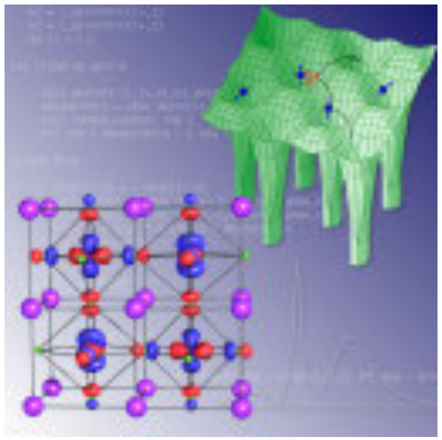

Making Use of Self-Energy Functionals: The Variational Cluster Approximation

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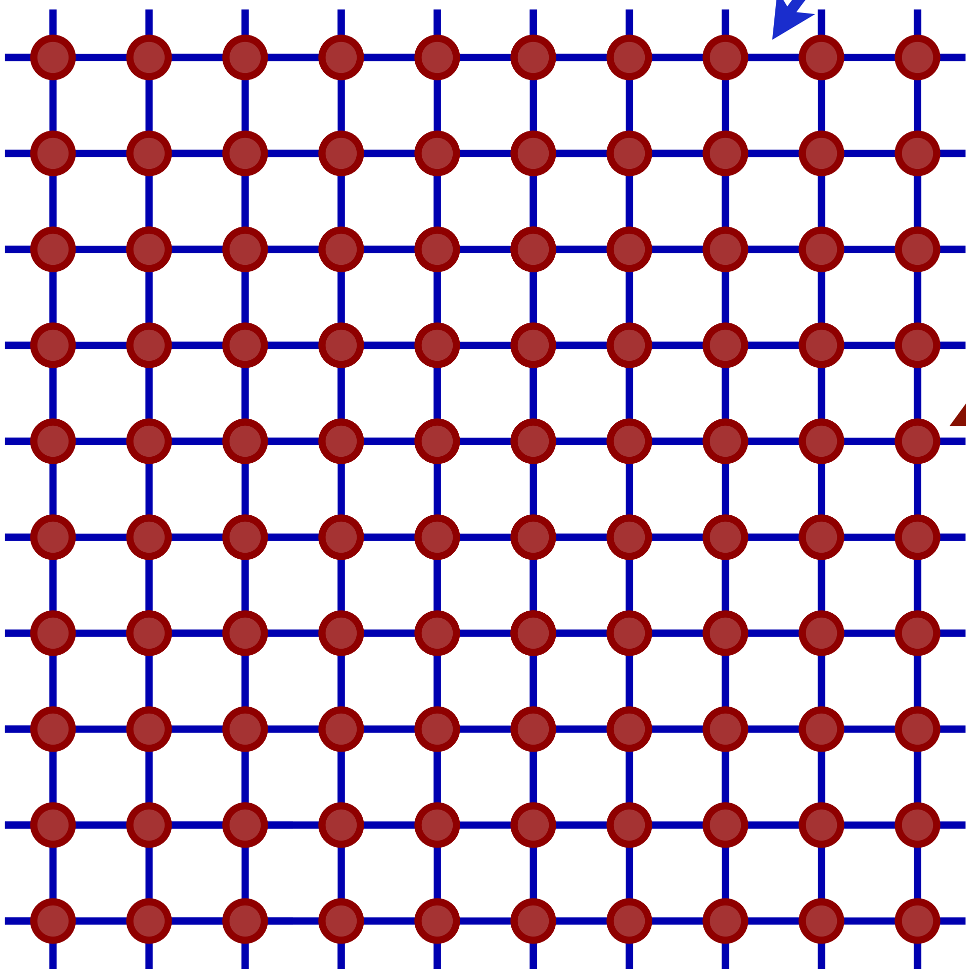
outline:
- the cluster approach
- diagrammatic perturbation theory
- self-energy-functional theory
- implementation of the variational cluster approximation
- selected results
- relation to other methods

The Hubbard model

$$H = H_0(\boldsymbol{t}) + H_1$$



kinetic and potential energy

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

interaction energy

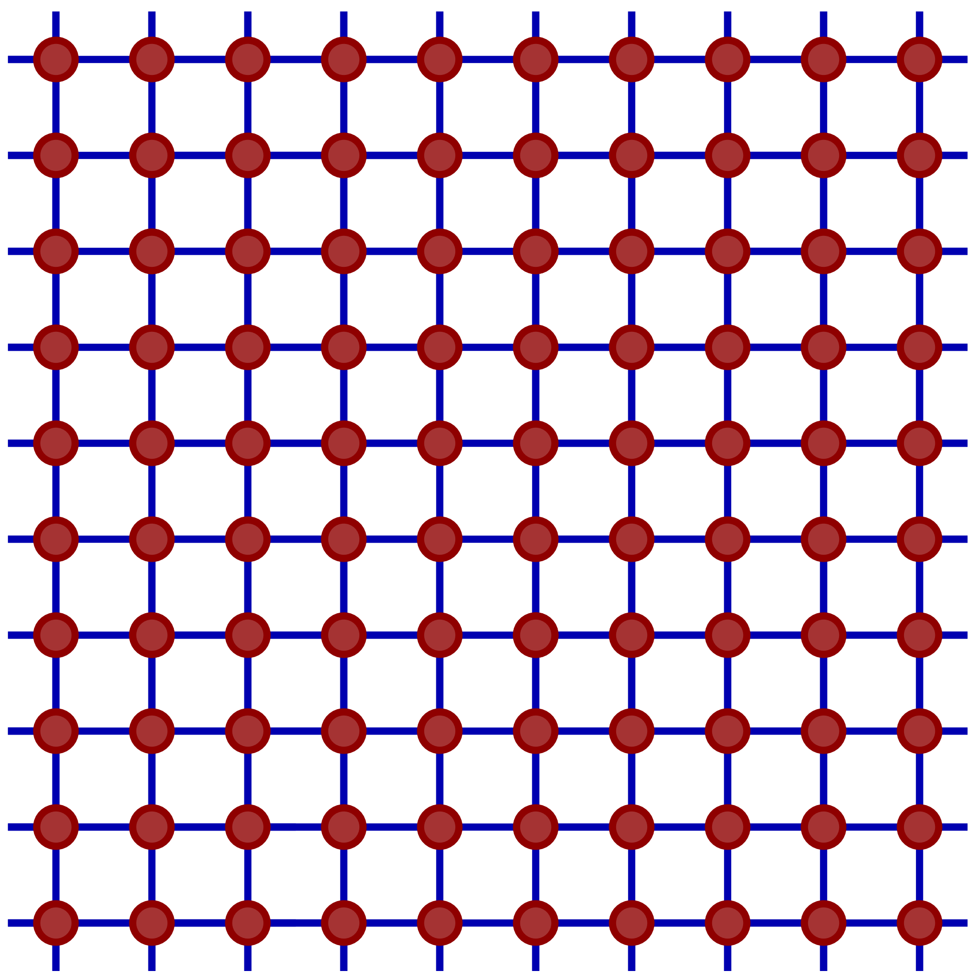
$$H_1 = \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

Why consider the Hubbard model ?

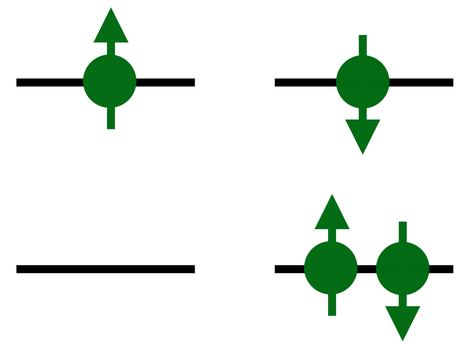
- generic many-body problem
- fermion statistics (second quant.)
- lattice model (vs. impurity model)
- Coulomb interaction
- most simple setup for the "correlation problem"

Hilbert space

$$H \;=\; H_0(\boldsymbol{t}) + H_1$$



single site: dimension 4



L sites: dimension $4^L = e^{\ln 4 \cdot L}$

using symmetries:
$N_\uparrow$ and $N_\downarrow$ are conserved

dimension $\begin{pmatrix} L \\ N_\uparrow \end{pmatrix} \begin{pmatrix} L \\ N_\downarrow \end{pmatrix}$

for L=10: 63504 (half-filling)
for L=12: 853776
accessible by Krylov-space methods

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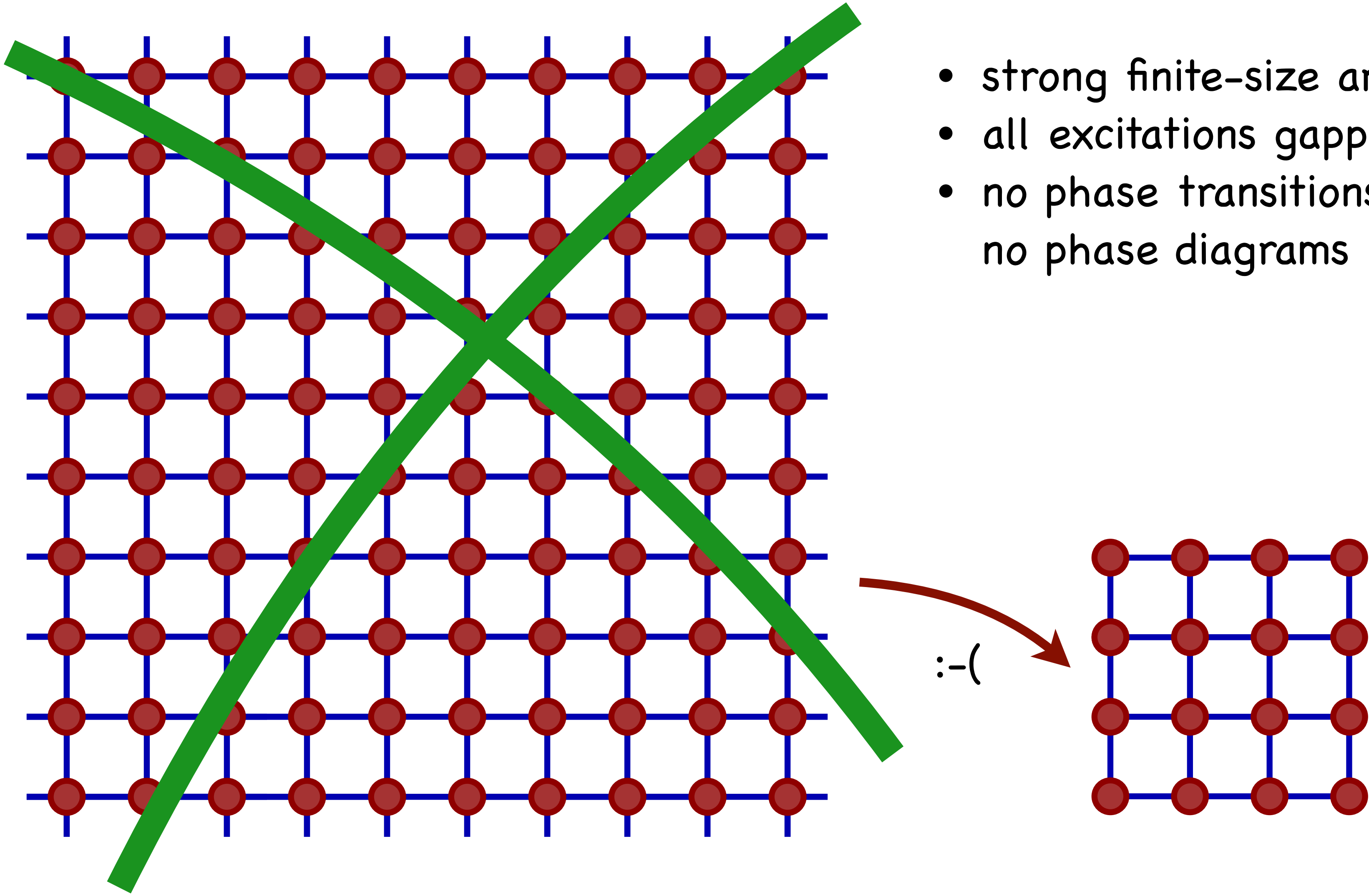
bad news

- strong finite-size artefacts
- all excitations gapped
- no phase transitions
  no phase diagrams



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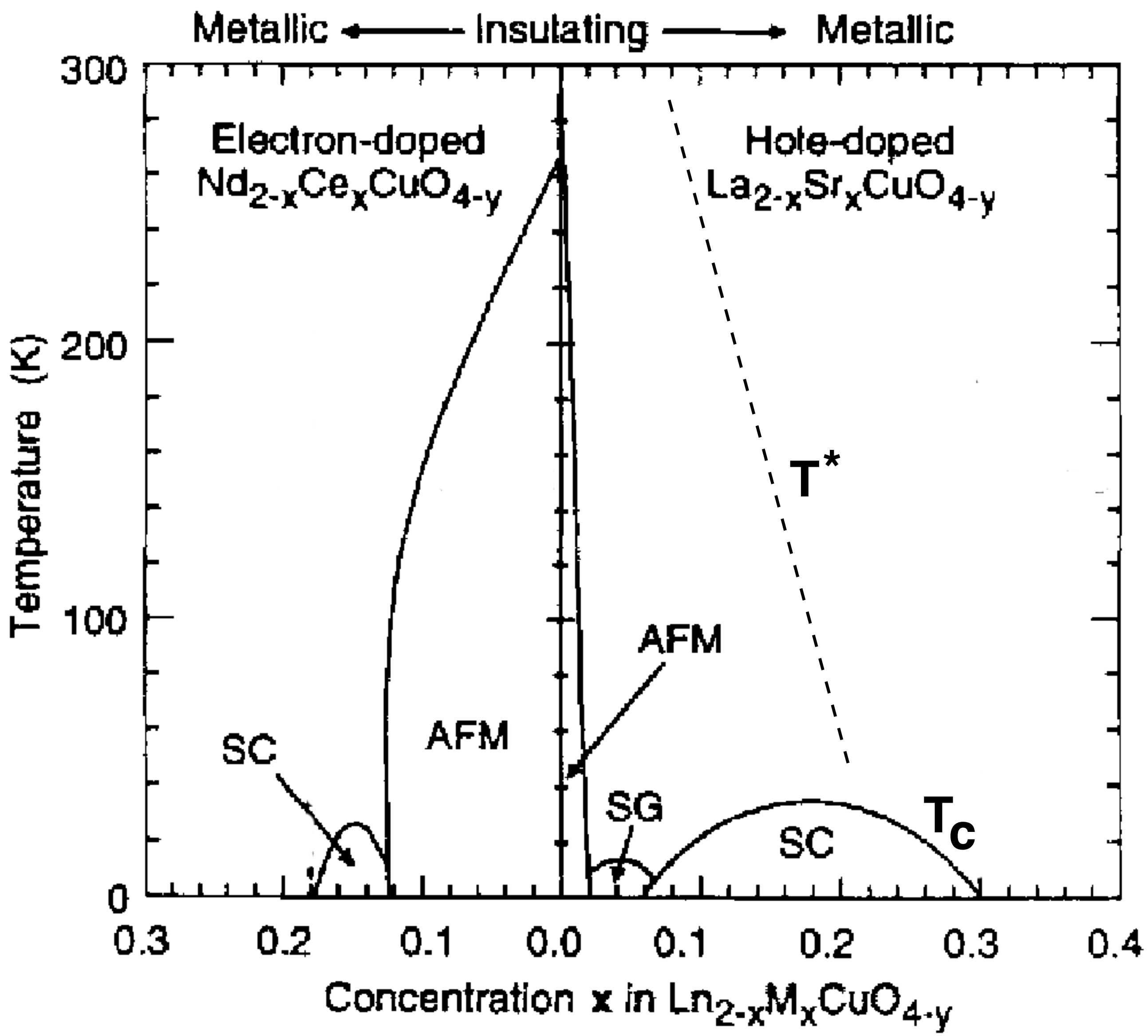
phase diagram of high-T_c materials



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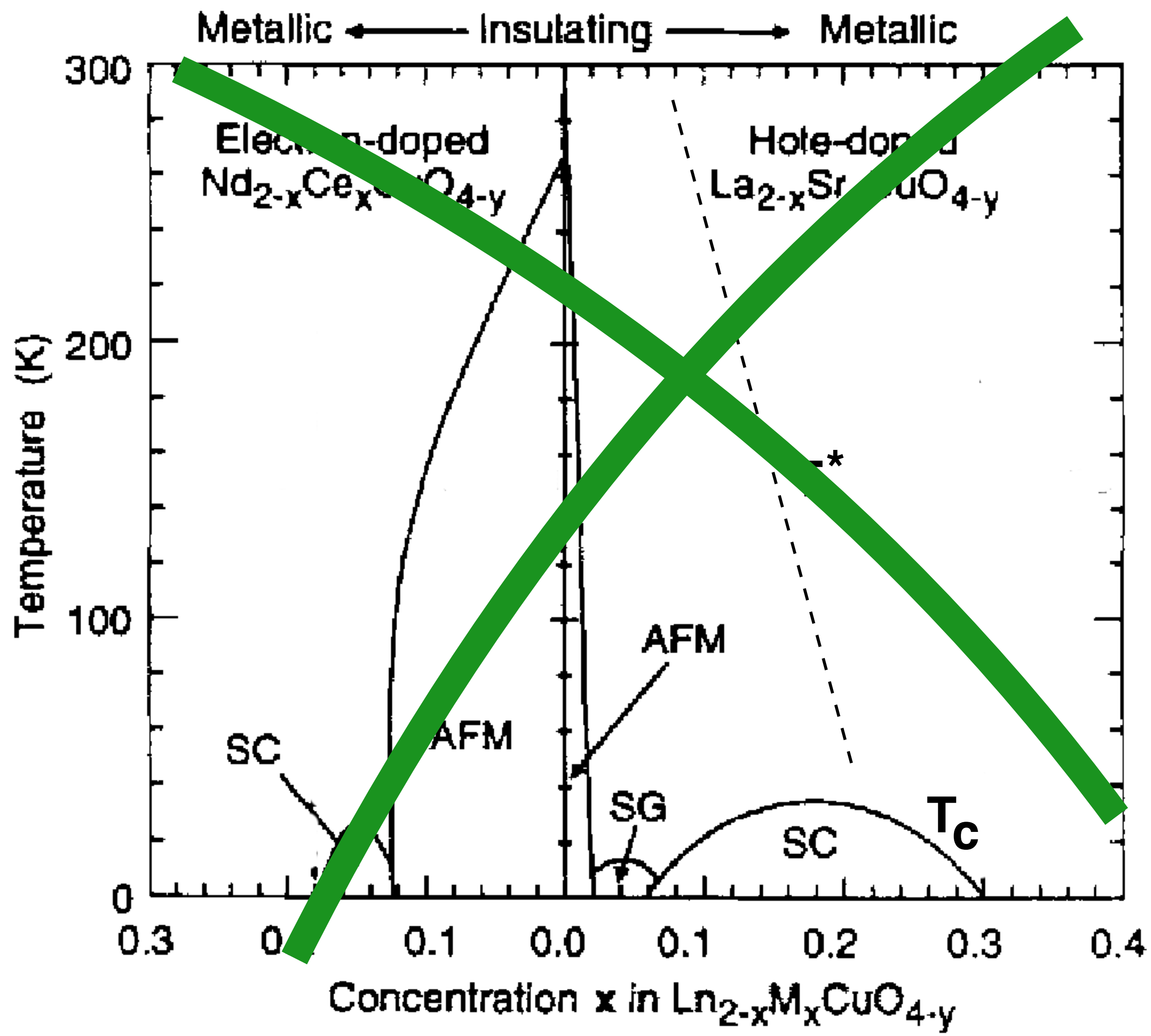
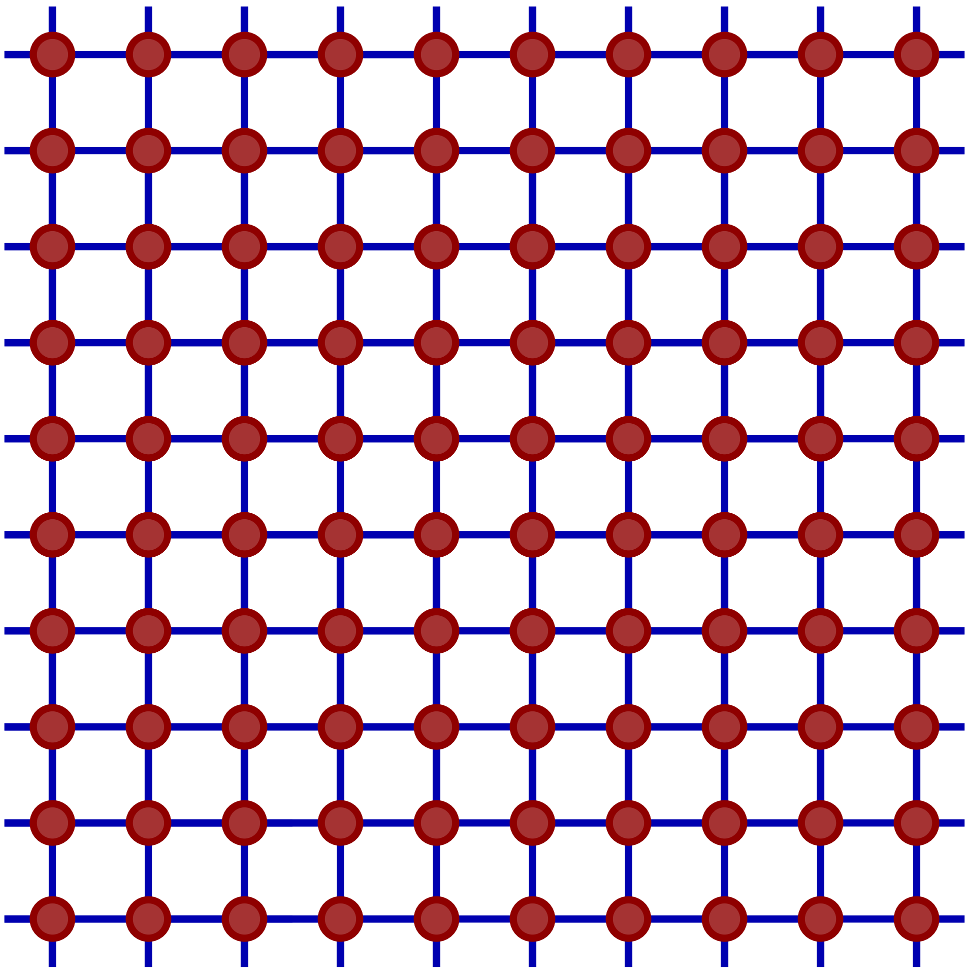
phase diagram of high-T_c materials

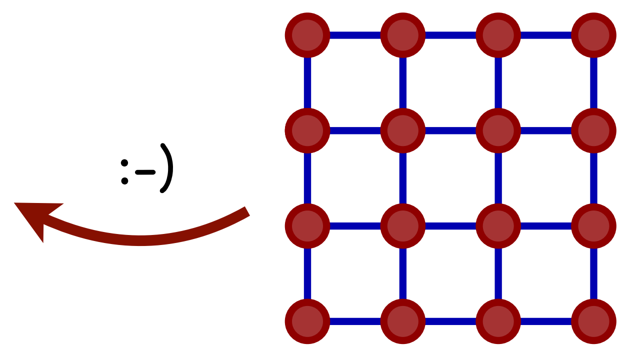


:-(

the main idea of a cluster approach

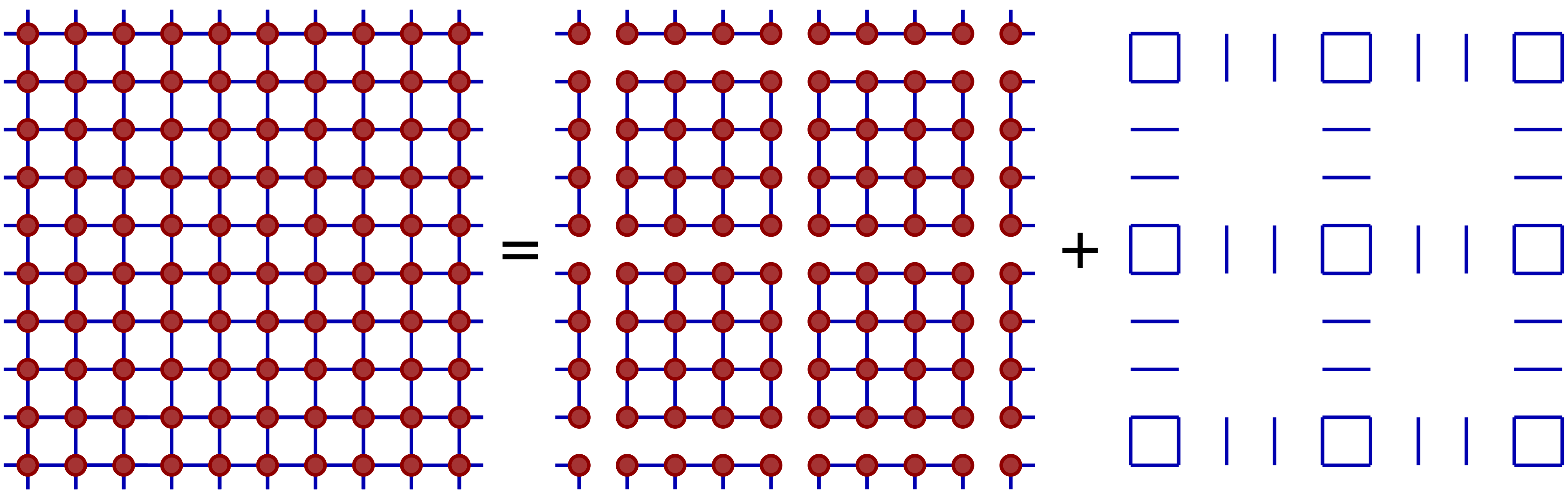


- solve the cluster problem exactly
- use the solution to reconstruct the solution for the full problem (this is approximate !)
- find a clever way how to do this step (“embedding problem”)
- Machiavelli: “divide et impera”?
- Goethe: “verein und leite”!



the cluster-perturbation theory (CPT)

original system reference system



hopping matrix **t** hopping matrix **t'** inter-cluster hopping V

$$\mathbf{t} = \mathbf{t}' + \mathbf{V}$$

treat this term perturbatively !

“free” systems and Green’s functions

- free system:

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

- reference system:

$$H'_0 = \sum_{ij\sigma} t'_{ij} c^\dagger_{i\sigma} c_{j\sigma} = H_0(\boldsymbol{t}')$$

- free Green’s function

$$\boldsymbol{G}_0(\omega) = \frac{1}{\omega + \mu - \boldsymbol{t}}$$

$$\boldsymbol{t} = \boldsymbol{t}' + \boldsymbol{V}$$

- Green’s function of the ref. system:

$$\boldsymbol{G}'_0(\omega) = \frac{1}{\omega + \mu - \boldsymbol{t}'}$$

we have: $$\mathbf{G}_0(\omega) = \frac{1}{\omega + \mu - \mathbf{t}' - \mathbf{V}} = \frac{1}{\omega + \mu - \mathbf{t}'} + \frac{1}{\omega + \mu - \mathbf{t}'} \mathbf{V} \frac{\mathbf{1}}{\omega + \mu - \mathbf{t}'} + \cdots$$

or: $$\boldsymbol{G}_0(\omega) = \boldsymbol{G}'_0(\omega) + \boldsymbol{G}'_0(\omega) \boldsymbol{V} \boldsymbol{G}'_0(\omega) + \cdots$$

sum **all** orders: $$\boldsymbol{G}_0(\omega) = \boldsymbol{G}'_0(\omega) + \boldsymbol{G}'_0(\omega) \boldsymbol{V} \boldsymbol{G}_0(\omega)$$ the “free” CPT equation !

solve: $$\boldsymbol{G}_0(\omega) = \frac{1}{\boldsymbol{G}'_0(\omega)^{-1} - \boldsymbol{V}}$$

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CPT using Green's functions

- "free" CPT equation:

$$G_0(\omega) = G_0'(\omega) + G_0'(\omega) V G_0(\omega) \qquad \text{(exact)}$$

- CPT equation:

$$G(\omega) = G'(\omega) + G'(\omega) V G(\omega) \qquad \text{(approximate)}$$

Gros, Valenti (1993), Senechal et al. (2000)

CPT:

- provides interacting G for (almost) arbitrarily large systems (large L)
- (in principle) controlled by $1/L_C$ (with L_C: number of cluster sites)
- with L_C=1, this is the "Hubbard-I approximation"

Hubbard (1963)

CPT in practice

- compute Green's function of the reference system, e.g., by exact diag.:

$$(H' - \mu N)|n'\rangle = E'_n|n'\rangle$$

$$G'_{ij\sigma}(\omega) = \frac{1}{Z'}\sum_{mn}\frac{(e^{-\beta E'_m} + e^{-\beta E'_n})\langle m'|c_{i\sigma}|n'\rangle\langle n'|c^\dagger_{j\sigma}|m'\rangle}{\omega - (E'_n - E'_m)}$$

- partition function

$$Z' = \sum_m e^{-\beta E'_m} \qquad \beta = 1/T$$

- CPT equation:

$$\boldsymbol{G}(\omega) = \boldsymbol{G}'(\omega) + \boldsymbol{G}'(\omega)\boldsymbol{V}\boldsymbol{G}(\omega) \qquad \text{with} \qquad \boldsymbol{t} = \boldsymbol{t}' + \boldsymbol{V}$$

- solve by matrix inversion for any frequency:

$$\boldsymbol{G}(\omega) = \frac{1}{\boldsymbol{G}'(\omega)^{-1} - \boldsymbol{V}}$$

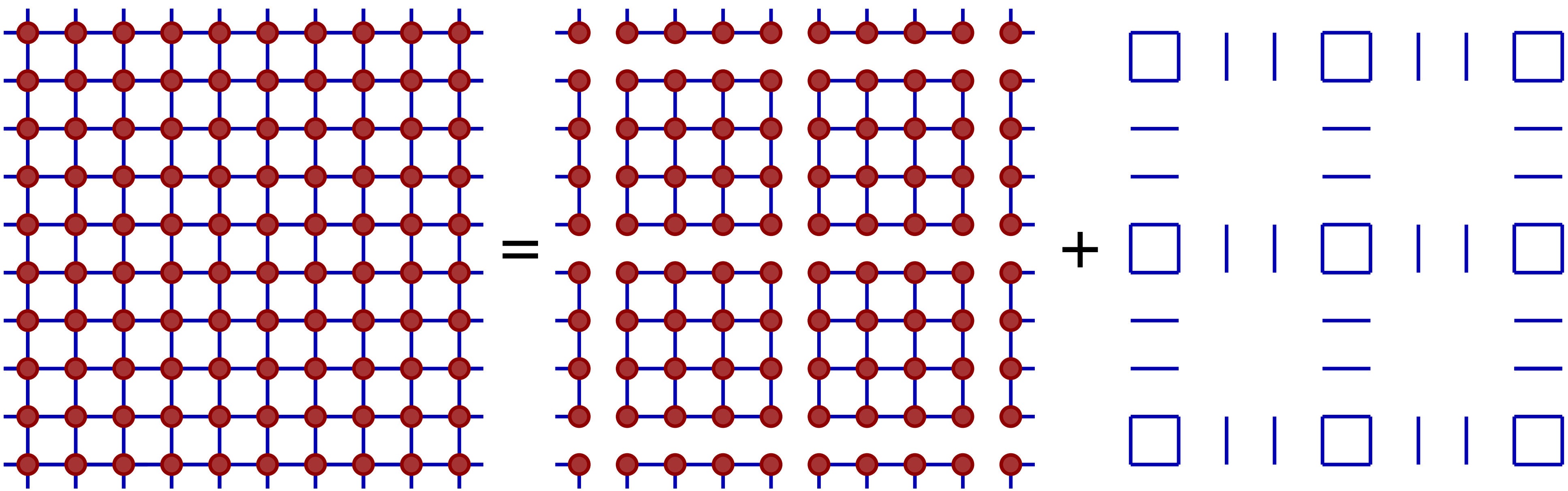
CPT in practice (cntd.)

- make use of translational symmetry (if present):

$$\boldsymbol{G}_{\boldsymbol{k}}(\omega) = \frac{1}{\boldsymbol{G}'_{\boldsymbol{k}}(\omega)^{-1} - \boldsymbol{V}(\boldsymbol{k})}$$

$$V_{IJ,ij} = V_{I-J,ij} \mapsto V_{ij}(\boldsymbol{k})$$

I: cluster index
i: site within a cluster
k: wave vector of reciprocal superlattice



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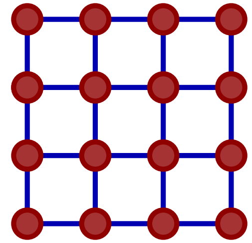
a big drawback of the CPT

finite cluster - finite Hilbert space - analytic functions



$$(H' - \mu N)|n'\rangle = E'_n |n'\rangle$$

$$G'_{ij\sigma}(\omega) = \frac{1}{Z'} \sum_{mn} \frac{(e^{-\beta E'_m} + e^{-\beta E'_n}) \langle m'|c_{i\sigma}|n'\rangle \langle n'|c^\dagger_{j\sigma}|m'\rangle}{\omega - (E'_n - E'_m)}$$

$$Z' = \sum_m e^{-\beta E'_m}$$

$$\Omega' = -T \ln Z' \qquad \text{analytic function of } \beta, \mu, U, \ldots$$

quantities of the lattice model:

$$\boldsymbol{G}(\omega) = \frac{1}{\boldsymbol{G}'(\omega)^{-1} - \boldsymbol{V}}$$

$$\boldsymbol{A}(\omega) = -\frac{1}{\pi} \mathrm{Im}\, \boldsymbol{G}(\omega + i0^+)$$

$$\langle c^\dagger_{j\sigma} c_{i\sigma} \rangle = \int_{-\infty}^{\infty} d\omega \frac{1}{e^{\beta\omega} + 1} A_{ij}(\omega)$$

no second-order phase transitions
e.g.: antiferromagnetism

$$m_{\mathrm{st.}} = \frac{1}{L} \sum_i (-1)^i (n_{i\uparrow} - n_{i\downarrow})$$

$$\chi = \frac{\partial m_{\mathrm{st.}}}{\partial B_{\mathrm{st.}}}\bigg|_{B_{\mathrm{st.}}=0} \neq \infty$$

freedom in the CPT construction

- original system

$$H = H_0(\boldsymbol{t}) + H_1 \qquad H_0 = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} = H_0(\boldsymbol{t})$$

- reference system

$$H' = H_0(\boldsymbol{t}') + H_1 \qquad H'_0 = \sum_{ij\sigma} t'_{ij} c^\dagger_{i\sigma} c_{j\sigma} = H_0(\boldsymbol{t}')$$

CPT:

$$\boldsymbol{G}_0(\omega) = \boldsymbol{G}'_0(\omega) + \boldsymbol{G}'_0(\omega)\boldsymbol{V}\boldsymbol{G}_0(\omega) \qquad \boldsymbol{V} = \boldsymbol{t} - \boldsymbol{t}'$$

- a different reference system

$$\widetilde{H}' = H_0(\widetilde{\boldsymbol{t}'}) + H_1 \qquad \widetilde{H}'_0 = \sum_{ij\sigma} \widetilde{t}'_{ij} c^\dagger_{i\sigma} c_{j\sigma} = H_0(\widetilde{\boldsymbol{t}'})$$

a different CPT ?

$$\boldsymbol{G}_0(\omega) = \widetilde{\boldsymbol{G}}'_0(\omega) + \widetilde{\boldsymbol{G}}'_0(\omega)\widetilde{\boldsymbol{V}}\boldsymbol{G}_0(\omega) \qquad \widetilde{\boldsymbol{V}} = \boldsymbol{t} - \widetilde{\boldsymbol{t}'} = \boldsymbol{V} - \Delta\boldsymbol{t}'$$

we have:

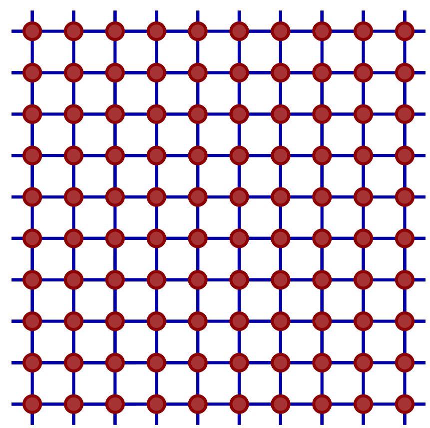
$$\boldsymbol{G}_0(\omega) = \widetilde{\boldsymbol{G}}'_0(\omega) + \widetilde{\boldsymbol{G}}'_0(\omega)\widetilde{\boldsymbol{V}}\boldsymbol{G}_0(\omega) = \widetilde{\boldsymbol{G}}'_0(\omega) + \widetilde{\boldsymbol{G}}'_0(\omega)\widetilde{\boldsymbol{V}}\widetilde{\boldsymbol{G}}'_0(\omega) + \cdots$$

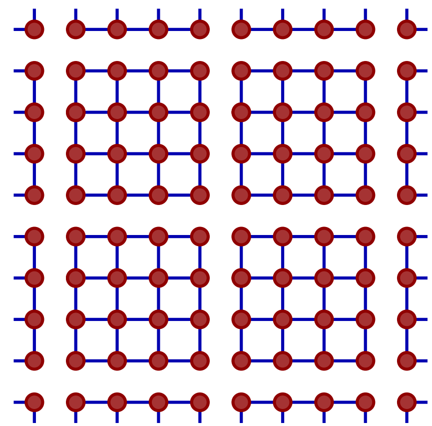
but:

$$\boxed{\widetilde{\boldsymbol{G}}(\omega) \equiv \widetilde{\boldsymbol{G}}'(\omega) + \widetilde{\boldsymbol{G}}'(\omega)\widetilde{\boldsymbol{V}}\widetilde{\boldsymbol{G}}'(\omega) + \cdots \neq \boldsymbol{G}'(\omega) + \boldsymbol{G}'(\omega)\boldsymbol{V}\boldsymbol{G}'(\omega) + \cdots \equiv \boldsymbol{G}(\omega)}$$

use the freedom to cure the drawback ?

e.g. spontaneous antiferromagnetic order





$B_{\text{st.}} = 0$ $\qquad$ $B'_{\text{st.}} > 0$

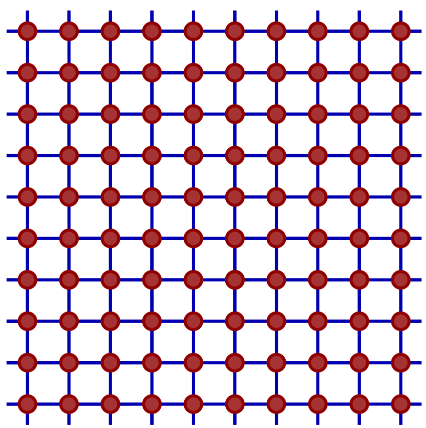
physical field $\qquad$ fictitious field

CPT construction with a **symmetry-broken** reference system !

$$\boldsymbol{G}(\omega) = \boldsymbol{G}'(\omega) + \boldsymbol{G}'(\omega)\boldsymbol{V}\boldsymbol{G}(\omega)$$

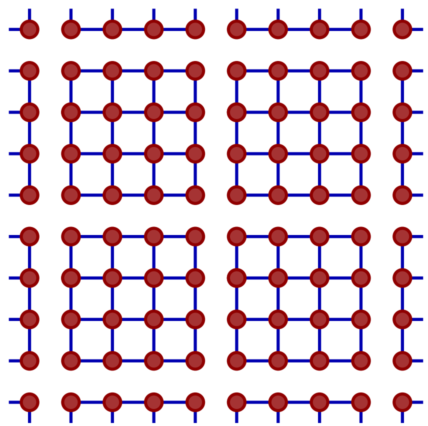
VCA - the main idea

e.g. spontaneous antiferromagnetic order



$B_{\mathrm{st.}} = 0$

physical field

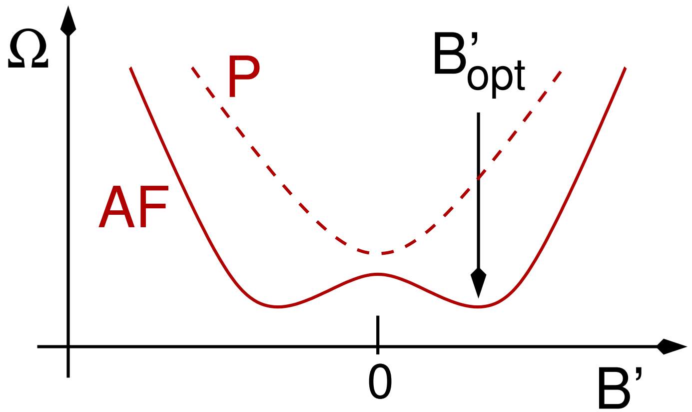


$B'_{\mathrm{st.}} > 0$

fictitious field

Q: how to find the "right" field ?

A: the optimal field should minimize the grand potential !



$$\Omega(B') = ? \quad \Omega(\boldsymbol{t}') = ?$$

the Ritz principle ?

we need a variational principle (consider T=0, ground state):

$$E(\boldsymbol{t}') = \min.$$

the Ritz principle ?

$$E[|\Psi\rangle] = \langle\Psi|H|\Psi\rangle = \min.$$

define:

$$E(\boldsymbol{t}') \equiv E[|\Psi(\boldsymbol{t}')\rangle]$$

optimal parameters:

$$\left.\frac{\partial E[|\Psi(\boldsymbol{t}')\rangle]}{\partial \boldsymbol{t}'}\right|_{\boldsymbol{t}'=\boldsymbol{t}'_{\mathrm{opt}}} \stackrel{!}{=} 0$$

we have:

$$|\Psi(\boldsymbol{t}')\rangle = |\Psi_1(\boldsymbol{t}'_1)\rangle \otimes |\Psi_2(\boldsymbol{t}'_2)\rangle \otimes \cdots \otimes |\Psi_{L/L_c}(\boldsymbol{t}'_{L/L_c})\rangle$$

this yields:

$$E[|\Psi(\boldsymbol{t}')\rangle] = \langle\Psi(\boldsymbol{t}')|(H_0(\boldsymbol{t}') + H_0(\boldsymbol{V}) + H_1)|\Psi(\boldsymbol{t}')\rangle = E_0(\boldsymbol{t}') + \langle\Psi(\boldsymbol{t}')|H_0(\boldsymbol{V})|\Psi(\boldsymbol{t}')\rangle$$

for decoupled clusters as a reference and with Hellmann-Feynman theorem:

$$\frac{\partial}{\partial \boldsymbol{t}'} E[|\Psi(\boldsymbol{t}')\rangle] = \frac{\partial}{\partial \boldsymbol{t}'} E_0(\boldsymbol{t}') = \frac{\partial}{\partial \boldsymbol{t}'} \langle\Psi(\boldsymbol{t}')|(H_0(\boldsymbol{t}') + H_1)|\Psi(\boldsymbol{t}')\rangle = \langle\Psi(\boldsymbol{t}')|\frac{\partial H_0(\boldsymbol{t}')}{\partial \boldsymbol{t}'}|\Psi(\boldsymbol{t}')\rangle$$

this yields:

- optimal parameters do not depend on V
- for optimal parameters: all one-particle correlations vanish

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define:

$$E(\boldsymbol{t}') = E[|\Psi(\boldsymbol{t}')\rangle]$$

optimal parameters:

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we have:

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this yields:
- optimal parameters do not depend on V
- for optimal parameters: all one-particle correlations vanish

unacceptable !

cannot make use of the Ritz principle!

need a variational principle based on Green functions

rather than on wave functions !

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a functional of the Green's function

wanted: $\Omega[\boldsymbol{G}]$ with $\dfrac{\delta\Omega[\boldsymbol{G}]}{\delta \boldsymbol{G}} = 0$

Luttinger, Ward (1960)
Baym, Kadanoff (1961)

$$\boxed{\Omega[\boldsymbol{G}] = \Phi[\boldsymbol{G}] + \operatorname{tr}\ln \boldsymbol{G} - \operatorname{tr}(\boldsymbol{G}_0^{-1} - \boldsymbol{G}^{-1})\boldsymbol{G}}$$

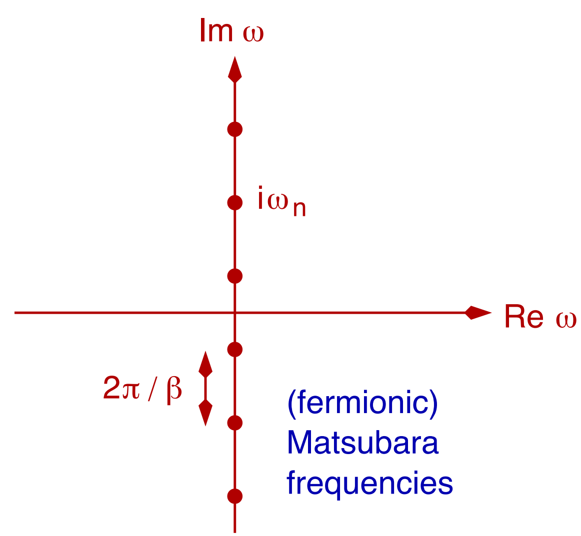
elements of $\boldsymbol{G}$: $G_{ij\sigma}(i\omega_n)$

$$G_{0,ij\sigma}(i\omega_n) = \left(\frac{1}{i\omega_n + \mu - \boldsymbol{t}}\right)_{ij\sigma}$$

$$\mathrm{Tr}\,\boldsymbol{A} \equiv \frac{1}{\beta}\sum_n \sum_{i\sigma} e^{i\omega_n 0^+} A_{ii\sigma}(i\omega_n)$$

Luttinger-Ward functional

grand potential



reminder: perturbation theory

- Hamiltonian:

$$\mathcal{H} = H - \mu N = \mathcal{H}_0 + H_1 = \mathcal{H}_0(\boldsymbol{t}) + H_1$$

- S-matrix:

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

- equation of motion:

$$-\frac{\partial}{\partial\tau} S(\tau,\tau') = H_{1,I}(\tau) S(\tau,\tau')$$ with free time dependence of $H_{1,I}$

- formal solution:

$$S(\tau,\tau') = \mathcal{T} \exp\left(-\int_{\tau'}^{\tau} d\tau'' H_{1,I}(\tau'')\right)$$

- partition function:

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

- starting point of perturbation theory:

$$\frac{Z}{Z_0} = \left\langle \mathcal{T} \exp\left(-\int_0^{\beta} d\tau'' H_{1,I}(\tau'')\right)\right\rangle^{(0)}$$

- expand, use Wick's theorem, and then …

- Green's function

$$G_{ij\sigma}(\tau) = -\langle \mathcal{T} c_{i\sigma}(\tau) c^\dagger_{j\sigma}(0)\rangle \qquad c_{i\sigma}(\tau) = e^{\mathcal{H}\tau} c_{i\sigma} e^{-\mathcal{H}\tau}$$

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

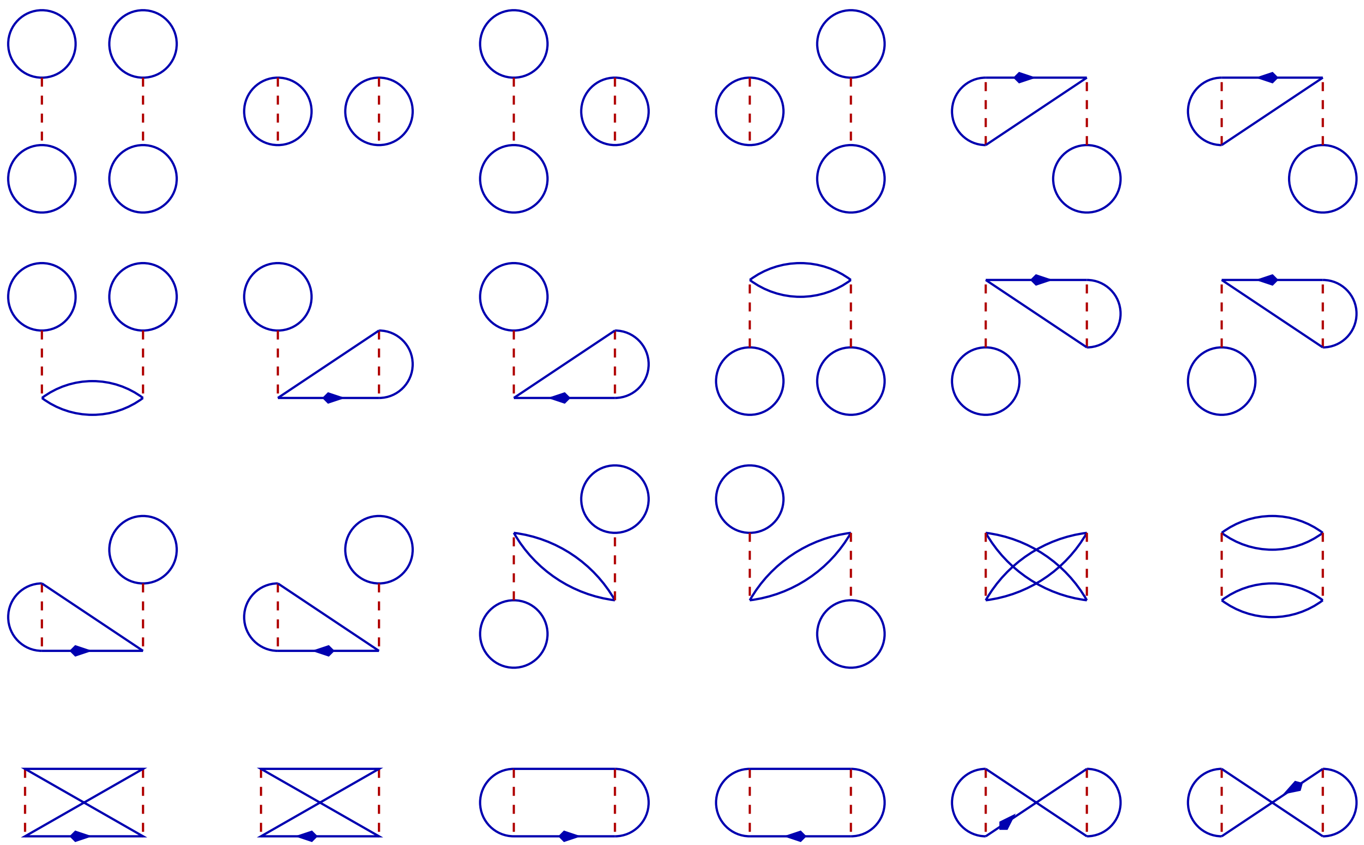
$$G_{ij\sigma}(i\omega_n) = \int_0^\beta d\tau\, G_{ij\sigma}(\tau)\, e^{i\omega_n\tau}$$

$$c_{i\sigma}(\tau) = S(0,\tau) c_{I,i\sigma}(\tau) S(\tau,0)$$

analogously: $$G_{ij\sigma}(\tau) = -\frac{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau H_{1,I}(\tau)\right) c_{I,i\sigma}(\tau) c^\dagger_{I,j\sigma}(0)\right\rangle^{(0)}}{\left\langle \mathcal{T} \exp\left(-\int_0^\beta d\tau H_{1,I}(\tau)\right)\right\rangle^{(0)}}$$

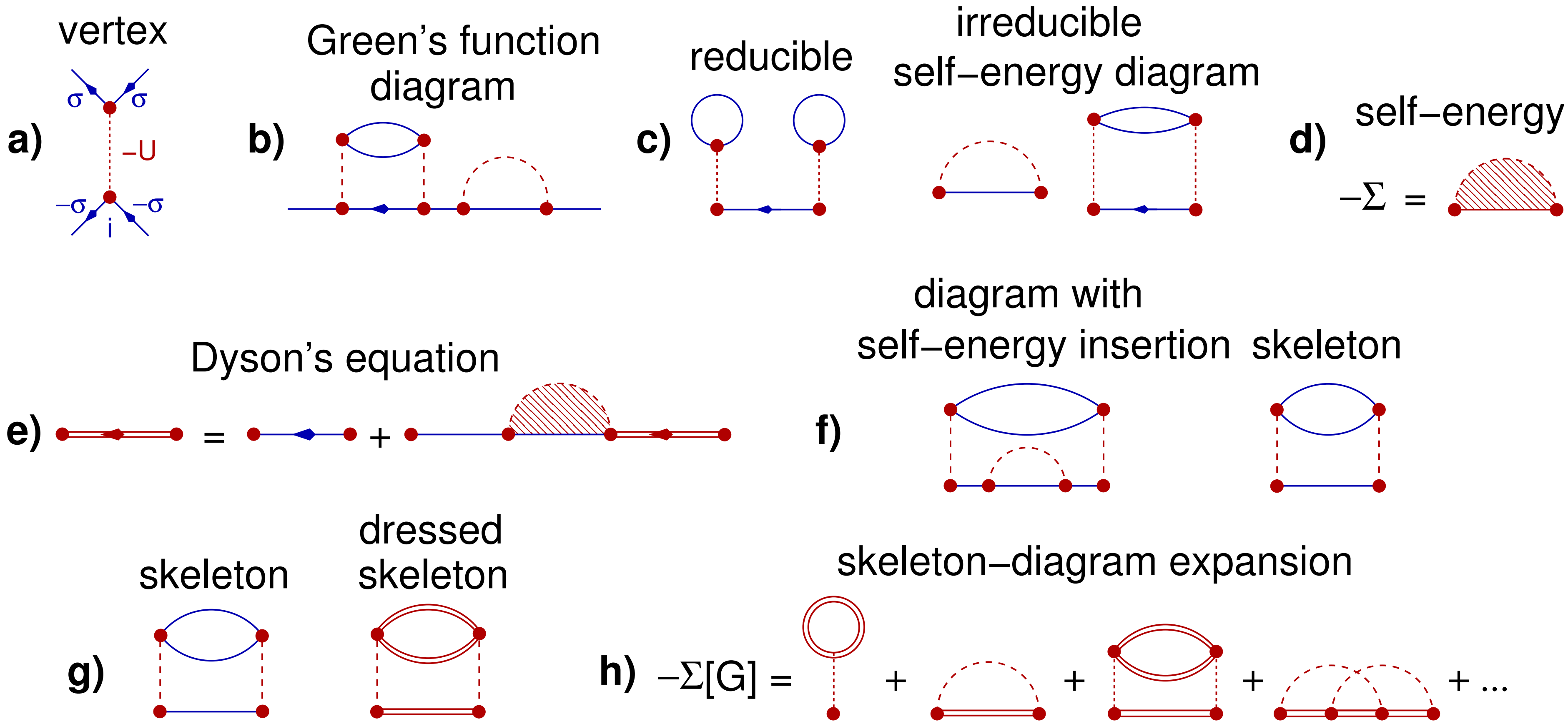
diagrammatic perturbation theory

... get, e.g., the second-order contribution to Z/Z_0 as:



- use the linked-cluster theorem, to get the grand potential as the sum of connected diagrams only, this yields: $\Omega - \Omega_0$

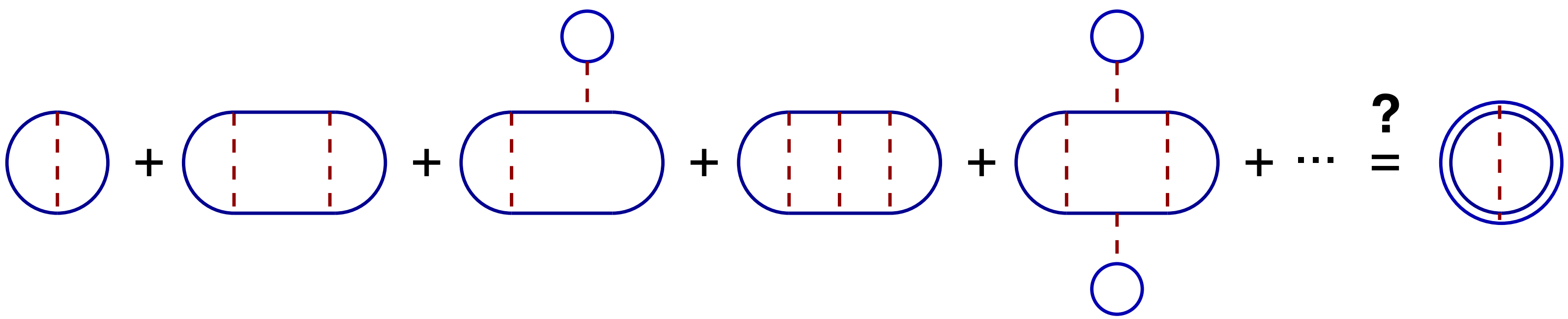
diagrams for the Green's function



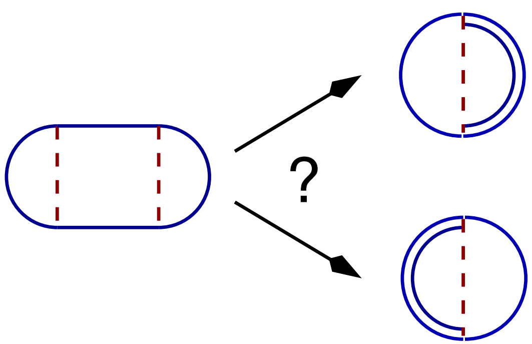
"renormalization"

renormalization of closed diagrams?

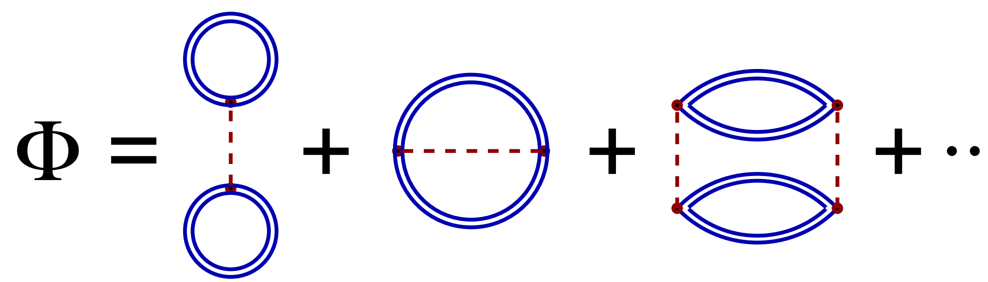
- remove self-energy insertions and replace free by interacting propagators ?



- this would imply a double counting of diagrams !



- don't care !
- sum all renormalized closed skeleton diagrams up to infinite order:



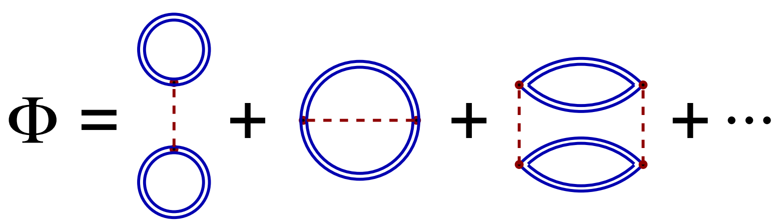
- Luttinger-Ward functional
(does not give the grand potential)

diagrams: summary

grand potential and LW functional:

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

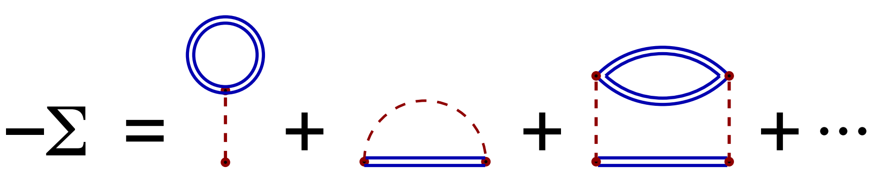
Luttinger-Ward functional:



derivative of the LW funct.:

$$\beta \frac{\delta \Phi[\boldsymbol{G}]}{\delta G_{ij\sigma}(i\omega_n)} = \Sigma_{ji\sigma}(i\omega_n)[\boldsymbol{G}]$$

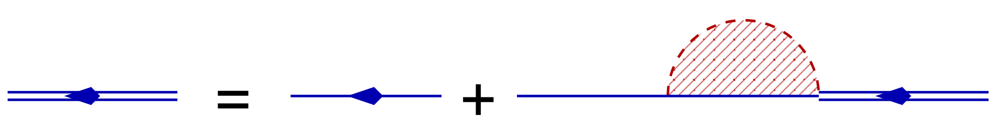
self-energy, skeleton-diagram expansion:



to be discussed:

- variational principle ?
- grand potential: proof ?
- tr ln (...) term is ill-defined !

Dyson's equation



variational principle

grand potential:

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

functional:

$$\Omega[\boldsymbol{G}] = \Phi[\boldsymbol{G}] + \mathrm{tr}\ln \boldsymbol{G} - \mathrm{tr}(\boldsymbol{G}_0^{-1} - \boldsymbol{G}^{-1})\boldsymbol{G}$$

$$\frac{\delta\Omega[\boldsymbol{G}]}{\delta\boldsymbol{G}} = 0 \quad ?$$

functional derivative:

$$\beta\frac{\delta\Omega[\boldsymbol{G}]}{\delta\boldsymbol{G}} = \beta\frac{\delta}{\delta\boldsymbol{G}}\left(\Phi[\boldsymbol{G}] + \mathrm{tr}\ln \boldsymbol{G} - \mathrm{tr}(\boldsymbol{G}_0^{-1} - \boldsymbol{G}^{-1})\boldsymbol{G}\right)$$

$$= \boldsymbol{\Sigma}[\boldsymbol{G}] + \boldsymbol{G}^{-1} - \boldsymbol{G}_0^{-1}$$

thus:

$$\beta\frac{\delta\Omega[\boldsymbol{G}]}{\delta\boldsymbol{G}} = 0 \quad \Leftrightarrow \quad \boldsymbol{\Sigma}[\boldsymbol{G}] = \boldsymbol{G}_0^{-1} - \boldsymbol{G}^{-1} \quad ✔$$

grand potential and LW functional

$$\Omega = \Phi + \mathrm{tr} \ln \boldsymbol{G} - \mathrm{tr}(\boldsymbol{\Sigma} \boldsymbol{G}) \quad ?$$

grand potential and LW functional

$$\Omega = \Phi + \mathrm{tr} \ln \boldsymbol{G} - \mathrm{tr}(\boldsymbol{\Sigma} \boldsymbol{G}) \quad ?$$

proof:

consider the derivative w.r.t. μ:

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

first term:

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

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

grand potential and LW functional

$$\Omega = \Phi + \mathrm{tr}\ln \boldsymbol{G} - \mathrm{tr}(\boldsymbol{\Sigma}\boldsymbol{G})$$?

proof:

consider the derivative w.r.t. μ:

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

first term:

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

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

second term:

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

grand potential and LW functional

$$\Omega = \Phi + \mathrm{tr} \ln \boldsymbol{G} - \mathrm{tr}(\boldsymbol{\Sigma G})$$?

proof:

consider the derivative w.r.t. μ:

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

first term:

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

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

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:

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

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grand potential and LW functional

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

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

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

$$= -\mathrm{Tr}\left[\frac{\partial \mathbf{G}_0^{-1}}{\partial \mu}\mathbf{G}\right]$$

with Dyson's equation $\mathbf{G} = 1/(\mathbf{G}_0^{-1} - \mathbf{\Sigma})$

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

grand potential and LW functional

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

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

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

$$= -\text{Tr}\left[\frac{\partial \mathbf{G}_0^{-1}}{\partial \mu}\mathbf{G}\right]$$

with Dyson's equat

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

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

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

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

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

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

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

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

$$= -\langle N \rangle$$

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

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grand potential and LW functional

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

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

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

$$= -\text{Tr}\left[\frac{\partial \mathbf{G}_0^{-1}}{\partial \mu}\mathbf{G}\right]$$

with Dyson's equat

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

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

q.e.d.

for $\mu \to -\infty$:

$$\boxed{\text{Tr} \ln \mathbf{G} = \Omega}$$

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

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

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

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

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

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

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

$$= -\langle N \rangle$$

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

proof that $\Omega = \mathrm{Tr}\ln \boldsymbol{G}$ for U=0

first step:

$$\frac{\partial}{\partial\mu}\mathrm{Tr}\ln\boldsymbol{G} = -\frac{\partial}{\partial\mu}\mathrm{Tr}\ln\boldsymbol{G}^{-1} = -\frac{\partial}{\partial\mu}\mathrm{Tr}\ln(i\omega_n+\mu-\boldsymbol{t}) = -\mathrm{Tr}\frac{1}{i\omega_n+\mu-\boldsymbol{t}} = -\langle N\rangle = \frac{\partial\Omega}{\partial\mu}$$

second step:

$$\Omega = 0 \quad \text{for} \quad \mu\to-\infty \quad \to \quad \text{need to show that} \quad \mathrm{Tr}\ln\boldsymbol{G} = 0 \quad \text{for} \quad \mu\to-\infty$$

$$\text{but} \quad \mathrm{Tr}\ln\boldsymbol{G} = -\mathrm{Tr}\ln(i\omega_n+\mu-\boldsymbol{t}) \mapsto \infty$$

third step:

$$\text{regularisation needed:} \quad \mathrm{Tr}\ln\boldsymbol{G} \mapsto \mathrm{Tr}\ln\boldsymbol{G} - \infty = \mathrm{Tr}\ln\boldsymbol{G} - \mathrm{Tr}\ln\frac{1}{i\omega_n+\mu-\varepsilon_0}$$

$$= \mathrm{Tr}\ln\frac{i\omega_n+\mu-\varepsilon_0}{i\omega_n+\mu-\boldsymbol{t}} \mapsto \mathrm{Tr}\ln 1 = 0 \quad \text{for} \quad \mu\mapsto-\infty$$

✔

regularization

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

well-defined ?

third term:

$$\mathrm{tr}(\boldsymbol{\Sigma G}) = \sum_{ij\sigma} \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{i\omega_n 0^+} \Sigma_{ij\sigma}(i\omega_n) G_{ji\sigma}(i\omega_n) \sim \sum_n e^{i\omega_n 0^+} \frac{1}{i\omega_n} \sim \sum_n e^{i2n0^+} \frac{1}{n} < \infty$$

second term:

$$\boldsymbol{G} \mapsto \frac{\mathbf{1}}{i\omega_n} \sim \frac{1}{2n+1} \sim \frac{1}{n} \qquad \sum_n \ln(1/n) \sim \sum_n n = \infty$$

add a (parameter-free) counter term:

$$\Omega \mapsto \Omega - \frac{1}{\beta} \sum_n \ln \frac{1}{i\omega_n + \mu - \varepsilon_0} \qquad \text{with } \varepsilon_0 \mapsto \infty \text{ eventually}$$

- infinite constant
- regularizes the tr ln (...) term
- all calculations unchanged

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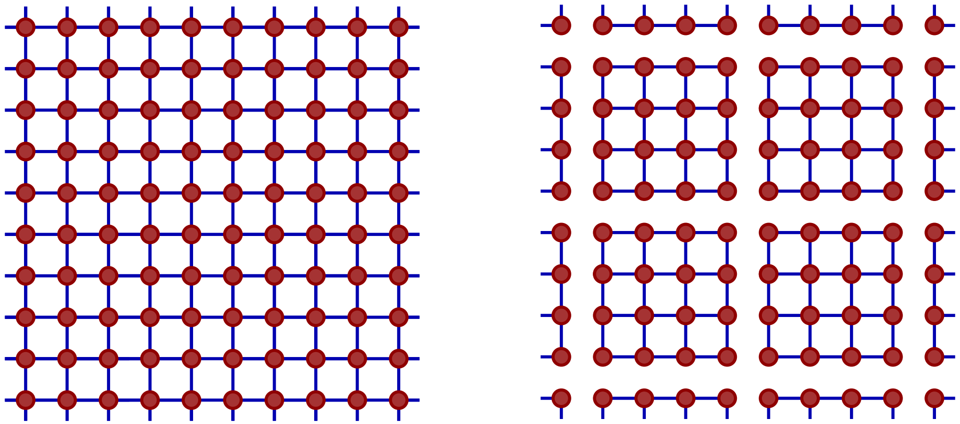
the general strategy



CPT:

$$\boldsymbol{G}(\omega) = \boldsymbol{G}'(\omega) + \boldsymbol{G}'(\omega)\boldsymbol{V}\boldsymbol{G}(\omega)$$

$$\boldsymbol{V} = \boldsymbol{t} - \boldsymbol{t}'$$

CPT with parameter optimization:

$$\boldsymbol{t}' \rightarrow H' = H_0(\boldsymbol{t}') + H_1 \rightarrow \boldsymbol{G}'(\omega) \rightarrow \boldsymbol{G}(\omega) = \boldsymbol{G}'(\omega) + \boldsymbol{G}'(\omega)\boldsymbol{V}\boldsymbol{G}(\omega) \rightarrow \Omega[\boldsymbol{G}]$$

$$\frac{\partial}{\partial \boldsymbol{t}'}\Omega[\boldsymbol{G}] = 0 \quad ?$$

more precisely: $\frac{\partial}{\partial \boldsymbol{t}'}\Omega[(\boldsymbol{G}'^{-1} - \boldsymbol{V})^{-1}] = 0$

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variational principle based on G ?

CPT with parameter optimization:

$$\boldsymbol{t}' \rightarrow H' = H_0(\boldsymbol{t}') + H_1 \rightarrow \boldsymbol{G}'(\omega) \rightarrow \boldsymbol{G}(\omega) = \boldsymbol{G}'(\omega) + \boldsymbol{G}'(\omega)\boldsymbol{V}\boldsymbol{G}(\omega) \rightarrow \Omega[\boldsymbol{G}]$$

$$\frac{\partial}{\partial \boldsymbol{t}'}\Omega[\boldsymbol{G}] = 0 \quad ?$$

conditional equation for the parameters t':

$$0 = \frac{\partial}{\partial \boldsymbol{t}'}\Omega[(\boldsymbol{G}'^{-1} - \boldsymbol{V})^{-1}] = \frac{\delta\Omega}{\delta \boldsymbol{G}} \cdot \frac{\partial \boldsymbol{G}}{\partial \boldsymbol{t}'} = (\boldsymbol{\Sigma}' + \boldsymbol{G}^{-1} - \boldsymbol{G}_0^{-1})\,\frac{\partial \boldsymbol{G}}{\partial \boldsymbol{t}'}$$

this must be **rejected** since:

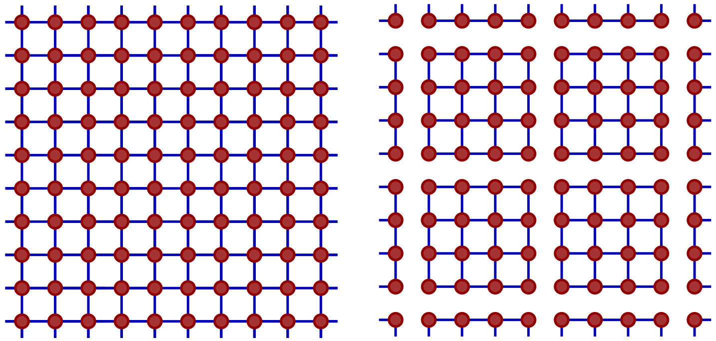
- it is ugly
- DMFT cannot be reproduced
  - DMFT: $G_{loc}=G'_{loc}$, but there is also a "bath"
  - if at all, then $(G^{-1})_{loc}=(G'^{-1})_{loc}$ ... see below

recall:

$$\Omega[\boldsymbol{G}] = \Phi[\boldsymbol{G}] + \mathrm{tr}\ln \boldsymbol{G} - \mathrm{tr}(\boldsymbol{G}_0^{-1} - \boldsymbol{G}^{-1})\boldsymbol{G}$$

$$\beta\frac{\delta\Omega[\boldsymbol{G}]}{\delta \boldsymbol{G}} = \boldsymbol{\Sigma}[\boldsymbol{G}] + \boldsymbol{G}^{-1} - \boldsymbol{G}_0^{-1}$$

new strategy



consider:

$$\boldsymbol{G} = \frac{1}{\boldsymbol{G}'^{-1} - \boldsymbol{V}} = \frac{1}{\omega + \mu - \boldsymbol{t}' - \boldsymbol{\Sigma}' - \boldsymbol{t} + \boldsymbol{t}'} = \frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}'}$$

a different way to do CPT !

parameter optimization:

$$\boldsymbol{t}' \longrightarrow H' = H_0(\boldsymbol{t}') + H_1 \longrightarrow \boldsymbol{\Sigma}'(\omega) \longrightarrow \boldsymbol{\Sigma}(\omega) = \boldsymbol{\Sigma}'(\omega) \longrightarrow \Omega[\boldsymbol{\Sigma}]$$

$$\frac{\partial}{\partial \boldsymbol{t}'}\Omega[\boldsymbol{\Sigma}] = 0 \quad ?$$

- this is nice ! construct approximations by choosing certain trial self-energies
- ... and it recovers DMFT ! (see below)
- we need a self-energy functional
- $\beta \frac{\delta \Phi}{\delta \boldsymbol{G}} = \boldsymbol{\Sigma}$: self-energy and Green's function are conjugate variables
- use Legendre transformation

the self-energy functional

Legrendre transformation:

$$F[\boldsymbol{\Sigma}] \equiv \Phi[\boldsymbol{G}[\boldsymbol{\Sigma}]] - \mathrm{Tr}(\boldsymbol{\Sigma}\boldsymbol{G}[\boldsymbol{\Sigma}])$$

immediately implies:

$$\frac{\delta F[\boldsymbol{\Sigma}]}{\delta \boldsymbol{\Sigma}} = -\frac{1}{\beta}\boldsymbol{G}[\boldsymbol{\Sigma}]$$

define self-energy functional:

$$\Omega[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} + \Phi[\boldsymbol{G}[\boldsymbol{\Sigma}]] - \mathrm{Tr}(\boldsymbol{\Sigma}\boldsymbol{G}[\boldsymbol{\Sigma}])$$

variational principle ?

$$\frac{\delta \Omega[\boldsymbol{\Sigma}]}{\delta \boldsymbol{\Sigma}} = 0$$

$$\mathrm{Tr}\,\boldsymbol{A} \equiv \frac{1}{\beta}\sum_n \sum_{i\sigma} e^{i\omega_n 0^+} A_{ii\sigma}(i\omega_n)$$

compute functional derivative:

$$\frac{\delta \Omega[\boldsymbol{\Sigma}]}{\delta \boldsymbol{\Sigma}} = \frac{1}{\beta}\left(\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} - \boldsymbol{G}[\boldsymbol{\Sigma}]\right)$$

this means:

$$\frac{\delta \Omega[\boldsymbol{\Sigma}]}{\delta \boldsymbol{\Sigma}} = 0 \quad \Leftrightarrow \quad \boldsymbol{G}[\boldsymbol{\Sigma}] = \frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} \quad \Leftrightarrow \quad \boldsymbol{G} = \frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}[\boldsymbol{G}]} \quad ✔$$

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alternatives ?

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

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

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

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

alternatives ?

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

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

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

alternatives ?

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

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

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alternatives ?

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

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

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

alternatives ?

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

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

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

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alternatives ?

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

(3) $\Omega_{\mathbf{t},}$

(4) $\Omega_{\mathbf{t},}$

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

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

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

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

alternatives ?

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

(3) $\Omega_{\mathbf{t},}$

(4) $\Omega_{\mathbf{t},}$

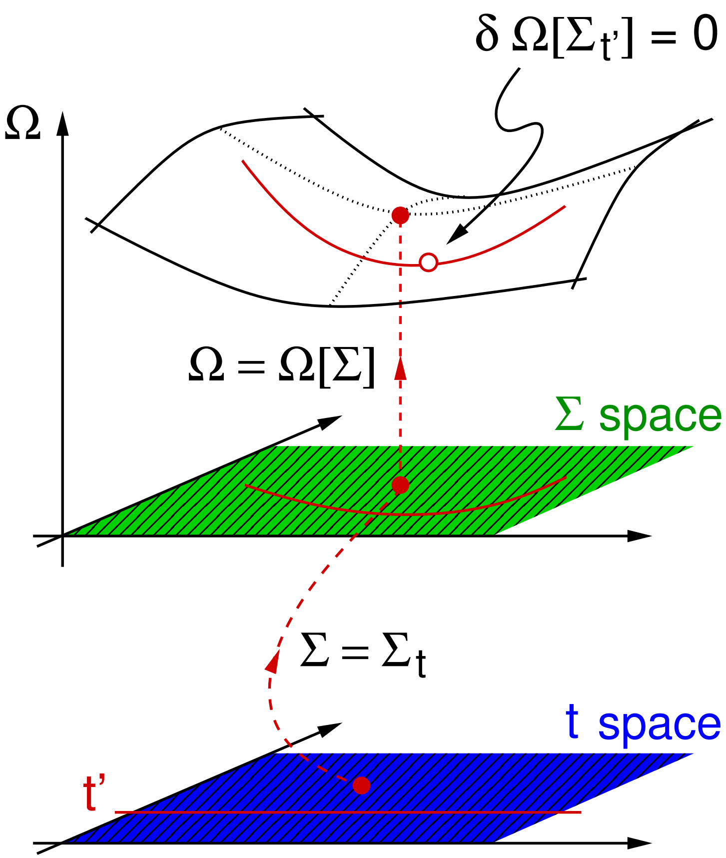
(5) $$\boxed{\Omega_{\mathbf{t},\mathbf{U}}[\mathbf{\Sigma}] = \Phi_{\mathbf{U}}[\mathbf{G}_{\mathbf{t},0}^{-1} - \mathbf{\Sigma}] + \mathrm{Tr}\ln \mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}] - \mathrm{Tr}(\mathbf{\Sigma}\mathbf{G}_{\mathbf{U}}[\mathbf{\Sigma}])}$$ ✖

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

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

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

self-energy-functional theory

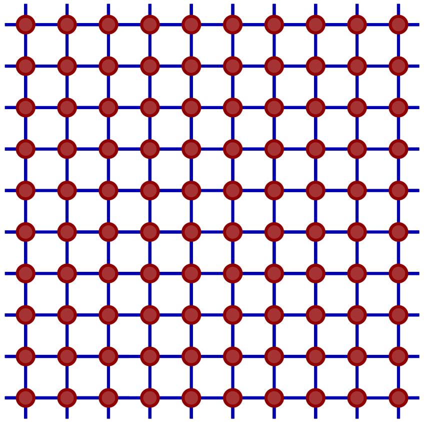


$$\Omega[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} + \Phi[\boldsymbol{G}[\boldsymbol{\Sigma}]] - \mathrm{Tr}(\boldsymbol{\Sigma}\boldsymbol{G}[\boldsymbol{\Sigma}])$$

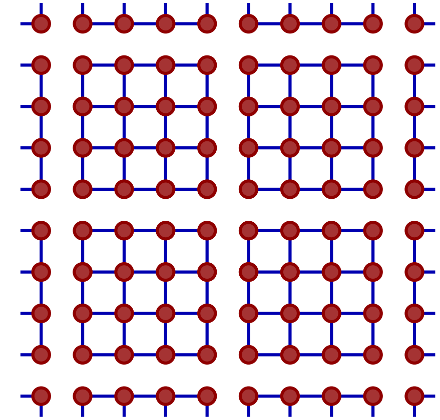
discussion:

- self-energy functional: saddle point vs. minimum
- how to define the domain ?
- where is the original idea of CPT ?
- why not insert an arbitrary self-energy ?
- what is the reference system good for?
- how to evaluate the functional on the restricted domain ?

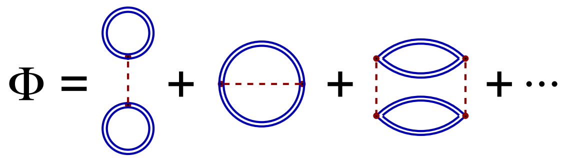
evaluation of the functional



$$\Omega[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1}-\boldsymbol{\Sigma}} + F[\boldsymbol{\Sigma}] \qquad \Omega'[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0'^{-1}-\boldsymbol{\Sigma}} + F[\boldsymbol{\Sigma}]$$

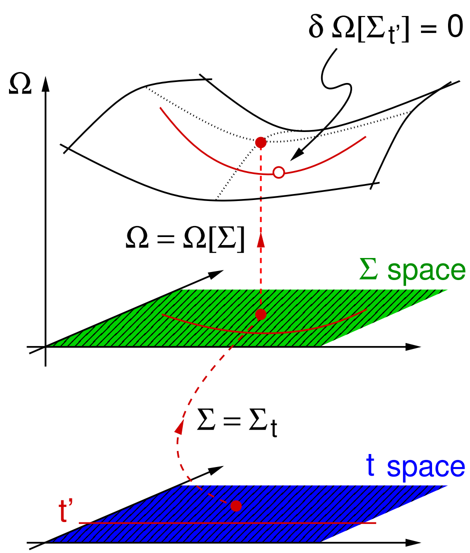


$$F[\boldsymbol{\Sigma}] \equiv \Phi[\boldsymbol{G}[\boldsymbol{\Sigma}]] - \mathrm{Tr}(\boldsymbol{\Sigma}\boldsymbol{G}[\boldsymbol{\Sigma}])$$



$$\Omega[\boldsymbol{\Sigma}] = \Omega'[\boldsymbol{\Sigma}] + \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1}-\boldsymbol{\Sigma}} - \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0'^{-1}-\boldsymbol{\Sigma}}$$

exact !



insert trial self-energy:

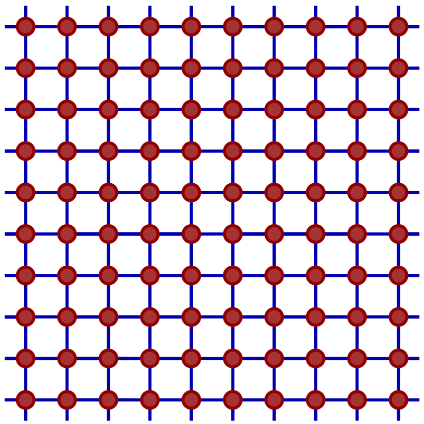
$$\Omega[\boldsymbol{\Sigma}_{t'}] = \Omega' + \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1}-\boldsymbol{\Sigma}_{t'}} - \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0'^{-1}-\boldsymbol{\Sigma}_{t'}}$$

(1) (2) (3)

SFT Euler equation:

$$\left.\frac{\partial\Omega[\boldsymbol{\Sigma}_{t'}]}{\partial \boldsymbol{t}'}\right|_{\boldsymbol{t}'=\boldsymbol{t}'_{\mathrm{opt}}} = 0$$

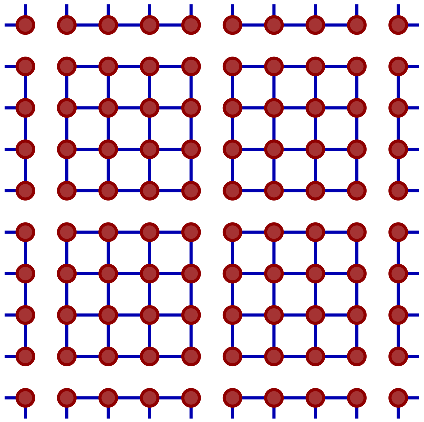
how to ...



$$\left.\frac{\partial\Omega[\boldsymbol{\Sigma}_{\boldsymbol{t}'}]}{\partial \boldsymbol{t}'}\right|_{\boldsymbol{t}'=\boldsymbol{t}'_{\mathrm{opt}}} = 0$$

$$\Omega[\boldsymbol{\Sigma}_{\boldsymbol{t}'}] = \Omega' + \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}'}} - \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0'^{\,-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}'}}$$

(1) (2) (3)



... get term (1) ?

$$(H'-\mu N)|n'\rangle = E'_n|n'\rangle$$

$$Z' = \sum_m e^{-\beta E'_m}$$

$$\Omega' = -T\ln Z'$$

... get term (2) ?

$$\frac{1}{{\boldsymbol{G}_0}^{-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}'}} = \frac{1}{\boldsymbol{G}'^{-1}-\boldsymbol{V}}$$

... get term (3) ?

$$\frac{1}{\boldsymbol{G}_0'^{\,-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}'}} = \boldsymbol{G}'$$

$$G'_{ij\sigma}(\omega) = \frac{1}{Z'}\sum_{mn}\frac{(e^{-\beta E'_m}+e^{-\beta E'_n})\langle m'|c_{i\sigma}|n'\rangle\langle n'|c^\dagger_{j\sigma}|m'\rangle}{\omega-(E'_n-E'_m)}$$

how to ...

$$\left.\frac{\partial \Omega[\boldsymbol{\Sigma}_{t'}]}{\partial \boldsymbol{t}'}\right|_{\boldsymbol{t}'=\boldsymbol{t}'_{\rm opt}} = 0$$

$$\Omega[\boldsymbol{\Sigma}_{t'}] = \Omega' + \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}_{t'}} - \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0'^{\,-1} - \boldsymbol{\Sigma}_{t'}}$$

(1) (2) (3)

... evaluate the Tr ln (...) terms ?

$$\mathrm{Tr}\ln\frac{1}{\boldsymbol{G}'^{-1} - \boldsymbol{V}} - \mathrm{Tr}\ln \boldsymbol{G}' = \frac{1}{\beta}\sum_n e^{i\omega_n 0^+}\left(\mathrm{tr}\ln\frac{1}{\boldsymbol{G}'^{-1}(i\omega_n) - \boldsymbol{V}} - \mathrm{tr}\ln \boldsymbol{G}'(i\omega_n)\right)$$

$$= \frac{1}{\beta}\sum_n e^{i\omega_n 0^+}\,\mathrm{tr}\ln\frac{1}{1 - \boldsymbol{V}\boldsymbol{G}'(i\omega_n)}$$

$$= -\frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{i\omega_n 0^+}\,\mathrm{tr}\ln(1 - \boldsymbol{V}\boldsymbol{G}'(i\omega_n))$$

$$\sim \sum_{n=-\infty}^{\infty} e^{i\omega_n 0^+}\,\ln(1 + \mathcal{O}(1/\omega_n)) \sim \sum_{n=-\infty}^{\infty} e^{i\omega_n 0^+}\,\mathcal{O}(1/\omega_n)$$

converges, and be coded this way, when combining +/- n-terms:

$$\mathrm{tr}\ln\left(1 - \boldsymbol{V}\frac{1}{i\omega_n}\right) + \mathrm{tr}\ln\left(1 + \boldsymbol{V}\frac{1}{i\omega_n}\right) = \mathrm{tr}\ln\left(1 - \boldsymbol{V}\frac{1}{i\omega_n}\right)\left(1 + \boldsymbol{V}\frac{1}{i\omega_n}\right) = \mathcal{O}(1/\omega_n^2)$$

cheap alternative using "Q-matrices":

do everything analytically:

$$\mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}'}}-\mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0'^{\,-1}-\boldsymbol{\Sigma}_{\boldsymbol{t}'}}=-\sum_m\frac{1}{\beta}\ln(1+e^{-\beta\omega_m})+\sum_m\frac{1}{\beta}\ln(1+e^{-\beta\omega'_m})$$

... only the poles of G and of G′ are needed !

Lehmann representation of G′, obtained by ED:

$$\boldsymbol{G}'(\omega)=\boldsymbol{Q}'\frac{1}{\omega-\boldsymbol{\Lambda}'}\boldsymbol{Q}'^{\dagger}\qquad \Lambda'_{mn}=\omega'_m\delta_{mn}\qquad Q'_{\alpha m}=\langle r|c_\alpha|s\rangle\sqrt{\frac{\exp(-\beta E'_r)+\exp(-\beta E'_s)}{Z'}}$$

orbitals   excitations

Lehmann representation of G:

$$\begin{aligned}\boldsymbol{G}(\omega) &= \frac{1}{\boldsymbol{G}'(\omega)^{-1}-\boldsymbol{V}}=\boldsymbol{G}'(\omega)+\boldsymbol{G}'(\omega)\boldsymbol{V}\boldsymbol{G}'(\omega)+\cdots\\ &= \boldsymbol{Q}'\left(\frac{1}{\omega-\boldsymbol{\Lambda}'}+\frac{1}{\omega-\boldsymbol{\Lambda}'}\boldsymbol{Q}'^{\dagger}\boldsymbol{V}\boldsymbol{Q}'\frac{1}{\omega-\boldsymbol{\Lambda}'}+\cdots\right)\boldsymbol{Q}'^{\dagger}=\boldsymbol{Q}'\frac{1}{\omega-\boldsymbol{M}}\boldsymbol{Q}'^{\dagger}\end{aligned}$$

to get poles of G, diagonalize

$$\boldsymbol{M}=\boldsymbol{\Lambda}'+\boldsymbol{Q}'^{\dagger}\boldsymbol{V}\boldsymbol{Q}'$$

matrix dimension: number of one-particle excitations in a cluster

Recipe for practical calculations

A typical VCA calculation is carried out as follows:

- Construct a reference system by tiling the original lattice into identical clusters.
- Choose a set of one-particle parameters $\boldsymbol{t}'$ of the reference system and compute $\boldsymbol{V} = \boldsymbol{t} - \boldsymbol{t}'$.
- Solve the problem for the reference system (U is fixed), i.e. compute the Green's function $\boldsymbol{G}'$ and find the poles ω'_m and the Q'-matrix.
- Get the poles ω_m of the approximate Green's function of the original system by diagonalization of the matrix $\boldsymbol{M} = \boldsymbol{\Lambda}' + \boldsymbol{Q}'^{\dagger}\boldsymbol{V}\boldsymbol{Q}$.
- Calculate the value of the SFT grand potential via Eq. (61) and Eq. (68) and by calculating the grand potential of the reference system Ω' from the eigenvalues of H'.
- Iterate this scheme for different $\boldsymbol{t}'$, such that one can solve

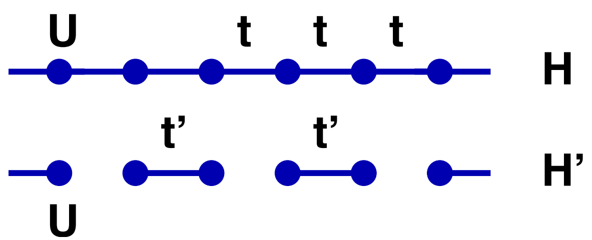
$$\left.\frac{\partial \Omega[\boldsymbol{\Sigma}_{\boldsymbol{t}'}]}{\partial \boldsymbol{t}'}\right|_{\boldsymbol{t}'=\boldsymbol{t}'_{\mathrm{opt}}} \stackrel{!}{=} 0 \qquad (69)$$

  for $\boldsymbol{t}'_{\mathrm{opt}}$.
- Evaluate observables, such as $\Omega[\boldsymbol{\Sigma}_{\boldsymbol{t}'_{\mathrm{opt}}}]$, $\boldsymbol{G}(\omega)$ and static expectation values derived from the SFT grand potential by differentiation, at the stationary point $\boldsymbol{t}'_{\mathrm{opt}}$.
- Redo the calculations for different parameters of the *original* system, e.g. a different U, filling or β to scan the interesting parameter space.

$$\Omega[\boldsymbol{\Sigma}_{t'}] = \Omega' + \mathrm{Tr}\ln\frac{1}{\mathbf{G}_0^{-1} - \boldsymbol{\Sigma}_{t'}} - \mathrm{Tr}\ln\frac{1}{\mathbf{G}_0'^{-1} - \boldsymbol{\Sigma}_{t'}}. \qquad (61)$$

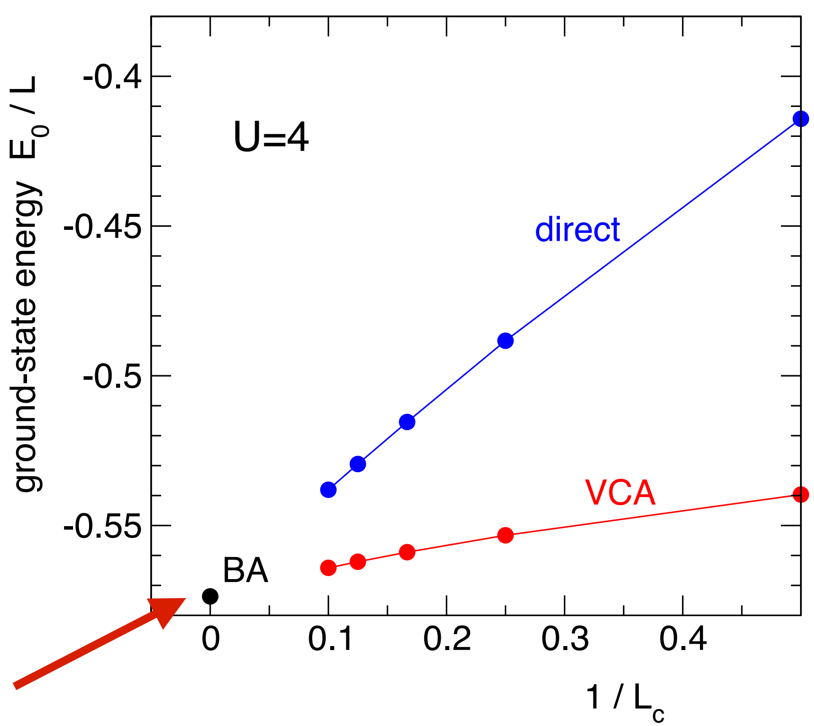
$$\mathrm{Tr}\ln\frac{1}{\mathbf{G}_0^{-1} - \boldsymbol{\Sigma}_{t'}} - \mathrm{Tr}\ln\frac{1}{\mathbf{G}_0'^{-1} - \boldsymbol{\Sigma}_{t'}} = -\sum_m \frac{1}{\beta}\ln(1+e^{-\beta\omega_m}) + \sum_m \frac{1}{\beta}\ln(1+e^{-\beta\omega'_m}), \qquad (68)$$

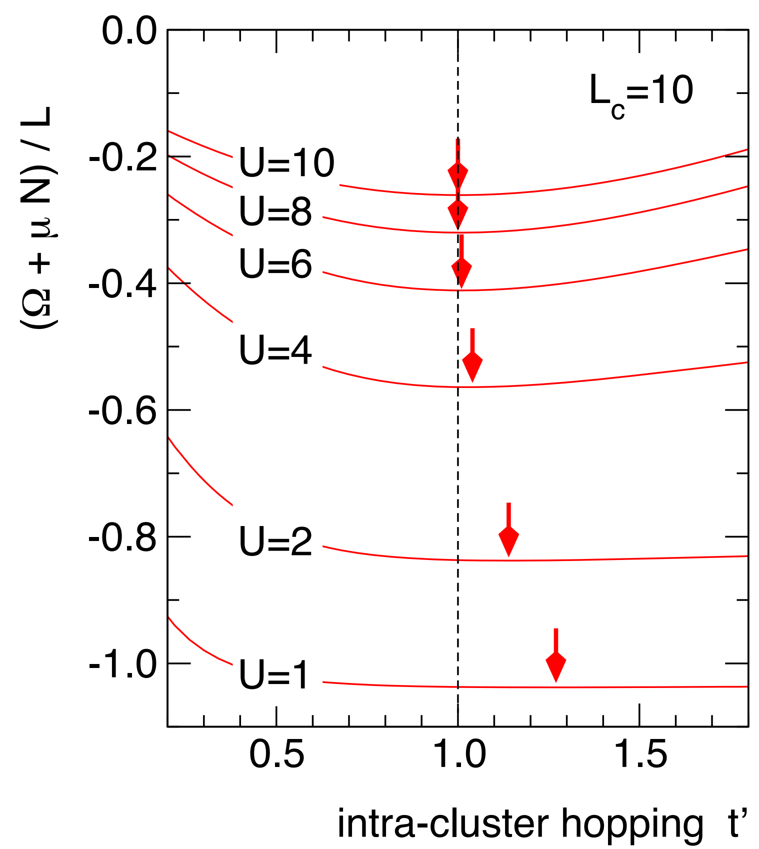
simple application: D=1 Hubbard model



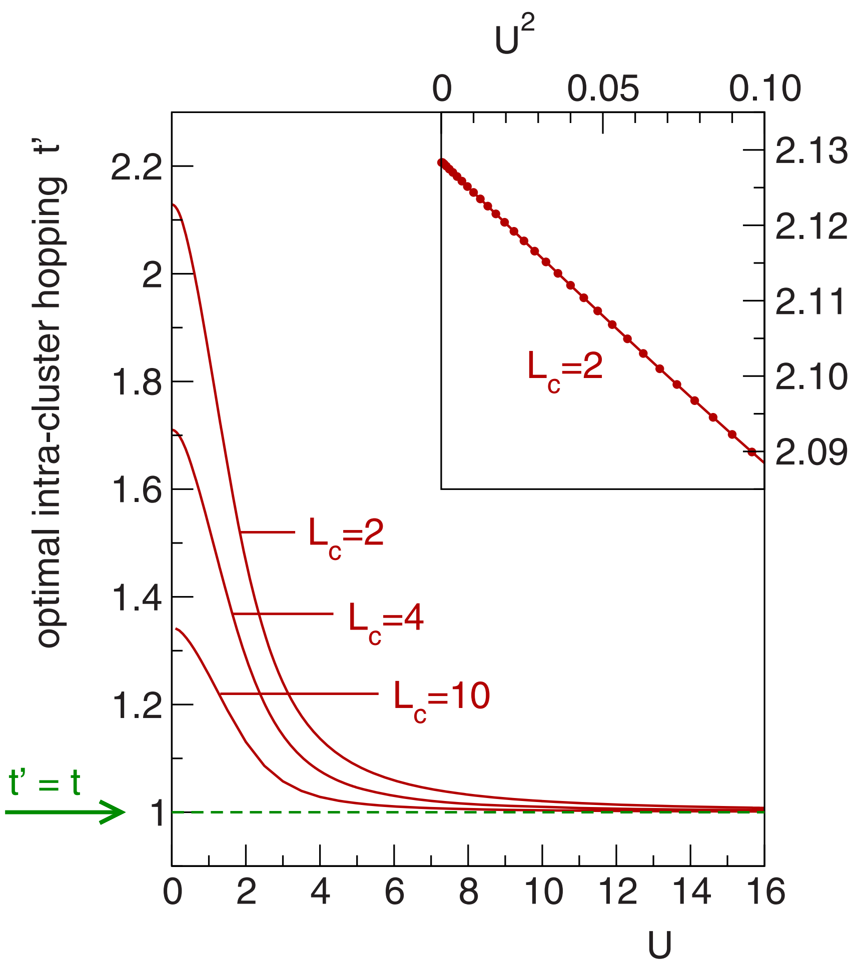
- half-filling, T=0, large L, small L_c
- a single variational parameter
- minimum or maximum

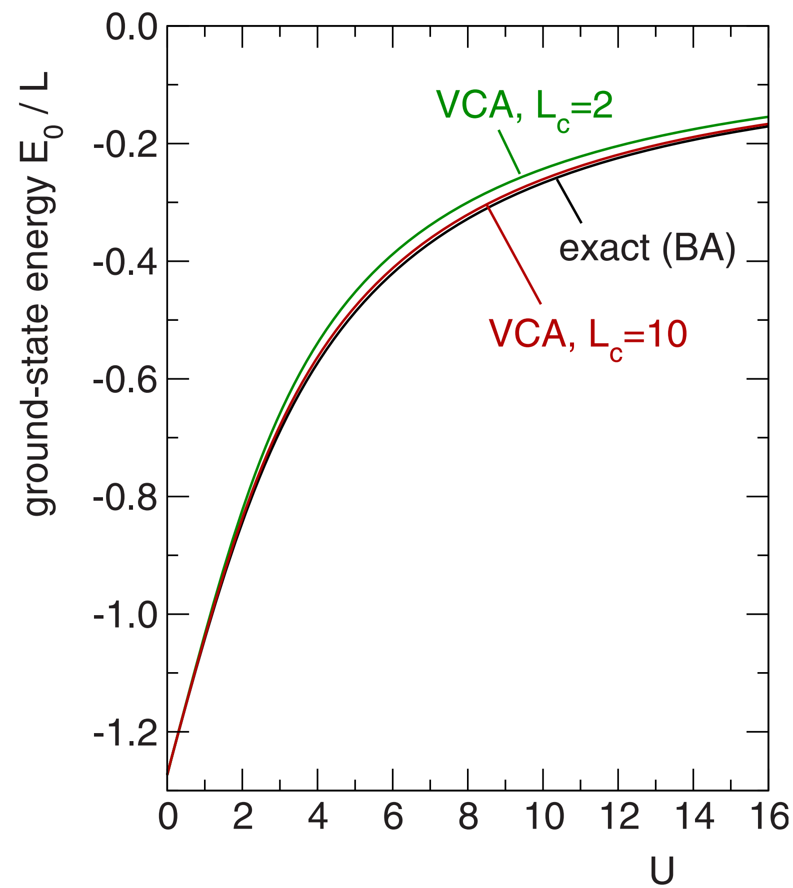
- shallow minimum for weak U
- strong U: t' close to t





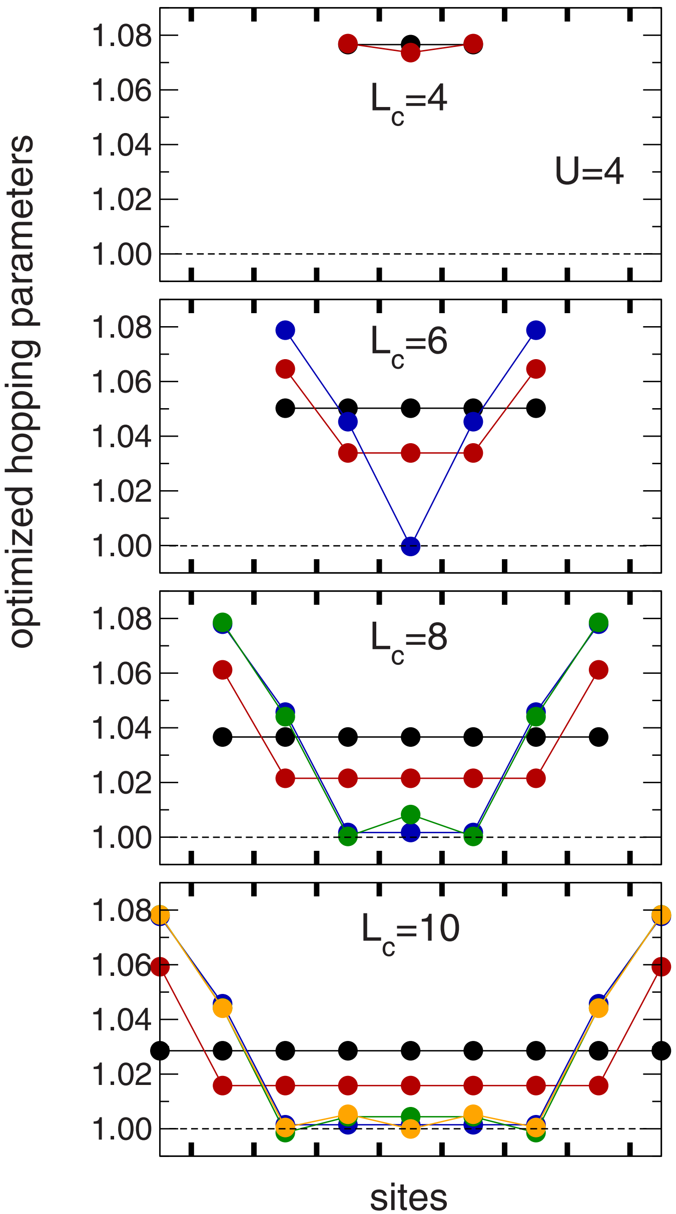
simple application: D=1 Hubbard model

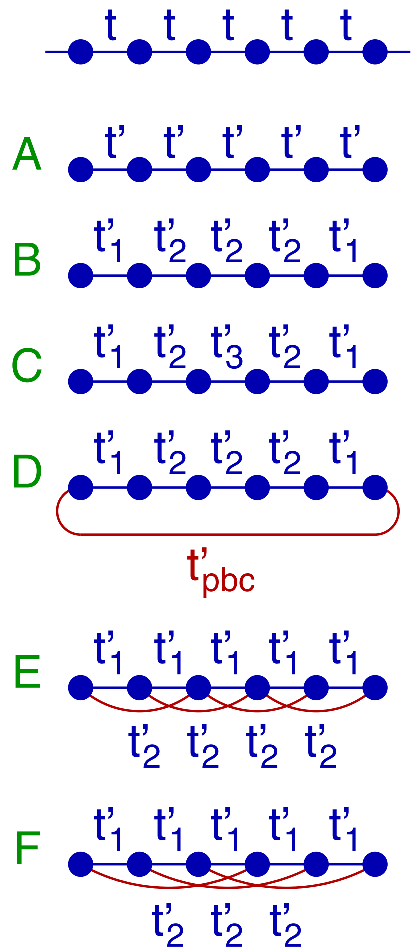




- best results for weak and strong U
  here: VCA is exact

more variational parameters





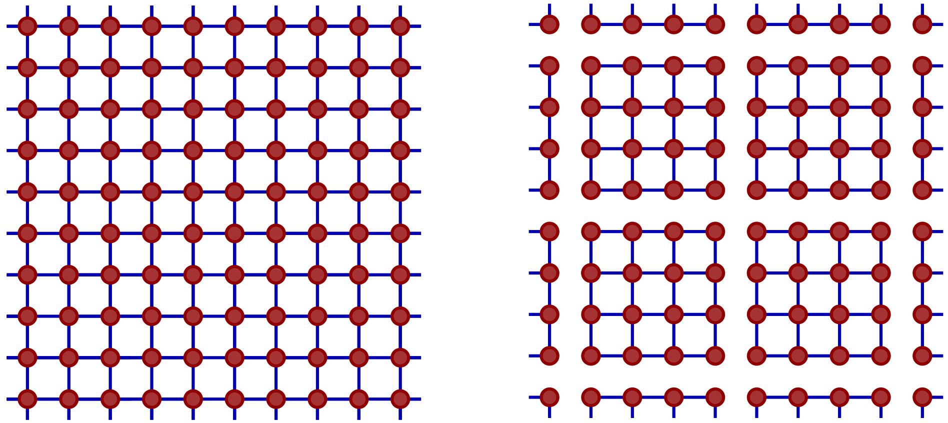
- larger clusters:
  larger Hilbert space AND more parameters
- find a stationary point in a high-dimensional space: e.g. minimize

$$|\partial \Omega[\boldsymbol{\Sigma}_{\boldsymbol{t}'}]/\partial \boldsymbol{t}'|^2.$$

- typically, the system makes use of more parameters
- effects are strongest at the edges
- VCA respects particle-hole symmetry
- VCA finds its own type of boundary conditions

recall: VCA – the main idea

e.g. spontaneous antiferromagnetic order

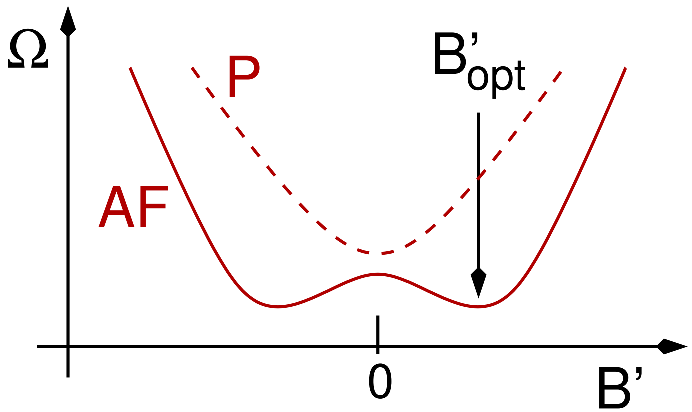


$B_{\mathrm{st.}} = 0$ $\qquad$ $B'_{\mathrm{st.}} > 0$

physical field $\qquad$ fictitious field

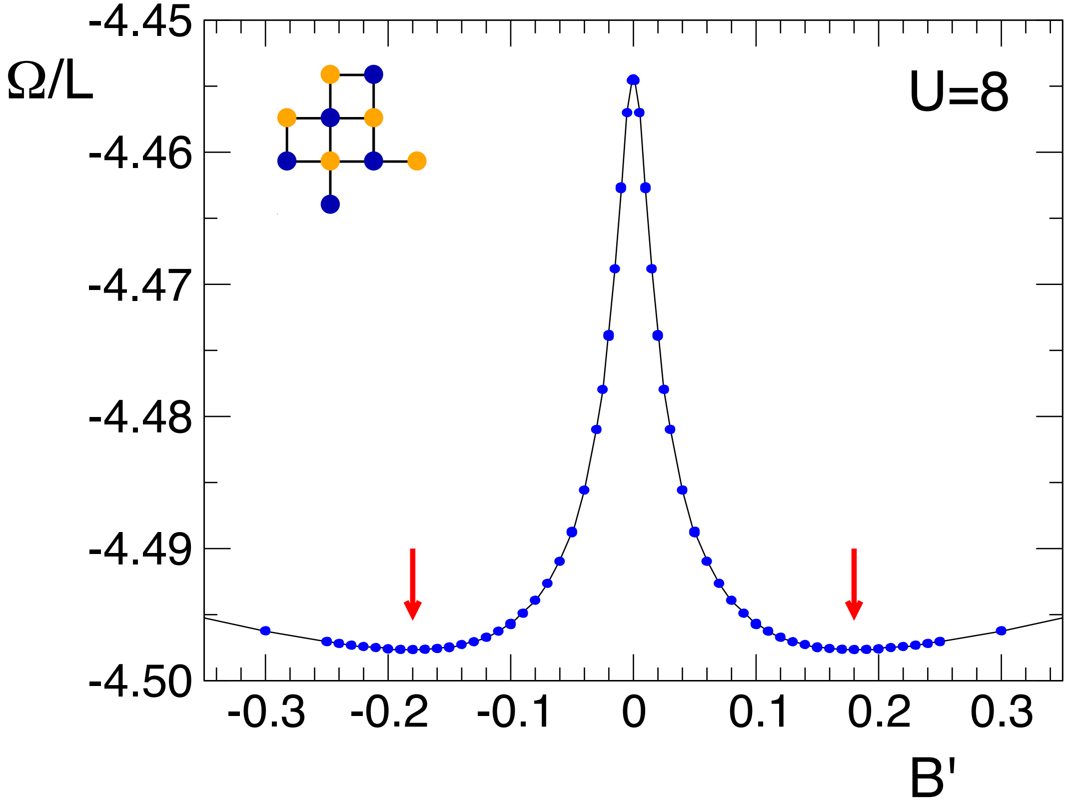
Q: how to find the "right" field ?

A: the optimal field should minimize the grand potential !



$$\Omega(B') = ? \quad \Omega(\boldsymbol{t}') = ?$$

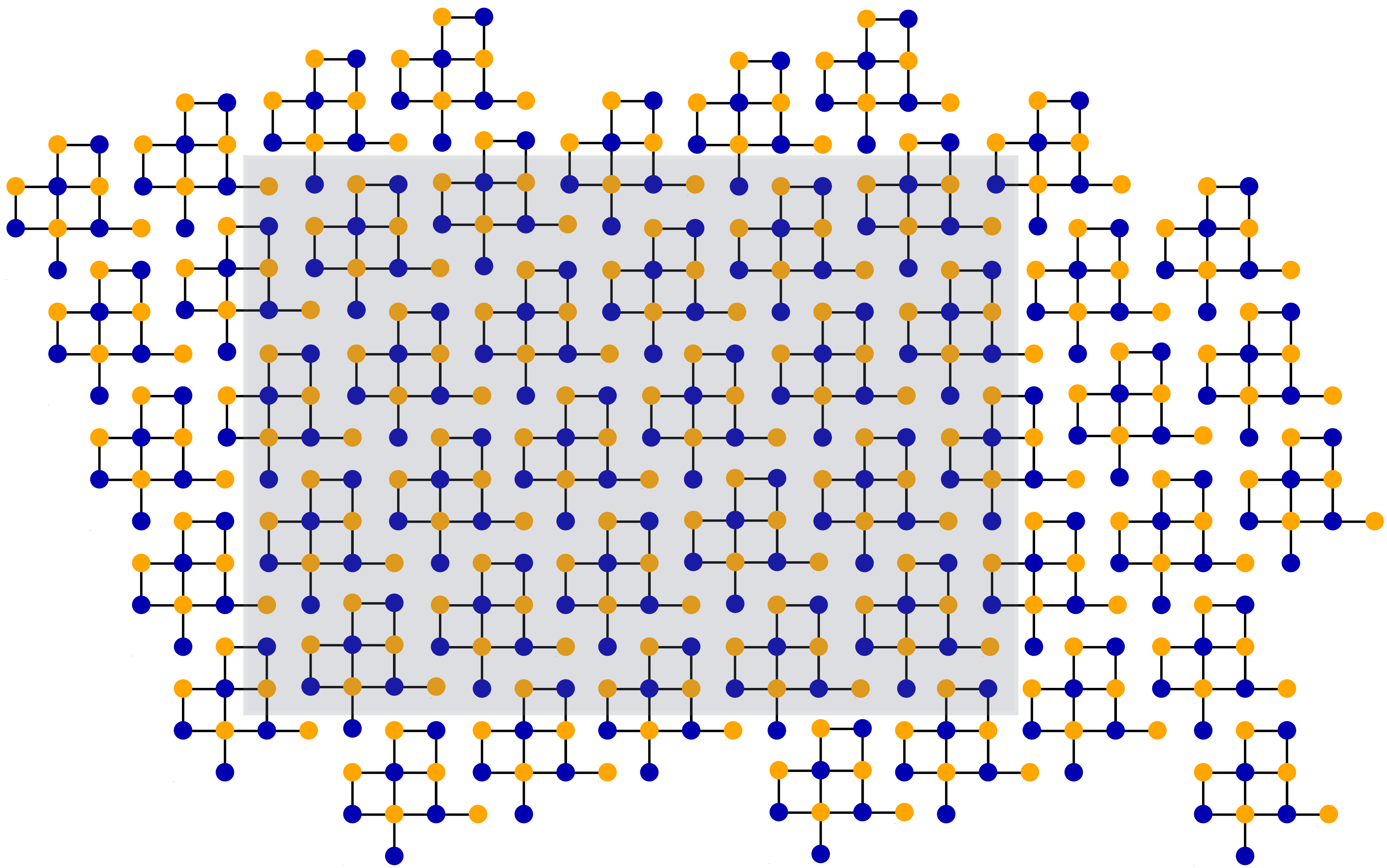
D=2: spontaneous order



$$H' = H'|_{B'=0} - B' \sum_{i\sigma} z_i (n_{i\uparrow} - n_{i\downarrow})$$

- D=2 Hubbard model, n=1, T=0
- cluster with L_C=10 sites
- low cluster symmetries favorable
- solver for the reference system: Lanczos
- fictitious staggered field (mean field, Weiss field)

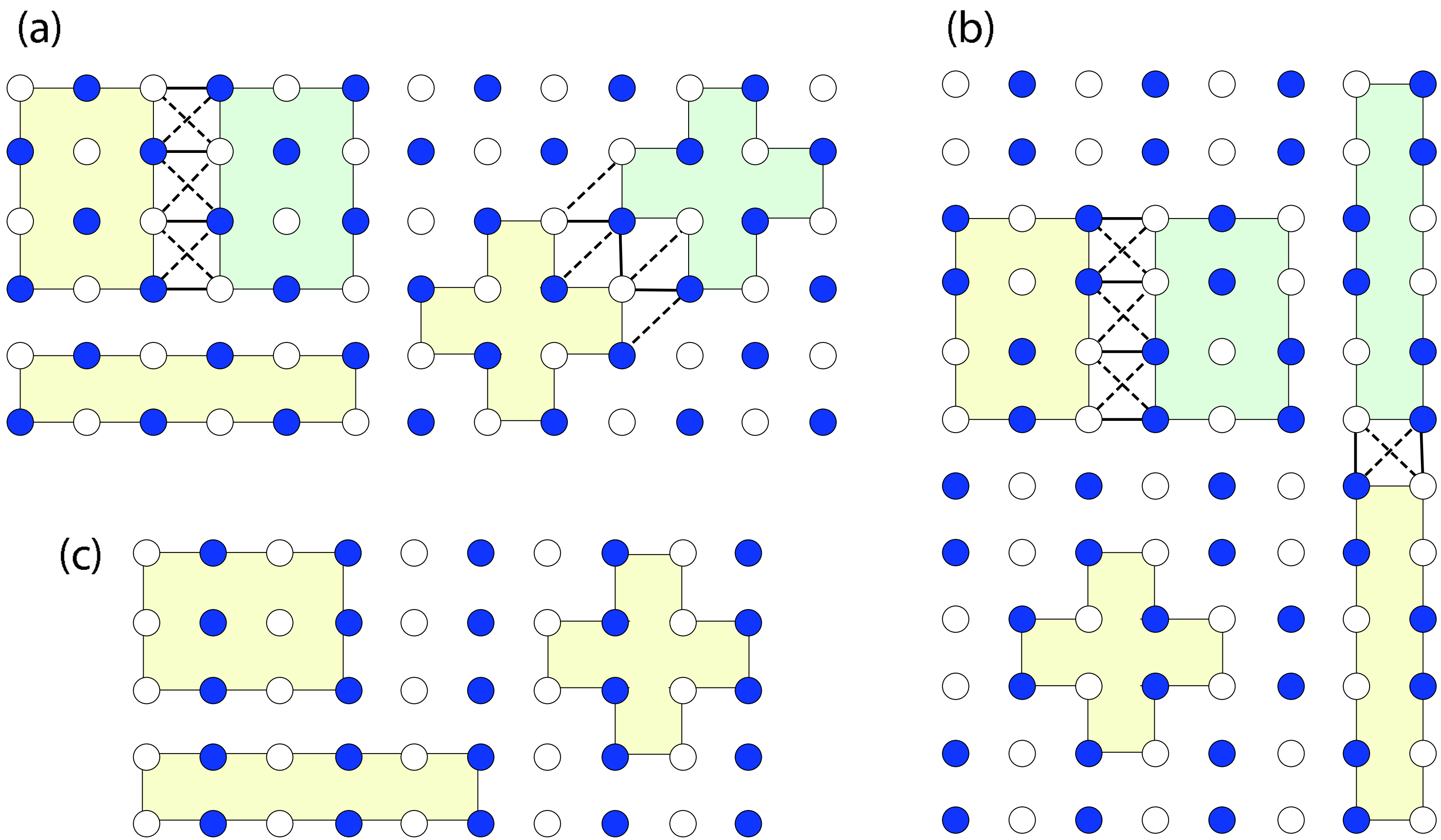
strange cluster ? but it works !



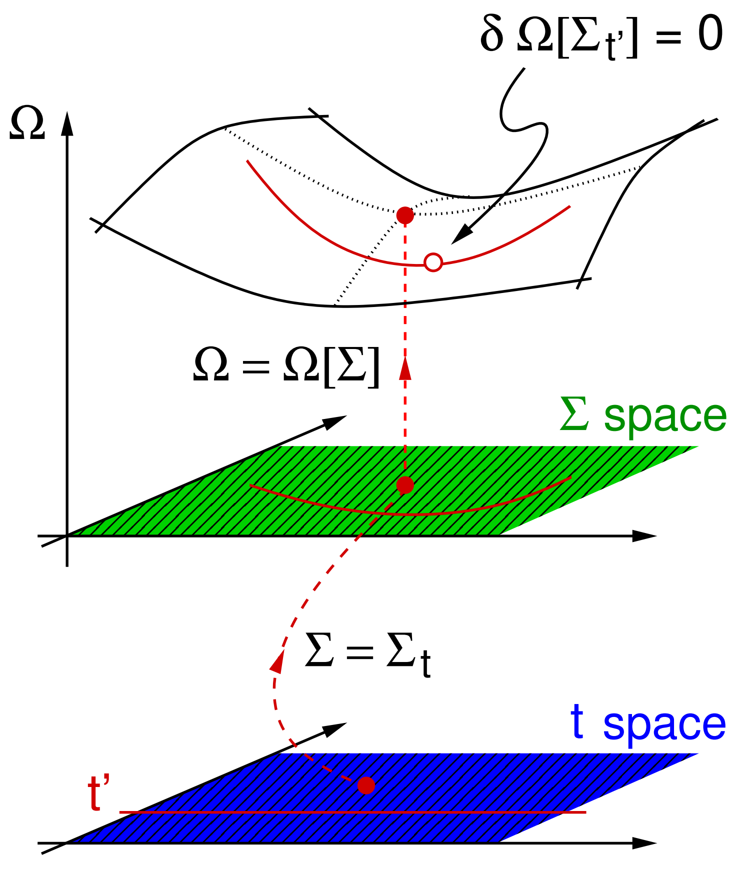
tiling of the lattice

- different clusters and pairs of clusters used for an A-B sublattice ordering

Yamada et al. (2013)



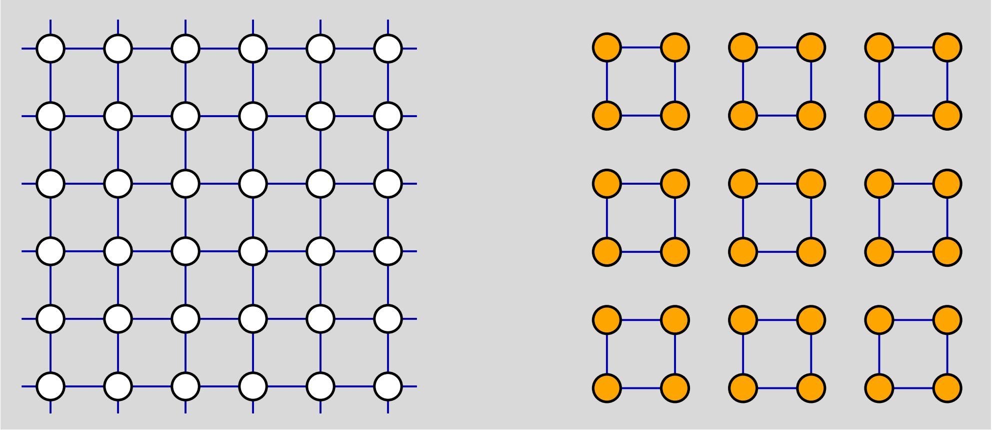
different reference systems: VCA



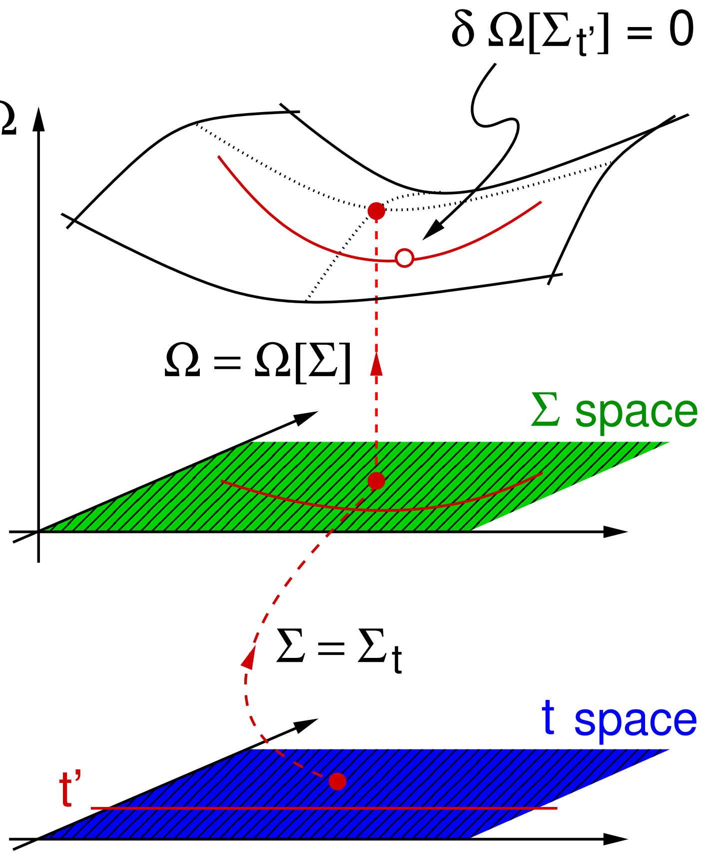
- VCA: cluster mean-field approach
- includes short-range spatial correlations
- mean-field-like on a scale beyond linear cluster extension

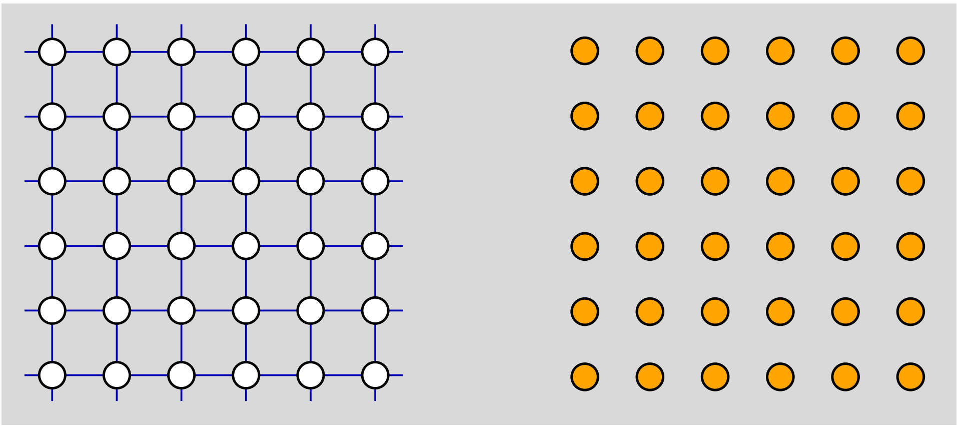
original system

reference system



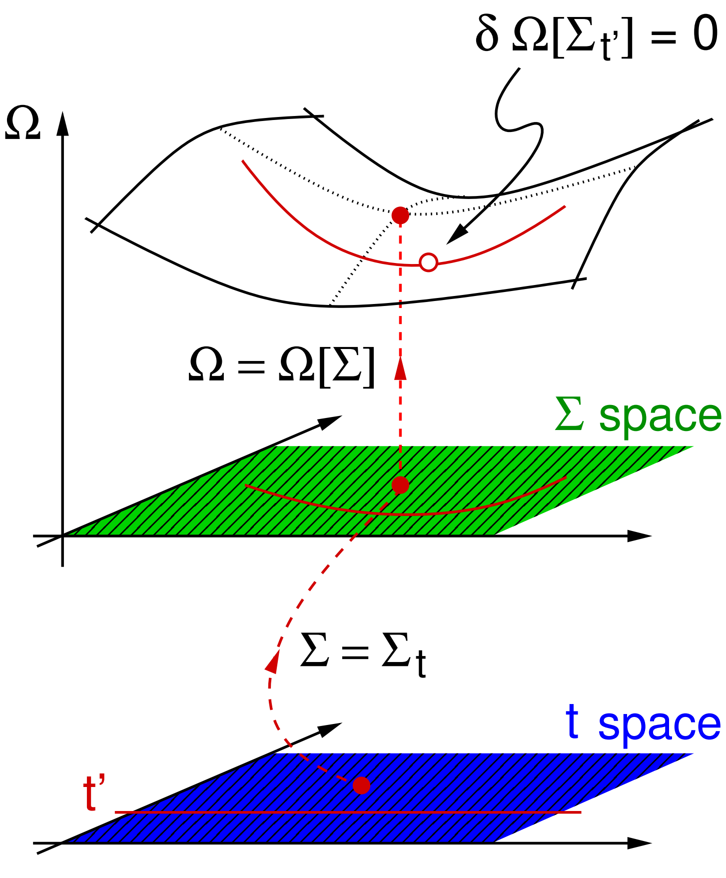
extreme case: single site

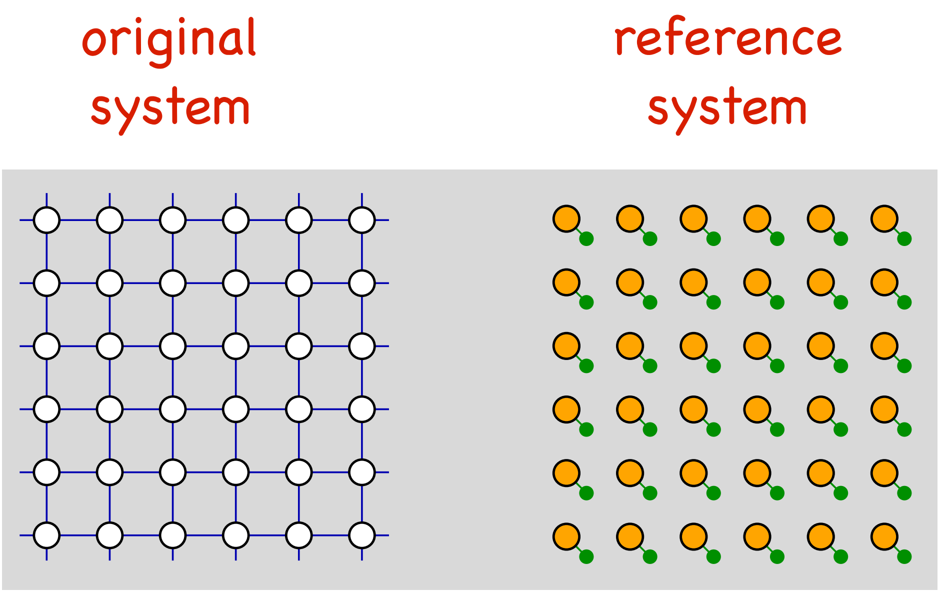




- single-site mean-field theory
- like Hubbard-I but with parameter optimization

bath sites

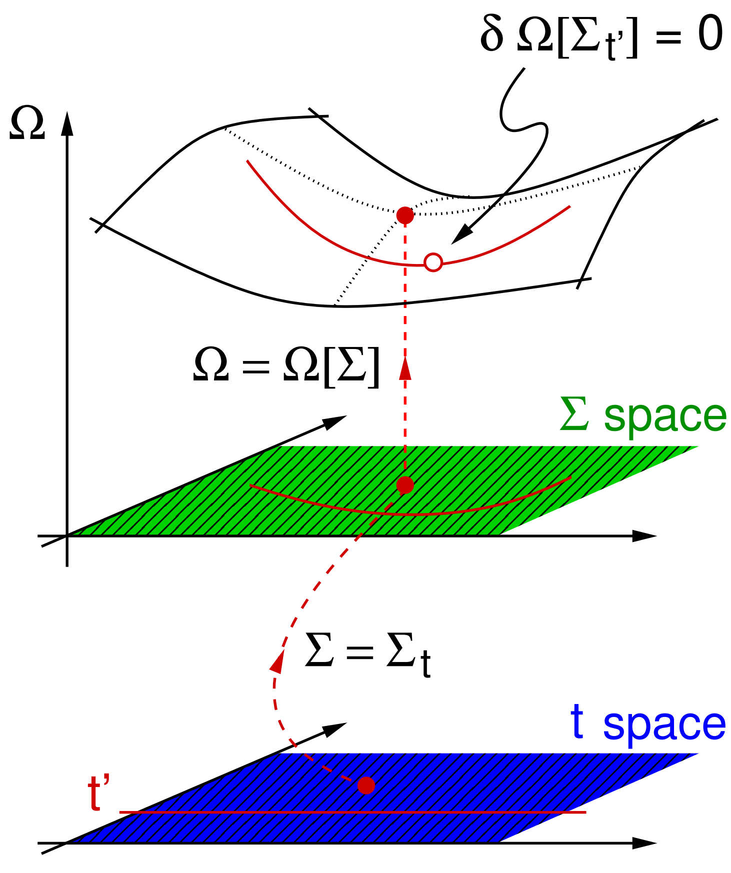




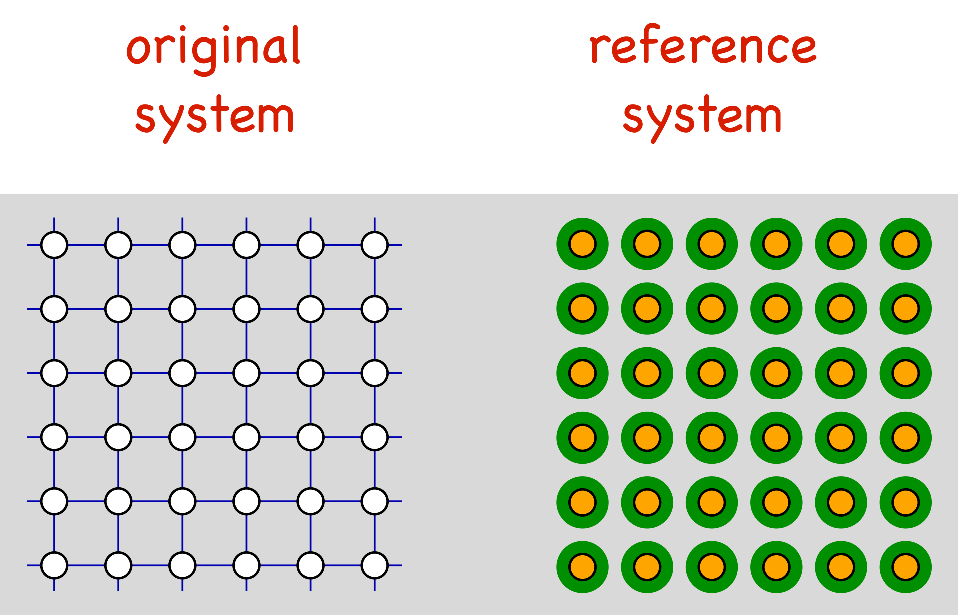
- choice of the reference system: same interaction part ! ("universality")
- bath sites: more variational degrees of freedom
- improve description of temporal fluctuations

$$\Omega[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} + F[\boldsymbol{\Sigma}] \qquad \Omega'[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0'^{\,-1} - \boldsymbol{\Sigma}} + F[\boldsymbol{\Sigma}]$$

best single-site mean-field theory ?



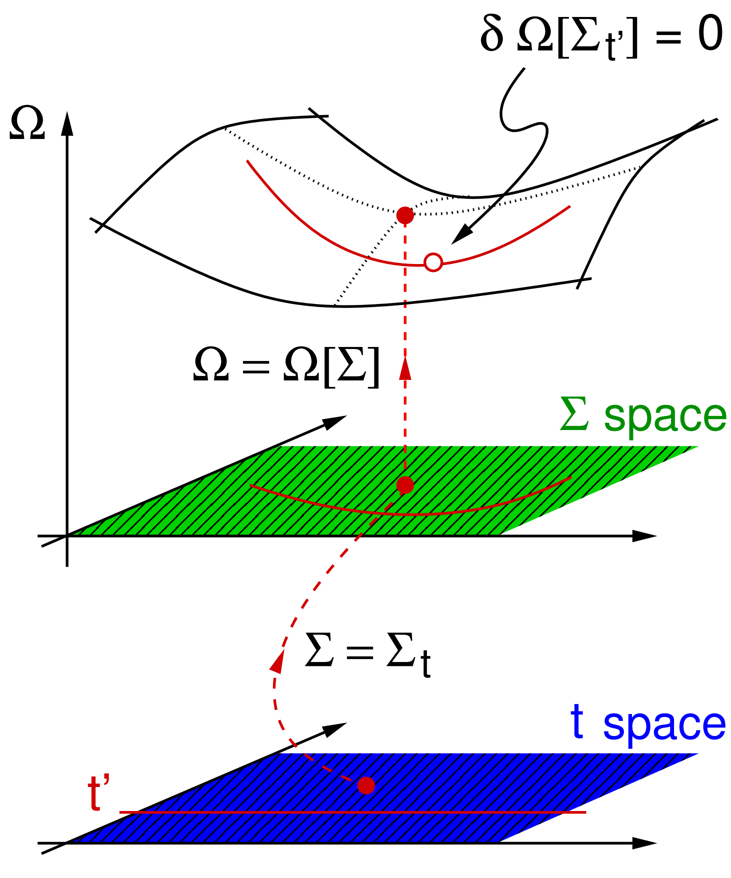
- continuum of bath sites
- this yields ...



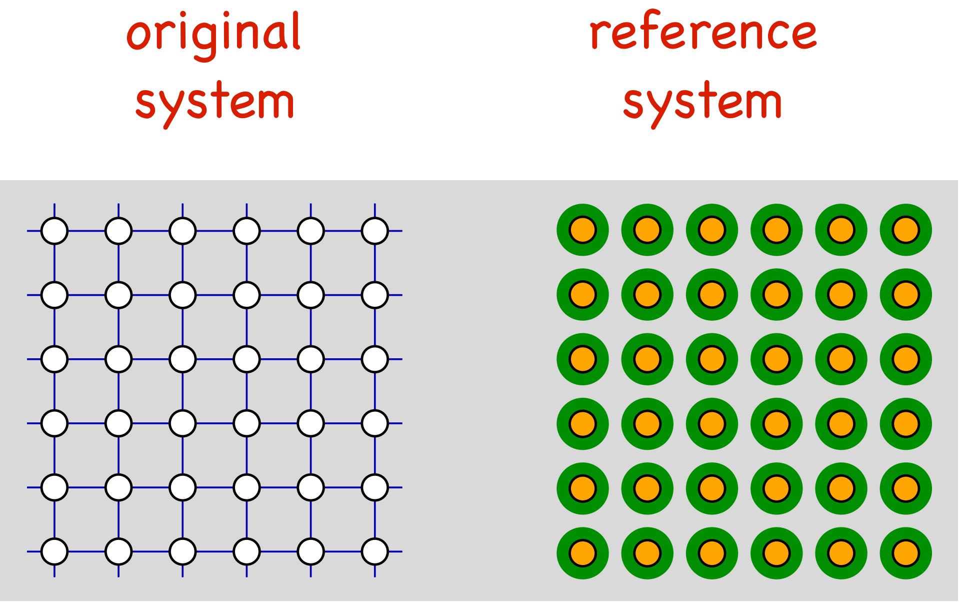
remember:

$$0 = \frac{\partial}{\partial \boldsymbol{t}'} \Omega[(\boldsymbol{G}'^{-1} - \boldsymbol{V})^{-1}] = \frac{\delta \Omega}{\delta \boldsymbol{G}} \cdot \frac{\partial \boldsymbol{G}}{\partial \boldsymbol{t}'} = \left(\boldsymbol{\Sigma}' + \boldsymbol{G}^{-1} - \boldsymbol{G}_0^{-1} \right) \frac{\partial \boldsymbol{G}}{\partial \boldsymbol{t}'}$$

best single-site mean-field theory ?



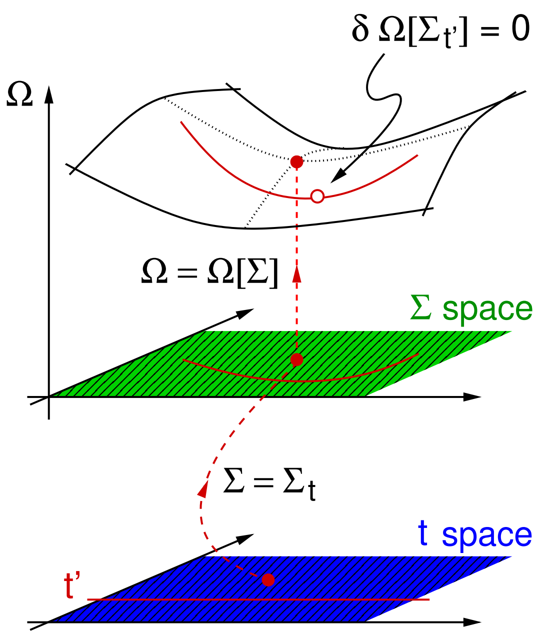
- continuum of bath sites
- this yields ... DMFT



remember:

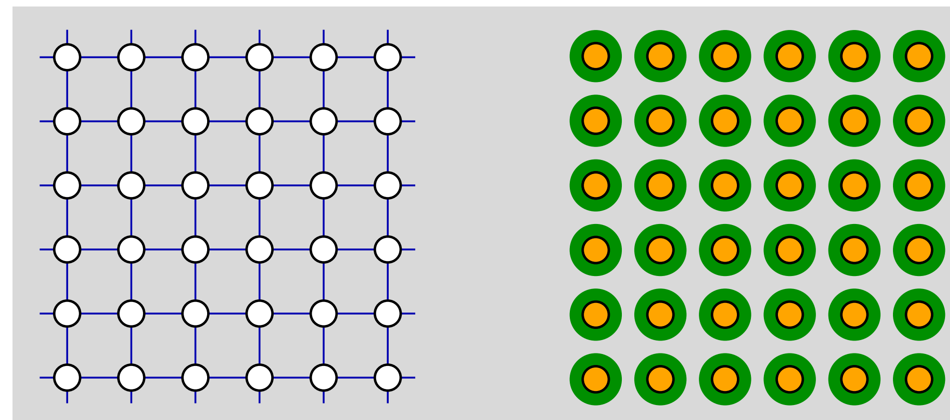
$$0 = \frac{\partial}{\partial \boldsymbol{t}'} \Omega[(\boldsymbol{G}'^{-1} - \boldsymbol{V})^{-1}] = \frac{\delta \Omega}{\delta \boldsymbol{G}} \cdot \frac{\partial \boldsymbol{G}}{\partial \boldsymbol{t}'} = \left(\boldsymbol{\Sigma}' + \boldsymbol{G}^{-1} - \boldsymbol{G}_0^{-1}\right) \frac{\partial \boldsymbol{G}}{\partial \boldsymbol{t}'}$$

DMFT



original system

reference system



here:

$$\Omega[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} + \Phi[\boldsymbol{G}[\boldsymbol{\Sigma}]] - \mathrm{Tr}(\boldsymbol{\Sigma}\boldsymbol{G}[\boldsymbol{\Sigma}])$$

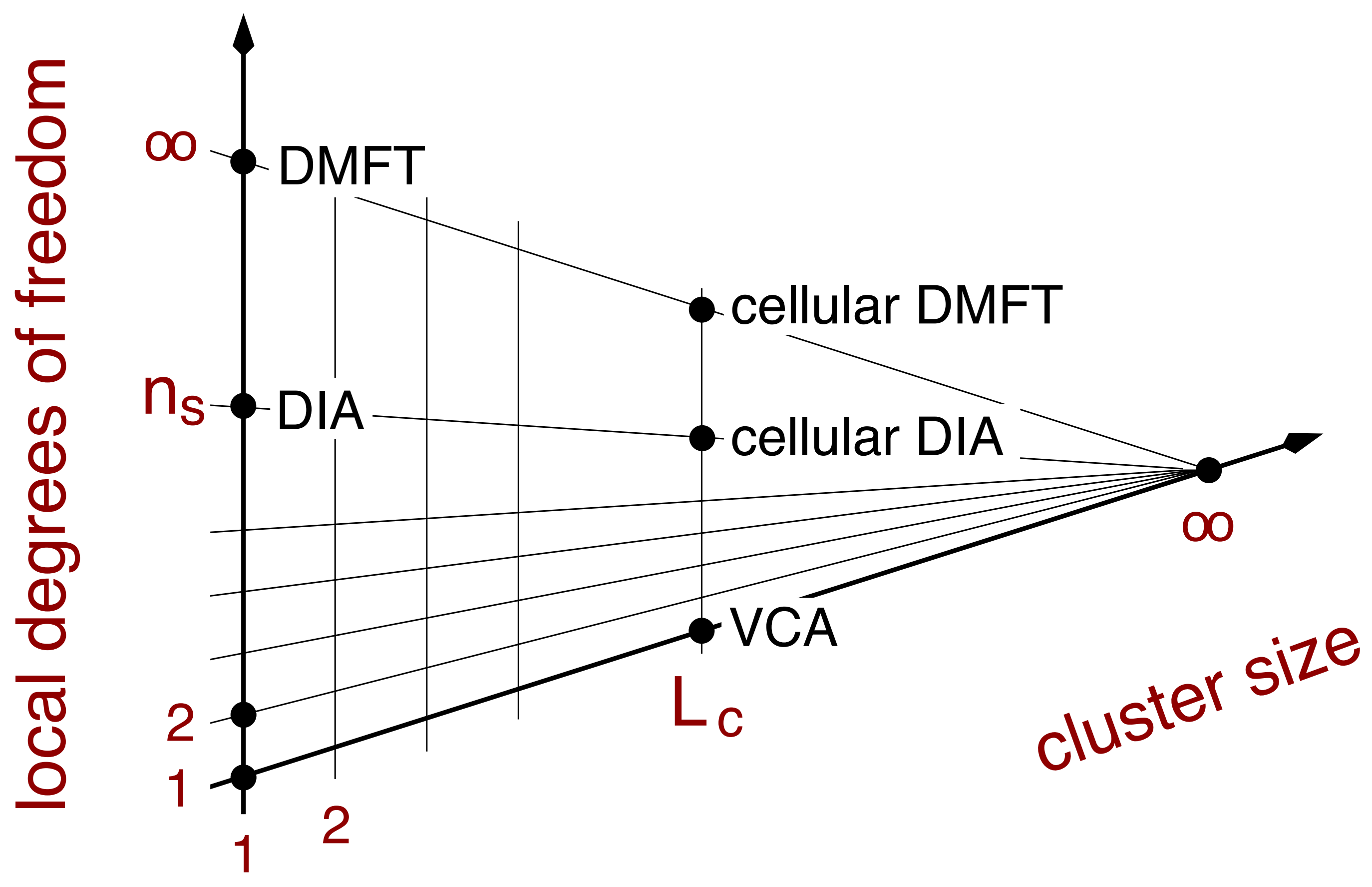
$$\frac{\delta\Omega[\boldsymbol{\Sigma}]}{\delta\boldsymbol{\Sigma}} = \frac{1}{\beta}\left(\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} - \boldsymbol{G}[\boldsymbol{\Sigma}]\right)$$

$$\frac{\partial}{\partial \boldsymbol{t}'}\Omega[\boldsymbol{\Sigma}_{\boldsymbol{t}'}] = \frac{\delta\Omega[\boldsymbol{\Sigma}]}{\delta\boldsymbol{\Sigma}} \cdot \frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{t}'}}{\partial \boldsymbol{t}'} \longrightarrow 0 = \frac{\partial\Omega[\boldsymbol{\Sigma}_{\boldsymbol{t}'}]}{\partial \boldsymbol{t}'} = \frac{1}{\beta}\sum_{\omega_n}\sum_{i\sigma}\left(\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} - \boldsymbol{G}'\right)_{ii,\sigma}\frac{\partial\Sigma_{ii,\sigma}}{\partial \boldsymbol{t}'}$$

DMFT self-consistency condition

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

VCA and its family



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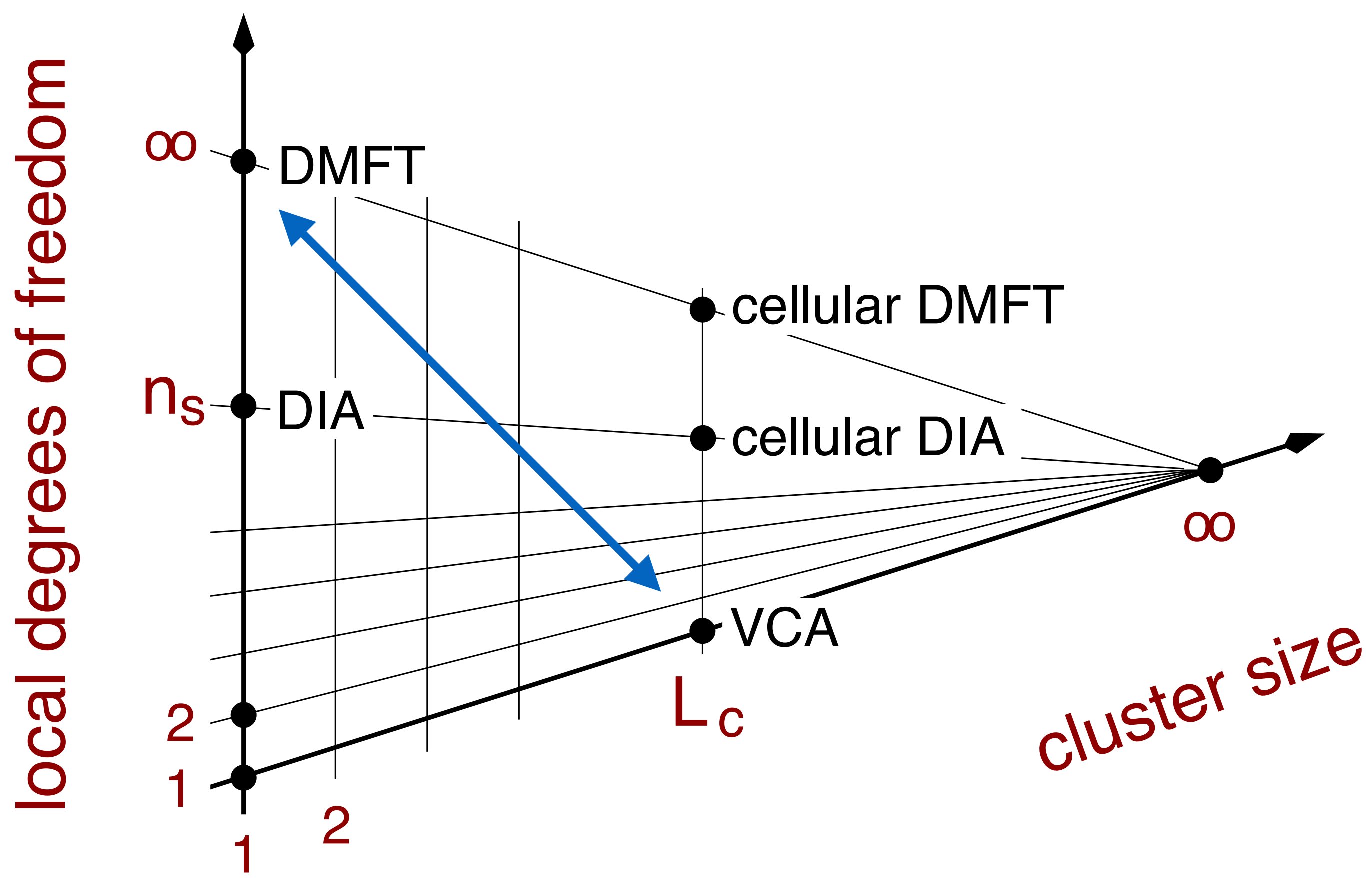
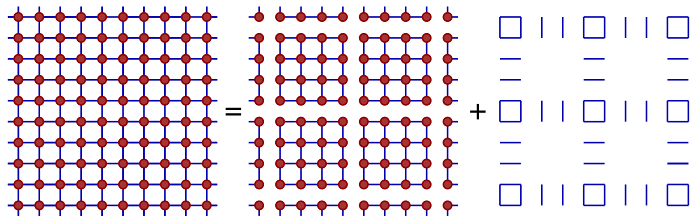
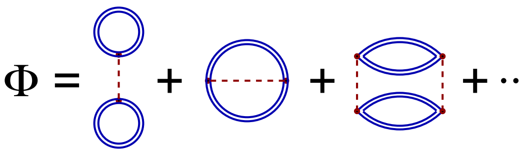
VCA and its family



conclusion

- CPT – a nice idea, but lacks self-consistency or variational character

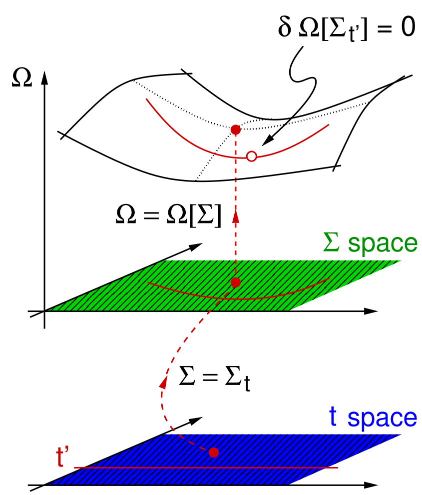




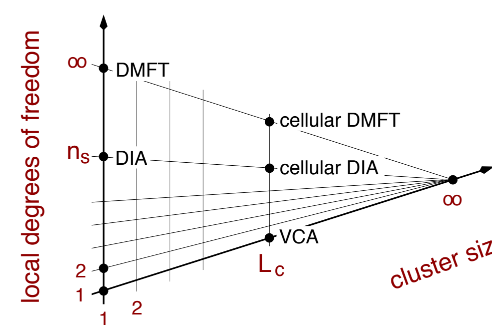
- Green's functions and perturbation theory are needed as a formal language
- variational principles can be constructed with functionals of dynamic (frequency-dependent) quantities (self-energy)

$$\Omega[\boldsymbol{\Sigma}] = \mathrm{Tr}\ln\frac{1}{\boldsymbol{G}_0^{-1} - \boldsymbol{\Sigma}} + \Phi[\boldsymbol{G}[\boldsymbol{\Sigma}]] - \mathrm{Tr}(\boldsymbol{\Sigma}\boldsymbol{G}[\boldsymbol{\Sigma}])$$

- the CPT-idea of a reference system saves the day



- the benefit: nice new cluster mean-field approximations
- and a new view on DMFT and related theories



VCA to the high-T_c problem

Senechal et al. (2004)

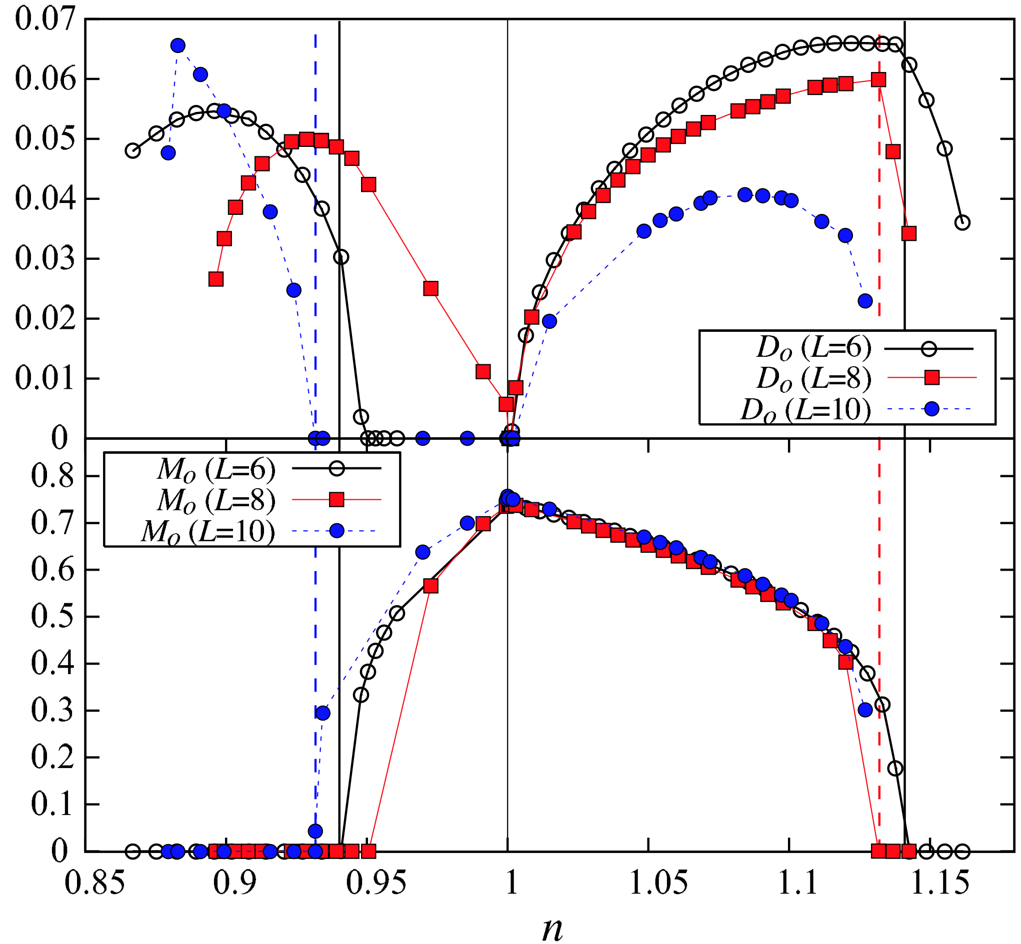
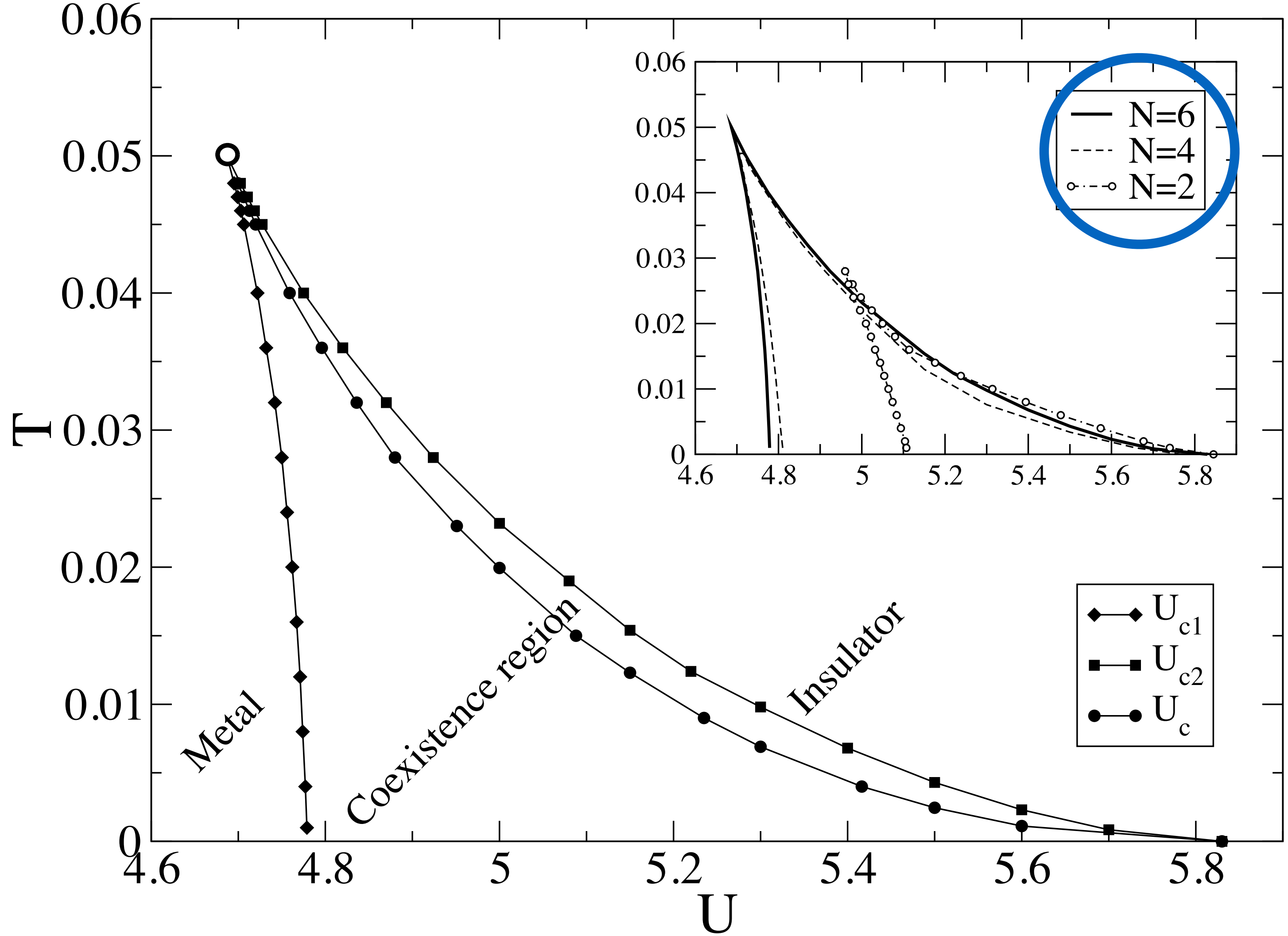


FIG. 1: AF (bottom) and dSC (top) order parameters for $U = 8t$ as a function of the electron density (n) for 2×3, 2×4 and 10-site clusters. Vertical lines indicate the first doping where only dSC order is non-vanishing.

bath sites

Pozgajcic (2004)



Mott transition