Nonperturbative conserving approximations and Luttinger's sum rule

Jutta Ortloff, Matthias Balzer, Michael Potthoff

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Luttinger's sum rule:

the volume in reciprocal space
enclosed by the Fermi surface
equals the average particle number

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HF, RPA, FLEX, ...

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HF, RPA, FLEX, ...

DMFT-based approximations

dynmical mean-field theory
dynamical cluster approximation
cellular DMFT
...

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different conserving approximations?

DIA, VCA
(self-energy-functional approach)

Fermi surface

non-interacting Fermi gas

Hamiltionian: $H = \sum_{\mathbf{k}} \sum_{\sigma=\uparrow,\downarrow} \varepsilon(\mathbf{k}) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$

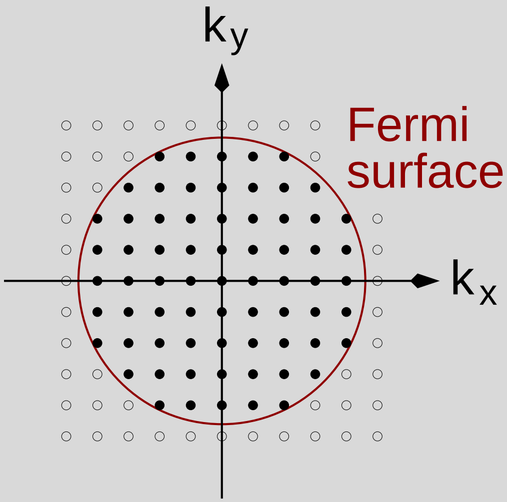
free dispersion:

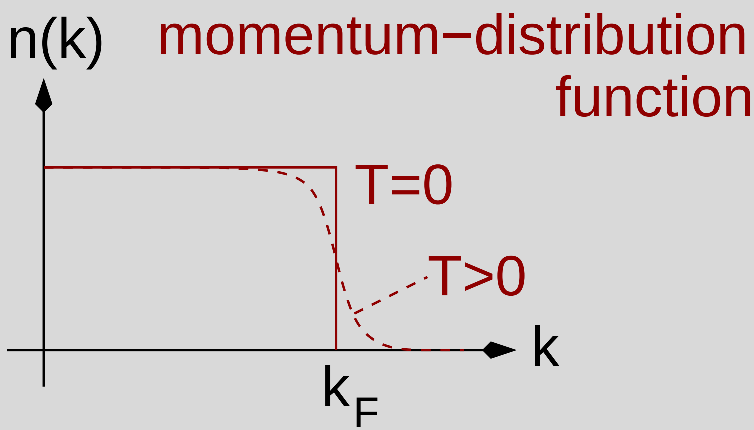
$$\varepsilon(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m}$$

tight-binding dispersion:

$$\varepsilon(\mathbf{k}) = -2t(\cos(k_x a) + \cos(k_y a))$$

Fermi surface: $\{\mathbf{k} | \varepsilon(\mathbf{k}) = \mu\}$





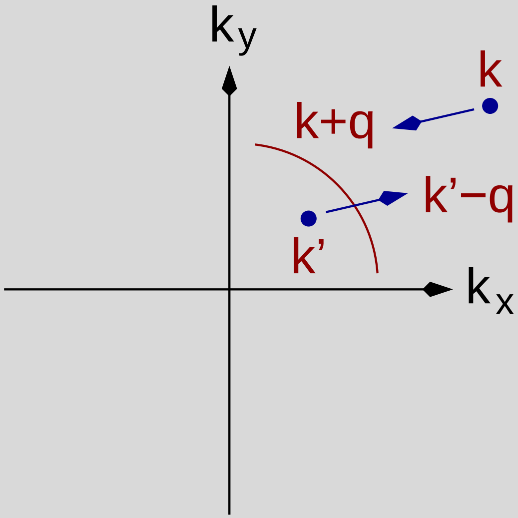
Fermi-surface volume: $V^{(0)}_{\mathrm{FS}} = 2 \sum_{\mathbf{k}} \Theta(\mu - \varepsilon(\mathbf{k}))$

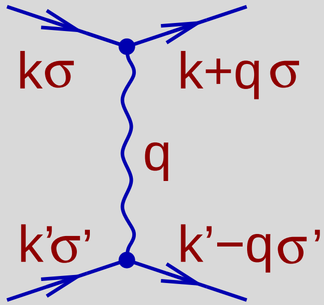
$$V^{(0)}_{\mathrm{FS}} = N$$

interactions

interacting Fermi system

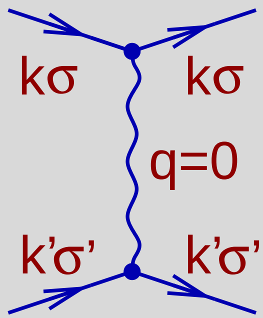
Hamiltonian: $$H = \sum_{\mathbf{k}} \sum_{\sigma=\uparrow,\downarrow} \varepsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{2L} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{\sigma\sigma'} c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}'-\mathbf{q}\sigma'}$$





Fermi liquid (Landau)

Hamiltonian: $$H_{\mathrm{FL}} = \sum_{\mathbf{k}} \sum_{\sigma} \varepsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2L} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma,\sigma'} F^{\sigma\sigma'}_{\mathbf{k}\mathbf{k}'} n_{\mathbf{k}\sigma} n_{\mathbf{k}'\sigma'}$$



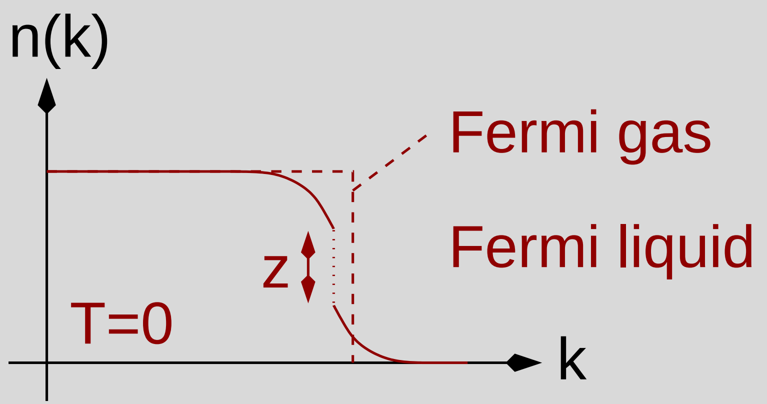
$\omega \longrightarrow 0$: no phase space for scattering

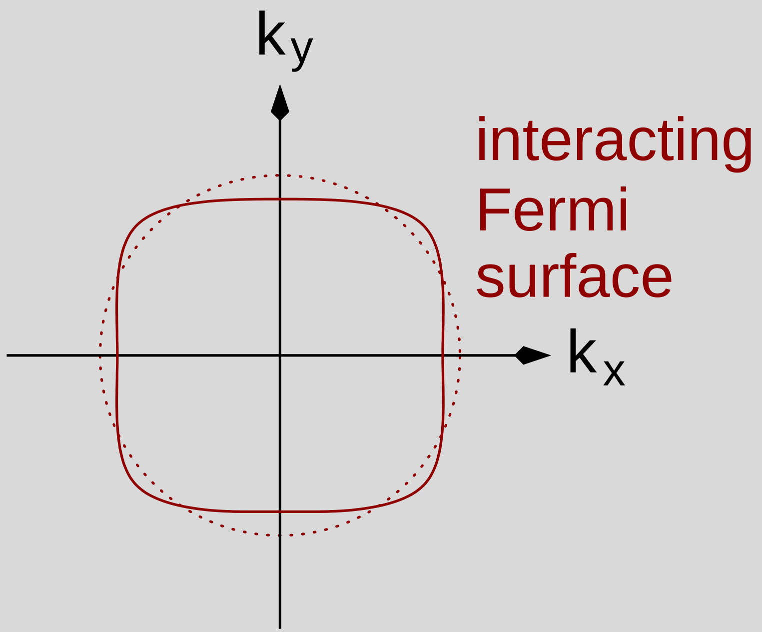
interacting Fermi surface

Fermi-liquid theory:

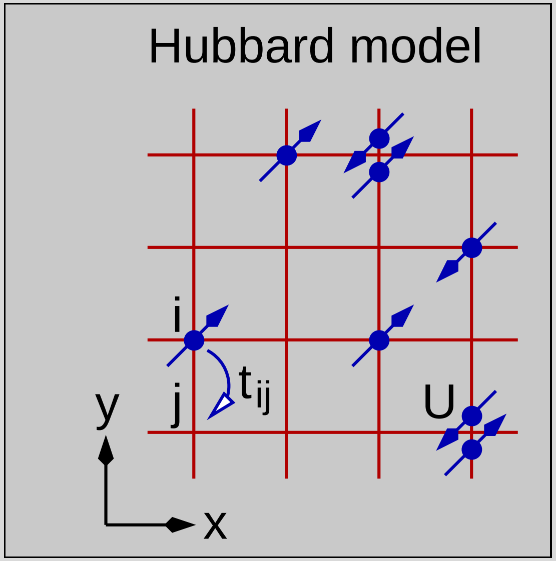
– there is a Fermi surface

– $V_{\mathrm{FS}} = N = V_{\mathrm{FS}}^{(0)}$ (Luttinger sum rule)





test of the sum rule

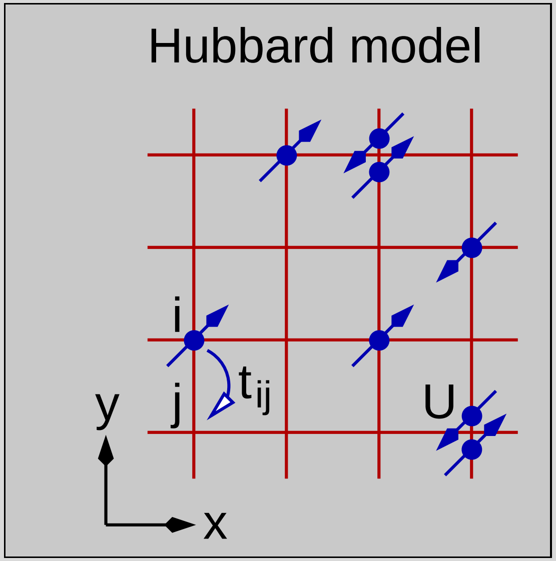


$$H = H_0 + H_1 = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow}$$

– nearest-neighbor hopping, amplitude: t_{ij}

– local (on-site) repulsion, strength U

test of the sum rule



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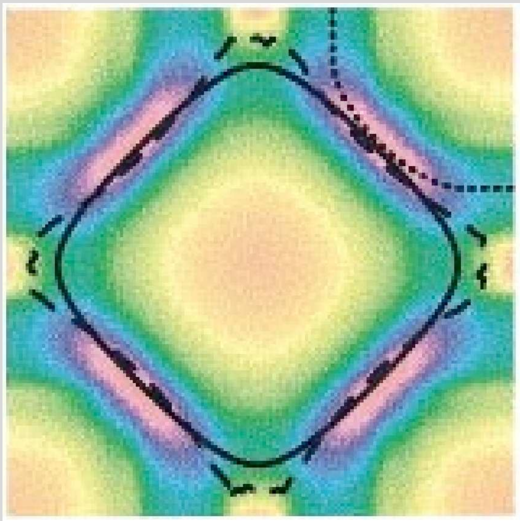
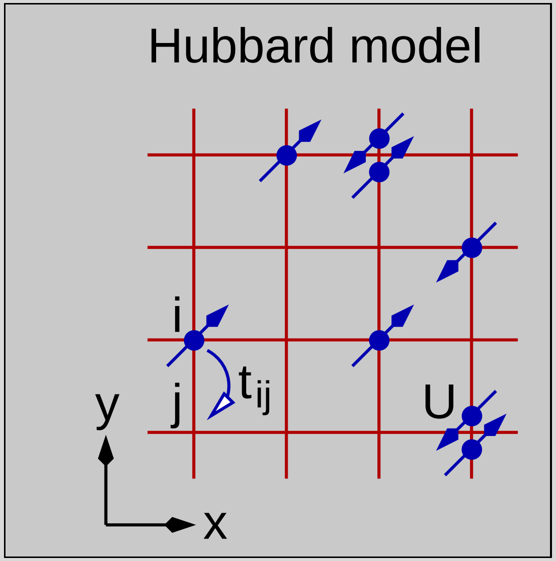


Puttika et al (1998)

t-J model:
expansion up to β^{12}, $J/t = 0.4$, $n = 0.8$, $T = 0.2J$,

criteria: $|\nabla n(\mathbf{k})| = $ max (dotted), $dn(\mathbf{k})/dT = 0$ (dashed)

test of the sum rule



$$H = H_0 + H_1 = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow}$$

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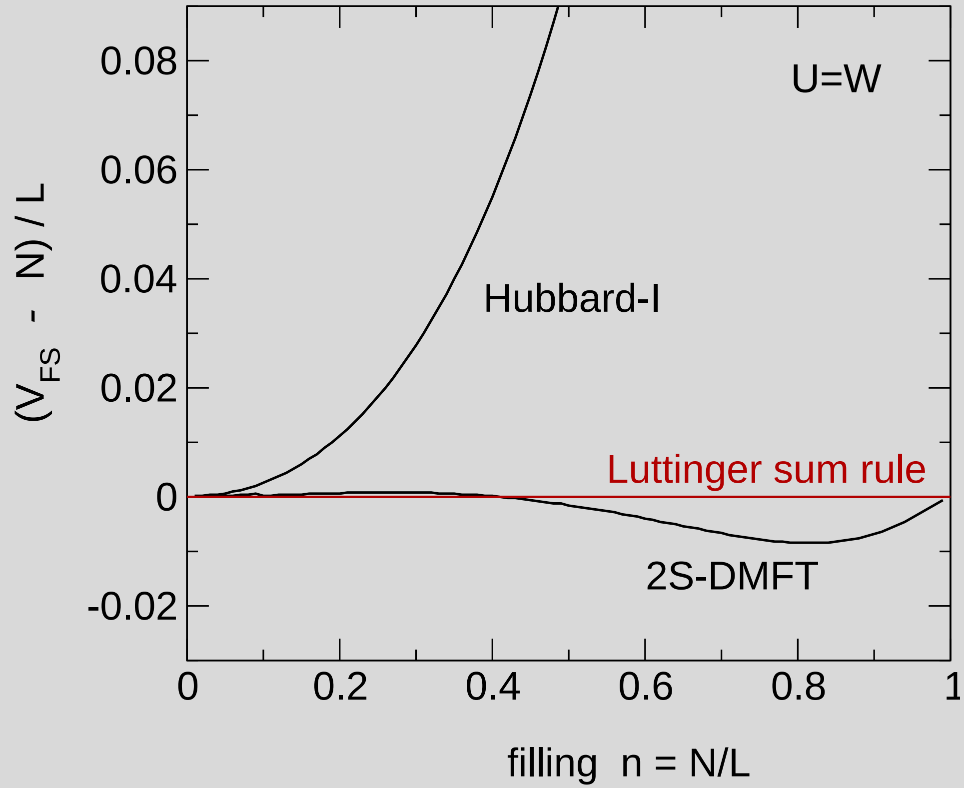
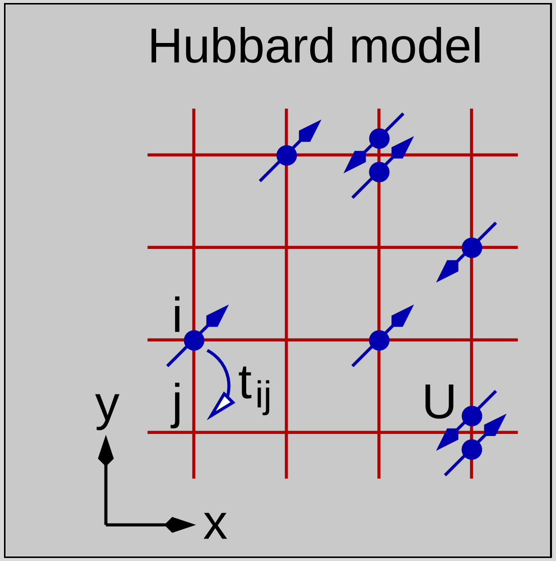


Hubbard model:
$T = 0$, $U = W$

ad hoc approximations

test of the sum rule



$$H = H_0 + H_1 = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow}$$

– nearest-neighbor hopping, amplitude: t_{ij}
– local (on-site) repulsion, strength U

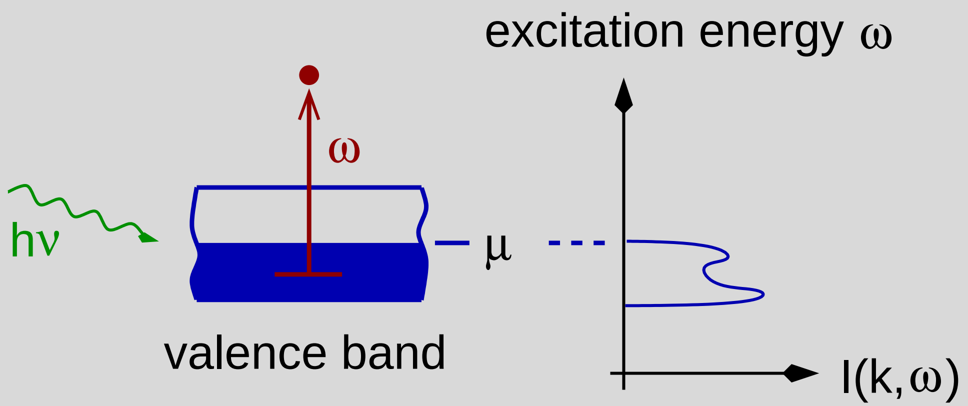
questions:

– are there violations of Luttinger's sum rule ?
– how to construct approximations satisfying the sum rule ?

– how to construct approximations not artificially satisfying the sum rule ?

Green's function

one-particle excitation / photoemission:

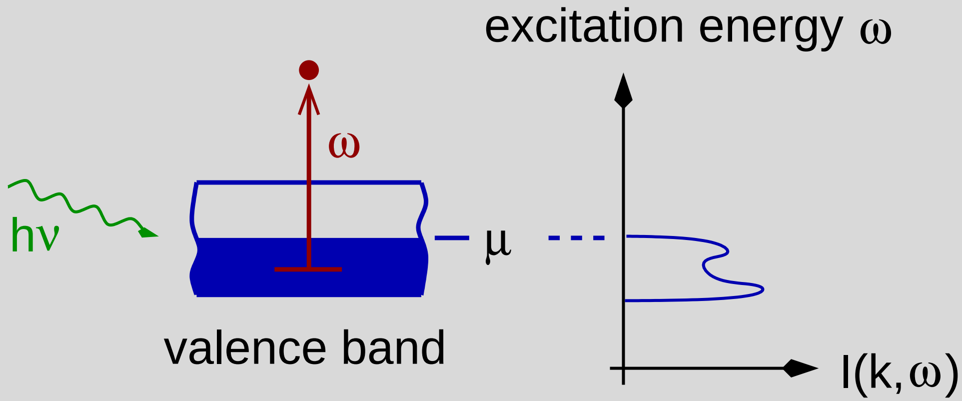


$$I(\mathbf{k},\omega) \propto \sum_m \left|\langle N-1,m \mid c_{\mathbf{k}} \mid N,0\rangle\right|^2 \delta\left(\omega - \left(E_m(N-1) - E_0(N)\right)\right) = A_{\mathbf{k}}(\omega)$$

Green's function: $G_{\mathbf{k}}(\omega) = \int dz \, \frac{A_{\mathbf{k}}(z)}{\omega - z}$ $\quad A_{\mathbf{k}}(\omega) = -\mathrm{Im}\, G(\mathbf{k},\omega + i0^+)/\pi$

Green's function

one-particle excitation / photoemission:



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

Green's function: $G_{\mathbf{k}}(\omega) = \int dz \, \frac{A_{\mathbf{k}}(z)}{\omega - z}$ $\qquad A_{\mathbf{k}}(\omega) = -\text{Im}\, G(\mathbf{k}, \omega + i0^+)/\pi$

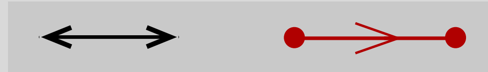
➜ Luttinger's sum rule: $N = V_{\text{FS}}$

➜ $N = \sum_{\mathbf{k}} \int_{-\infty}^{0} d\omega \; A_{\mathbf{k}}(\omega) = -\frac{1}{\pi} \text{Im} \sum_{\mathbf{k}} \int_{-\infty}^{0} d\omega \; G_{\mathbf{k}}(\omega + i0^+)$ $\qquad N = \text{Tr}\, \mathbf{G}$

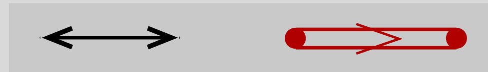
➜ FS: $G_{\mathbf{k}}(\omega = 0)^{-1} = 0 \qquad V_{\text{FS}} = \sum_{\mathbf{k}} \Theta(G_{\mathbf{k}}(\omega = 0)^{-1})$ $\qquad V_{\text{FS}} = \text{Tr} \frac{\partial}{\partial \omega} \ln \mathbf{G}^{-1}$

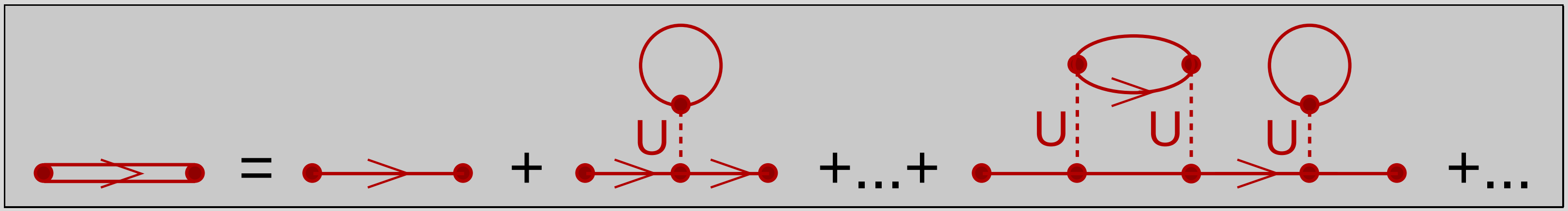
perturbation theory

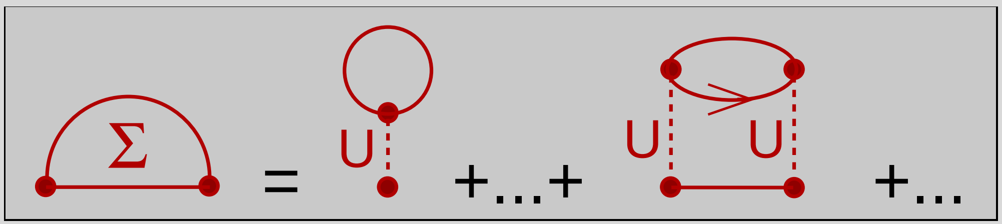
$H = H_0$ ➜ $G^{(0)}_{\mathbf{k}}(\omega)$ (free system)



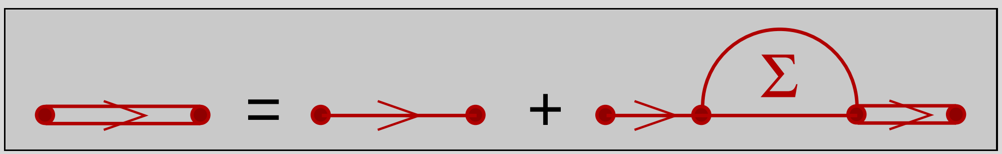
$H = H_0 + H_1$ ➜ $G_{\mathbf{k}}(\omega)$ (interacting system)







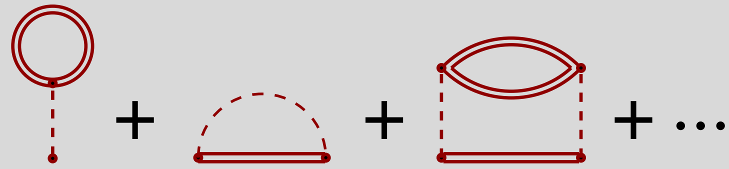
$\Sigma_{\mathbf{k}}(\omega)$: self-energy



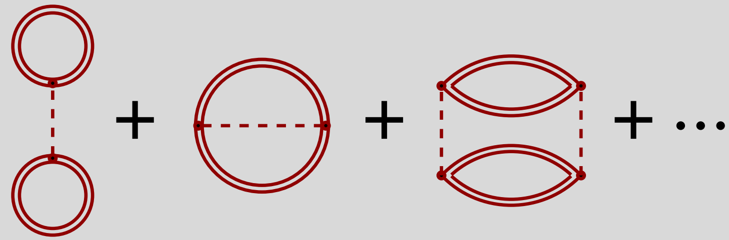
$$G_{\mathbf{k}}(\omega) = G^{(0)}_{\mathbf{k}}(\omega) + G^{(0)}_{\mathbf{k}}(\omega)\Sigma_{\mathbf{k}}(\omega)G_{\mathbf{k}}(\omega)$$ (Dyson's equation)

proof of the sum rule

expansion of the self-energy: $\Sigma =$



define Luttinger-Ward functional: $\Phi =$



hence: $\mathbf{\Sigma}[\mathbf{G}] = \dfrac{\delta \Phi[\mathbf{G}]}{\delta \mathbf{G}}$

consider shift transformation $\mathbf{G}(\omega) \to \mathbf{G}(\omega + \nu) \equiv \mathbf{G}_\nu(\omega)$

$$\boxed{\Phi[\mathbf{G}] = \Phi[\mathbf{G}_\nu]}$$

invariant!

exploiting the invariance:

$$0 = \frac{d}{d\nu} \Phi[\mathbf{G}_\nu] \bigg|_{\nu=0} = \int d\omega \frac{\delta \Phi}{\delta \mathbf{G}} \frac{\partial \mathbf{G}}{\partial \omega} = \mathrm{Tr} \left(\mathbf{\Sigma} \frac{\partial \mathbf{G}}{\partial \omega} \right)$$

some algebra:

$$N = \mathrm{Tr}\, \mathbf{G} = \mathrm{Tr} \left(\mathbf{G} \frac{\partial \mathbf{G}^{(0)\,-1}}{\partial \omega} \right) = \mathrm{Tr} \left(\mathbf{G} \frac{\partial}{\partial \omega} (\mathbf{G}^{-1} + \mathbf{\Sigma}) \right)$$

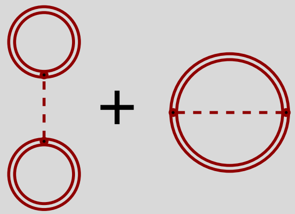
$$= \mathrm{Tr} \left(\frac{\partial}{\partial \omega} \ln \mathbf{G}^{-1} \right) - \mathrm{Tr} \left(\mathbf{\Sigma} \frac{\partial \mathbf{G}}{\partial \omega} \right) = V_{\mathrm{FS}}$$

Luttinger, Ward (1963)

conserving approximations

recipe:

- write down a truncated Luttinger-Ward functional: $\Phi[\mathbf{G}] \mapsto \Phi_{\text{trunc}}[\mathbf{G}]$
  e.g. Hartree-Fock approximation:

$\Phi_{\text{HF}} =$ 

- derive self-energy: ("Φ derivable")
  $$\mathbf{\Sigma}[\mathbf{G}] = \frac{\delta\Phi[\mathbf{G}]}{\delta\mathbf{G}}$$
- use Dyson's equation
  $$\mathbf{G} = \frac{1}{\mathbf{G}^{(0)}{}^{-1} - \mathbf{\Sigma}}$$

result: *Baym, Kadanoff (1961)*

- macroscopic conservations laws respected (energy, momentum, spin, ...)
- thermodynamical consistency
- Luttinger's sum rule satisfied (same proof)

➜ non-perturbative conserving approximations?

non-perturbative construction of Φ

$$\Omega_{\mathbf{U}}[\mathbf{G}_0^{-1}] = -T \ln \int D[c^*, c]\, e^{-S_{\mathbf{U}}[\mathbf{G}_0^{-1}]}$$

$$\mathbf{G}[\mathbf{G}_0^{-1}] = -\frac{1}{T} \frac{\delta \Omega_{\mathbf{U}}[\mathbf{G}_0^{-1}]}{\delta \mathbf{G}_0^{-1}} \quad \text{(one-to-one)}$$

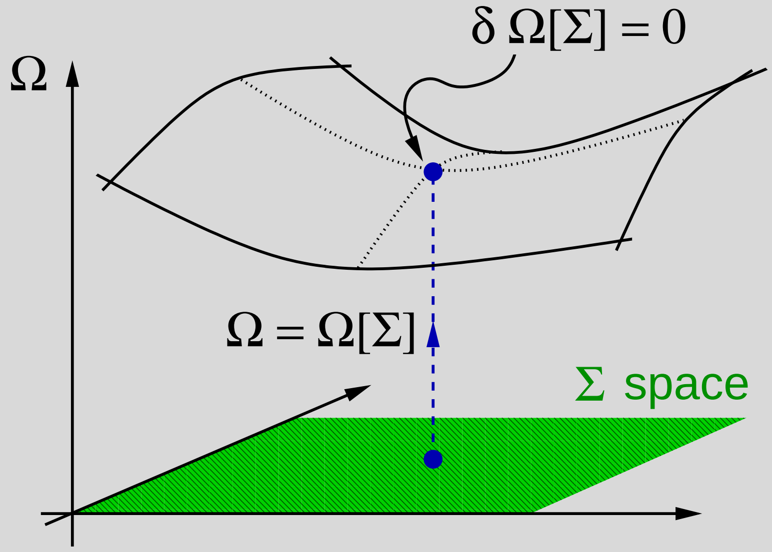
$$\Phi_{\mathbf{U}}[\mathbf{G}] = \Omega_{\mathbf{U}}[\mathbf{G}_{0,U}^{-1}[\mathbf{G}]] + \text{Tr}(\mathbf{G}\mathbf{G}_{0,\mathbf{U}}^{-1}[\mathbf{G}]) - \text{Tr} \ln \mathbf{G}$$

➜ Luttinger-Ward functional, universal

$\Lambda_{\mathbf{U}}[\mathbf{\Sigma}]$: Legendre transform of $\Phi_{\mathbf{U}}[\mathbf{G}]$

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

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



self-energy-functional theory (SFT)

non-perturbative construction of Φ

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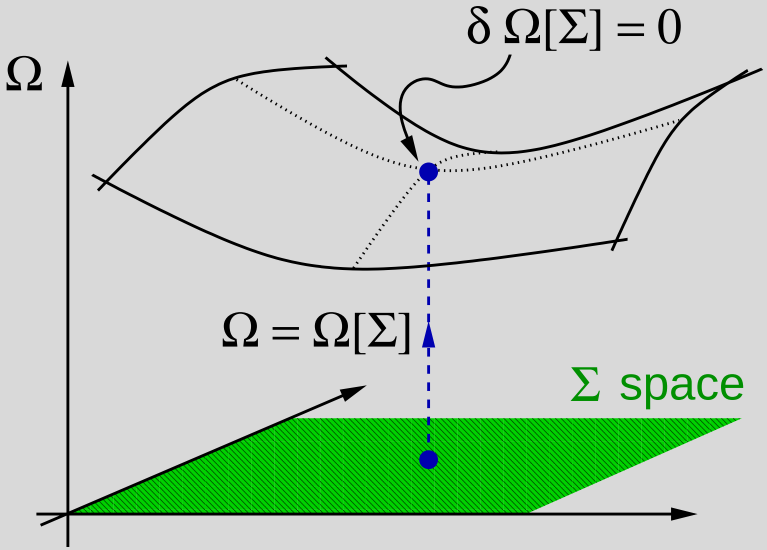
$$\delta \Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = 0 \Leftrightarrow \frac{-1}{\mathbf{G}_{0,\mathbf{t}}^{-1} - \mathbf{\Sigma}} = \frac{\delta \Lambda_{\mathbf{U}}[\mathbf{\Sigma}]}{\delta \mathbf{\Sigma}}$$

➜ $\Omega[\Sigma]$ stationary at physical self-energy

➜ $\Lambda_U[\Sigma]$ construced formally, but unknown

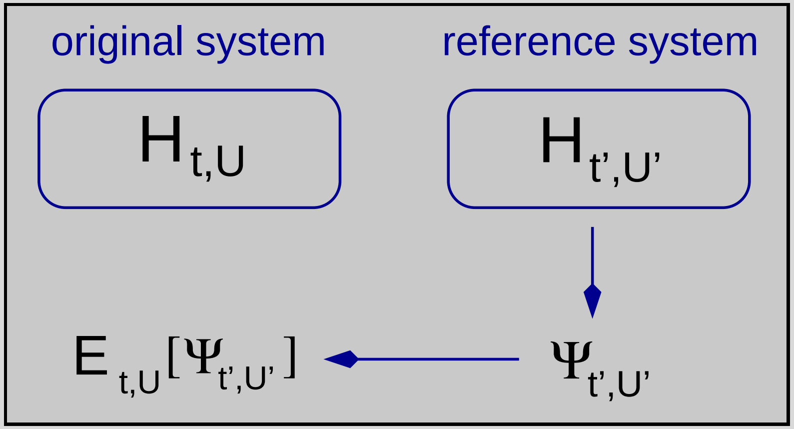
SFT	DFT
$\delta\Omega[\mathbf{\Sigma}] = 0$	$\delta\Omega[\mathbf{n}] = 0$



self-energy-functional theory (SFT)

reference system

Rayleigh, Ritz



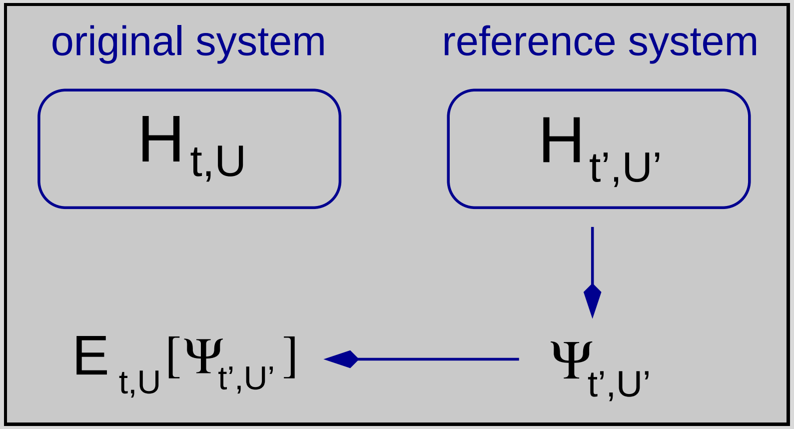
$$E_{\mathbf{t},\mathbf{U}}[|\Psi\rangle] = \langle\Psi|H_{\mathbf{t},\mathbf{U}}|\Psi\rangle$$

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

➜ Hartree-Fock approximation

reference system

Rayleigh, Ritz



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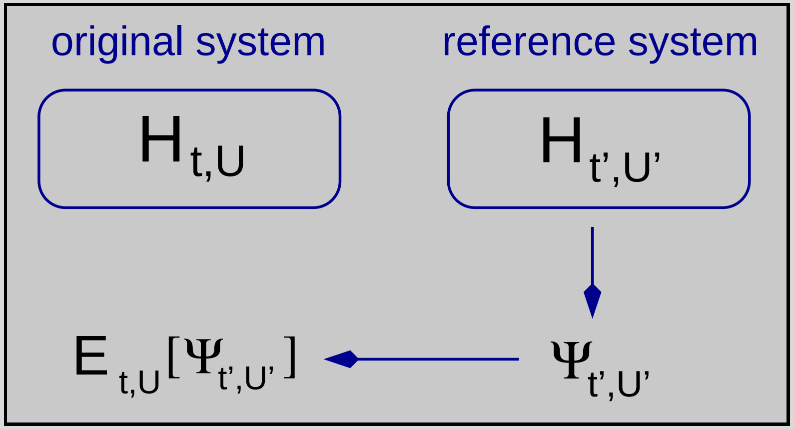
➜ **Hartree-Fock approximation**

type of approximation ⇔ choice of reference system

reference system

Rayleigh, Ritz



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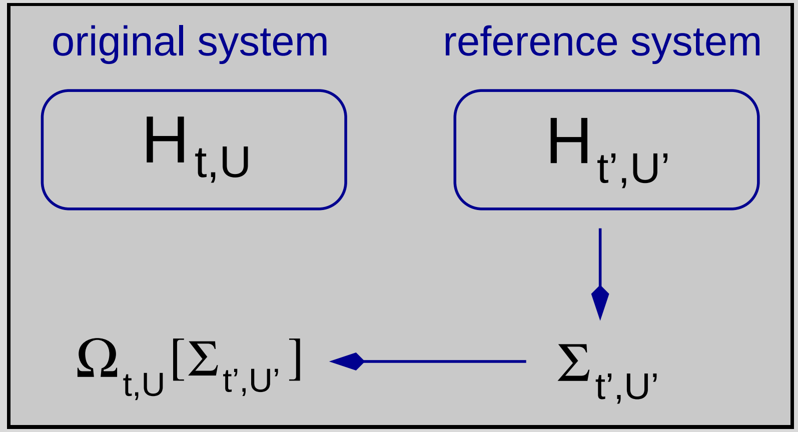
$$\frac{\partial E_{\mathbf{t},\mathbf{U}}[|\Psi_{\mathbf{t}',\mathbf{U}'=0}\rangle]}{\partial \mathbf{t}'} \stackrel{!}{=} 0$$

➜ **Hartree-Fock approximation**

SFT



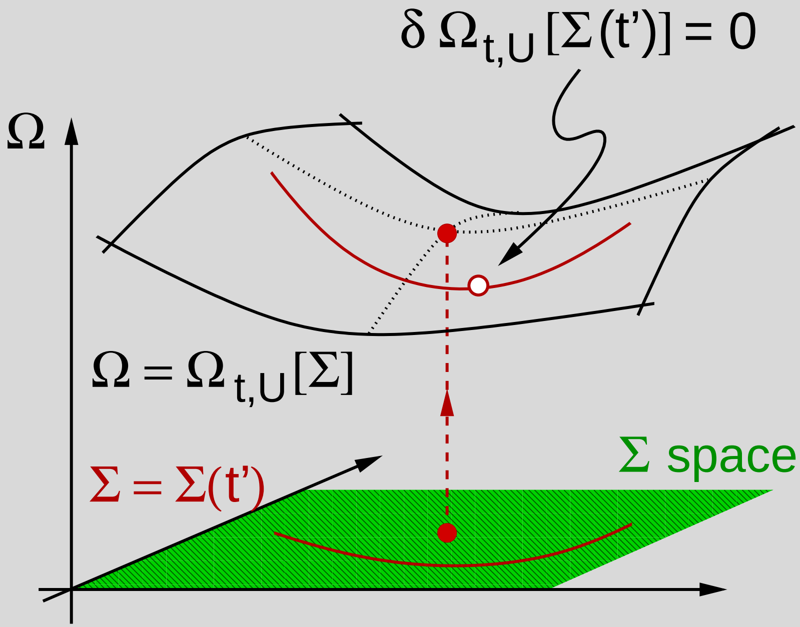
$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \text{?}$$

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

➜ **new approximations ?**

type of approximation ⇔ choice of reference system

evaluation of the self-energy functional



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

original system:

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

reference system:

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

combination:

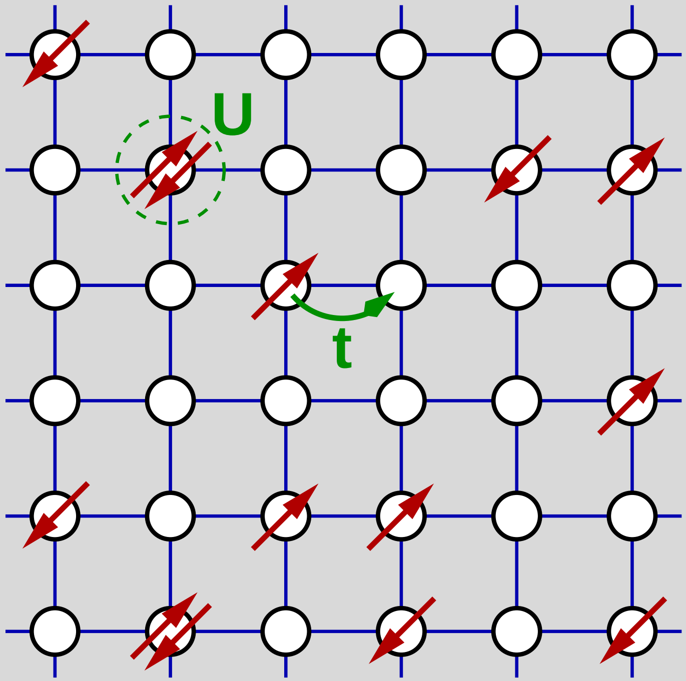
$$\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \Omega_{\mathbf{t}',\mathbf{U}}[\mathbf{\Sigma}] + \text{Tr}\ln\frac{1}{\mathbf{G}_{0,\mathbf{t}}^{-1} - \mathbf{\Sigma}} - \text{Tr}\ln\frac{1}{\mathbf{G}_{0,\mathbf{t}'}^{-1} - \mathbf{\Sigma}}$$

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

➜ **Φ-derivable, conserving, respecting Luttinger sum rule?**

cluster approximations

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

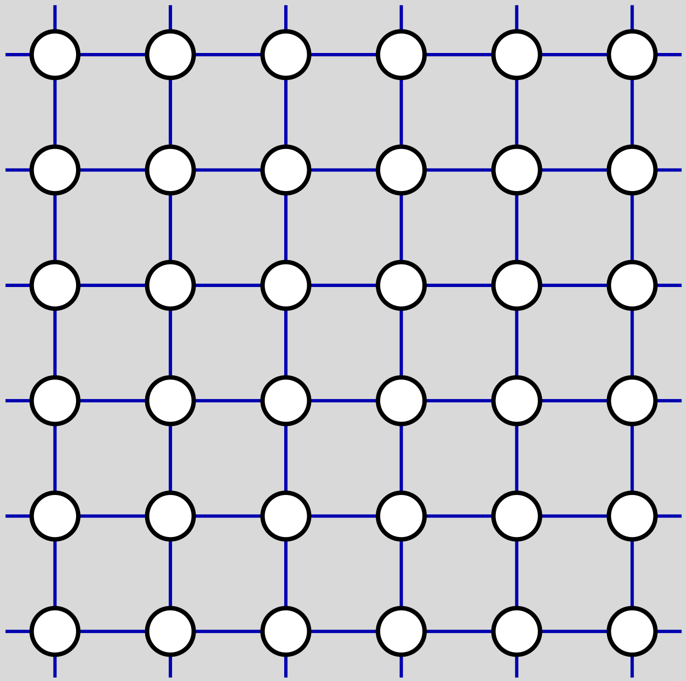


lattice model ($D = 2$) in
the thermodynamic limit

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

cluster approximations

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



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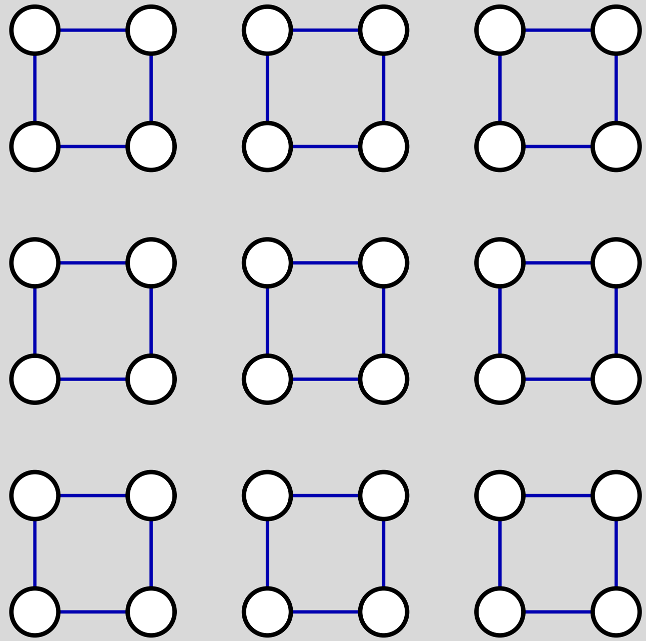


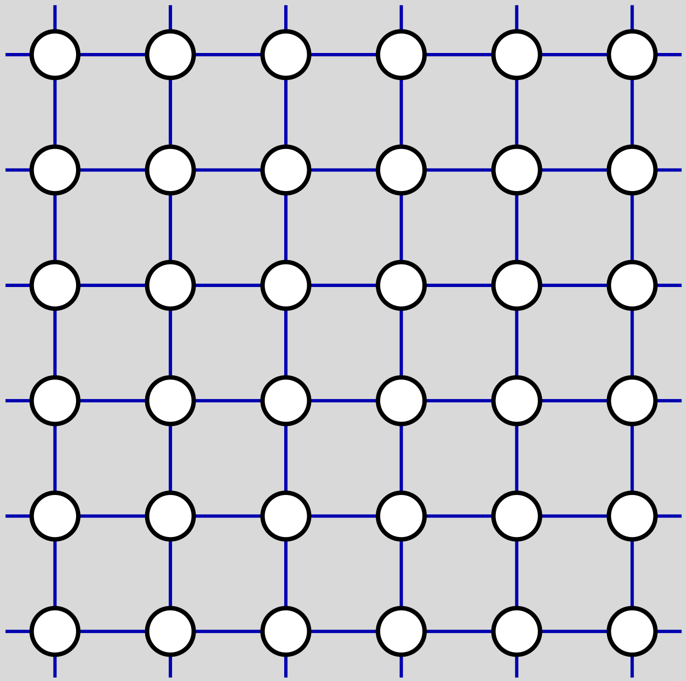
system of decoupled clusters

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

stationary point: $\dfrac{\partial}{\partial \mathbf{t}'}\Omega_{\mathbf{t}}[\mathbf{\Sigma}(\mathbf{t}')] = 0$

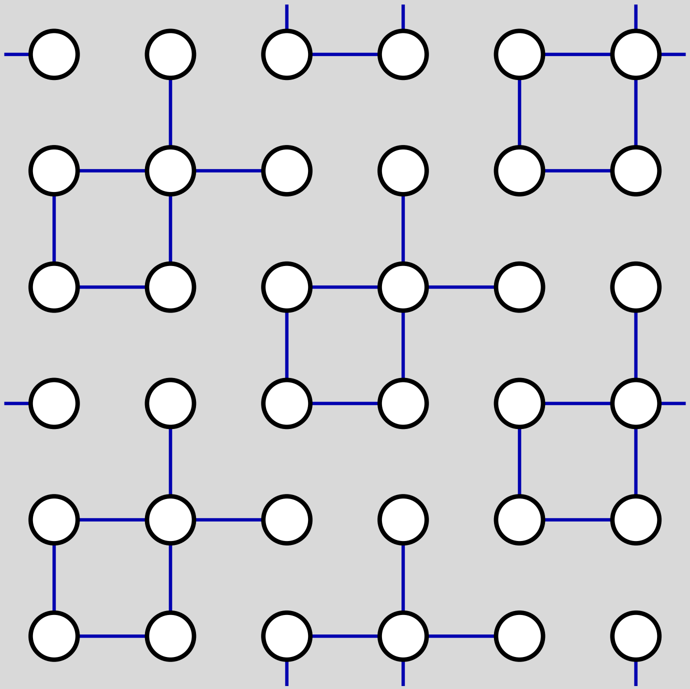
cluster approximations

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



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

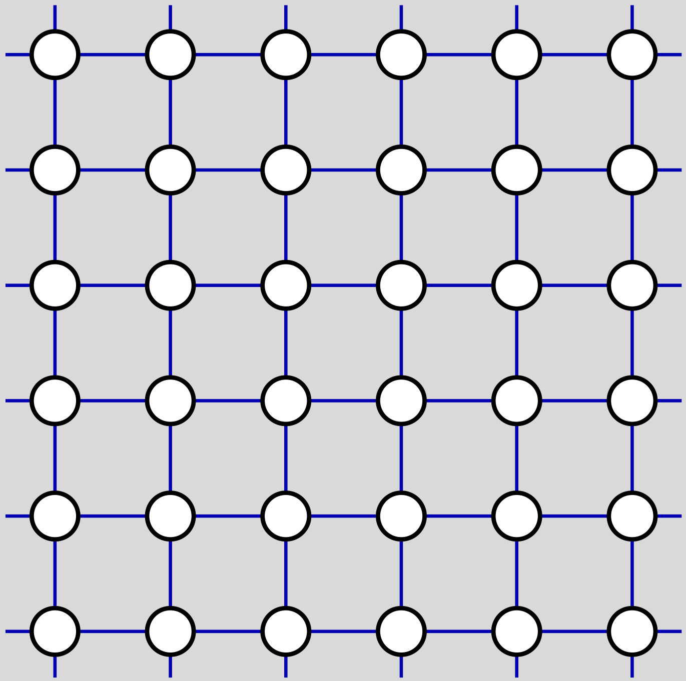
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

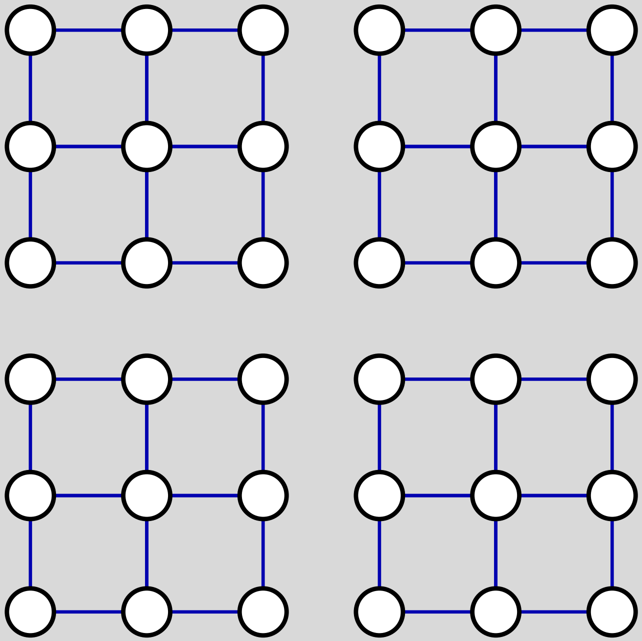
cluster approximations

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



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

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

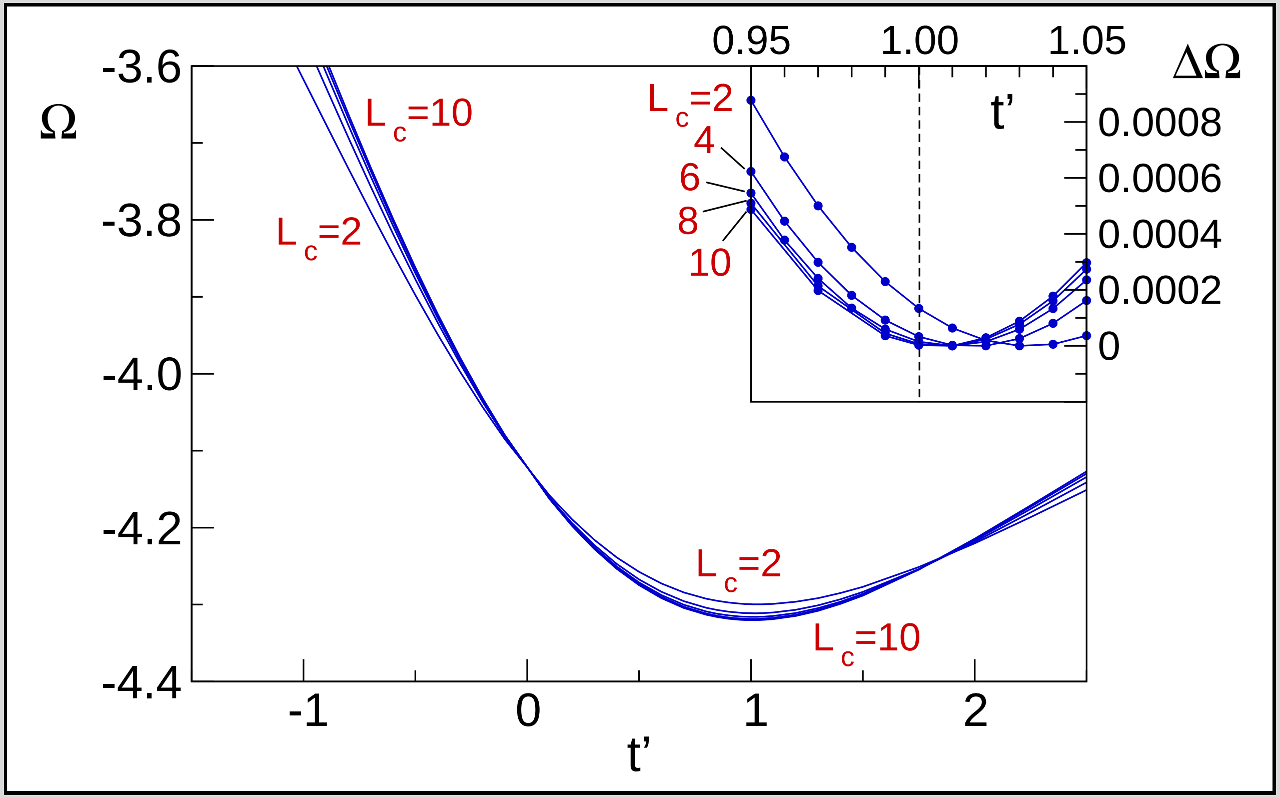


system of decoupled clusters
cluster size: L_c
$L_c \leq 2$: analytic
$L_c \leq 6$: exact diagonalization
$L_c \leq 12$: Lanczos method
$L_c \leq 100$: stochastic techniques

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

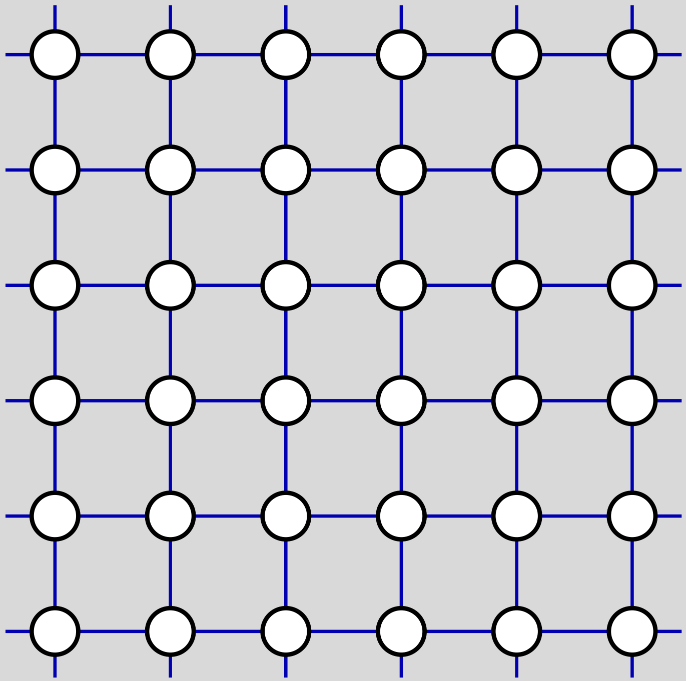


➜ $\Omega(t') \equiv \Omega[\mathbf{\Sigma}(t')]$ **stationary at** $t'_{\mathrm{min}} \neq t$

➜ $t'_{\mathrm{min}} \approx t$

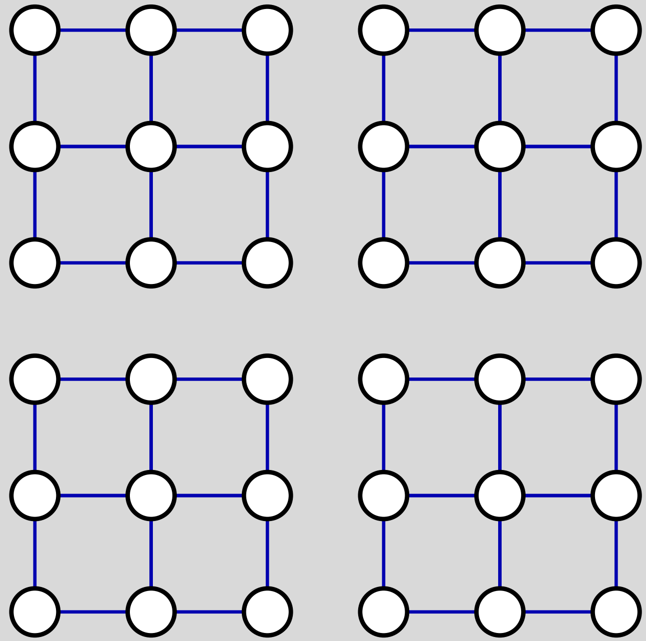
cluster approximations

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



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

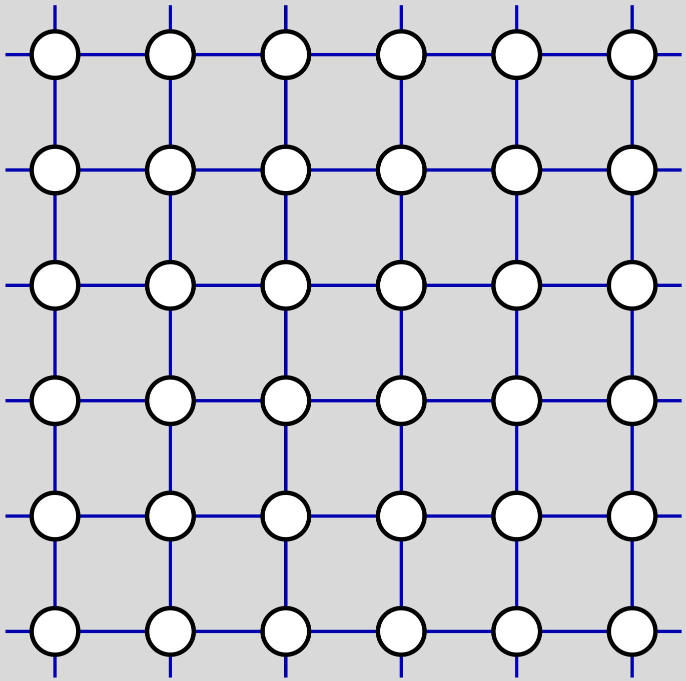
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

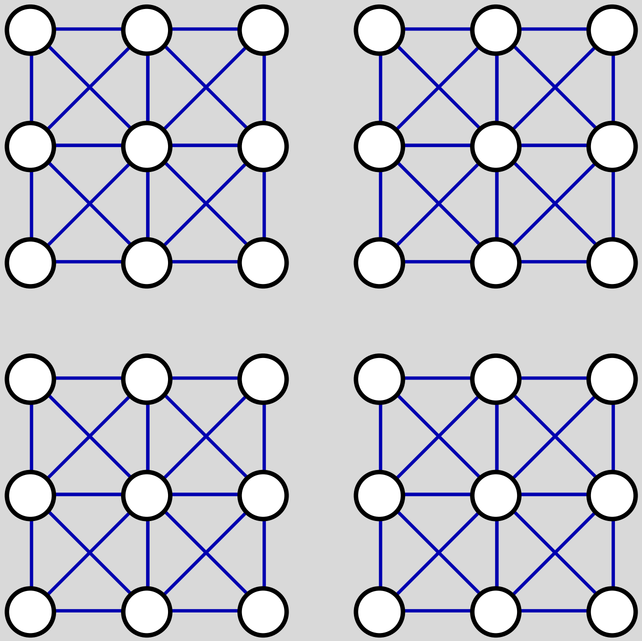
cluster approximations

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



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

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

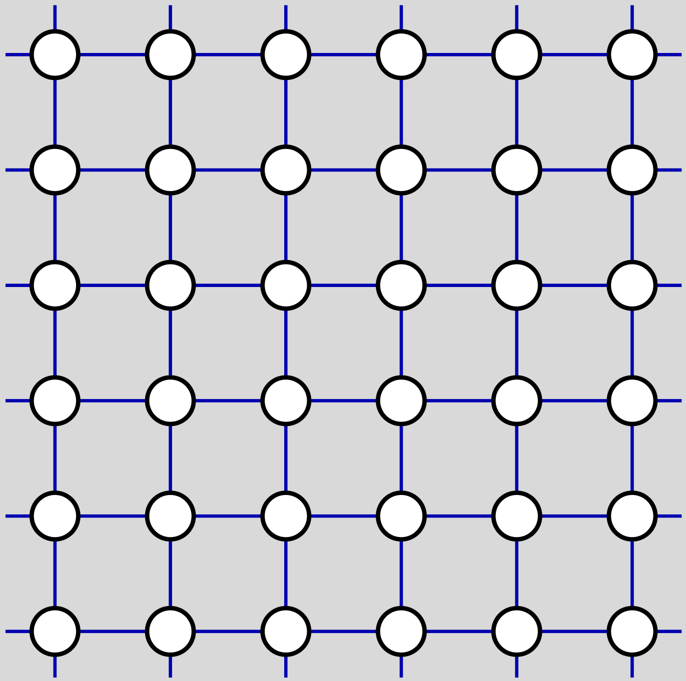


system of decoupled clusters

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

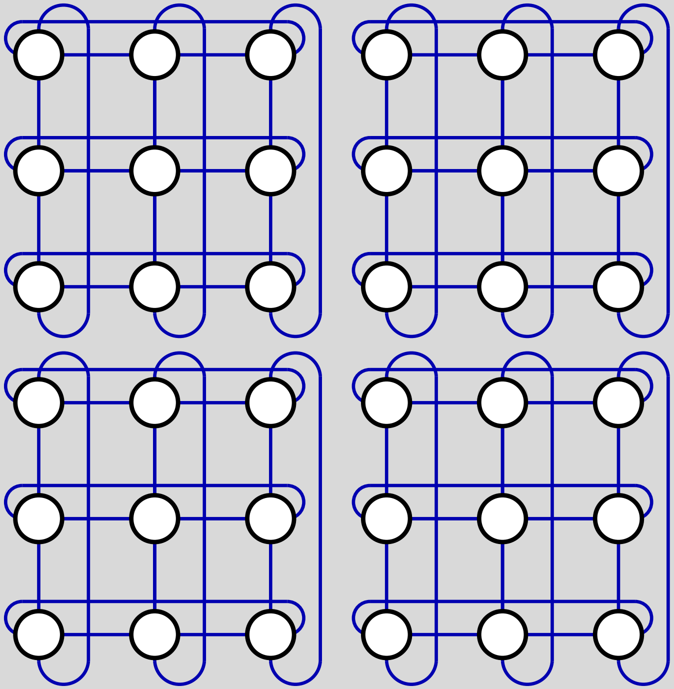
cluster approximations

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



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

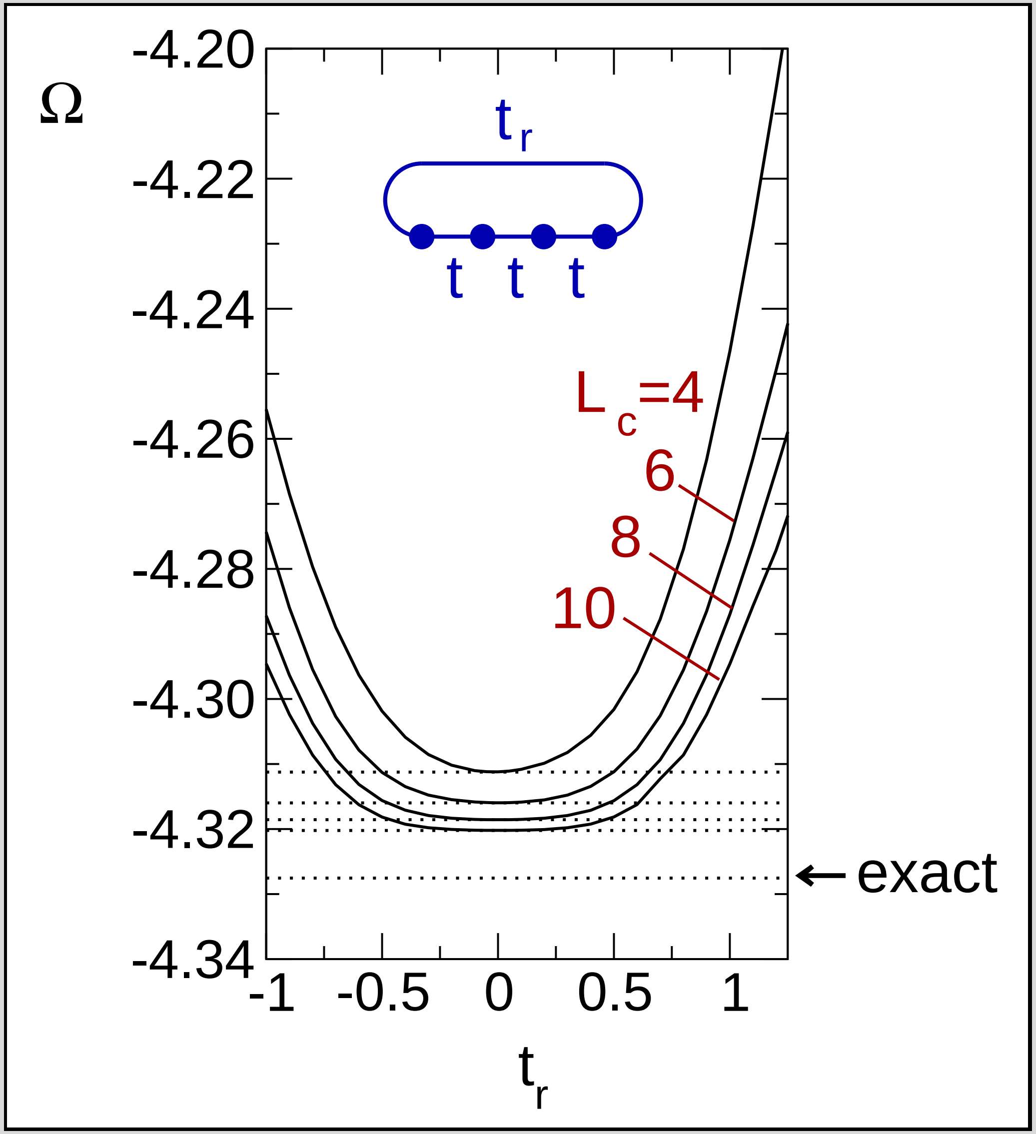
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

variational parameters:
hopping between cluster boundaries
boundary conditions

boundary conditions



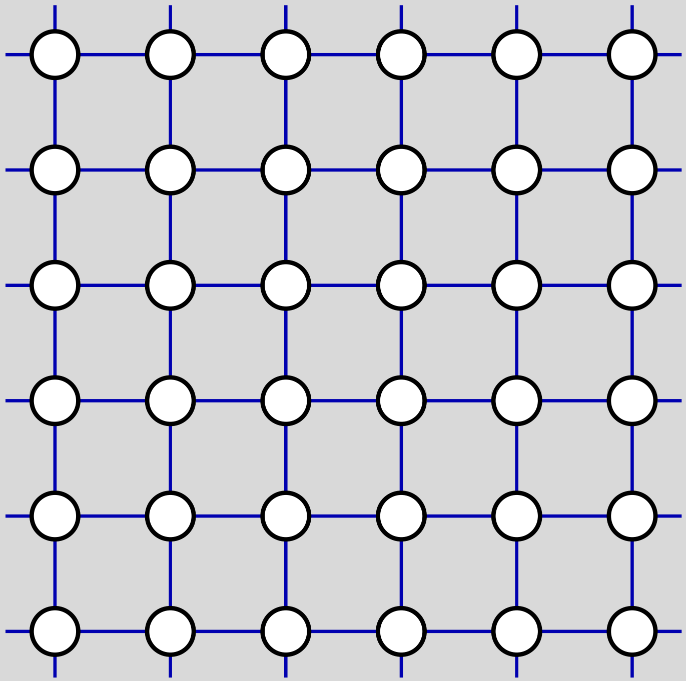
exact: *Lieb, Wu (1968)*

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

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

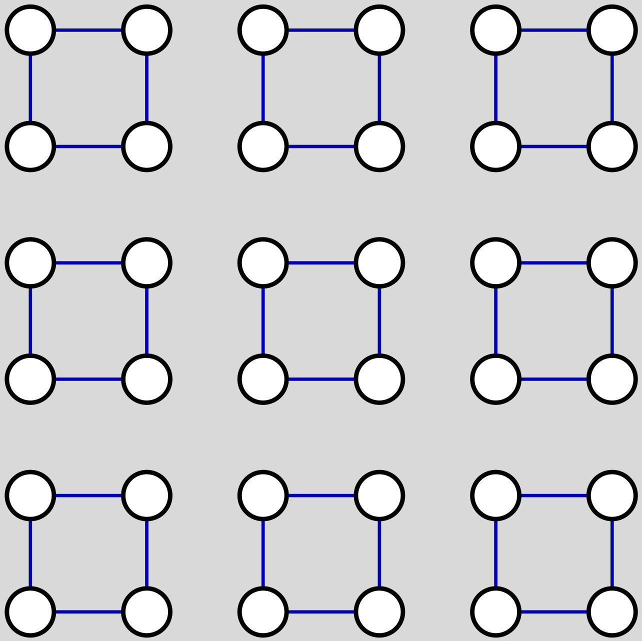
cluster approximations

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



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

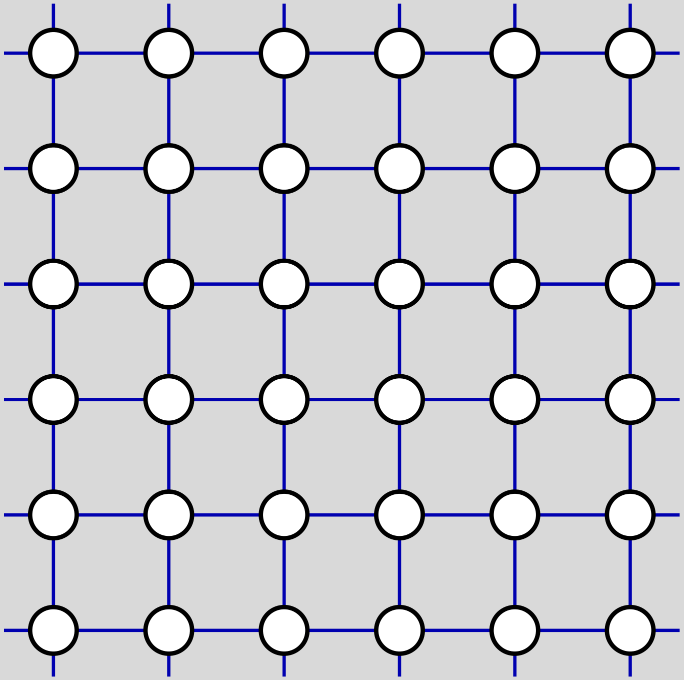
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



system of decoupled clusters

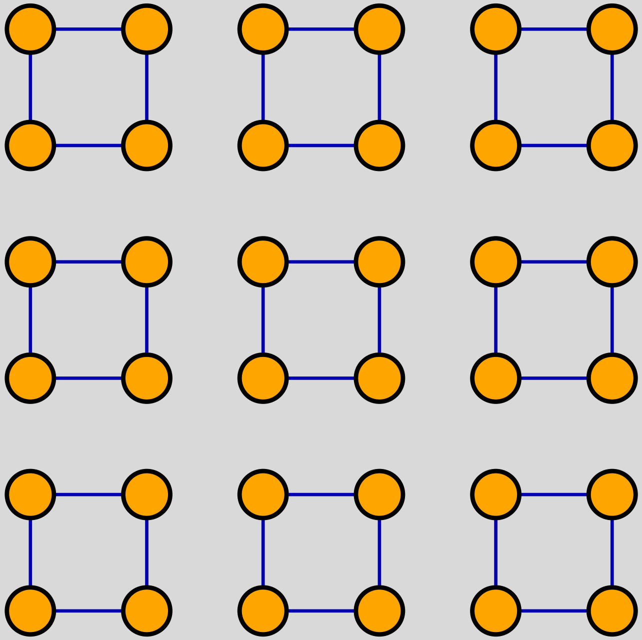
cluster approximations

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



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

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

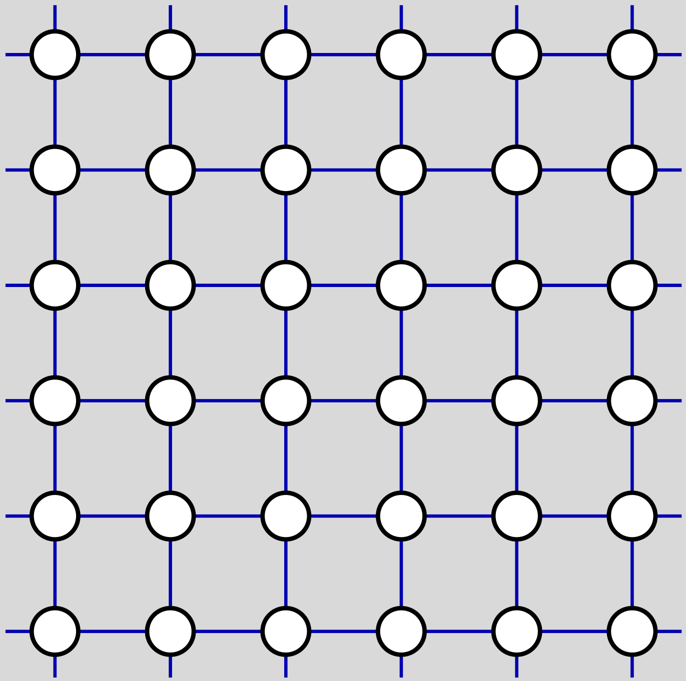


system of decoupled clusters

variational parameters:
on-site energies
thermodynamic consistency

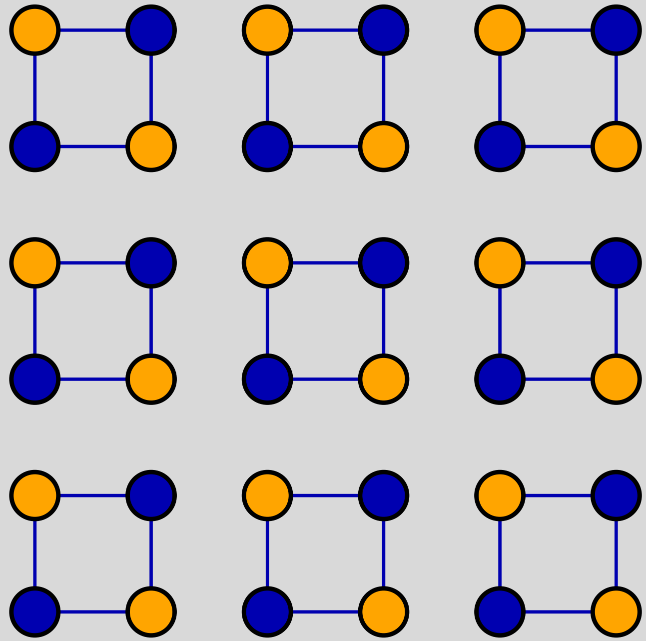
cluster approximations

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



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

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

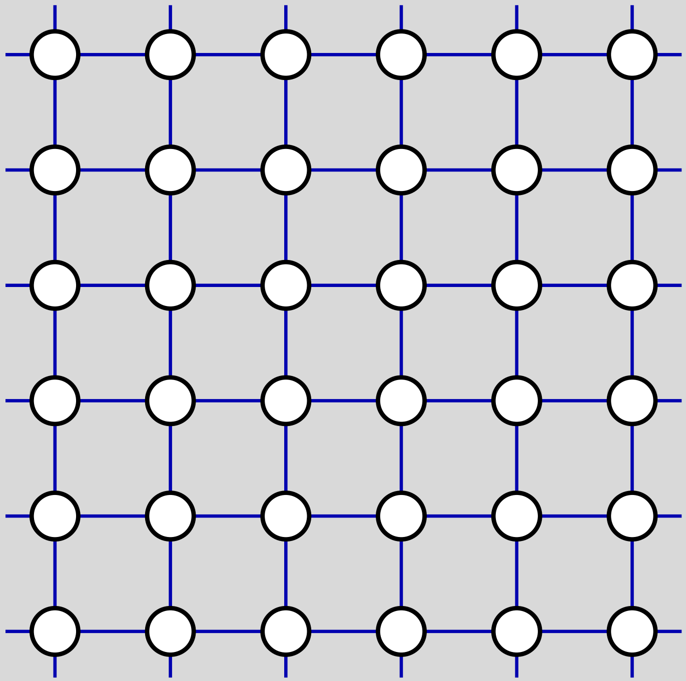


system of decoupled clusters

variational parameters:
ficticious symmetry-breaking fields
spontaneous symmetry breaking

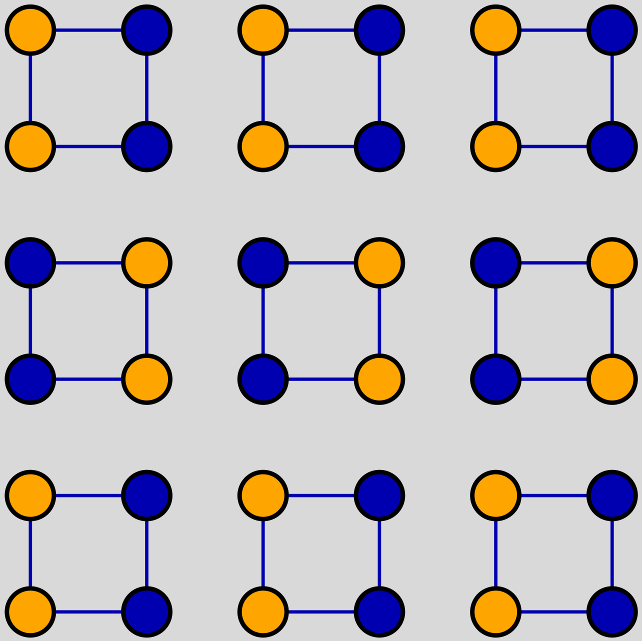
cluster approximations

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



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

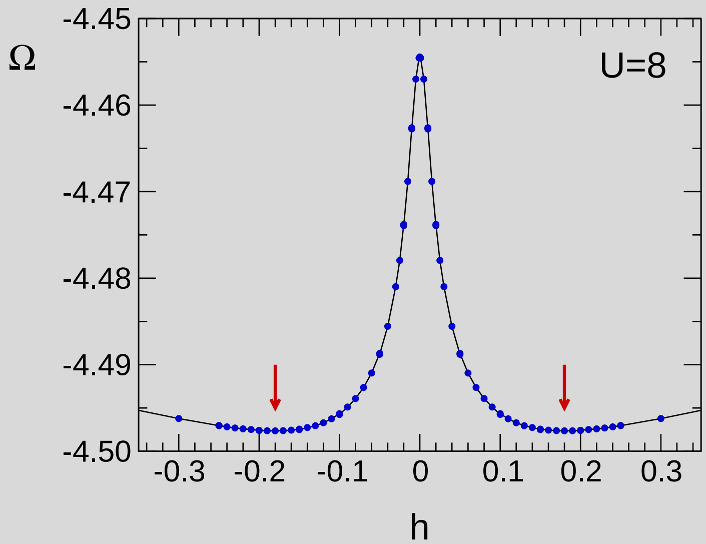
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



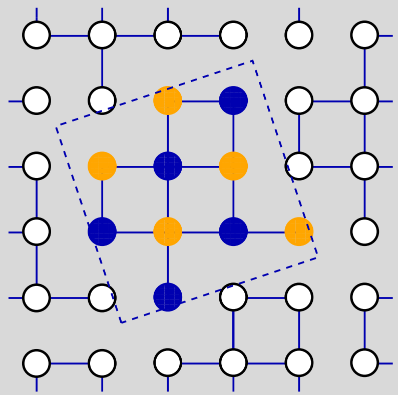
system of decoupled clusters

variational parameters:
ficticious symmetry-breaking fields
different order parameters

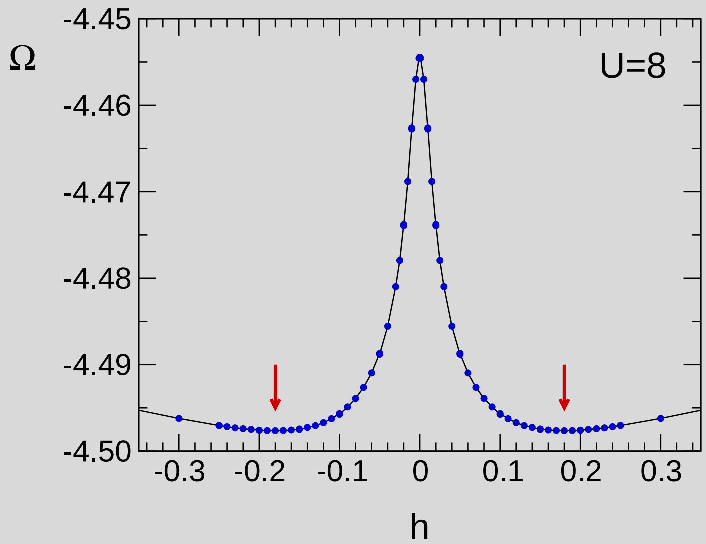
antiferromagnetism



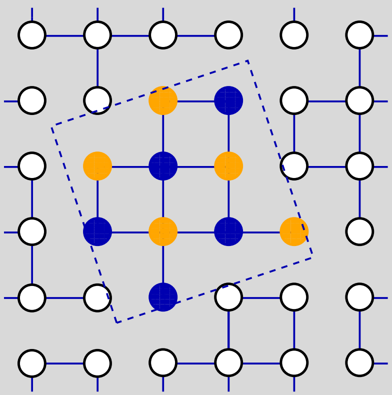
$D = 2$ Hubbard model, half-filling



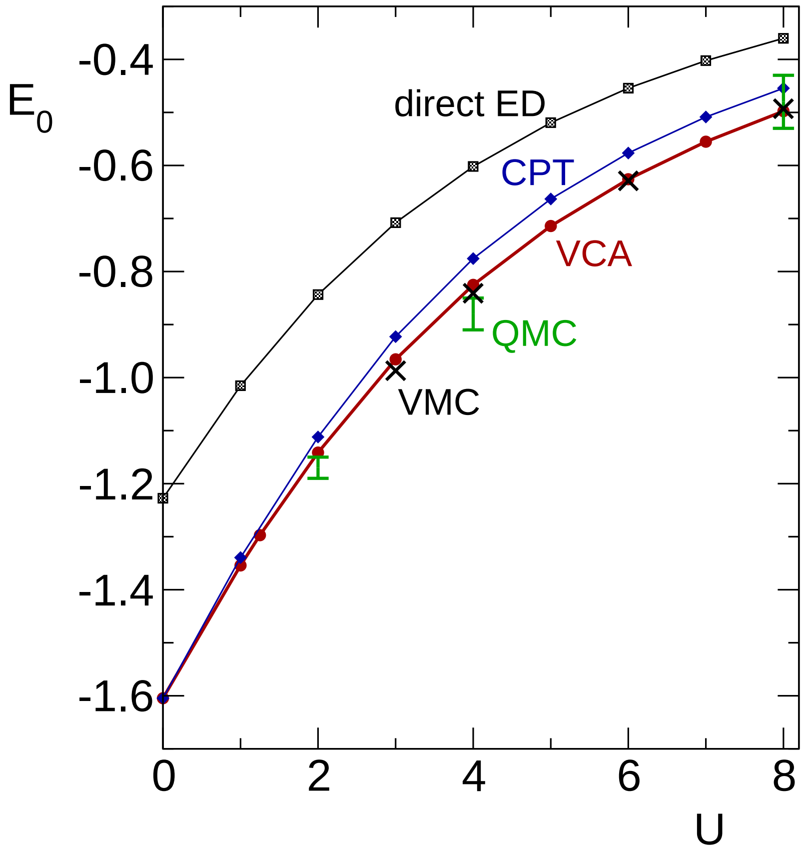
antiferromagnetism



$D = 2$ Hubbard model, half-filling



ground-state energy per site:

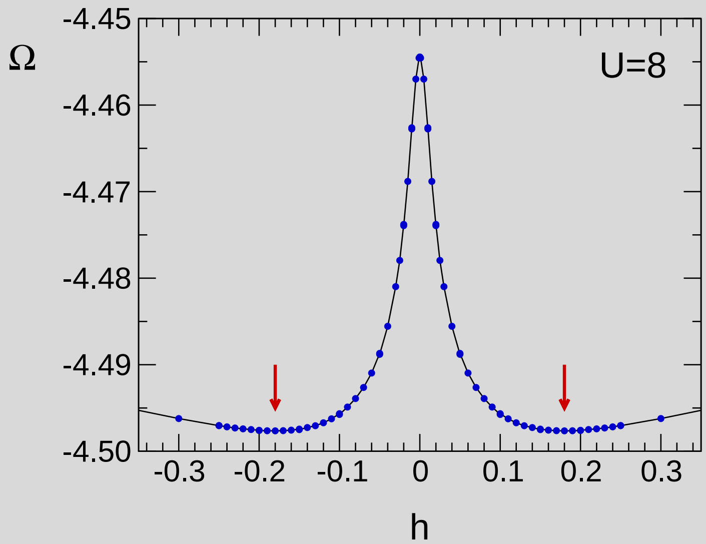


QMC, VMC: extrapolated to $L \to \infty$, $T \to 0$

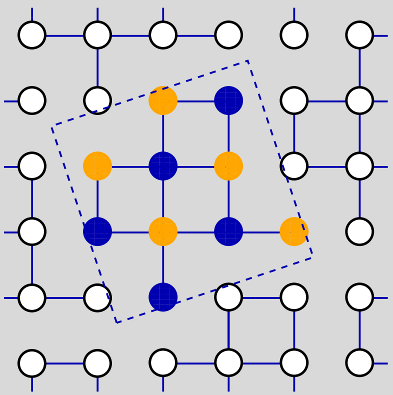
QMC: *Hirsch (1985)*

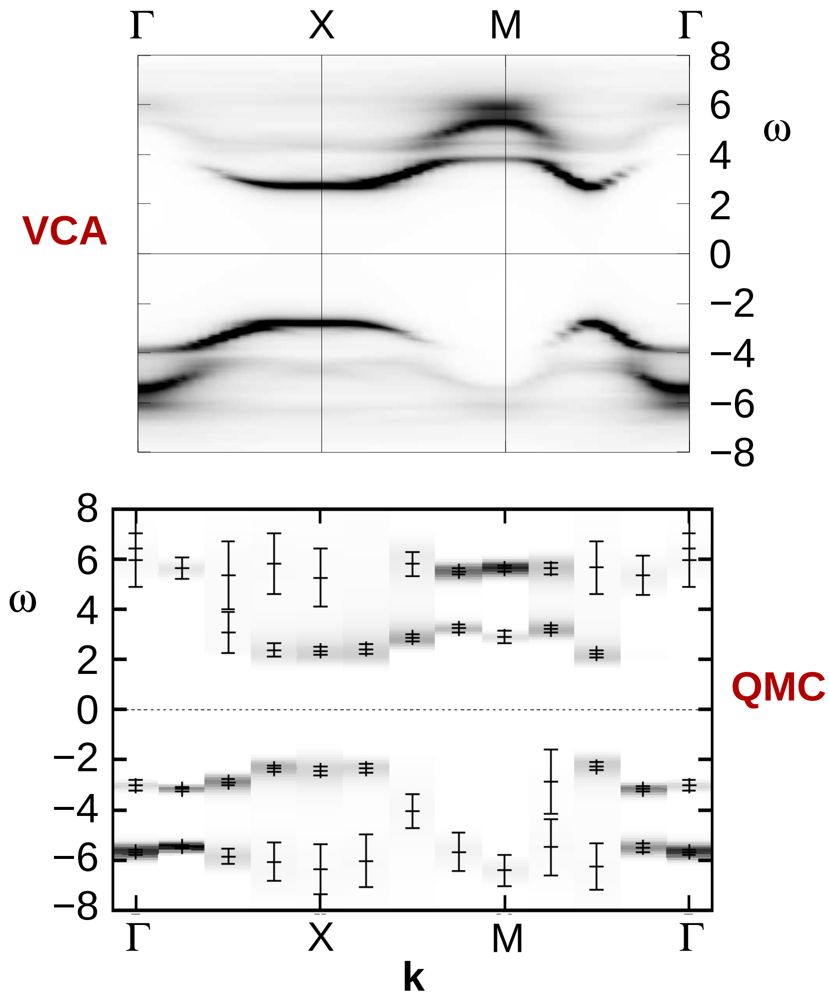
VMC: *Yokoyama, Shiba (1987)*

antiferromagnetism



$D = 2$ Hubbard model, half-filling

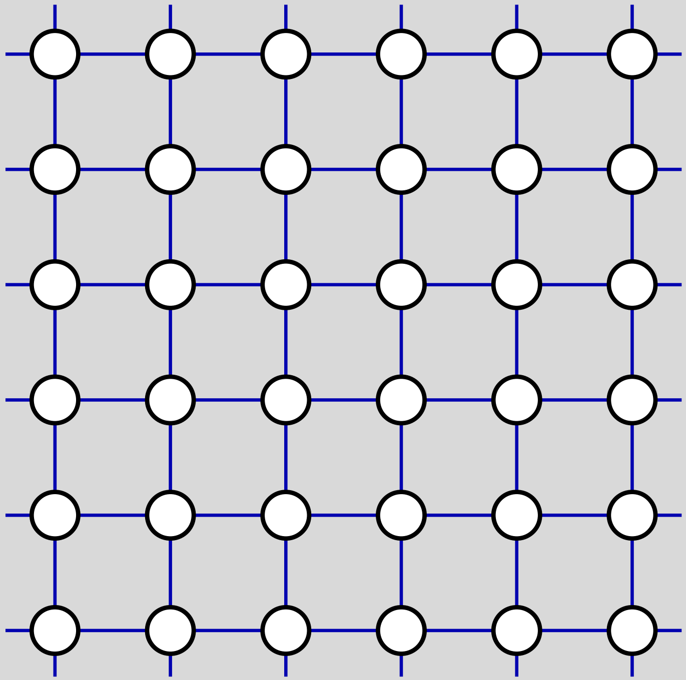




QMC / MaxEnt: $\beta = 10$, 8 $\times$ 8 cluster

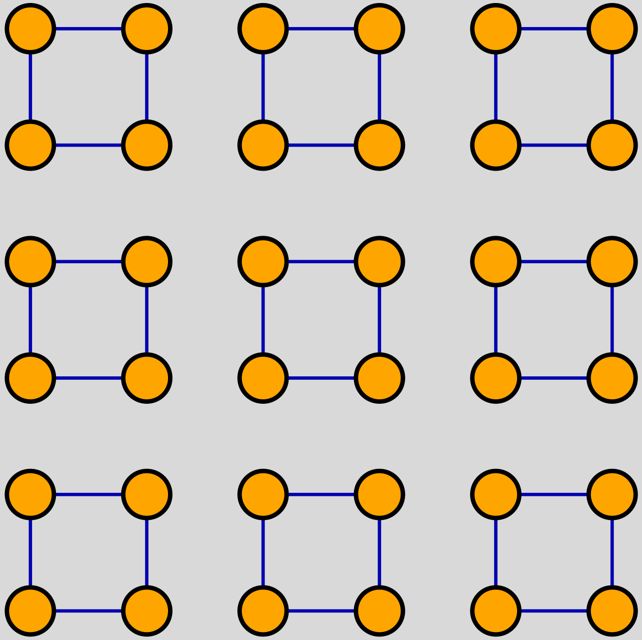
classification of approximations

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



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

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

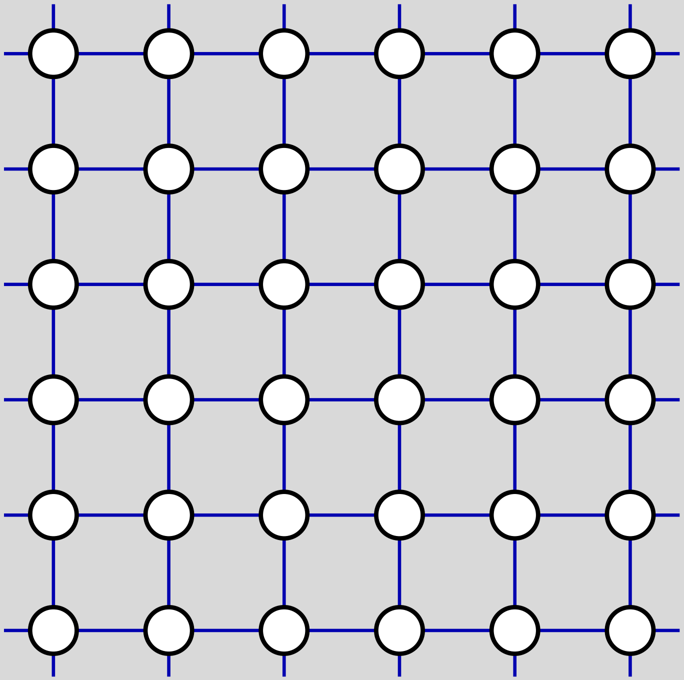


system of decoupled clusters

$L_c = 4$

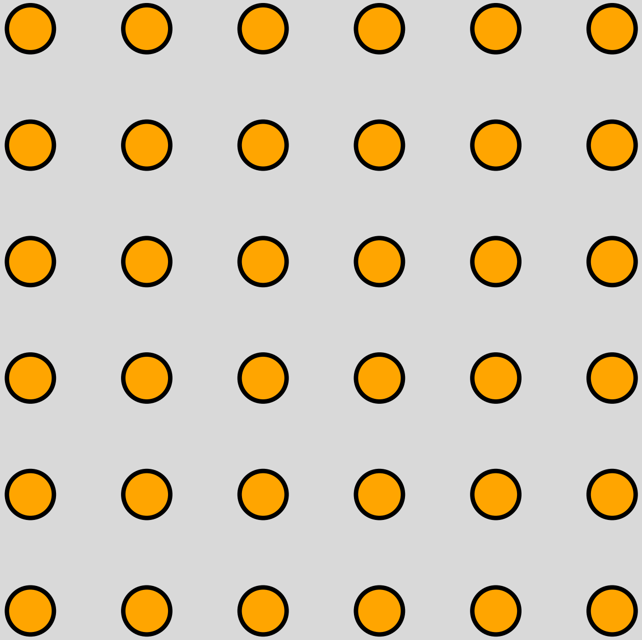
classification of approximations

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



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

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



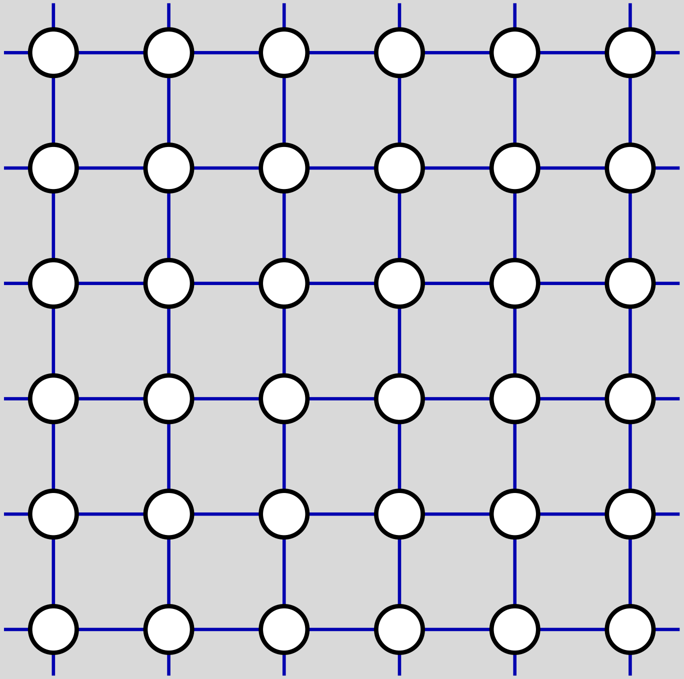
system of decoupled clusters

$L_c = 1$

Hubbard-I-type approximation

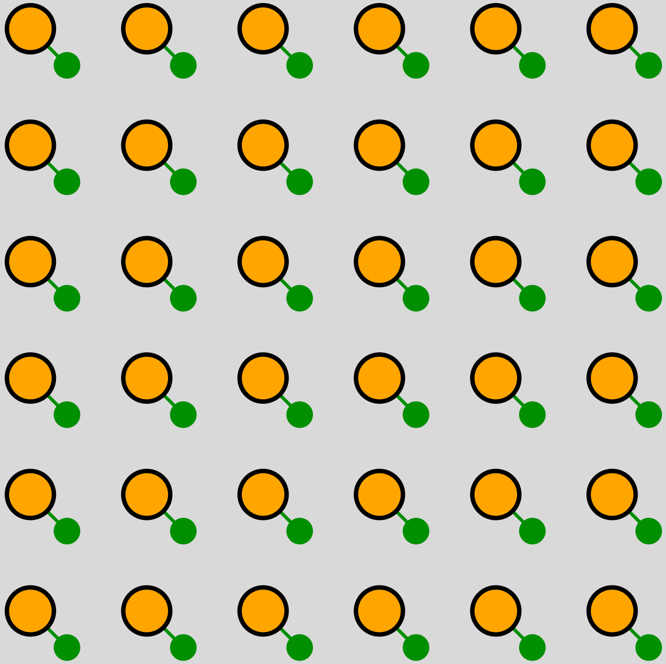
classification of approximations

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



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

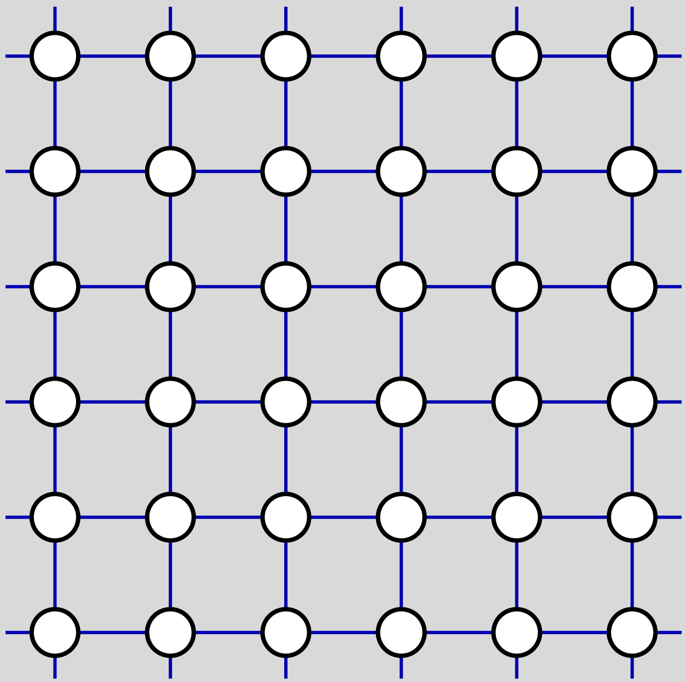
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

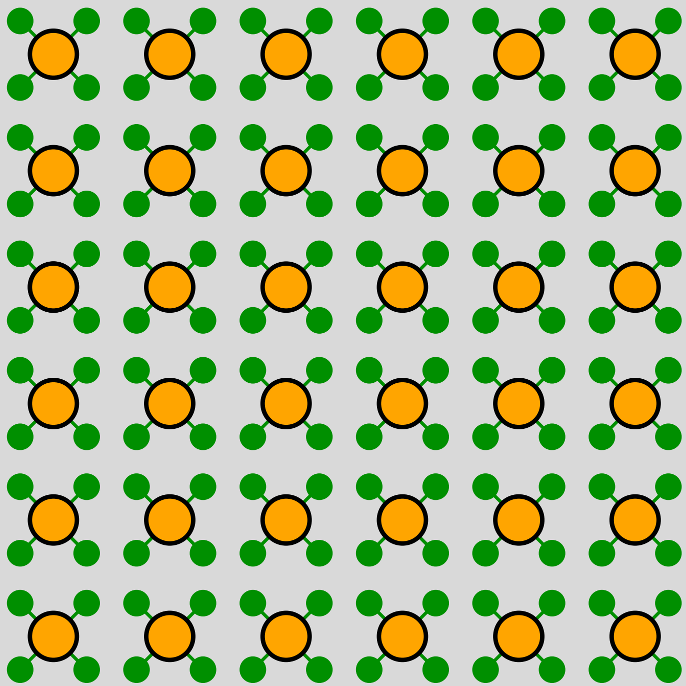
classification of approximations

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



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

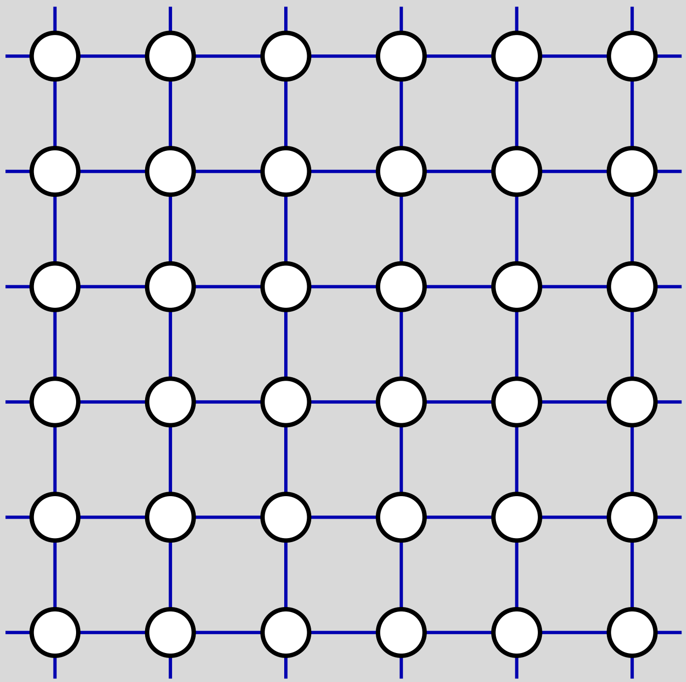
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

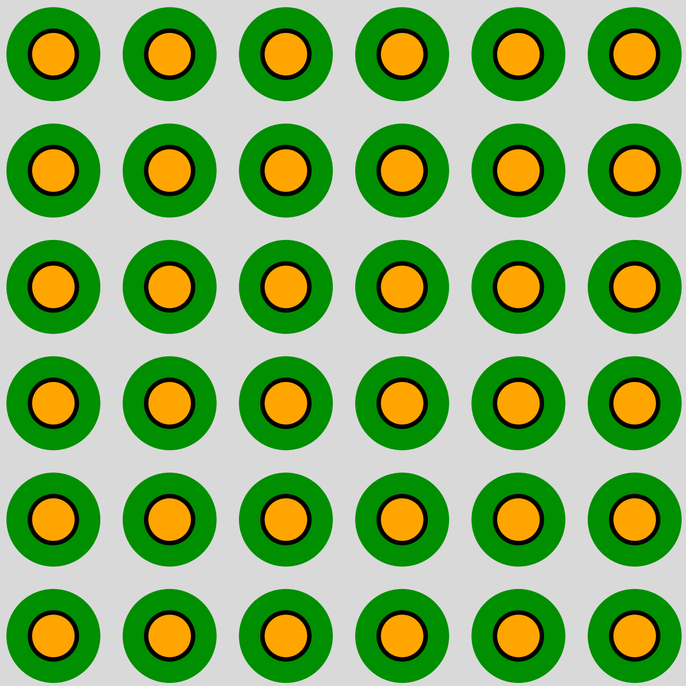
classification of approximations

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

with additional bath sites

$L_c = 1$, $L_b = \infty$

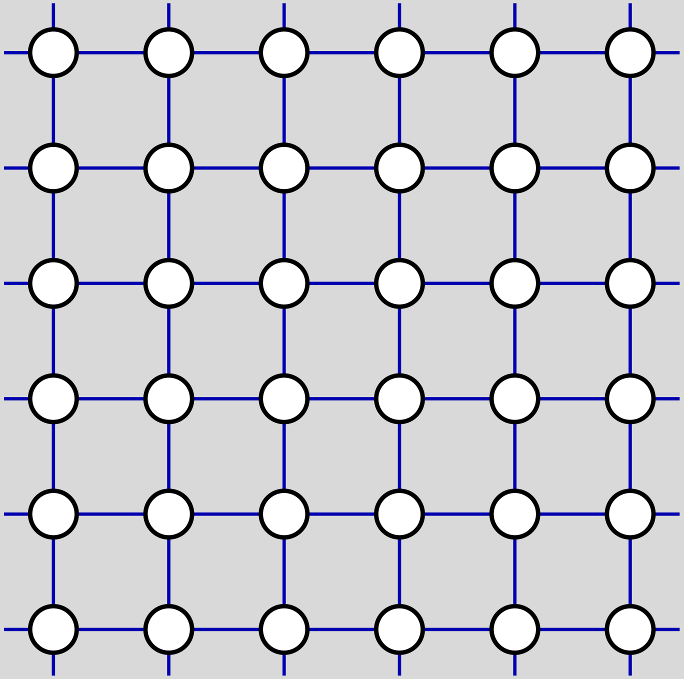
optimum mean-field theory, DMFT

Metzner, Vollhardt (1989)

Georges, Kotliar, Jarrell (1992)

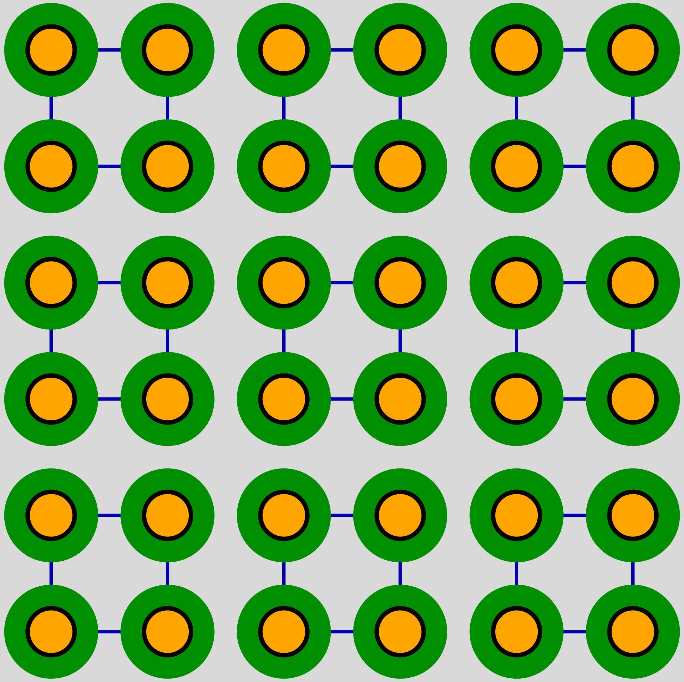
classification of approximations

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



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

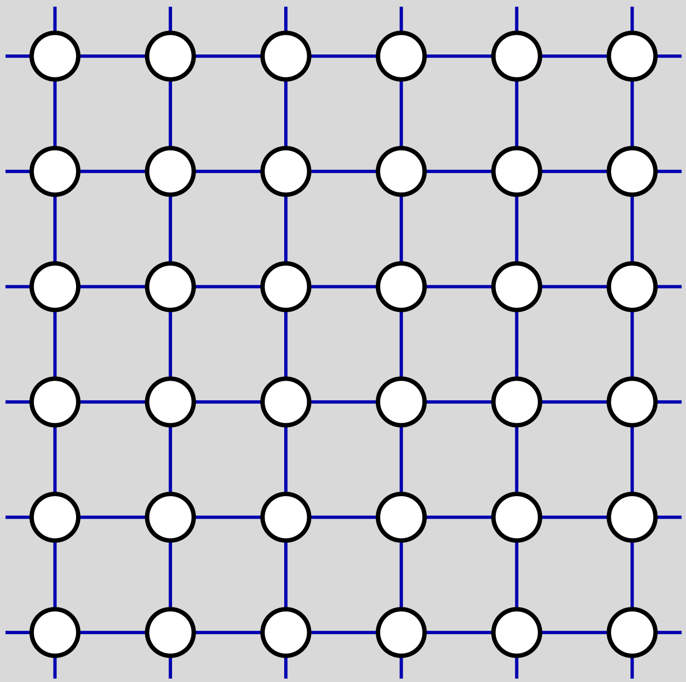
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

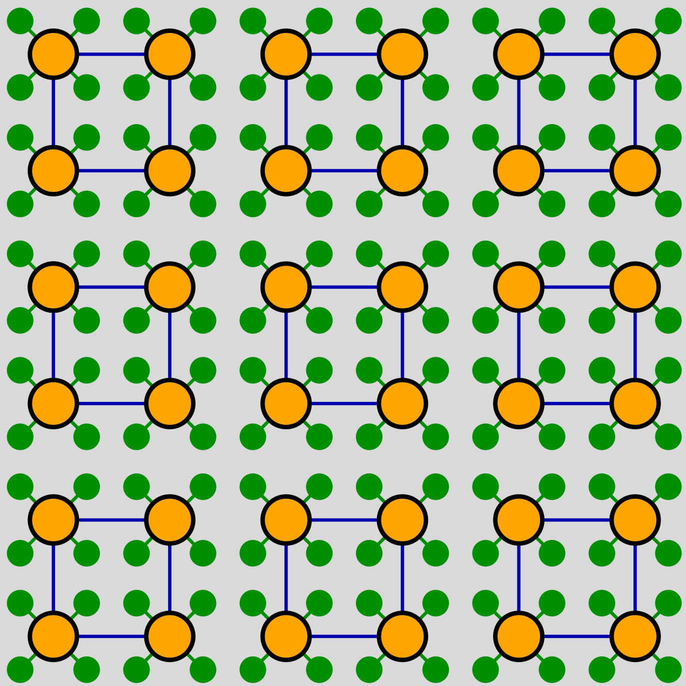
classification of approximations

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



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

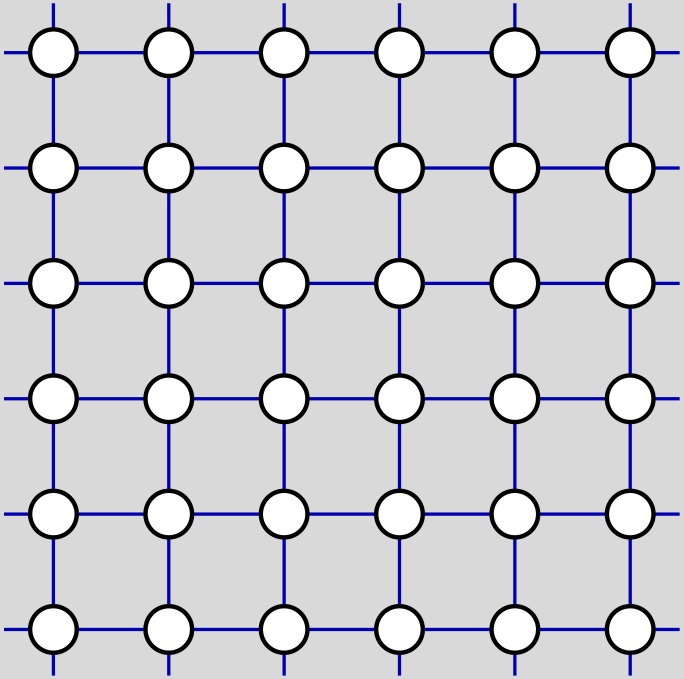
reference system, $H_{\mathbf{t}',\mathbf{U}}$**:**



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

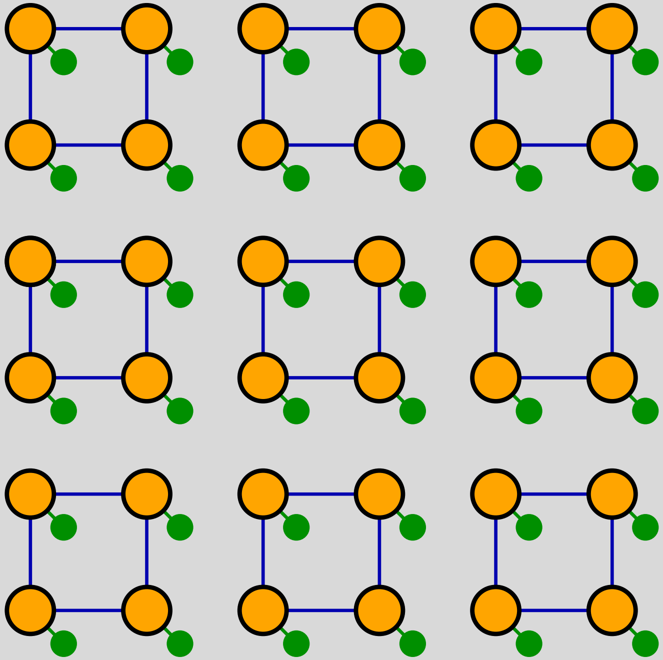
classification of approximations

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



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

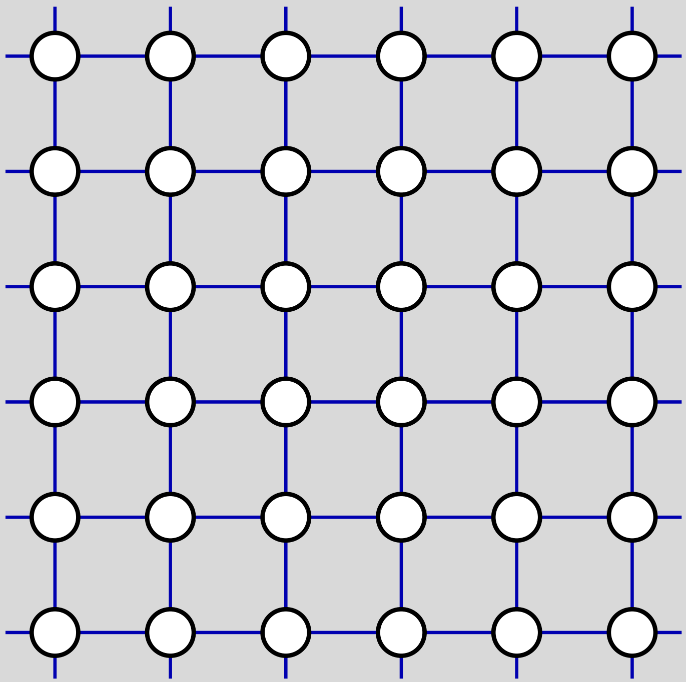
reference system, $H_{\mathbf{t}',\mathbf{U}}$:



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

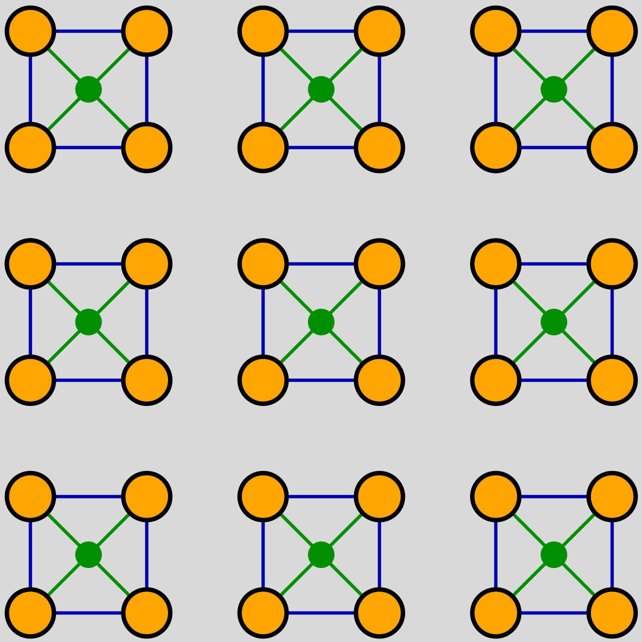
classification of approximations

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



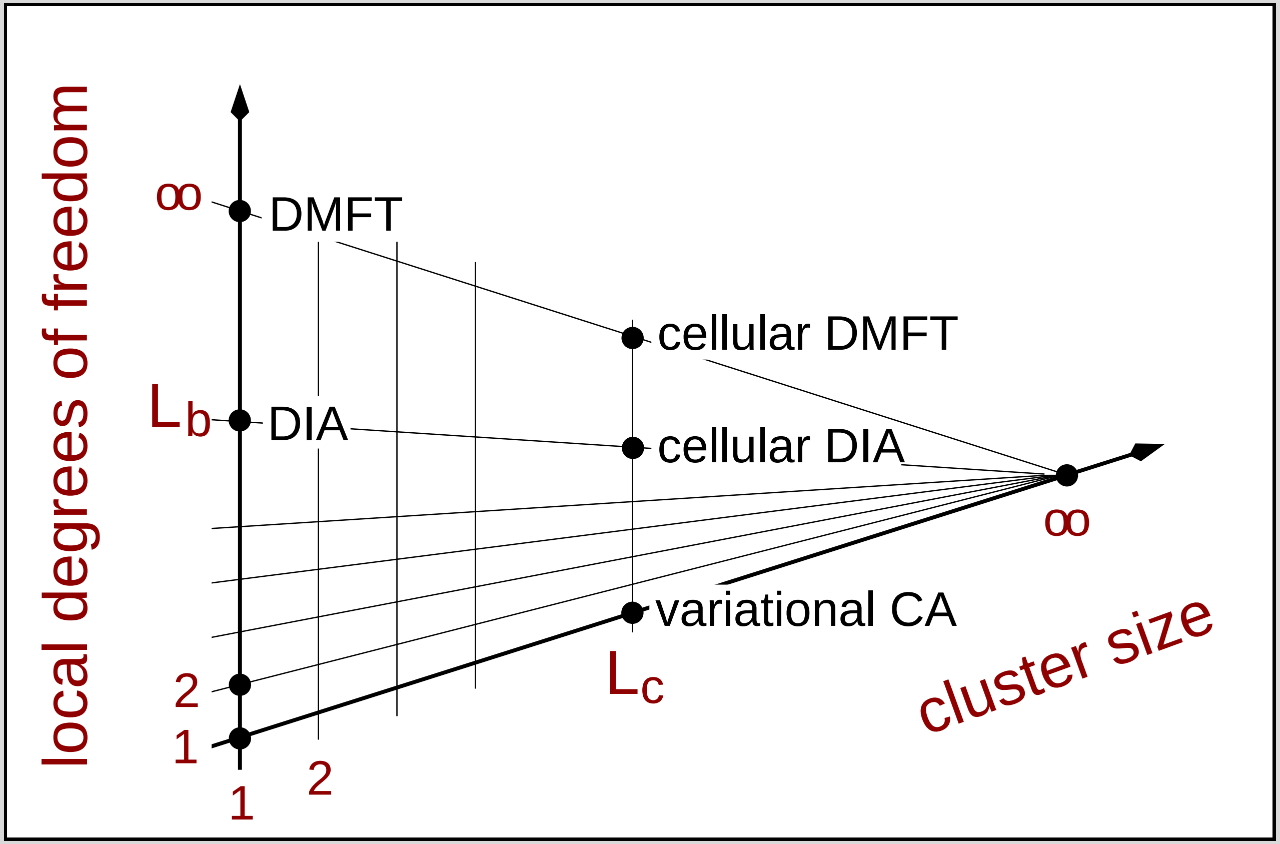
lattice model ($D = 2$) in
the thermodynamic limit

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



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

classification of 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)*

Luttinger sum rule

self-energy functional:

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

μ derivative:

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

particle number and FS volume:

$$N = N' - V'_{\mathrm{FS}} + V_{\mathrm{FS}}$$

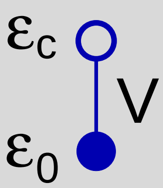
proliferation of the sum rule:

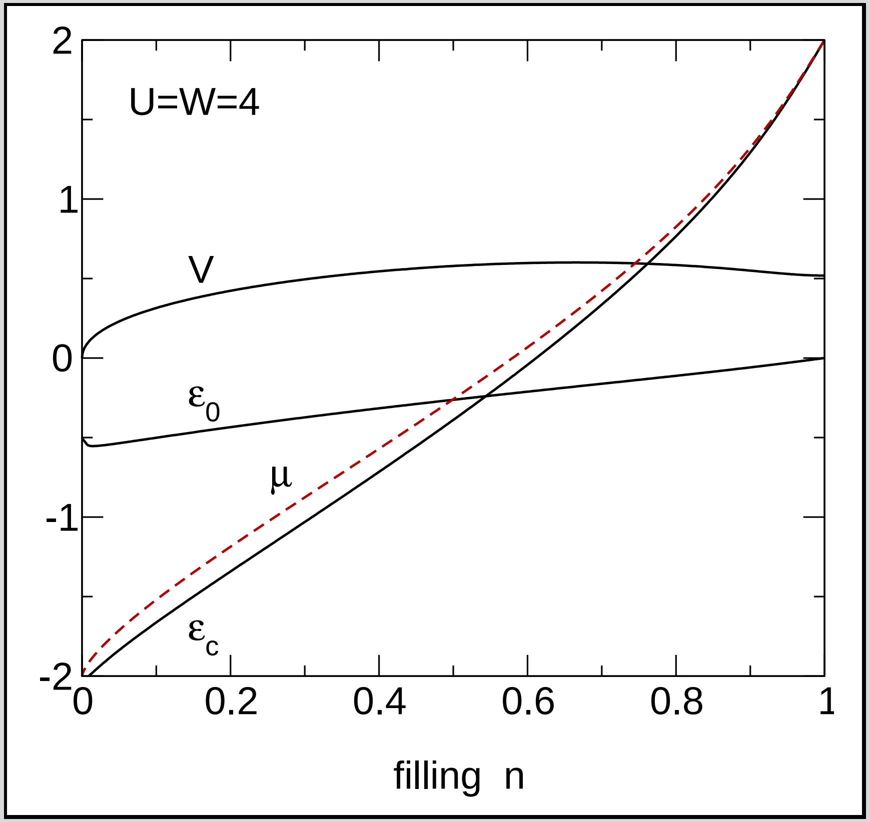
$$N = V_{\mathrm{FS}} \Leftrightarrow N' = V'_{\mathrm{FS}}$$

dynamical impurity approximation

Hubbard model, semielliptical free DOS ($W = 4$)

two-site DIA:





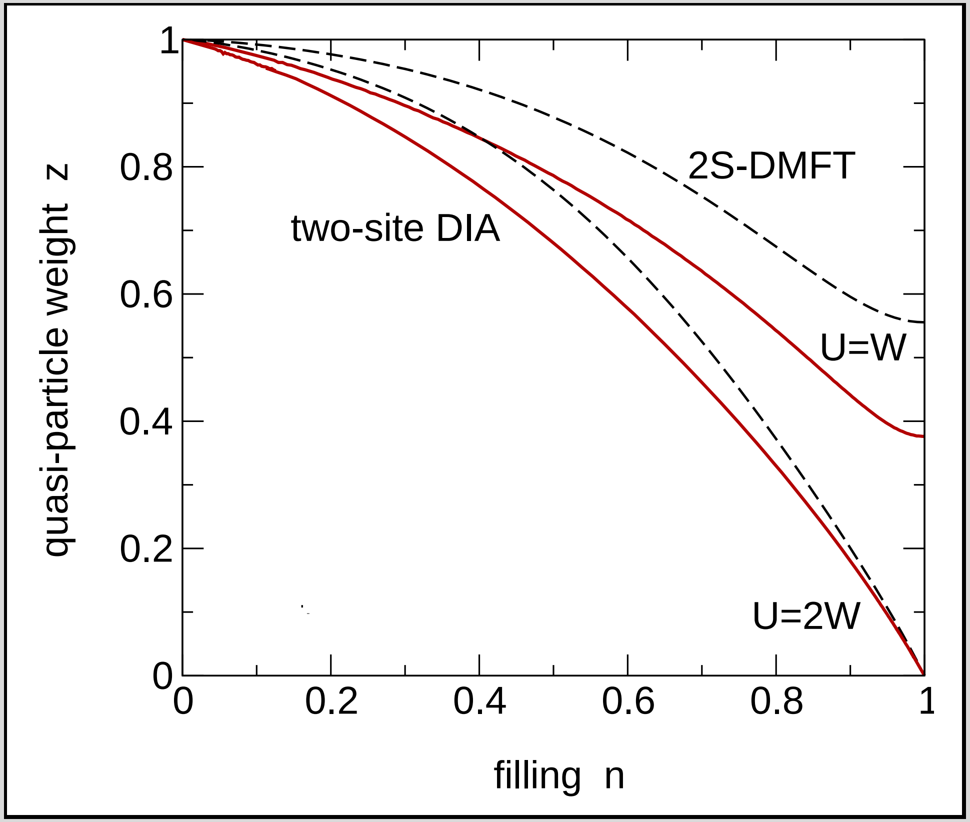
– total particle number: (2-site reference system) $N' = 2$

– Kondo regime: $\varepsilon_0 \ll \varepsilon_c, \mu \ll \varepsilon_0 + U$

– DMFT: $\varepsilon_0 =$ const $= 0$

effective mass

mass enhancement: $\dfrac{m^*}{m} = z^{-1} = 1 - \Sigma'(\omega = 0)$

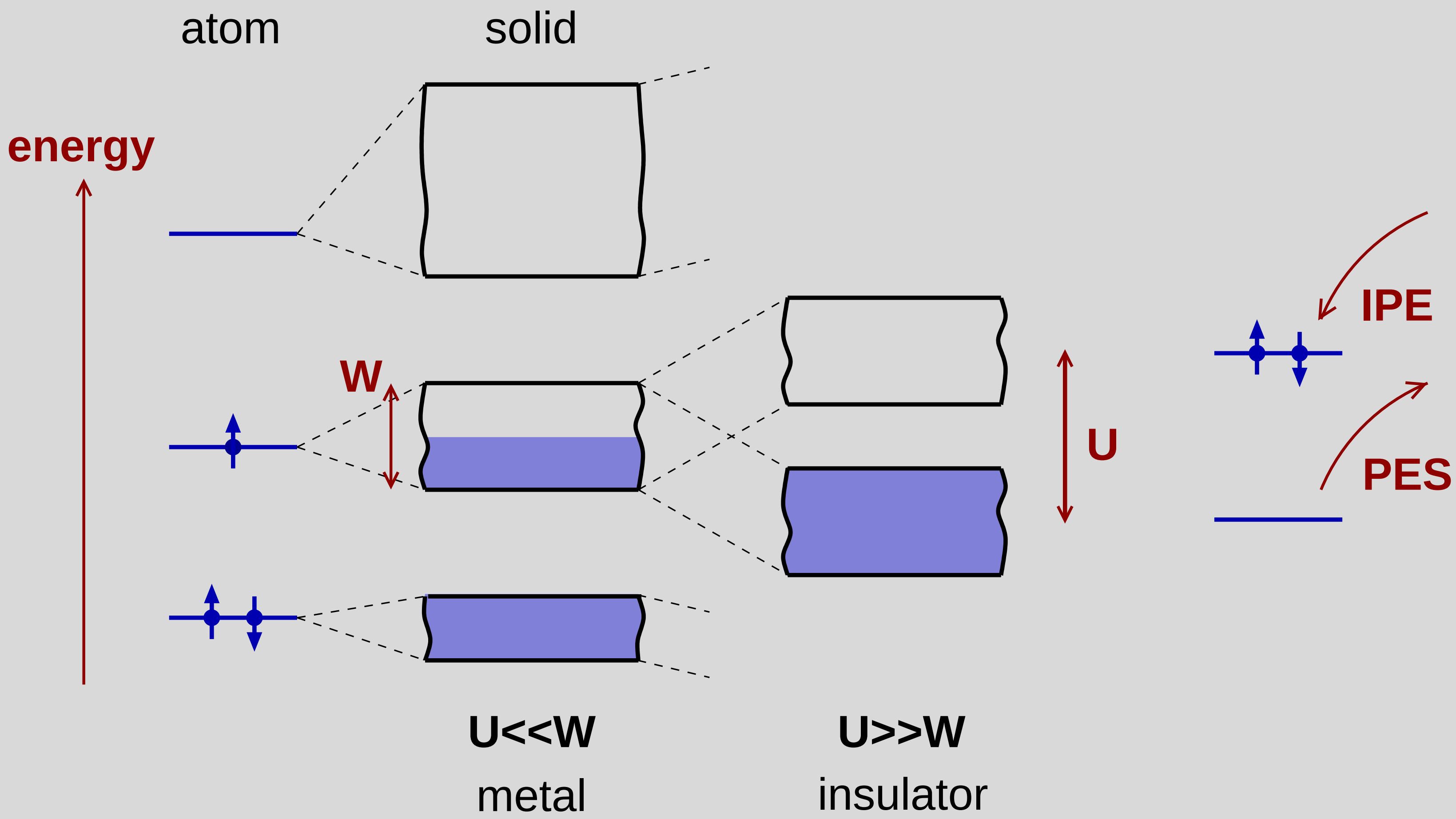


Hubbard model
semielliptical DOS, $W = 4$

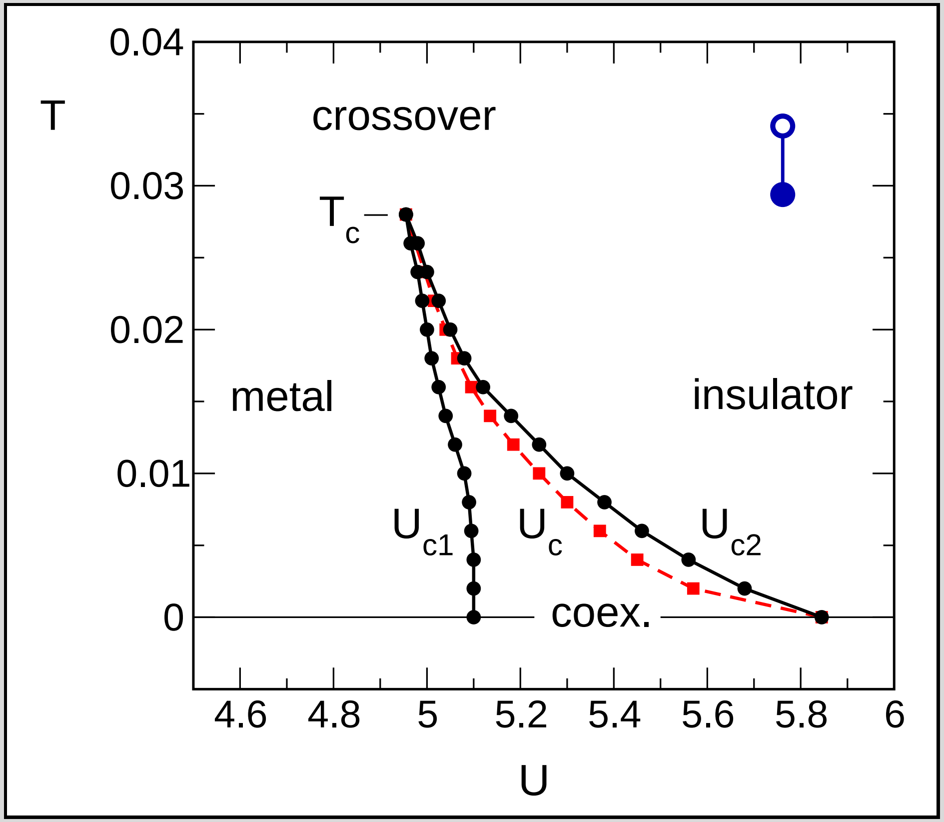
two-site DIA ($L_b = 2$)

➜ **Mott transition for $n \to 1$ and strong U**
➜ **2S-DMFT: non-conserving two-site approximation**

Mott transition



Mott transition: phase diagram



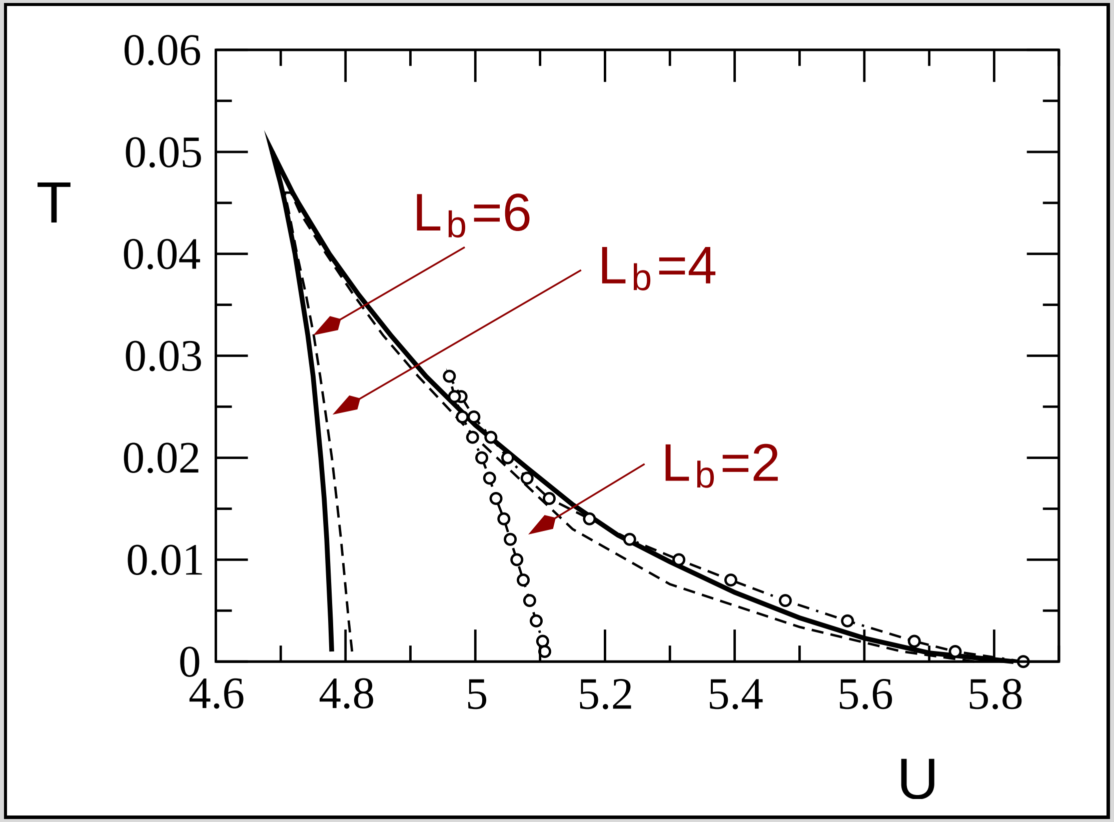
Hubbard model
half-filling
semielliptical DOS, $W = 4$

two-site DIA ($L_b = 2$)

➜ **qualitative** agreement wit DMFT (QMC, NRG)

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

convergence with increasing L_b



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

DIA

Pozgajcic (2004)

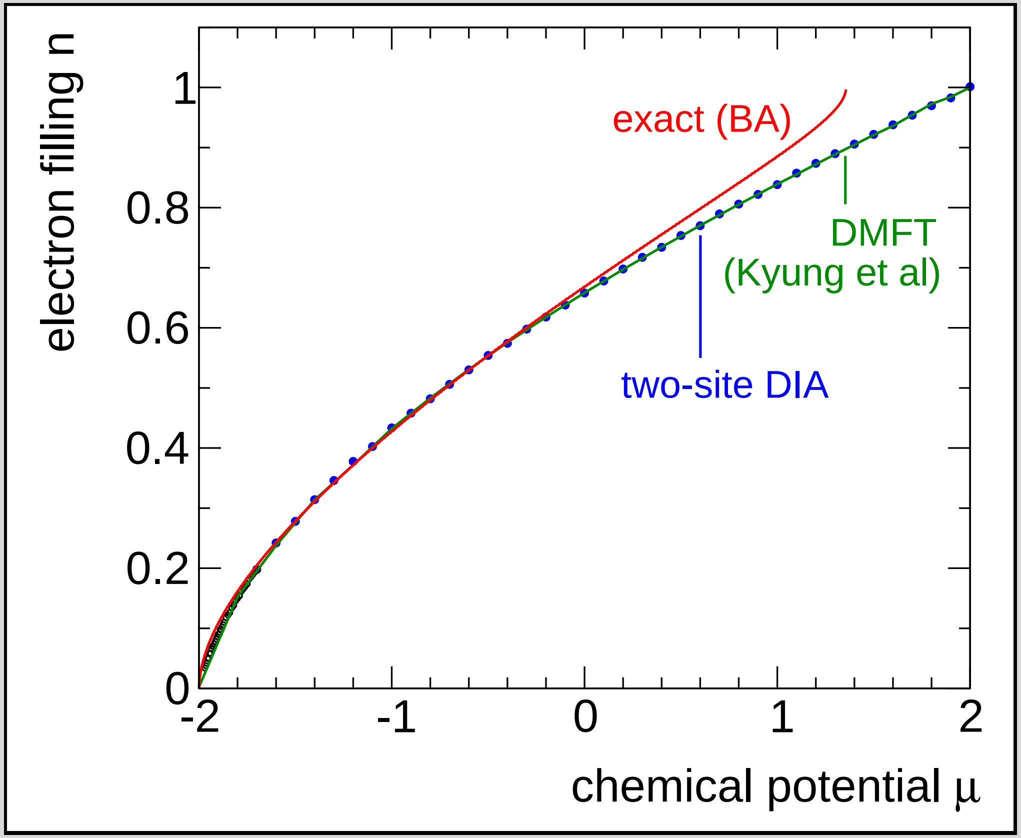
➜ **quantitative** agreement with DMFT (QMC, NRG)

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

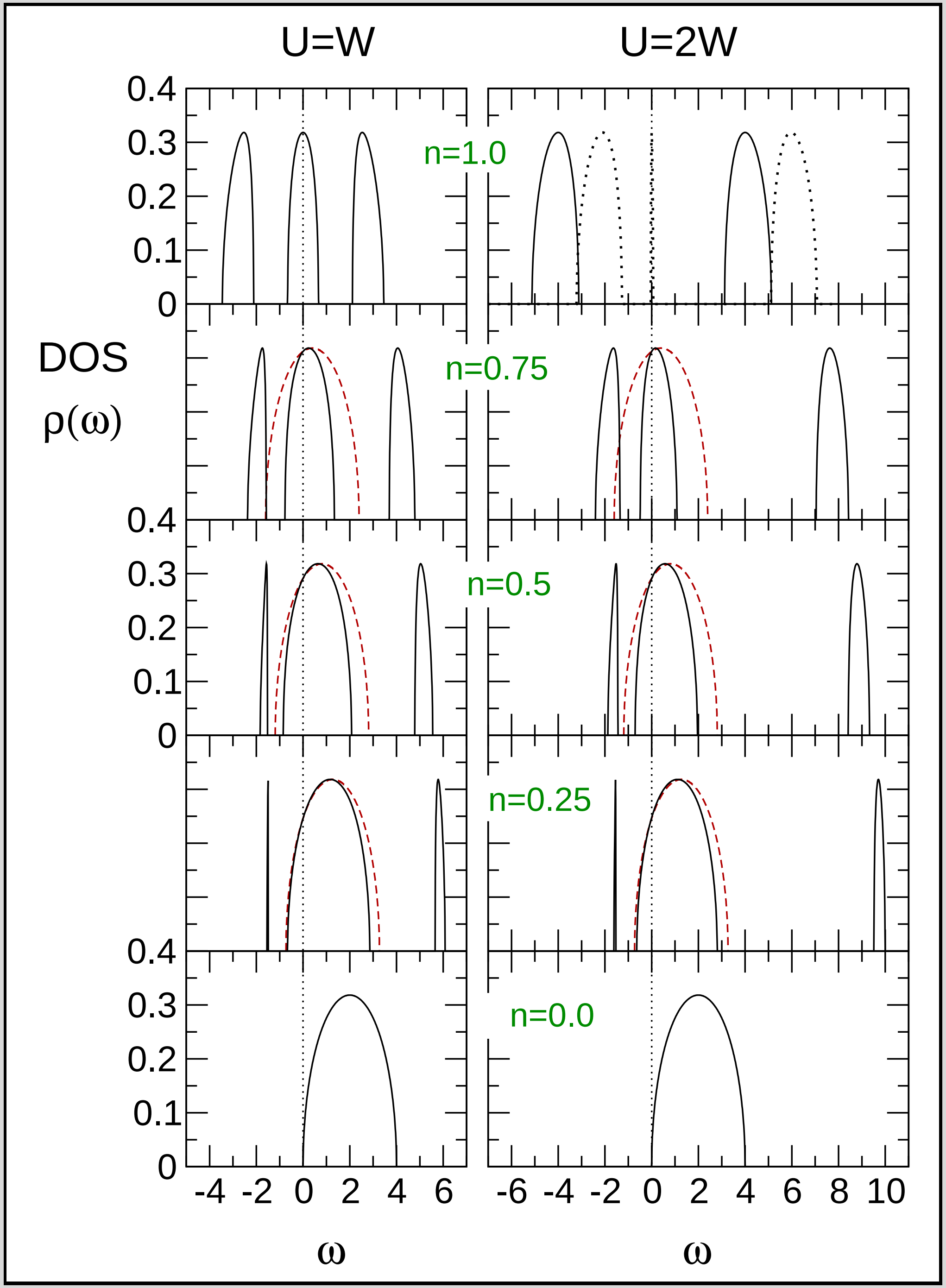
➜ **extremely fast convergence** with increasing L_b

one dimension: two-site DIA

Hubbard model, $D = 1$, $U = 4 = W$, $T = 0$: exact (Bethe ansatz) vs. DMFT vs. 2S-DIA



density of states



Luttinger sum rule for a $\mathbf{k}$-independent self-energy:

➜ $V_{\mathrm{FS}} = V_{\mathrm{FS}}^{(0)}$

$$V_{\mathrm{FS}} = 2\sum_{\mathbf{k}} \Theta(\mu - \varepsilon(\mathbf{k}) - \Sigma(0))$$

$$V_{\mathrm{FS}}^{(0)} = 2\sum_{\mathbf{k}} \Theta(\mu_0 - \varepsilon(\mathbf{k}))$$

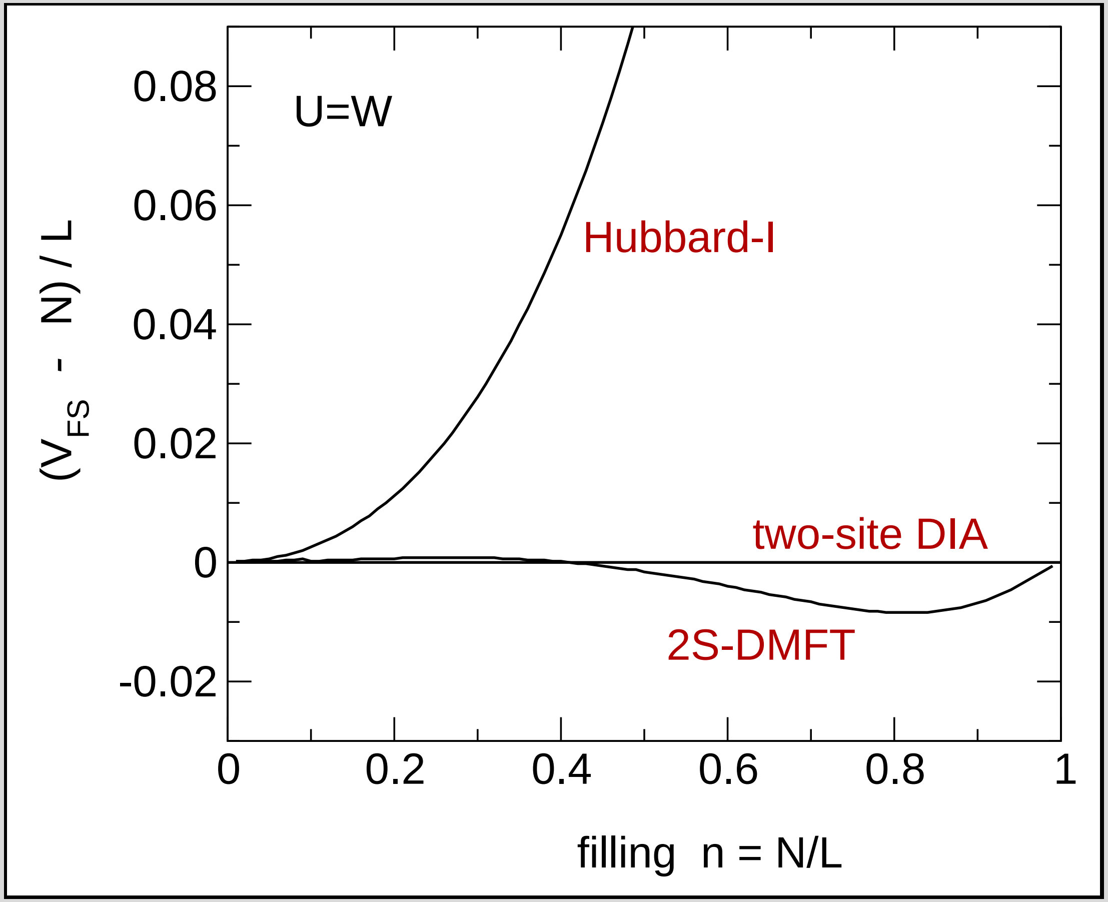
➜ $\mu = \mu_0 + \Sigma(0)$

$$\rho(\omega) = \sum_{\mathbf{k}} \delta(\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(\omega))$$

$$\rho_0(\omega) = \sum_{\mathbf{k}} \delta(\omega + \mu_0 - \varepsilon(\mathbf{k}))$$

➜ $\rho(0) = \rho_0(0)$

Fermi-surface volume



➜ non-conserving approximations: Hubbard-I, 2S-DMFT

➜ conserving approximation: two-site DIA

single-impurity Anderson model

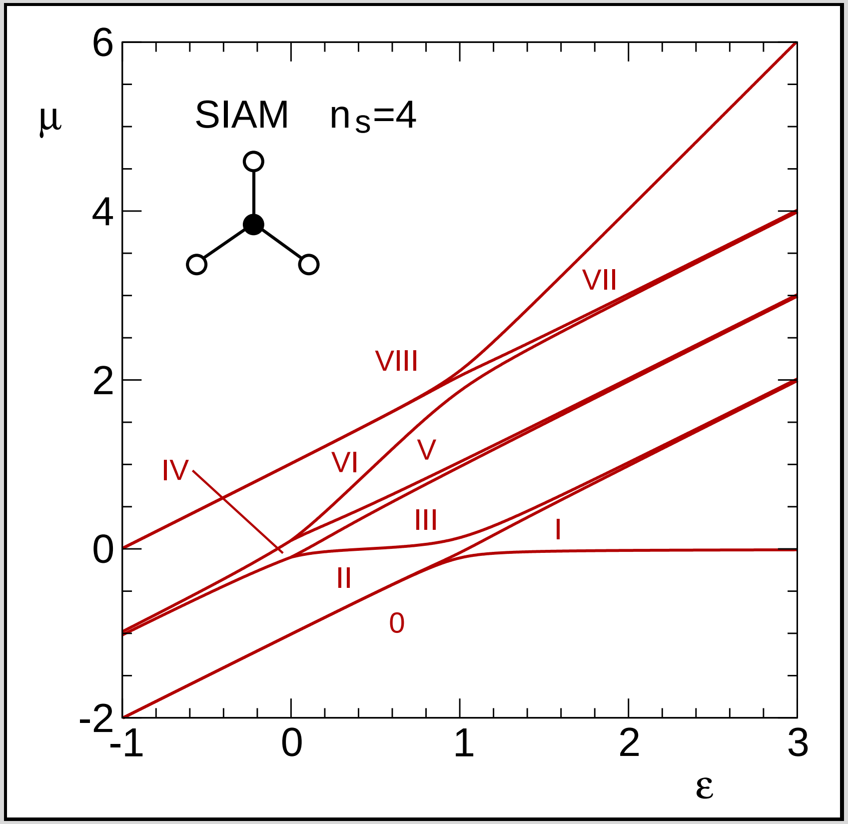
sum rule fulfilled within 2S-DIA ➜ sum rule fulfilled exactly for reference system

$$N = V_{\mathrm{FS}} \Leftrightarrow N' = V'_{\mathrm{FS}}$$

direct check:

1) $L_b = 2$: analytically
2) $L_b = 4$: full diagonalization
3) $L_b \leq 10$: Lanczos

➜ sum rule never violated



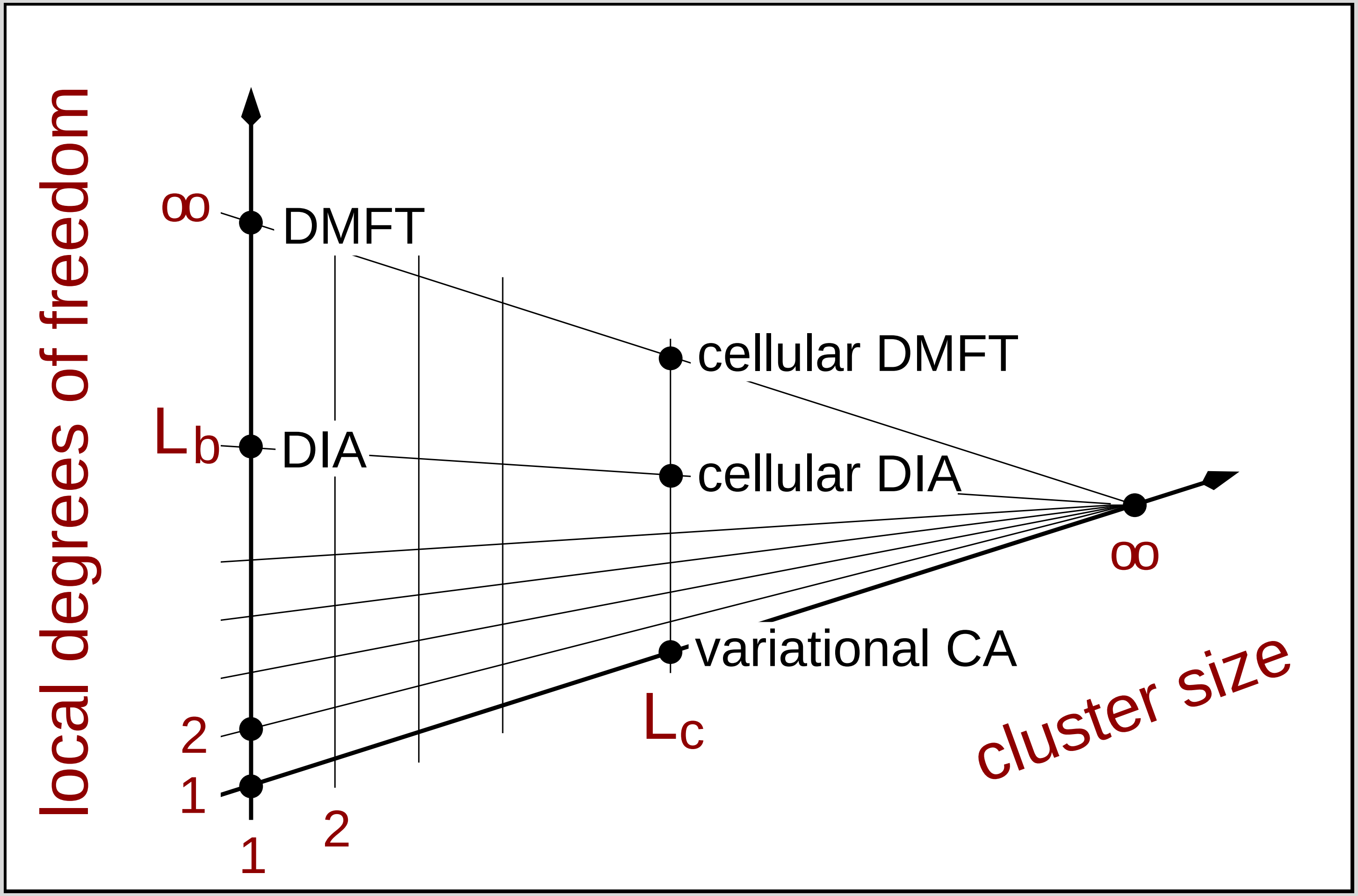
$U = 2\varepsilon, V_k = 0.1, \varepsilon_k = \varepsilon + (k-3), k = 2,3,4$

Green's function: $G_{\alpha\beta}(\omega)$
diagonalized Green's function: $G_k(\omega)$
Luttinger sum rule:

$$\sum_{k,m} \alpha_m^{(k)} \Theta(\mu - \omega_m^{(k)}) = \sum_{k,m} \Theta(\mu - \omega_m^{(k)}) - \sum_{k,n} \Theta(\mu - \zeta_n^{(k)})$$

cluster approximations

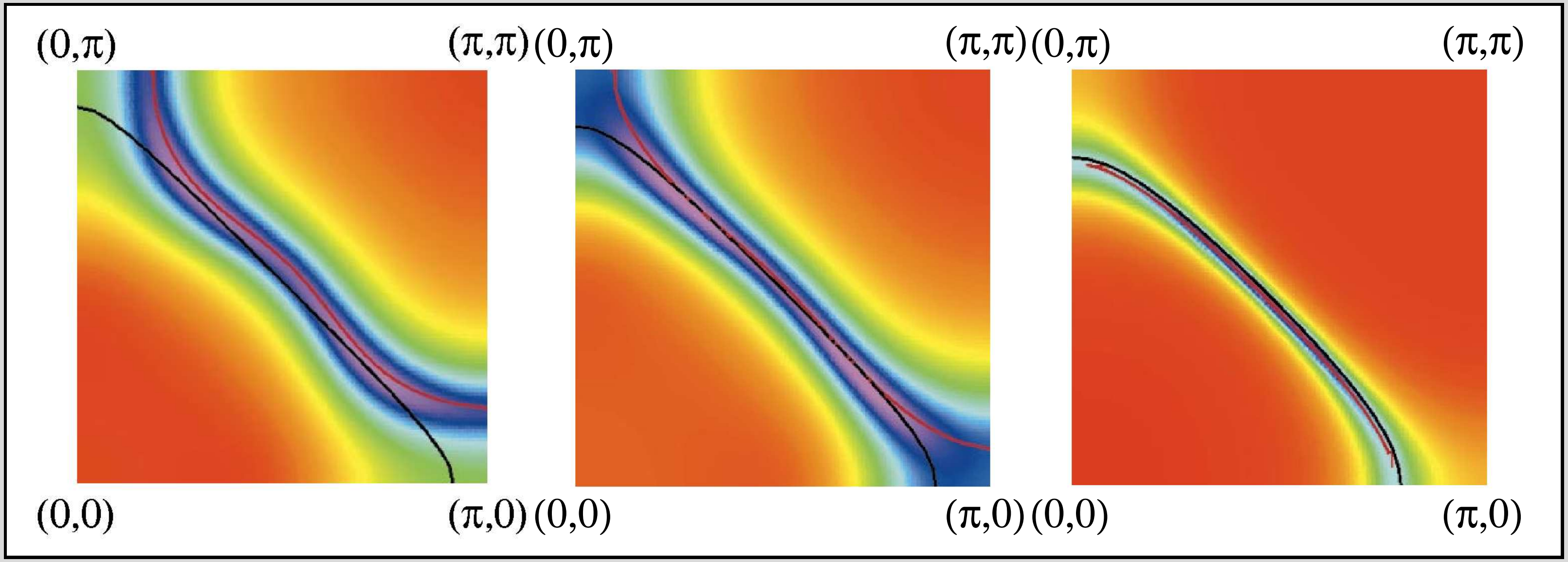
$$N = V_{\mathrm{FS}} \Leftrightarrow N' = V'_{\mathrm{FS}}$$



dynamical cluster approximation (DCA)

Hubbard model, $D = 2$, n.n. hopping t, $U = W = 8t$, $T = W/60$, $L_c = 16$, QMC

$n = 0.95$ $n = 0.9$ $n = 0.8$



$A(\mathbf{k}, \omega = 0)$ *Maier, Pruschke, Jarrell (2002)*

➜ sum rule violated close to Mott insulator

finite Hubbard clusters

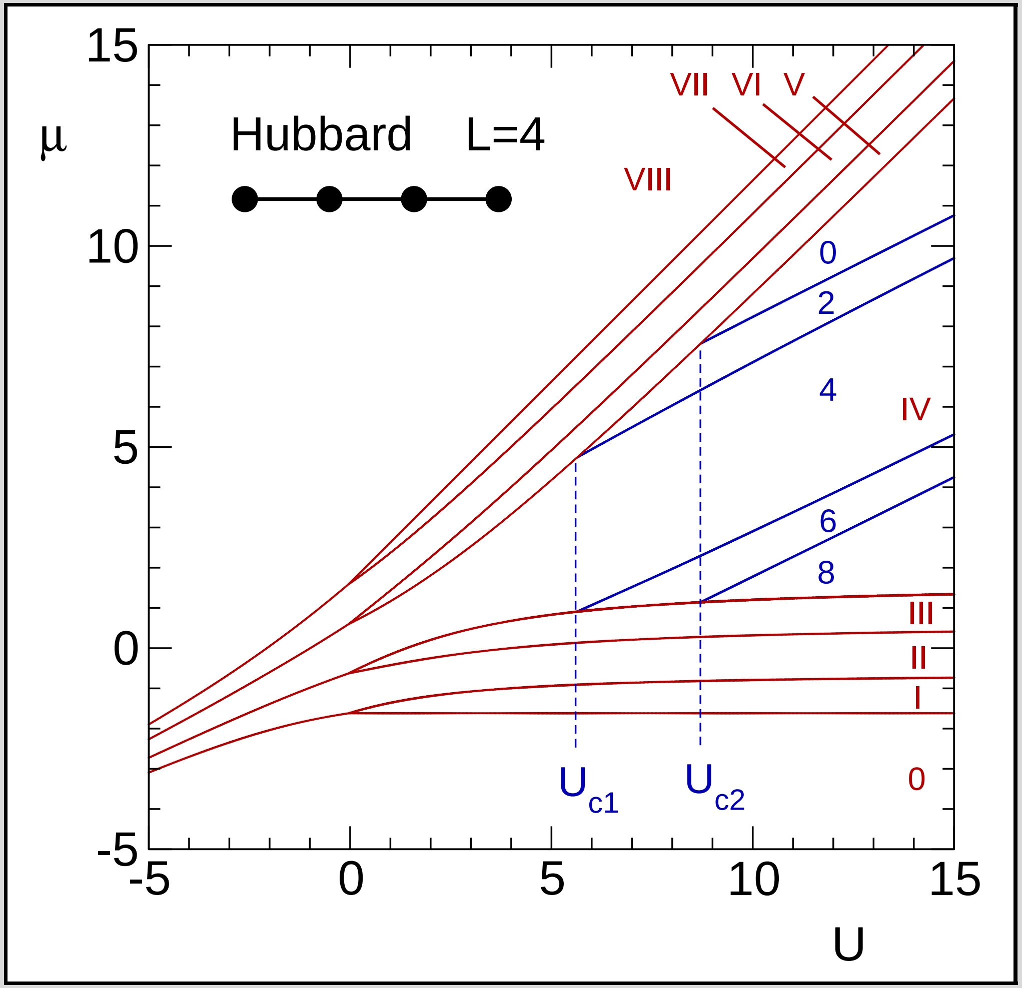
sum rule violated for Hubbard clusters?

$$N = V_{\rm FS} \Leftrightarrow N' = V'_{\rm FS}$$

direct check:

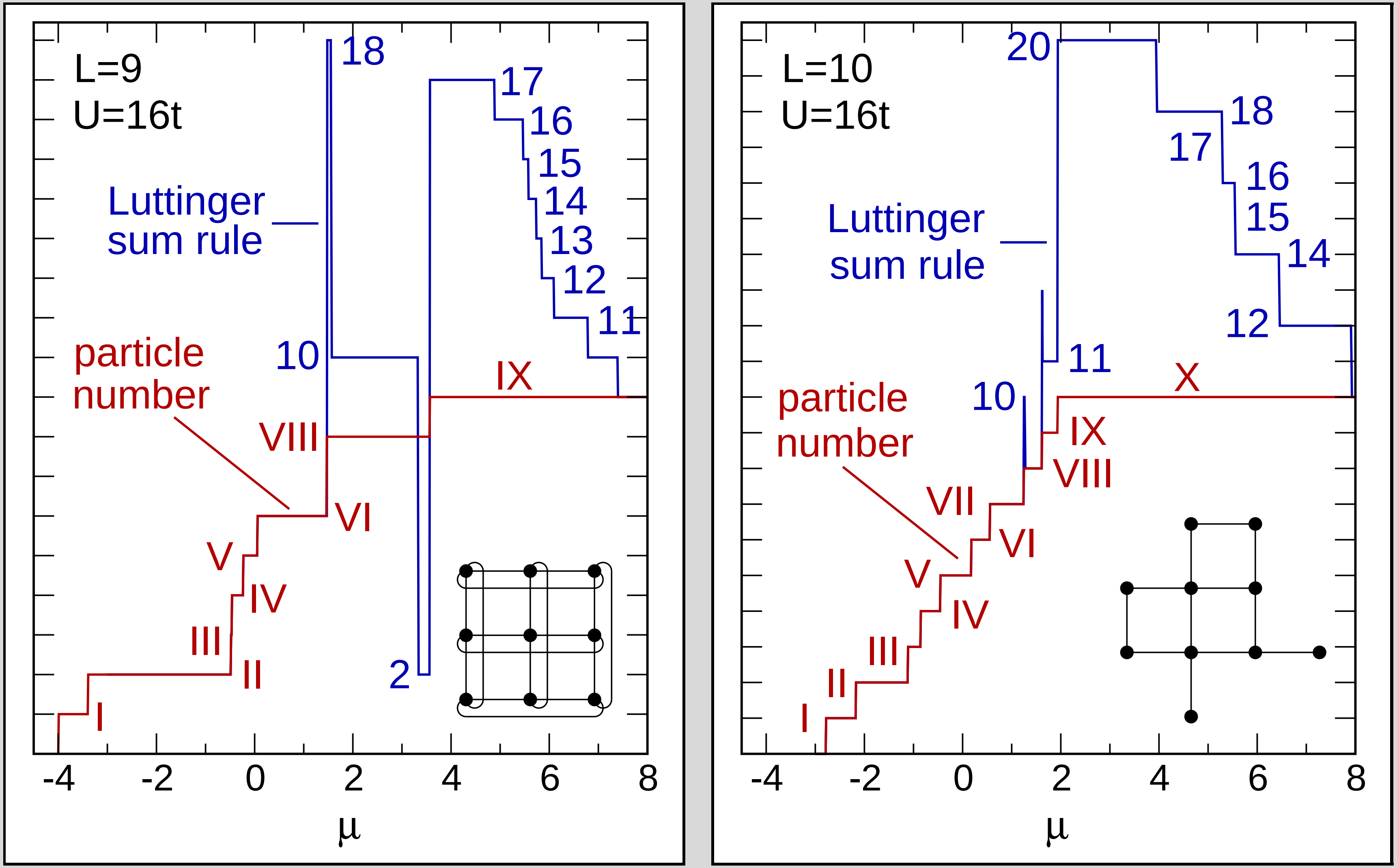
1) $L_c = 2$: analytically
2) $L_c = 4$: full diagonalization
3) $L_c \leq 10$: Lanczos

➜ sum rule violated
for the Mott insulator



$$\sum_{k,m} \alpha_m^{(k)} \Theta(\mu - \omega_m^{(k)}) = \sum_{k,m} \Theta(\mu - \omega_m^{(k)}) - \sum_{k,n} \Theta(\mu - \zeta_n^{(k)})$$

finite Hubbard clusters



➜ sum rule violated close to Mott insulator

conclusions

- **Fermi-liquid theory:** $N = V_{\rm FS}$
- **proof: perturbation theory to all orders** n **(**$n \to \infty$**) for** $T \to 0$
- **(weak-coupling) conserving approximations: truncation of** $\Phi[\mathbf{G}]$
  – macroscopic conservation laws respected
  – thermodynamically consistent
  – Luttinger's sum rule respected
- **non-perturbative construction of** $\Phi[\mathbf{G}]$ **possible (**$T > 0$**)**
- **self-energy-functional theory: non-perturbative conserving approximations**
  – dynamical impurity approximation (DIA)
  – variational cluster approximation (VCA)
  – DMFT, C-DMFT/DCA
- **sum rule:** $N = V_{\rm FS} \Leftrightarrow N' = V'_{\rm FS}$
- **sum rule respected by DMFT, DIA** $\Leftrightarrow$ **sum rule holds for the (finite) single-impurity Anderson model (Friedel sum rule)**
- **sum rule violated by DCA, VCA** $\Leftrightarrow$ **sum rule violated for Hubbard clusters**
- **where is the defect in the proof? proposal:** $\lim\limits_{T\to 0}\lim\limits_{n\to\infty} \neq \lim\limits_{n\to\infty}\lim\limits_{T\to 0}$