Dynamic cluster quantum Monte Carlo simulations of cuprate superconductors

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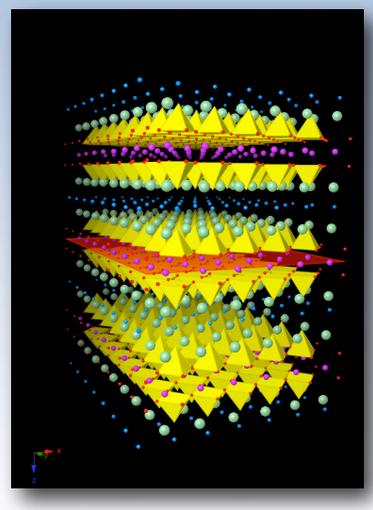
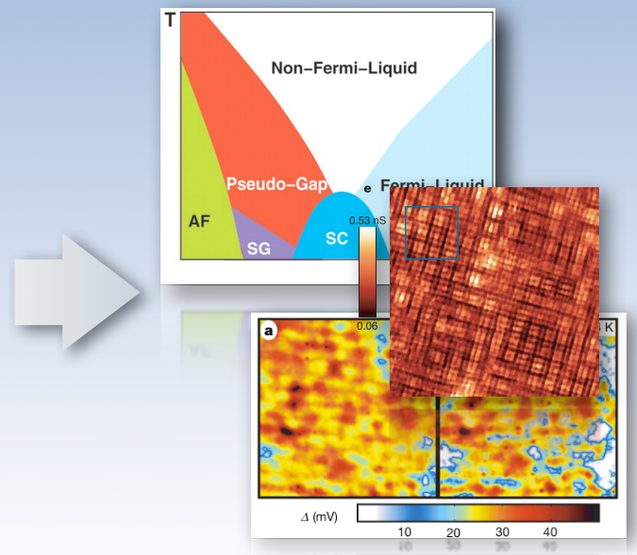
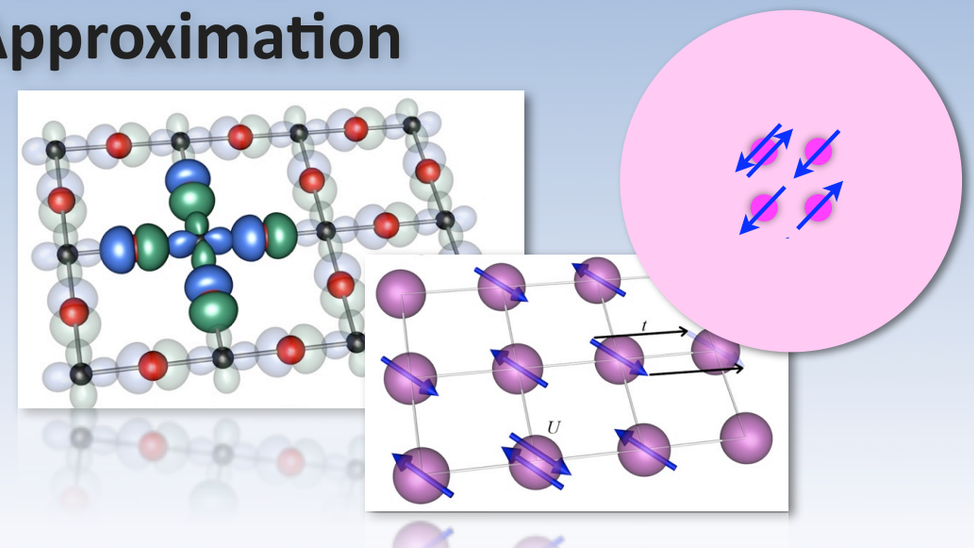
Outline

HTSC cuprates

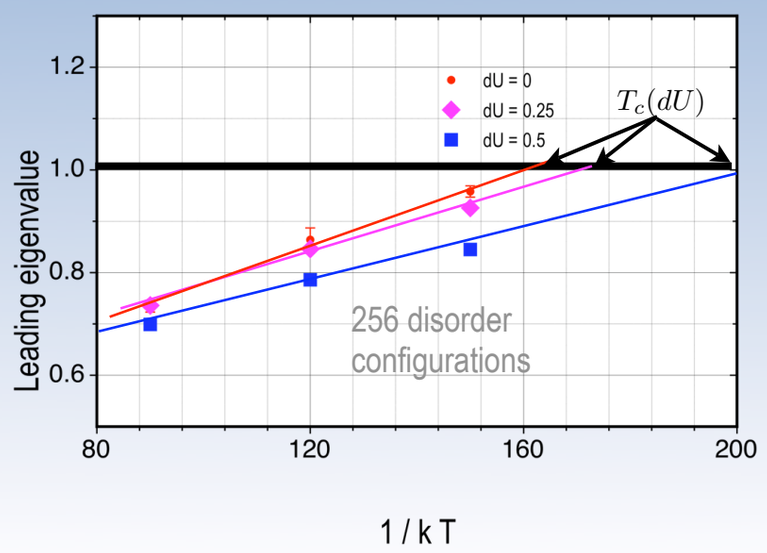




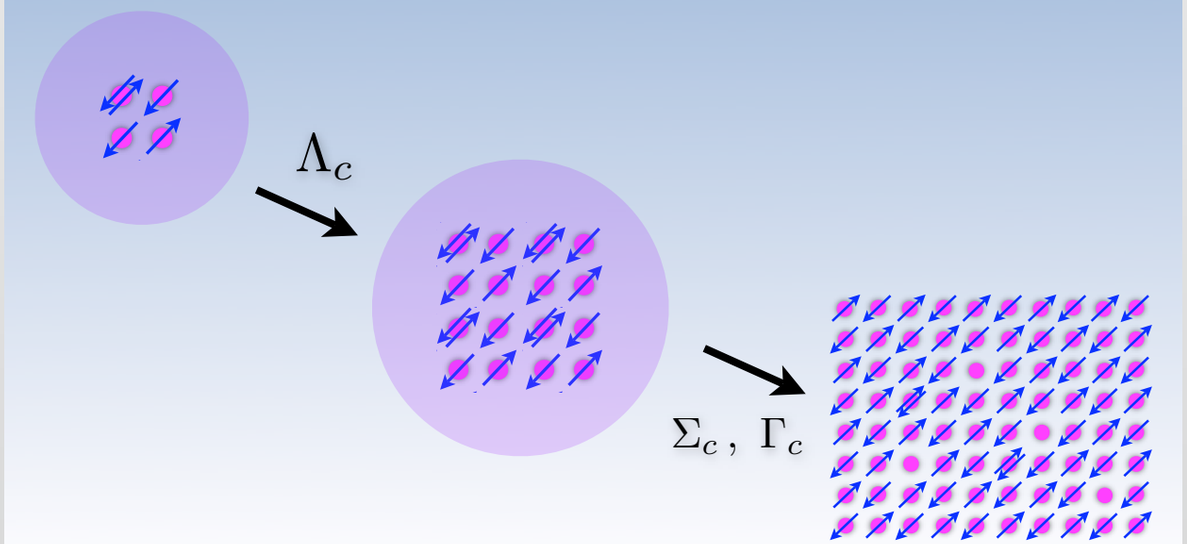
Optimizing the Dynamic Cluster QMC Approximation



Effects of disorder



Avoiding the sign problem



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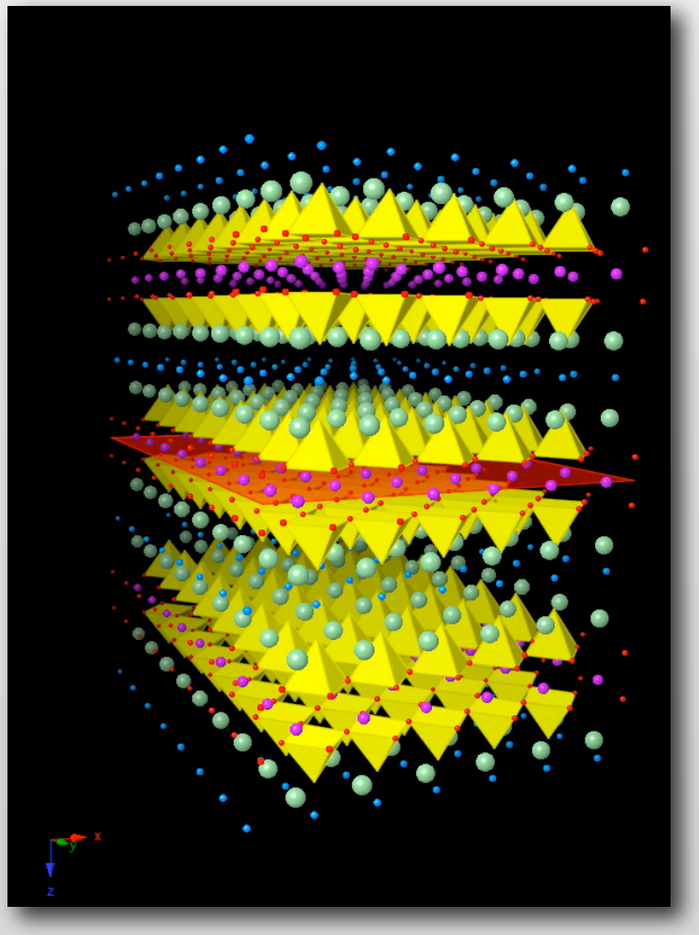
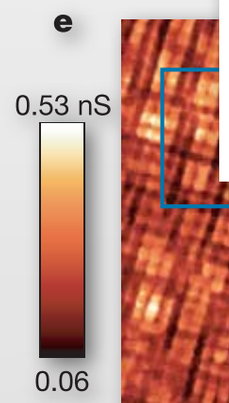
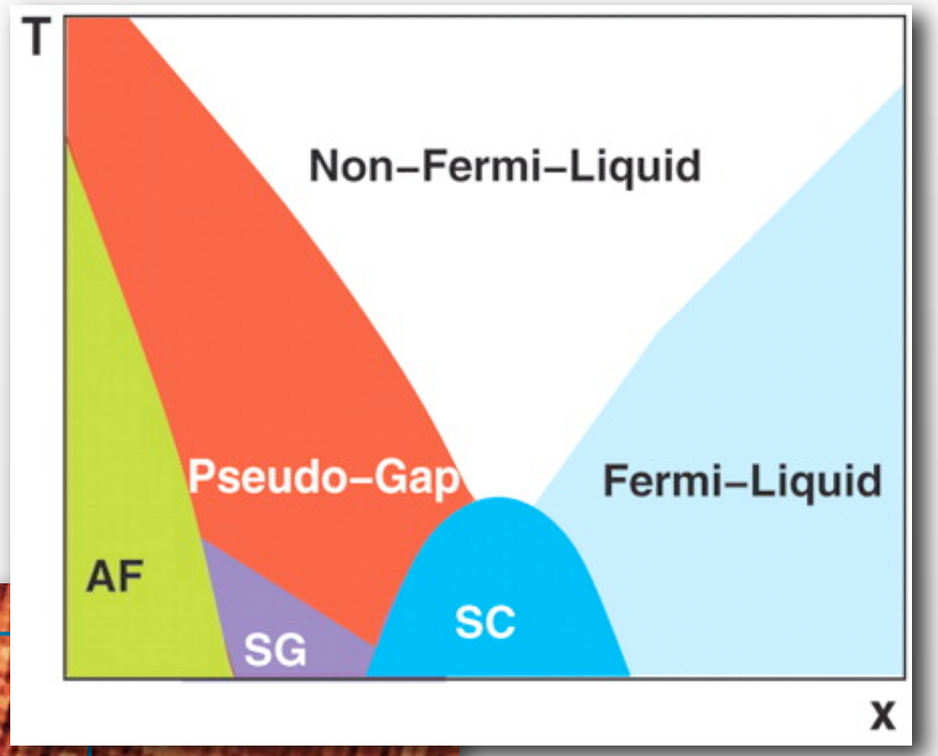
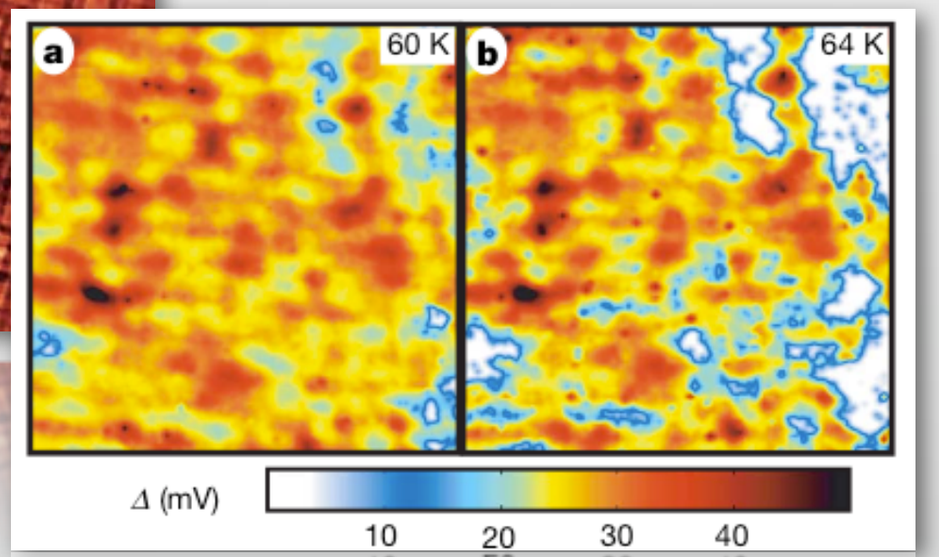
HTSC cuprates

- <U> ≈ <T>
- Competing states
- Rich phase diagram
- Nanoscale inhomogeneities
- Superconductivity



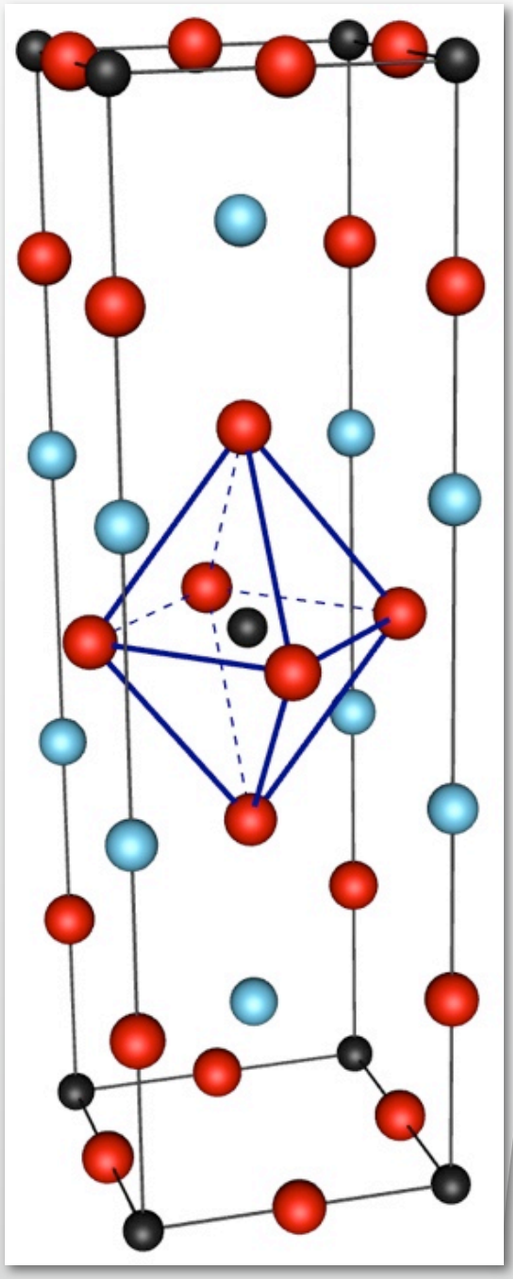




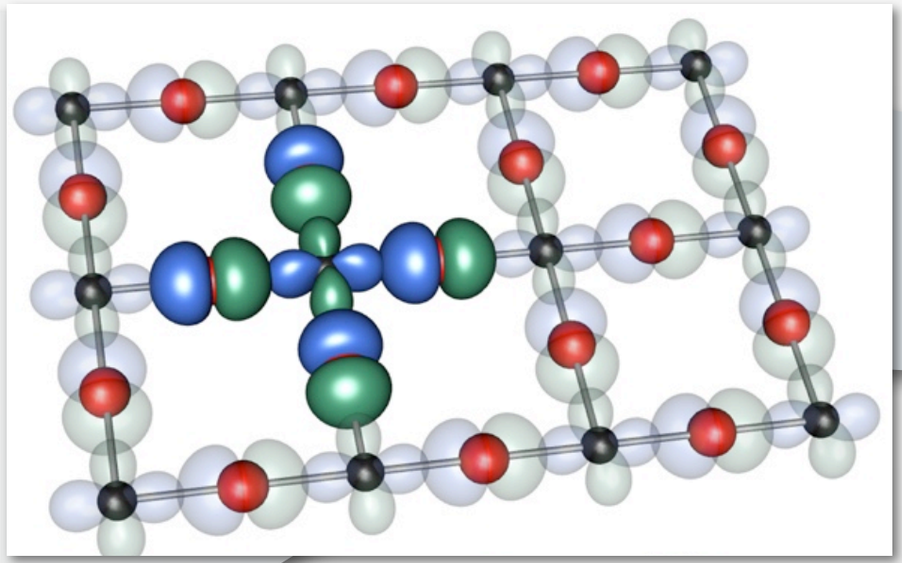


2D Hubbard Model for Cuprates

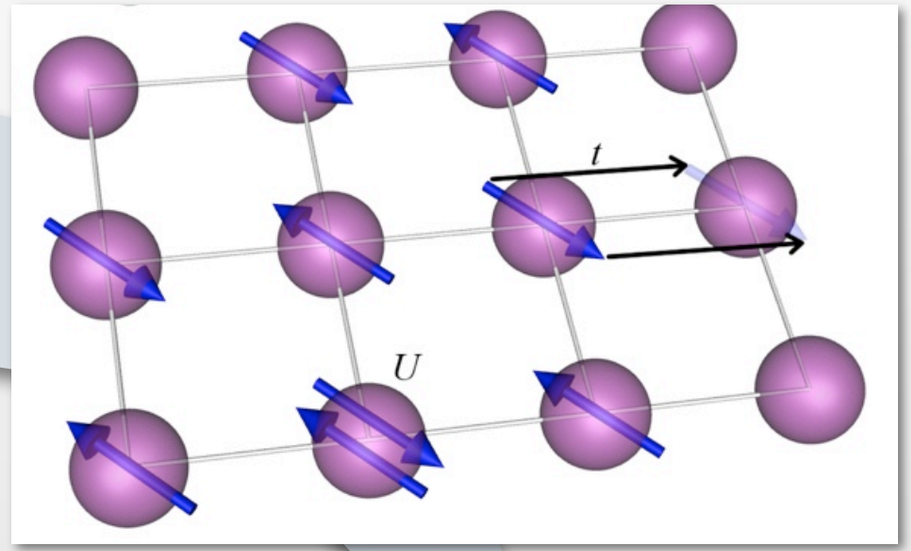
Cuprate structure



CuO-planes



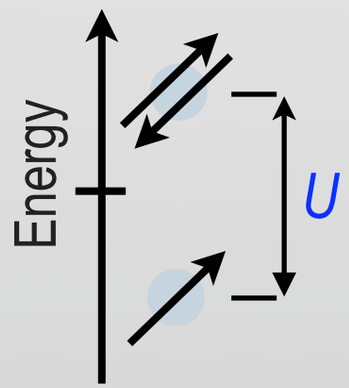
2D Hubbard Model



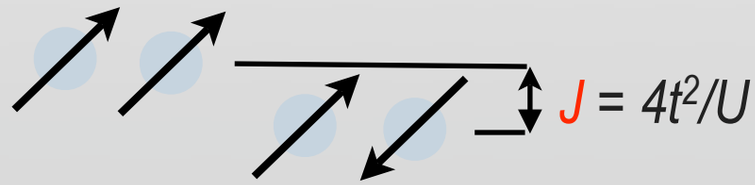
$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Basic properties:

- Moment formation



- Antiferromagnetic exchange



Cuprate Superconductivity = Multi-Scale Problem

Atomic scale

- Strong local correlations
- Moment formation

~ nm

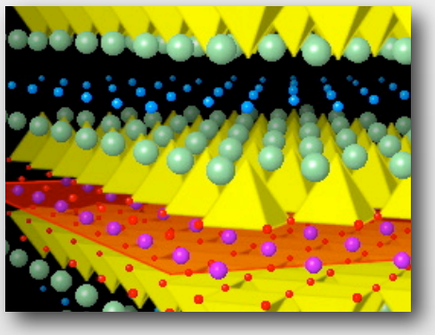
Nano-scale

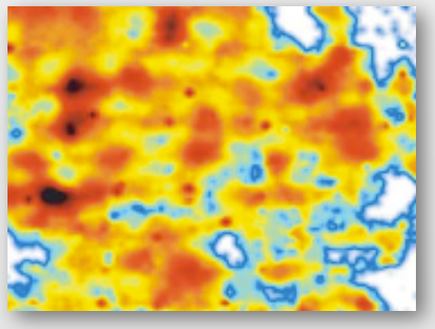
- Antiferromagnetic correlations
- Cooper pairs
- Inhomogeneities

~ µm

Macro-scale

- Macroscopic quantum effects





Theory:

Atomistic description → Complexity ~ 4^N

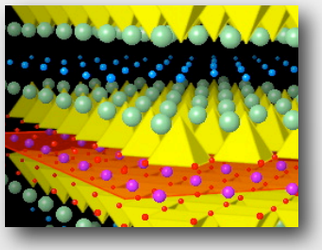
Thermodynamics Continuum description → $N \sim 10^{23}$

Quantum Cluster Theories

Quantum cluster theories:
Maier, Jarrell, Pruschke & Hettler, RMP '05

Atomic scale

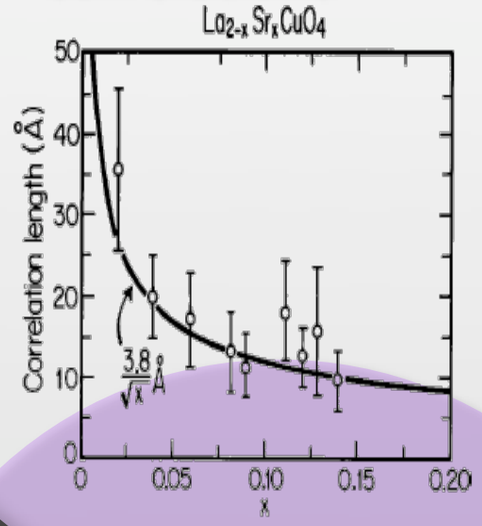
- Strong local correlations
- Moment formation



~ nm

Nano-scale

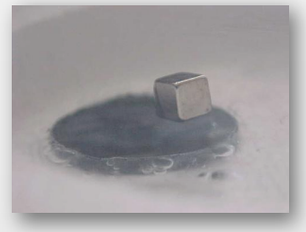
- Antiferromagnetic correlations



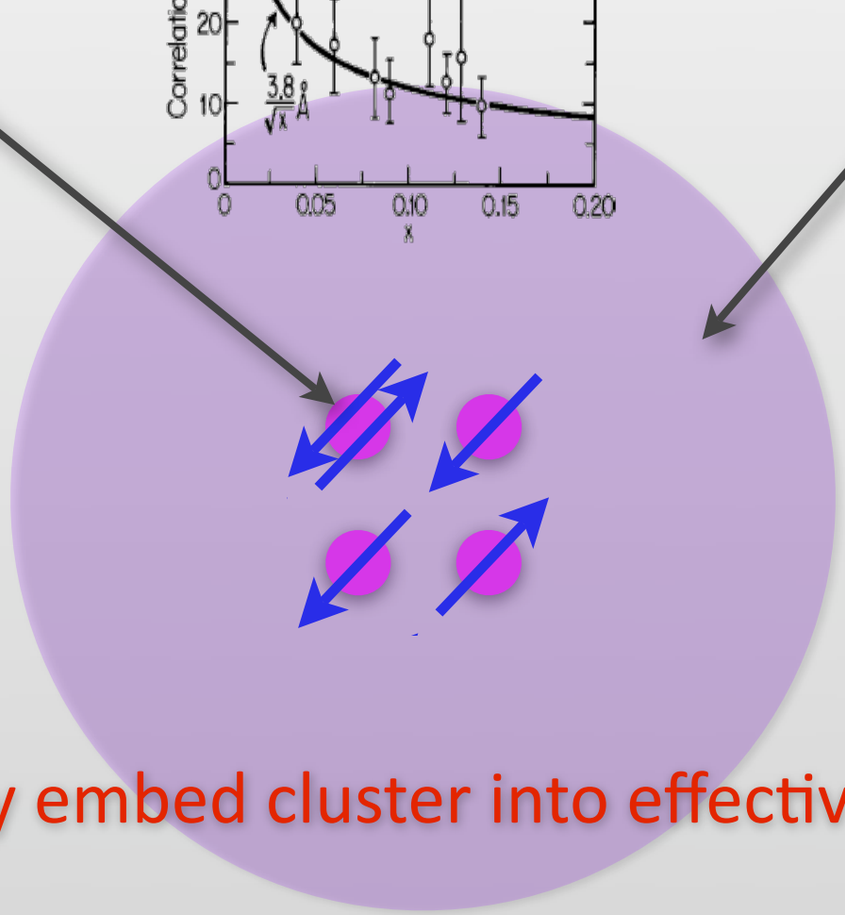
~ µm

Macro-scale

- Macroscopic quantum effects



Explicitly treat correlations within a localized cluster

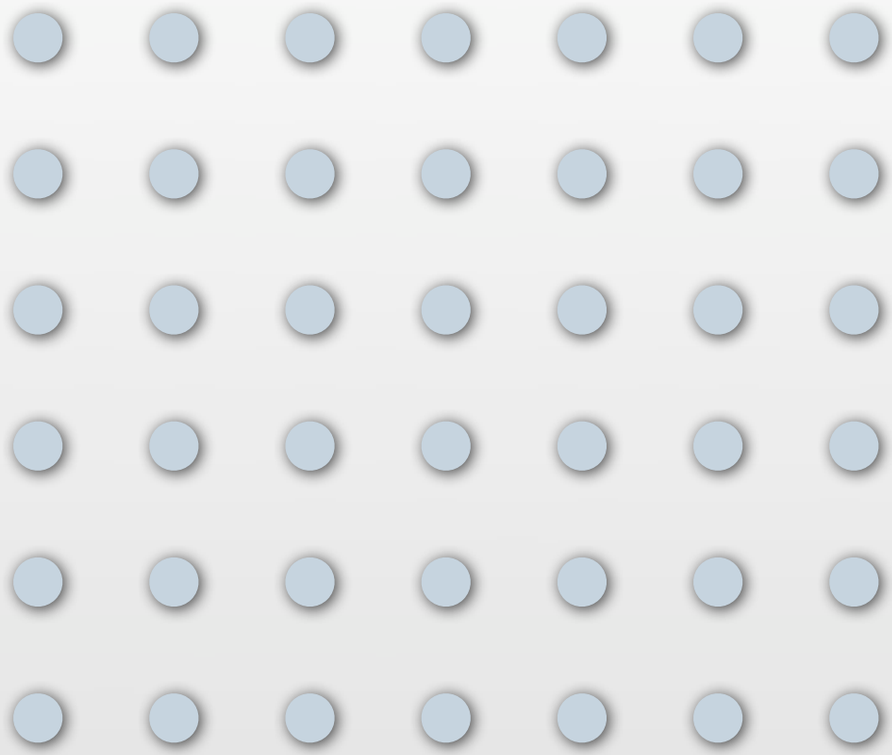


Treat macroscopic scales within mean-field

Coherently embed cluster into effective medium

Dynamic cluster approximation: Coarse-graining the reciprocal space

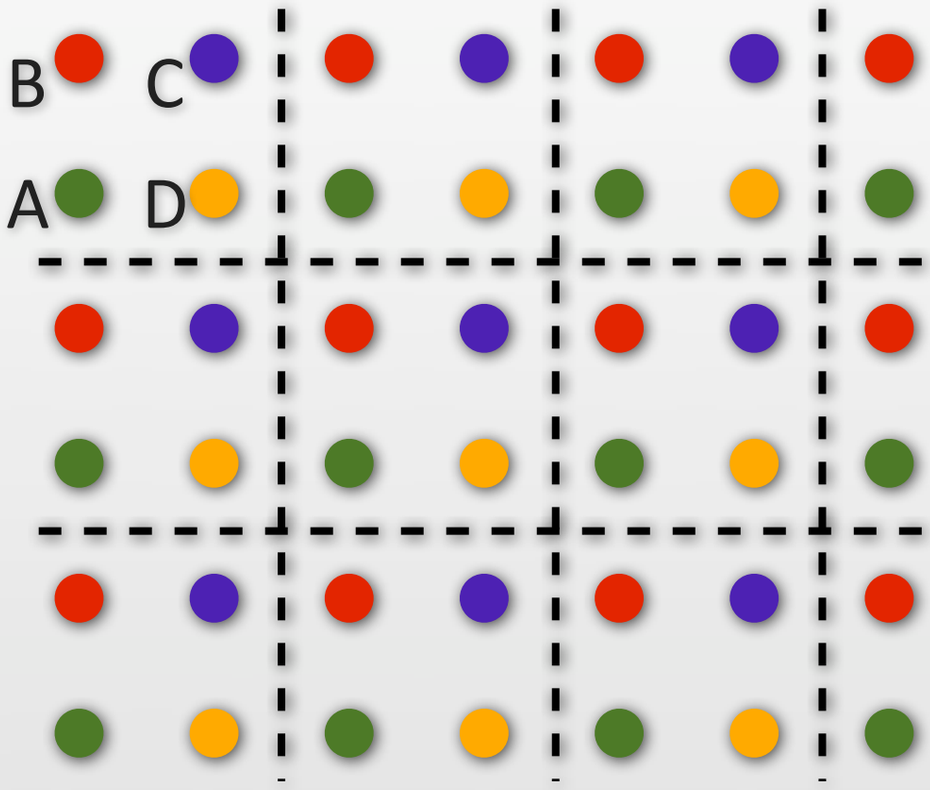
Hettler *et al.*, PRB '98



Dynamic cluster approximation: Coarse-graining the reciprocal space

Hettler *et al.*, PRB '98

Split lattice into clusters/sublattices



Dynamic cluster approximation: Coarse-graining the reciprocal space

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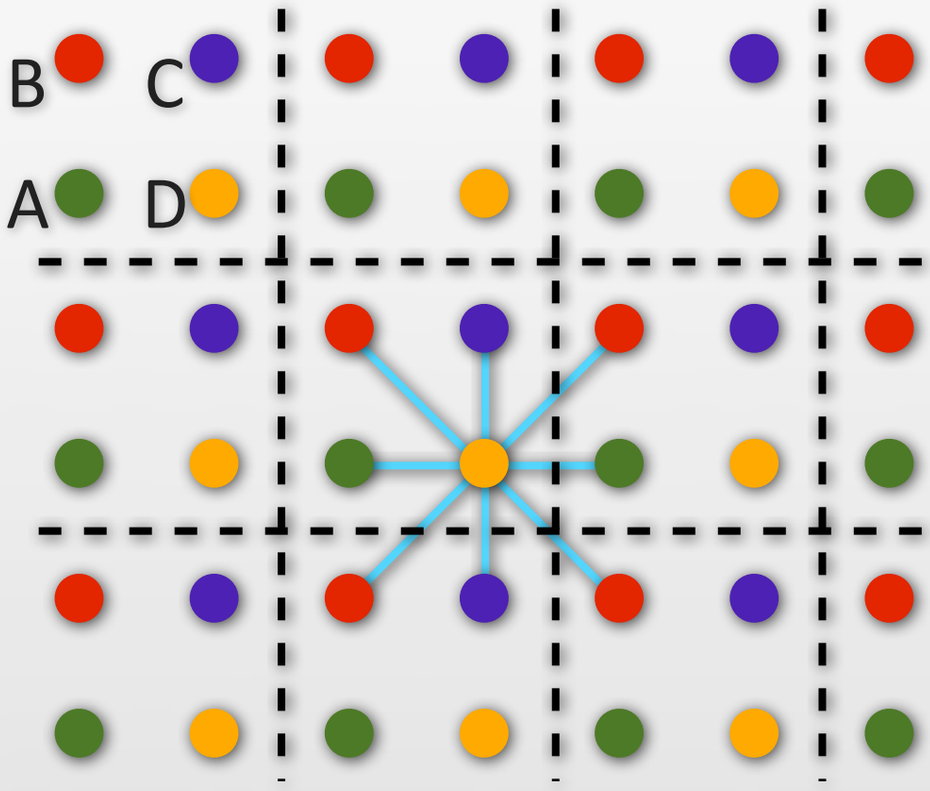

Self-energy finite between nn sites on different sublattices

Dynamic cluster approximation: Coarse-graining the reciprocal space

Hettler *et al.*, PRB '98

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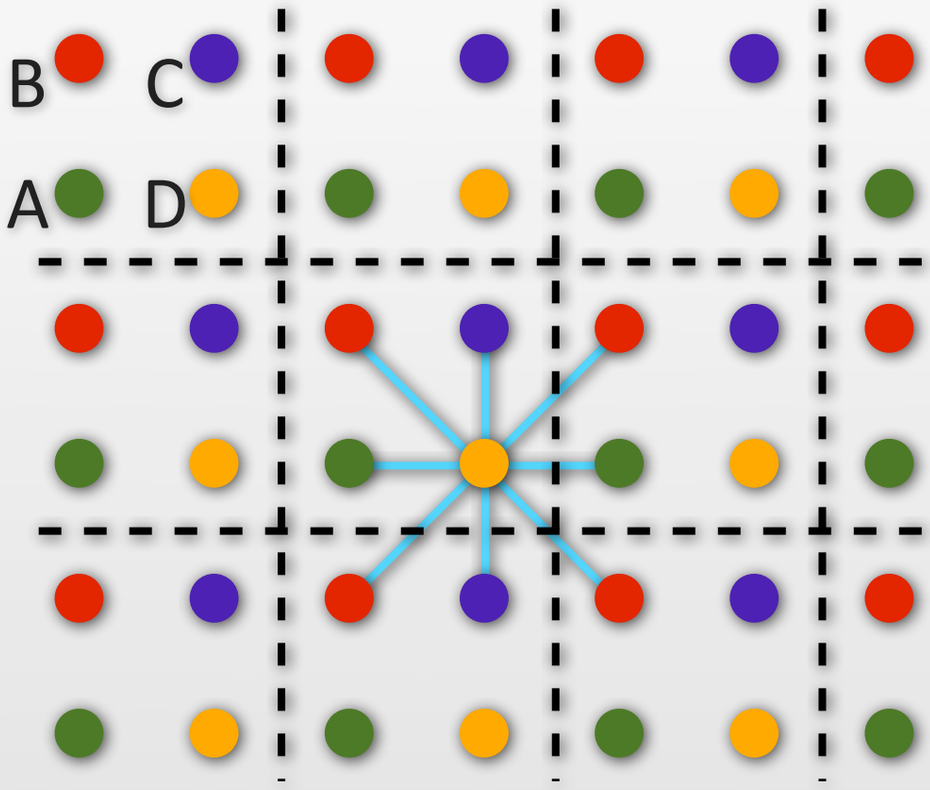
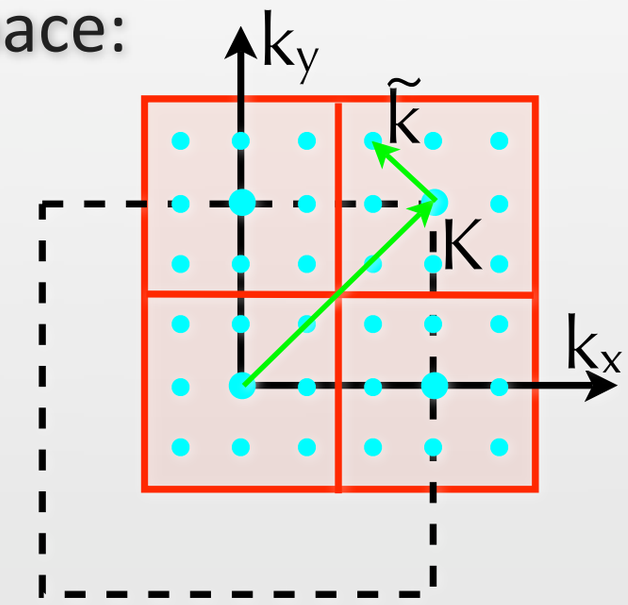


Self-energy finite between nn sites on different sublattices

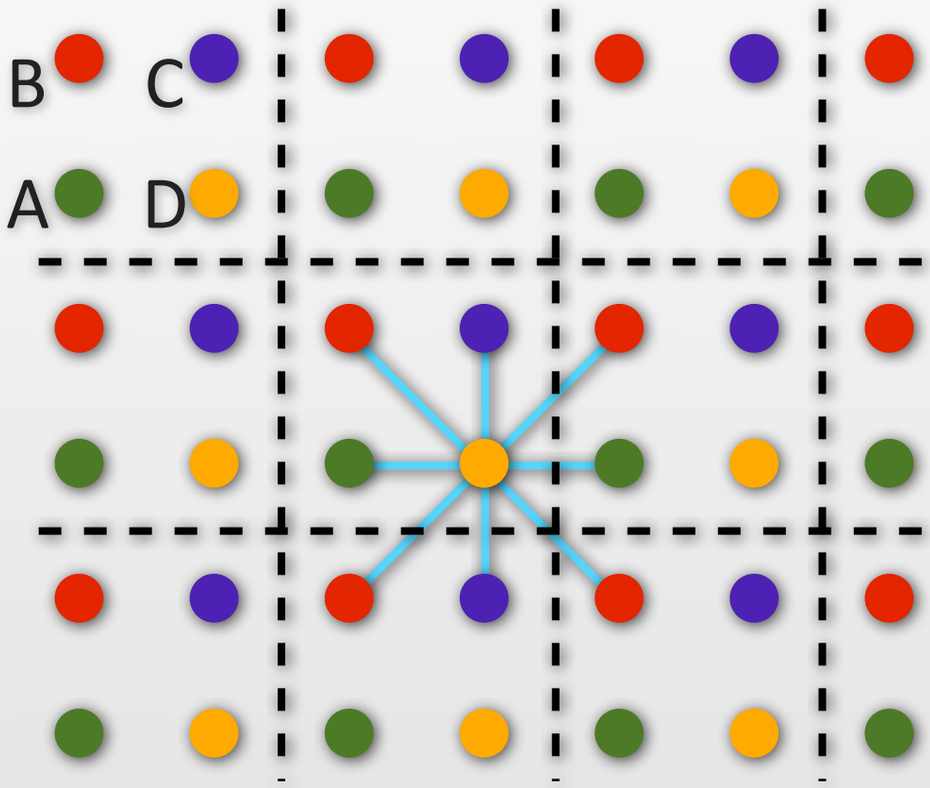
→ In reciprocal space:



Dynamic cluster approximation: Coarse-graining the reciprocal space

Hettler *et al.*, PRB '98

Split lattice into clusters/sublattices



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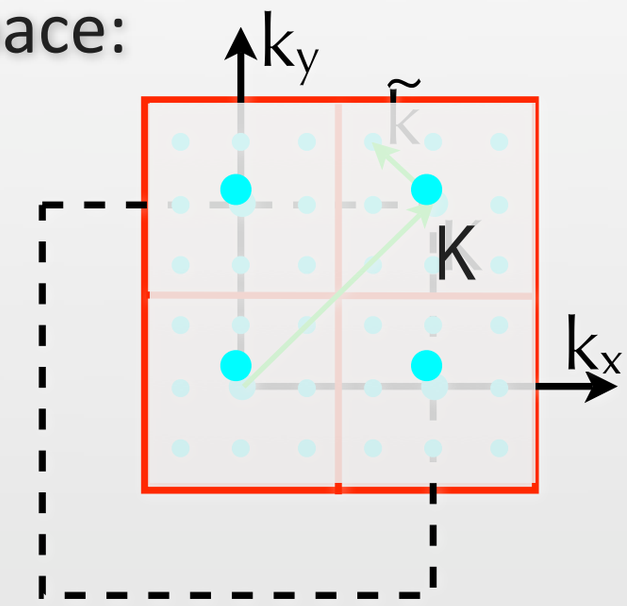


$$\Sigma(k,z) \approx \Sigma(K,z)$$

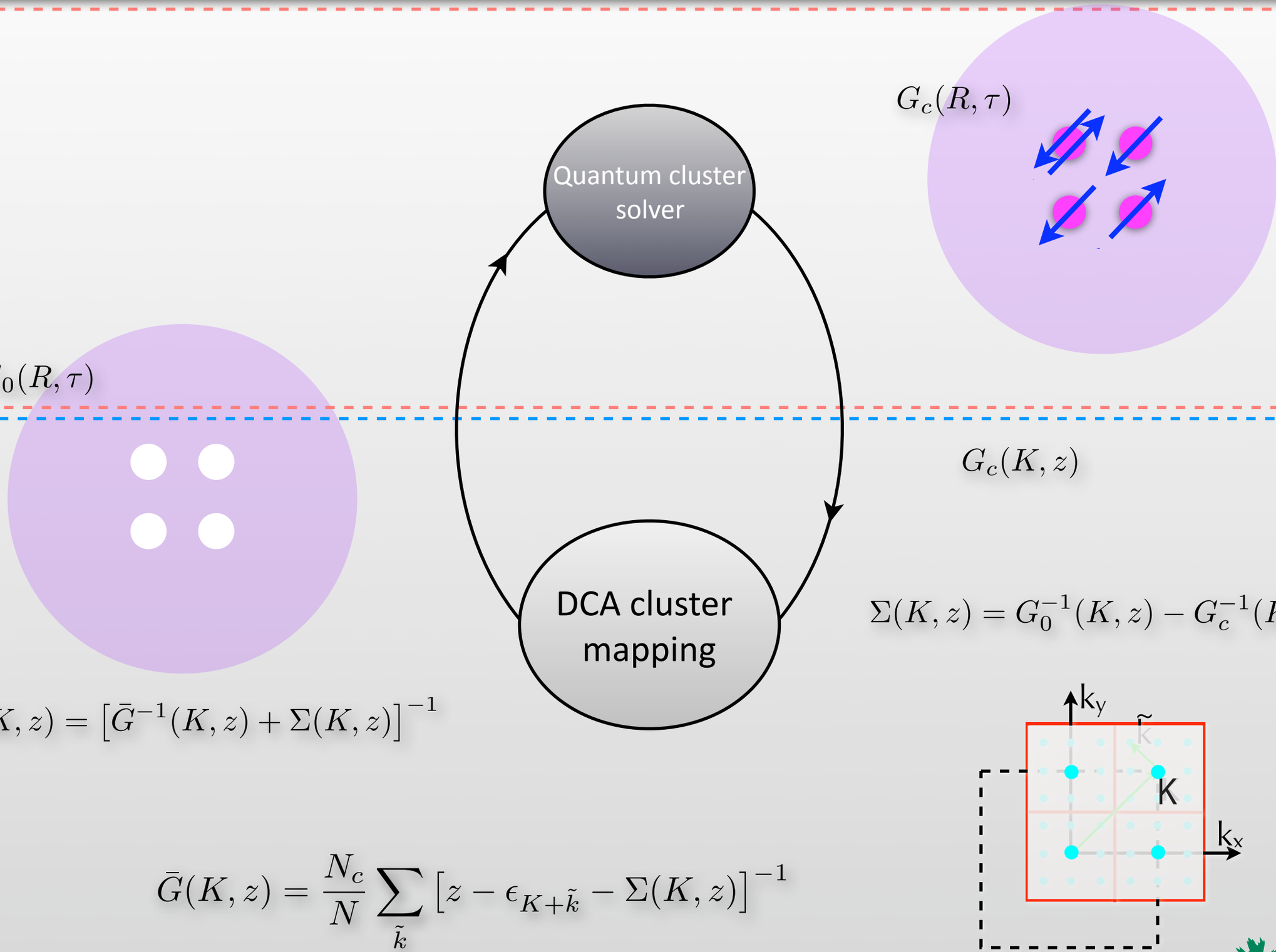
calculate Σ on coarse-grid: $\Sigma(K,z) = \mathcal{F}[\bar{G}(K,z)]$

coarse-grained propagator:

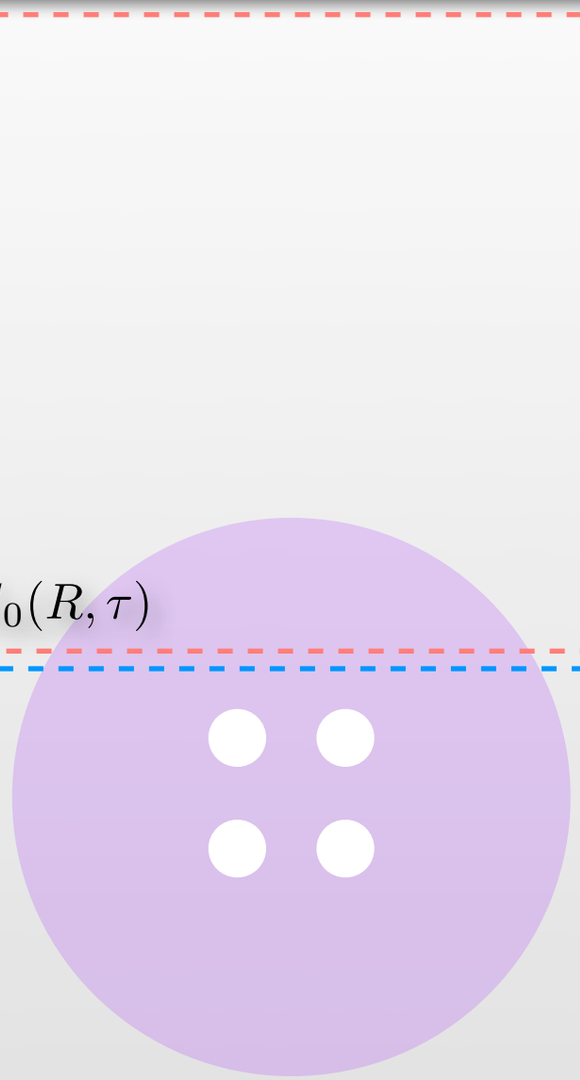
$$\bar{G}(K,z) = \frac{N_c}{N}\sum_{\tilde{k}} G(K+\tilde{k},z) = \frac{N_c}{N}\sum_{\tilde{k}} \frac{1}{z-\epsilon_{K+\tilde{k}}-\Sigma(K,z)}$$

→ Cluster with periodic BC embedded in mean-field host

DCA self-consistent cluster mapping and cluster solver



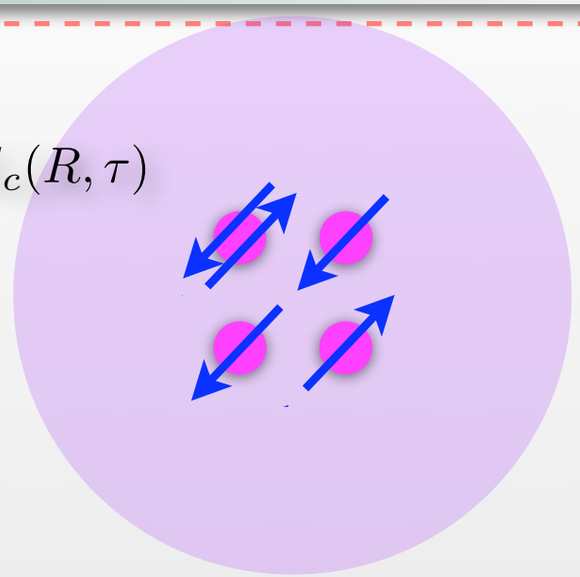
DCA self-consistent cluster mapping and cluster solver



$G_0(R,\tau)$

Quantum cluster solver

DCA cluster mapping



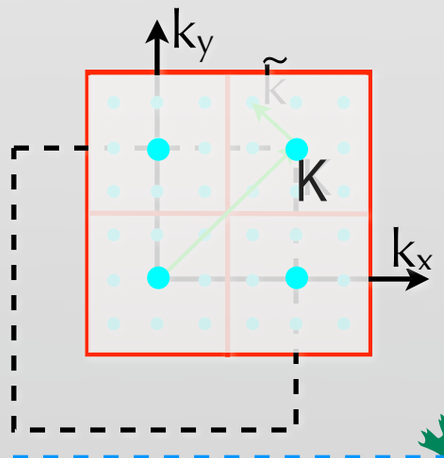
$G_c(R,\tau)$

$G_c(K,z)$

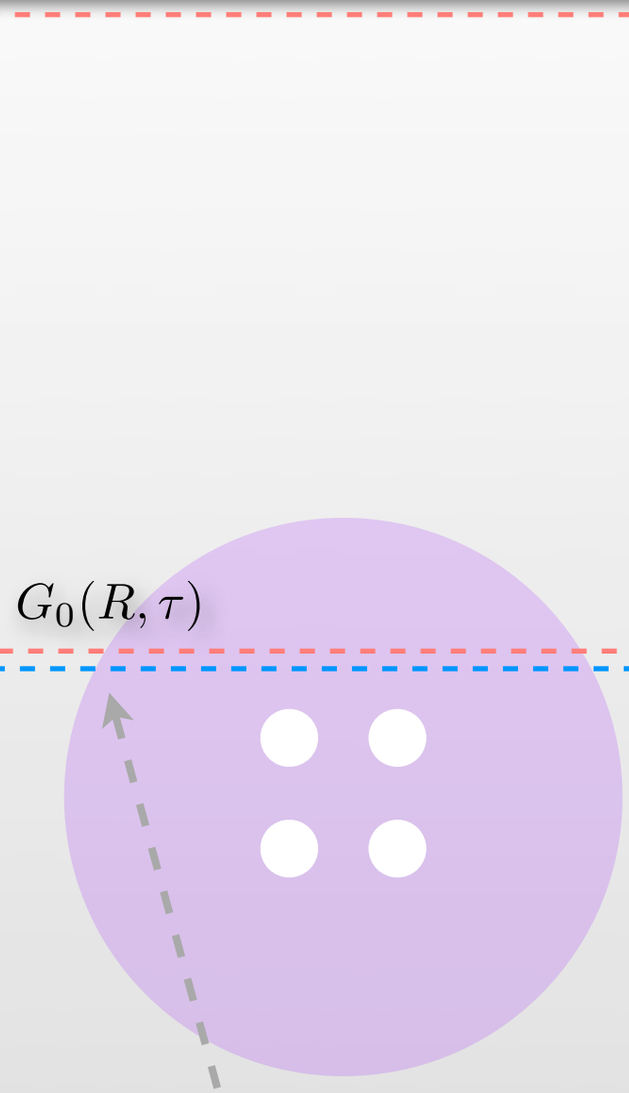
$$\Sigma(K,z) = G_0^{-1}(K,z) - G_c^{-1}(K,z)$$

$$G_0(K,z) = \left[\bar{G}^{-1}(K,z) + \Sigma(K,z)\right]^{-1}$$

$$\bar{G}(K,z) = \frac{N_c}{N}\sum_{\tilde{k}}\left[z - \epsilon_{K+\tilde{k}} - \Sigma(K,z)\right]^{-1}$$



DCA self-consistent cluster mapping and cluster solver



$G_0(R,\tau)$

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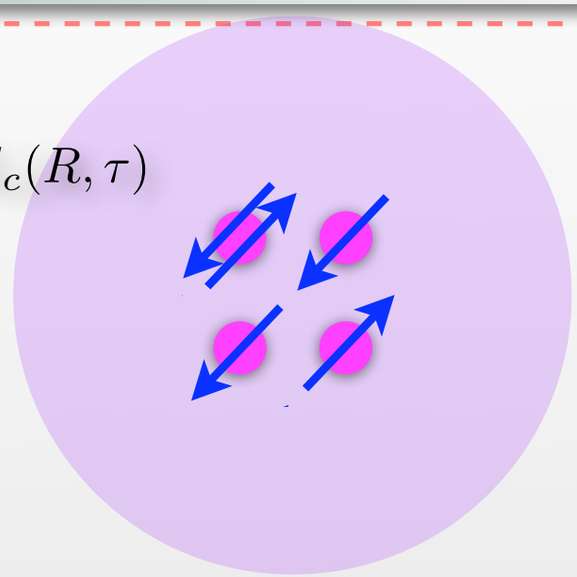
Quantum cluster solver

DCA cluster mapping



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$G_c(K,z)$

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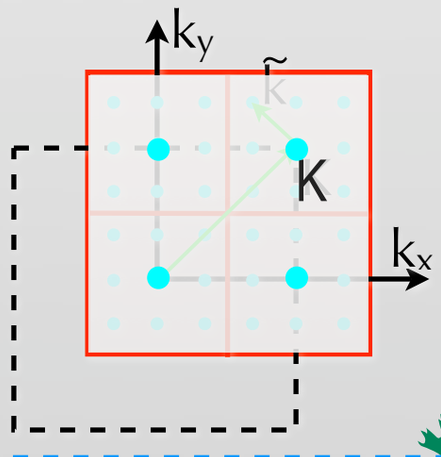
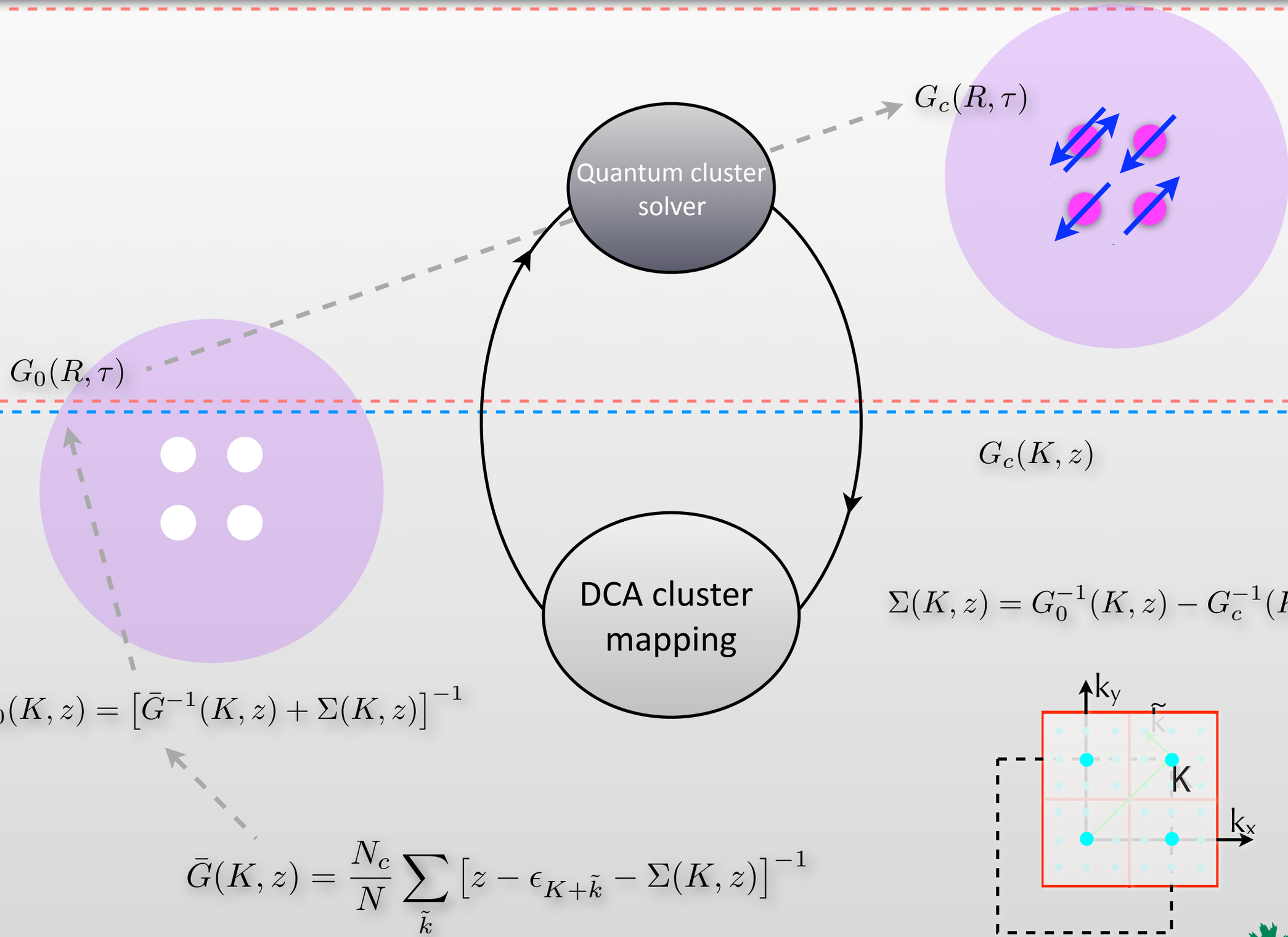


DCA self-consistent cluster mapping and cluster solver



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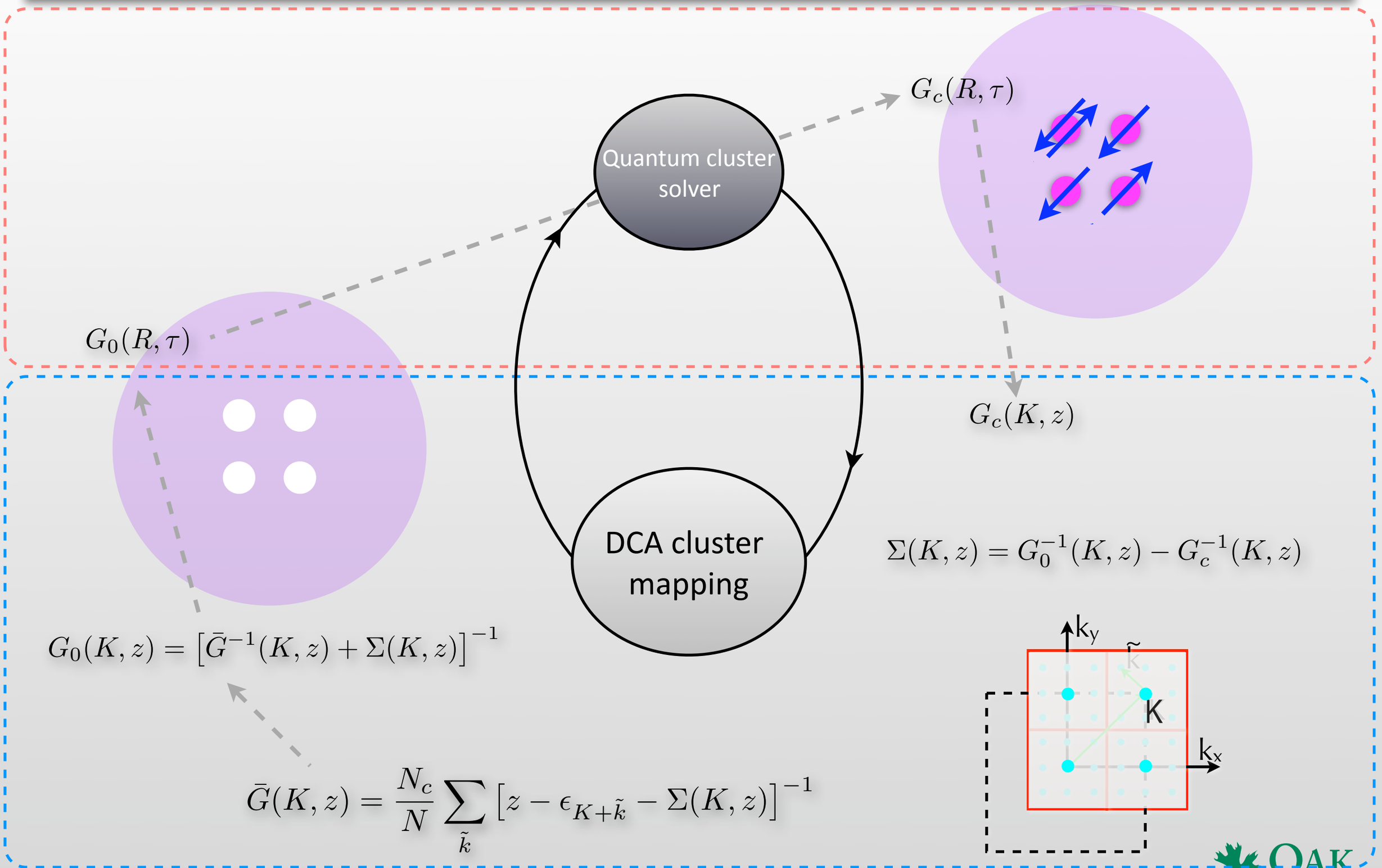

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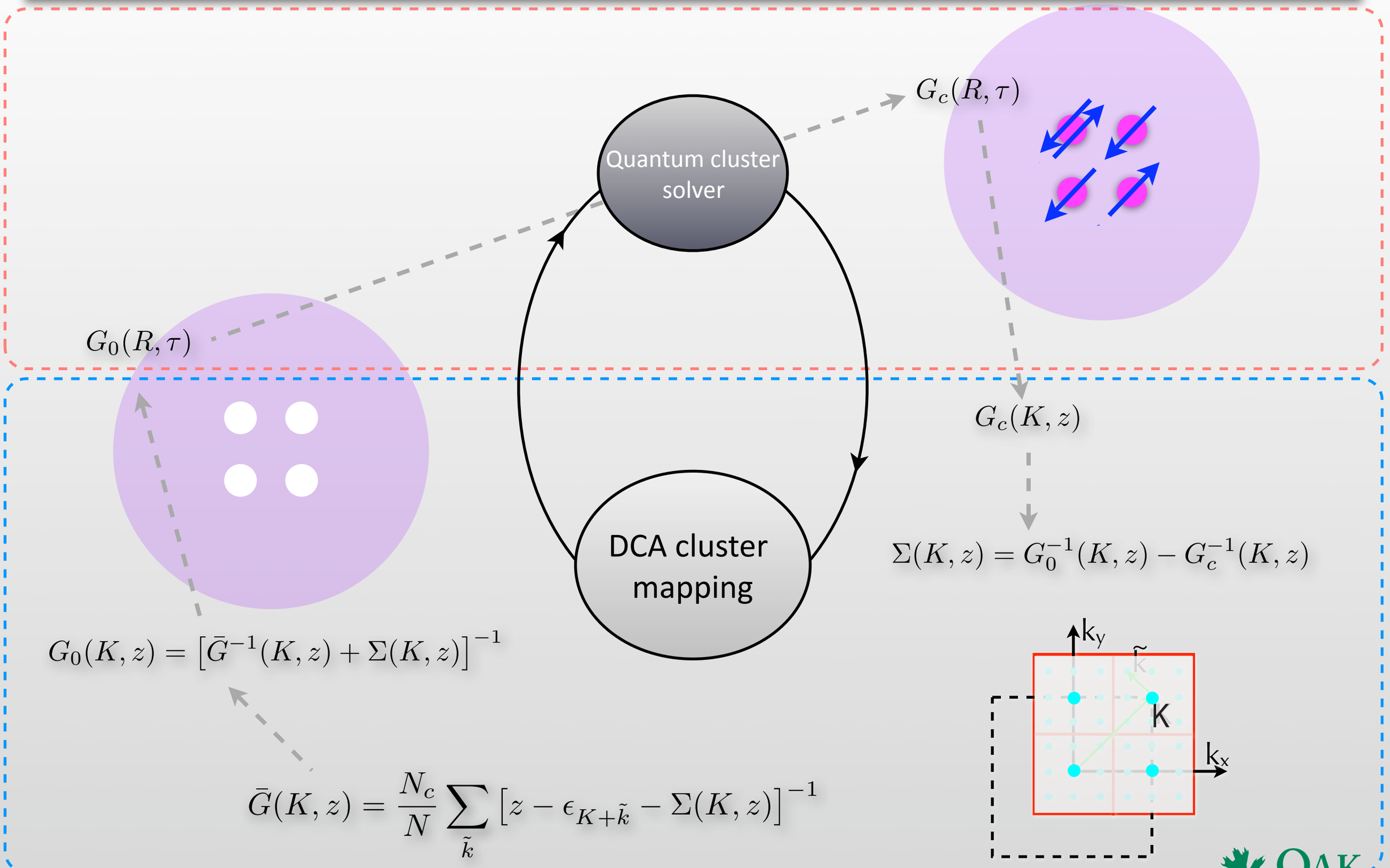

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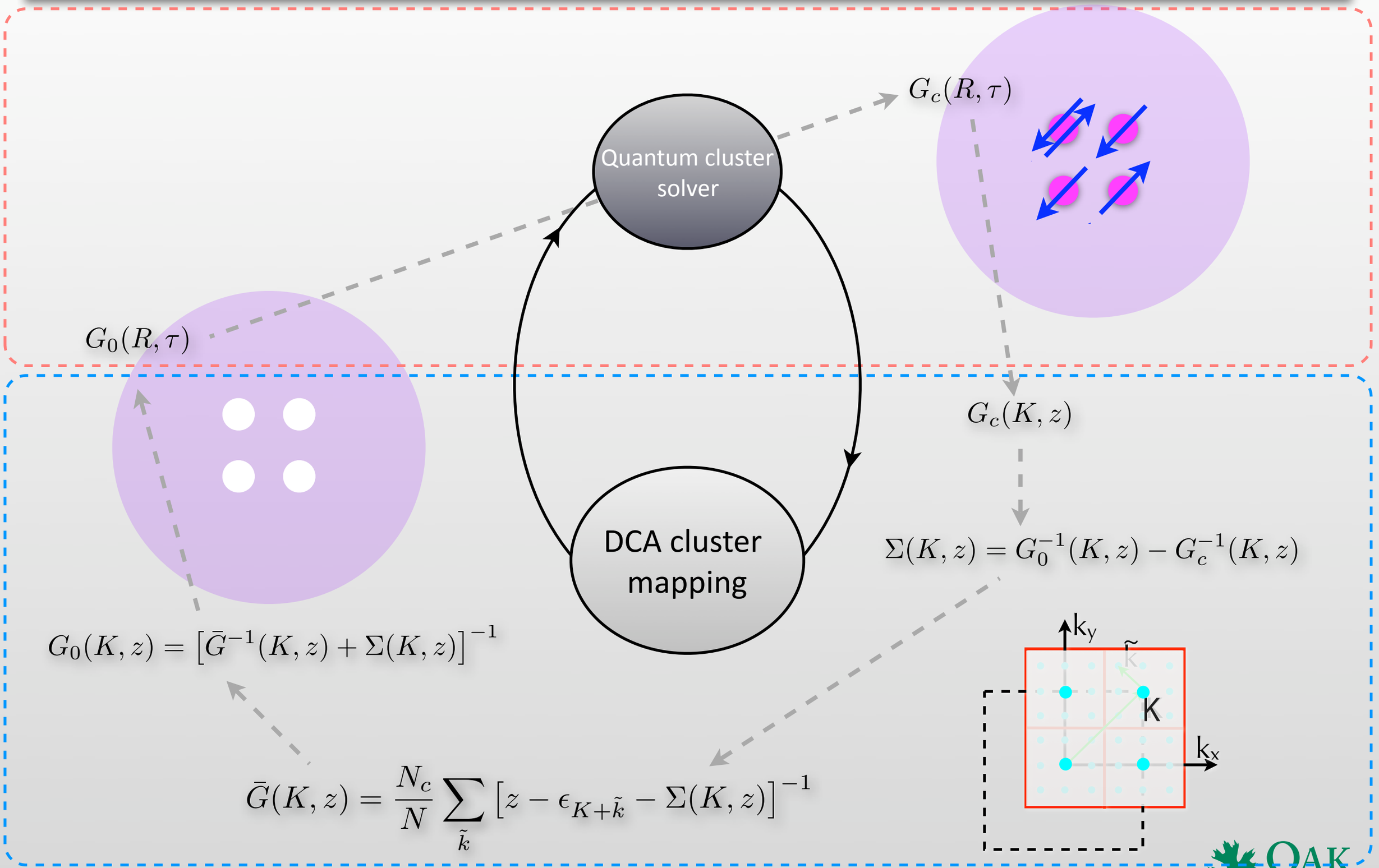


DCA: Some properties

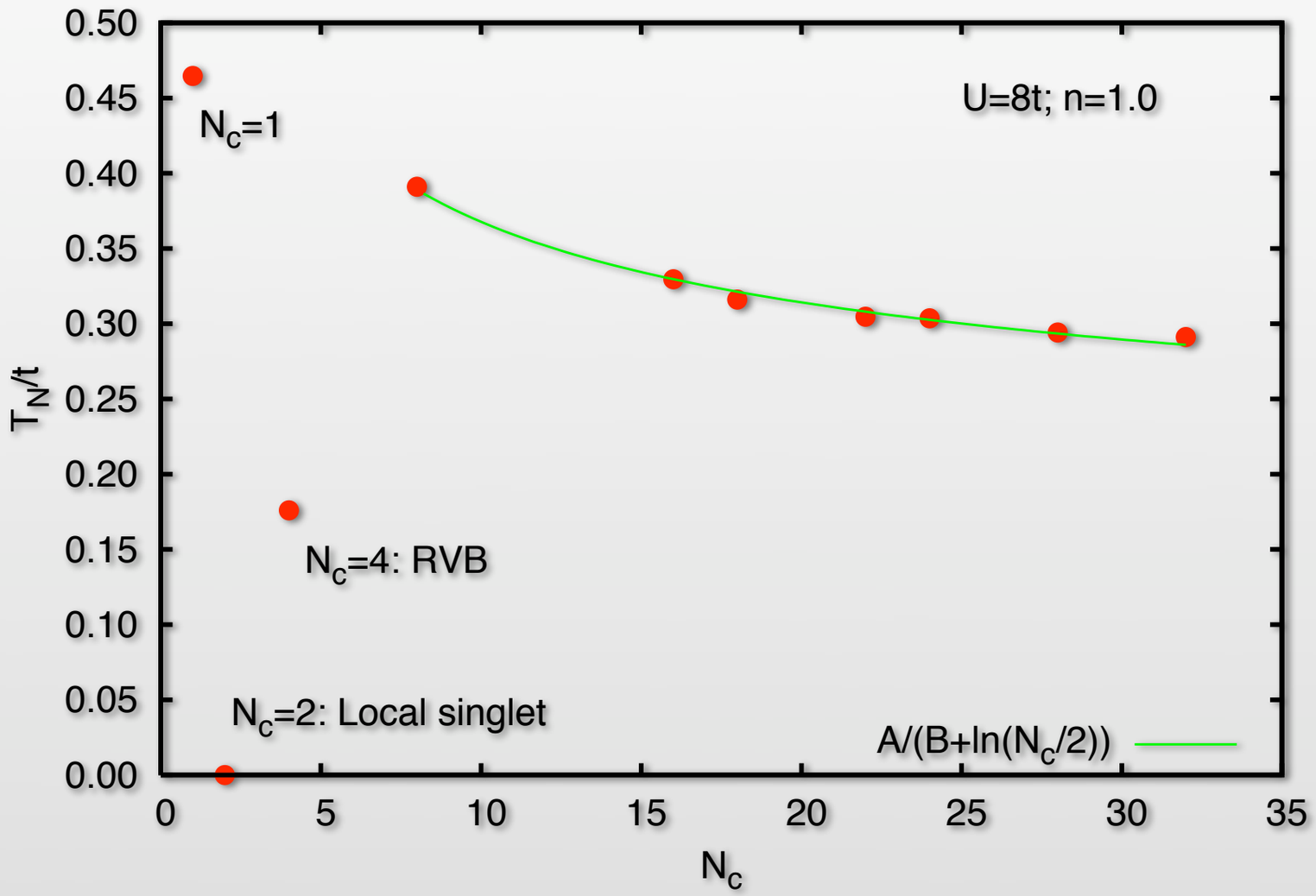
Basic approximation:

- Treats spatial correlations beyond cluster size in a mean-field
- Completely retains temporal fluctuations
- Non-perturbative!

Consequences:

- Can describe broken symmetry phases
- Transitions are mean-field (mean-field exponents etc.)
- Transition occurs when correlation length exceeds cluster size (finite size scaling)
- Systematic improvements by increasing cluster size

Antiferromagnetism in half-filled 2D Hubbard model



Scaling ansatz:

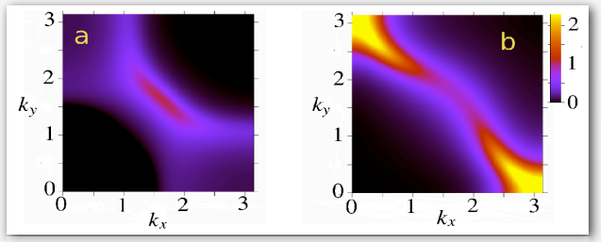
$$\xi(T_N) = L_c$$

$$\xi(T) \propto e^{A/T}$$

$$\rightarrow \quad T_N \sim \frac{A}{B + \ln(N_c)/2}$$

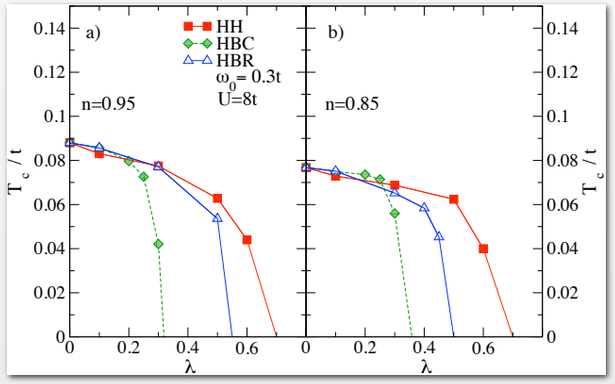
Overview of DCA calculations for 2D Hubbard model

Pseudogap



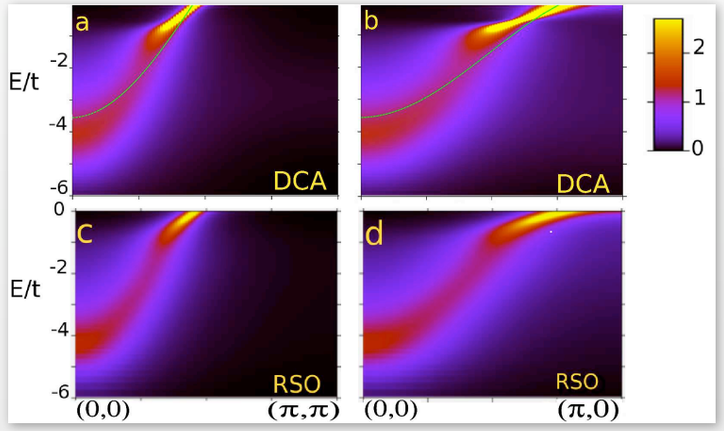
Maier *et al.*, EPJ B 13 '00
Huscroft *et al.*, PRL 86 '01
Macridin *et al.*, PRL 97 '06

Phonons



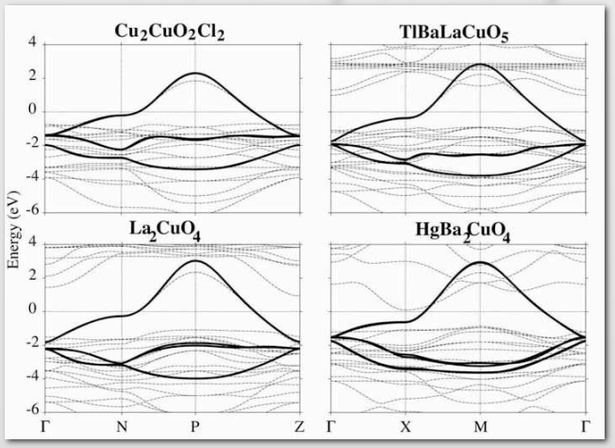
Macridin *et al.*, PRL 97 '06

High-energy kink/Waterfall



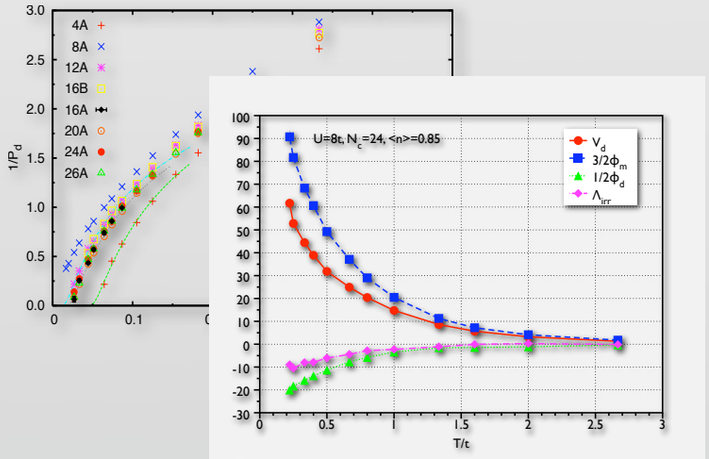
Macridin *et al.*, PRL 76 '07

Material specificity



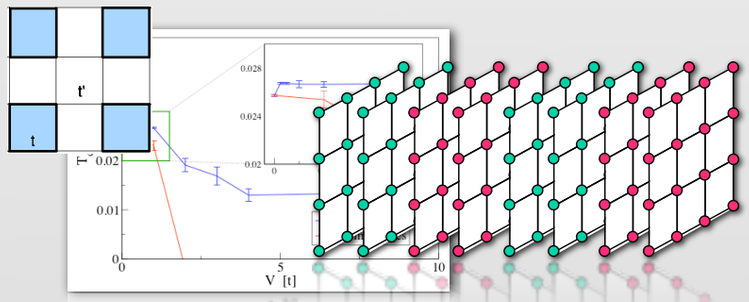
Macridin *et al.*, PRB 71 '05
Kent *et al.*, PRB 78 '08
Wang *et al.*, preprint '08

Superconductivity & pairing mechanism



Maier *et al.*, many papers

Inhomogeneities/disorder



Doluweera *et al.*, PRB 78 '08
Kemper *et al.*, preprint '08
Okamoto & Maier, PRL 101 '08

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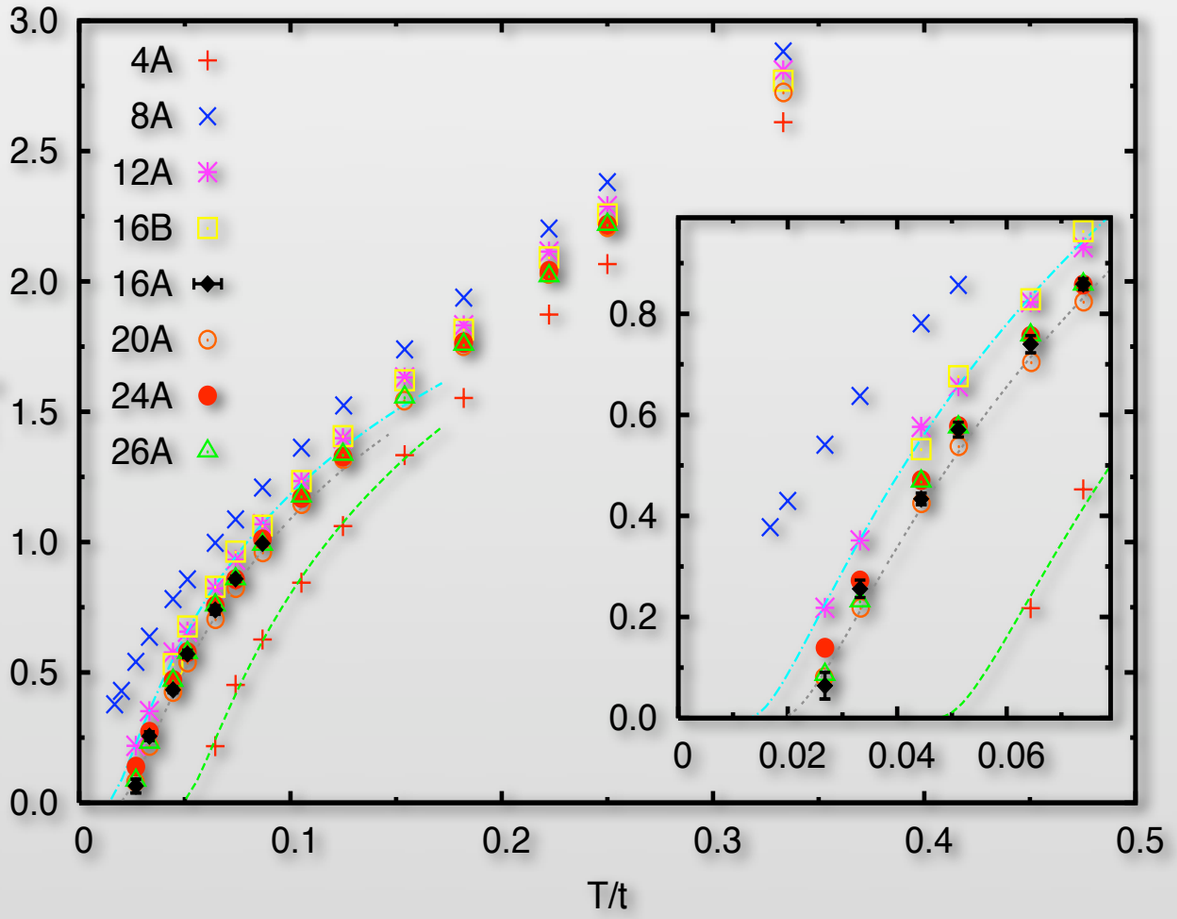
Overview of DCA calculations for 2D Hubbard model

Superconductivity in 2D Hubbard Model

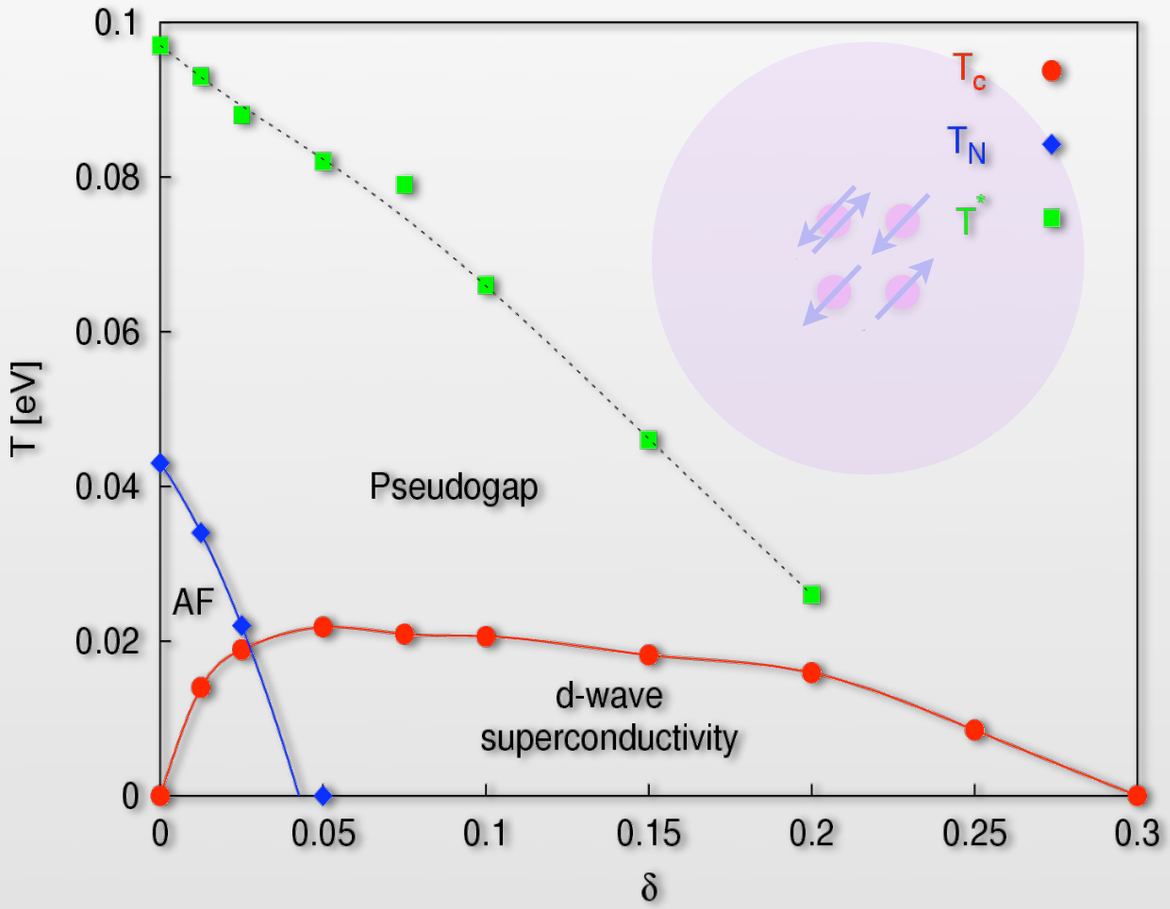
d-wave pair-field susceptibility

$P_d = \int_0^\beta d\tau \langle \Delta_d(\tau) \Delta_d^\dagger(0) \rangle$ diverges in large clusters



Maier, Jarrell, Schulthess, Kent & White, PRL '05

Jarrell, Maier *et al.*, EPL '01



4-site cluster: Rich phase diagram with competing phases including antiferromagnetism, pseudogap and superconductivity

Pairing matrix formalism

- Bethe-Salpeter equation for pair-field susceptibility

$$\begin{aligned} P &= \chi_0^{pp} + \Gamma^{pp}\chi_0^{pp}P \\ &= \chi_0^{pp}[1 - \Gamma^{pp}\chi_0^{pp}]^{-1} \end{aligned}$$

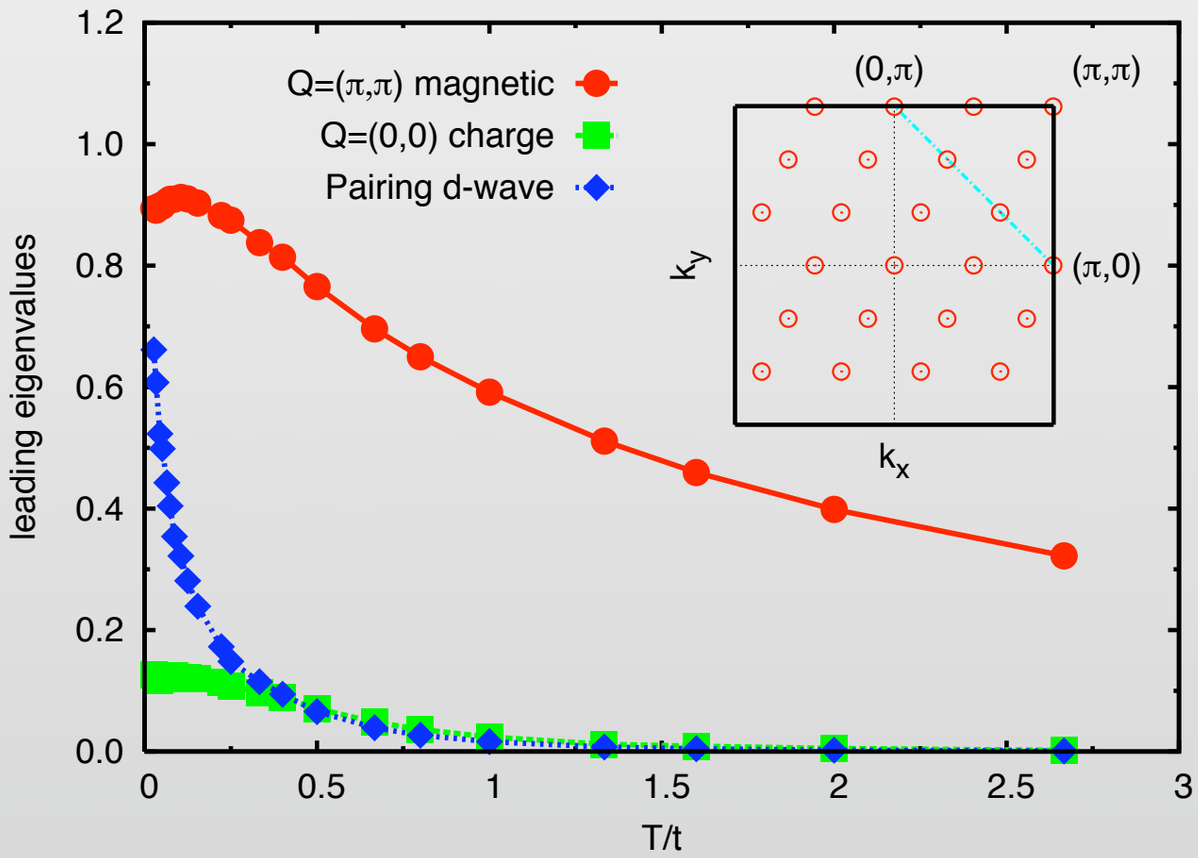
- Instead of calculating *P*, calculate eigenvalues and eigenvectors of

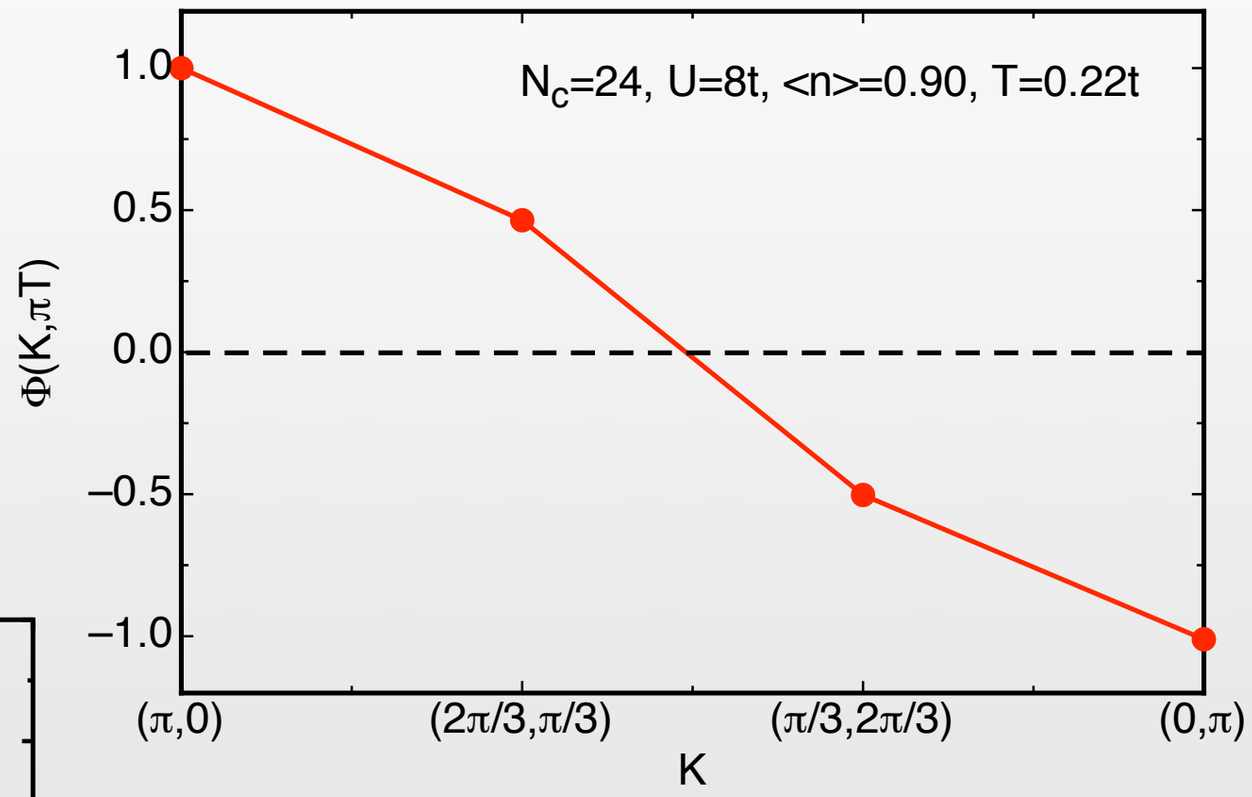
$$-\frac{T}{N_c}\sum_K \Gamma^{pp}(K,K')\chi_0^{pp}(K')\Phi_\alpha(K') = \lambda_\alpha\Phi_\alpha(K)$$

- *P* diverges when leading eigenvalue λ_α becomes one
- Symmetry of superconducting state is given by $K=(K,\omega_n)$ dependence of $\phi_\alpha(K)$

Leading eigenvalue and eigenvector

- *U=4t, <n> = 0.85, N_c=24*
- AF correlations dominate
- Leading particle-particle eigenvalue corresponds to d-wave singlet





d-wave harmonics:

$$d_i = \sum_k g_i(k)\Phi_d(k,\pi T)$$

$$g_1(k) = \cos k_x - \cos k_y$$

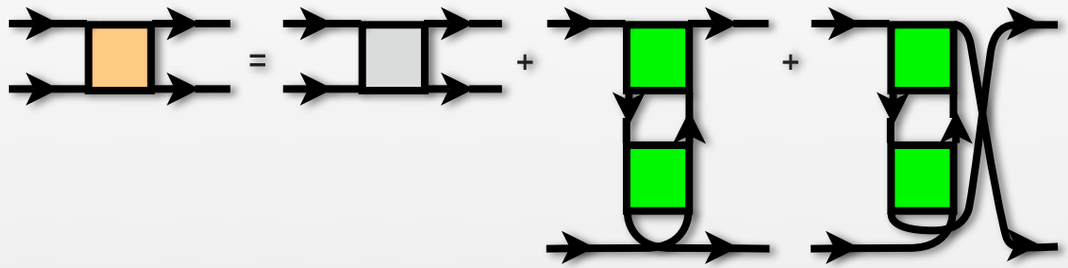
$$g_2(k) = \cos 2k_x - \cos 2k_y$$

U/t	d_2/d_1
4	0.064
6	0.128
8	0.157

TAM *et al.*, PRL '06

Pairing mechanism

- Analyze particle-particle vertex



Maier *et al.*, PRL '06, PRB '06, Physica C '07

- Spin susceptiblity representation of the pairing interaction

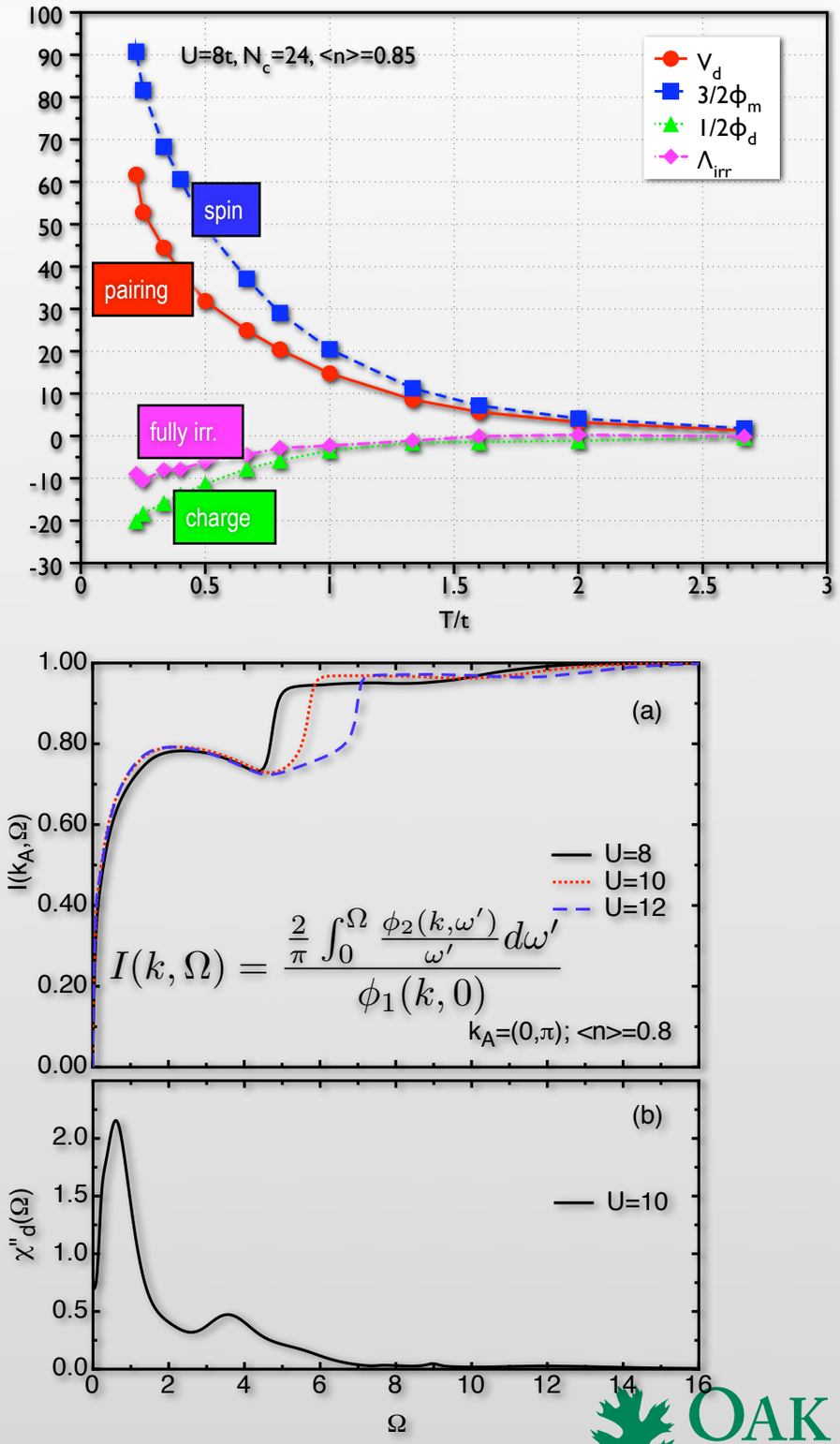
$$V_d(k,k',\omega,\omega') \approx \frac{3}{2}\bar{U}^2\chi(k-k',\omega-\omega')$$

Maier *et al.*, PRB '07 x 2

- Relative importance of spin fluctuations and RVB mechanism

$$\begin{aligned} V_d &\approx \frac{3}{2}\bar{U}^2\chi(k-k',\omega-\omega') \\ &- \bar{J}(\cos k_x - \cos k_y)(\cos k'_x - \cos k'_y) \end{aligned}$$

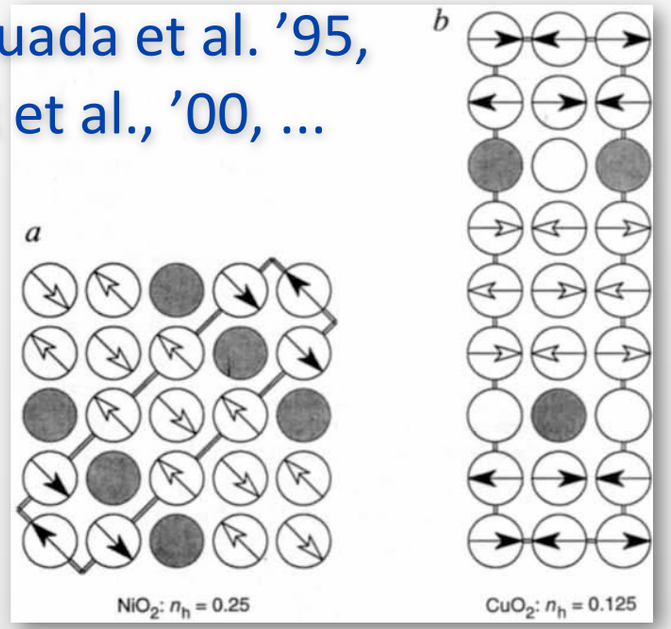
Maier *et al.*, PRL '08



Nanoscale inhomogeneities in cuprates

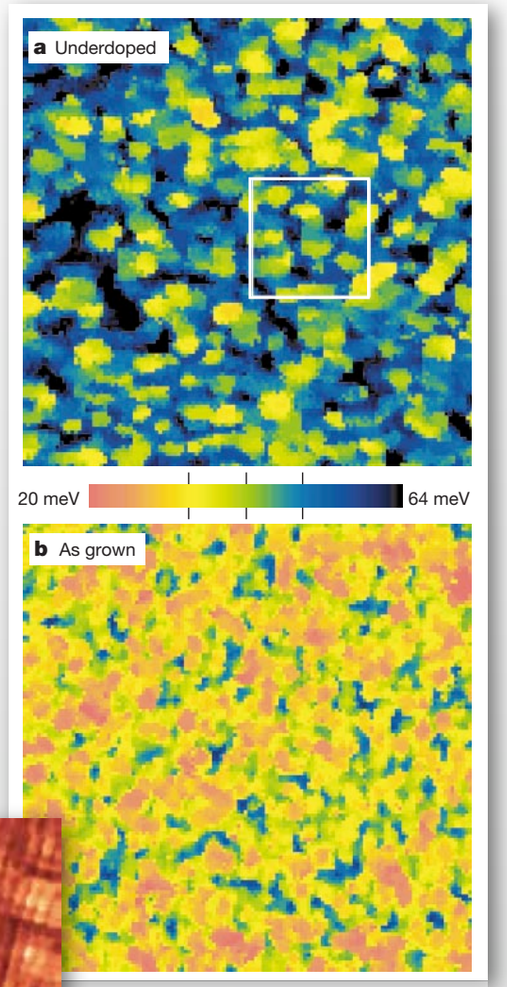
Stripes in neutron scattering:

Tranquada et al. ’95,
Mook et al., ’00, ...



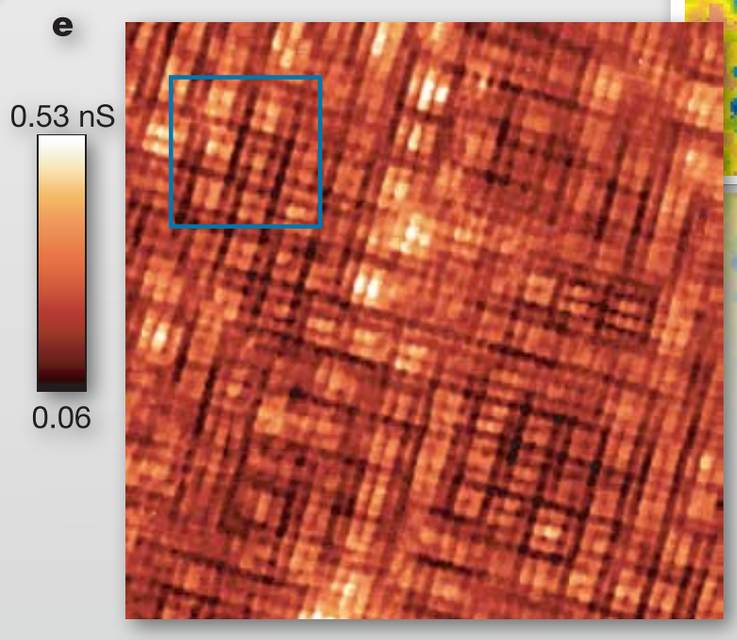
Random SC gap modulations in STM (BSCCO):

Lang et al. ‘02



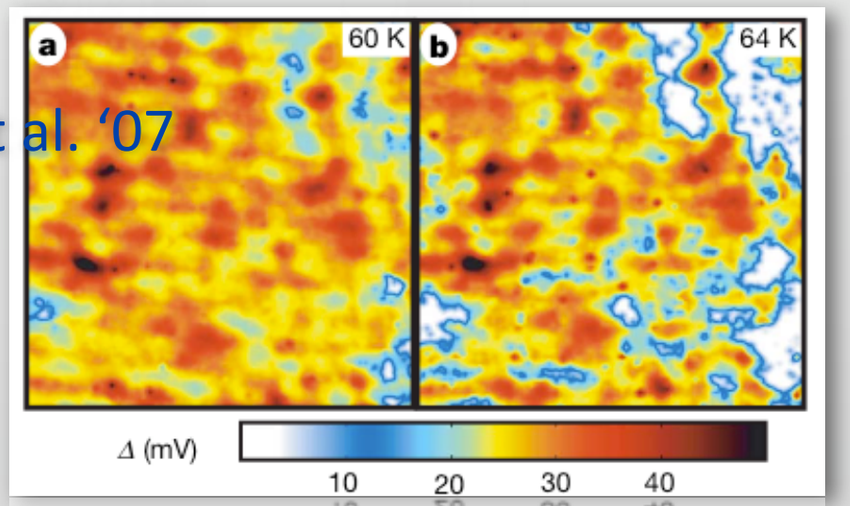
Charge ordered “checkerboard” state (Na doped cuprates):

Hanaguri et al. ‘04



Random gap modulations above T_c (BSCCO):

Gomes et al. ‘07



Hirsch-Fye quantum Monte Carlo (HF-QMC) solver

Partition function & Metropolis Monte Carlo $$Z = \int e^{-E[\mathbf{x}]/k_{\mathrm{B}}T} d\mathbf{x}$$

Acceptance criterion for M-MC move: $$\min\{1, e^{E[\mathbf{x}_k]-E[\mathbf{x}_{k+1}]}\}$$

Partition function & HF-QMC: $$Z \sim \mathrm{Tr}_{\{s_{i,l}\}} \prod_{\sigma} \det[\mathbf{G}_{c,\sigma}(\{s_{i,l}\})^{-1}]$$

Acceptance: $$\min\{1, \prod_{\sigma} \det[\mathbf{G}_{c,\sigma}(\{s_{i,l}\}_k)/\det[\mathbf{G}_{c,\sigma}(\{s_{i,l}\}_{k+1})\}$$

Update of Green's function after acceptance:

$$\mathbf{G}_{c,\sigma}(\{s_{i,l}\}_{k+1}) = \mathbf{G}_{c,\sigma}(\{s_{i,l}\}_k) + \mathbf{a}_k \times \mathbf{b}_k$$

Scaling of HF-QMC algortihm

Green's function update at step *k* after acceptance of spin flip at position p_k:

size $N_t \times N_t; \quad N_t = N_c \times N_l \sim 4000$

$$\begin{aligned} \mathbf{G}_{k+1} &= \mathbf{G}_k + \alpha_k(\mathbf{G}_k(:,p_k) - \mathbf{e}_{p_k})\mathbf{G}_k(p_k,:) \\ &= \mathbf{G}_k + \mathbf{a}_k\mathbf{b}_k^t \\ &= \mathbf{G}_0 + \mathbf{a}_0\mathbf{b}_0^t + \mathbf{a}_1\mathbf{b}_1^t + \cdots + \mathbf{a}_k\mathbf{b}_k^t \end{aligned}$$ (rank 1 update)

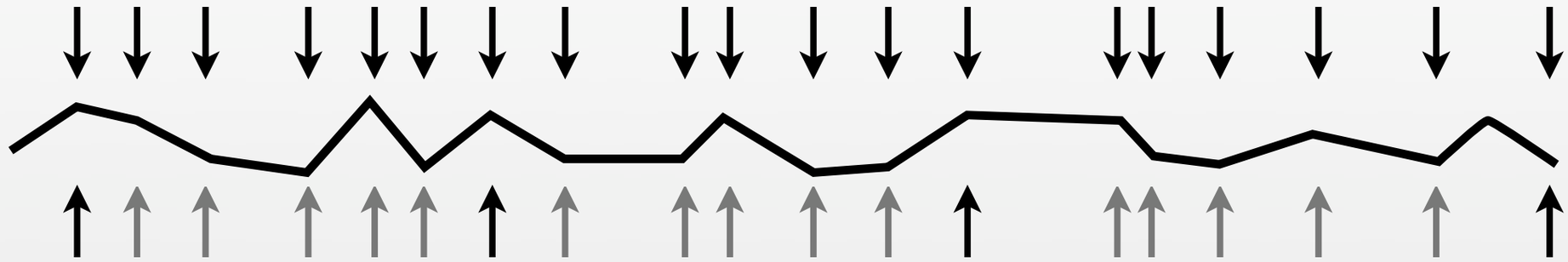
Transition probability from state *k* to state *k*+1:

$$R = \frac{\det(\mathbf{G}_k)}{\det(\mathbf{G}_{k+1})} = 1 + \gamma_k(1 - \mathbf{G}_k(p_k,p_k))\,.$$

→ Computing *R* requires $O(N_t^2)$ operations

Acceleration through delayed (Ed) updates

Delay multiple rank 1 updates to perform more efficient rank *k* update



At step *k*, regenerate row p_k and column p_k of G_k

$$\mathbf{col}_k = \mathbf{col}_0 + \sum_{i=0}^{k-1} \mathbf{a}_i \mathbf{b}_i(p_i)$$

$$\mathbf{row}_k = \mathbf{row}_0 + \sum_{i=0}^{k-1} \mathbf{a}_i(p_i) \mathbf{b}_i \, .$$

Obtain diagonal entries of G_k from

$$\mathbf{d}_{k+1}(p) = \mathbf{G}_{k+1}(p,p) = \mathbf{d}_k(p) + \mathbf{a}_k(p)\mathbf{b}_k(p), \quad \text{for } p = 1 : N_t.$$

→ Computing *R* requires O(kN_t) operations (as opposed to O(N_t^2))

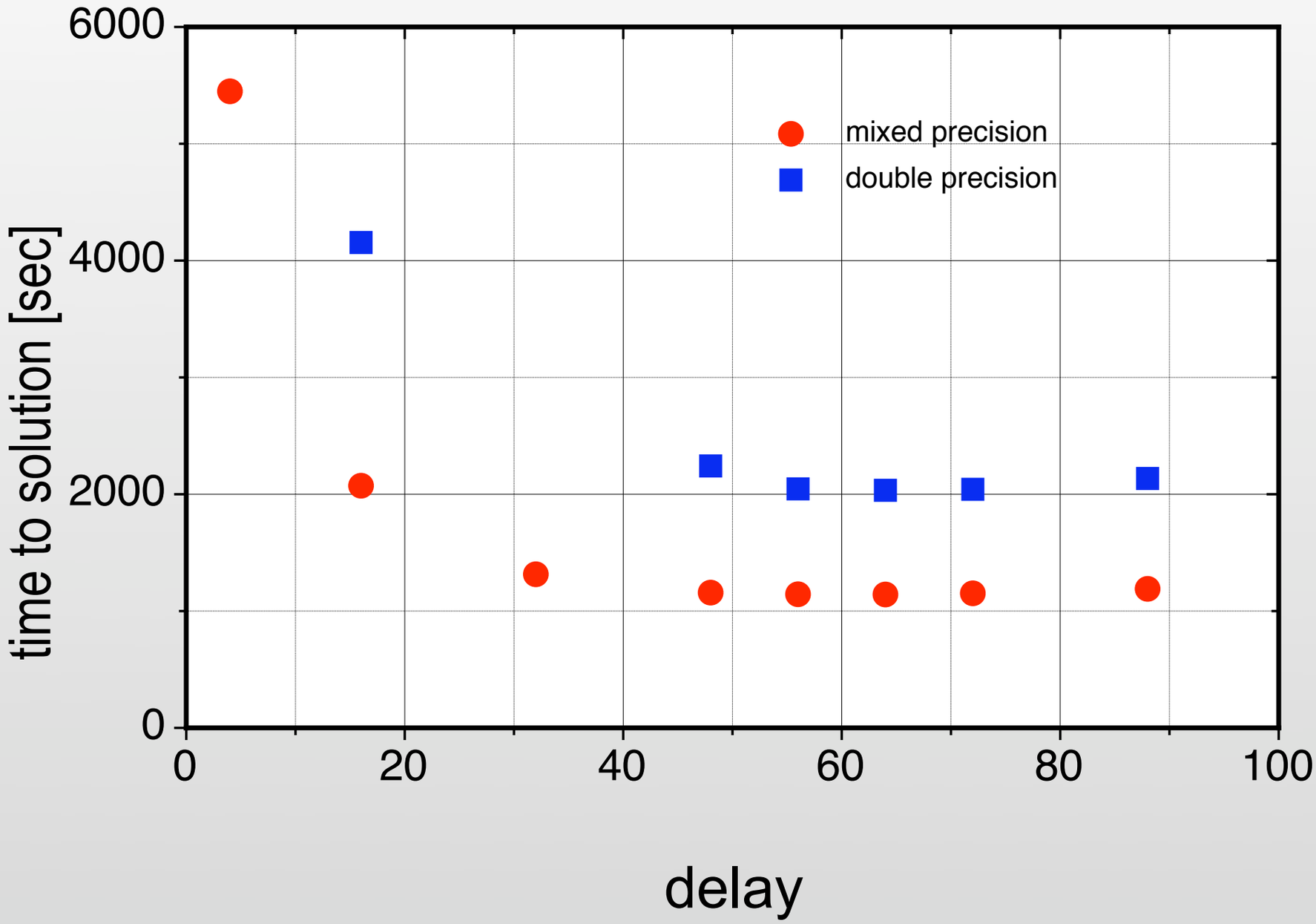
Green's function update after *k* steps

$$\mathbf{G}_{k+1} = \mathbf{G}_0 + [\mathbf{a}_0|\mathbf{a}_1|\cdots|\mathbf{a}_k]\,[\mathbf{b}_0|\mathbf{b}_1|\cdots|\mathbf{b}_k]^t \, .$$ (rank *k* update)

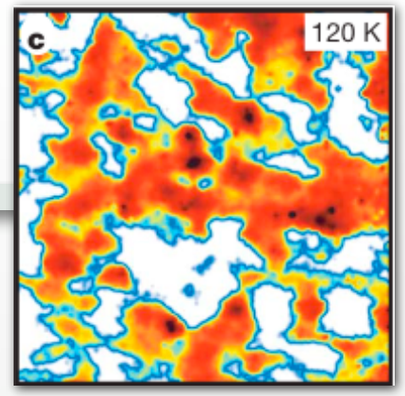
→ Comlexity for *k* updates remains O(kN_t^2), but rank-1 update is replaced by rank-*k* update (+ bookkeeping)

Performance improvement for delayed updates

$$N_c = 16 \qquad N_l = 150 \qquad N_t = 2400$$



Disorder and inhomogeneities



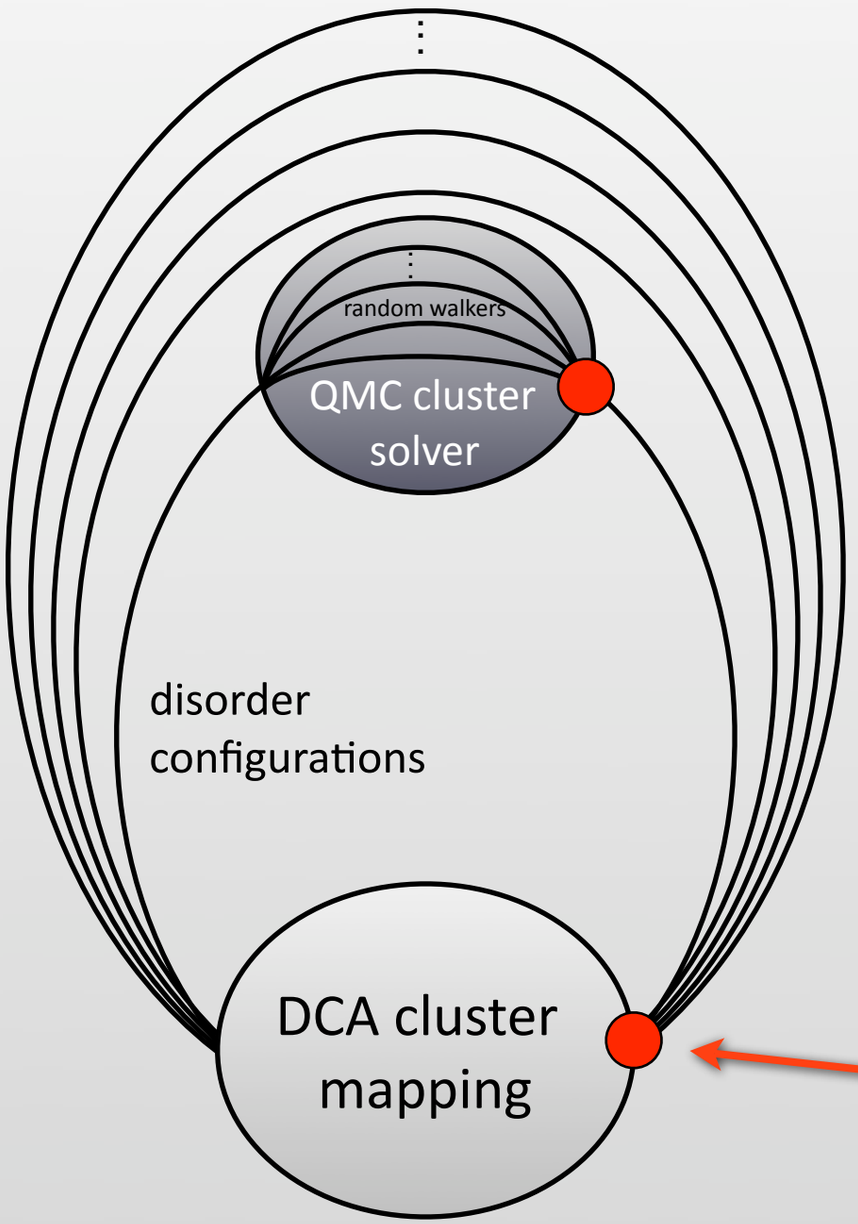
- Hubbard model with diagonal disorder

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U_i n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} V_i n_{i\sigma}$$

$$U_i \in \{U + \Delta U, U - \Delta U\}$$

$$V_i \in \{V, 0\}$$

$$N_c = 16 \rightarrow N_d = 2^{16}$$



required communication

Disorder-average cluster Green's function:

$$G_c(X_i - X_j, z) = \frac{1}{N_c} \sum_{\nu=1}^{N_d} G_c^{\nu}(X_i, X_j, z)$$

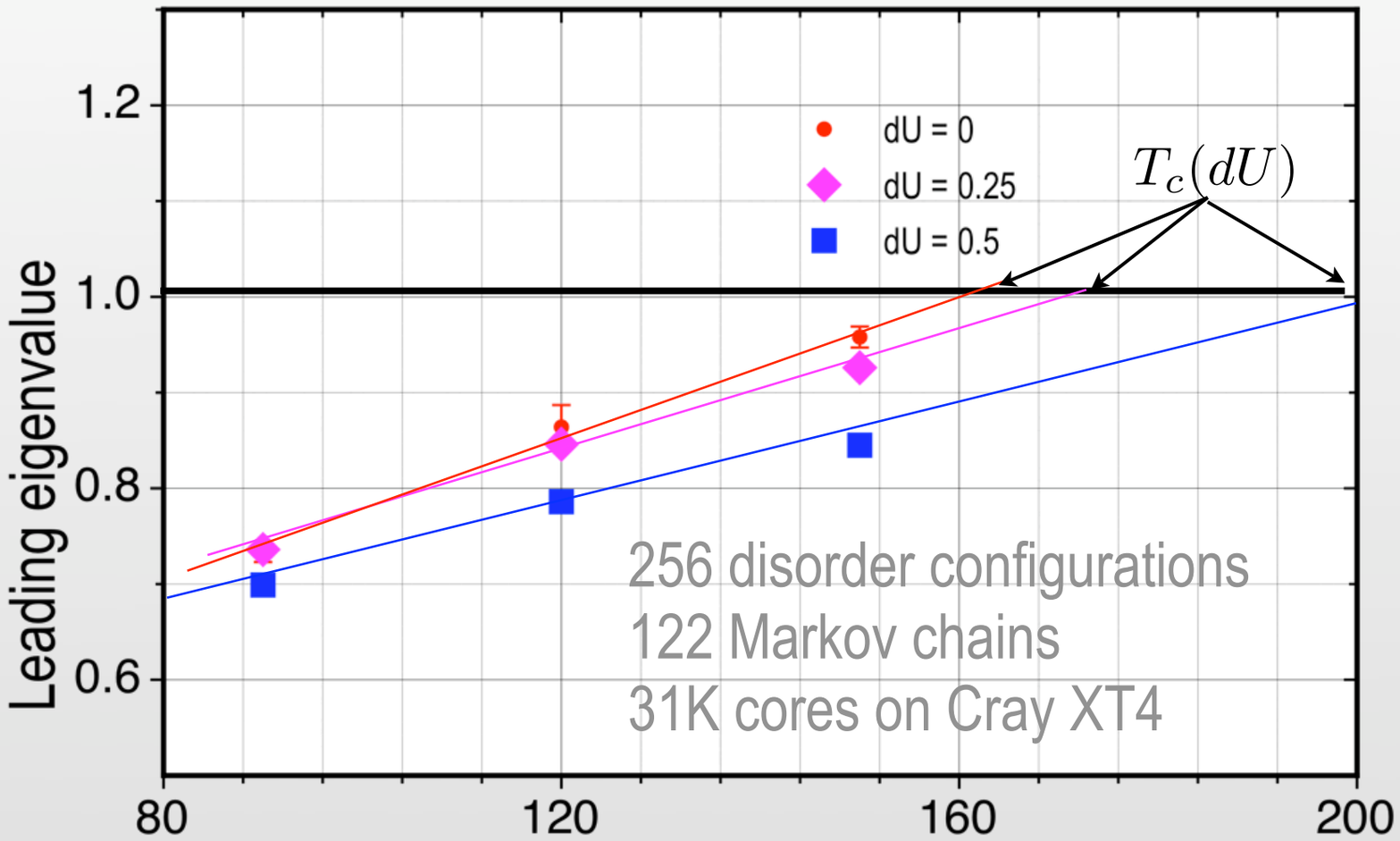
Effect of random disorder in U

$$U_i = U \pm \Delta U$$

$$P(\{U_i\}) = \prod_{i=1}^{N_c} P_i(U_i)$$

$$P_i(U_i = U \pm \Delta U) = 1/2$$

N_c = 16, <n> = 0.9, U=4t



→ Random disorder reduces transition temperature

Effect on the pairing interaction?

Spatial variation of pairing strength?

Relation to chemistry? → $P_i(U_i = U + \Delta U) = x$

Limit of small impurity concentration

Kemper, Doluweera, Maier, Jarrell, Hirschfeld, Cheng, preprint '08

- Hubbard model with diagonal disorder

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} V_i n_{i\sigma}$$

- For small impurity concentrations *x*, consider only configurations with zero or one impurity $V_i = V$

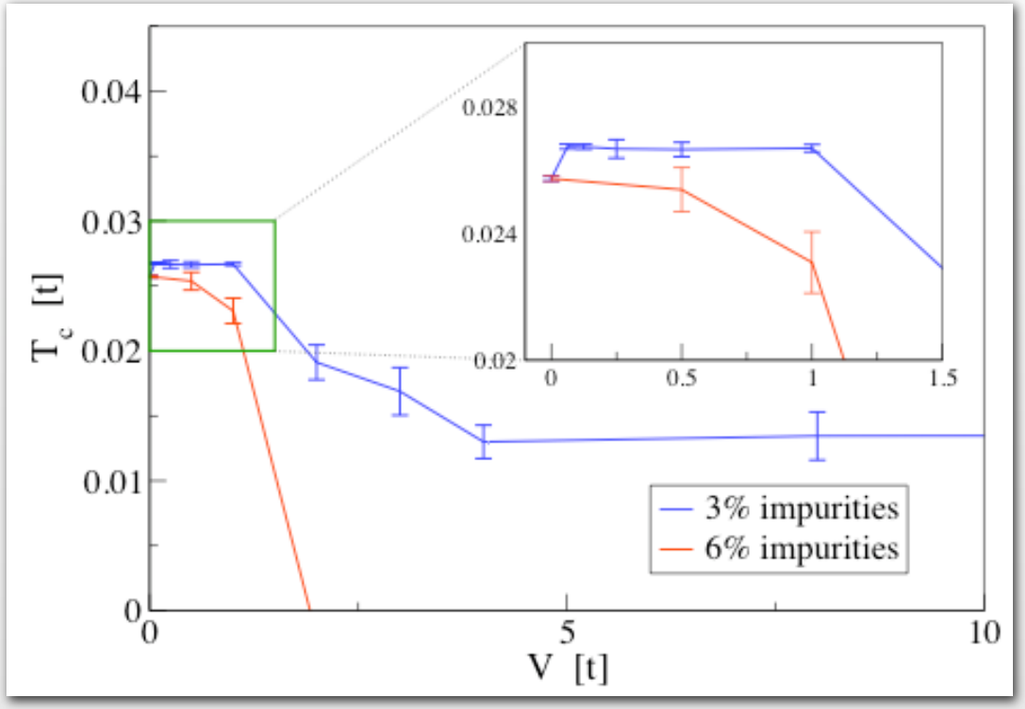
$$G^c_{ij} = x N_c G^c_{1,ij} + (1 - x N_c) G^c_{0,ij}$$

16-site cluster with one impurity

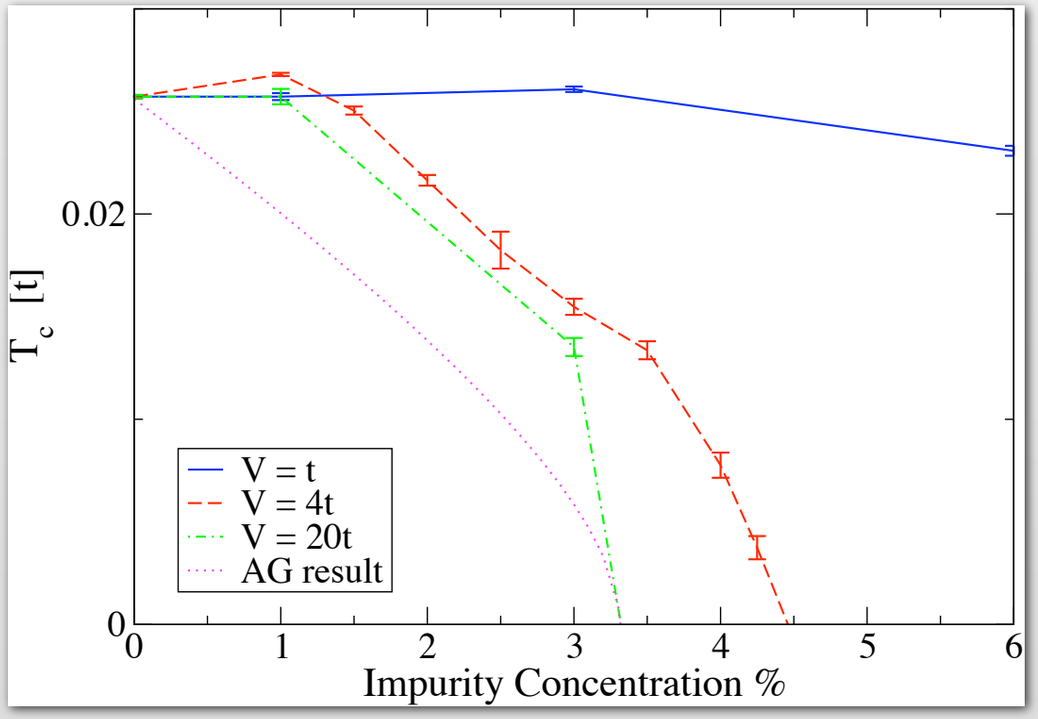
Clean 16-site cluster

Effect of single impurity

Kemper, Doluweera, Maier, Jarrell, Hirschfeld, Cheng, preprint '08



- Initial rise of T_c with impurity potential
  - Due to enhancement of antiferromagnetic spin correlations

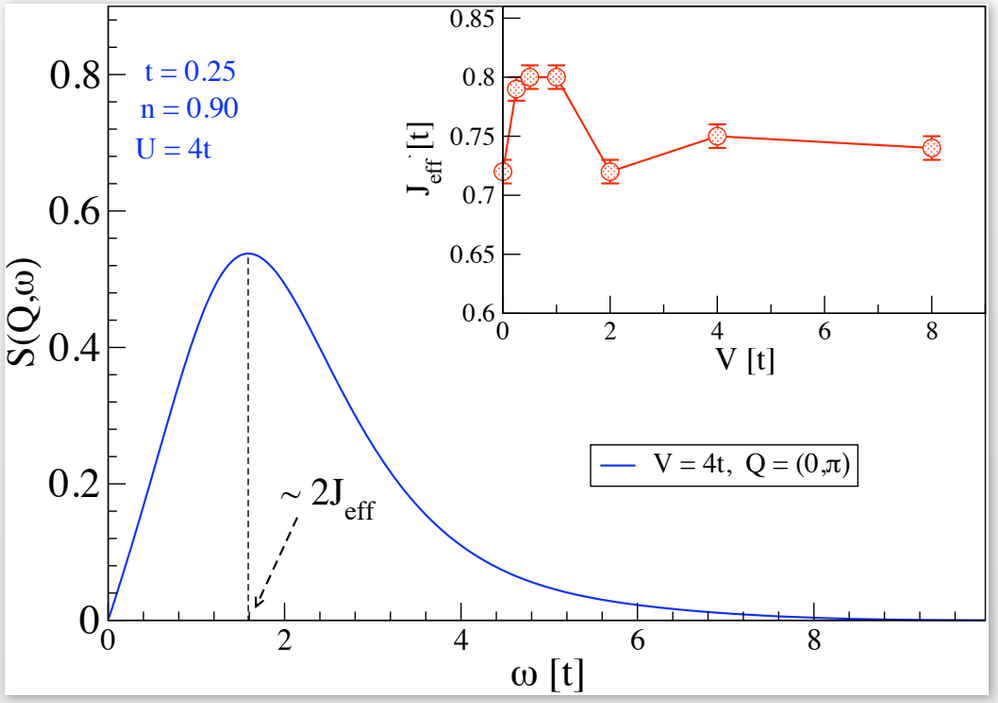


- Decrease of T_c for strong scattering
  - Due to scattering from impurity-induced magnetic moments and ordinary pair-breaking

- Robustness of superconductivity against weak disorder due to correlations (consistent with Garg, Randeria, Trivedi, Nature Physics '08)

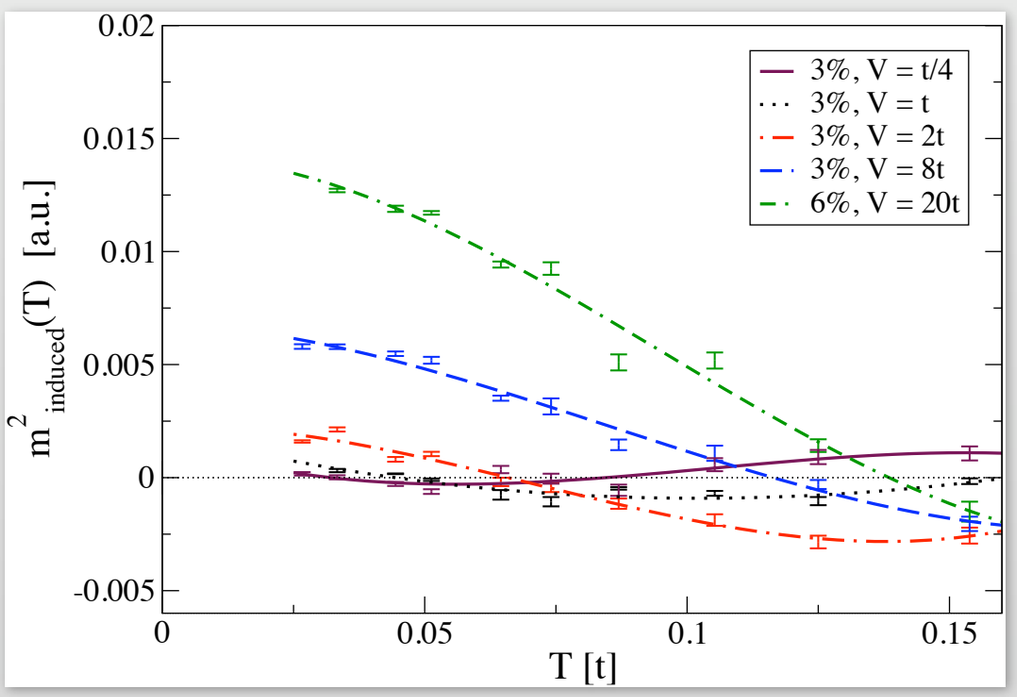
Mechanism

Cluster spin susceptibility



- Increase in T_c due to enhancement of AF spin correlations

Induced magnetic moment



- Decrease of T_c for strong scattering due to moment formation
- Induced moment for strong scattering: $m^2 \sim 1/4$
  - > Valence bond solid??

DCA & Stripes?

Doping a Mott insulator:
Physics dominated by Coulomb energy, kinetic energy is frustrated

DCA & Stripes?

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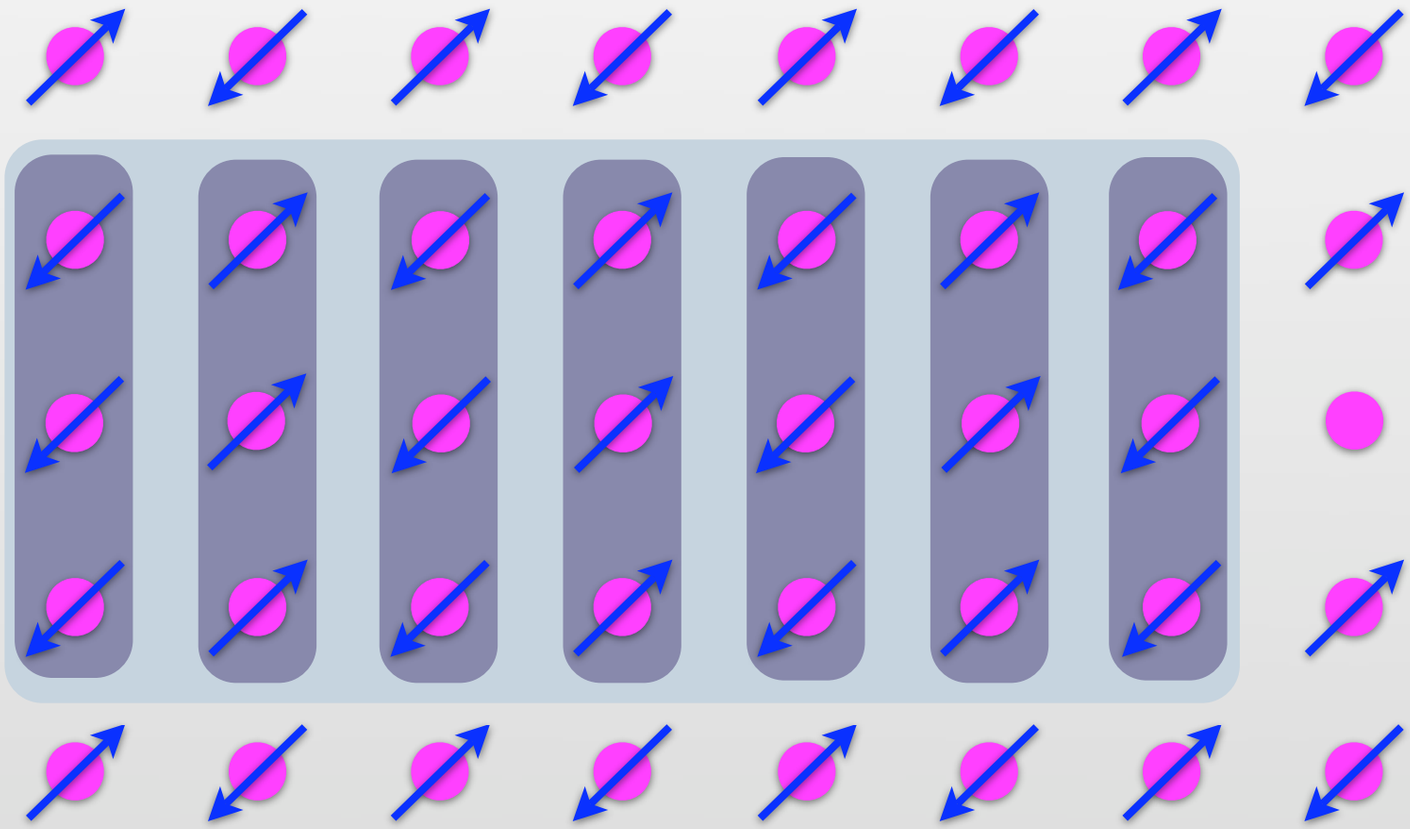


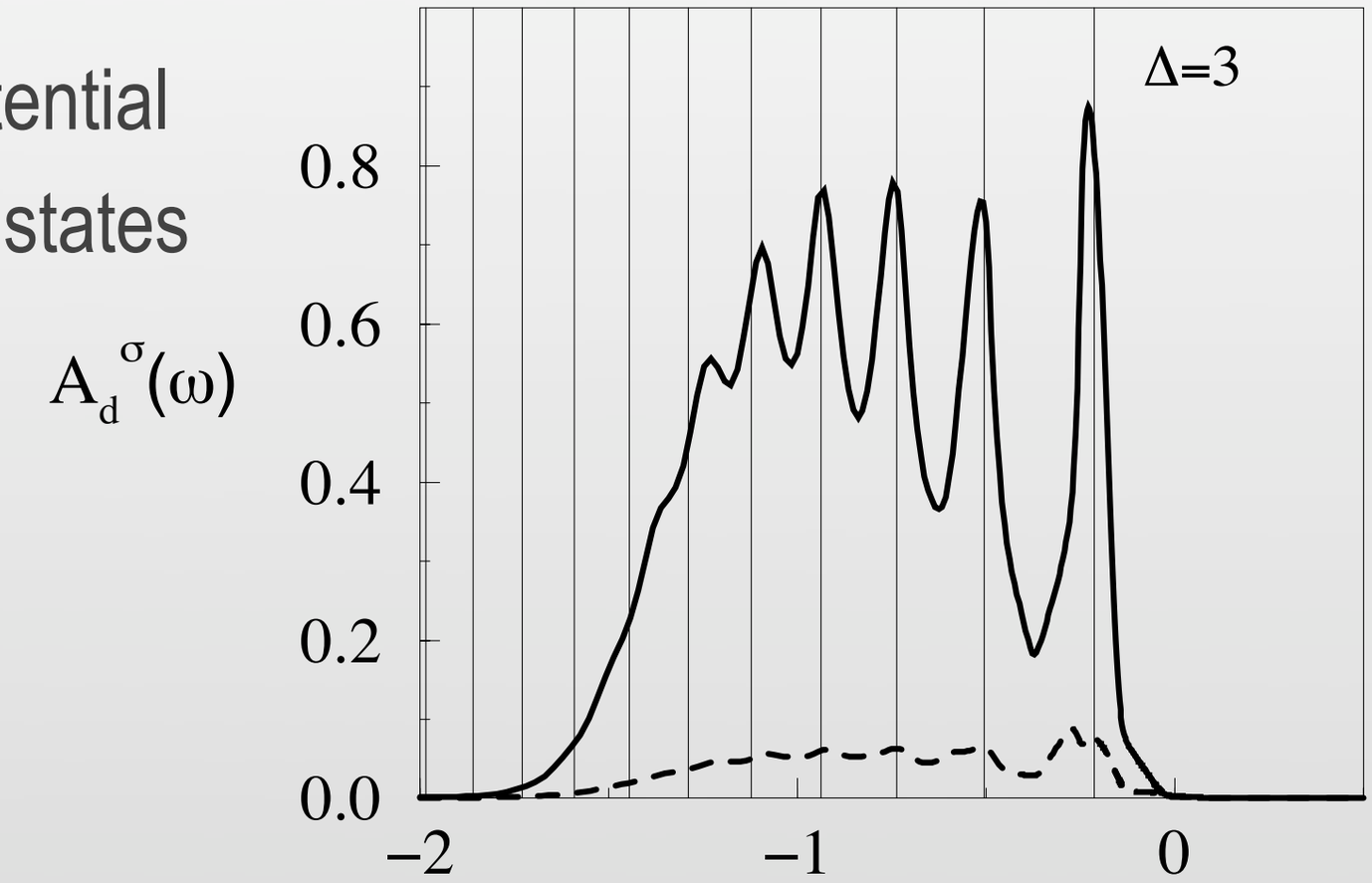
Hole localization due to increase in exchange energy!

DCA & Stripes?

Doping a Mott insulator:
Physics dominated by Coulomb energy, kinetic energy is frustrated

> Confining potential

> D=∞: Bound states



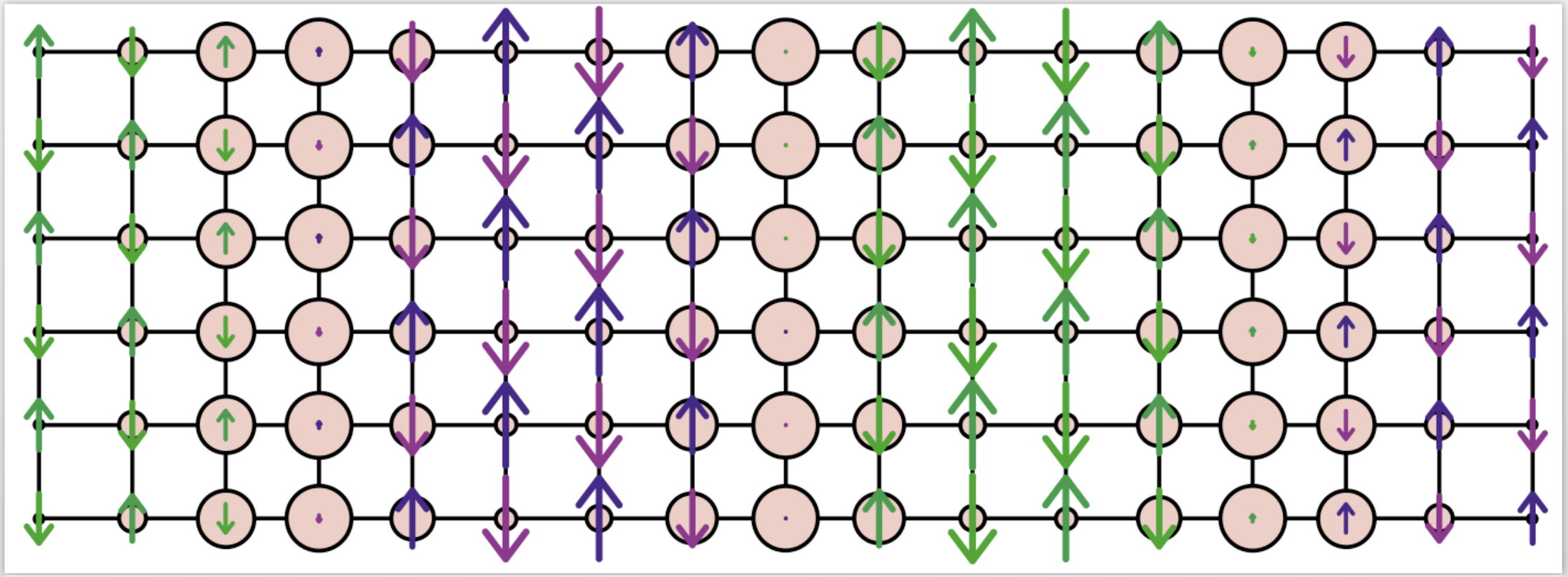
TAM *et al.*, Eur. Phys. J. B, '99

Hole localization due to increase in exchange energy!

Stripes: A way to relieve kinetic energy frustration

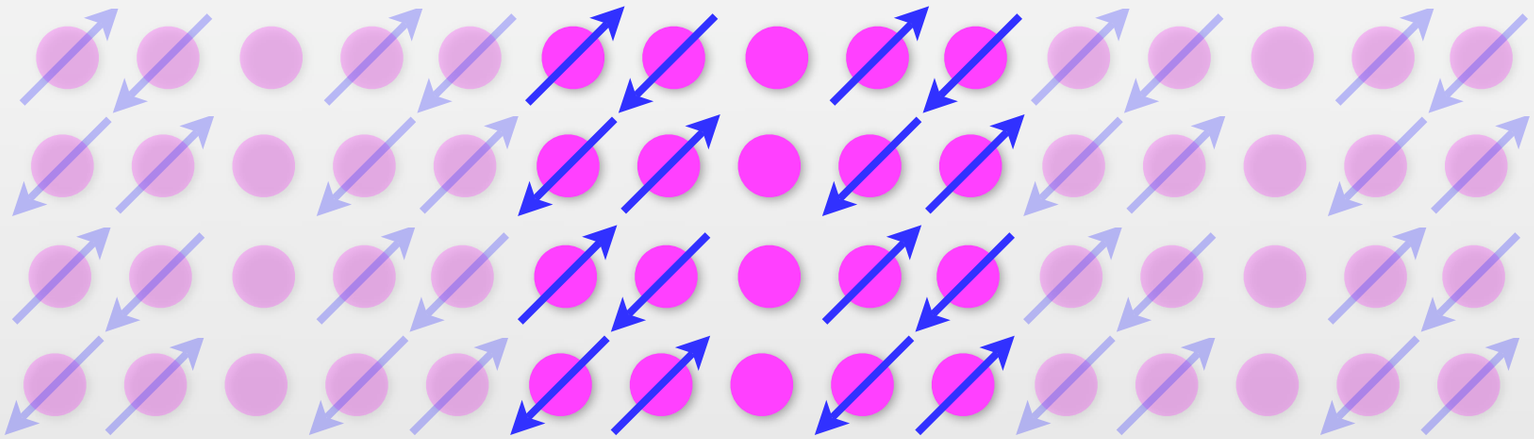
System phase separates into hole rich and hole poor regions

Gor'kov, Sokol '87; Zaanen, Gunnarson '89; Emory, Kivelson, Lin '90;
Emery, Kivelson '93; White, Scalapino '98, Zaanen, Nature '00

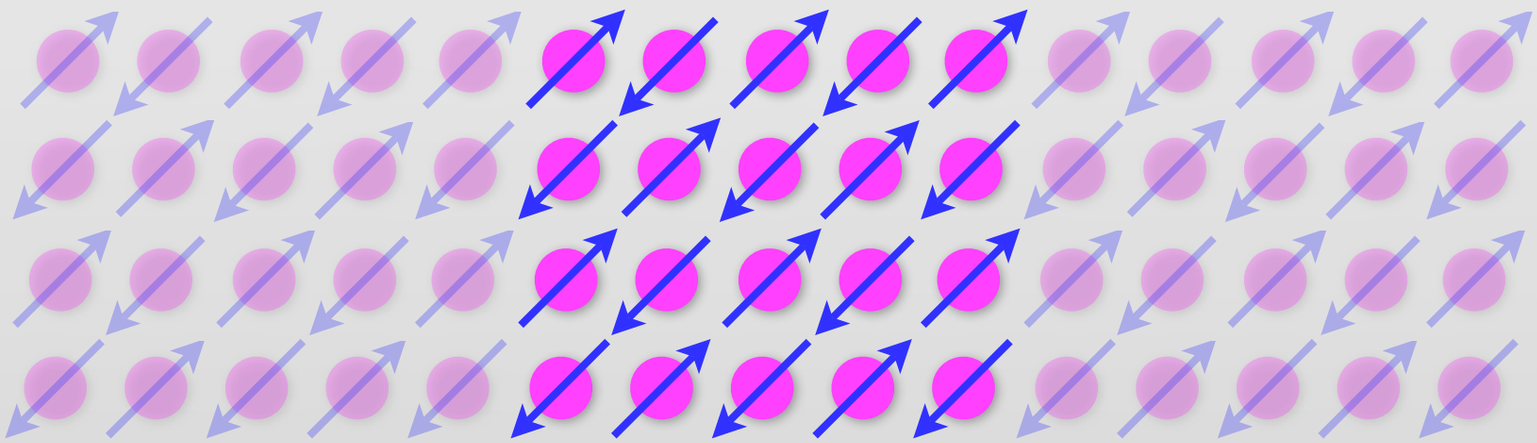


DCA & Stripes?

- DCA cluster has periodic boundary conditions
  - Stripes are easily frustrated
  - 20-site 5 x 4 cluster should accommodate exactly one stripe without frustrating it



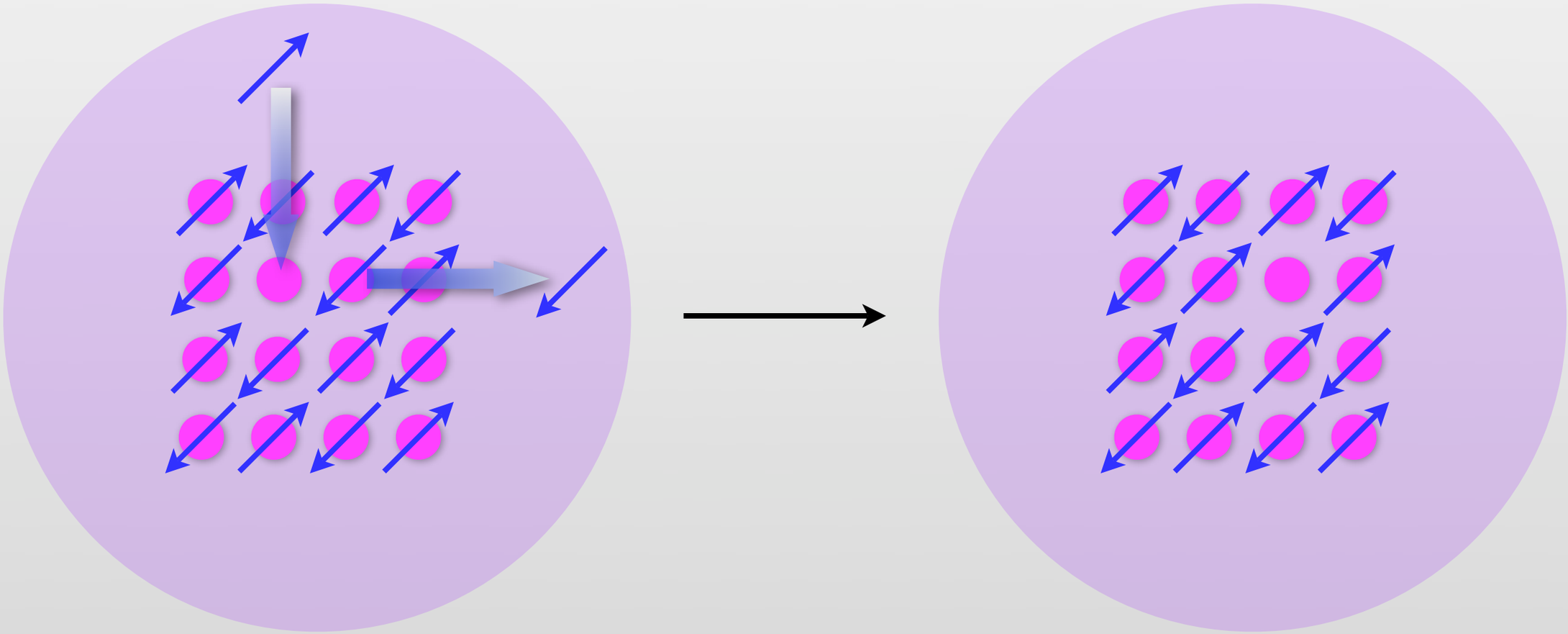
  - But half-filled unstriped cluster frustrates AF correlations - (π,π) is not cluster K-point



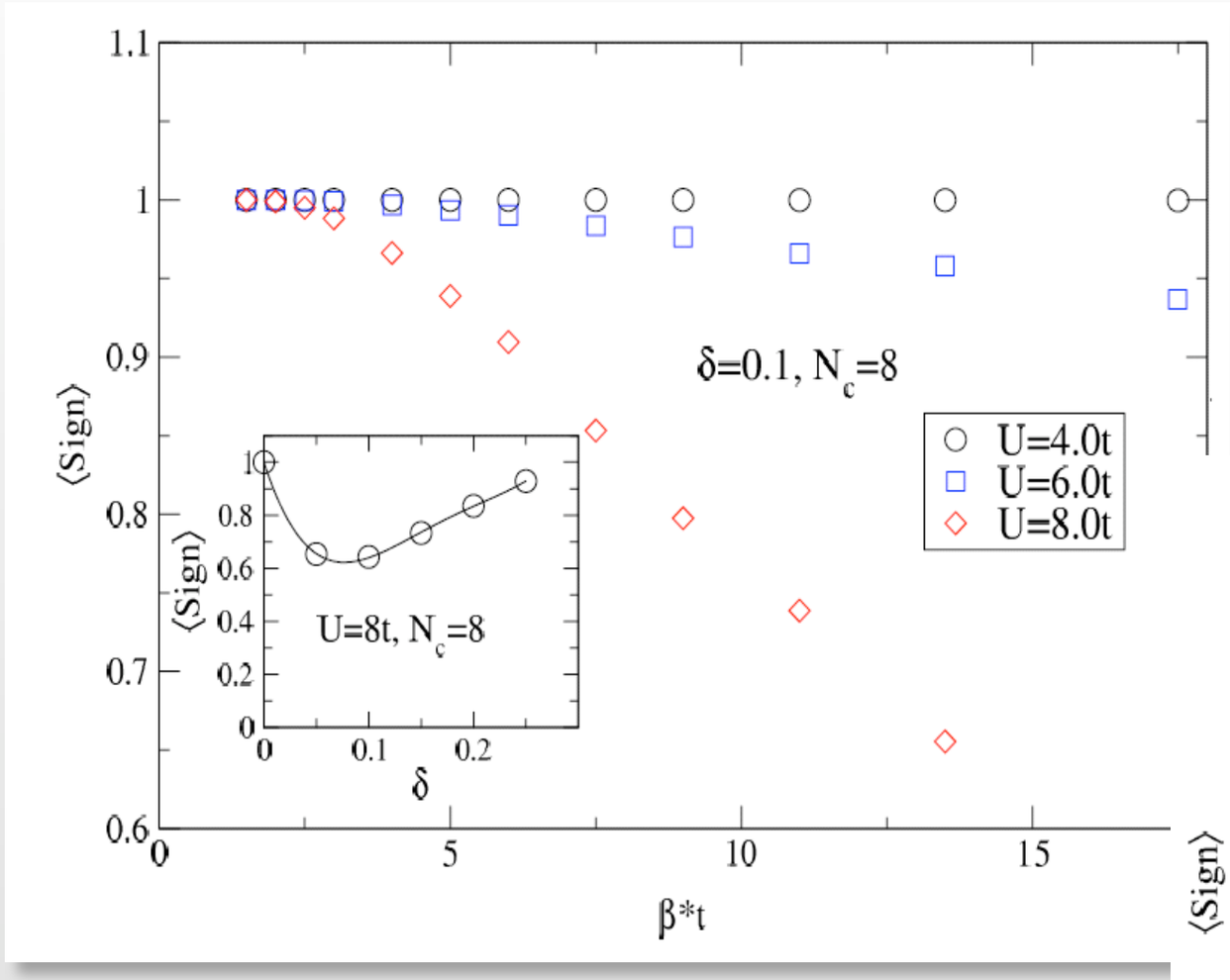
  - Average over boundary conditions?

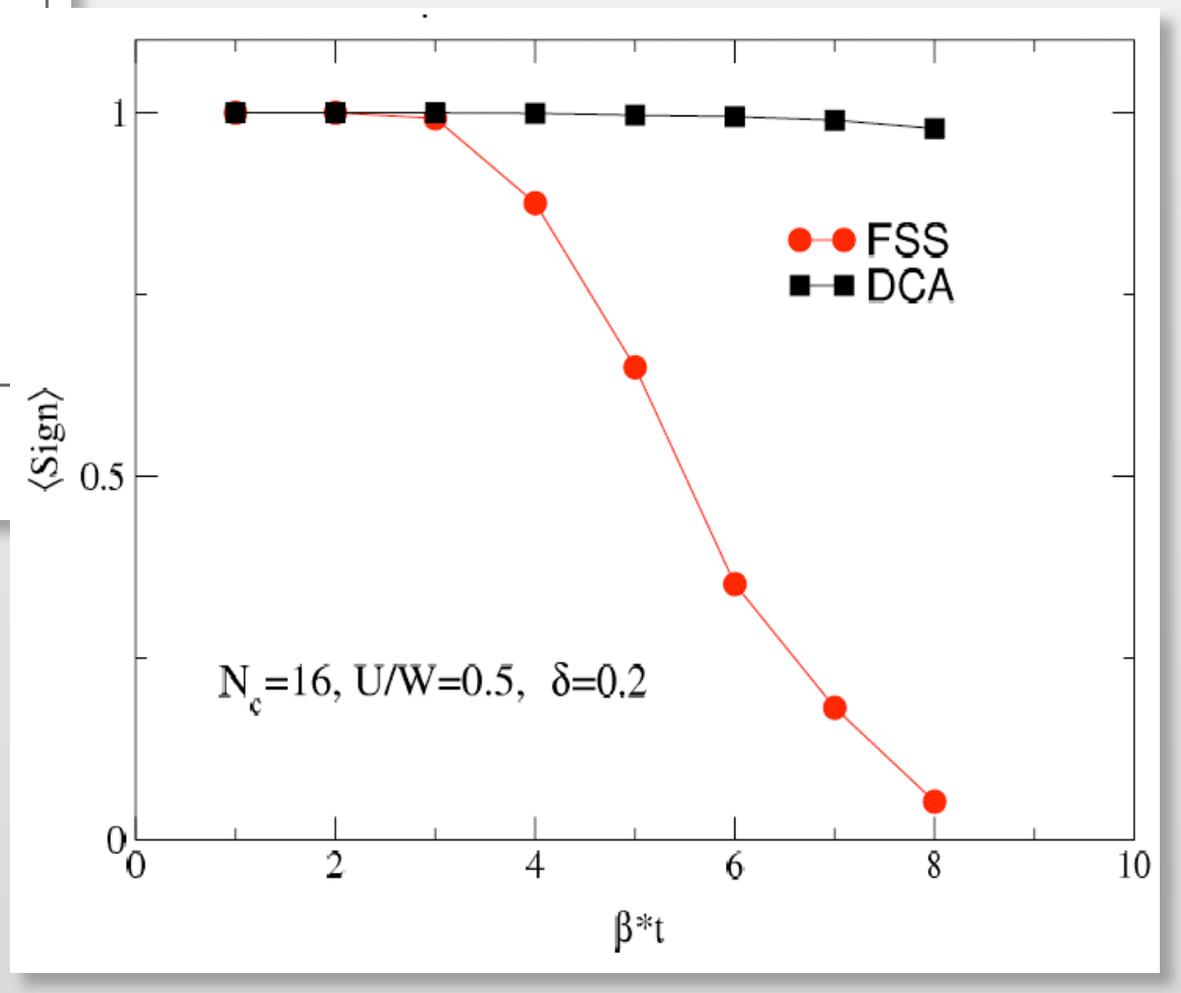
DCA & Stripes?

- DCA cluster is translationally invariant
  - Every site in the cluster couples to the mean-field
  - Holes can move in the cluster via mean-field without frustrating AF bonds



DCA/QMC sign problem





Better than finite size QMC!

Avoiding the sign-problem with parquet

- Present approach (DMFT,CDMFT, DCA, ...)
  - Calculate self-energy and irreducible vertices in cluster

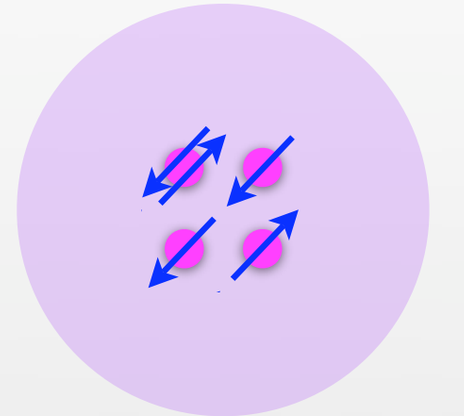
Cluster:

$$G_c = [G_{c,0}^{-1} - \Sigma_c]^{-1} \qquad \chi_c = [\chi_{c,0}^{-1} - \mathbf{\Gamma}_c]^{-1}$$

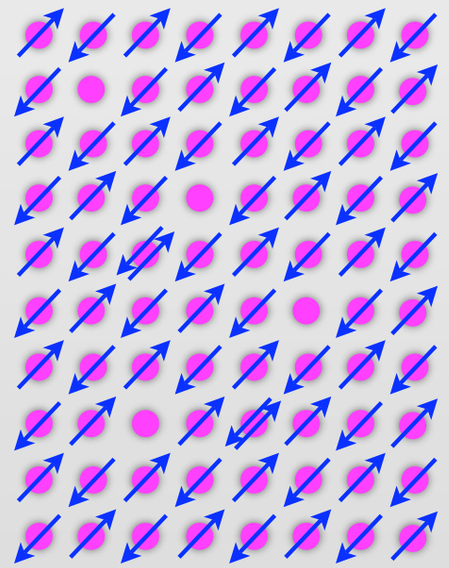
$\downarrow$

Lattice:

$$G = [G_0^{-1} - \Sigma_c]^{-1} \qquad \chi = [\chi_0^{-1} - \mathbf{\Gamma}_c]^{-1}$$



$\Sigma_c\,,\ \Gamma_c$

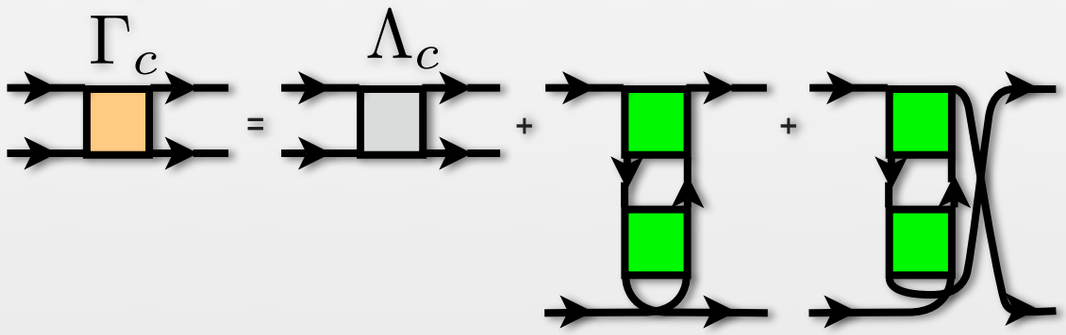


  - Use cluster self-energy and vertices in lattice Green's functions
  - Assumes that self-energy and vertices are local or weakly momentum dependent

Avoiding the sign problem ...

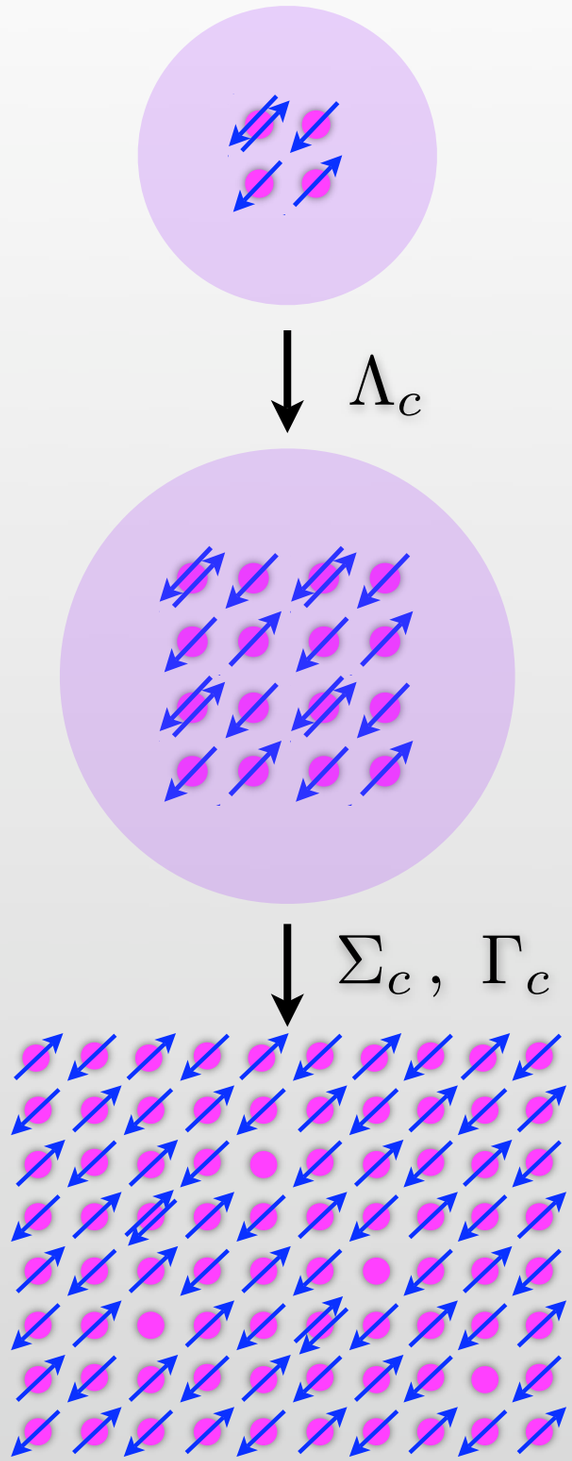
SciDAC-2: Jarrell, Tomko, Bai, Savrasov, Scalettar, Maier, D'Azevedo

- New multi-scale many-body approach
  - Calculate fully irreducible vertex Λ_c on small cluster using QMC



  - Use parquet equations to calculate Σ_c , Γ_c on larger cluster
  - No sign problem → scales algebraically
  - Λ_c more local than Σ_c , Γ_c
  - Short-ranged correlations on small cluster treated explicitly with QMC
  - Intermediate-ranged correlations on larger cluster treated with parquet
  - Long-ranged correlations treated in mean-field

(see also K. Held: Dynamical vertex approximation, PRB '07, Rubtsov *et al.*: dual Fermions arXiv:0810.3819v2)



Summary

Optimizations of Dynamic Cluster quantum Monte Carlo

- Ten-fold speedup through delayed (Ed) updates and mixed precision

DCA simulations of homogeneous 2D Hubbard model

- Superconductivity, antiferromagnetism,pseudogap behavior
- Insights into the pairing mechanism - RVB vs. spin fluctuations

DCA simulations of disordered Hubbard model

- Disorder reduces transition temperature
- Robustness of superconductivity against weak disorder due to correlations

Multi-scale many-body approach

- Treat correlations on different length-scales with different accuracy