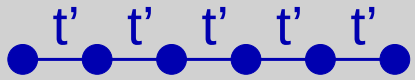
➜ **enhanced t' compensates for missing inter-cluster hopping**

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

VCA: optimal intra-cluster hopping

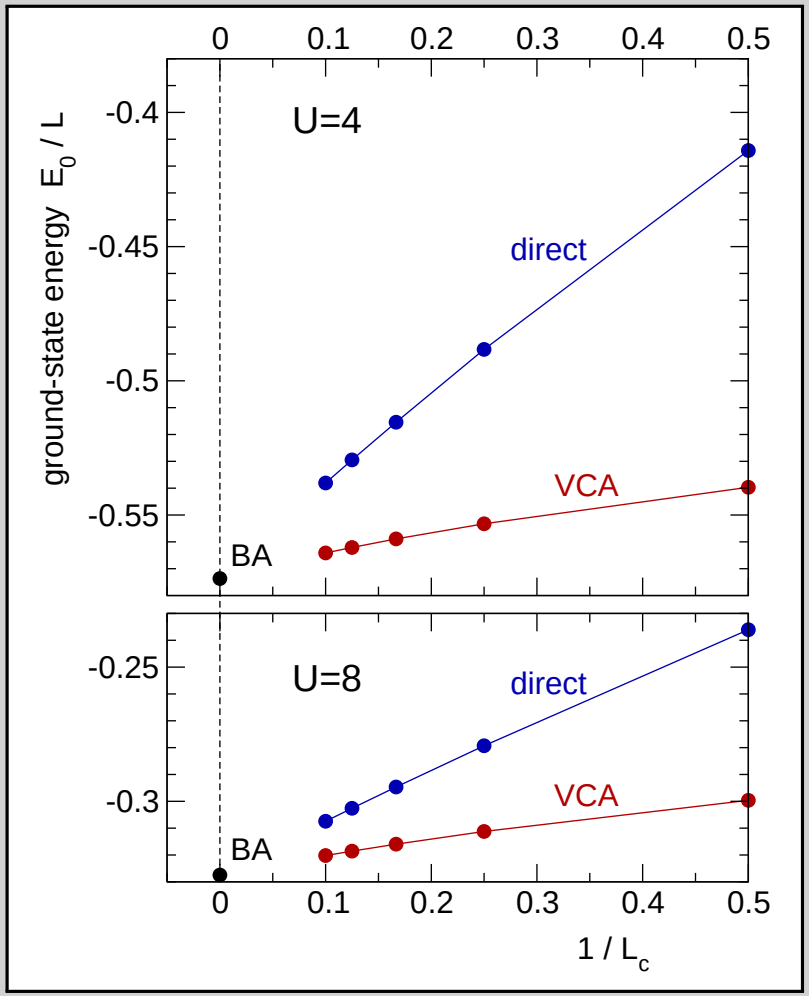


- $t = 1, \mu = U/2$
- $\Omega(t') \equiv \Omega[\mathbf{\Sigma}(t')]$

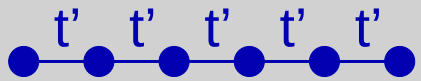


➜ **weak coupling: strong renormalization of t' vs. small self-energy**

finite-size scaling



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



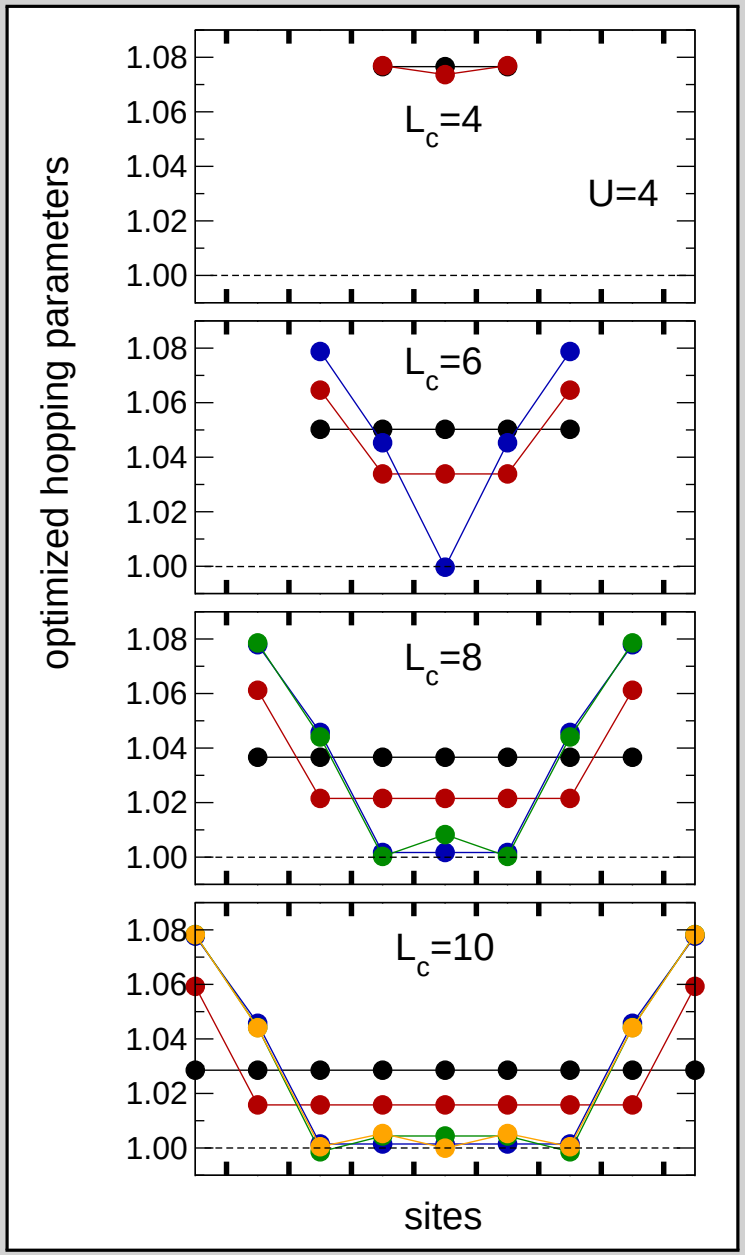
➜ **VCA: faster convergence**

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

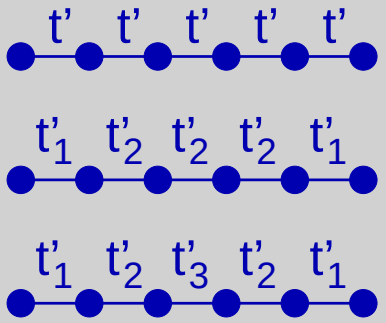
VCA: recipe for practical calculations

- 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%**

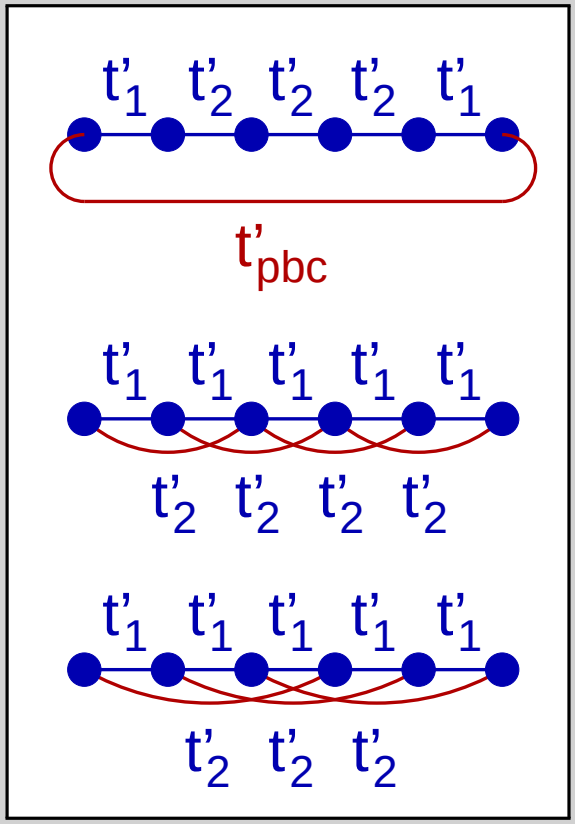
➜ **significant effects at chain edges**

➜ **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)

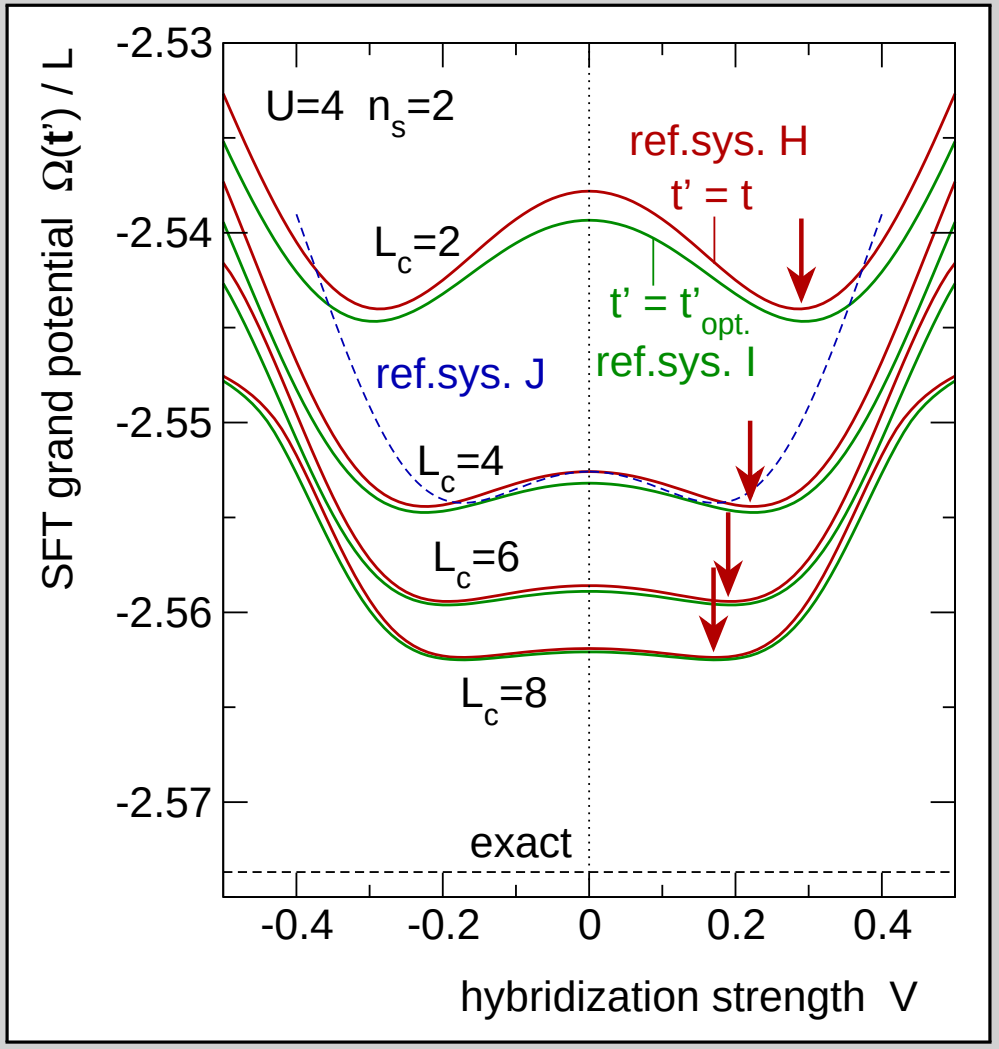
third-neareast-neighbor hopping

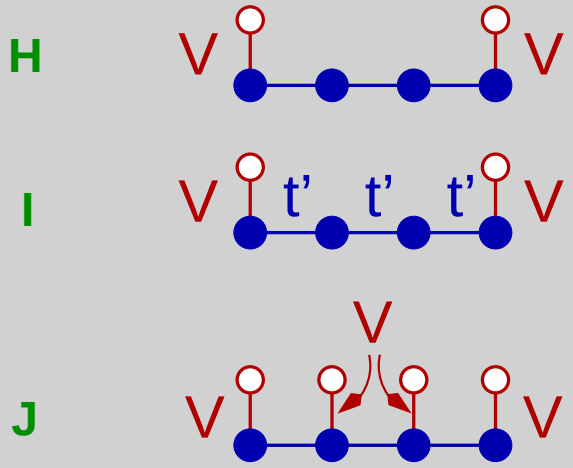
➜ **hopping parameters not present in original system: almost vanishing**

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

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

bath sites



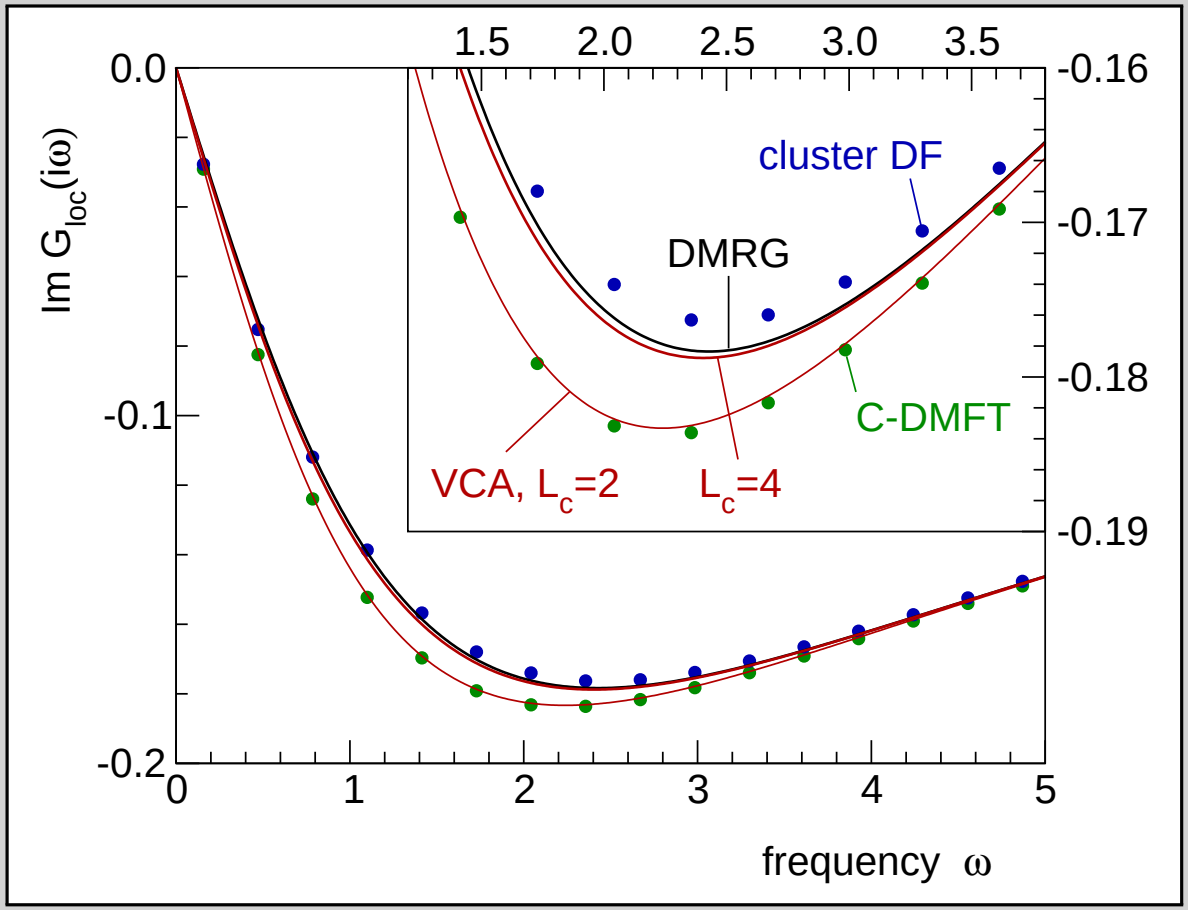


➜ **I vs. H: optimization of bath sites more effective than hopping**

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

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

local Matsubara Green's function



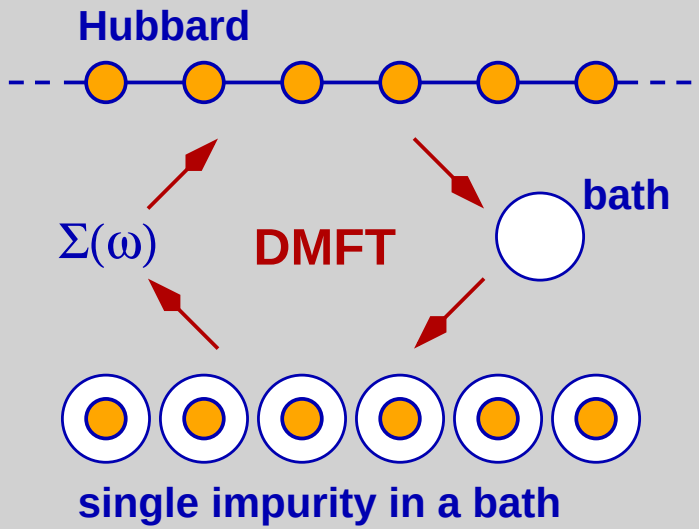
- $t = 1$, $\mu = U/2$, $U = 6$
- VCA with $n_s = 3$
- C-DMFT with $n_s = \infty$ ($\beta = 20$)
- cluster DF for $L_c = 2$ ($\beta = 20$)
- (dynamical) DMRG: numerically exact

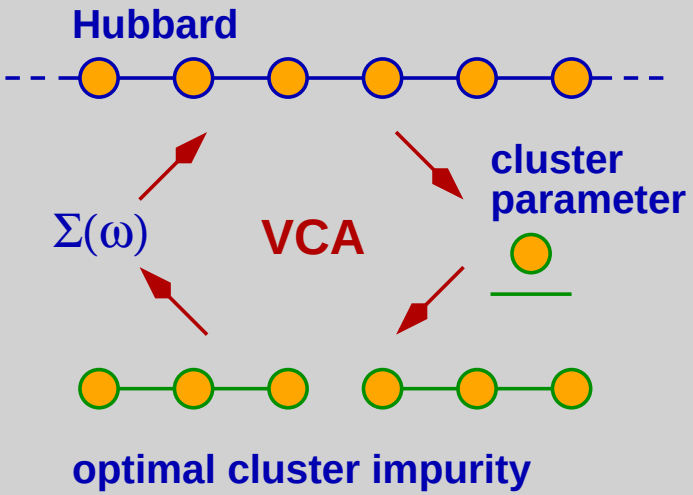
➜ **VCA comparable to C-DMFT**

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

Mott Transition in $D = 2$

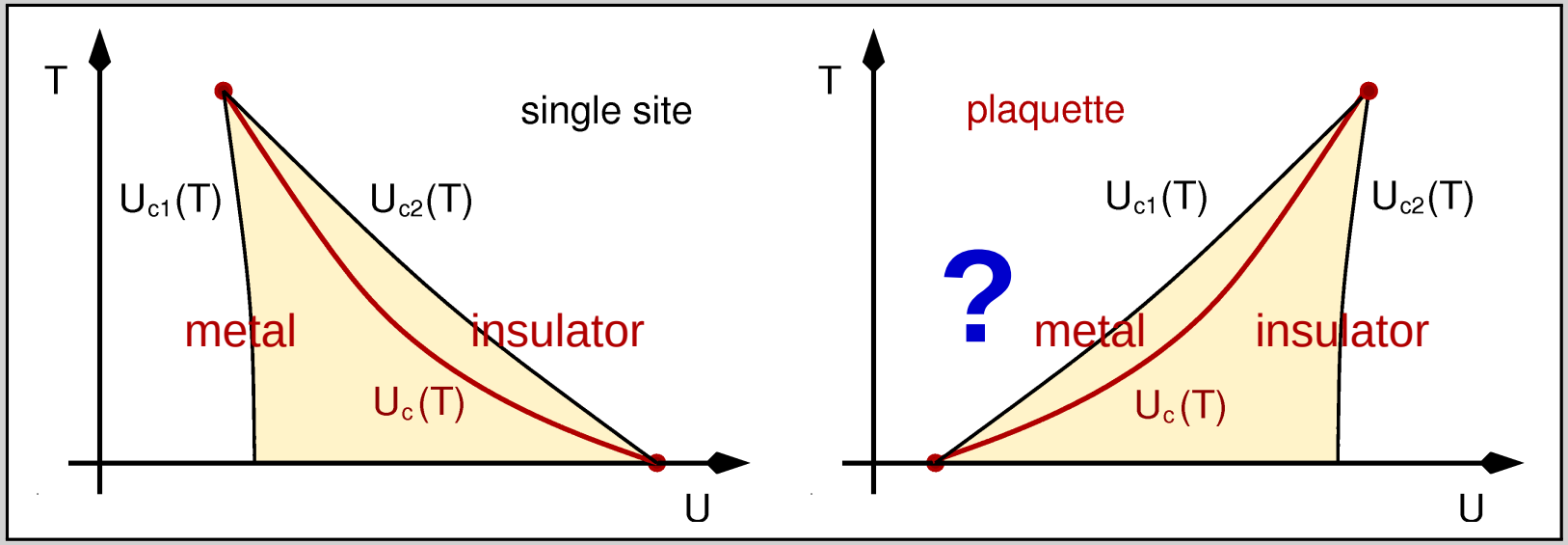
plaquette VCA





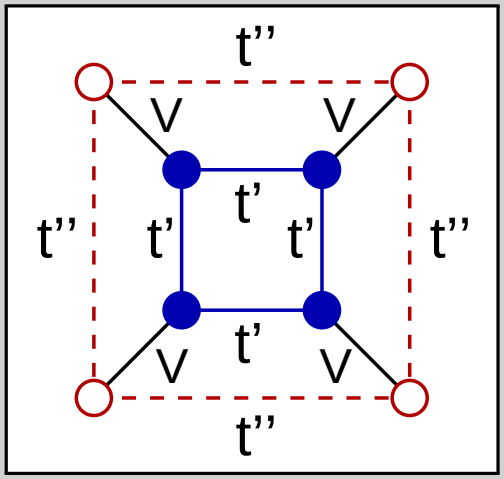
the insulator wins at higher temperatures

the metal wins at higher temperatures ?



parameter optimization

reference system
for plaquette VCA

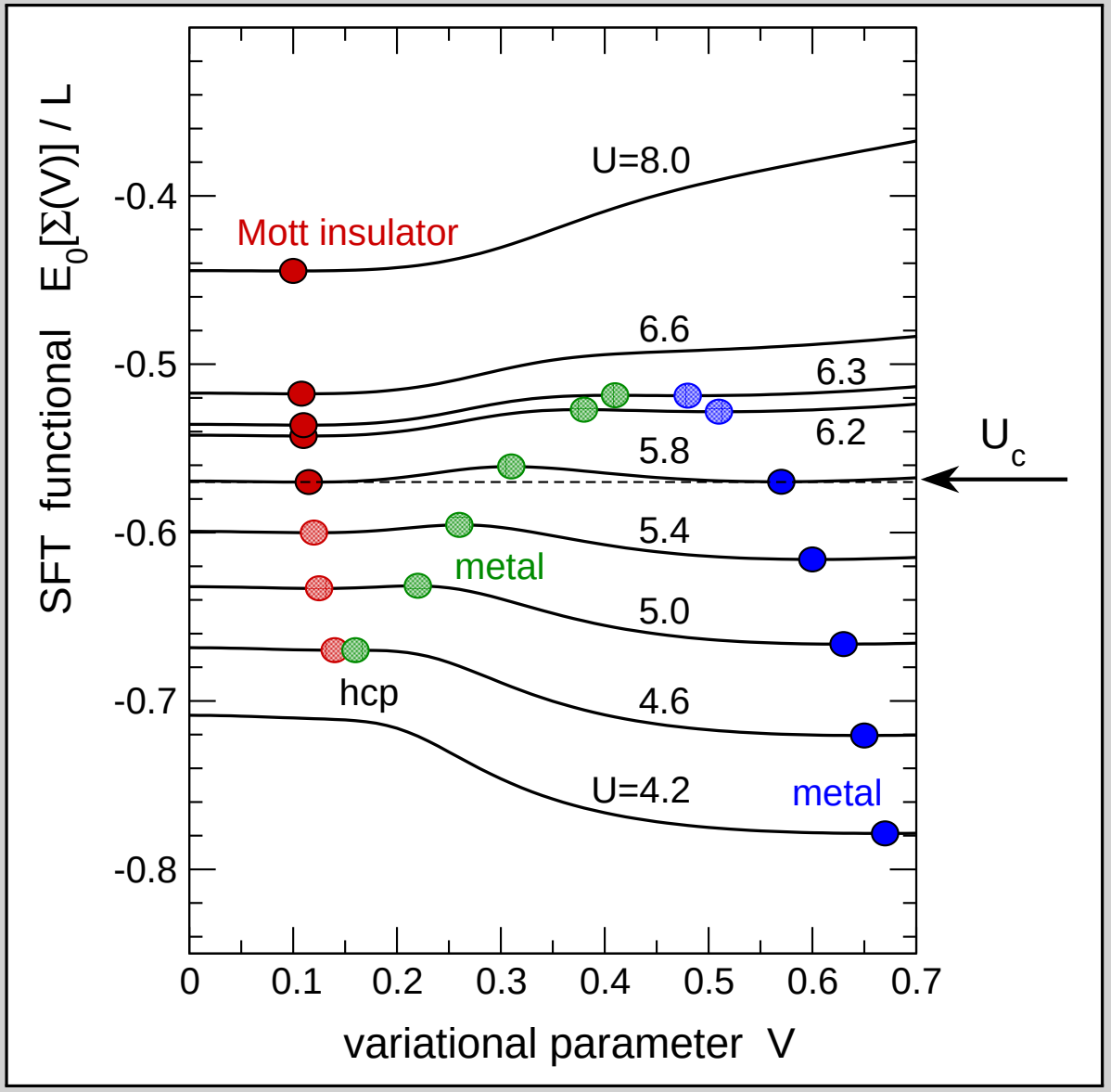


- on-site energies at correlated sites: $\varepsilon_c = 0$ (particle-hole symmetry)
- on-site energies at bath sites: $\varepsilon_b = U/2 = \mu$ (particle-hole symmetry)
- t'': optimal value small, $|t''_{\rm opt}| < t/25$ (t'' irrelevant for $L_b \to \infty$)
- t': optimal value $t'_{\rm opt} = t + \Delta t'_{\rm opt}$ 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

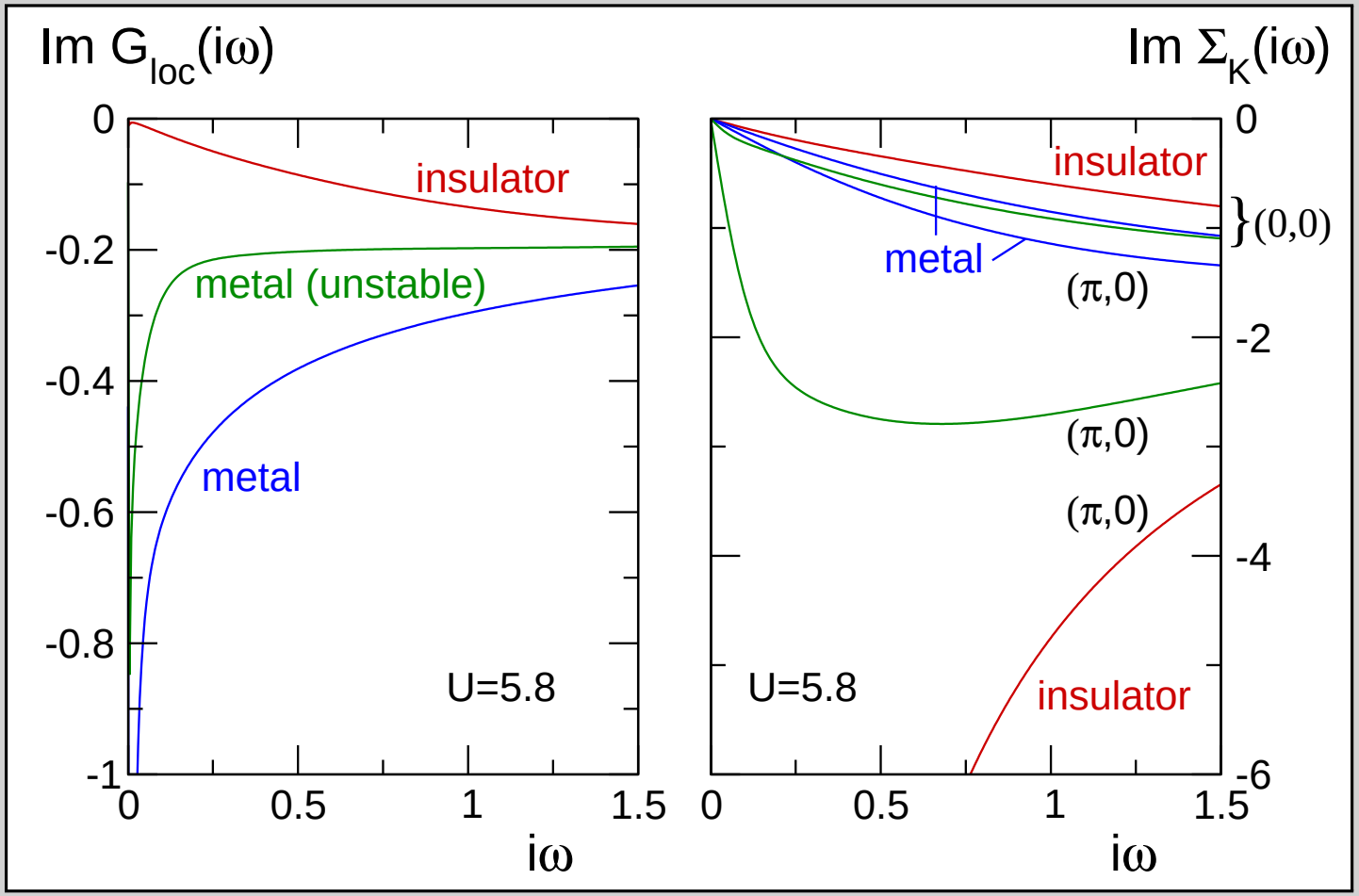
large $V_{\rm opt}$: metal

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

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

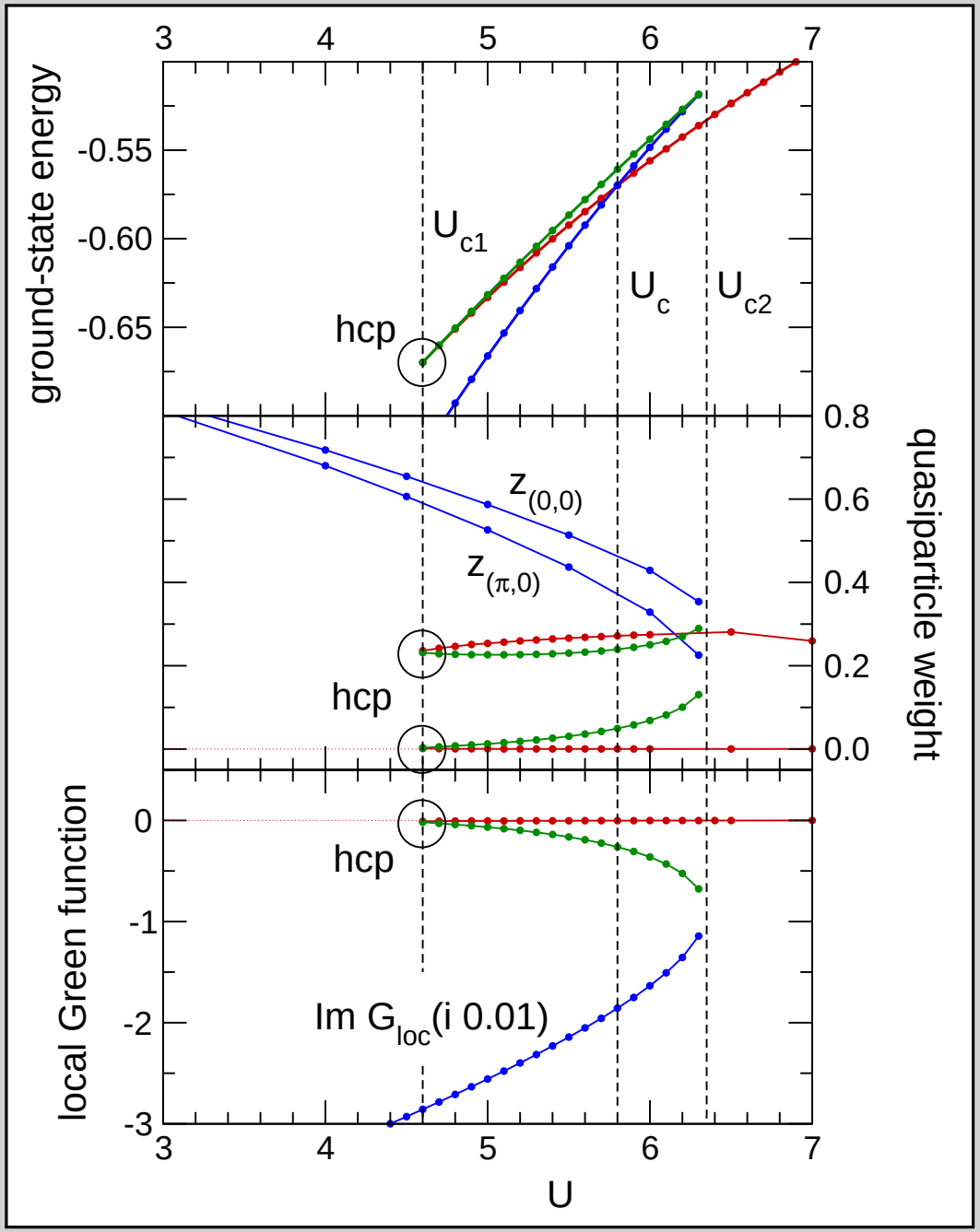
hidden critical point

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



➜ **third, metastable solution is metallic**

physical quantities in the coexistence range



hidden critical point scenario