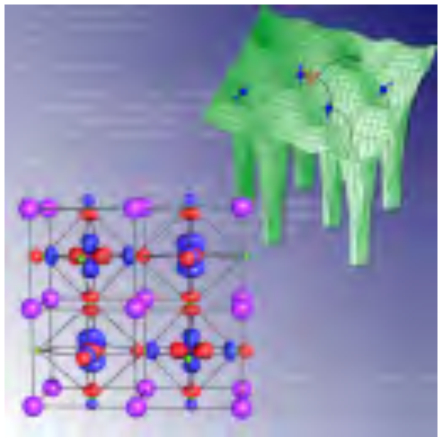

Cluster Extensions of Dynamical Mean-Field Theory

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outline:

- motivation
- geometry
- Green's functions
- cluster-perturbation theory
- periodization schemes
- self-consistent cluster embedding approaches
- applications

MOTIVATION

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timeline

1966: Hubbard-I approximation

|

1993: cluster-perturbation theory (CPT)

|

1989 - 1992: dynamical mean-field theory (DMFT)

|

1998: dynamical cluster approximation (DCA)

|

2000 - 2001: cellular dynamical mean-field theory (C-DMFT)

|

2003: variational cluster approach (VCA)

|

2004: periodized cellular dynamical mean-field theory (PC-DMFT)

|

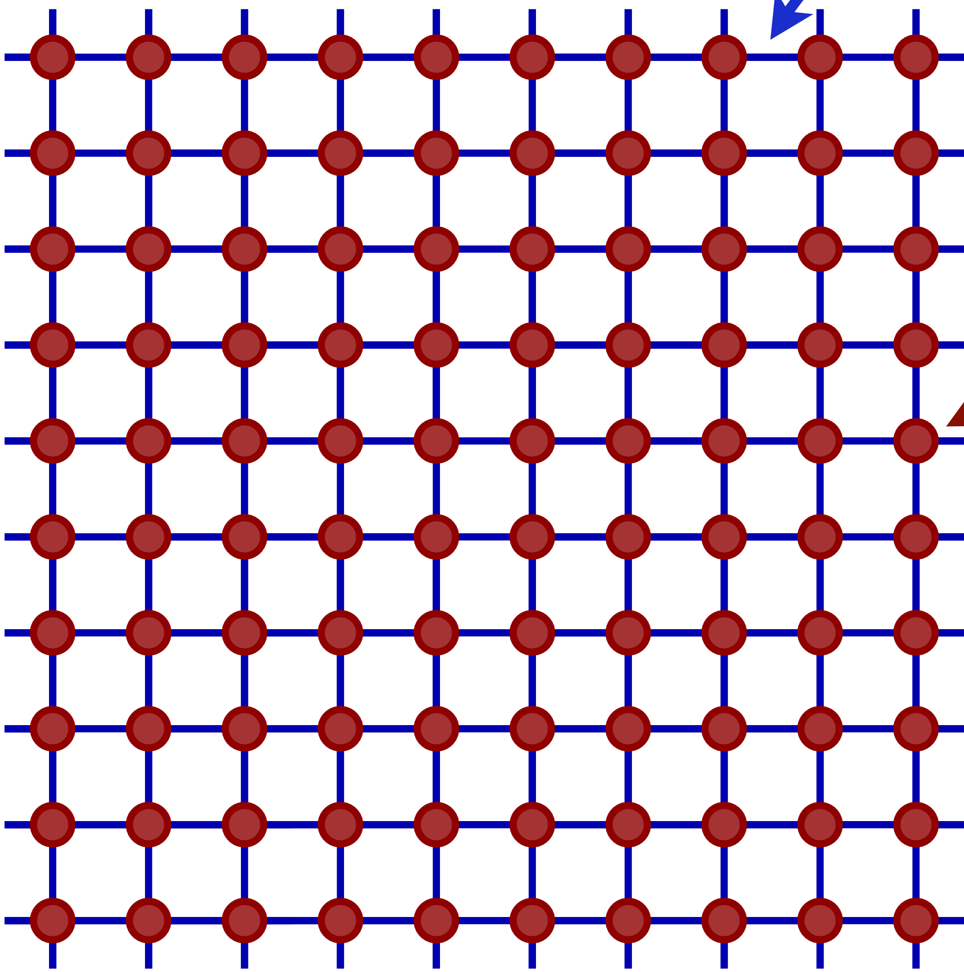
2006: periodic cluster-perturbation theory

|

lattice models

$$H = H_0 + H_1$$

e.g.: Hubbard model



kinetic and potential energy

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

interaction energy

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

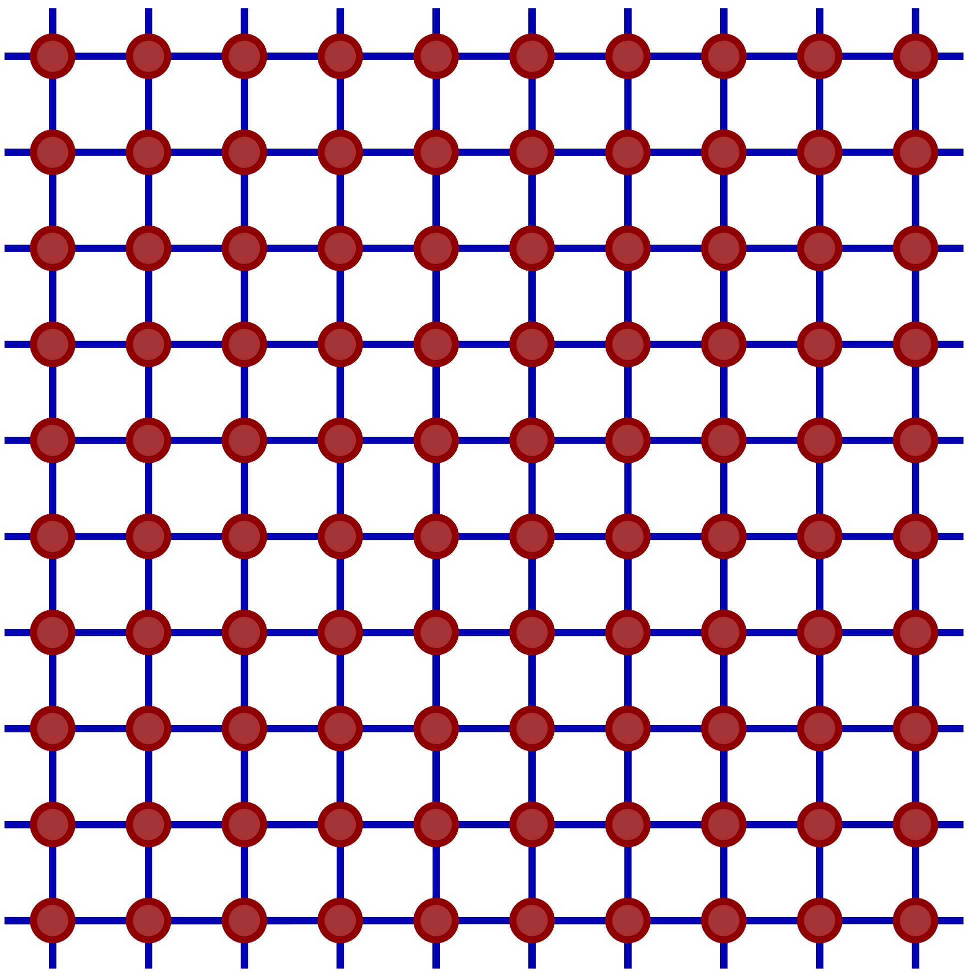
Why consider the Hubbard model ?

- generic many-body problem
- most simple setup for the "correlation problem"

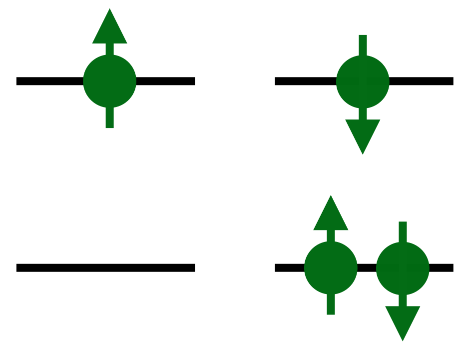
Hilbert space

$H = H_0 + H_1$

e.g.: Hubbard model



single site: dimension 4



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

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

dimension $\binom{L}{N_\uparrow}\binom{L}{N_\downarrow}$

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

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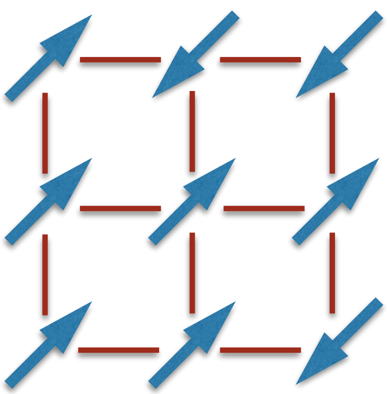
quantum statistics

S=1/2 Heisenberg model



$$H = \sum_{i,j} J_{ij} \boldsymbol{S}_i \boldsymbol{S}_j - B \sum_i S_{iz}$$

$$|m_i\rangle = |\uparrow\rangle\,,\,|\downarrow\rangle$$

compute the ground state?

$$|\Psi_0\rangle = \sum_{m_1, m_2, \ldots, m_L} c_{m_1,\ldots,m_L} |m_1\rangle \otimes \cdots \otimes |m_L\rangle$$

coefficients cannot be stored for large L!

quantum statistics:
compute the partition function / free energy

$$Z(T, x) = \mathrm{tr}\, \exp(-\beta H(x))$$

$$F(T, x) = -T \ln Z(T, x)$$

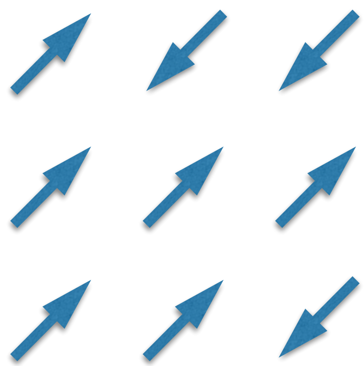
gives access to thermodynamics!

DMFT: provides the thermodynamics (and excitations)

correlated lattice models

Heisenberg model, J=0

$$Z = \mathrm{tr}\exp\left(\beta B \sum_i S_{iz}\right) = \sum_{m_1,\dots,m_L} \exp\left(\beta B \sum_i m_i\right)$$
$$= \sum_{m_1,\dots,m_L} \prod_i \exp\left(\beta B m_i\right) = \prod_i \sum_{m_i} \exp\left(\beta B m_i\right)$$
$$= \left(\exp(\beta B/2) + \exp(-\beta B/2)\right)^L = Z_1 \cdots Z_L = Z_1^L$$



$$H = -B \sum_i S_{iz}$$

noninteracting system can be treated easily

no correlations

magnetic phase diagram??

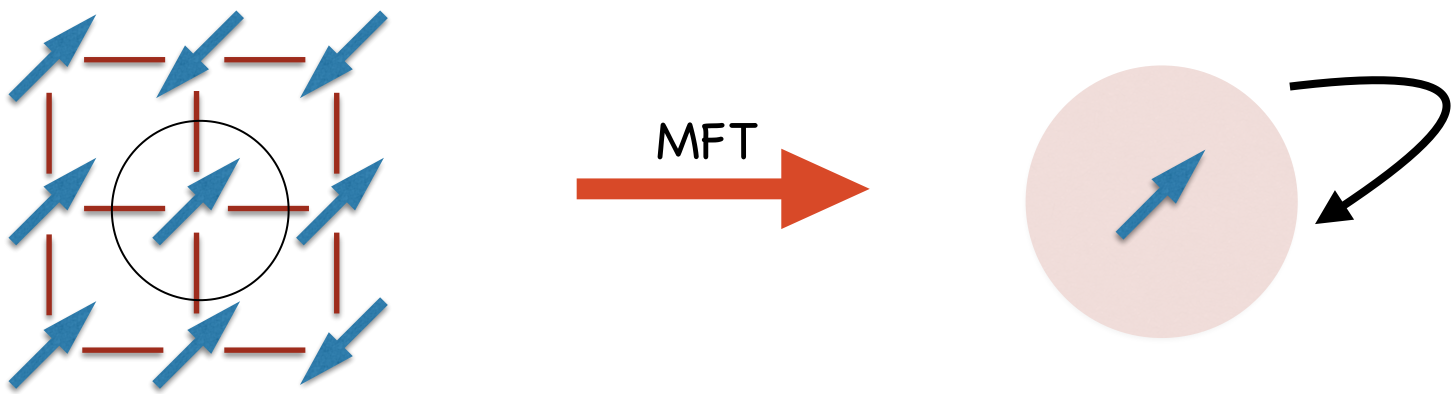
DMFT: aims at strongly correlated lattice fermion models

phenomena:
Kondo effect, Mott transition, collective order of spin, charge, orbital degrees of freedom, superconductivity, heavy-fermion behavior, etc.

mean-field approach

$$H = \sum_{i,j} J_{ij} \boldsymbol{S}_i \boldsymbol{S}_j - B \sum_i S_{iz}$$

$$H_{\mathsf{MF}} = -B \sum_i S_{iz} - B_{\mathsf{MF}} \sum_i S_{iz}$$



fluctuating local field

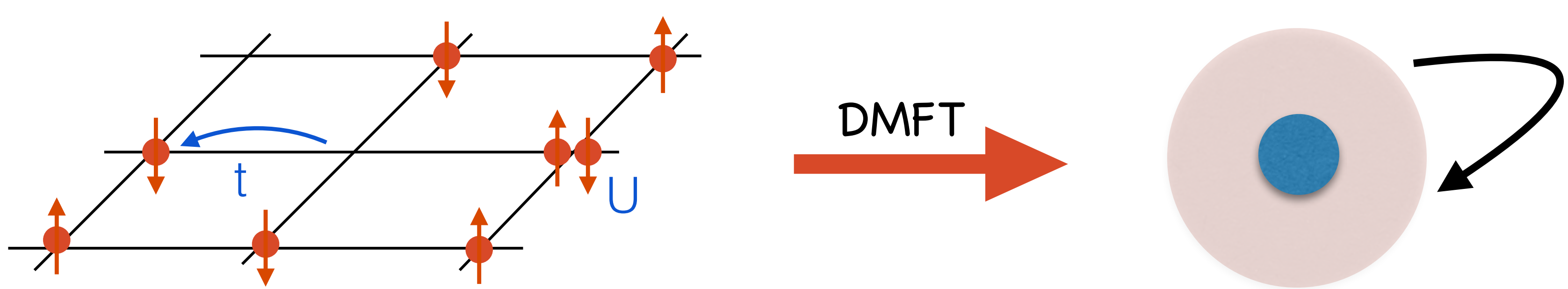
constant mean field

- mean field represents the environment
- should be determined (at best) from the solution of the lattice model
- pragmatically from the solution of H_{MF}, i.e.: $B_{MF} = -2qJ\langle S_{iz}\rangle$
- requires selfconsistent solution

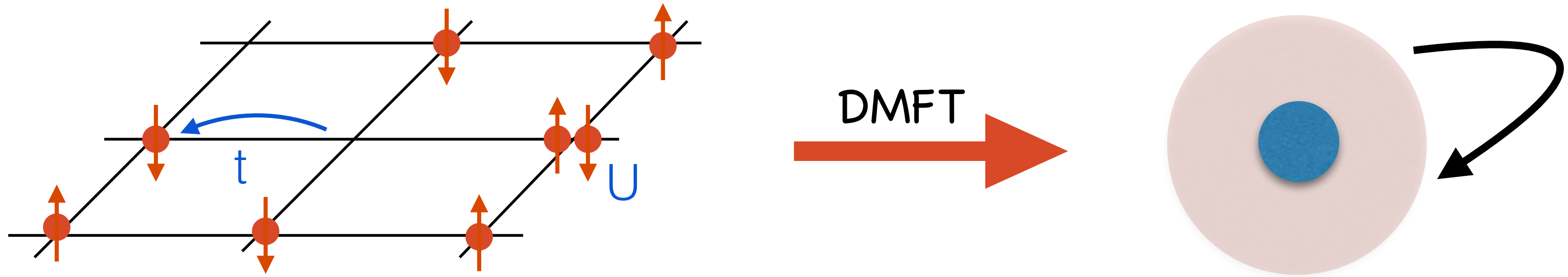
MFT: impurity model selfconsistently embedded in a bath

dynamical mean-field theory

- much more complicated as compared to Weiss MFT
  self-consistency equation formulated in terms of Green's functions
- optimal mean-field theory for lattice-fermion models (e.g. Hubbard model)
  point of orientation in the landscape of various MFT's
- no internal inconsistencies, not restricted to a certain parameter range (weak / strong interaction etc.), nonperturbative theory
- exact theory in the (carefully defined) limit of infinite dimensions
  but usually applied for $D < \infty$ as an approximation
- is able to describe spontaneous symmetry breaking (magnetism, SC, ...)
- can be derived in various way
- and highly successful, including applications to real materials (LDA+DMFT)



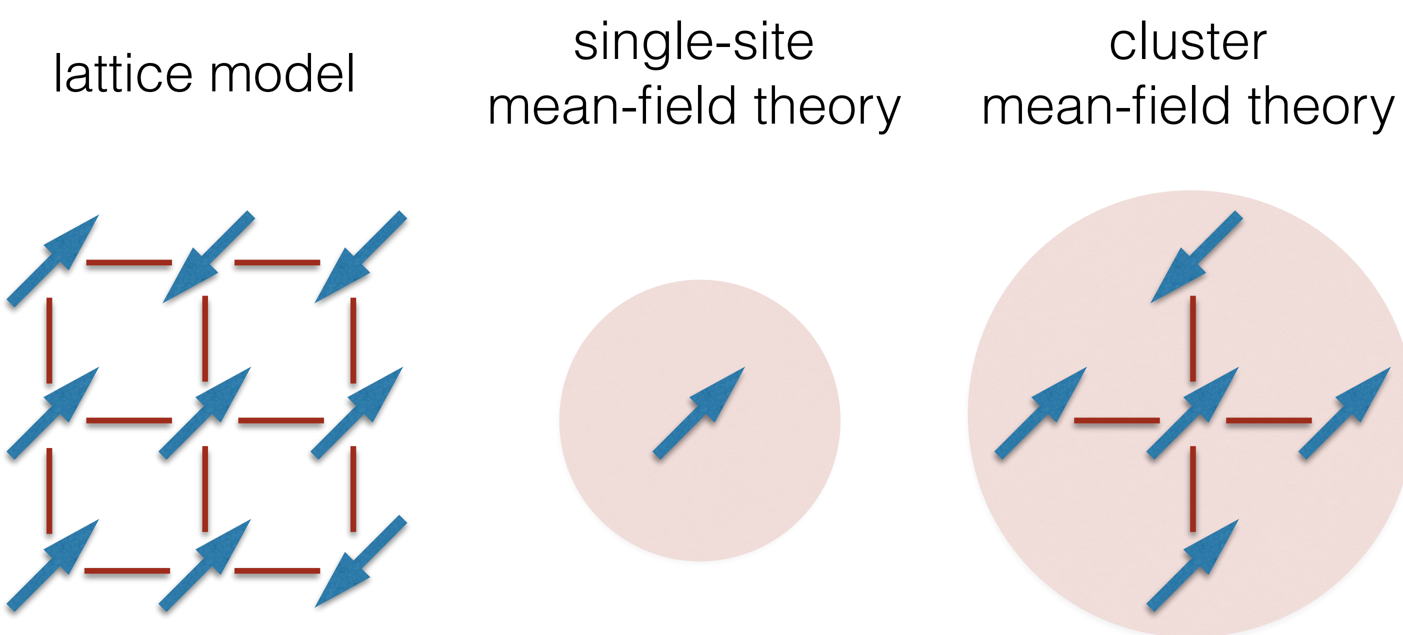
but ...



- short-range correlations are treated insufficiently
- no feedback of nonlocal two-particle (e.g. magnetic) correlation on the Green's function
- consequence: e.g. qualitatively wrong phase diagram in two dimensions
- no symmetry-broken phases with nonlocal order parameters including unconventional (d-wave) superconductivity
- incorrect critical behavior close to second-order phase transitions
- violation of exact identities and sum rules, violation of the Mermin-Wagner theorem, etc.
- DMFT (if applied to finite-D models) is approximate

WANTED: systematic route from DMFT to the exact solution

cluster mean-field approach



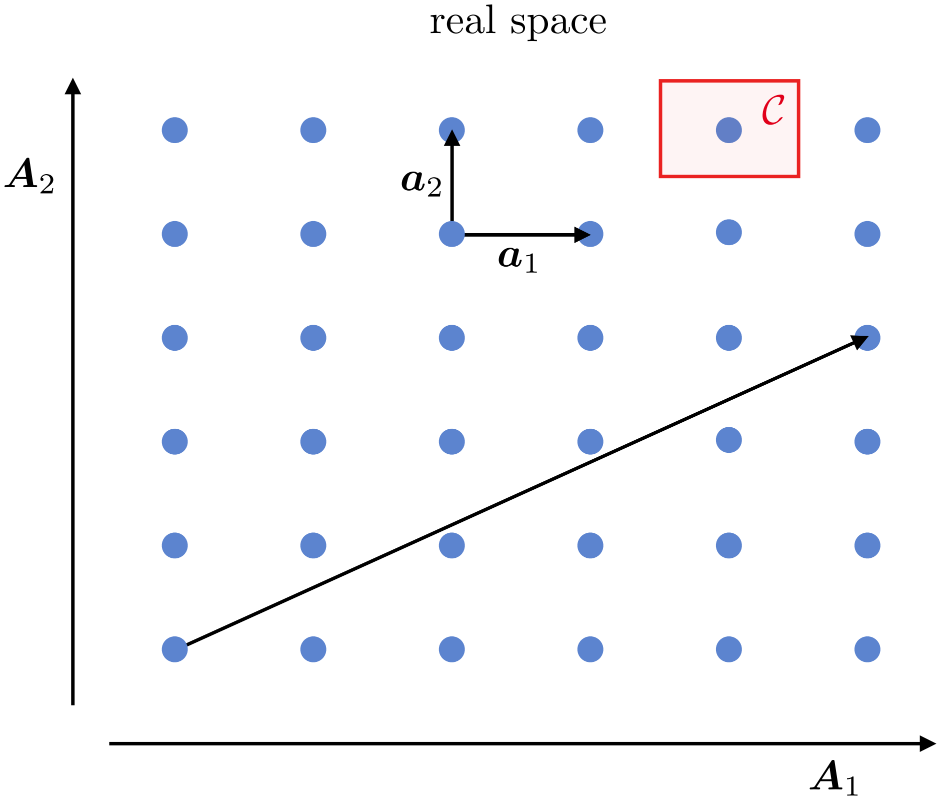
self-consistent embedding of a cluster with L_c sites in a bath

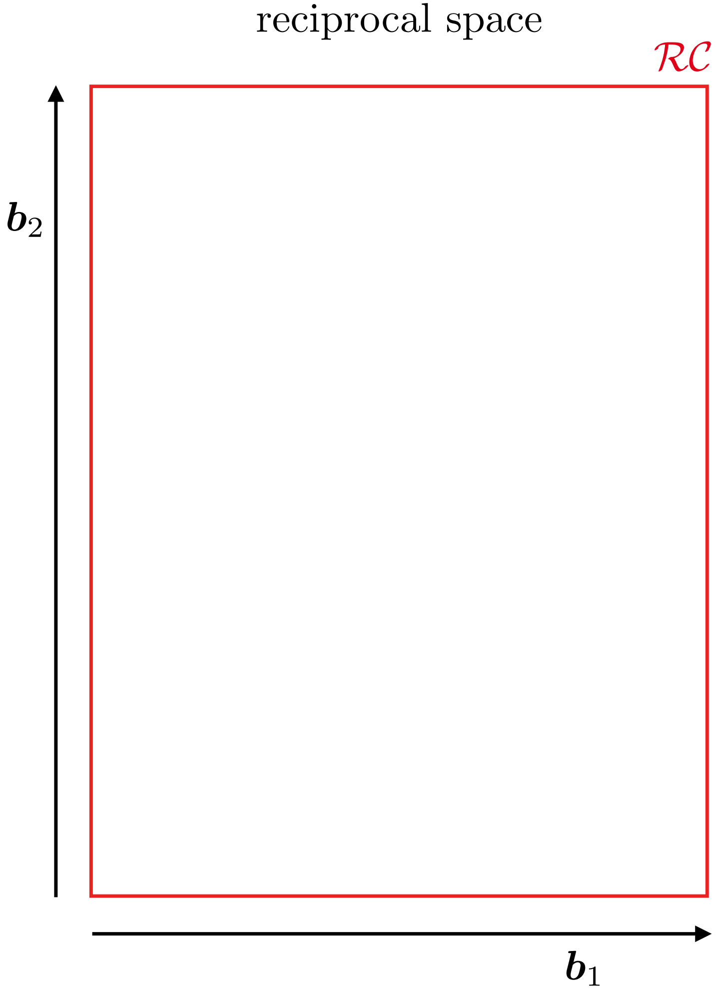
systematic, exact for infinite L_c
computational effort expected to increase strongly with L_c

GEOMETRY

lattice and reciprocal lattice

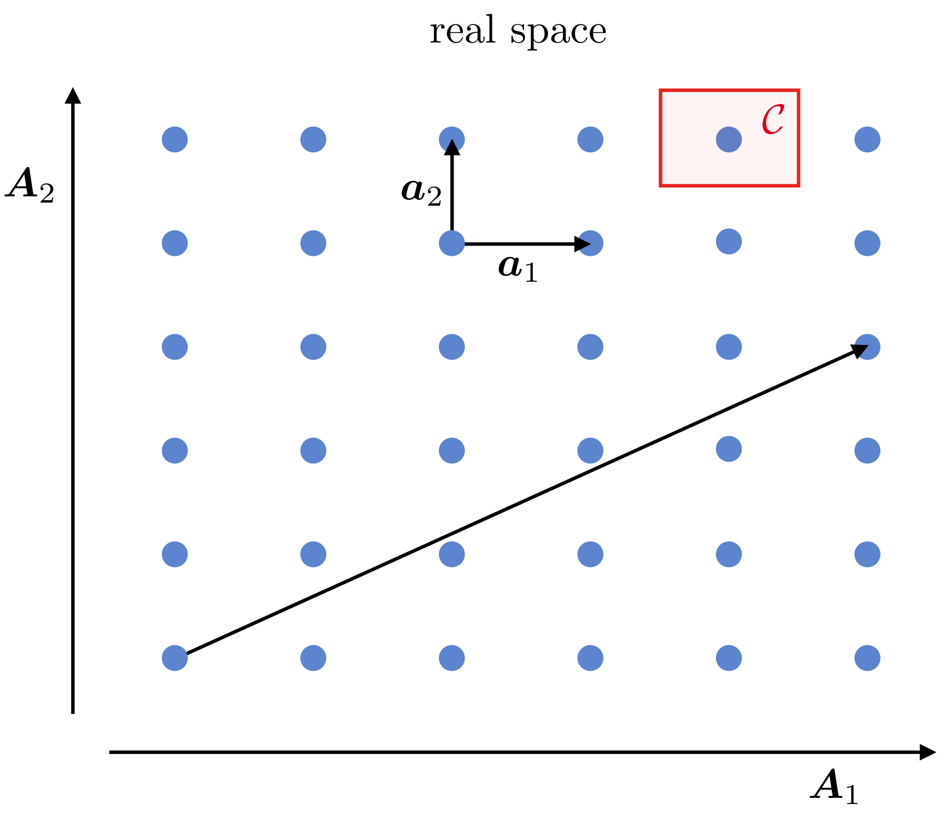
$$\boldsymbol{R} = \sum_{\alpha=1}^{D} i_\alpha \boldsymbol{a}_\alpha \qquad \boldsymbol{G} = \sum_{\beta=1}^{D} j_\beta \boldsymbol{b}_\beta \qquad \exp(i\boldsymbol{G}\boldsymbol{R}) = 1 \qquad \boldsymbol{a}_\alpha \boldsymbol{b}_\beta = 2\pi\delta_{\alpha\beta} \qquad V_{\mathcal{C}} V_{\mathcal{RC}} = (2\pi)^D$$

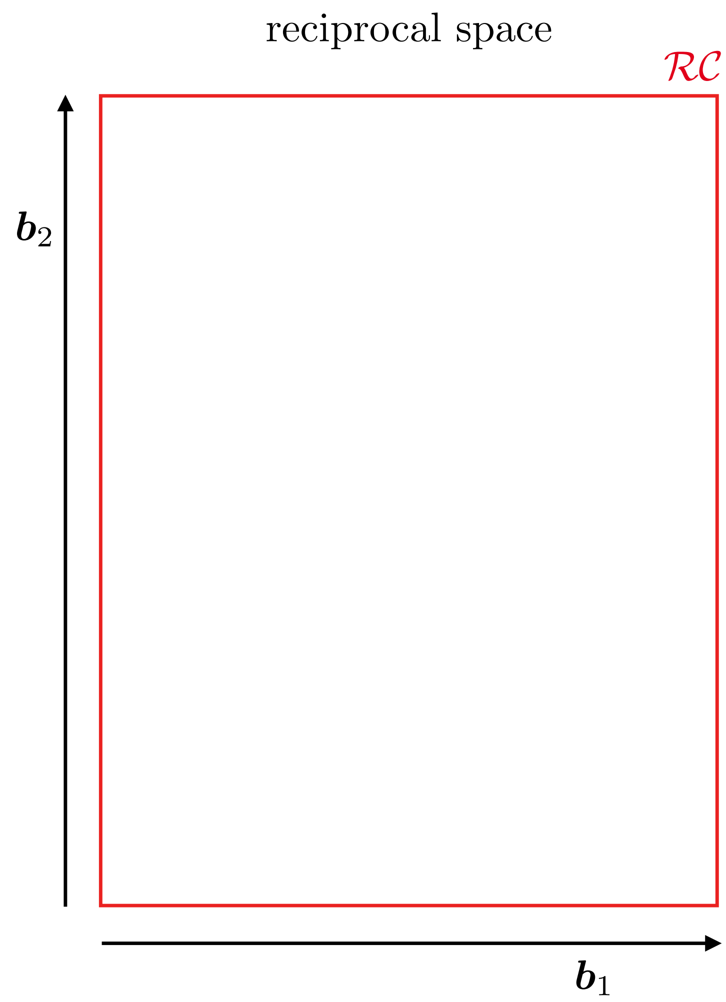




discrete Fourier series

$$f(\boldsymbol{x}) = f(\boldsymbol{x}+\boldsymbol{R}) \;\Rightarrow\; f(\boldsymbol{x}) = \sum_{\boldsymbol{G}} f_{\boldsymbol{G}} e^{i\boldsymbol{G}\boldsymbol{x}}\,, \quad f_{\boldsymbol{G}} = \frac{1}{V_{\mathcal{C}}}\int_{\mathcal{C}} d^D x\, f(\boldsymbol{x}) e^{-i\boldsymbol{G}\boldsymbol{x}}$$





periodic boundaries

$$L = L_1 \times \cdots \times L_D$$

$$V = \det(\boldsymbol{A}_1, ..., \boldsymbol{A}_D)$$

$$\boldsymbol{A}_\alpha = L_\alpha \boldsymbol{a}_\alpha$$

$$\boldsymbol{x} \equiv \boldsymbol{x} + \boldsymbol{A}_\alpha$$

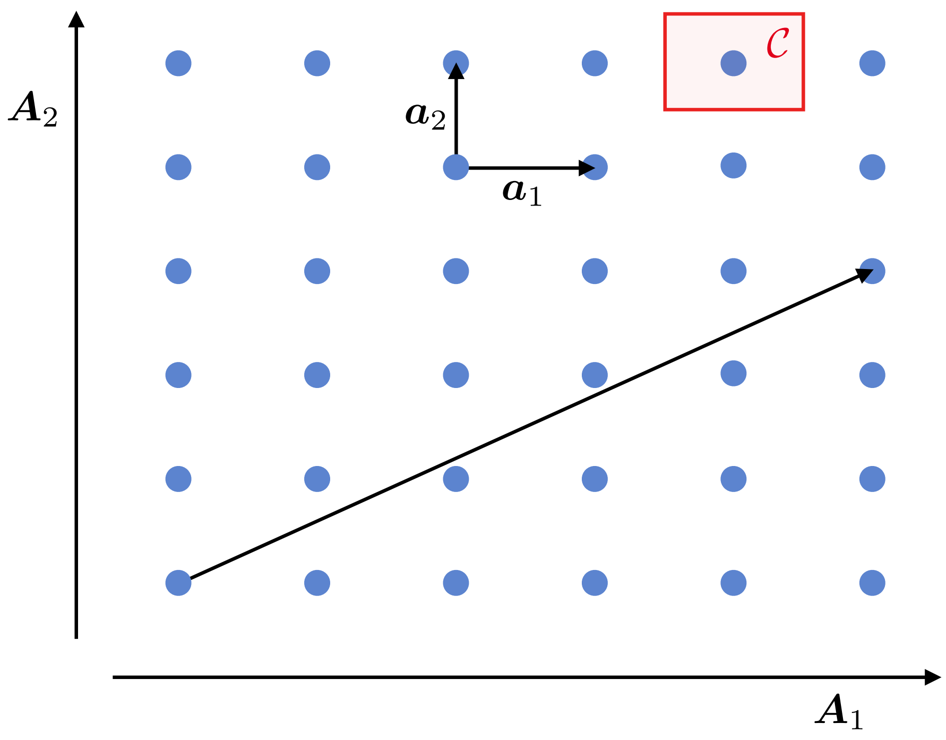
$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{x}} f_{\boldsymbol{k}}$$

$$e^{i\boldsymbol{k}\boldsymbol{A}_\alpha} = 1$$

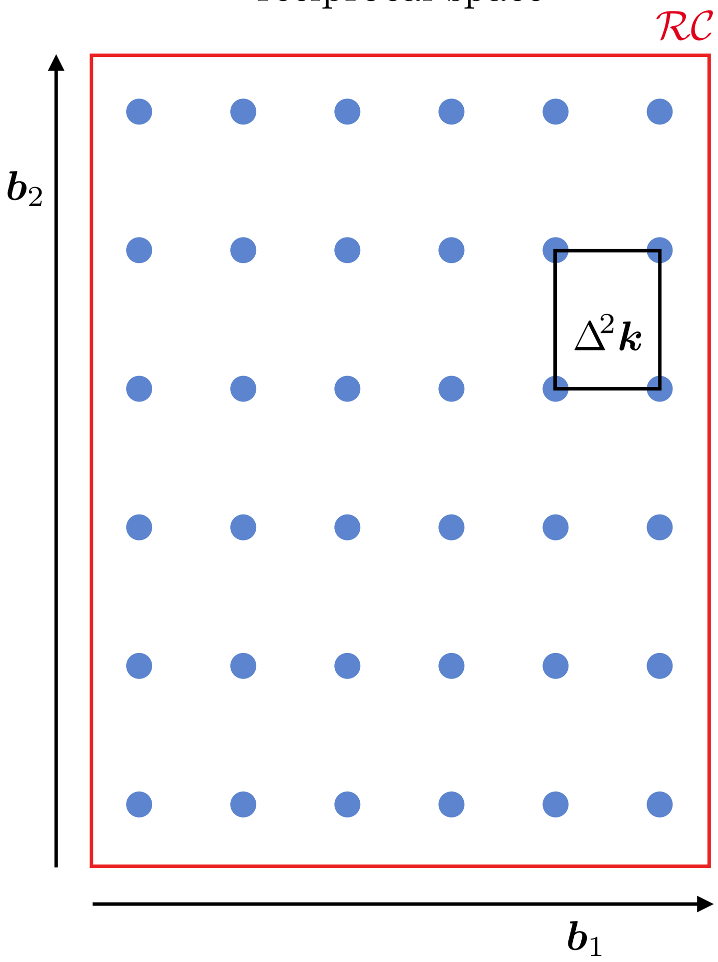
$$V\,\Delta^D k = (2\pi)^D$$

$$L = V_{\mathcal{RC}}/\Delta^D k$$

real space

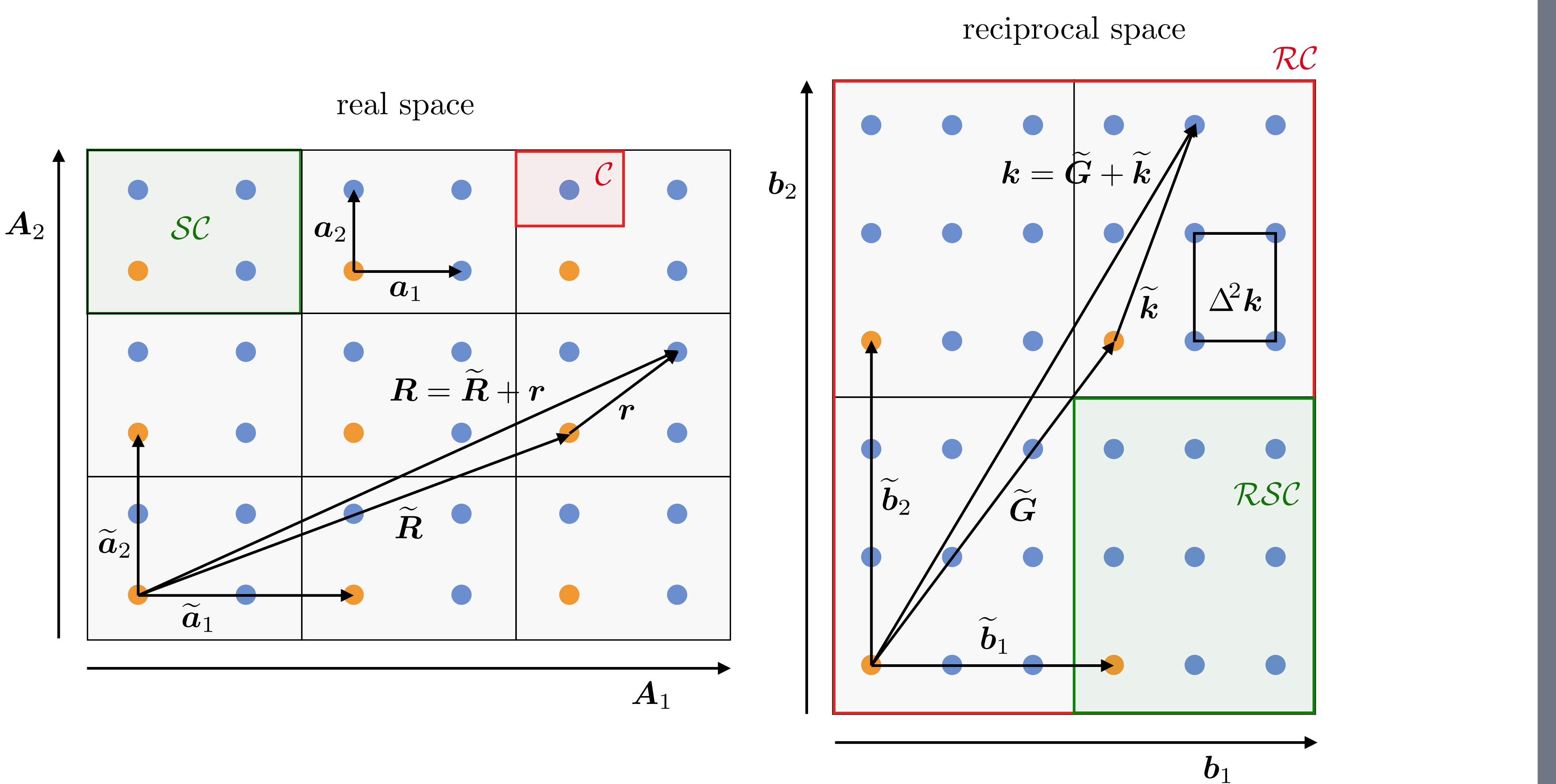


reciprocal space



superlattice and reciprocal superlattice

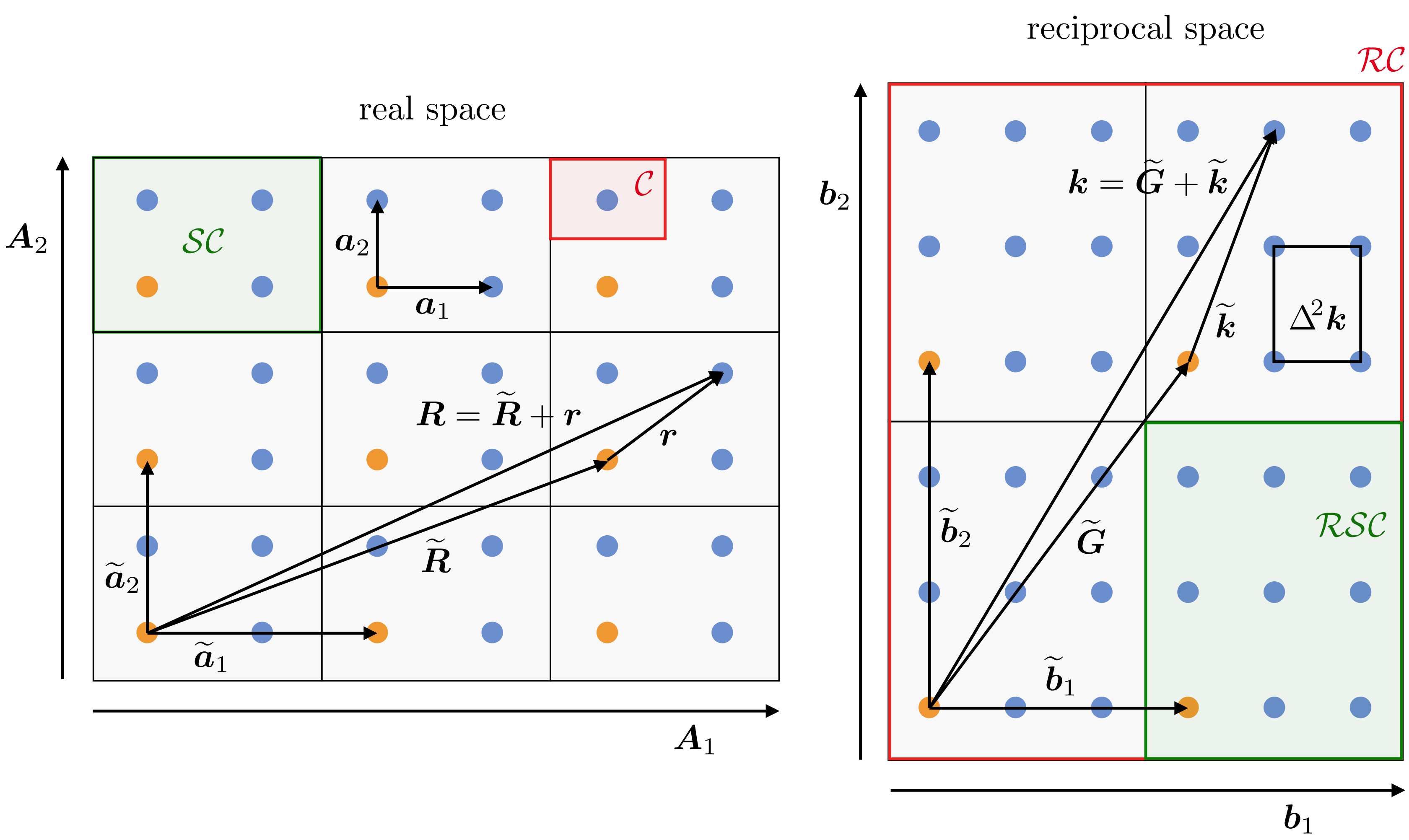
$$\widetilde{\boldsymbol{R}} = \sum_{\alpha=1}^{D} i_\alpha \widetilde{\boldsymbol{a}}_\alpha \qquad \widetilde{\boldsymbol{G}} = \sum_{\beta=1}^{D} j_\beta \widetilde{\boldsymbol{b}}_\beta \qquad \exp(i\widetilde{\boldsymbol{G}}\widetilde{\boldsymbol{R}}) = 1 \qquad \widetilde{\boldsymbol{a}}_\alpha \widetilde{\boldsymbol{b}}_\beta = 2\pi\delta_{\alpha\beta} \qquad V_{\mathcal{SC}} V_{\mathcal{RSC}} = (2\pi)^D$$



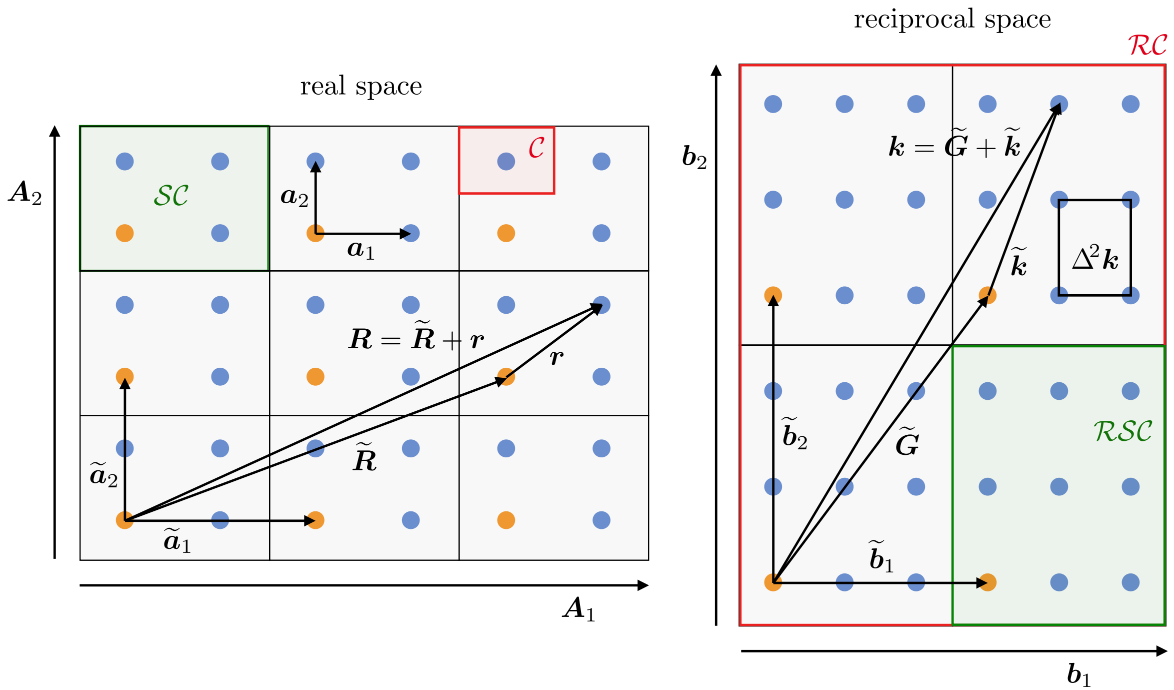
cluster and reciprocal cluster vectors

$\boldsymbol{R} = \widetilde{\boldsymbol{R}} + \boldsymbol{r}$

$\boldsymbol{k} = \widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}$



Fourier transformations



$$\boldsymbol{R} = \widetilde{\boldsymbol{R}} + \boldsymbol{r}$$

$$\boldsymbol{k} = \widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}$$

lattice F.T. (L x L)

$$U_{\boldsymbol{R},\boldsymbol{k}} = \frac{1}{\sqrt{L}} \exp(i\boldsymbol{k}\boldsymbol{R})$$

superlattice F.T. (L/L_c x L/L_c)

$$V_{\widetilde{\boldsymbol{R}},\widetilde{\boldsymbol{k}}} = \frac{1}{\sqrt{L/L_c}} \exp(i\widetilde{\boldsymbol{k}}\widetilde{\boldsymbol{R}})$$

cluster F.T. (L_c x L_c)

$$W_{\boldsymbol{r},\widetilde{\boldsymbol{G}}} = \frac{1}{\sqrt{L_c}} \exp(i\widetilde{\boldsymbol{G}}\boldsymbol{r})$$

note: $\boldsymbol{U} \neq \boldsymbol{V}\boldsymbol{W} = \boldsymbol{W}\boldsymbol{V}$

overview

object, quantity	symbol, definition	properties, relations
basis spanning the lattice	$\boldsymbol{a}_\alpha$	$\alpha = 1, ..., D$
volume of a primitive cell	$V_\mathcal{C} = \det(\{\boldsymbol{a}_\alpha\})$	
lattice vectors	$\boldsymbol{R} = \boldsymbol{R}_i = \sum_\alpha i_\alpha \boldsymbol{a}_\alpha$	$i_\alpha \in \mathbb{Z}$, $1 \le i_\alpha \le L_\alpha$
basis vectors of reciprocal lattice	$\boldsymbol{b}_\beta$	$\boldsymbol{a}_\alpha \boldsymbol{b}_\beta = 2\pi\delta_{\alpha\beta}$
volume of a reciprocal unit cell	$V_{\mathcal{RC}} = \det(\{\boldsymbol{b}_j\})$	$V_{\mathcal{RC}} = (2\pi)^D / V_\mathcal{C}$
reciprocal lattice vectors	$\boldsymbol{G} = \boldsymbol{G}_j = \sum_\beta j_\beta \boldsymbol{b}_\beta$	$j_\beta \in \mathbb{Z}$, $\boldsymbol{GR} \in 2\pi\mathbb{Z}$
basis spanning the superlattice	$\widetilde{\boldsymbol{a}}_\alpha$	$\widetilde{\boldsymbol{a}}_\alpha = L_{c,\alpha} \boldsymbol{a}_\alpha$
volume of a superlattice cell	$V_{\mathcal{SC}} = \det(\{\widetilde{\boldsymbol{a}}_\alpha\})$	$V_{\mathcal{SC}} = L_c V_\mathcal{C}$
superlattice vectors	$\widetilde{\boldsymbol{R}} = \widetilde{\boldsymbol{R}}_i = \sum_\alpha i_\alpha \widetilde{\boldsymbol{a}}_\alpha$	$i_\alpha \in \mathbb{Z}$, $1 \le i_\alpha \le L/L_{c,\alpha}$
basis of reciprocal superlattice	$\widetilde{\boldsymbol{b}}_\beta$	$\widetilde{\boldsymbol{a}}_\alpha \widetilde{\boldsymbol{b}}_\beta = 2\pi\delta_{\alpha\beta}$
volume of a rec. superlattice cell	$V_{\mathcal{RSC}} = \det(\{\widetilde{\boldsymbol{b}}_j\})$	$V_{\mathcal{RSC}} = (2\pi)^D / V_{\mathcal{SC}}$
reciprocal superlattice vectors	$\widetilde{\boldsymbol{G}} = \widetilde{\boldsymbol{G}}_j = \sum_\beta j_\beta \widetilde{\boldsymbol{b}}_\beta$	$\widetilde{\boldsymbol{G}}\widetilde{\boldsymbol{R}} \in 2\pi\mathbb{Z}$
vectors spanning the system	$\boldsymbol{A}_\alpha$	$\boldsymbol{A}_\alpha = L_\alpha \boldsymbol{a}_\alpha = (L/L_{c,\alpha})\widetilde{\boldsymbol{a}}_\alpha$
system volume	$V = \det(\{\boldsymbol{A}_i\})$	$V = L V_\mathcal{C}$
.	.	.
discrete wave vectors	$\boldsymbol{k}$	$\boldsymbol{k}\boldsymbol{A}_\alpha \in 2\pi\mathbb{Z}$
volume element in $\boldsymbol{k}$-space	$\Delta^D k$	$\Delta^D k = (2\pi)^D / V$
.	.	.

GREEN'S FUNCTION

single-electron Green's function

single-electron Green's function (at temperature T=0)

$$G_{\boldsymbol{R},\boldsymbol{R}'}(\omega) = \langle 0|c^\dagger_{\boldsymbol{R}',\sigma} \frac{1}{\omega - E_0 + H} c_{\boldsymbol{R},\sigma}|0\rangle + \langle 0|c_{\boldsymbol{R},\sigma} \frac{1}{\omega + E_0 - H} c^\dagger_{\boldsymbol{R}',\sigma}|0\rangle$$

H invariant under lattice translations:

$$c_{\boldsymbol{R},\sigma} \to c_{\boldsymbol{R}+\boldsymbol{R}_0,\sigma} \qquad c^\dagger_{\boldsymbol{R},\sigma} \to c^\dagger_{\boldsymbol{R}+\boldsymbol{R}_0,\sigma}$$

implies:

$$G_{\boldsymbol{R}+\boldsymbol{R}_0,\boldsymbol{R}'+\boldsymbol{R}_0}(\omega) = G_{\boldsymbol{R},\boldsymbol{R}'}(\omega)$$

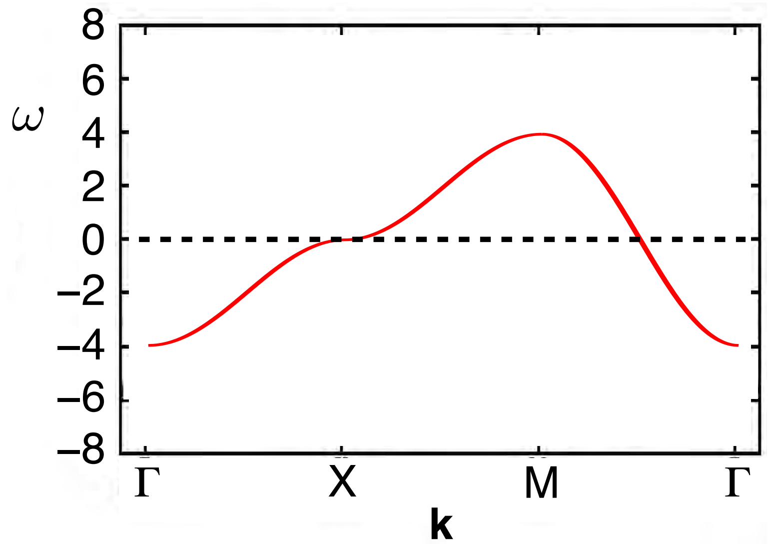
hence: G can be diagonalized using U

$$(\boldsymbol{U}^\dagger \boldsymbol{G}(\omega)\boldsymbol{U})_{\boldsymbol{k}\boldsymbol{k}'} = G(\boldsymbol{k},\omega)\delta_{\boldsymbol{k},\boldsymbol{k}'}$$

spectral density: (the central observable, related to PES, IPE)

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

noninteracting spectral density



$$H_0 = \sum_{\boldsymbol{R}\boldsymbol{R}'\sigma} t_{\boldsymbol{R}\boldsymbol{R}'} c^\dagger_{\boldsymbol{R}\sigma} c_{\boldsymbol{R}'\sigma}$$

$$A(\boldsymbol{k},\omega) = \delta(\omega - \epsilon(\boldsymbol{k}))$$

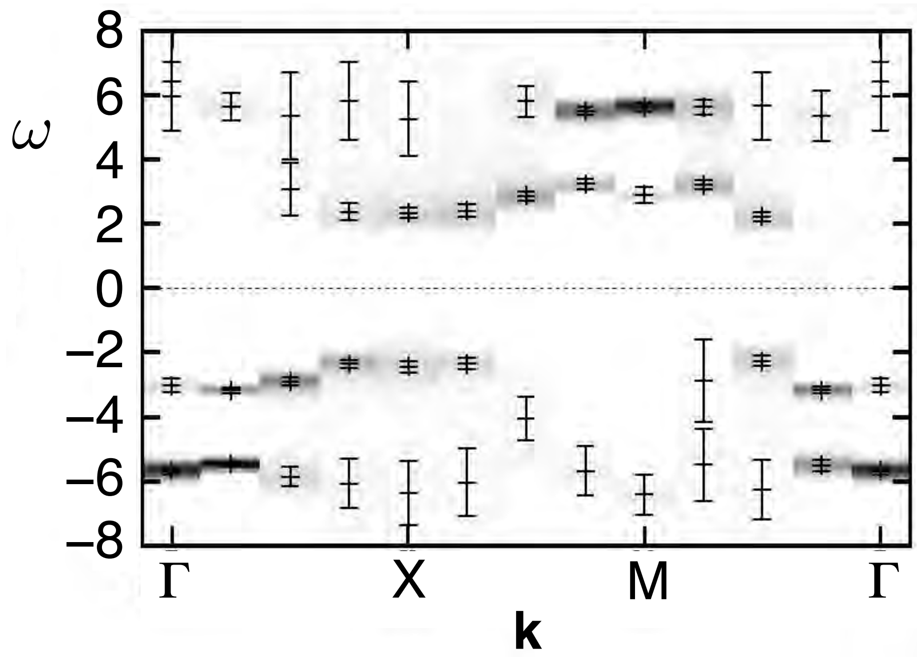
$$\varepsilon(\boldsymbol{k}) = -2t(\cos k_x + \cos k_y)$$

- half-filling, else: $H \to H - \mu N$
- occupied states - PES
- unoccupied states - IPE
- Fermi surface

What happens when adding an interaction? (e.g. single-band Hubbard model)

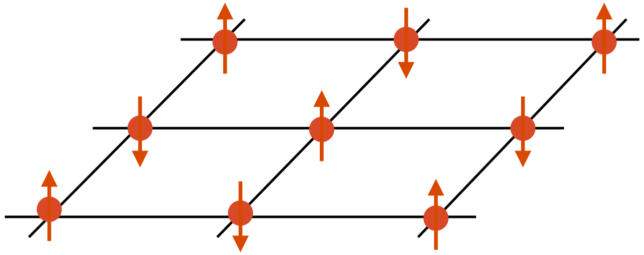
$$H_1 = \frac{U}{2} \sum_{\boldsymbol{R}\sigma} n_{\boldsymbol{R}\sigma} n_{\boldsymbol{R}-\sigma}$$

interacting spectral density

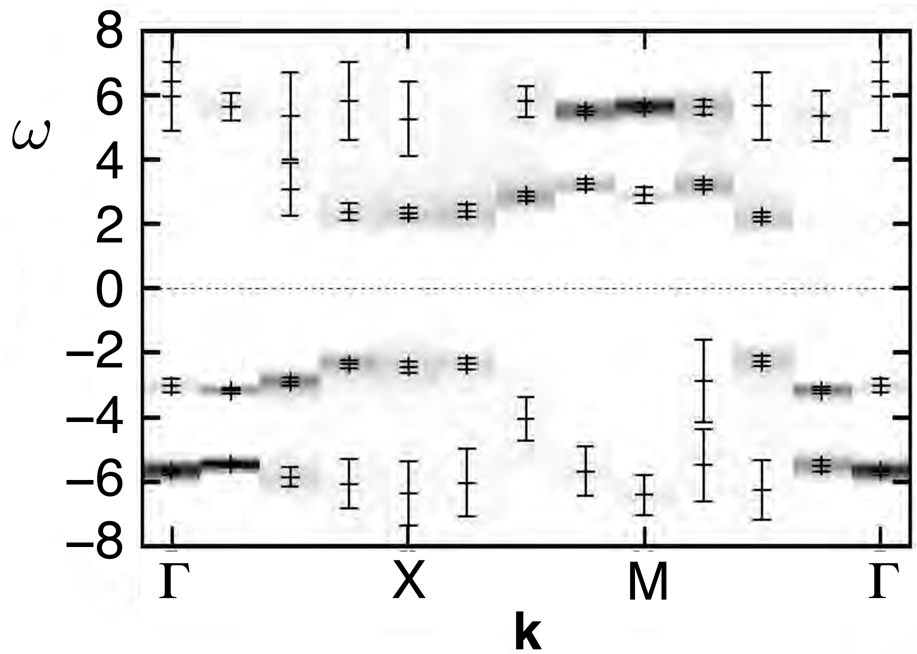


- 2D Hubbard model, n=1, low T=0.1
- U=W=8
- L=8x8 sites, PBC
- QMC results

Gröber et al. (2000)



interacting spectral density



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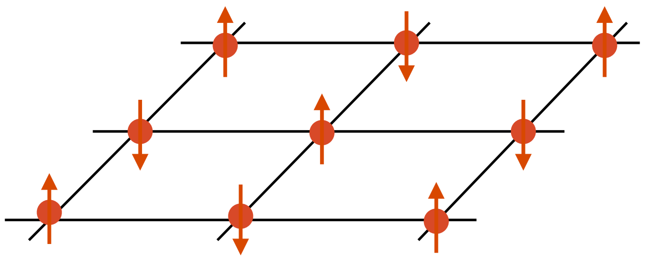
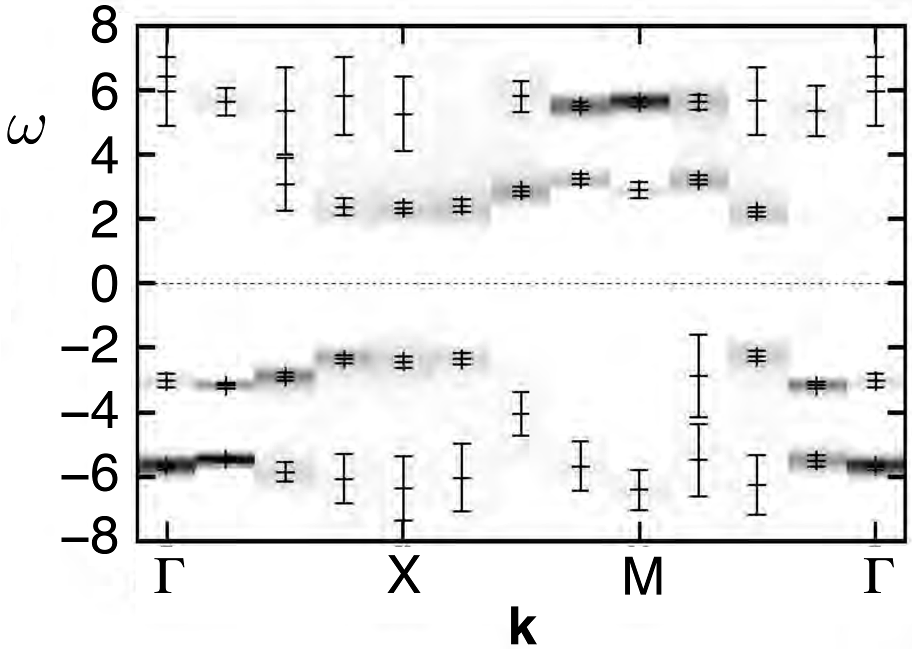


technical problems:

- k resolution
- thermal broadening
- thermally induced decay of correlations
- MaxEnt must be used to get real-frequency data: broadening

many-body effects



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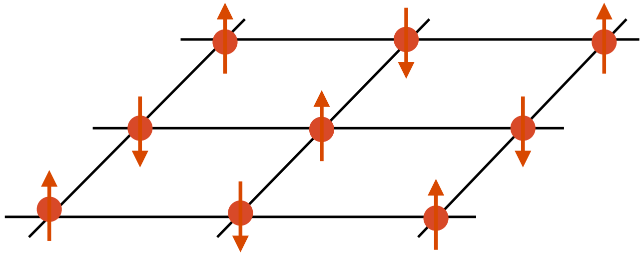
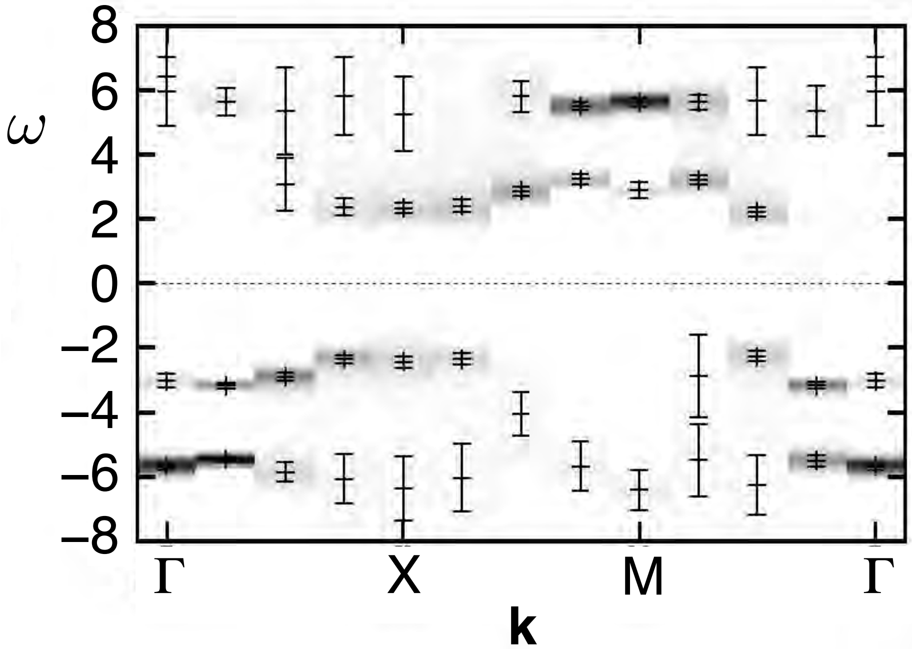


many-body effects:

- gapped single-particle excitations -> interaction-driven (Mott) insulator
- finite lifetime of excitations
- incoherent background: complicated high-order decay processes

Hubbard bands



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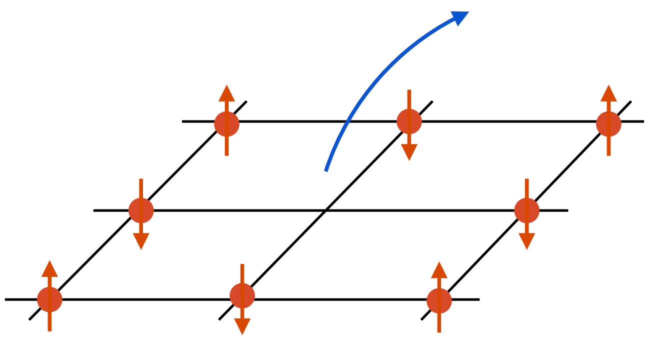
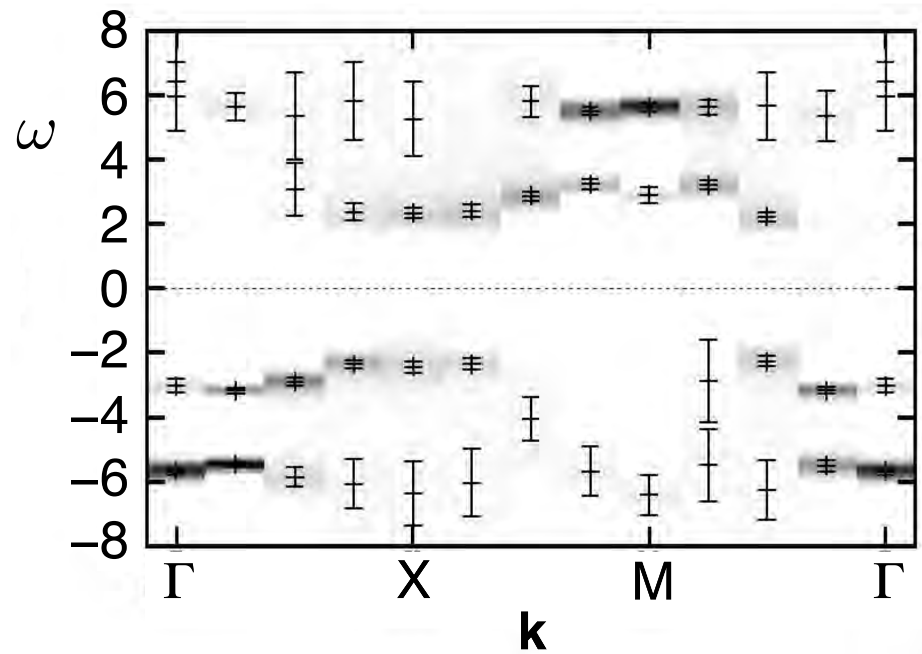


many-body effects:

- Hubbard bands: correlation-induced satellites
- LHB: PES $\omega = E_0 - E_n - \mu \approx -\mu = -U/2$
- **LOCAL CORRELATIONS**

$$A_{\boldsymbol{R},\boldsymbol{R}'}(\omega) = \langle 0 | c^\dagger_{\boldsymbol{R}',\sigma} \delta(\omega - E_0 + H) c_{\boldsymbol{R},\sigma} | 0 \rangle + \langle 0 | c_{\boldsymbol{R},\sigma} \delta(\omega + E_0 - H) c^\dagger_{\boldsymbol{R}',\sigma} | 0 \rangle$$

Hubbard bands



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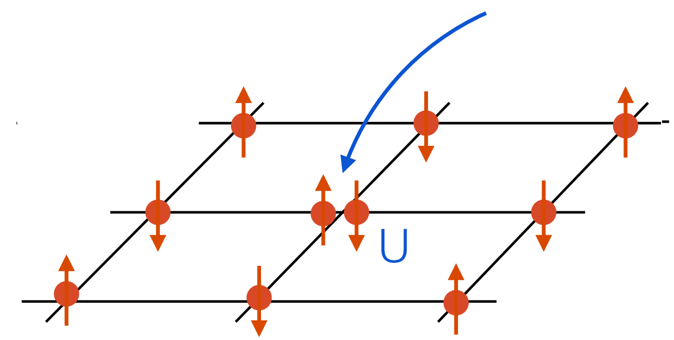
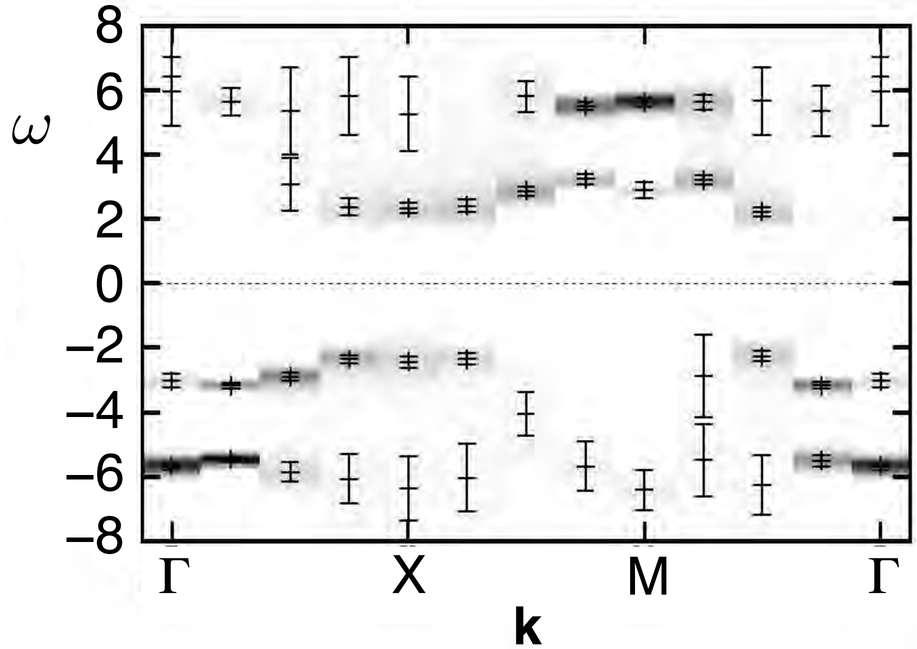


many-body effects:

- Hubbard bands: correlation-induced satellites
- UHB: IPE $\omega = E_n - E_0 - \mu \approx U - \mu = U/2$
- **LOCAL CORRELATIONS**

$$A_{\boldsymbol{R},\boldsymbol{R}'}(\omega) = \langle 0|c^\dagger_{\boldsymbol{R}',\sigma}\delta(\omega - E_0 + H)c_{\boldsymbol{R},\sigma}|0\rangle + \langle 0|c_{\boldsymbol{R},\sigma}\delta(\omega + E_0 - H)c^\dagger_{\boldsymbol{R}',\sigma}|0\rangle$$

low-energy excitations



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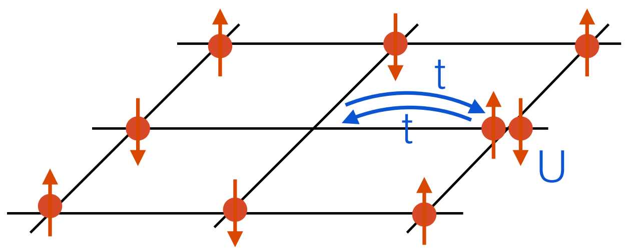
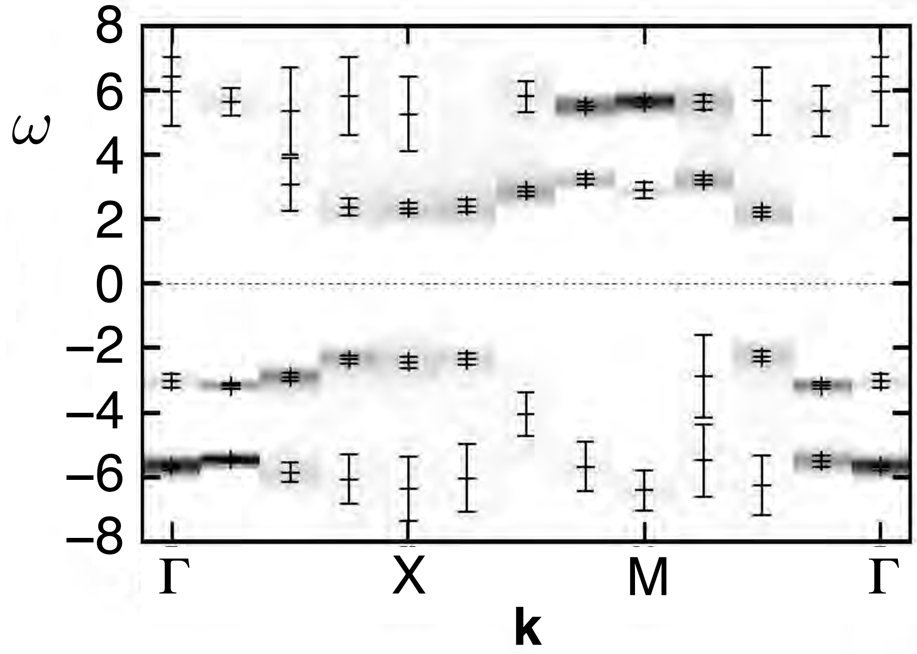


many-body effects:

- well-defined low-energy structure
- infinite U: fully localized electrons - 2^L-fold degenerate ground state
- finite U: delocalization via second-order hopping processes mapping onto AF Heisenberg model with $J=4t^2/U$
- low-energy excitations: nonlocal spin excitations, band width 2J

low-energy excitations



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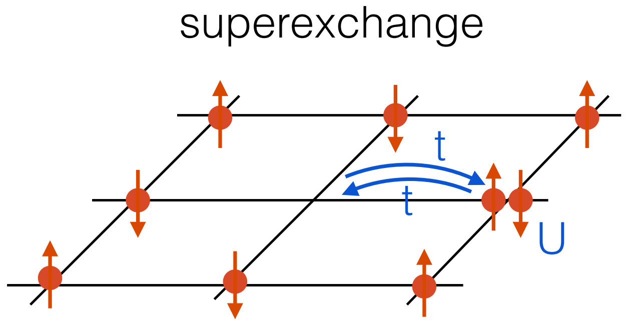
Gröber et al. (2000)



many-body effects:

- low-energy excitations: nonlocal spin excitations, band width 2J
- spin excitations couple to single-particle excitations:
  moving hole (PES) or doublon (IPE) dressed, emit/absorb spin excitations
- renormalization of the Hubbard bands AND new satellites
- **NONLOCAL CORRELATIONS**

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local and nonlocal correlations

LOCAL CORRELATIONS

- high-energy spectral features
- high spectral weight
- Hubbard bands

- accessible within mean-field theories with a proper treatment of the local excitations and their delocalization in the lattice
- DMFT

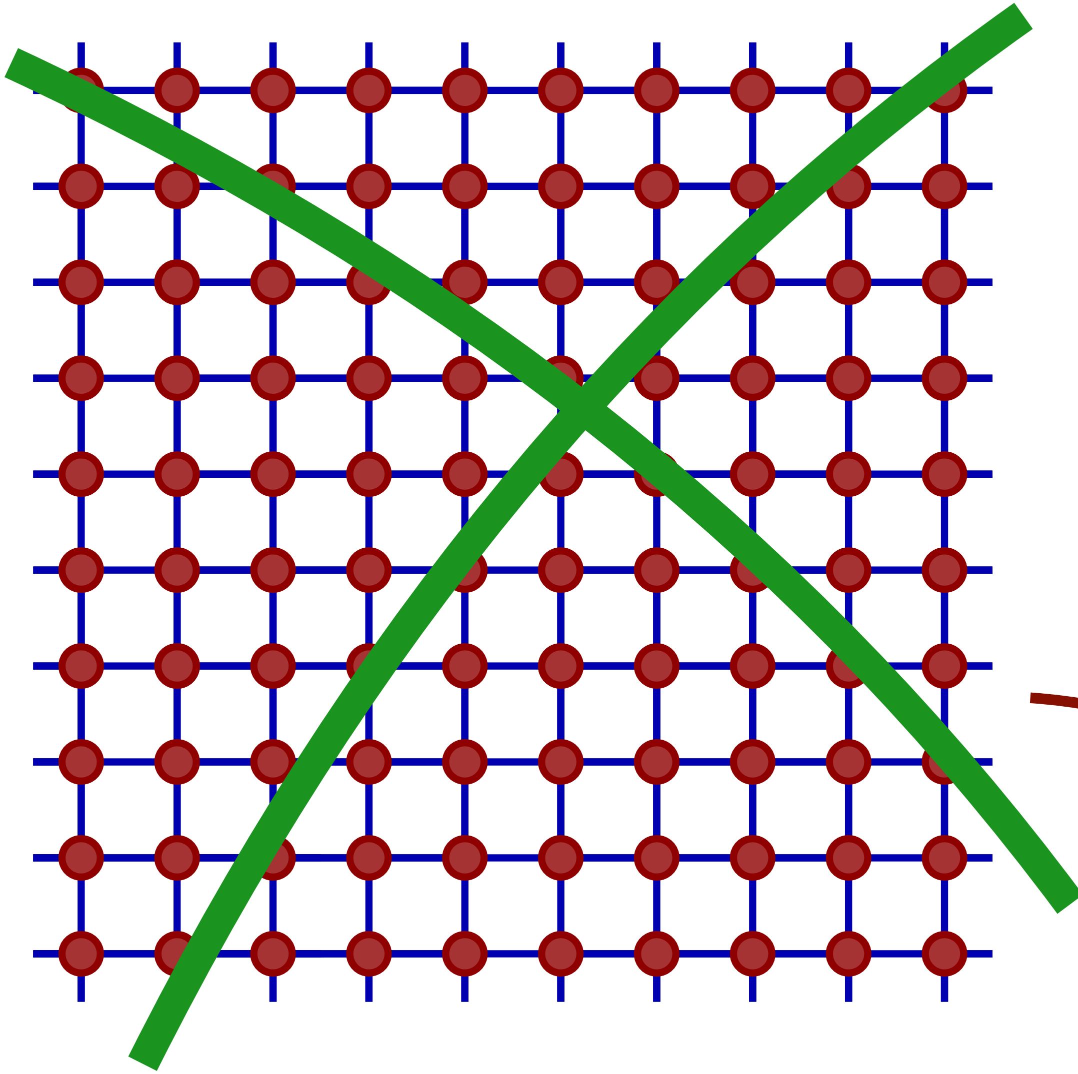
NONLOCAL CORRELATIONS

- low-energy spectral features
- lower spectral weight
- hole/doublon after emission/ absorption of a spin excitation

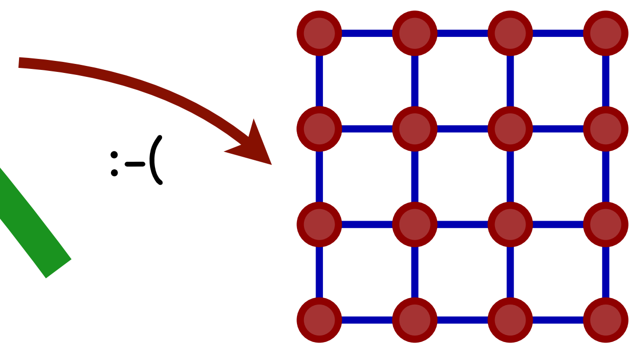
- requires feedback of two-particle (e.g. AF magnetic) correlations to the single-particle excitations
- beyond mean-field theory
- cluster extensions of DMFT

CLUSTER-PERTURBATION THEORY

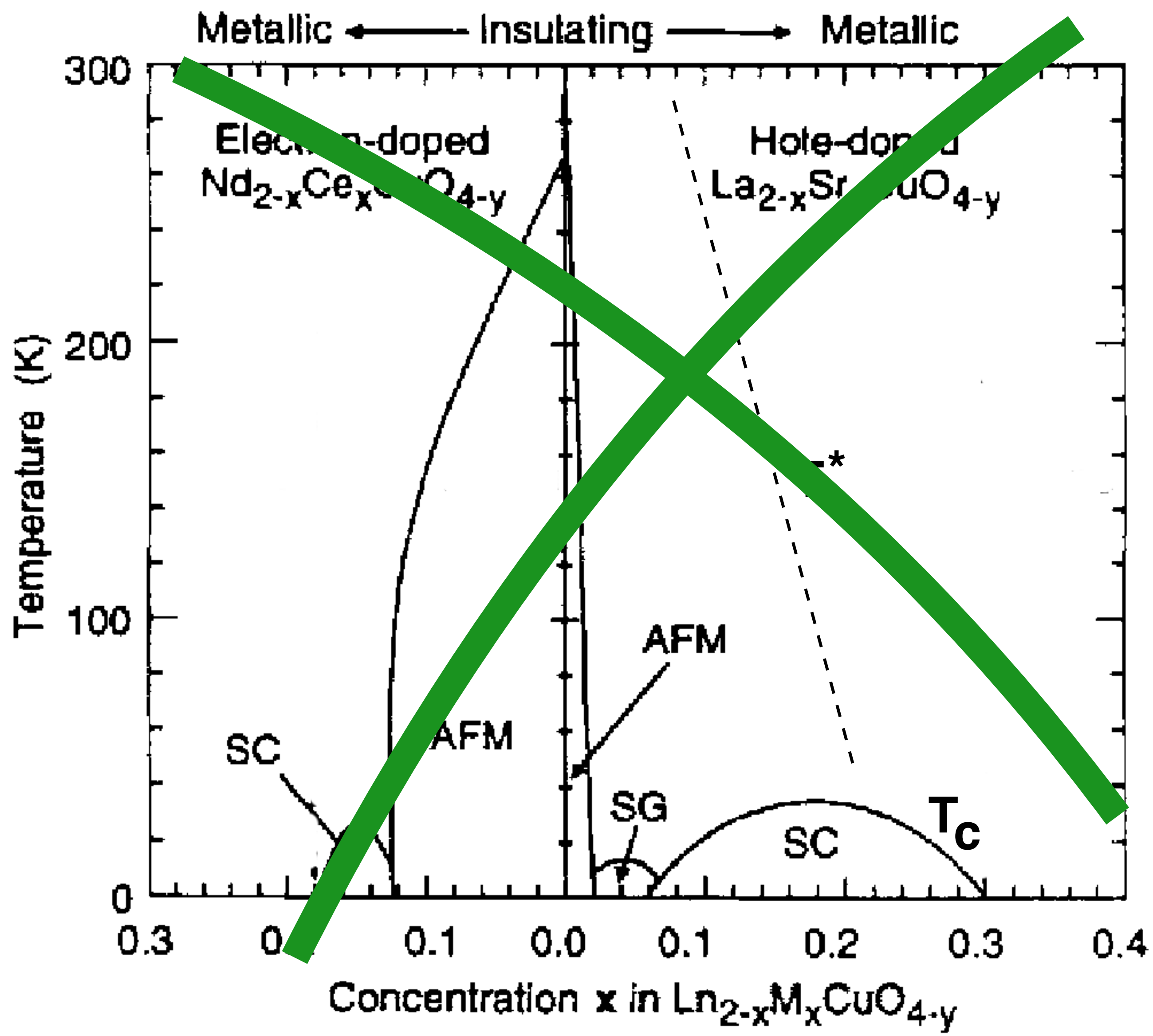
bad news



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

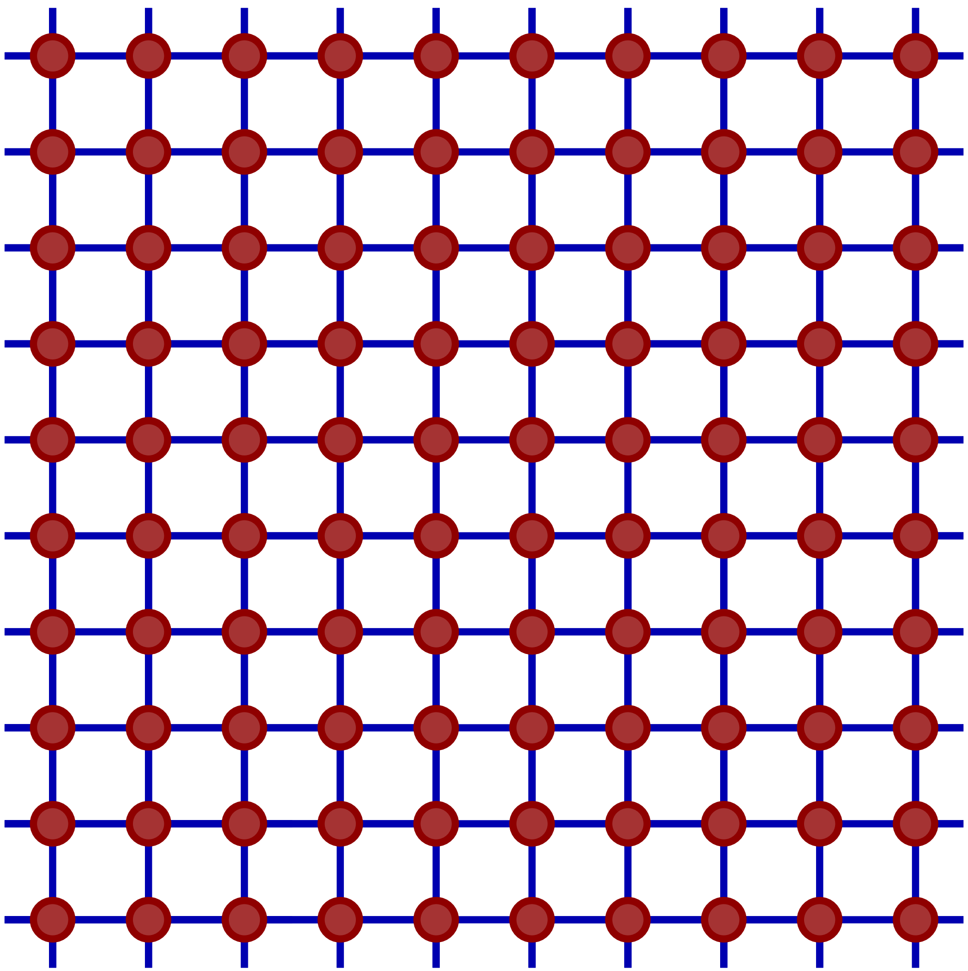


phase diagram of high-T_C materials

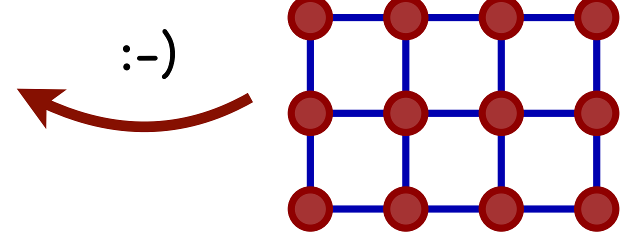


:-(

the main idea of a cluster approach



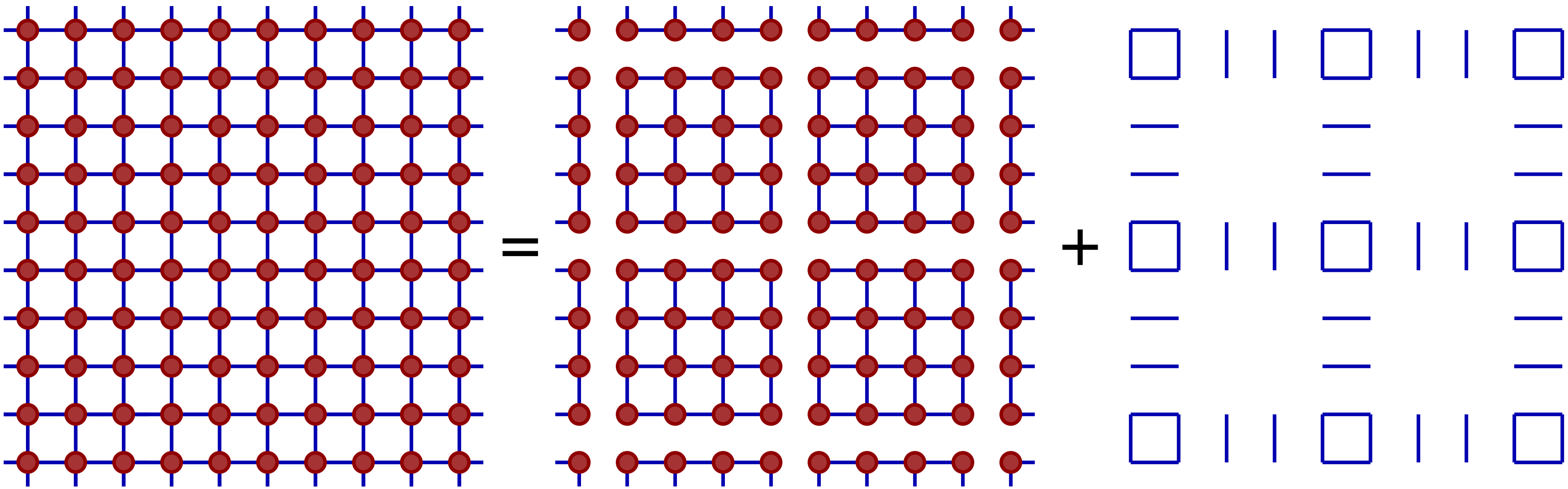
- solve the cluster problem exactly
- use the solution to reconstruct the solution for the full problem (this is approximate !)
- find a clever way how to do this step ("embedding problem")
- "divide and conquer strategy"



cluster-perturbation theory (CPT)

original system (L sites)

reference system (L/L_c clusters with L_c sites each)



hopping matrix **t**

hopping matrix **t'**

inter-cluster hopping V

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

treat this term perturbatively !

"free" system and Green's functions

- free system:

$$H_0 = \sum_{\boldsymbol{R}_1 \boldsymbol{R}_2 \sigma} t_{\boldsymbol{R}_1 \boldsymbol{R}_2} c^\dagger_{\boldsymbol{R}_1 \sigma} c_{\boldsymbol{R}_2 \sigma}$$

- reference system:

$$H'_0 = \sum_{\boldsymbol{R}_1 \boldsymbol{R}_2 \sigma} t'_{\boldsymbol{R}_1 \boldsymbol{R}_2} c^\dagger_{\boldsymbol{R}_1 \sigma} c_{\boldsymbol{R}_2 \sigma}$$

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

CPT for interacting systems

- "free" CPT equation:

$$G_0(\omega) = G_0'(\omega) + G_0'(\omega) V G_0(\omega)$$ (exact)

- CPT equation:

$$G(\omega) = G'(\omega) + G'(\omega) V G(\omega)$$ (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: alternative derivation

- Dyson equation of the reference systems

$$\boldsymbol{G}'(\omega) = \boldsymbol{G}'_0(\omega) + \boldsymbol{G}'_0(\omega)\boldsymbol{\Sigma}'(\omega)\boldsymbol{G}'(\omega)$$

- Dyson equation of the original system:

$$\boldsymbol{G}(\omega) = \boldsymbol{G}_0(\omega) + \boldsymbol{G}_0(\omega)\boldsymbol{\Sigma}(\omega)\boldsymbol{G}(\omega)$$

- assume that

$$\boldsymbol{\Sigma}'(\omega) = \boldsymbol{\Sigma}(\omega)$$ (approximate)

- this yields

$$\boldsymbol{G}'_0(\omega)^{-1} - \boldsymbol{G}'(\omega)^{-1} = \boldsymbol{G}_0(\omega)^{-1} - \boldsymbol{G}(\omega)^{-1}$$

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

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

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

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:

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

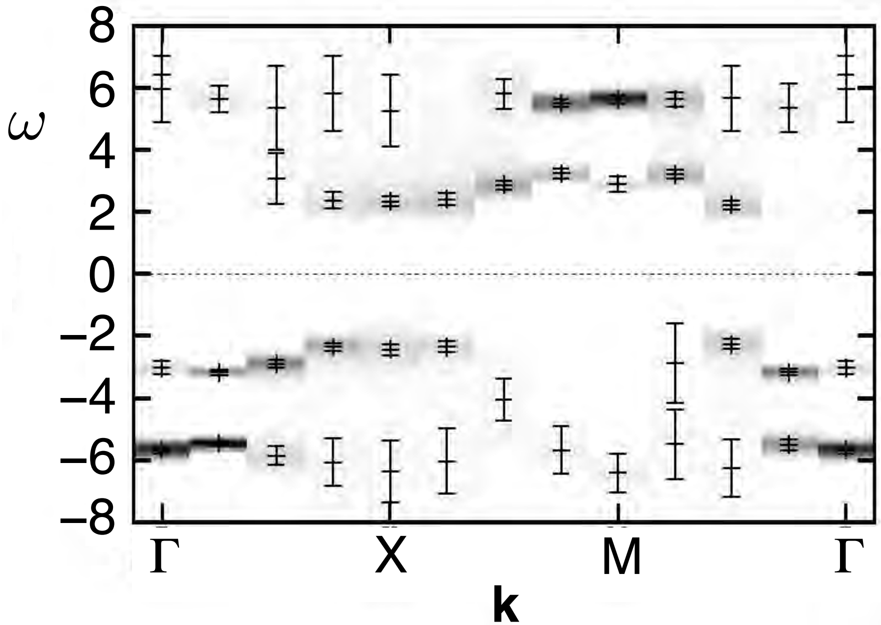
- solve by matrix inversion for any frequency:

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

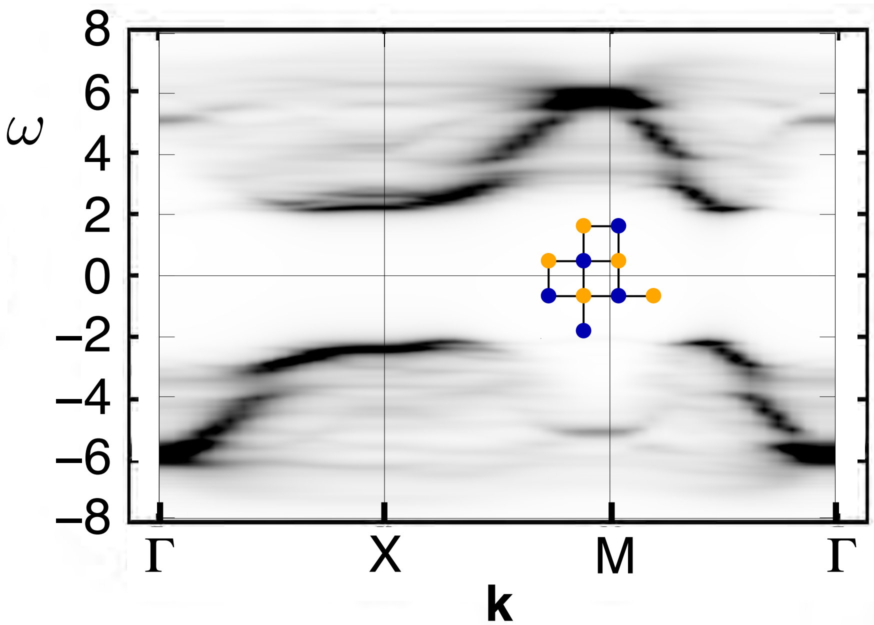
QMC vs. CPT

2D Hubbard model, n=1, U=8

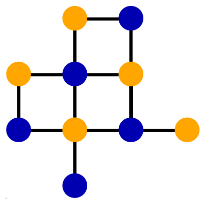
L=8x8 sites, T=0.1, QMC



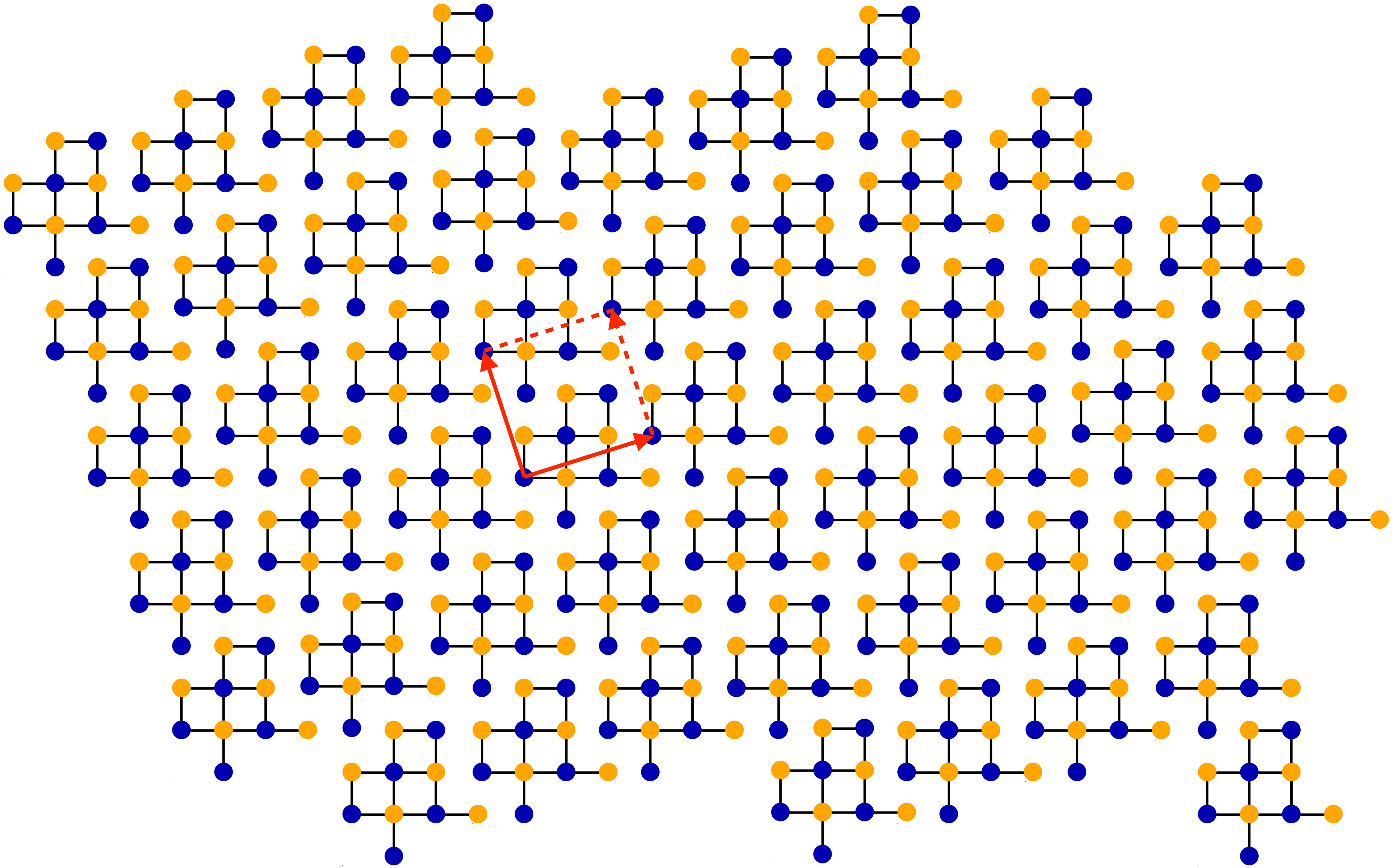
L=O(10⁴) sites, L_c=10, T=0, CPT



strange cluster?



strange cluster? but it works!



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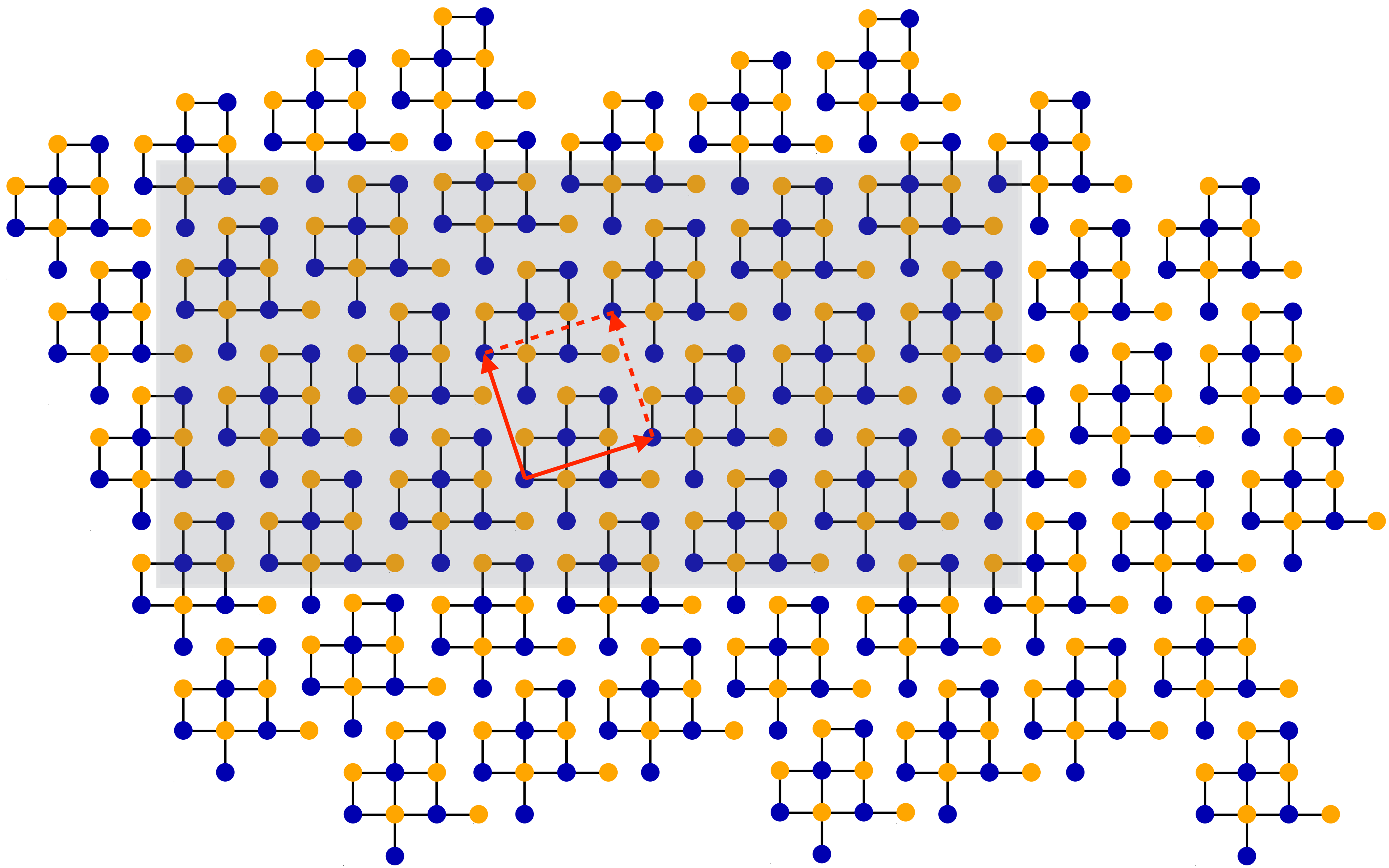
strange cluster? but it works!



PERIODIZATION

translation symmetries

CPT Green's function

$$G_{\boldsymbol{R},\boldsymbol{R}'}(\omega) = G_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}',\boldsymbol{r}\boldsymbol{r}'}(\omega)$$

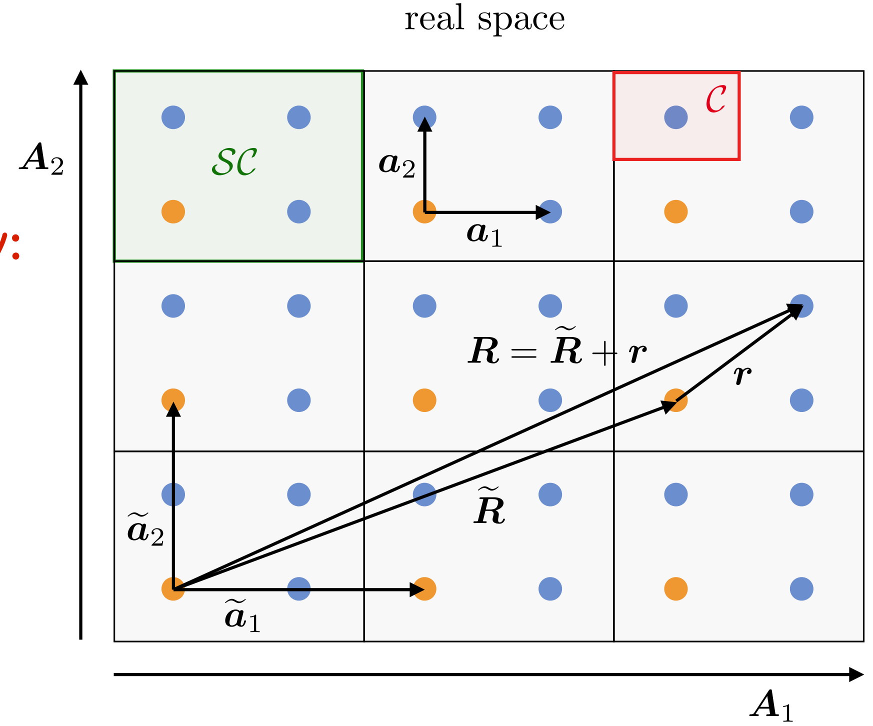
invariant under superlattice translations only:

$$G_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}',\boldsymbol{r}\boldsymbol{r}'}(\omega) = G_{\widetilde{\boldsymbol{R}}+\Delta\widetilde{\boldsymbol{R}},\widetilde{\boldsymbol{R}}'+\Delta\widetilde{\boldsymbol{R}},\boldsymbol{r},\boldsymbol{r}'}(\omega)$$

(partial) diagonalization by superlattice Fourier transformation V

$$\frac{L_c}{L}\sum_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}'} V^{\dagger}_{\widetilde{\boldsymbol{k}},\widetilde{\boldsymbol{R}}} G_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}',\boldsymbol{r}\boldsymbol{r}'}(\omega) V_{\widetilde{\boldsymbol{R}}',\widetilde{\boldsymbol{k}}'} = G_{\boldsymbol{r}\boldsymbol{r}'}(\widetilde{\boldsymbol{k}},\omega)\delta_{\widetilde{\boldsymbol{k}}\widetilde{\boldsymbol{k}}'}$$

$$G_{\boldsymbol{r}\boldsymbol{r}'}(\widetilde{\boldsymbol{k}},\omega) = \left(\frac{1}{\omega+\mu-\boldsymbol{t}(\widetilde{\boldsymbol{k}})-\boldsymbol{\Sigma}(\omega)}\right)_{\boldsymbol{r}\boldsymbol{r}'}$$



cluster-local elements:

$$G^{(\mathrm{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega) = \frac{L_c}{L}\sum_{\widetilde{\boldsymbol{k}}\in\mathcal{RSC}}\left(\frac{1}{\omega+\mu-\boldsymbol{t}(\widetilde{\boldsymbol{k}})-\boldsymbol{\Sigma}(\omega)}\right)_{\boldsymbol{r}\boldsymbol{r}'}$$

local density of states:

$$A_{\boldsymbol{R}}(\omega) = -\frac{1}{\pi}\mathrm{Im}\, G_{\boldsymbol{r}\boldsymbol{r}}(\omega+i0^+) \neq A(\omega)$$

translation symmetries

CPT Green's function

$$G_{\boldsymbol{R},\boldsymbol{R}'}(\omega) = G_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}',\boldsymbol{r}\boldsymbol{r}'}(\omega)$$

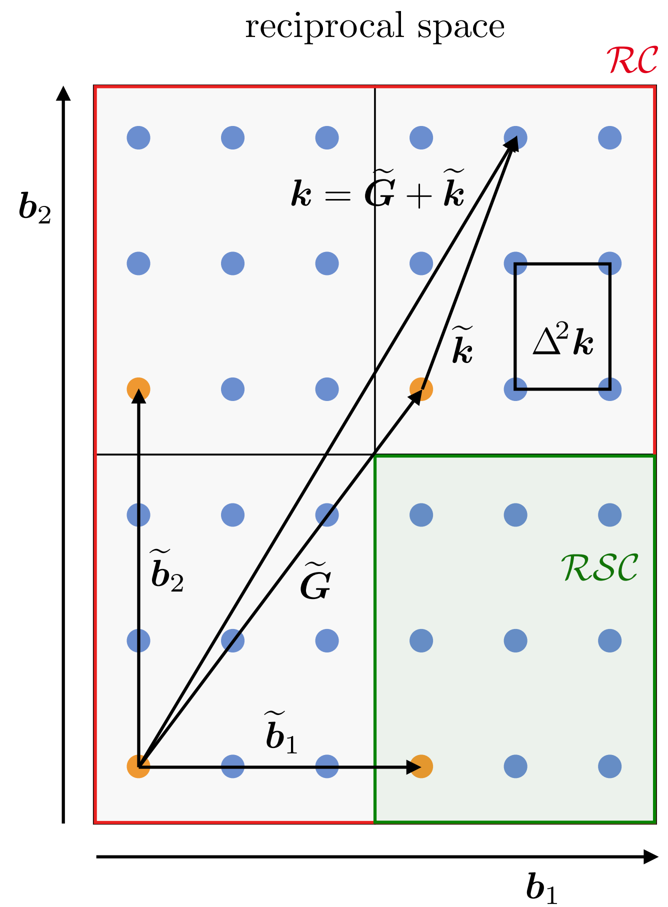
invariant under superlattice translations only:

$$G_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}',\boldsymbol{r}\boldsymbol{r}'}(\omega) = G_{\widetilde{\boldsymbol{R}}+\Delta\widetilde{\boldsymbol{R}},\widetilde{\boldsymbol{R}}'+\Delta\widetilde{\boldsymbol{R}},\boldsymbol{r},\boldsymbol{r}'}(\omega)$$

(partial) diagonalization by superlattice Fourier transformation V

$$\frac{L_c}{L}\sum_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}'} V^{\dagger}_{\widetilde{\boldsymbol{k}},\widetilde{\boldsymbol{R}}} G_{\widetilde{\boldsymbol{R}}\widetilde{\boldsymbol{R}}',\boldsymbol{r}\boldsymbol{r}'}(\omega) V_{\widetilde{\boldsymbol{R}}',\widetilde{\boldsymbol{k}}'} = G_{\boldsymbol{r}\boldsymbol{r}'}(\widetilde{\boldsymbol{k}},\omega)\delta_{\widetilde{\boldsymbol{k}}\widetilde{\boldsymbol{k}}'}$$

$$G_{\boldsymbol{r}\boldsymbol{r}'}(\widetilde{\boldsymbol{k}},\omega) = \left(\frac{1}{\omega+\mu-\boldsymbol{t}(\widetilde{\boldsymbol{k}})-\boldsymbol{\Sigma}(\omega)}\right)_{\boldsymbol{r}\boldsymbol{r}'}$$



cluster-local elements:

$$G^{(\mathrm{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega) = \frac{L_c}{L}\sum_{\widetilde{\boldsymbol{k}}\in\mathcal{RSC}}\left(\frac{1}{\omega+\mu-\boldsymbol{t}(\widetilde{\boldsymbol{k}})-\boldsymbol{\Sigma}(\omega)}\right)_{\boldsymbol{r}\boldsymbol{r}'}$$

local density of states:

$$A_{\boldsymbol{R}}(\omega) = -\frac{1}{\pi}\mathrm{Im}\, G_{\boldsymbol{r}\boldsymbol{r}}(\omega+i0^+) \neq A(\omega)$$

how to restore the translation symmetry?

(1) use periodic boundary conditions on each cluster

Zacher et al. (2000)

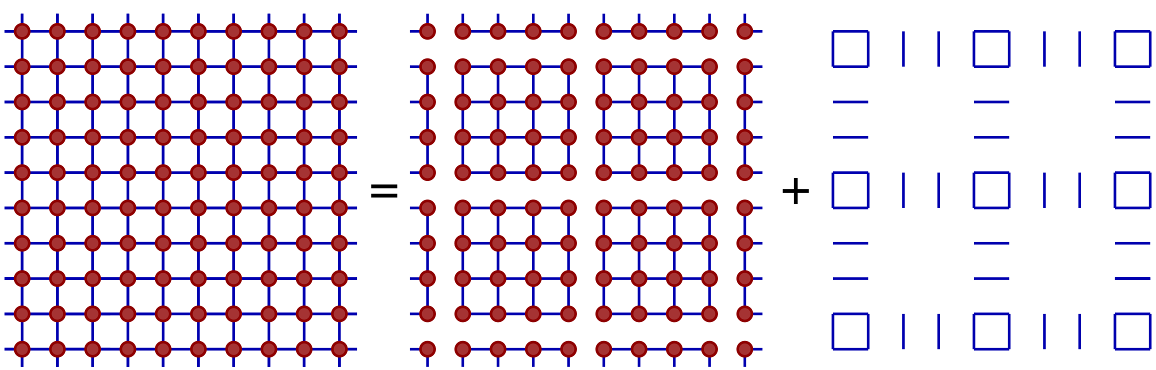
$$A_{\boldsymbol{R}}(\omega) = A(\omega) \qquad G_{\boldsymbol{R},\boldsymbol{R}}(\omega) = G(\omega) \qquad G_{\tilde{\boldsymbol{R}},\tilde{\boldsymbol{R}},\boldsymbol{r}+\Delta r,\boldsymbol{r}'+\Delta r}(\omega) = G_{\tilde{\boldsymbol{R}},\tilde{\boldsymbol{R}},\boldsymbol{r},\boldsymbol{r}'}(\omega)$$

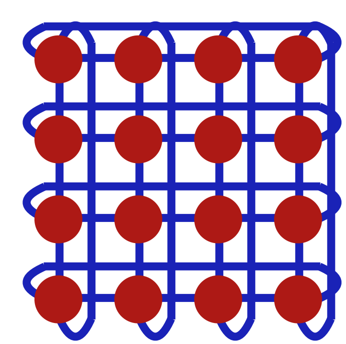
and: $G_{\tilde{\boldsymbol{R}}\tilde{\boldsymbol{R}}',\boldsymbol{r}\boldsymbol{r}'}(\omega) = G_{\tilde{\boldsymbol{R}}+\Delta\tilde{\boldsymbol{R}},\tilde{\boldsymbol{R}}'+\Delta\tilde{\boldsymbol{R}},\boldsymbol{r},\boldsymbol{r}'}(\omega)$

but: $G_{\boldsymbol{R}+\Delta\boldsymbol{R},\boldsymbol{R}'+\Delta\boldsymbol{R}}(\omega) \neq G_{\boldsymbol{R},\boldsymbol{R}'}(\omega)$

since: $\boldsymbol{U} \neq \boldsymbol{V}\boldsymbol{W}$

in practice: results are worse compared to clusters with open b.c.





how to restore the translation symmetry?

(2) take the average

$$A(\omega) \equiv \frac{1}{L_c} \sum_{\boldsymbol{r}} A_{(\tilde{\boldsymbol{R}},\boldsymbol{r})}(\omega) = \frac{1}{L} \sum_{\boldsymbol{R}} A_{\boldsymbol{R}}(\omega)$$

"physical spectral density" "CPT spectral density"

(3) periodization

in k-space: $U_{\boldsymbol{R},\boldsymbol{k}} = \frac{1}{\sqrt{L}} e^{i\boldsymbol{k}\boldsymbol{R}}$ $\quad G_{\boldsymbol{k}\boldsymbol{k}'}(\omega) \mapsto G_{\boldsymbol{k}\boldsymbol{k}}(\omega)\delta_{\boldsymbol{k},\boldsymbol{k}'} \equiv \widehat{T}[\boldsymbol{G}]_{\boldsymbol{k}\boldsymbol{k}'}(\omega)$

in real space: $\widehat{T}[\boldsymbol{G}]_{\boldsymbol{R}\boldsymbol{R}'} = \frac{1}{L} \sum_{\boldsymbol{R}''\boldsymbol{R}'''} \delta_{\boldsymbol{R}-\boldsymbol{R}',\boldsymbol{R}''-\boldsymbol{R}'''} G_{\boldsymbol{R}''\boldsymbol{R}'''}$ $\quad \widehat{T}$: periodization operator

we have:

$$\widehat{T}[\boldsymbol{G}]_{\boldsymbol{R}\boldsymbol{R}}(\omega) = \frac{1}{L} \sum_{\boldsymbol{R}''\boldsymbol{R}'''} \delta_{\boldsymbol{R}''\boldsymbol{R}'''} G_{\boldsymbol{R}''\boldsymbol{R}'''}(\omega) = \frac{1}{L} \sum_{\boldsymbol{R}} G_{\boldsymbol{R}\boldsymbol{R}}(\omega) = \frac{1}{L_c} \sum_{\boldsymbol{r}} G_{\boldsymbol{r}\boldsymbol{r}}(\omega)$$

how to restore the translation symmetry?

(4) periodization of the self-energy

$$\boldsymbol{\Sigma}(\omega) \mapsto \widehat{T}[\boldsymbol{\Sigma}](\omega) \qquad \widehat{T}[\boldsymbol{\Sigma}]_{(\widetilde{\boldsymbol{R}},\boldsymbol{r}),(\widetilde{\boldsymbol{R}}',\boldsymbol{r}')}(\omega) = \frac{1}{L_c} \sum_{\boldsymbol{r}'',\boldsymbol{r}'''} \delta_{\widetilde{\boldsymbol{R}}+\boldsymbol{r}-\widetilde{\boldsymbol{R}}'-\boldsymbol{r}',\boldsymbol{r}''-\boldsymbol{r}'''} \Sigma_{\boldsymbol{r}'',\boldsymbol{r}'''}(\omega)$$

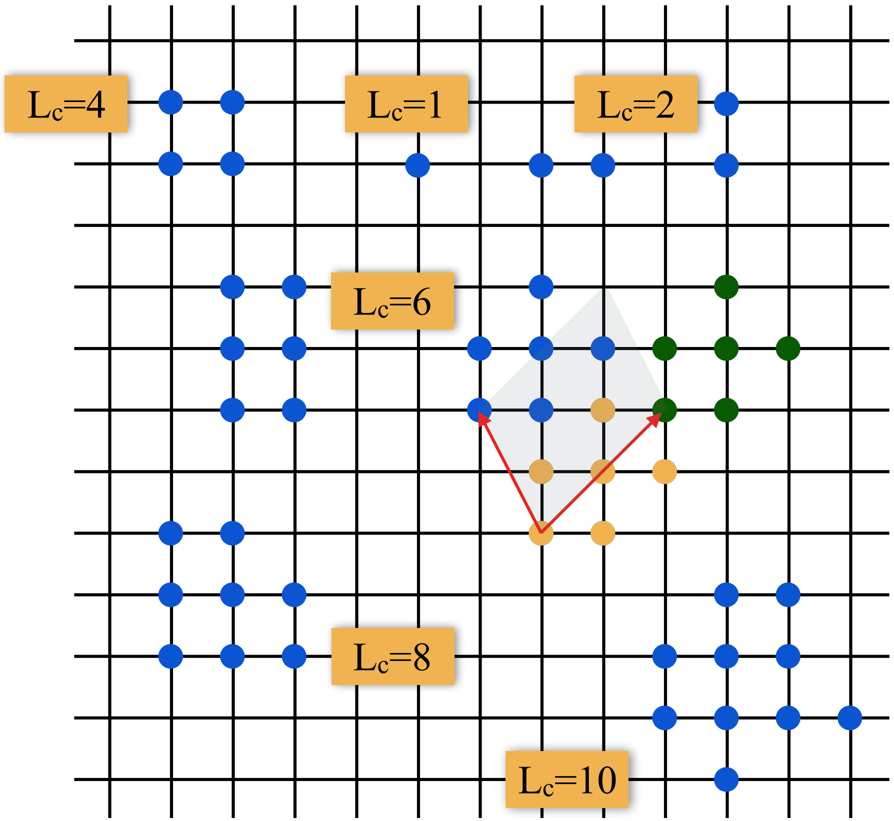
G-periodization:

standard procedure, see CPT result

Σ-periodization:

also ad hoc, but more artificial
as performed at an earlier stage

both can be generalized to restore
the correct **rotational** (point-group)
symmetries as well!



how to restore the translation symmetry?

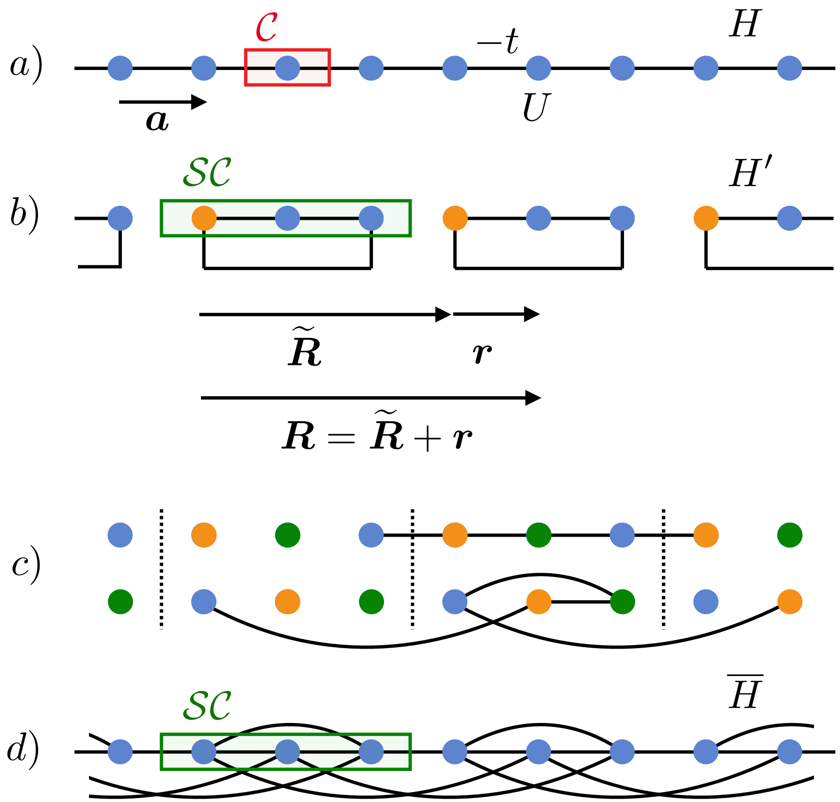
(5) periodic CPT

Tran Minh-Tien (2006)
Biroli et al. (2004)

t′: disconnected clusters with periodic b.c.
modify the parameters of H rather than H′:

$$\boldsymbol{t} \mapsto \overline{\boldsymbol{t}}$$

- such that the symmetries of H and H′ are the same
- superlattice translations: ✓
- cluster translations: X
- add the necessary hopping parameters
- irrelevant for $L_c \to \infty$!
- explicitly: $\overline{\boldsymbol{t}} = (\boldsymbol{V}\boldsymbol{W})\boldsymbol{U}^\dagger \boldsymbol{t} \boldsymbol{U}(\boldsymbol{V}\boldsymbol{W})^\dagger$



how to restore the translation symmetry?

(5) periodic CPT

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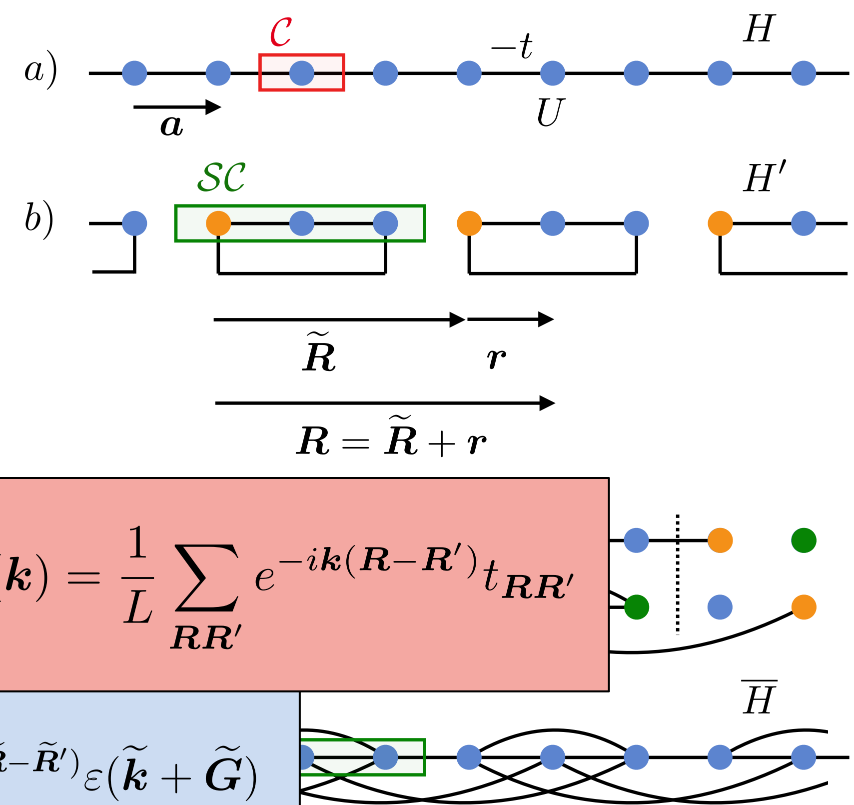


- such that the symmetries of H and H′ are the same
- superlattice translations: ✓
- cluster translations: X
- add the necessary hopping parameters
- irrelevant for $L_c \to \infty$!
- explicitly: $\overline{\boldsymbol{t}} = (\boldsymbol{V}\boldsymbol{W})\boldsymbol{U}^\dagger \boldsymbol{t} \boldsymbol{U} (\boldsymbol{V}\boldsymbol{W})^\dagger$

$$\varepsilon(\boldsymbol{k}) = \frac{1}{L} \sum_{\boldsymbol{R}\boldsymbol{R}'} e^{-i\boldsymbol{k}(\boldsymbol{R}-\boldsymbol{R}')} t_{\boldsymbol{R}\boldsymbol{R}'}$$

$$\overline{t}_{\boldsymbol{R}\boldsymbol{R}'} = t_{\widetilde{\boldsymbol{R}},\boldsymbol{r};\widetilde{\boldsymbol{R}}',\boldsymbol{r}'} = \frac{1}{L_c} \sum_{\widetilde{\boldsymbol{G}}} e^{i\widetilde{\boldsymbol{G}}(\boldsymbol{r}-\boldsymbol{r}')} \frac{L_c}{L} \sum_{\widetilde{\boldsymbol{k}}} e^{i\widetilde{\boldsymbol{k}}(\widetilde{\boldsymbol{R}}-\widetilde{\boldsymbol{R}}')} \varepsilon(\widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}})$$

how to restore the translation symmetry?

(5) periodic CPT, contd.

t': disconnected clusters with periodic b.c.
modify the parameters of H rather than H':

$$\boldsymbol{t} \mapsto \overline{\boldsymbol{t}}$$

- apply CPT to $\overline{H}$ using ref.sys. H'

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

- this is diagonalized by **VW**:

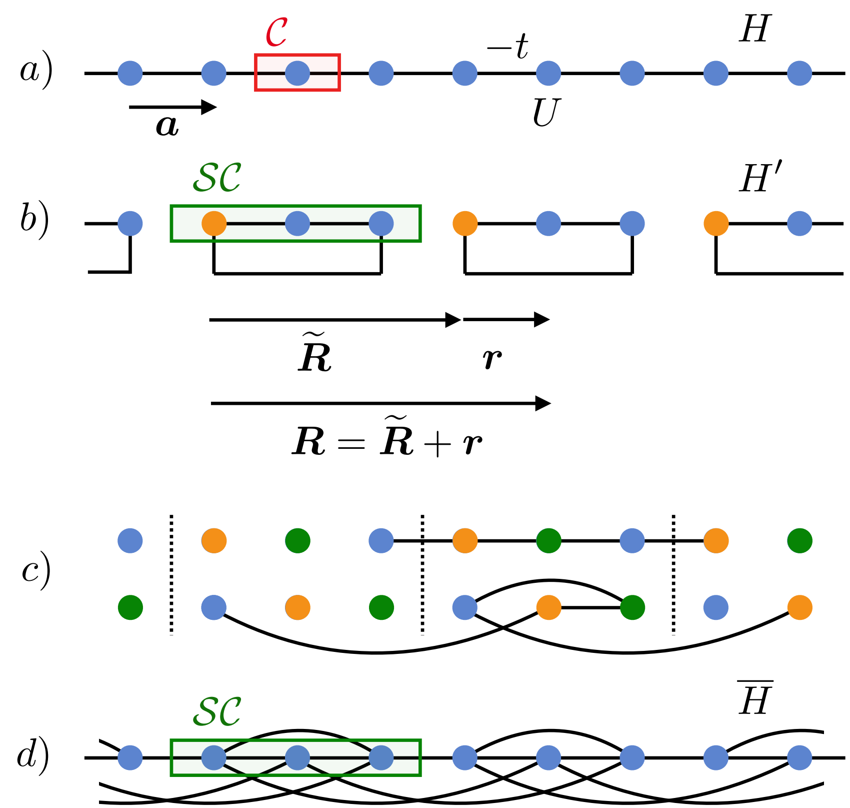
$$G(\widetilde{\boldsymbol{k}}, \widetilde{\boldsymbol{G}}, \omega) = \frac{1}{\omega + \mu - \varepsilon(\widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}) + \Sigma(\widetilde{\boldsymbol{G}}, \omega)}$$

- implicit periodization, identifying

$$G(\widetilde{\boldsymbol{k}}, \widetilde{\boldsymbol{G}}, \omega) \equiv G(\boldsymbol{k}, \omega)$$

- self-energy is discontinuous:

$$\Sigma(\widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}, \omega) = \Sigma(\widetilde{\boldsymbol{k}}, \omega)$$



how to restore the translation symmetry?

(5) periodic CPT, contd.

t': disconnected clusters with periodic b.c.
modify the parameters of H rather than H':

$$\boldsymbol{t} \mapsto \bar{\boldsymbol{t}}$$

- apply CPT to $\overline{H}$ using ref.sys. H'

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

- this is diagonalized by **VW**:

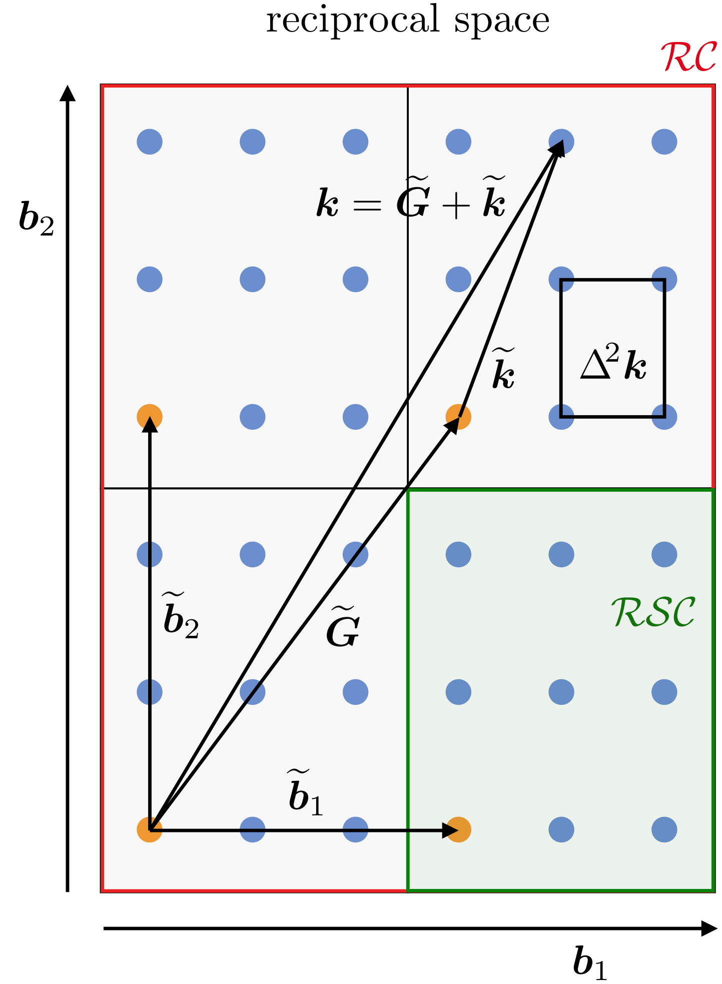
$$G(\widetilde{\boldsymbol{k}}, \widetilde{\boldsymbol{G}}, \omega) = \frac{1}{\omega + \mu - \varepsilon(\widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}) + \Sigma(\widetilde{\boldsymbol{G}}, \omega)}$$

- implicit periodization, identifying

$$G(\widetilde{\boldsymbol{k}}, \widetilde{\boldsymbol{G}}, \omega) \equiv G(\boldsymbol{k}, \omega)$$

- self-energy is discontinuous:

$$\Sigma(\widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}, \omega) = \Sigma(\widetilde{\boldsymbol{G}}, \omega)$$



SELF-CONSISTENT CLUSTER EMBEDDING

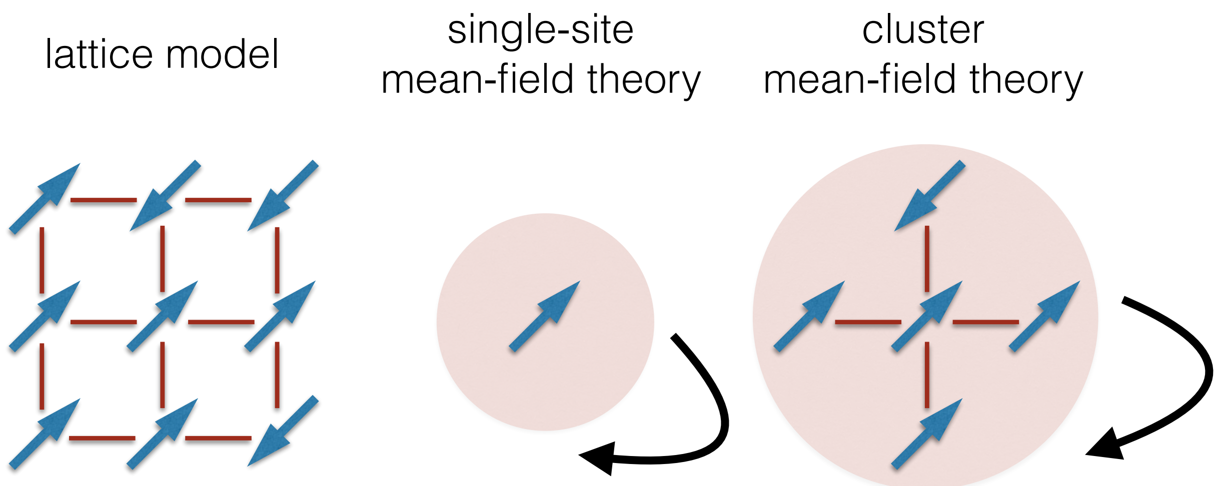
cluster extensions of DMFT

impurity / cluster approach

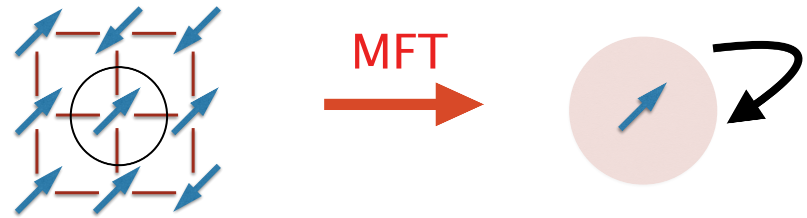
Hubbard-I approximation
CPT
periodic CPT

with self-consistent embedding

DMFT
cellular DMFT
DCA



recall DMFT



local self-energy generated by

$$H' = \sum_\sigma \varepsilon_{\mathrm{imp}} c_\sigma^\dagger c_\sigma + \frac{U}{2} \sum_\sigma n_{\mathrm{imp},\sigma} n_{\mathrm{imp},-\sigma} + \sum_{k\sigma} \varepsilon_k a_{k\sigma}^\dagger a_{k\sigma} + \sum_{k\sigma} (V_k c_\sigma^\dagger a_{k\sigma} + \mathrm{H.c.})$$

local Green's function on the impurity site:

$$G^{(\mathrm{imp})}(\omega) = \frac{1}{\omega + \mu - \varepsilon_{\mathrm{imp}} - \Delta(\omega) - \Sigma'(\omega)}$$

hybridization function:

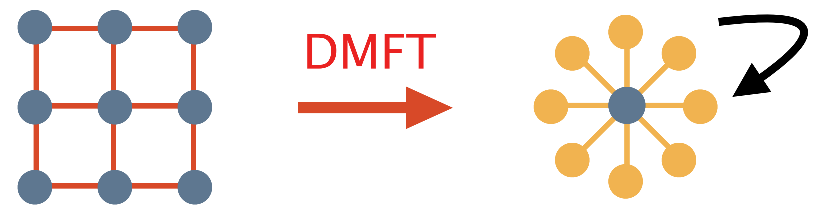
$$\Delta(\omega) = \sum_k \frac{V_k^2}{\omega + \mu - \varepsilon_k}$$

use SIAM as reference system:

$$\Sigma(\omega) = \Sigma'(\omega)$$

derive self-consistency condition to fix the parameters of H' !

recall DMFT



local self-energy generated by

$$H' = \sum_{\sigma} \varepsilon_{\text{imp}} c_{\sigma}^{\dagger} c_{\sigma} + \frac{U}{2} \sum_{\sigma} n_{\text{imp},\sigma} n_{\text{imp},-\sigma} + \sum_{k\sigma} \varepsilon_k a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_{k\sigma} (V_k c_{\sigma}^{\dagger} a_{k\sigma} + \text{H.c.})$$

local Green's function on the impurity site:

$$G^{(\text{imp})}(\omega) = \frac{1}{\omega + \mu - \varepsilon_{\text{imp}} - \Delta(\omega) - \Sigma'(\omega)}$$

hybridization function:

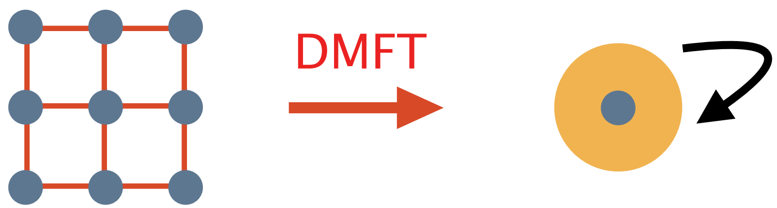
$$\Delta(\omega) = \sum_{k} \frac{V_k^2}{\omega + \mu - \varepsilon_k}$$

use SIAM as reference system:

$$\Sigma(\omega) = \Sigma'(\omega)$$

derive self-consistency condition to fix the parameters of H' !

recall DMFT



local self-energy generated by

$$H' = \sum_{\sigma} \varepsilon_{\text{imp}} c^{\dagger}_{\sigma} c_{\sigma} + \frac{U}{2} \sum_{\sigma} n_{\text{imp},\sigma} n_{\text{imp},-\sigma} + \sum_{k\sigma} \varepsilon_k a^{\dagger}_{k\sigma} a_{k\sigma} + \sum_{k\sigma} (V_k c^{\dagger}_{\sigma} a_{k\sigma} + \text{H.c.})$$

local Green's function on the impurity site:

$$G^{(\text{imp})}(\omega) = \frac{1}{\omega + \mu - \varepsilon_{\text{imp}} - \Delta(\omega) - \Sigma'(\omega)}$$

hybridization function:

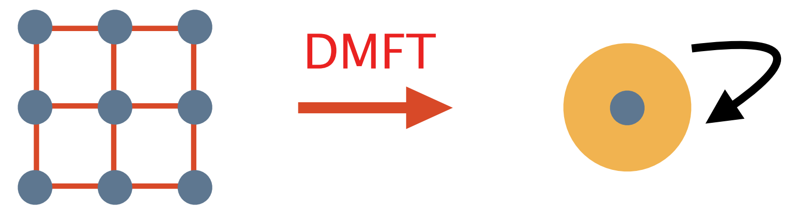
$$\Delta(\omega) = \sum_{k} \frac{V_k^2}{\omega + \mu - \varepsilon_k}$$

use SIAM as reference system:

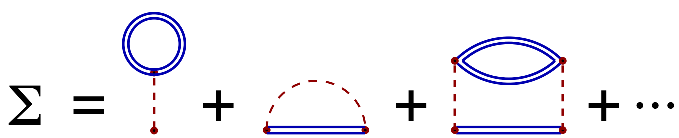
$$\Sigma(\omega) = \Sigma'(\omega)$$

derive self-consistency condition to fix the parameters of H' !

self-consistency condition



skeleton-diagram expansion:



functional relation for the Hubbard model (infinite D)

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}[\boldsymbol{G}^{(\mathrm{loc})}]$$

functional relation for the impurity Anderson model

$$\boldsymbol{\Sigma}' = \boldsymbol{\Sigma}[\boldsymbol{G}^{(\mathrm{imp})}]$$

with $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}'$ this implies:

$$G^{(\mathrm{imp})}(\omega) = G^{(\mathrm{loc})}(\omega) \qquad \text{where} \qquad G^{(\mathrm{imp})}(\omega) = \frac{1}{\omega + \mu - \varepsilon_{\mathrm{imp}} - \Delta(\omega) - \Sigma'(\omega)}$$

solving for the hybridization function:

$$\Delta(\omega) = \sum_k \frac{V_k^2}{\omega + \mu - \varepsilon_k} = \omega + \mu - \varepsilon_{\mathrm{imp}} - \Sigma(\omega) - \frac{1}{G^{(\mathrm{loc})}(\omega)}$$

DMFT self-consistency condition

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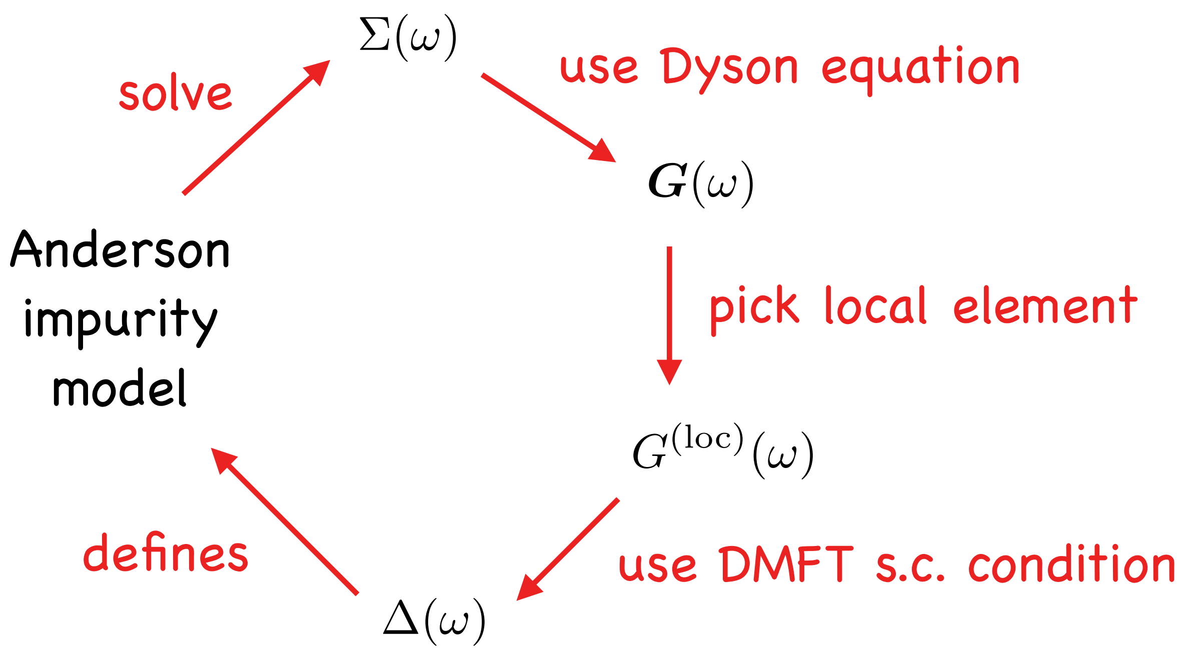
DMFT self-consistency cycle



cellular DMFT

Lichtenstein, Katsnelson (2000)

Kotliar et al. (2001)

$\Sigma(\omega)$ — use Dyson equation → $\boldsymbol{G}(\omega)$

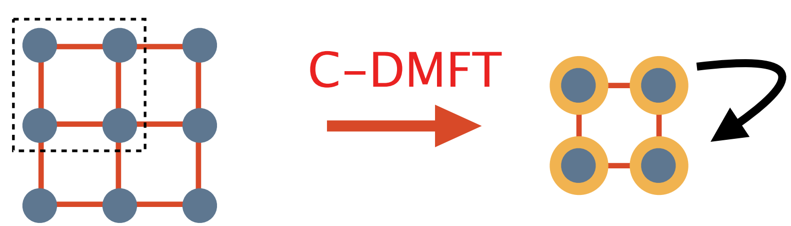
$\boldsymbol{G}(\omega)$ — pick local element → $G^{(\mathrm{loc})}(\omega)$

$G^{(\mathrm{loc})}(\omega)$ — use DMFT s.c. condition → $\Delta(\omega)$

$\Delta(\omega)$ — defines → Anderson cluster model

Anderson cluster model — solve → $\Sigma(\omega)$

$$H' = \sum_{\boldsymbol{r}\boldsymbol{r}'\sigma} t_{\boldsymbol{r}\boldsymbol{r}'} c^\dagger_{\boldsymbol{r}\sigma} c_{\boldsymbol{r}'\sigma} + \frac{U}{2} \sum_{\boldsymbol{r}\sigma} n_{\boldsymbol{r}\sigma} n_{\boldsymbol{r}-\sigma} + \sum_{k\sigma} \varepsilon_{\boldsymbol{r}k} a^\dagger_{\boldsymbol{r}k\sigma} a_{\boldsymbol{r}k\sigma} + \sum_{\boldsymbol{r}k\sigma} (V_{\boldsymbol{r}k} c^\dagger_{\boldsymbol{r}\sigma} a_{\boldsymbol{r}k\sigma} + \mathrm{H.c.})$$



cellular DMFT

$\Sigma(\omega)$

use Dyson equation

$G(\omega)$

pick elements of G on the cluster

$G^{(\mathrm{loc})}_{rr'}(\omega)$

use DMFT s.c. condition

$\Delta(\omega)$

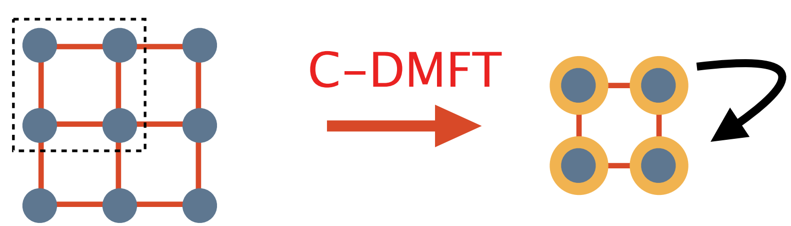
defines

Anderson cluster model

solve

$$\Sigma_{\widetilde{R}\widetilde{R},rr'}(\omega) = \Sigma'_{rr'}(\omega)$$

$$G^{(\mathrm{loc})}_{rr'}(\omega) = \frac{L_c}{L} \sum_{\widetilde{k} \in \mathcal{RSC}} \left(\frac{1}{\omega + \mu - \boldsymbol{t}(\widetilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}(\omega)} \right)_{rr'}$$



cellular DMFT

$\Sigma(\omega)$

use Dyson equation

$G(\omega)$

pick elements of G on the cluster

$G^{(\mathrm{loc})}_{\boldsymbol{rr'}}(\omega)$

use C-DMFT s.c. condition

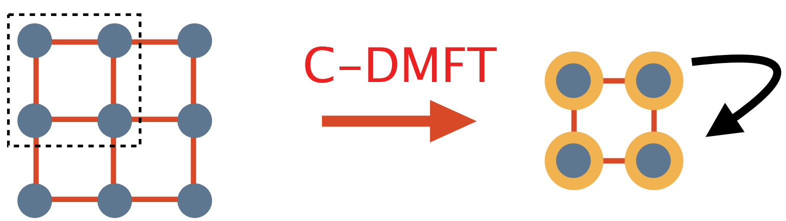
$$G^{(\mathrm{cluster})}_{\boldsymbol{rr'}}(\omega) = G^{(\mathrm{loc})}_{\boldsymbol{rr'}}(\omega)$$

$\Delta(\omega)$

defines

Anderson cluster model

solve



cellular DMFT

$\boldsymbol{\Sigma}(\omega)$

use Dyson equation

$\boldsymbol{G}(\omega)$

pick elements of G on the cluster

$\boldsymbol{G}^{(\text{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega)$

use C-DMFT s.c. condition

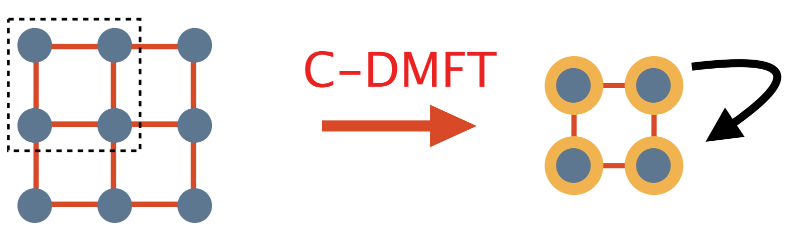
$\boldsymbol{\Delta}(\omega)$

defines

Anderson cluster model

solve

$$\varDelta_{\boldsymbol{r}}(\omega) = \sum_{k\sigma} \frac{V_{\boldsymbol{r}k}^2}{\omega + \mu - \varepsilon_{\boldsymbol{r}k}} = \omega + \mu - t_{\boldsymbol{r}\boldsymbol{r}} - \varSigma_{\boldsymbol{r}\boldsymbol{r}}(\omega) - (\boldsymbol{G}^{(\text{cluster})})^{-1}_{\boldsymbol{r}\boldsymbol{r}}(\omega)$$



periodized cellular DMFT

Biroli et al. (2004)

$\Sigma(\omega)$

use Dyson equation

$\boldsymbol{G}(\omega)$

pick elements of G on the cluster

$G^{(\mathrm{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega)$

use C-DMFT s.c. condition

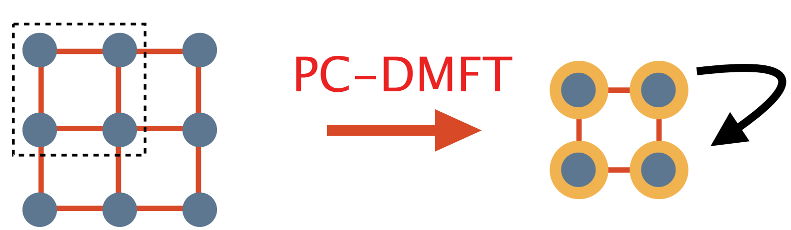
$\boldsymbol{\Delta}(\omega)$

defines

Anderson cluster model

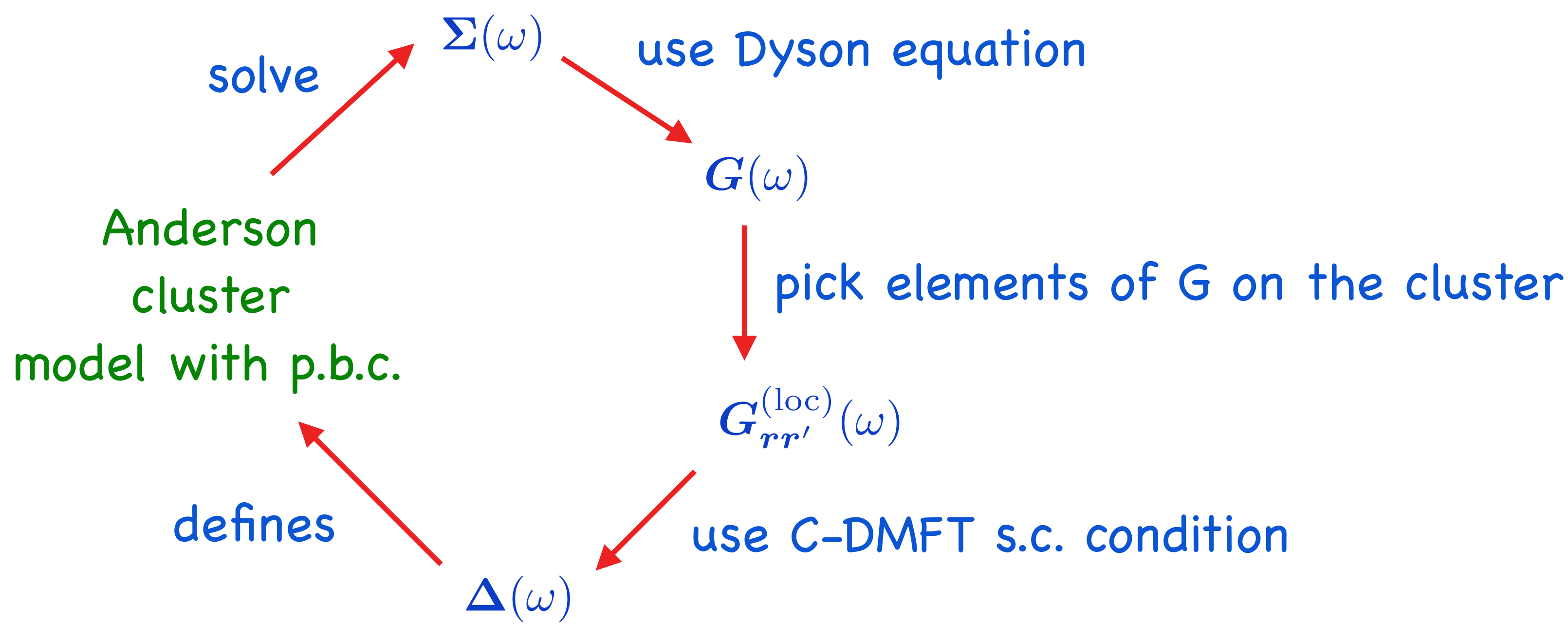
solve

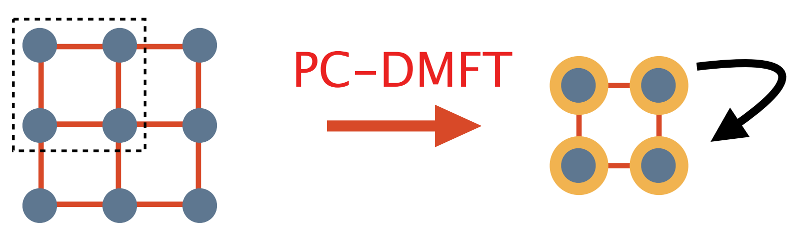
$$G^{(\mathrm{cluster})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega) = G^{(\mathrm{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega) = \frac{1}{L}\sum_{\boldsymbol{k}} \frac{e^{i\boldsymbol{k}(\boldsymbol{r}-\boldsymbol{r}')}}{\omega + \mu - \varepsilon(\boldsymbol{k}) - \widehat{T}[\boldsymbol{\Sigma}](\boldsymbol{k},\omega)}$$



dynamical cluster approximation

Hettler et al. (1998)





dynamical cluster approximation

Hettler et al. (1998)

$\boldsymbol{\Sigma}(\omega)$

use Dyson equation with $t \mapsto \bar{t}$

$\boldsymbol{G}(\omega)$

pick elements of G on the cluster

$\boldsymbol{G}^{(\mathrm{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega)$

use C-DMFT s.c. condition

$\boldsymbol{\Delta}(\omega)$

defines

Anderson cluster model with p.b.c.

solve

$$G^{(\mathrm{cluster})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega) = G^{(\mathrm{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega) = \frac{L_c}{L} \sum_{\widetilde{\boldsymbol{k}} \in \mathcal{RSC}} \left(\frac{1}{\omega + \mu - \bar{\boldsymbol{t}}(\widetilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}(\omega)} \right)_{\boldsymbol{r}\boldsymbol{r}'}$$

dynamical cluster approximation

Hettler et al. (1998)

$\Sigma(\omega)$

use Dyson equation with $t \mapsto \bar{t}$

$\boldsymbol{G}(\omega)$

pick elements of G on the cluster

$\boldsymbol{G}^{(\mathrm{loc})}_{\boldsymbol{r}\boldsymbol{r}'}(\omega)$

use C-DMFT s.c. condition

$\boldsymbol{\Delta}(\omega)$

defines

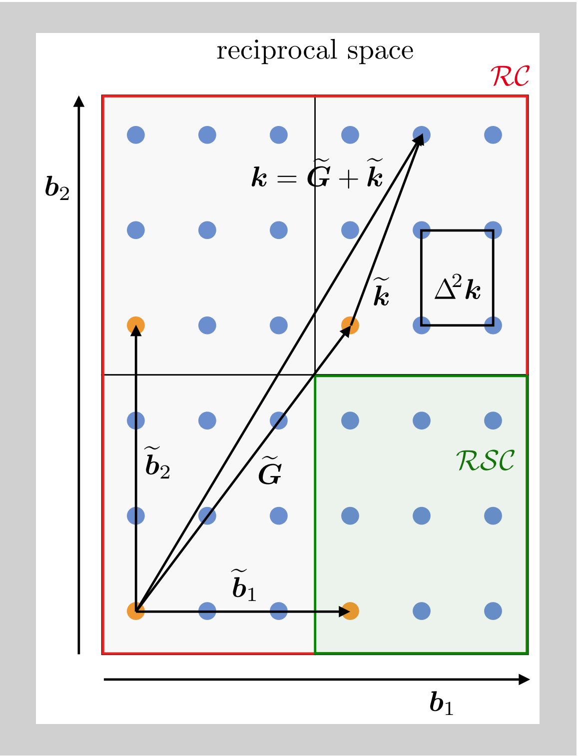
Anderson cluster model with p.b.c.

solve

DCA self-consistency equation:

$$G^{(\mathrm{cluster})}(\widetilde{\boldsymbol{G}},\omega) = \frac{L_c}{L}\sum_{\widetilde{\boldsymbol{k}}} \frac{1}{\omega+\mu-\varepsilon(\widetilde{\boldsymbol{k}}+\widetilde{\boldsymbol{G}})-\Sigma(\widetilde{\boldsymbol{G}},\omega)}$$

DCA: k-space perspective



completely neglect the momentum dependence of the self-energy

DMFT self-consistency equation:

$$G^{(\mathrm{imp})}(\omega) = G^{(\mathrm{loc})}(\omega) = \frac{1}{L} \sum_{\boldsymbol{k}} \frac{1}{\omega + \mu - \varepsilon(\boldsymbol{k}) - \Sigma(\omega)}$$

DCA self-consistency equation:

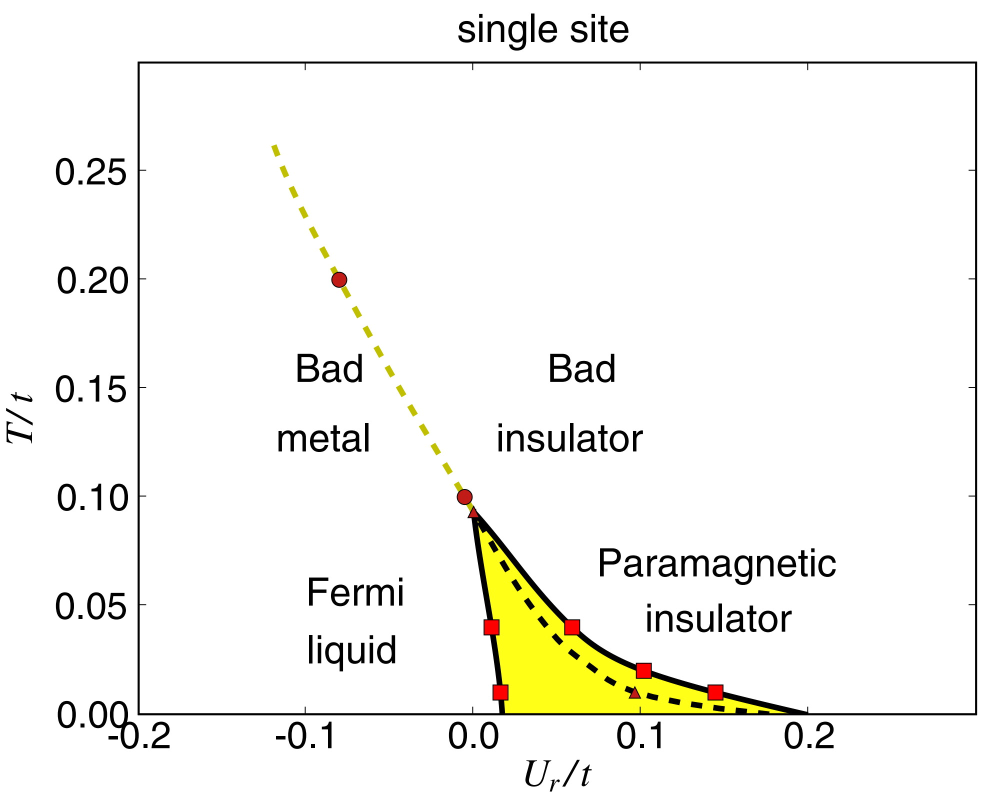
$$G^{(\mathrm{cluster})}(\widetilde{\boldsymbol{G}}, \omega) = \frac{L_c}{L} \sum_{\widetilde{\boldsymbol{k}}} \frac{1}{\omega + \mu - \varepsilon(\widetilde{\boldsymbol{k}} + \widetilde{\boldsymbol{G}}) - \Sigma(\widetilde{\boldsymbol{G}}, \omega)}$$

discard information on the fine structure of the momentum dependence of the self-energy

keep overall, rough information on the momentum dependence

APPLICATIONS

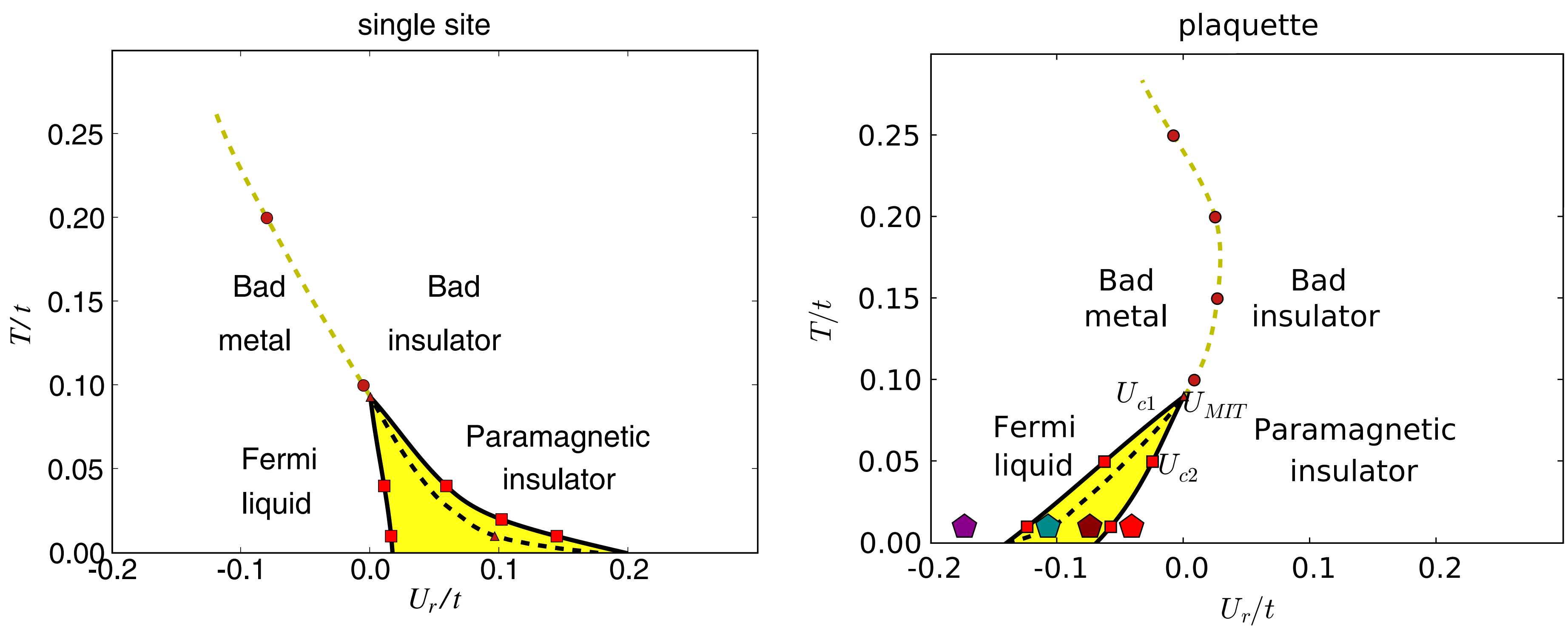
Mott transition - DMFT



- DMFT phase diagram (paramagnetic)
- Mott insulator at T=0: macroscopic entropy L log2
- superexchange does not lift the ground-state degeneracy
- missing feedback of nonlocal (magnetic) correlations
- consequence: at T>0 the high entropy stabilizes the insulator $F = E-TS$

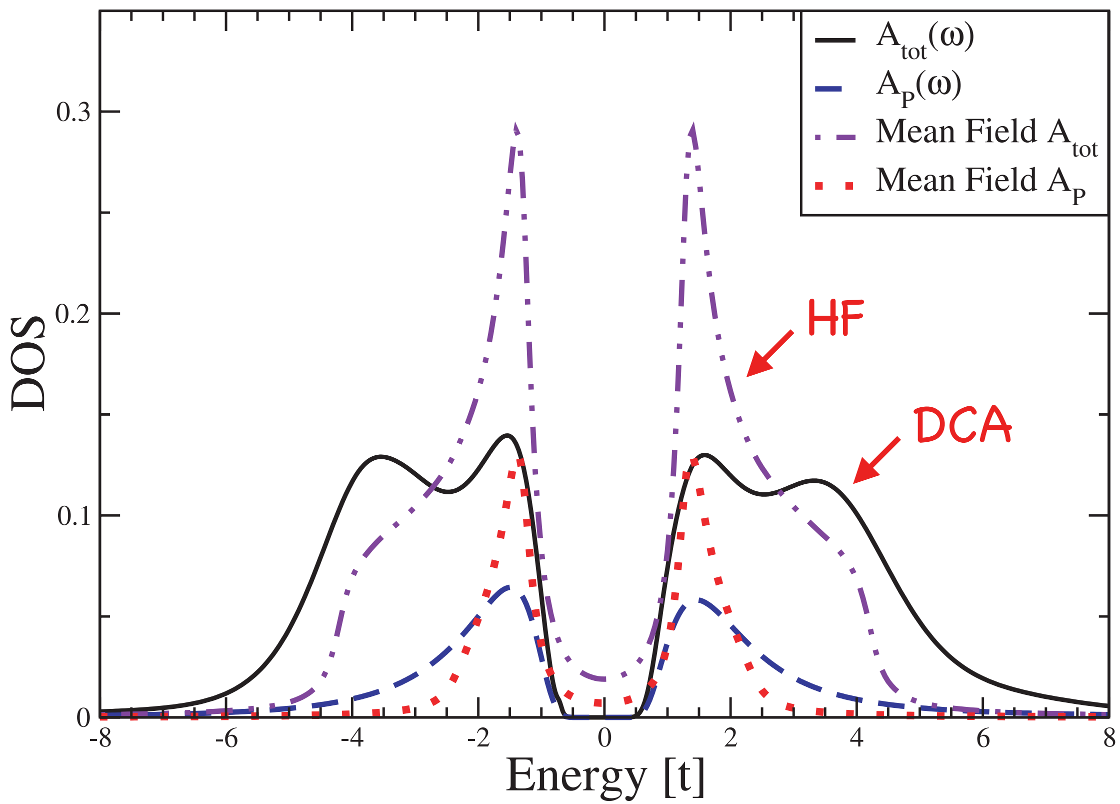
Mott transition: cellular DMFT

Park et al. (2008)



- DMFT correct at high temperatures: nonlocal correlations attenuated
- the transition line $U_c(T)$ bends back at low T
- U_c lower by roughly a factor two
- nonlocal (short-range) correlations allow for nonlocal singlet formation
- unique ground state of the Mott insulator

nonlocal correlations: DCA

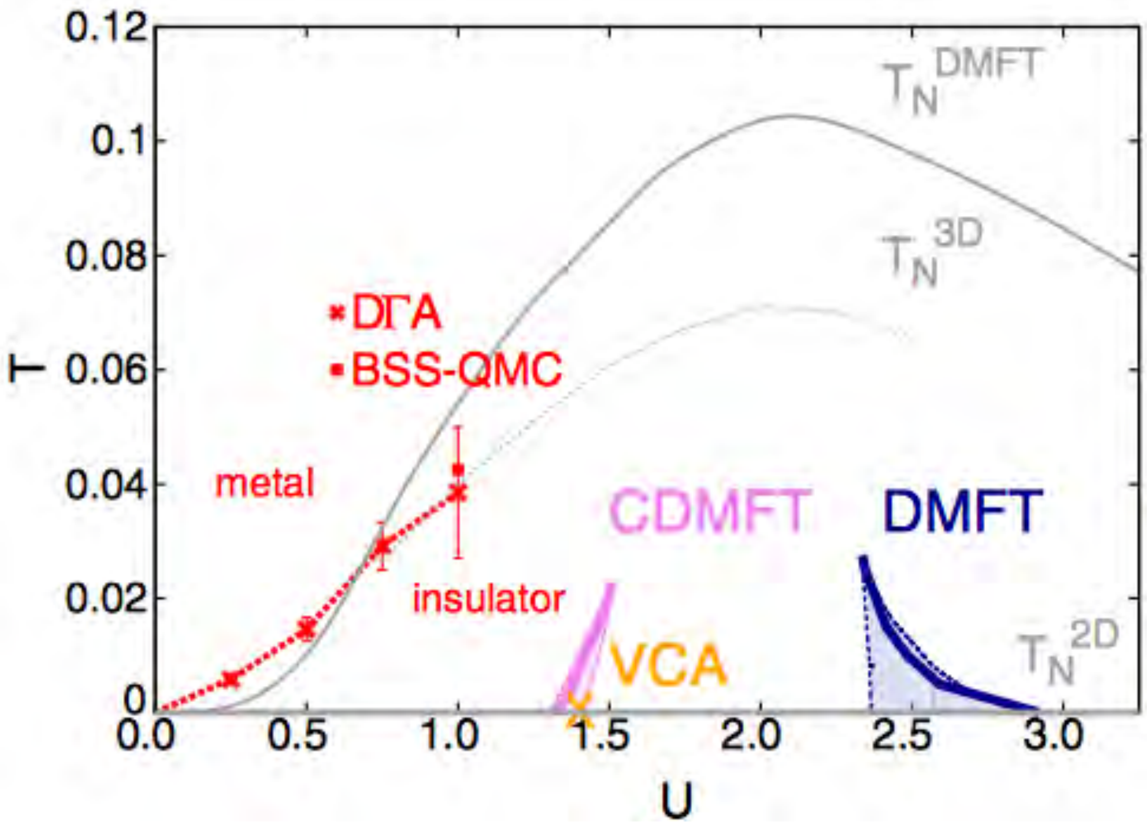


Gull et al. (2008)

- paramagnetic insulator
- plaquette, L_c=4
  note: o.b.c. = p.b.c.
  still C-DMFT ≠ DCA
- QMC solver, MaxEnt
- four-peak structure
  cf. lattice-QMC results !
- low-energy peaks:
  nonlocal correlations
- consistent with AF
  Hartree-Fock calculations
- HF: LRO -> doubling of unit cell, gap opening at the boundary of the reduced BZ

- Mott gap or Slater gap ?
- k = (pi,0), (0.pi): Mott (pole of self-energy)
  k = (0,0), (pi,pi): Slater-type transition
- k-selective transition

diagrammatic extension of DMFT



Schäfer et al. (2015)

- dynamical vertex approx. (and lattice QMC)
- gapped spectra for all U (due to scattering from extended AF fluctuations)
- no metal-insulator transition
- crossover from Slater to Heisenberg physics (but no symmetry breaking, consistent with MW66)

- is this the final answer?
- diagrammatic approaches: there is no control parameter (like L_c)

unconventional superconductivity

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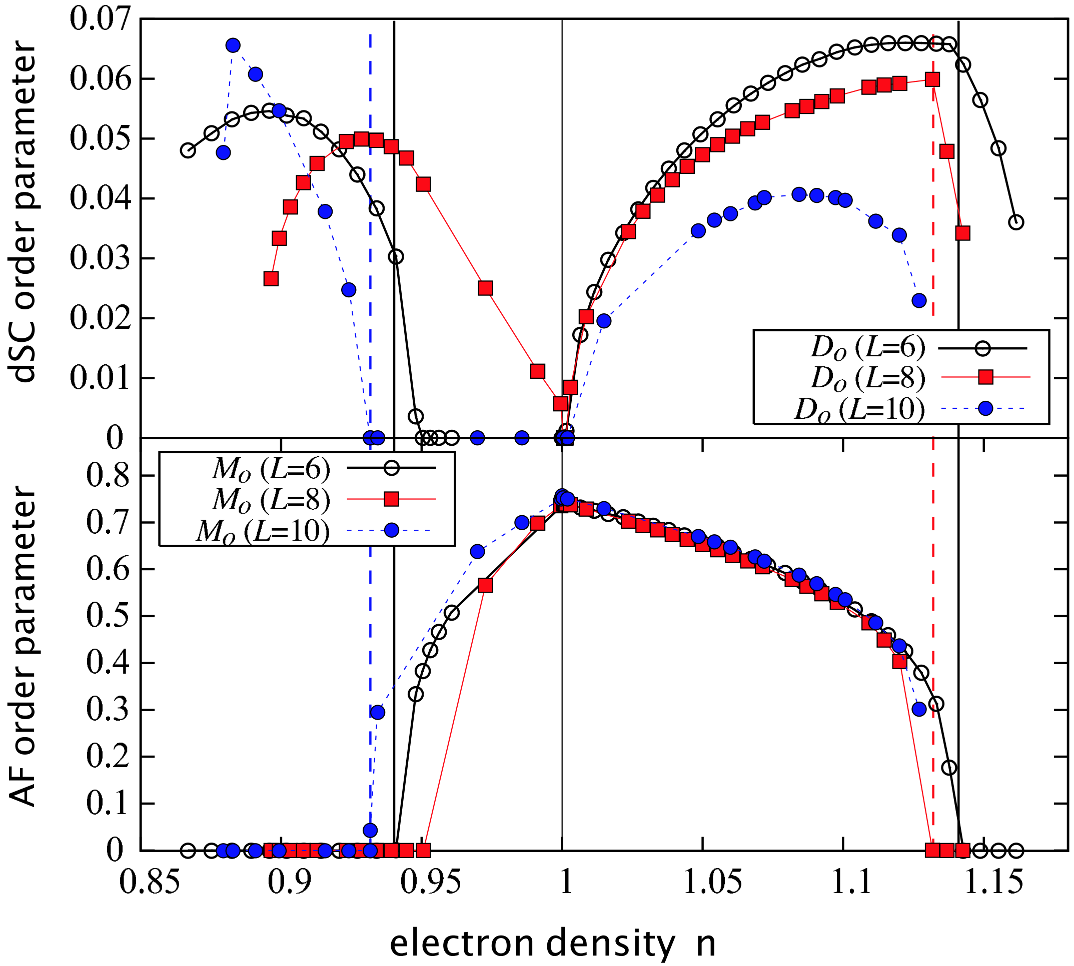

Senechal et al. (2005)

- T=0, L_c=6,8,10, VCA ("simplified C-DMFT") U=8, t=1, t'=-0.3, t''=0.2
- spontaneous symmetry breaking with nonlocal order parameter (not accessible to DMFT)
- SC coexists with AF
- pure SC at higher hole doping levels
- artificial finite-size and cluster-geometry effects

- are cluster approaches efficient to solve the high-T_c problem ?

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conclusions

DMFT

useful
beautiful
requires extensions

cluster extensions

systematic
limited in practice
artificial symmetry breaking and restoration

diagrammatic extensions

not systematic
respect symmetries
can be motivated physically

conclusions

cluster extensions

systematic
limited in practice
artificial symmetry breaking and restoration

not unique

C-DMFT	DCA
real-space perspective	k-space perspective

convergence with $L_c = L_1^D$:

C-DMFT	DCA
for local observables: exponential for extended observables: $1/L_1$	for extended observables: $1/L_1^2$
breaks translational symmetries SSB: "automatic"	respects translational symmetries SSB: must be anticipated

conclusions

cluster extensions

which type of physics is dominated
by local and short-range correlations?

Mott transition

there is a DMFT scenario
cluster approaches: this is incorrect in D=2
cluster approaches themselves not reliable in D=2 ?

high-T_c superconductivity

cannot be explained within DMFT
cluster approaches: short-range correlations are essential
likely: longer-range correlations important as well

conclusions

cluster extensions

systematic
limited in practice
artificial symmetry breaking and restoration

more issues

efficient cluster solver: QMC only (?)
systems with nonlocal or even long-range interactions
there is no straightforward real-space cluster DMFT !

THE END.