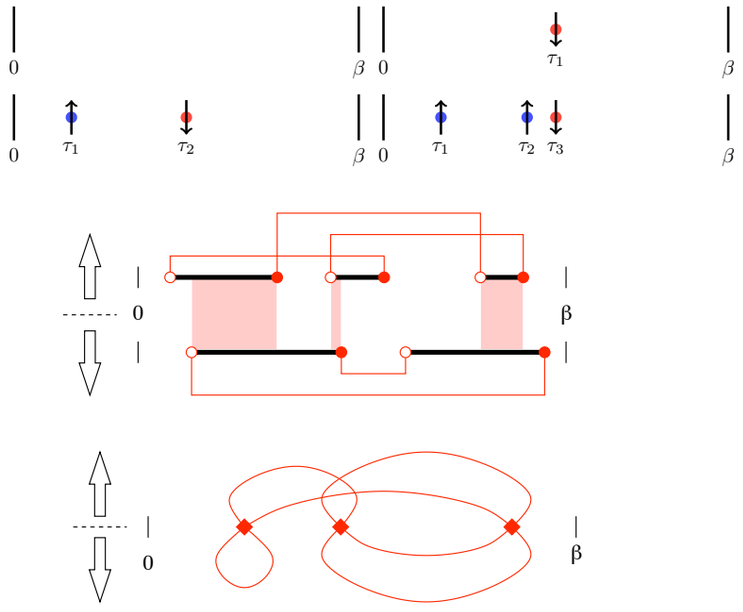
Continuous-Time Quantum Monte Carlo Algorithms



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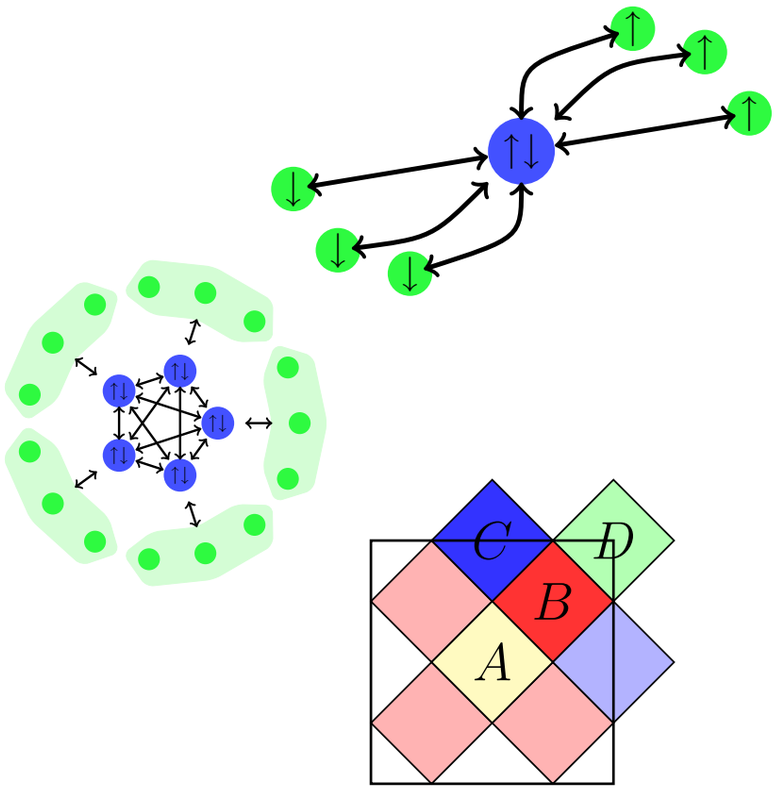


Overview

Quick introduction to the Dynamical Mean Field Theory (DMFT)

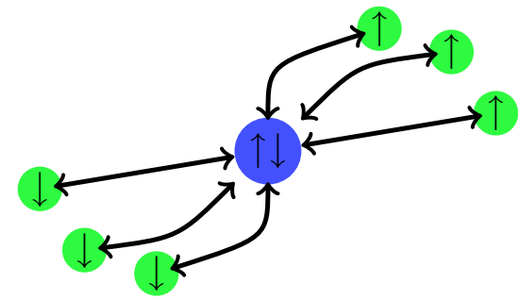
Continuous-Time Quantum Monte Carlo Methods and comparison to other methods

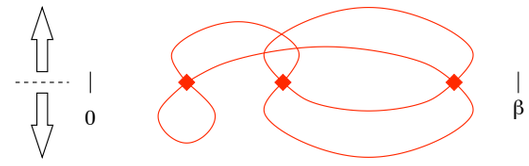
The Weak Coupling method

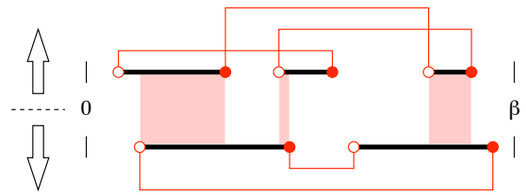
They Hybridization Expansion

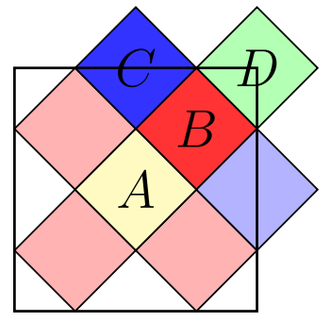
Continuous-Time Auxiliary Field impurity solver algorithm and large clusters

Some (very few) results (see P. Werner's talk for more applications)



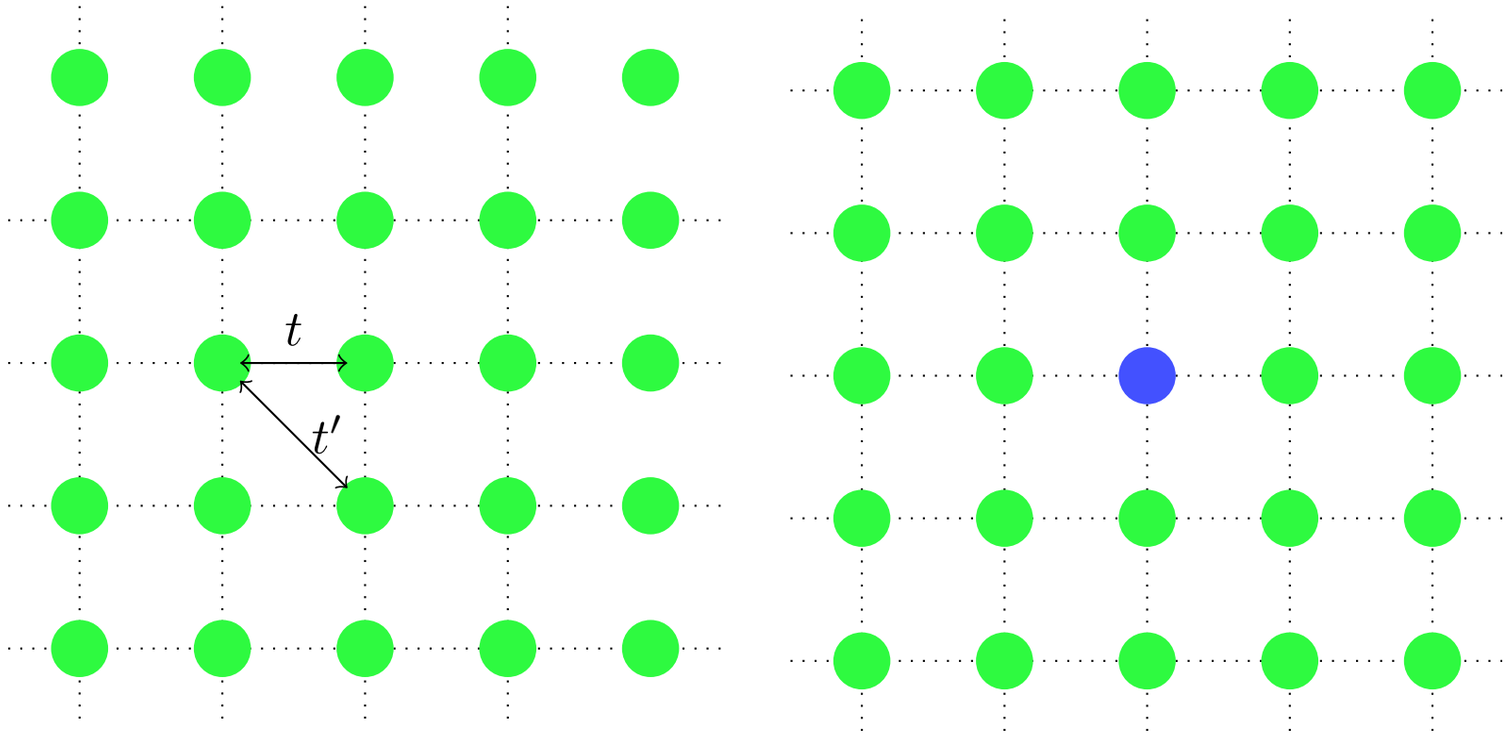






DMFT and Impurity Problem

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow}.$$

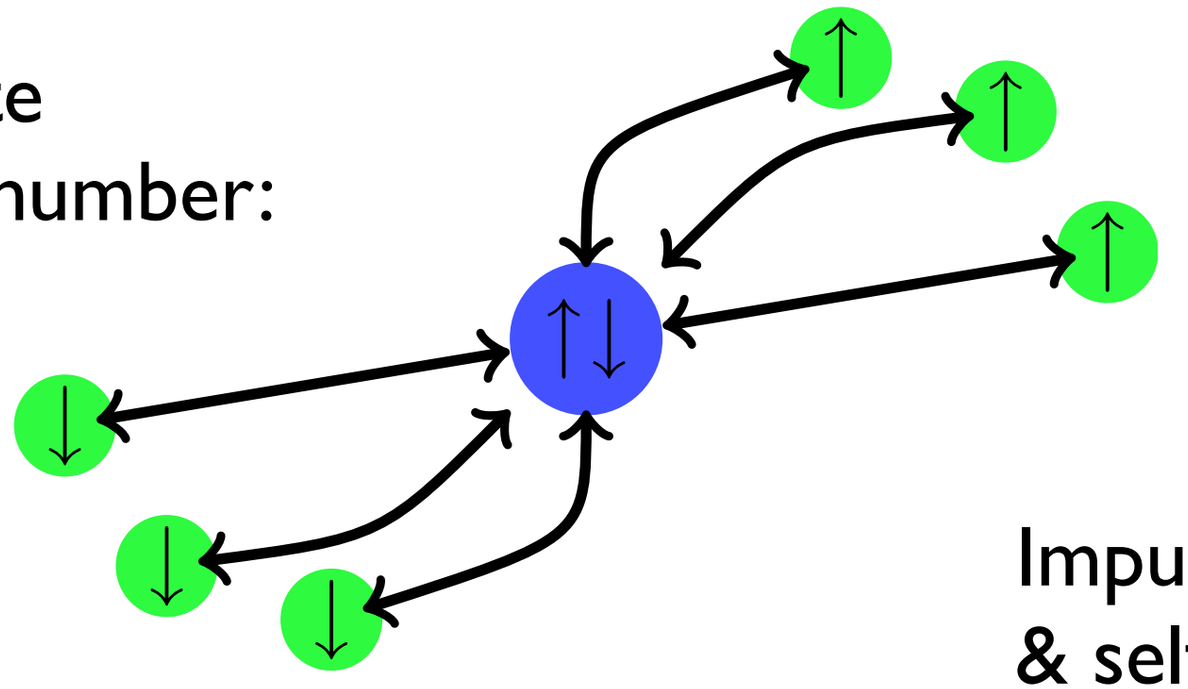


Impurity Problem: $S_{\text{eff}} = -\sum_\sigma \int\int_0^\beta d\tau d\tau' c^\dagger_\sigma(\tau)\mathcal{G}^{-1}_{0\sigma}(\tau-\tau')c_\sigma(\tau) + U\int_0^\beta d\tau n_\uparrow(\tau)n_\downarrow(\tau)$

Self Consistency: $G(i\omega_n) = \sum_{\vec{k}\in BZ} \frac{1}{i\omega_n + \mu - \epsilon(\vec{k}) - \Sigma(i\omega_n)}.$

DMFT and Impurity Problem

Limit of infinite coordination number:

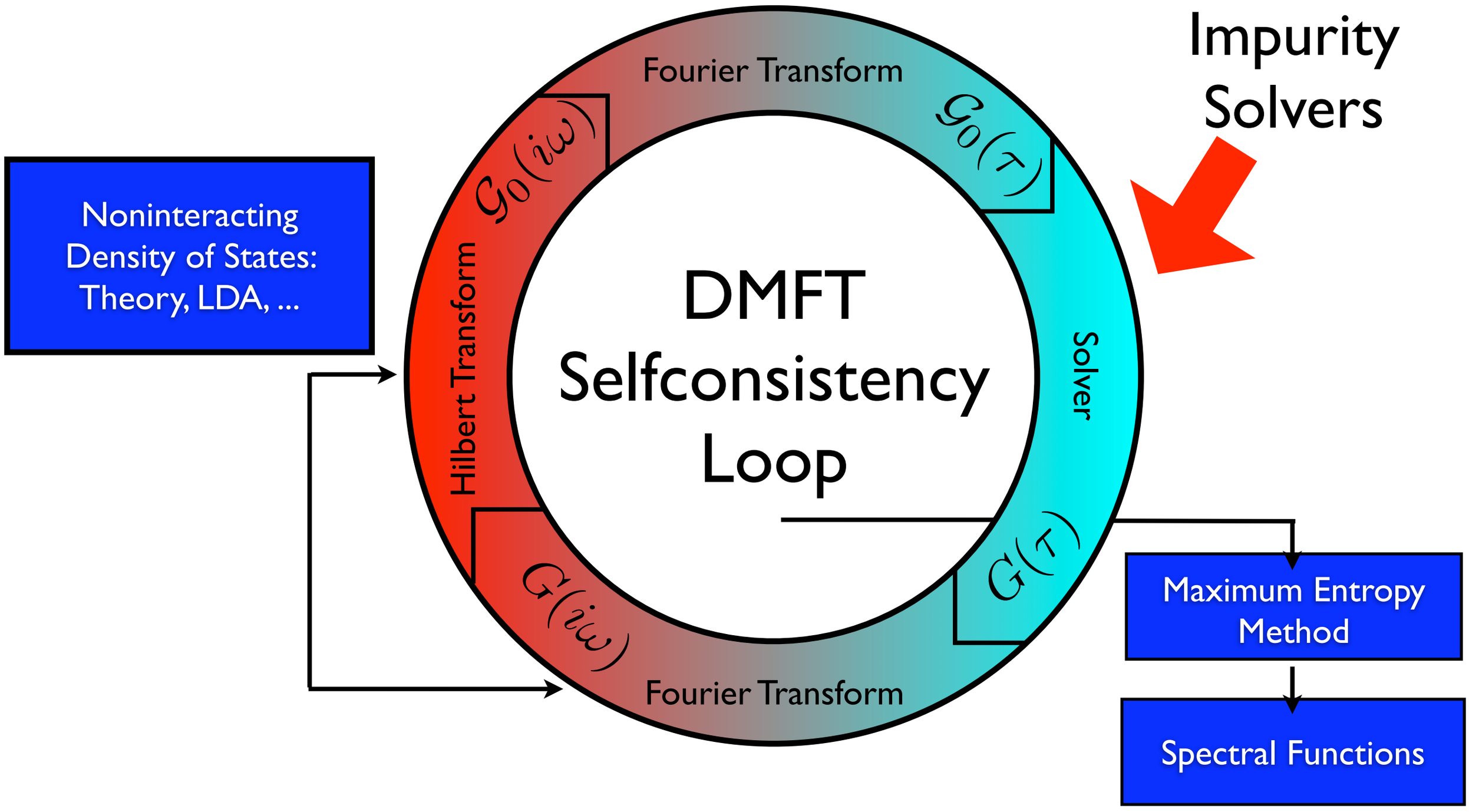


Impurity coupled to a bath & self consistency condition

Impurity Problem: $$S_{\rm eff} = -\sum_{\sigma} \int\int_0^\beta d\tau d\tau' c_\sigma^\dagger(\tau) \mathcal{G}_{0\sigma}^{-1}(\tau - \tau') c_\sigma(\tau) + U \int_0^\beta d\tau n_\uparrow(\tau) n_\downarrow(\tau)$$

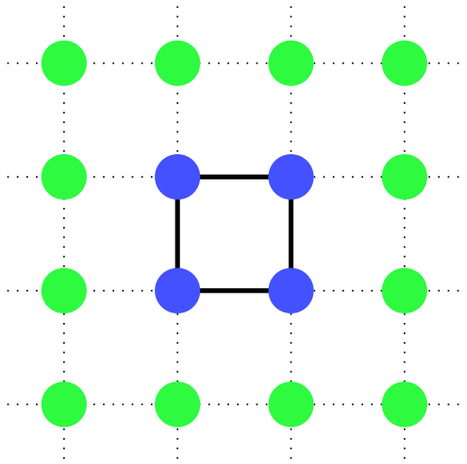
Self Consistency: $$G(i\omega_n) = \sum_{\vec{k} \in BZ} \frac{1}{i\omega_n + \mu - \epsilon(\vec{k}) - \Sigma(i\omega_n)}.$$

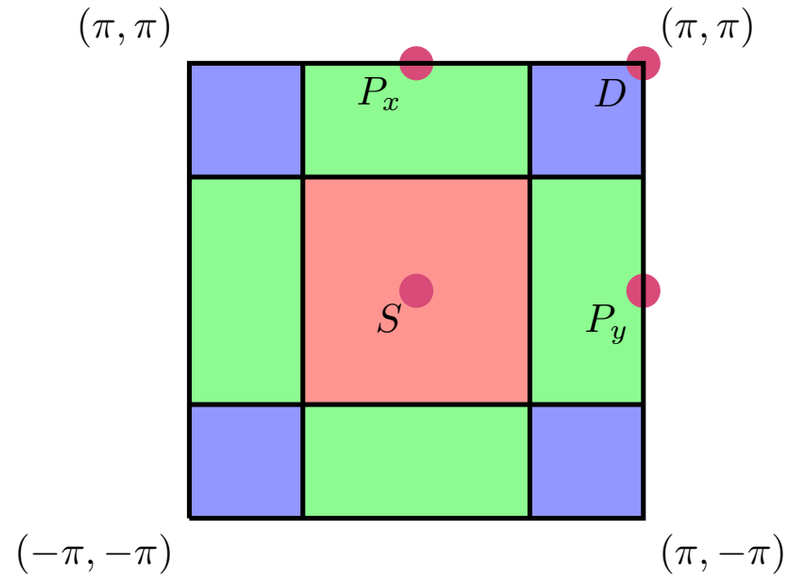
DMFT Self Consistency



Cluster DMFT

Various variants developed by Lichtenstein *et al.*, Jarrell *et al.*, Kotliar *et al.*





Infinite coordination number: momentum independent self energy.

Dynamic Cluster Approximation (DCA): reintroduce momentum dependence to DMFT.

DCA self energy is chosen to be constant within patches of the Brillouin zone

Cluster impurity problem

$$S_{\text{eff}} = -\int\int_0^\beta d\tau \sum_{ij\sigma} c^\dagger_{i\sigma}(\tau)\mathcal{G}^0_{ij,\sigma}(\tau-\tau')^{-1}c_{j\sigma}(\tau') + \int_0^\beta d\tau \sum_{j=1}^{N_c} U n_{j\uparrow}(\tau)n_{j\downarrow}(\tau)$$

Self consistency condition

$$\Sigma_K = \mathcal{G}^0_K(i\omega_n)^{-1} - G^{-1}_{\text{imp}}$$

$$\overline{G}(K,i\omega_n) = \int_{\text{BZ patch}} \frac{dk}{i\omega_n + \mu - \epsilon(k) - \Sigma_K}$$

$$\mathcal{G}^0_K(i\omega_n)^{-1} = \Sigma_K + \overline{G}^{-1}_K(i\omega_n)$$

Hirsch Fye QMC Impurity Solver

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow}. \quad Z = \mathrm{Tr}e^{-\beta H} = \mathrm{Tr}\prod_{l=1}^{L} e^{-\Delta\tau(H_0+V)}$$

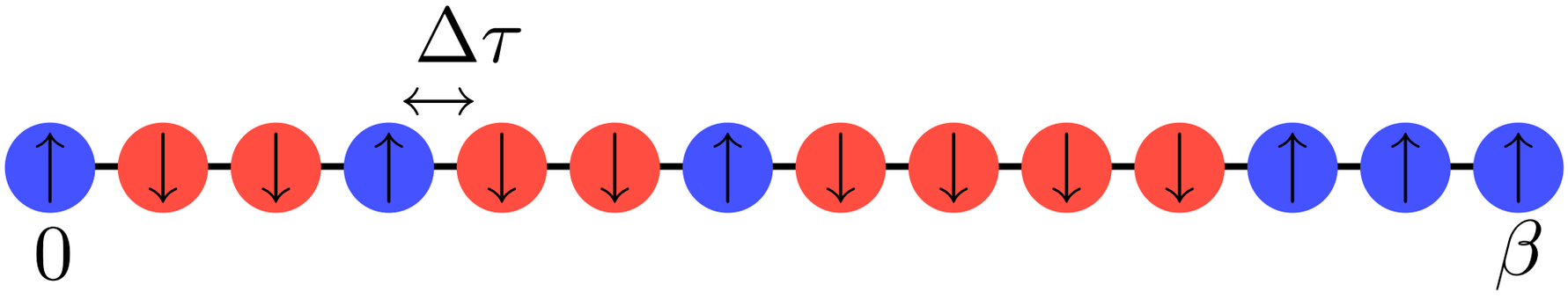
$$Z \simeq \prod_{l=1}^{L} e^{-\Delta\tau H_0}e^{-\Delta\tau V}$$

Trotter breakup: discretization of the integral, introduces Trotter errors

Auxiliary field decomposition

$$\exp\left[-\Delta\tau\left(Un_\uparrow n_\downarrow - \frac{1}{2}(n_\uparrow + n_\downarrow)\right)\right] = \frac{1}{2}\sum_{\sigma=\pm1}\exp\left[\lambda\sigma(n_\uparrow - n_\downarrow)\right]$$

$$\cosh(\lambda) = \exp(\Delta\tau U/2)$$



Sampling of partition function integral on discretized time slices

Continuous-Time Algorithms

Partition function in the interaction representation:

$$Z = \mathrm{Tr}\left[e^{-\beta H_0} T_\tau e^{-\int_0^\beta d\tau V(\tau)}\right]$$

Expansion into perturbation series (powers of the interaction *V*):

$$Z = \sum_{k=0}^{\infty} \int d\tau_1 \cdots \int_{\tau_{k-1}}^{\beta} d\tau_k \mathrm{Tr}\left[e^{-\beta H_0} e^{\tau_k H_0}(-V) \cdots e^{-(\tau_2-\tau_1)H_0}(-V) e^{-\tau_1 H_0}\right].$$

Graphical representation of terms of the integral at different orders:

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Graphical representation of terms of the integral at different orders:

$W_0 = \mathrm{Tr}\left[e^{-\beta H_0}\right]$ a)

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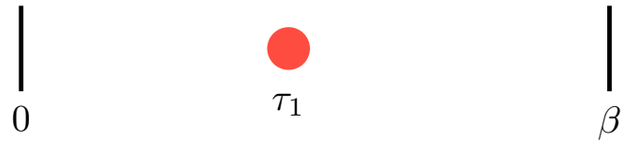
Graphical representation of terms of the integral at different orders:

$$W_0 = \mathrm{Tr}\left[e^{-\beta H_0}\right]$$

a)

$$W_1(\tau_1) = \mathrm{Tr}\left[e^{-(\beta-\tau_1)H_0} V e^{-\tau_1 H_0}\right]$$

b)



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Graphical representation of terms of the integral at different orders:

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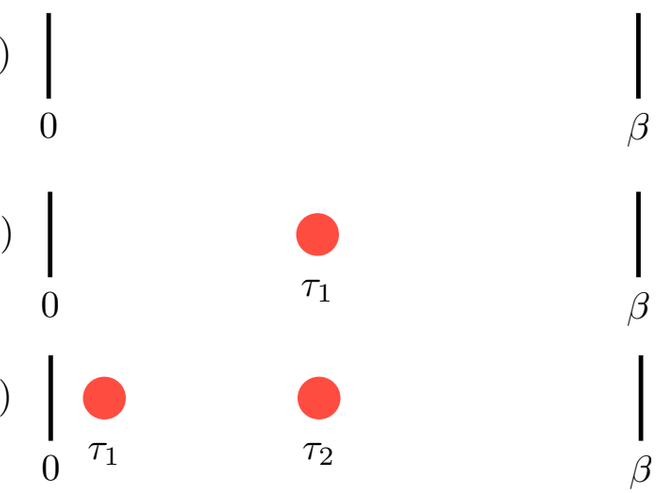
$$W_1(\tau_1) = \mathrm{Tr}\left[e^{-(\beta-\tau_1)H_0} V e^{-\tau_1 H_0}\right]$$

$$W_2(\tau_1,\tau_2) = \mathrm{Tr}\left[e^{-(\beta-\tau_1)H_0} V e^{-(\tau_1-\tau_2)H_0} V e^{-\tau_2 H_0}\right]$$



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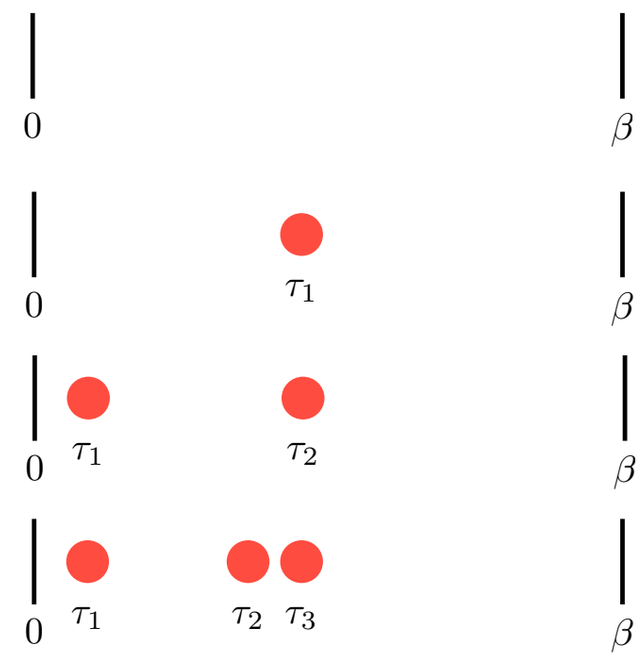
$$W_3(\tau_1,\tau_2,\tau_3) = \mathrm{Tr}\left[e^{-(\beta-\tau_1)H_0} V e^{-(\tau_1-\tau_2)H_0} V e^{-(\tau_2-\tau_3)H_0} V e^{-\tau_3 H_0}\right]$$

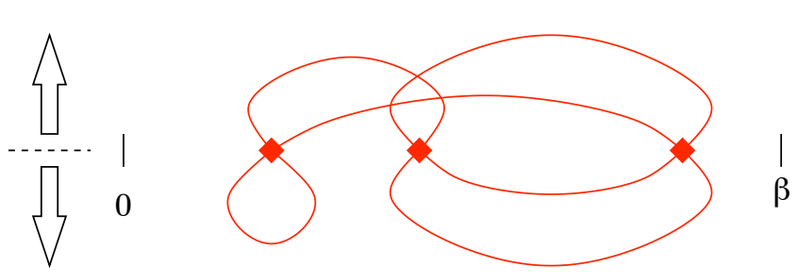


A. N. Rubtsov and A. I. Lichtenstein, JETP Letters **80**, 61 (2004);
Werner *et al.*, PRL **97**, 076405 (2006)

Weak Coupling and Hybridization Expansion

$$Z = \sum_{k=0}^{\infty} \int d\tau_1 \cdots \int_{\tau_{k-1}}^{\beta} d\tau_k \, \mathrm{Tr} \left[e^{-\beta H_0} e^{\tau_k H_0} (-V) \cdots e^{-(\tau_2 - \tau_1) H_0} (-V) e^{-\tau_1 H_0} \right].$$

Two complementary approaches: Expansion in the interaction (e.g. the 'Hubbard U')

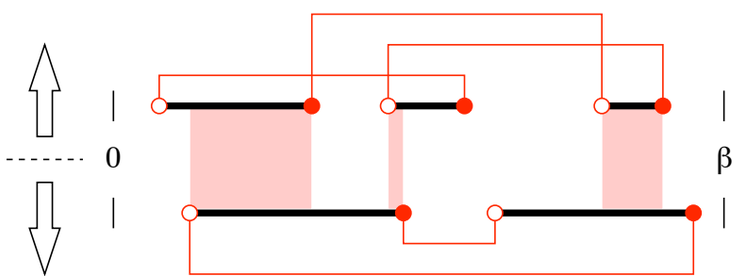


$$H = -\sum_{\langle ij \rangle, \sigma} t_{ij} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

Hopping exact

Expansion in the hybridization

Local Hamiltonian exact

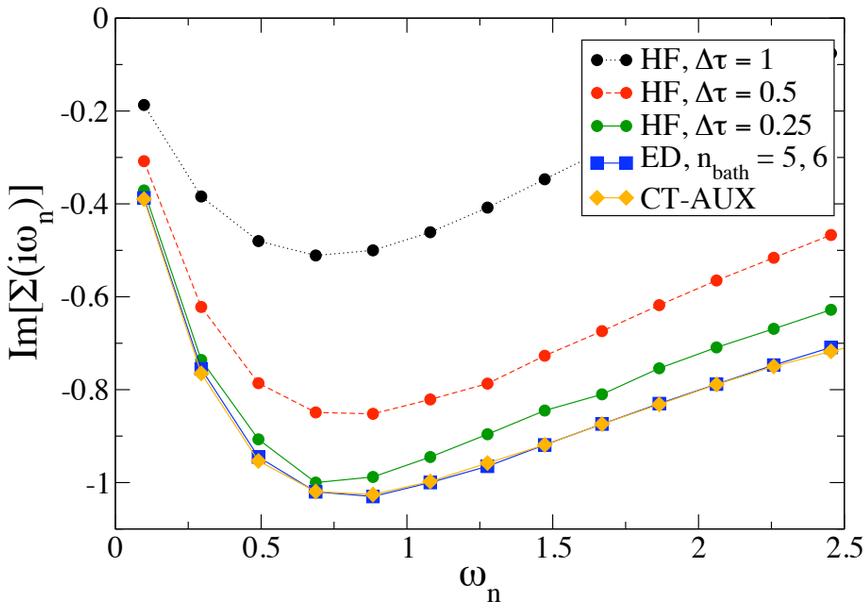


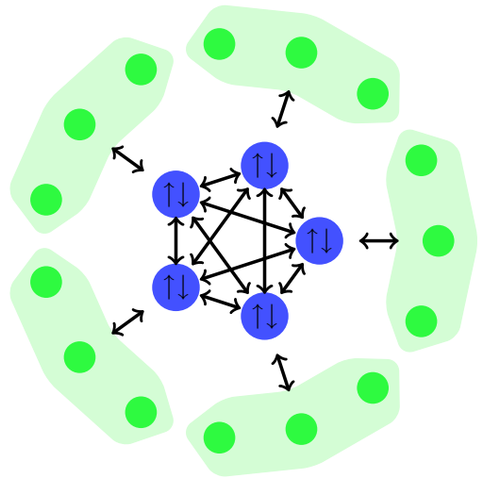
$$H = -\sum_{\langle ij \rangle, \sigma} t_{ij} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

Any analytical diagrammatic expansion can be converted into a QMC algorithm!

Advantages of Continuous Time QMC

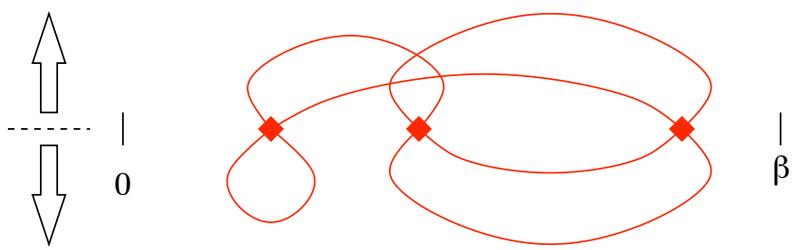
No Approximations



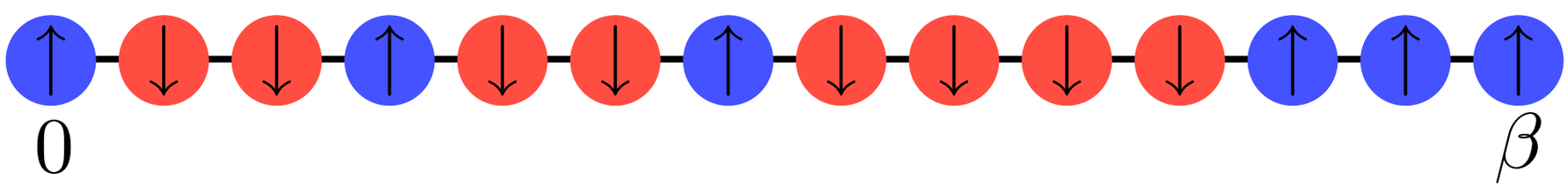


General interactions (e.g. exchange & pair hopping), new physics

Speedup of about a factor of 10^3:

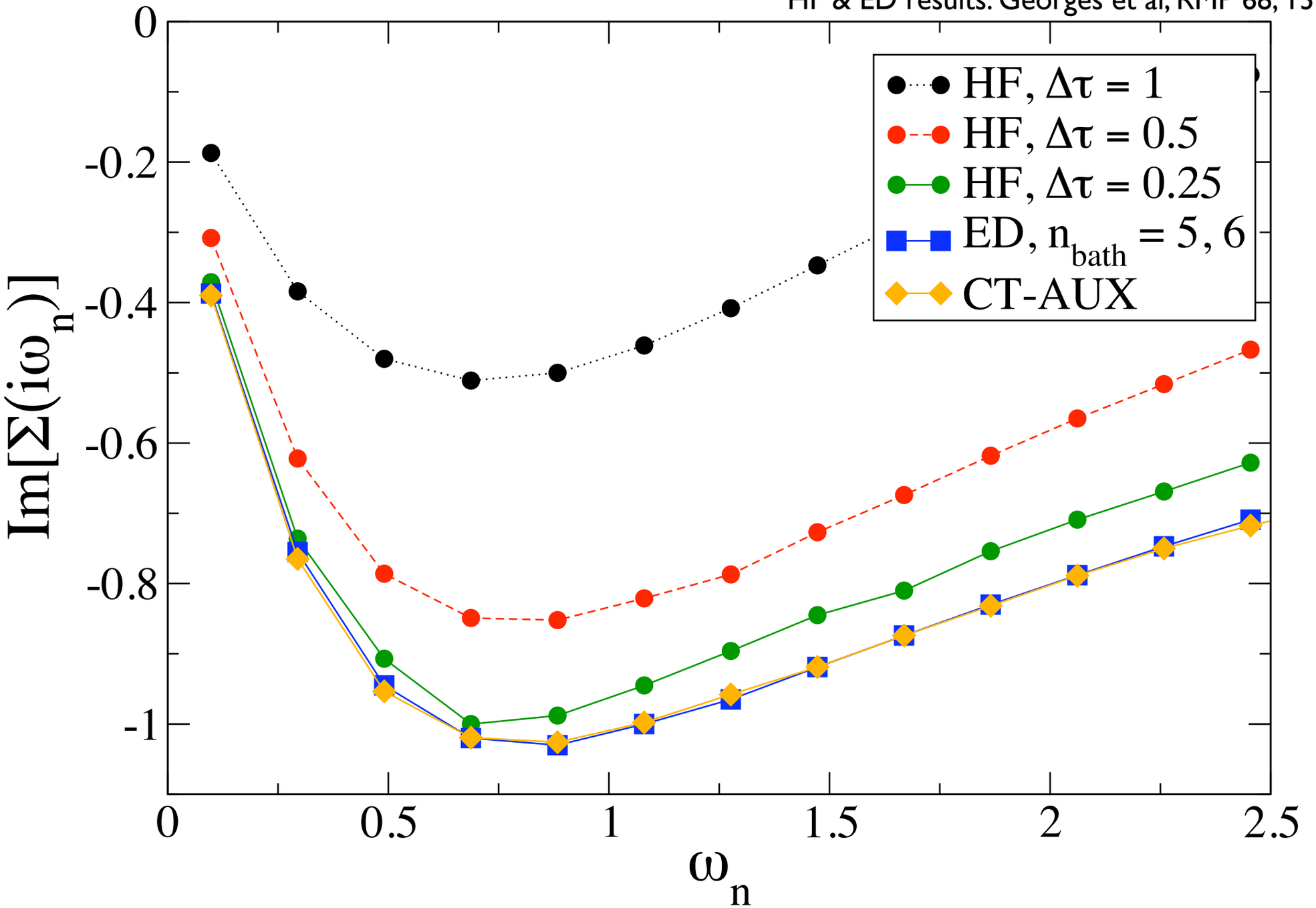


Intuitive picture: Smooth functions (diagrams) need to be approximated by a discretized version; resolution needs to be about 10 times larger than the features. Numerical effort is cubic ($O(N^3)$) for all algorithms



Discretization Errors

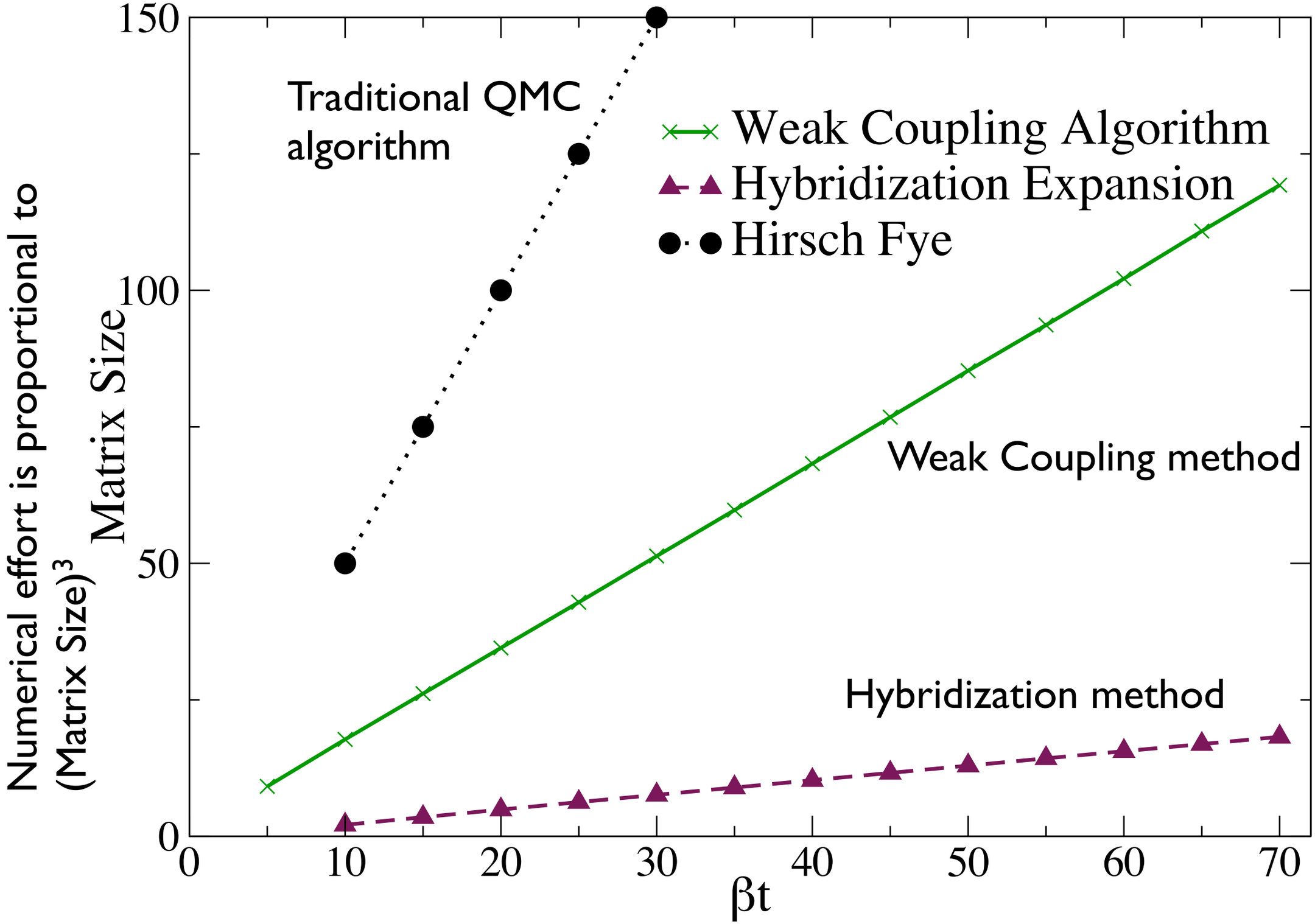
HF & ED results: Georges et al, RMP 68, 13 (1996)



No discretization of the imaginary time interval as in Hirsch-Fye is necessary, extrapolation is avoided from the start.

Gull, Werner, Troyer, Millis, Phys. Rev. B **76**, 235123 (2007)

Performance Comparison



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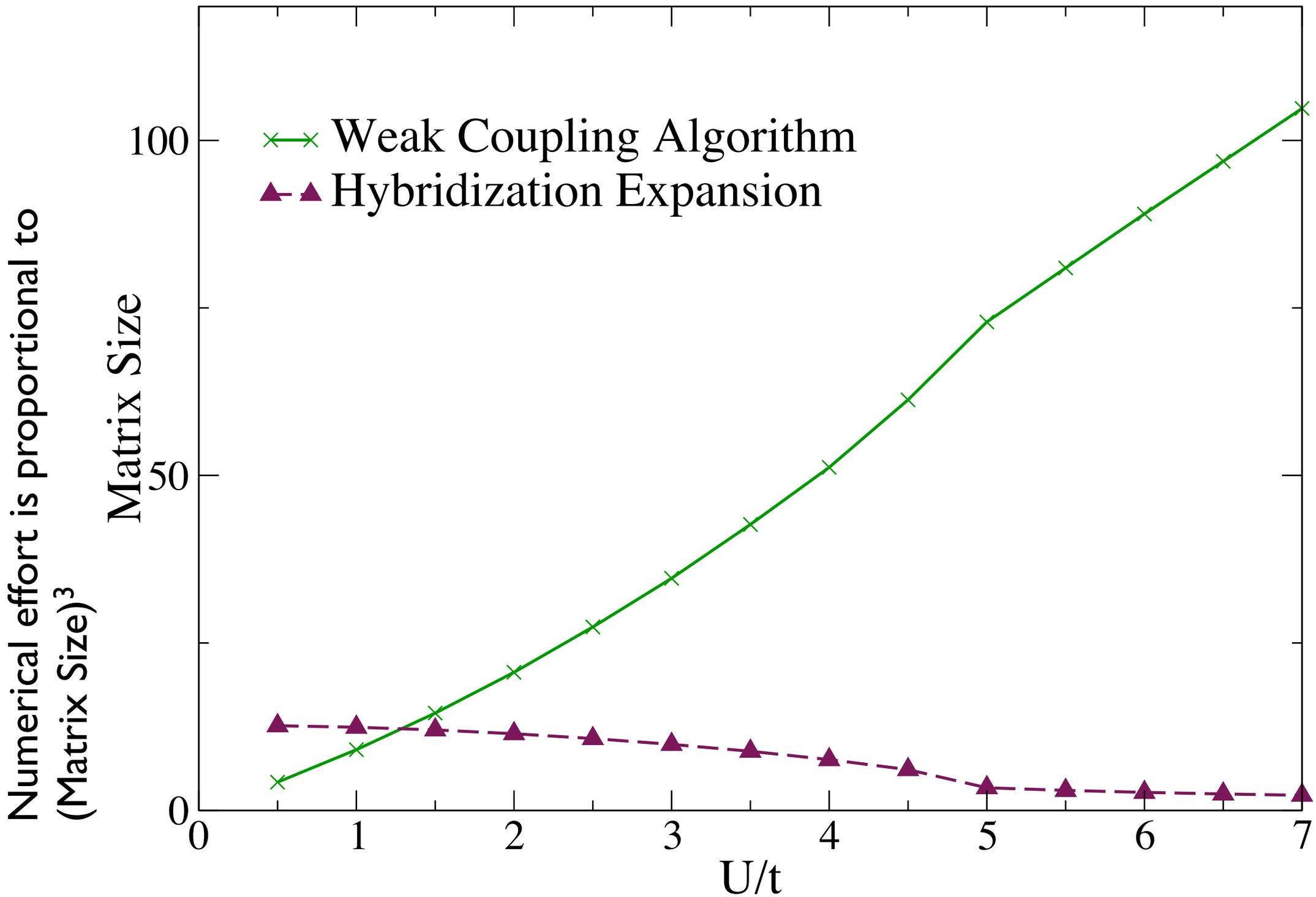

A. N. Rubtsov and A. I. Lichtenstein, JETP Letters **80**, 61 (2004)

Weak Coupling Algorithm

Weak coupling partition function expansion (SIAM):

$$\frac{Z}{Z_0} = \sum_{k=0}^{\infty} \frac{(-U)^k}{k!} \iiint_0^\beta d\tau_1 \cdots d\tau_k \sum_{s_1 \cdots s_k} \prod_{\sigma} \langle T_\tau [n_{\sigma_1}(\tau_1) - \alpha_{s_1 \sigma_1}] \cdots [n_{\sigma_k}(\tau_k) - \alpha_{s_k \sigma_k}] \rangle$$

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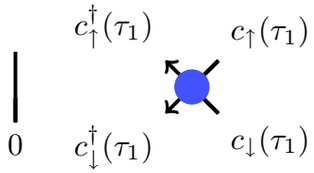

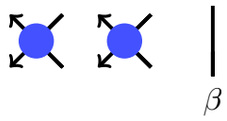

Location of interaction vertices

A. N. Rubtsov and A. I. Lichtenstein, JETP Letters **80**, 61 (2004)

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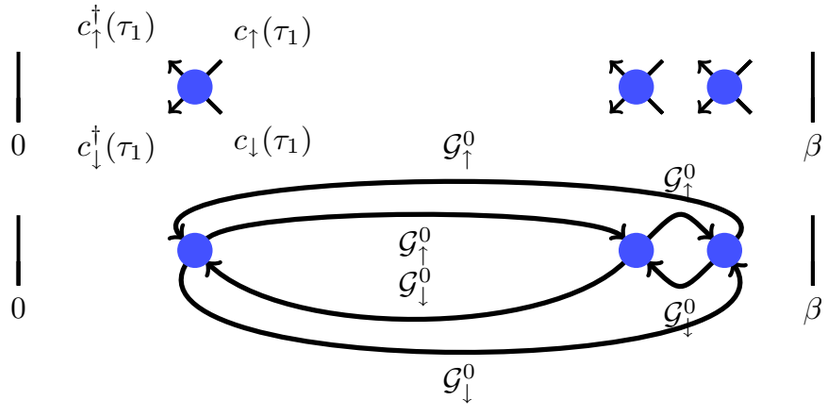

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Green's function lines

A. N. Rubtsov and A. I. Lichtenstein, JETP Letters **80**, 61 (2004)

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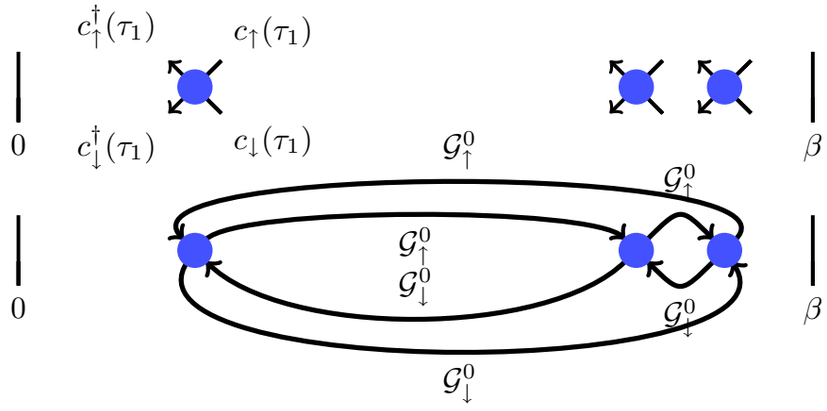

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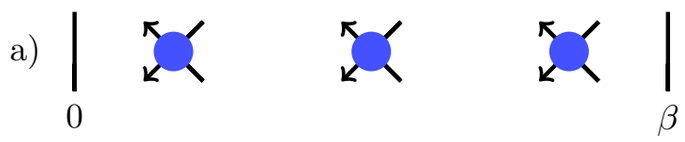
Monte Carlo sampling process:



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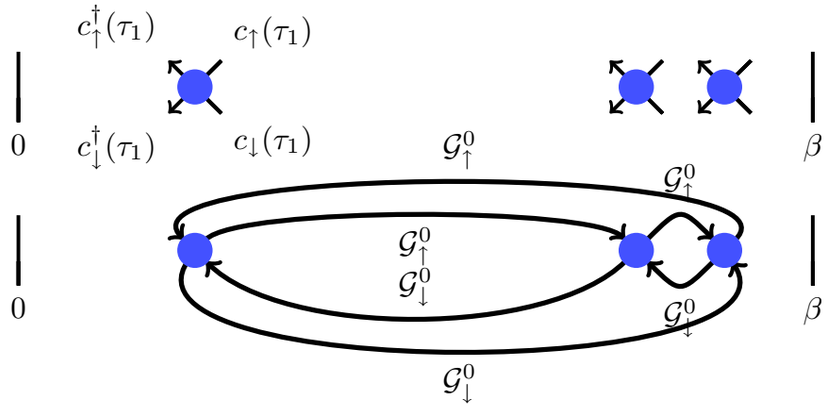
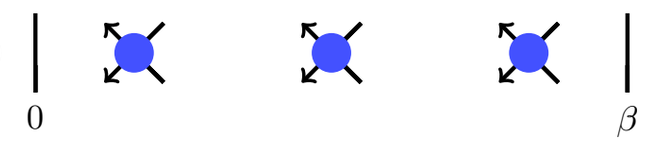


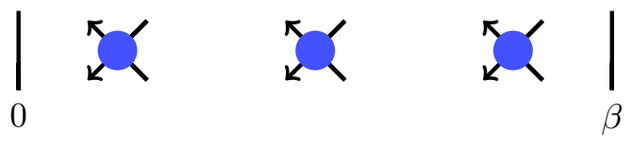
Location of interaction vertices

Green's function lines

b) 

Vertex insertion.

Monte Carlo sampling process:

a) 

A. N. Rubtsov and A. I. Lichtenstein, JETP Letters **80**, 61 (2004)

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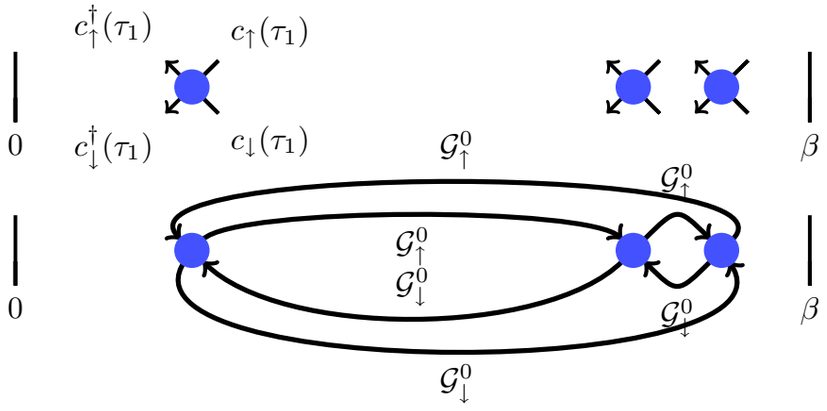

Location of interaction vertices

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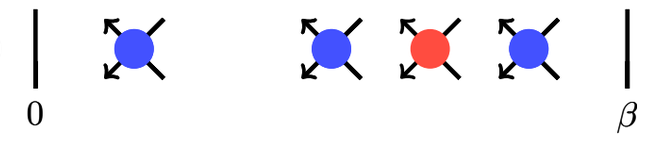
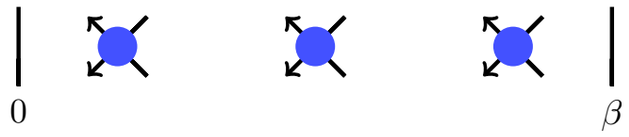
b) 

Vertex insertion.

Monte Carlo sampling process:

a) 

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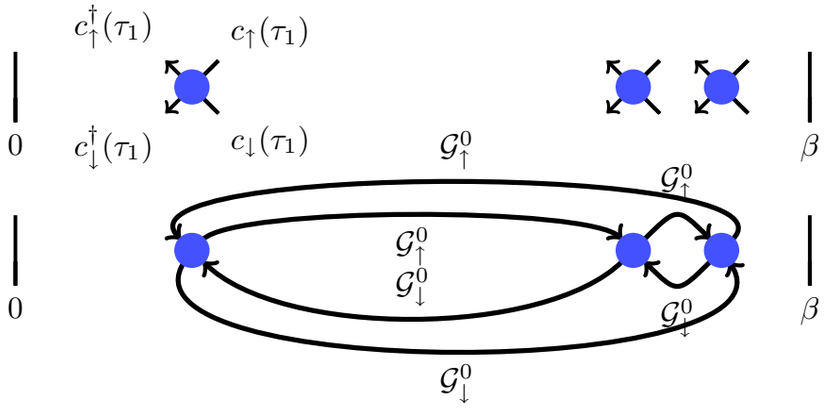

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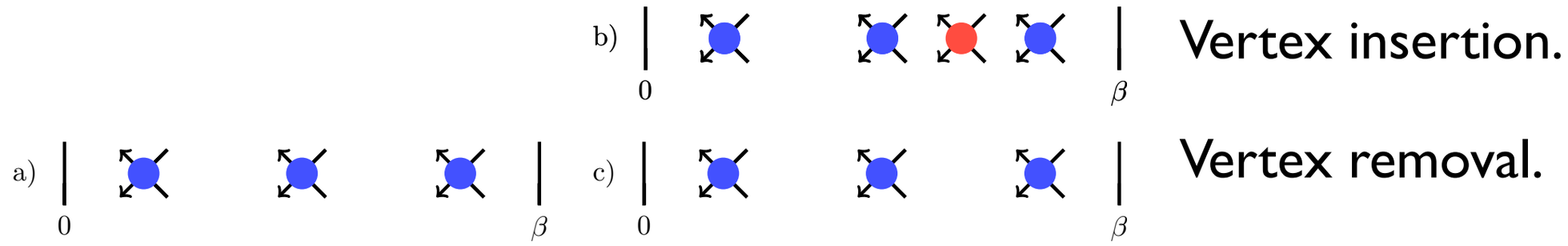

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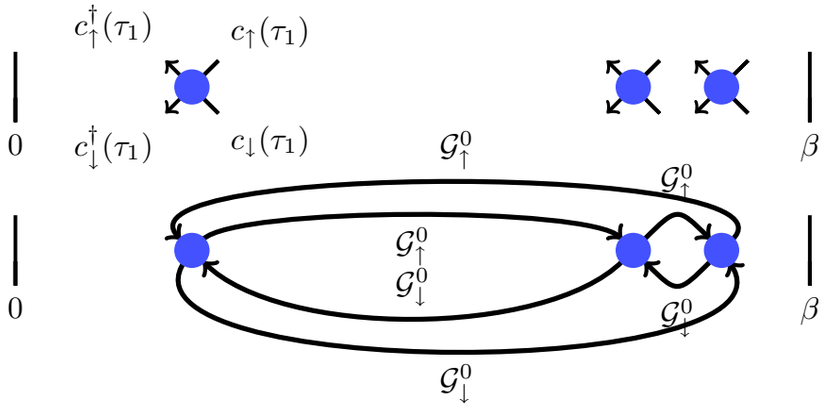

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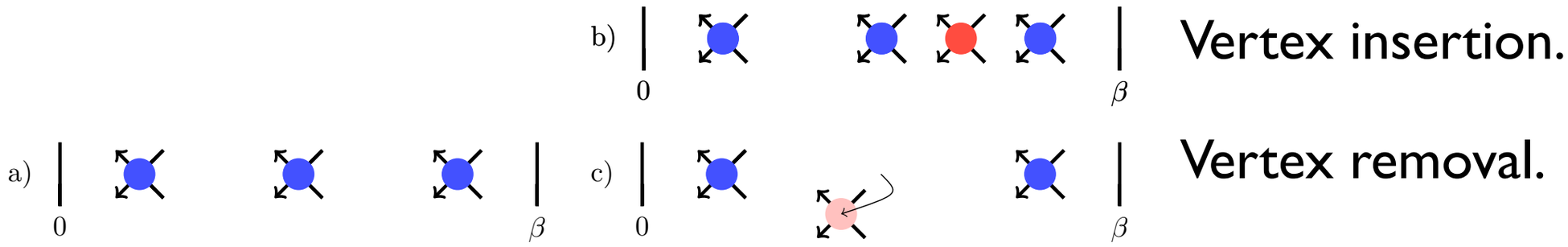

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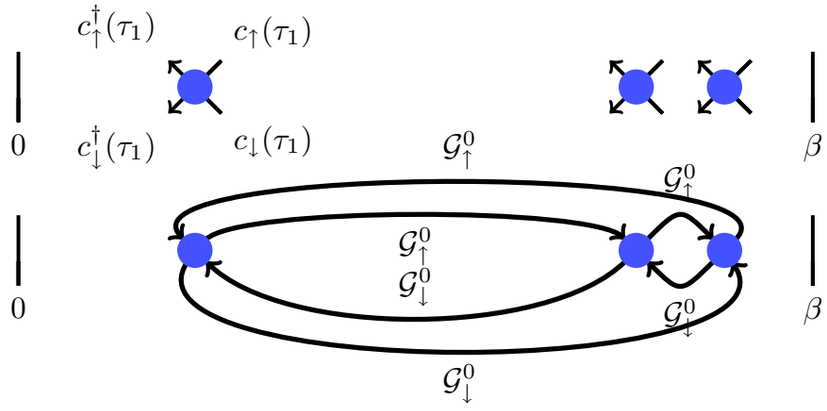

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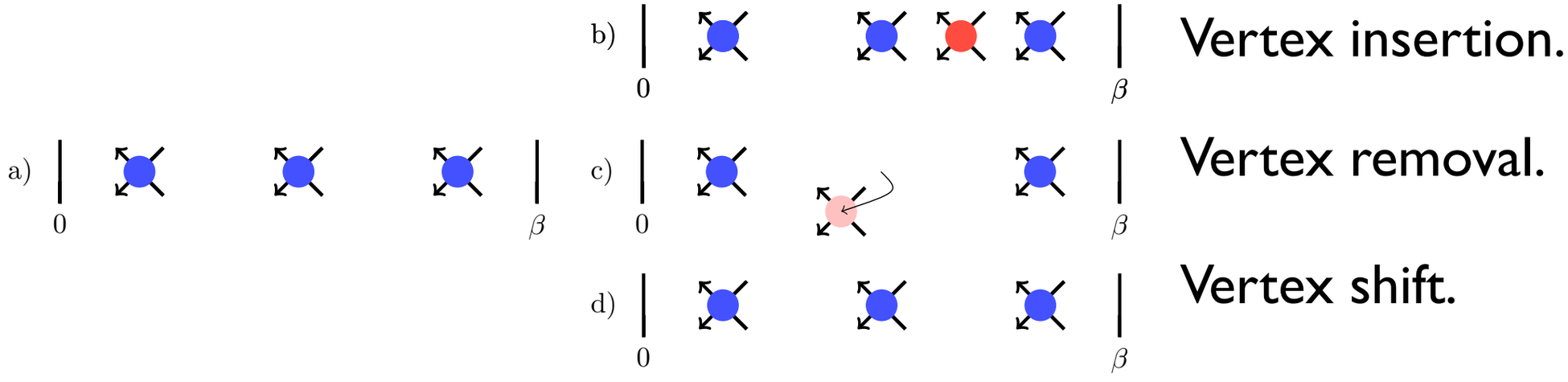

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Vertex shift.

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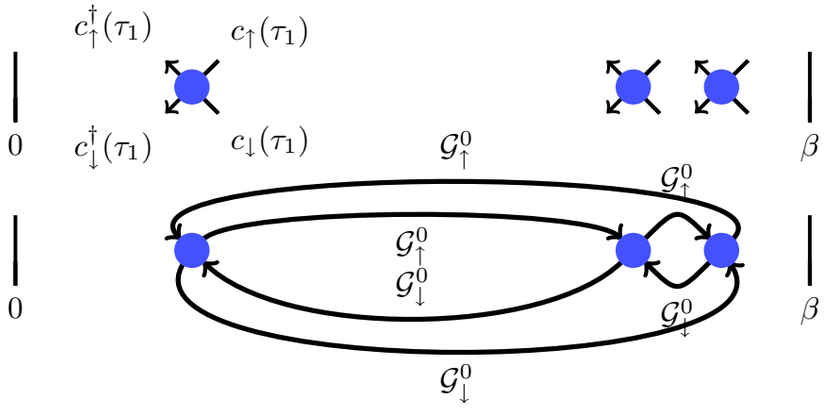

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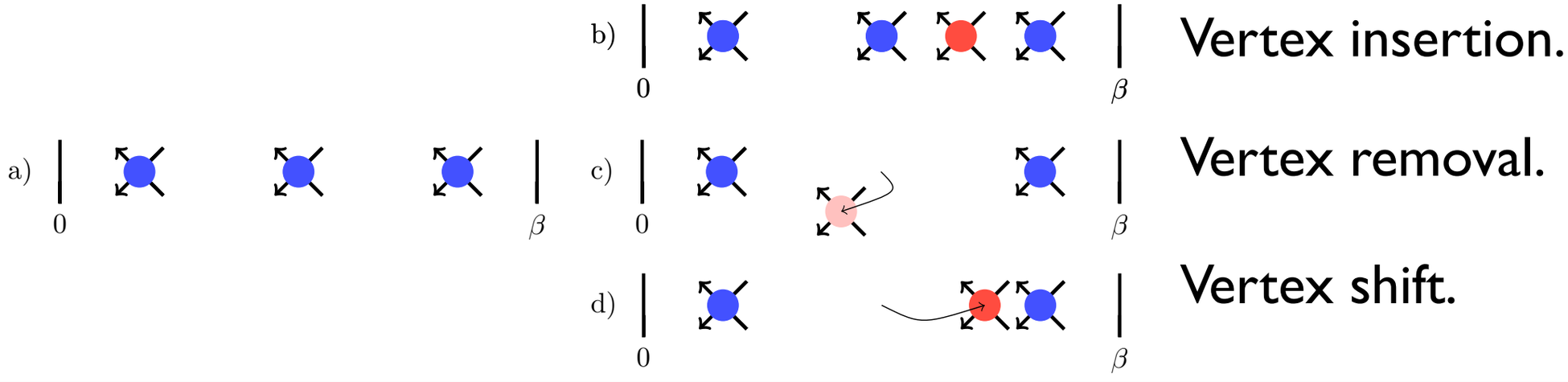

Vertex insertion.

Vertex removal.

Vertex shift.

Continuous-Time Auxiliary Field

Decoupling of the interaction with an auxiliary field:

$$1 - \frac{\beta U}{K}\left(n_{i\uparrow}n_{i\downarrow} - \frac{n_{i\uparrow}+n_{i\downarrow}}{2}\right) = \frac{1}{2}\sum_{s=\pm 1}\exp\left(\gamma s(n_{i\uparrow}-n_{i\downarrow})\right),$$

$$\cosh(\gamma) = 1 + \frac{U\beta}{2K}.$$

Partition function expansion in the interaction representation:

$$Z = \sum_{k=0}^{\infty}\sum_{s_1,\cdots s_k=\pm 1}\int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \left(\frac{K}{2\beta}\right)^k Z_k(\{s_k,\tau_k\}),$$

$$Z_k(\{s_i,\tau_i\}) \equiv \mathrm{Tr}\prod_{i=k}^{1}\exp(-\Delta\tau_i H_0)\exp(s_i\gamma(n_\uparrow - n_\downarrow)).$$

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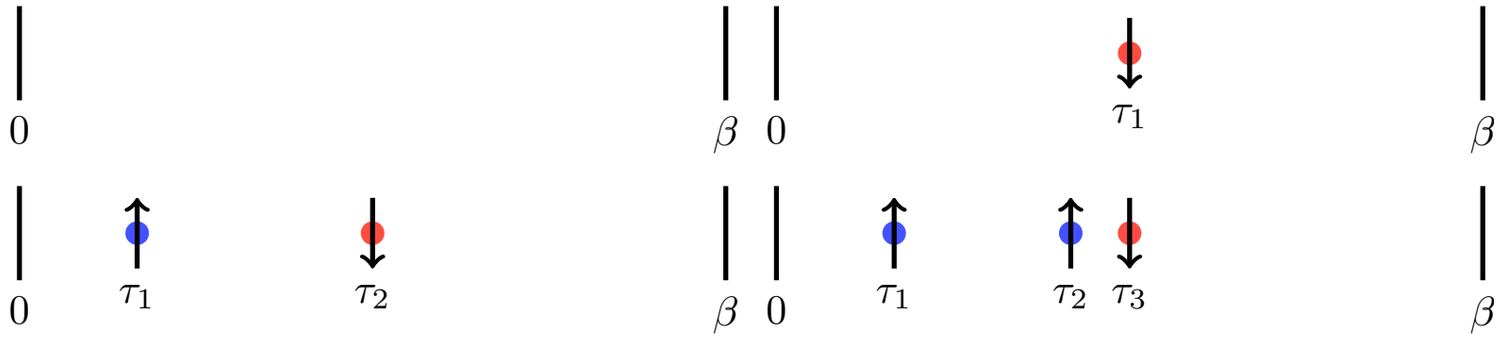
Diagrams of the partition function:



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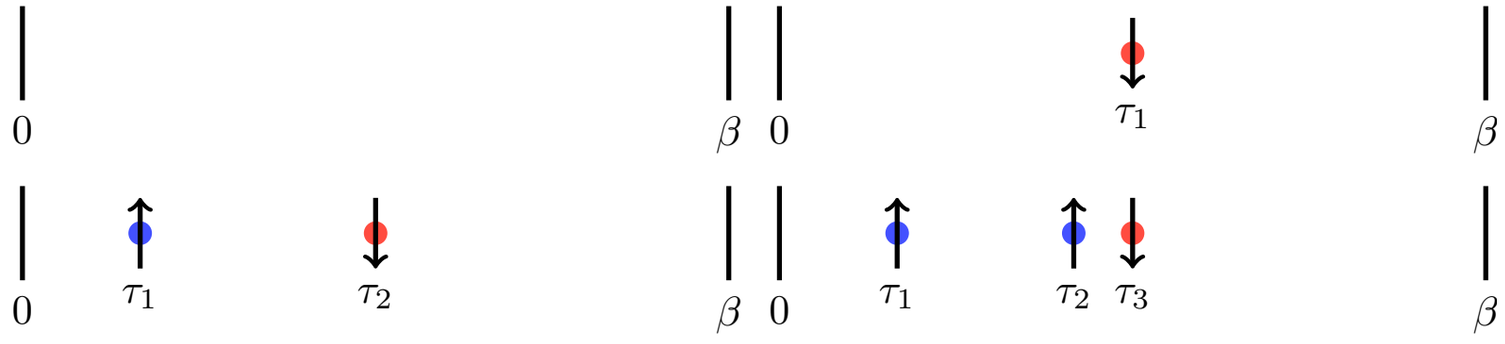
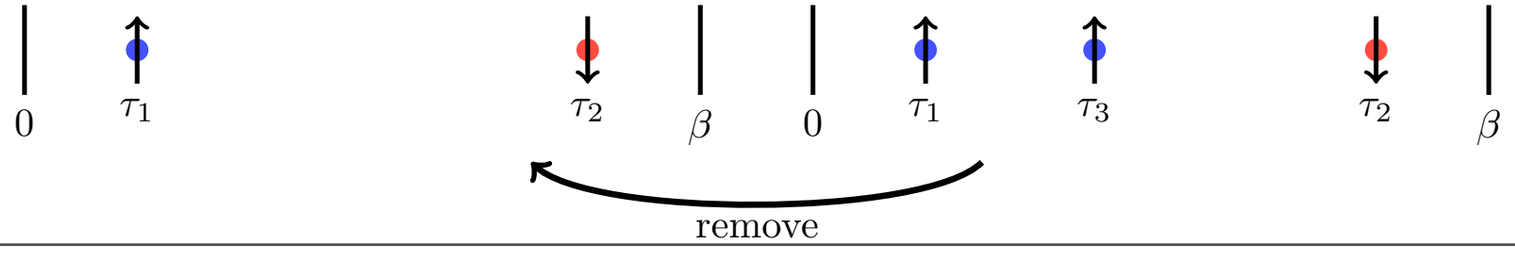


Monte Carlo Sampling:



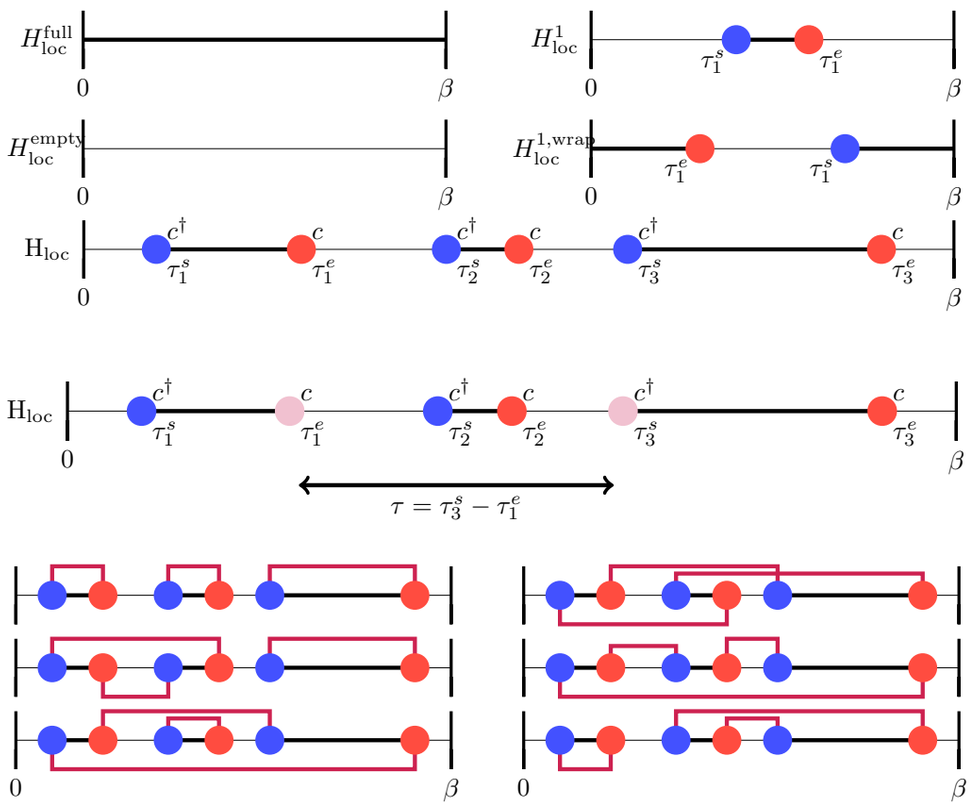
Hybridization Expansion

Expansion in the interaction representation, where $V = H_{mix}$, $H_0 = H_{loc}$. Density - density interactions.

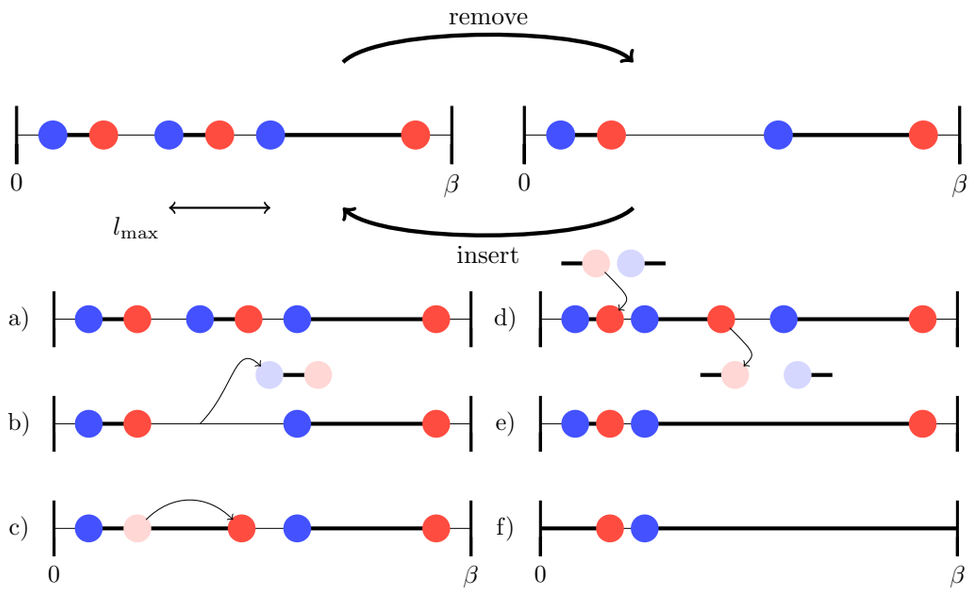
$$Z = \mathrm{Tr} e^{-\beta H} = \mathrm{Tr}\left[e^{-\beta H_0} T_\tau e^{-\int_0^\beta d\tau H_{\mathrm{mix}}(\tau)}\right]$$

$$= \sum_{k=0}^{\infty} \int d\tau_1 \cdots \int_{\tau_{k-1}}^{\beta} d\tau_k \mathrm{Tr}\left[e^{-\beta H_0} e^{\tau_k H_0}(-H_{\mathrm{mix}}) \cdots e^{-(\tau_2-\tau_1)H_0}(-H_{\mathrm{mix}}) e^{-\tau_1 H_0}\right]$$

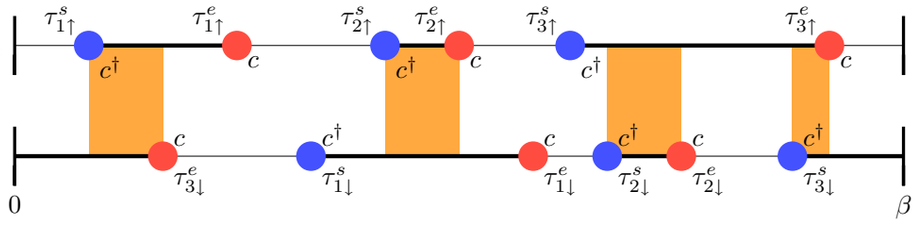
Configurations



Sampling Process



Interactions (density density)



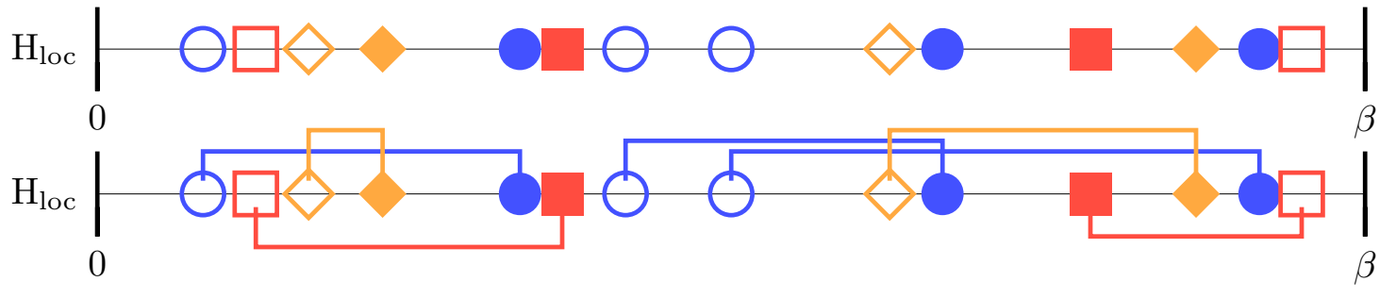
P. Werner and A.J. Millis, PRB **74**, 155107 (2006)
K. Haule, Phys. Rev. B **75**, 155113 (2007)

Hybridization - General Interactions

More complicated interactions (clusters, multiorbital, phonons, ...)?

Configuration of H_{loc}

Configuration of V



Matrix exponentials

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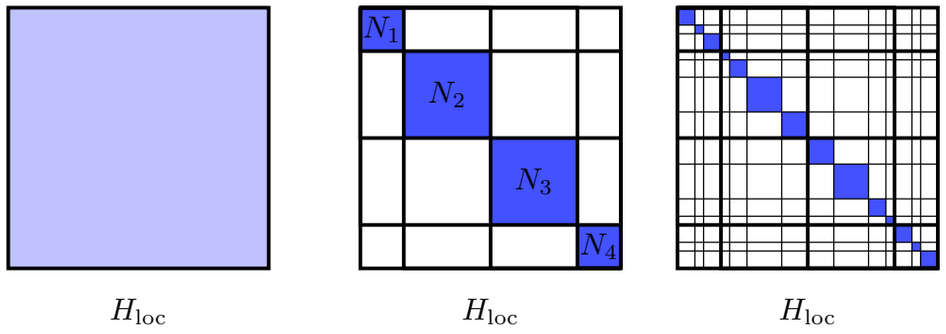
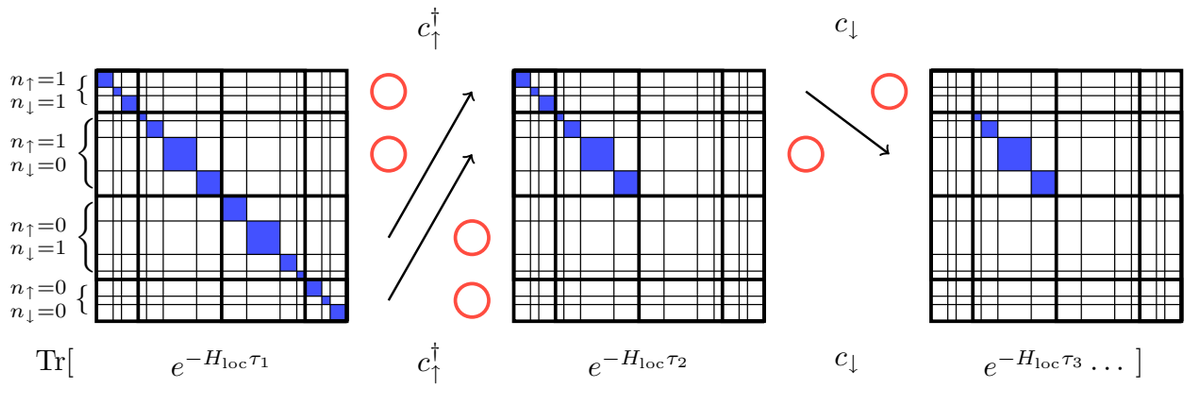
$$= \sum_{k=0}^{\infty} \int d\tau_1 \cdots \int_{\tau_{k-1}}^{\beta} d\tau_k \mathrm{Tr}\left[e^{-\beta H_0} e^{\tau_k H_0}(-H_{\mathrm{mix}}) \cdots e^{-(\tau_2-\tau_1)H_0}(-H_{\mathrm{mix}}) e^{-\tau_1 H_0}\right]$$

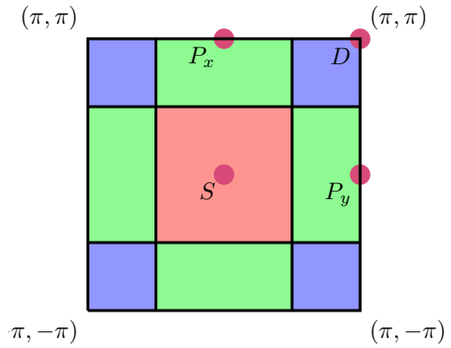
occupation number basis $[H_{\mathrm{loc}}, S_z] = 0 = [H_{\mathrm{loc}}, N]$ further symmetries

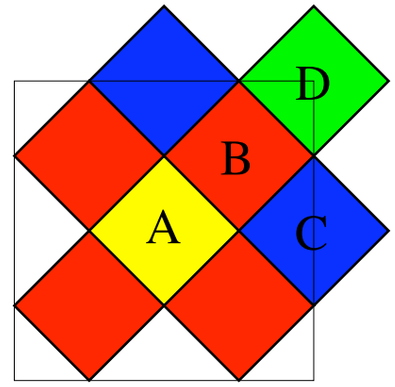


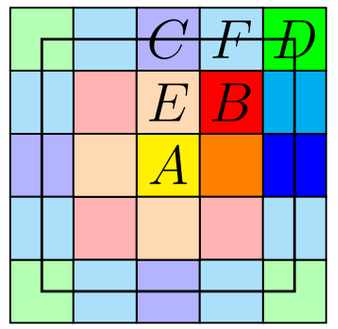


Choosing the appropriate Algorithm

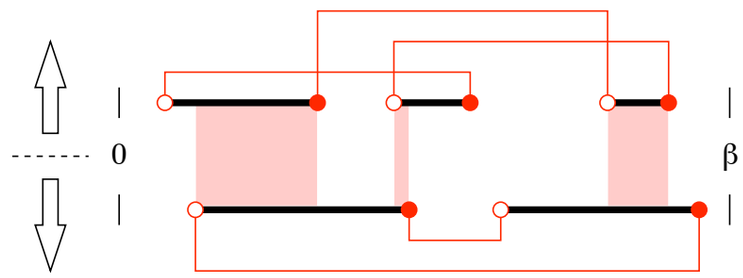
Large cluster calculations: Continuous-time auxiliary field method (up to 10x10 clusters)





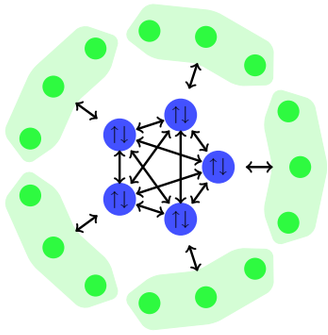


Problems with density density interactions, many orbitals: Hybridization expansion (linear in the number of orbitals)



Problems with general but weak interactions: Weak Coupling expansion

Problems with general interactions but few orbitals: Hybridization expansion.

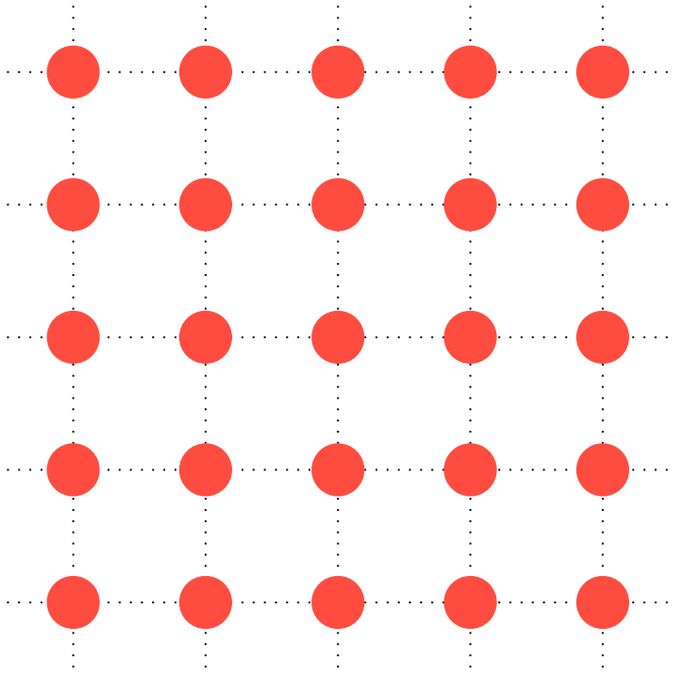


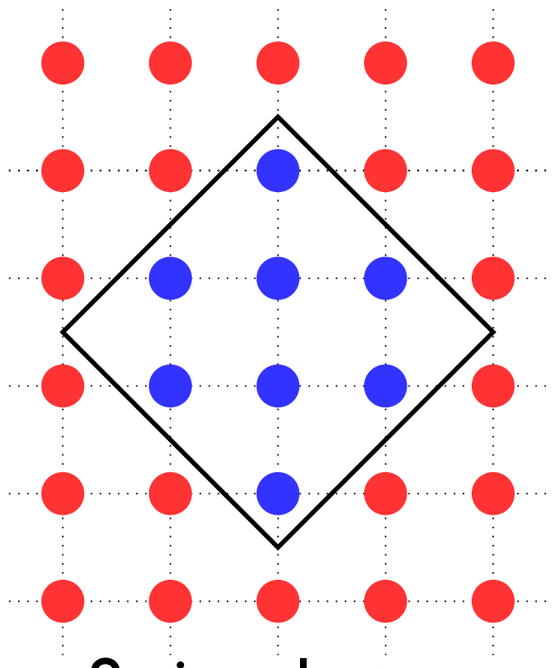
Cluster Dynamical Mean Field Theory

Maier et al., Rev. Mod. Phys. 77, 1027 (2005)

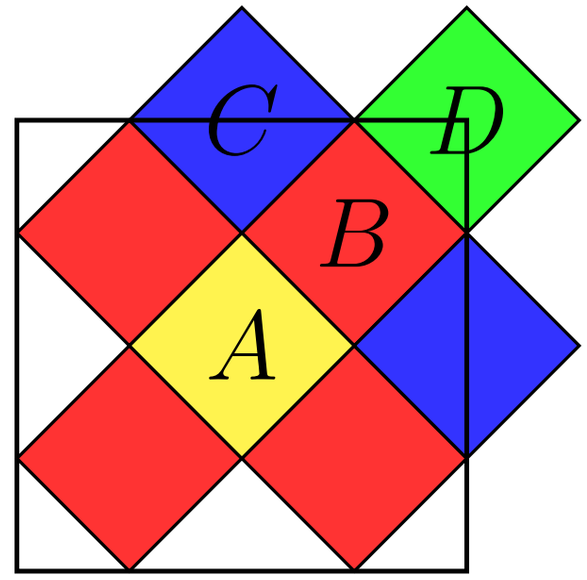
Hubbard model on 2d square lattice:

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow}.$$





8-site cluster



Tiling of the BZ

DCA: Hettler et al., Phys. Rev. B 58, R 7475 (1998)

Restriction to paramagnetic bath $\epsilon_p = -2t(\cos(p_x) + \cos(p_y)) - 4t' \cos(p_x)\cos(p_y)$

DCA self energy is chosen to be constant within patches of the Brillouin zone.

8-site (cluster): clear node / antinode distinction. Regions away from the Fermi surface (at zero and (π,π)) are not mixed in with regions around the FS.

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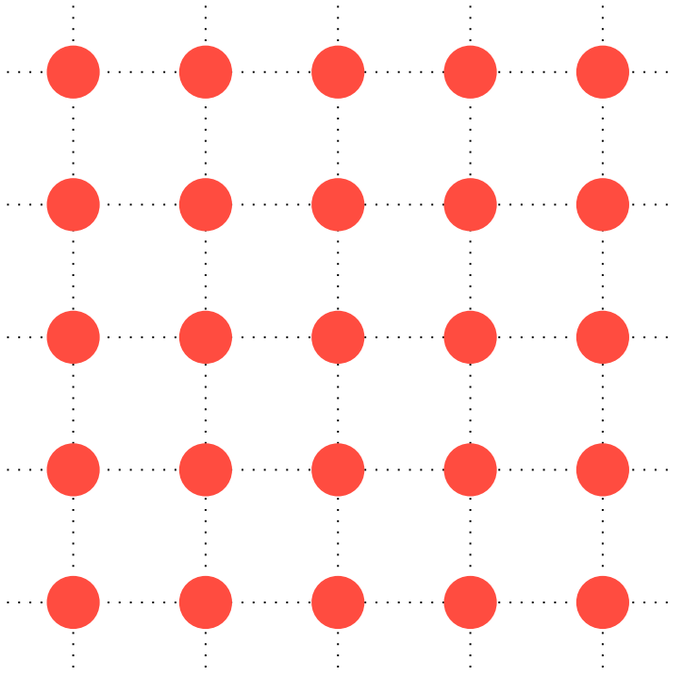

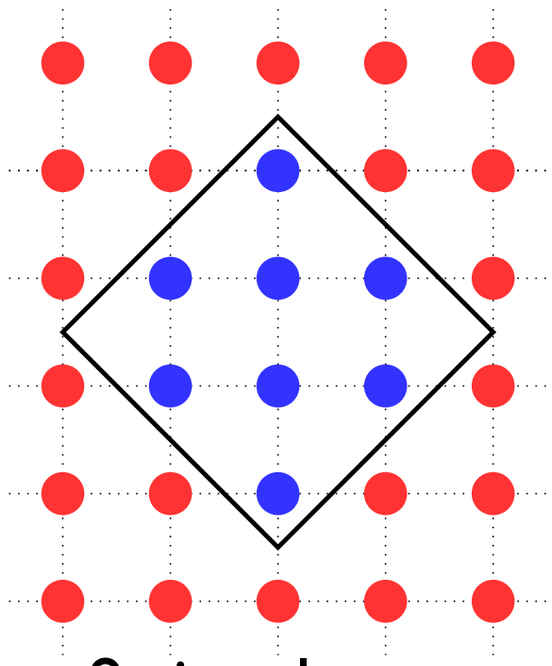

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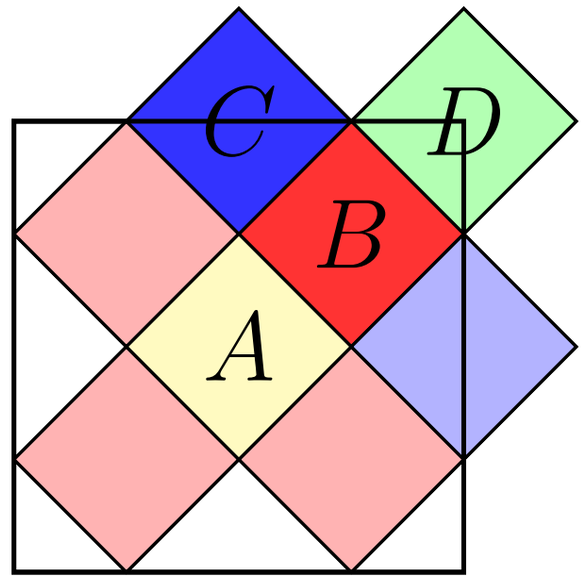

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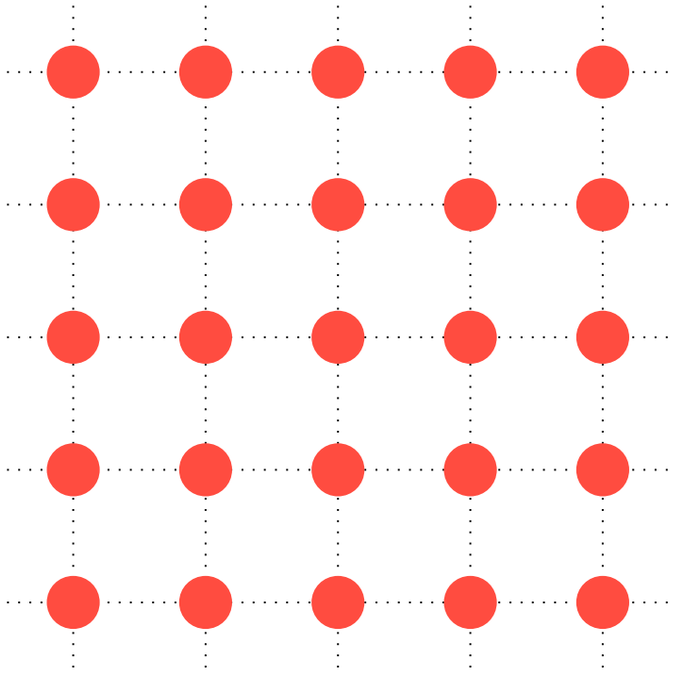
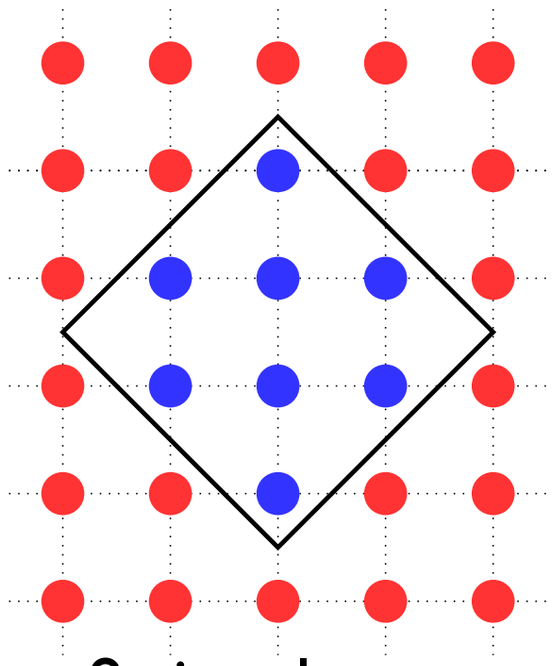
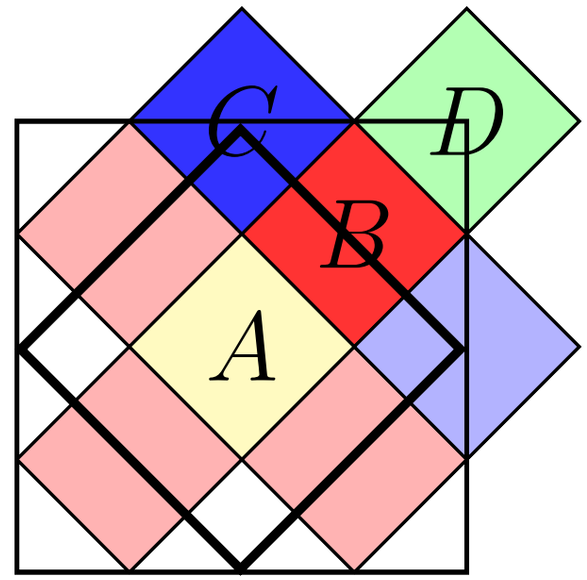




8-site cluster



t'=0
Tiling of the BZ

DCA: Hettler et al., Phys. Rev. B 58, R 7475 (1998)

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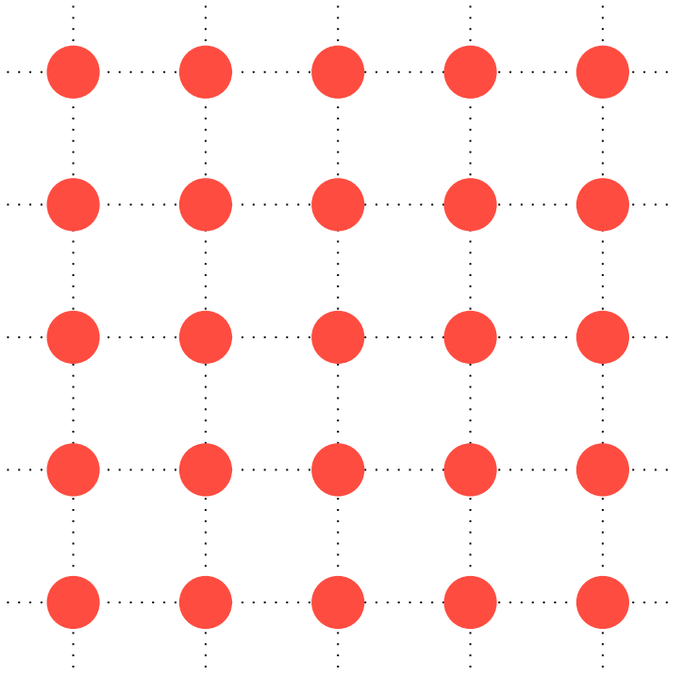

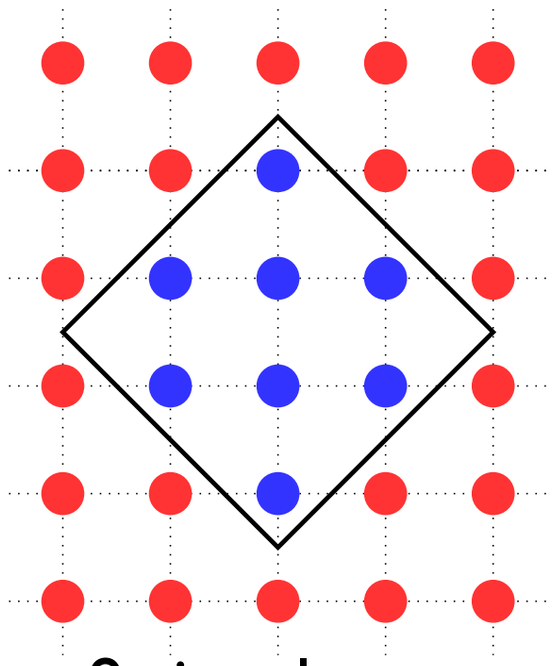

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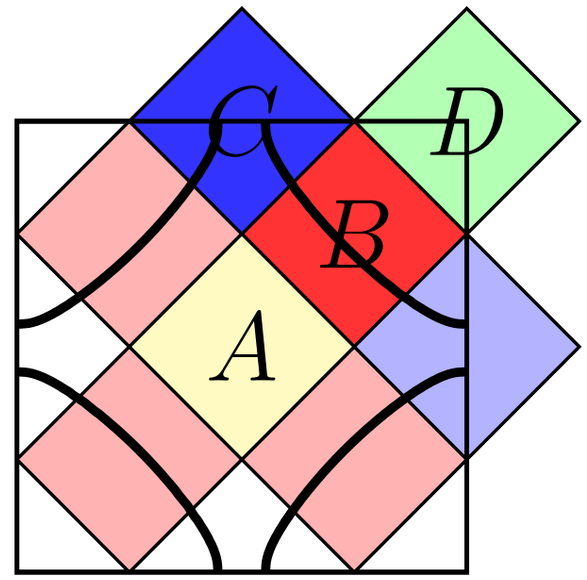

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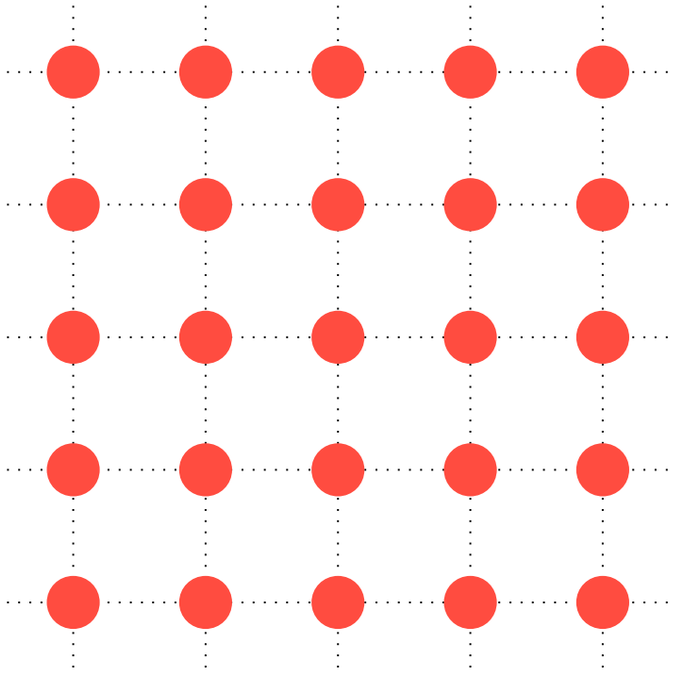

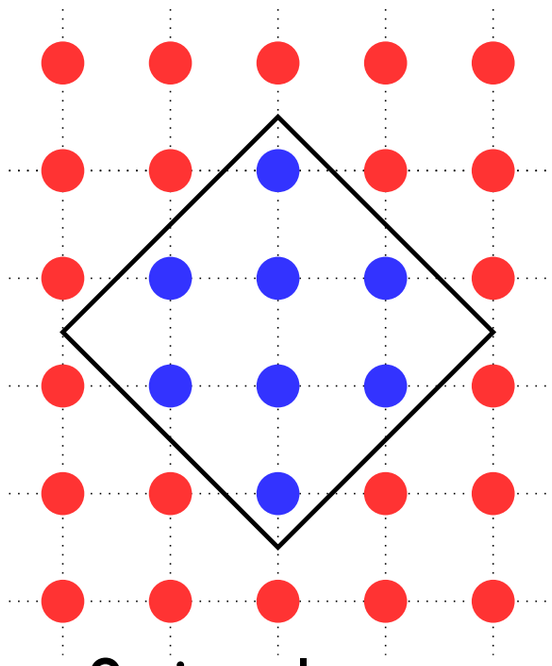

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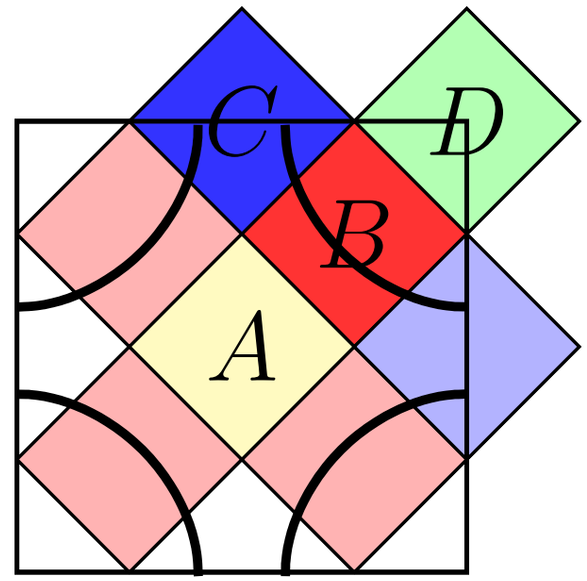

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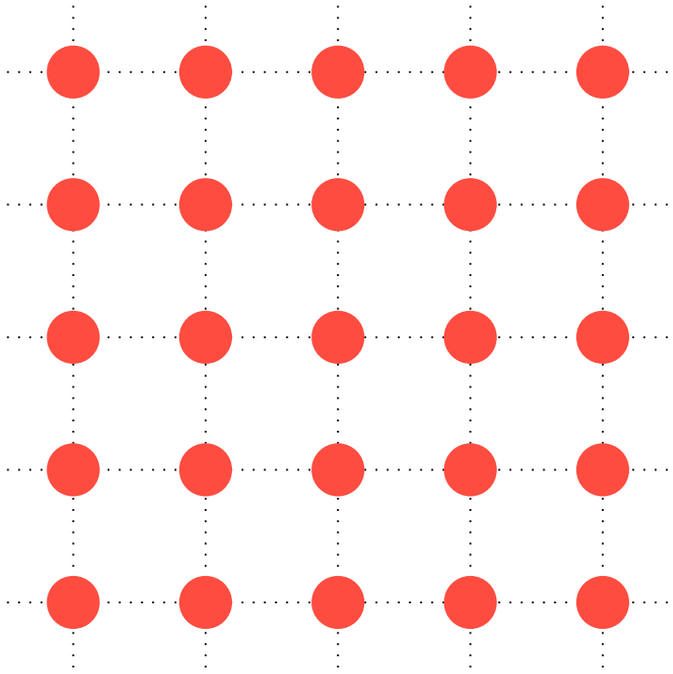

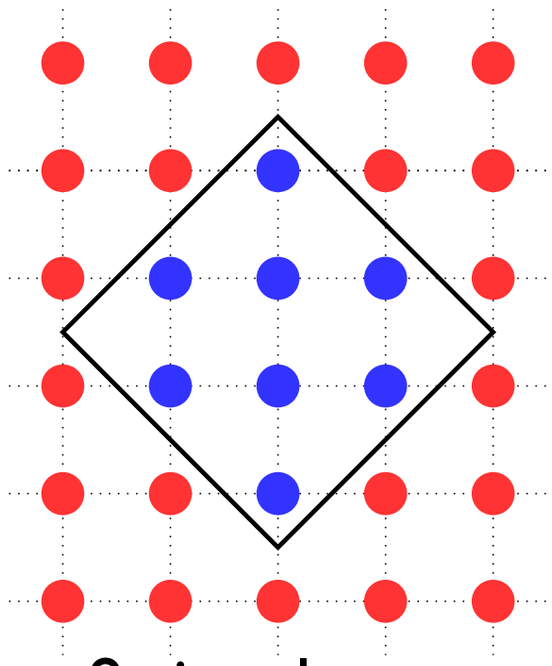

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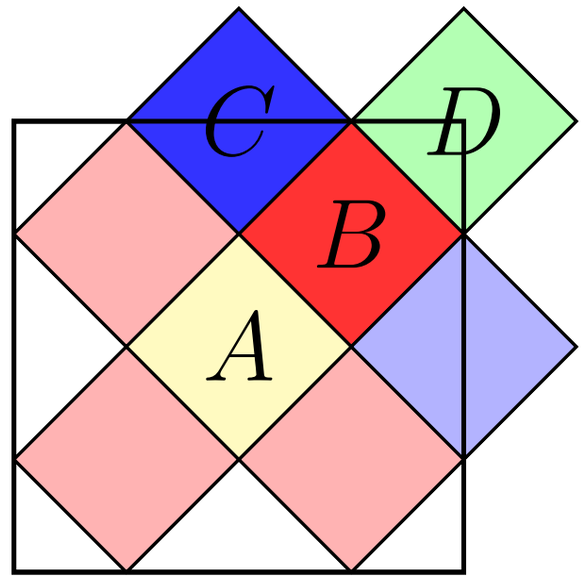

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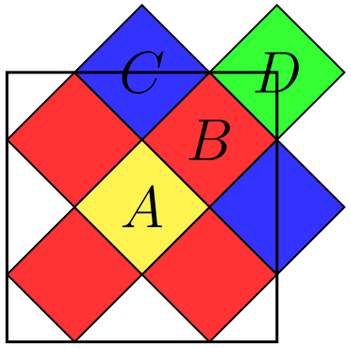
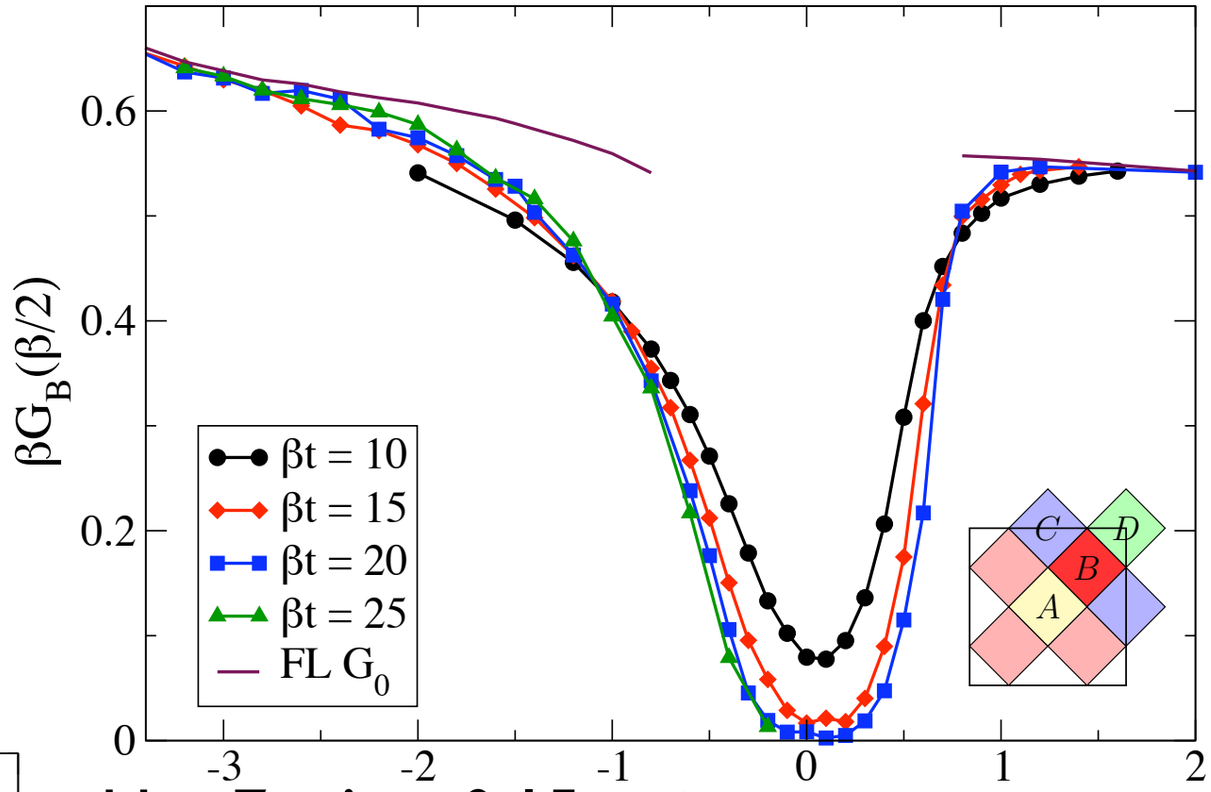


Results: Doping Driven Transition

Spectral function A(0) at the Fermi energy as a function of chemical potential exhibits clear crossing points.

Sector C transition occurs before sector B transition. Transitions coalesce on the electron doped side for larger t', but not on the hole doped side.



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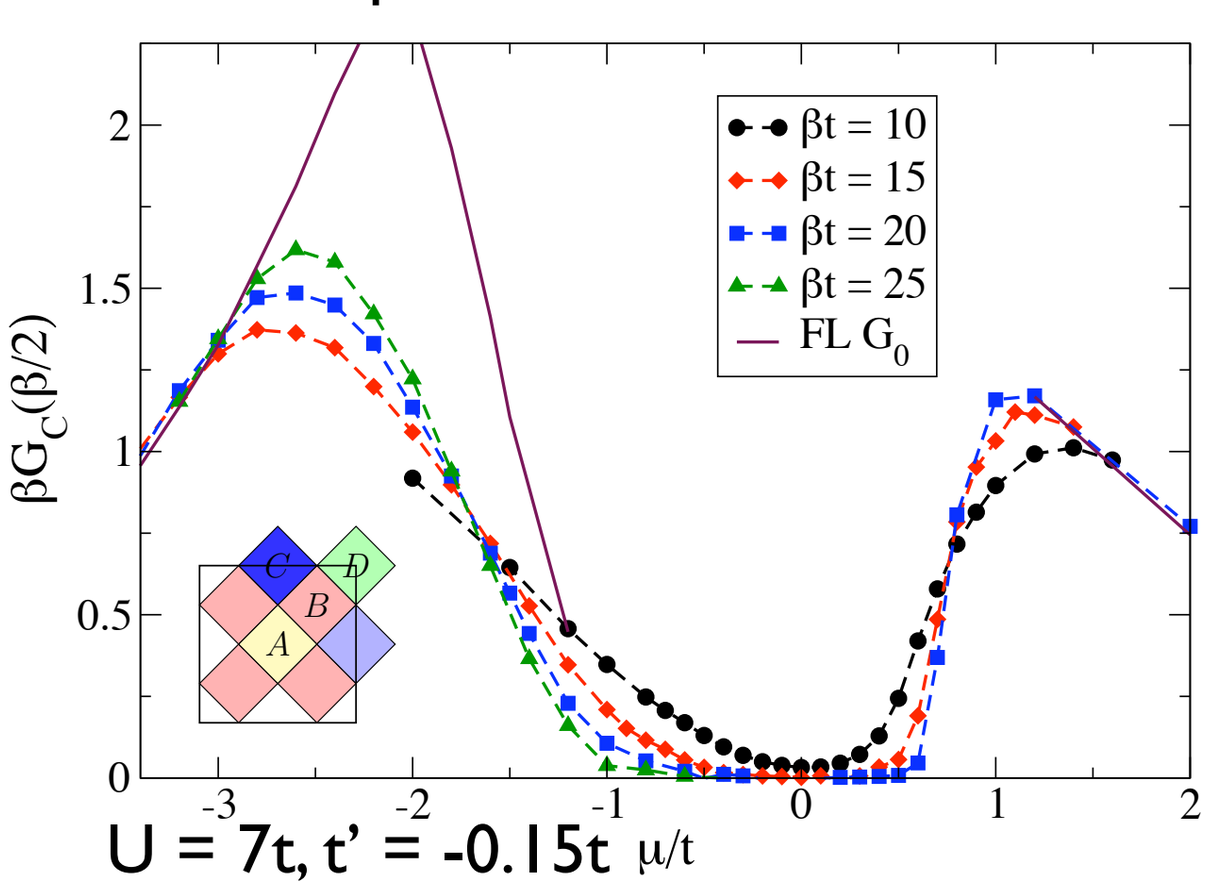

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For large electron and hole doping: behavior consistent with Fermi liquid theory.

For intermediate doping: A(0) is suppressed in comparison with FL, possible Non-FL phase in sector B.

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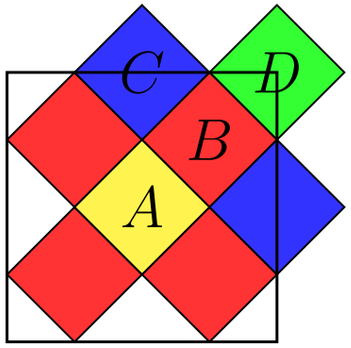

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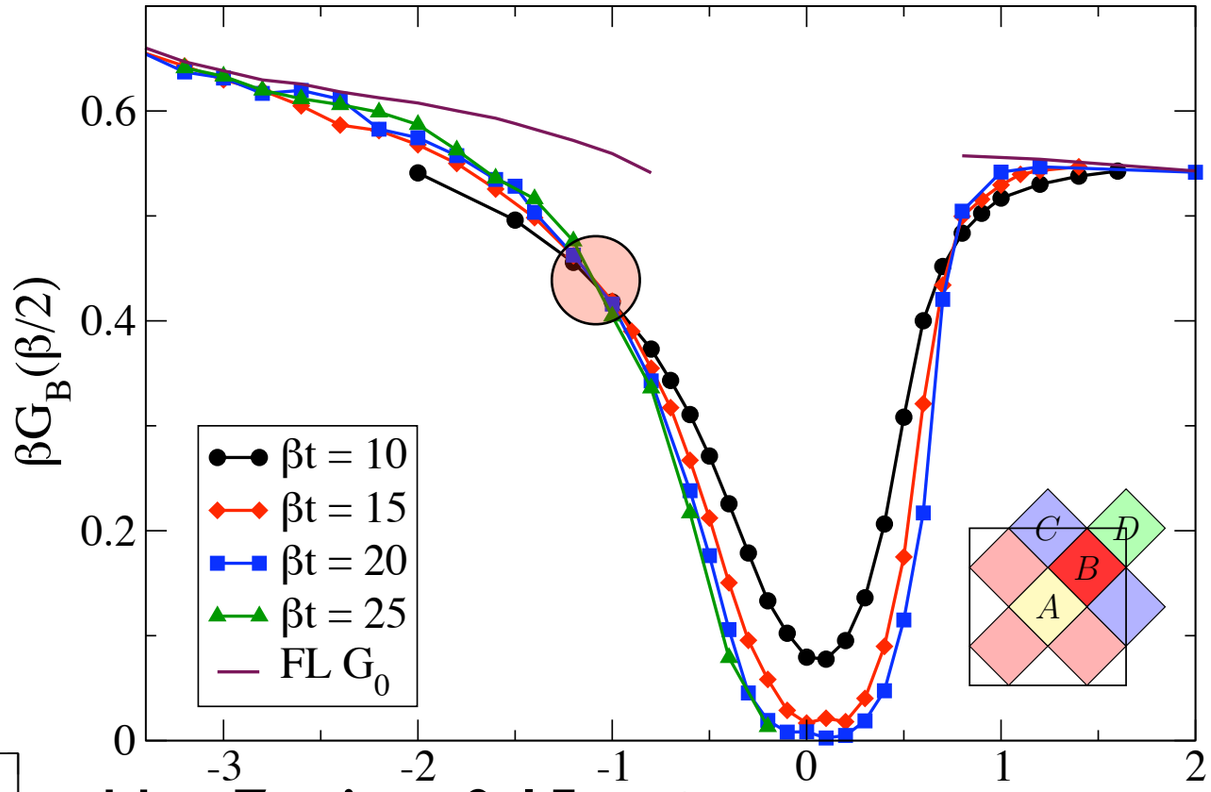

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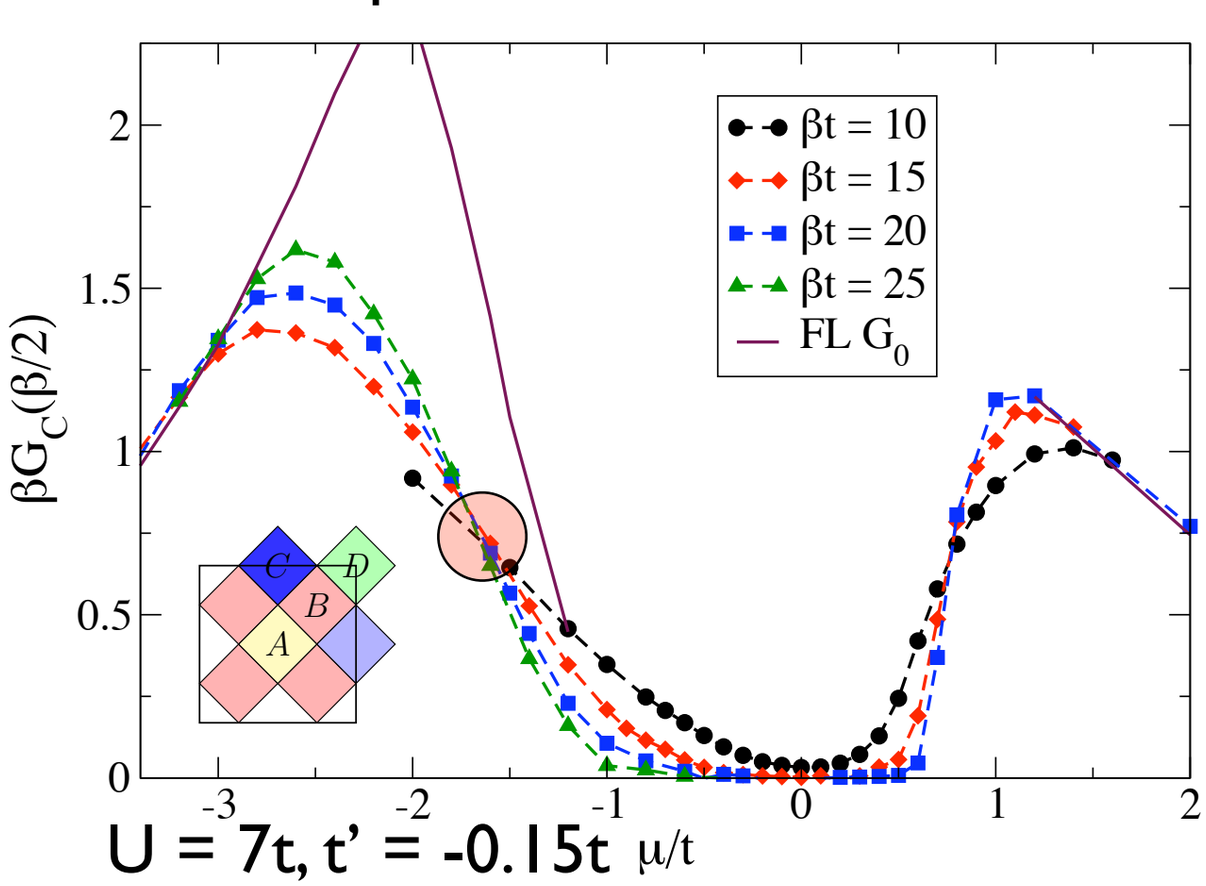

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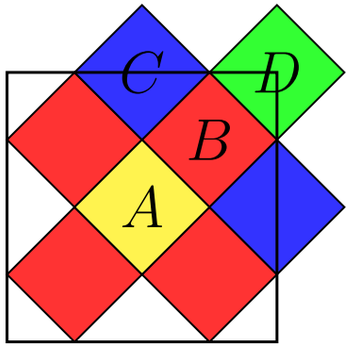

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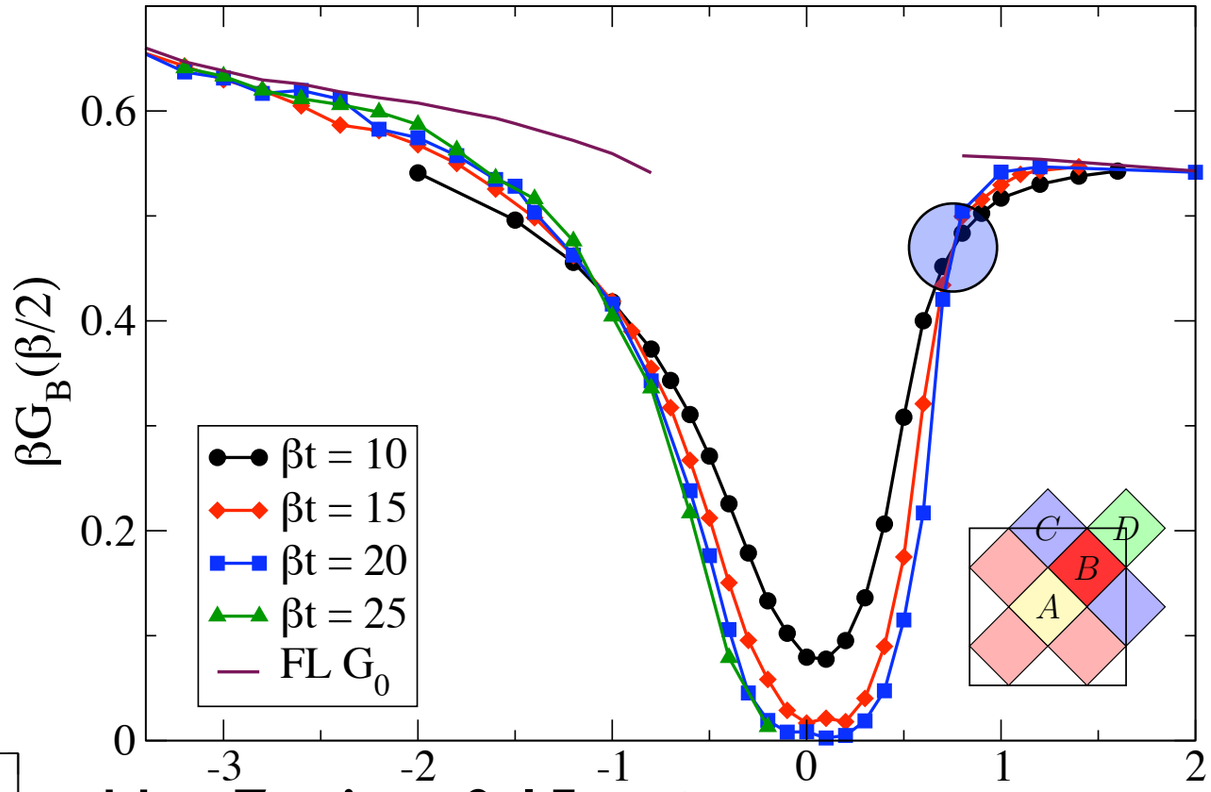

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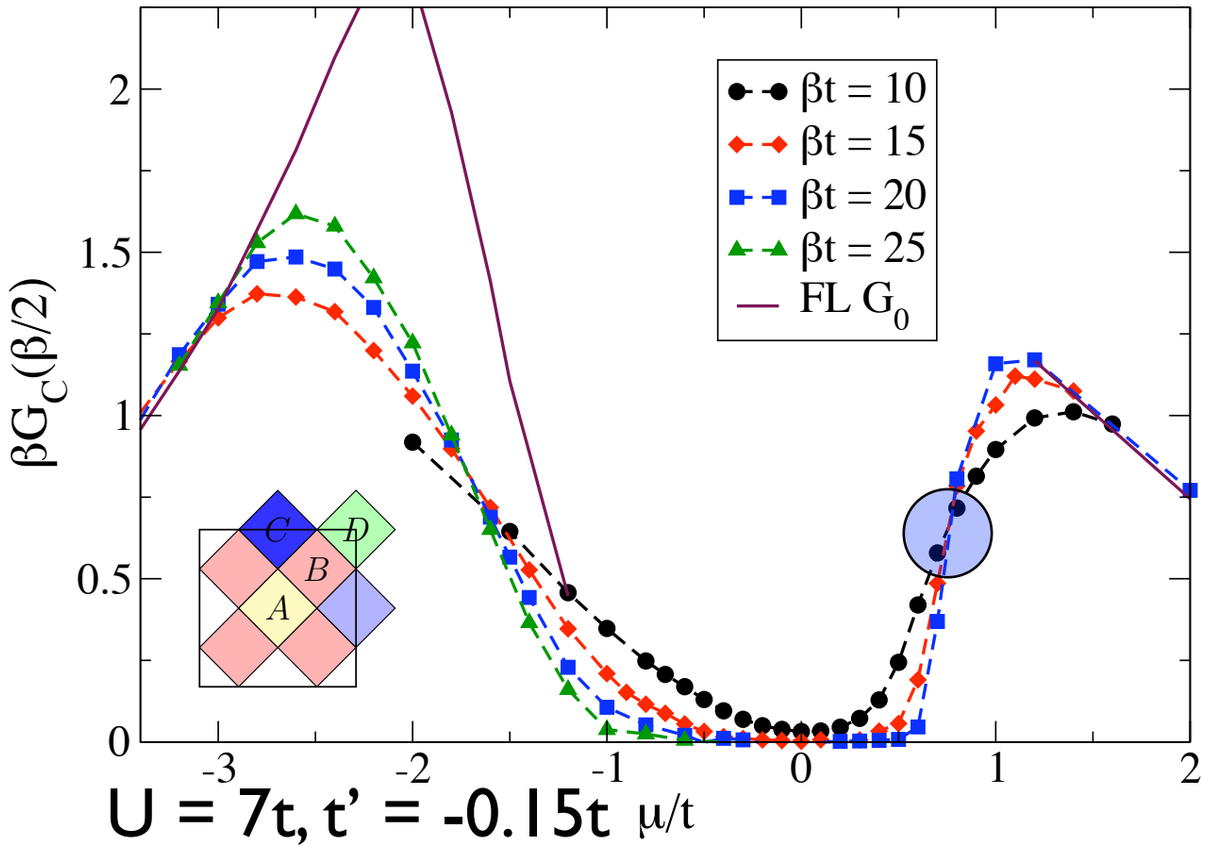

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Conclusions

For a review on continuous-time algorithms see my PhD thesis
http://e-collection.ethbib.ethz.ch/view/eth:31103

Open source codes: In preparation, will be published this summer as part of the ALPS (alps.comp-phys.org) libraries.

New algorithms allow access to new physics: Larger systems, extrapolation to the infinite system, general interactions, and more orbitals.