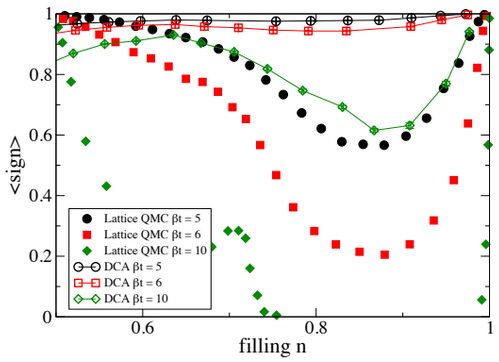
Introduction to CT-QMC

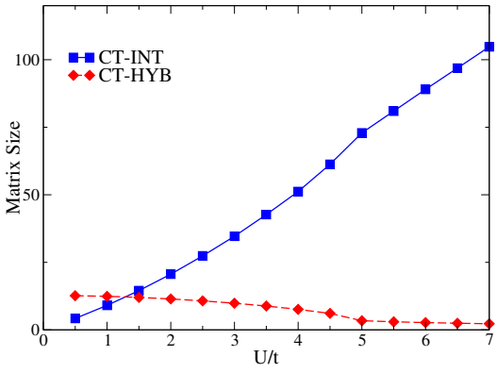
Emanuel Gull

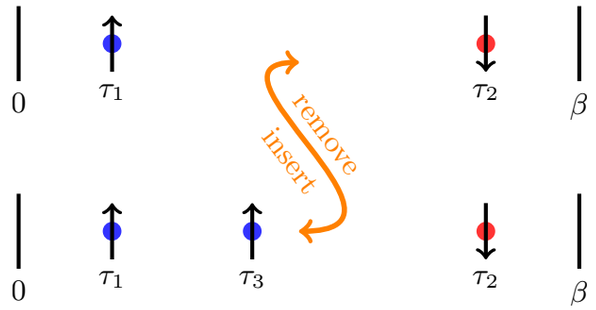
Vienna, September 01 2013

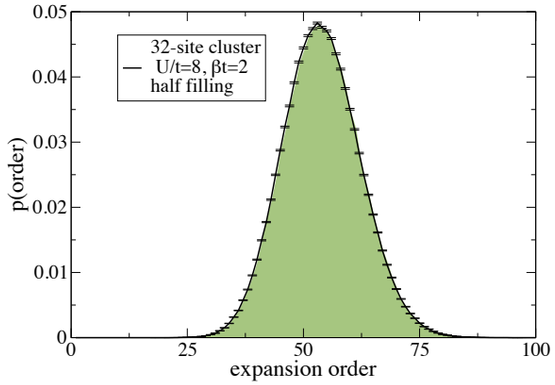
Outline

What is CT-QMC?

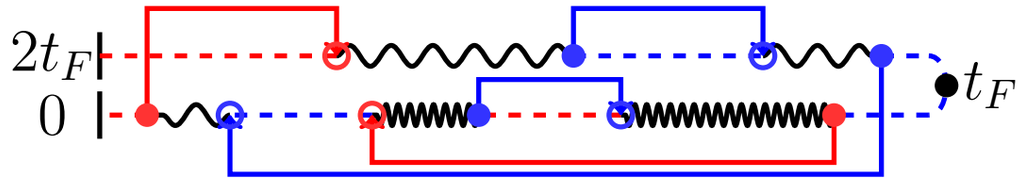




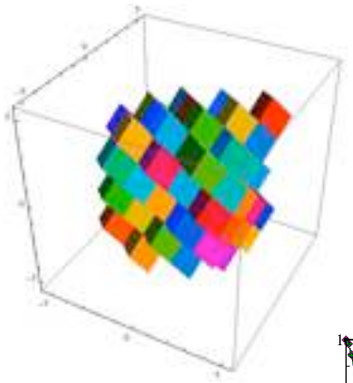


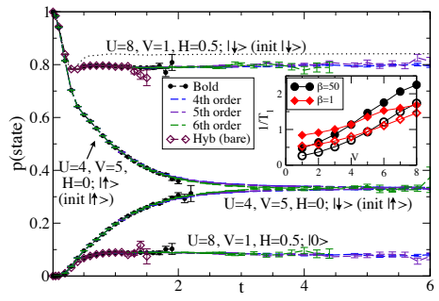


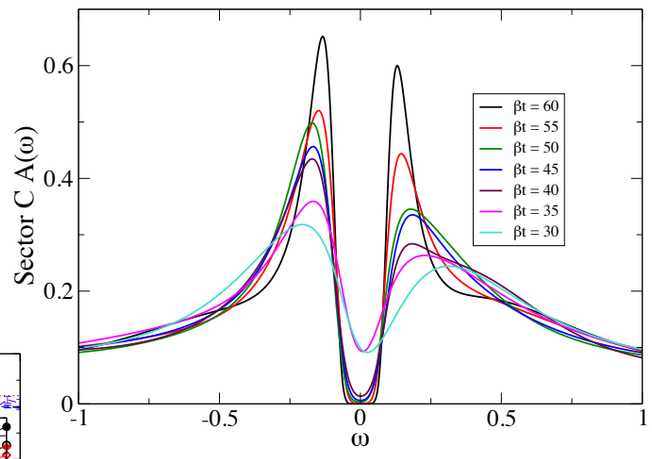
Advantages over other types of QMC

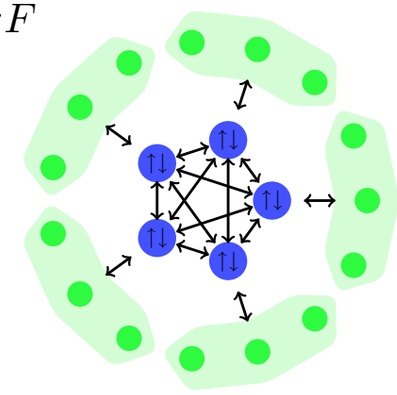


Various Formulations





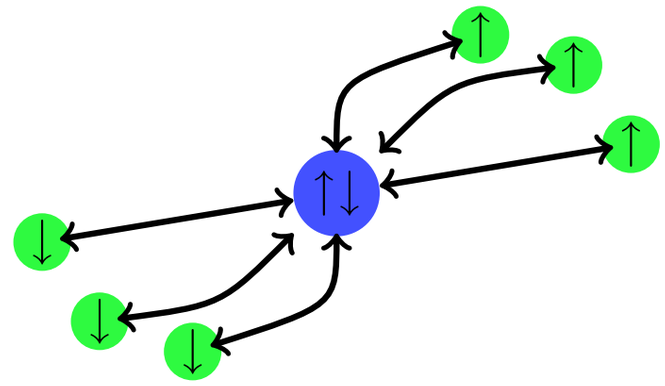




A couple of applications (time permitting)

What is CT-QMC?

Take an interacting quantum system



Write down its Hamiltonian (or action) in two parts

$$H = H_1 + H_2$$

Write down the partition function

$$Z = \mathrm{Tr} e^{-\beta H}$$

Go to interaction representation and expand H with respect to H_1 to infinite order on a computer

$$Z = \sum_{k=0}^{\infty} Z_k = \sum_{k=0}^{\infty} \sum_{p_k q_k r_k s_k} \int_0^\beta d\tau_1 \int_0^\beta d\tau_1' \cdots \int_0^\beta d\tau_{2k}' \Omega^{\tau_1 \tau_1' \cdots \tau_{2k} \tau_{2k'}}_{k,(p_1,q_1,r_1,s_1)\cdots(p_k,q_k,r_k,s_k)}$$

Expansion order

Orbitals that interact

Imaginary time integration

Expansion coefficient

Literature

Diagrammatic Monte Carlo

- Prokof'ev, Svistunov and Tupitsyn, Exact quantum Monte Carlo process for the statistics of discrete systems, JETP Lett 64, 911 (1996)
- Prokof'ev, Svistunov and Tupitsyn, Exact, Complete, and Universal Continuous-Time Worldline Monte Carlo Approach to the Statistics of Discrete Quantum Systems, JETP Lett 87, 310 (1998)
- Prokof'ev, Svistunov and Tupitsyn, Polaron Problem by Diagrammatic Quantum Monte Carlo, Phys. Rev. Lett. 81, 2514 (1998)

Interaction expansions

- Rubtsov and Lichtenstein, Continuous-time quantum Monte Carlo method for fermions: Beyond auxiliary field framework, JETP Lett 80, 61 (2004)
- Rubtsov, Savkin, and Lichtenstein, Continuous-time quantum Monte Carlo method for fermions, Phys. Rev. B 72, 035122 (2005)
- Gull, Werner, Parcollet, and Troyer, Continuous-time auxiliary-field Monte Carlo for quantum impurity models, EPL 82, 57003 (2008)

Hybridization expansion

- Werner, Comonac, de Medici, Troyer, Millis, Continuous-Time Solver for Quantum Impurity Models, Phys. Rev. Lett. 97, 076405 (2006)
- Werner and Millis, Hybridization expansion impurity solver: General formulation and application to Kondo lattice and two-orbital models, Phys. Rev. B 74, 155107 (2006)
- Läuchli and Werner, Krylov implementation of the hybridization expansion impurity solver and application to 5-orbital models, Phys. Rev. B 80, 235117 (2009)

Review

- Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner, Continuous-time Monte Carlo methods for quantum impurity models, Rev. Mod. Phys. 83, 349 (2011)

Potentially also useful

- Gull, PhD thesis, ETH Zurich 2008
- Werner, Lecture notes of the International Summer School on Numerical Methods for Correlated Systems in Condensed Matter (CIFAR/PITP), 2008

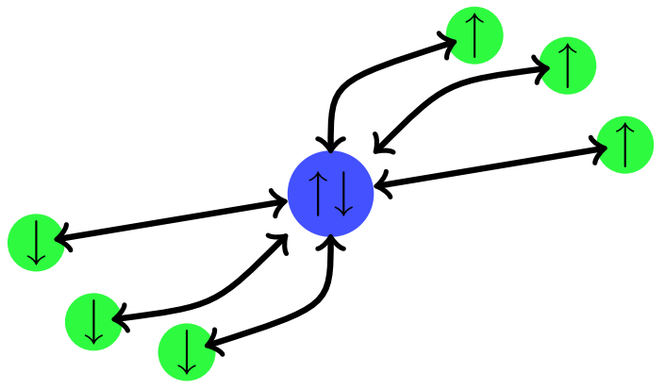
Excerpts of a derivation

Werner, Lecture notes of the International Summer School on Numerical Methods for Correlated Systems in Condensed Matter (CIFAR/PITP), 2008

Problem Setup

$$H = H_0 + H_U + H_{\rm bath} + H_{\rm mix}$$

$$\begin{aligned} H_0 &= -(\mu - U/2)(n_\uparrow + n_\downarrow), \\ H_U &= U(n_\uparrow n_\downarrow - (n_\uparrow + n_\downarrow)/2 \\ H_{\rm bath} &= \sum_{\sigma,p} \epsilon_p a^\dagger_{p,\sigma} a_{p,\sigma}, \\ H_{\rm mix} &= \sum_{\sigma,p} (V^\sigma_p d^\dagger_\sigma a_{p,\sigma} + h.c.). \end{aligned}$$



$$Z = Tr\left[e^{-\beta H}\right] \qquad g(\tau) = \frac{1}{Z} Tr\left[e^{-(\beta-\tau)H} d e^{-\tau H} d^\dagger\right]$$

Series and Series Expansion

$$H = H_1 + H_2$$

$$A(\beta) = e^{\beta H_1} e^{-\beta H}$$

$$\begin{aligned} Z &= Tr\left[e^{-\beta H_1} T e^{-\int_0^\beta d\tau H_2(\tau)}\right] \\ &= \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \ldots \int_{\tau_{n-1}}^\beta d\tau_n Tr\left[e^{-(\beta-\tau_n)H_1}(-H_2)\ldots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1}\right] \end{aligned}$$

$$dA/d\beta = e^{\beta H_1}(H_1 - H)e^{-\beta H} = -H_2(\beta)A(\beta)$$

$$A(\beta) = T\exp[-\int_0^\beta d\tau H_2(\tau)] \qquad Z = Tr[e^{-\beta H_1} A(\beta)].$$

Excerpts of a derivation

Werner, Lecture notes of the International Summer School on Numerical Methods for Correlated Systems in Condensed Matter (CIFAR/PITP), 2008

$$Z = Tr\left[e^{-\beta H_1} T e^{-\int_0^\beta d\tau H_2(\tau)}\right]$$

$$= \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \ldots \int_{\tau_{n-1}}^\beta d\tau_n Tr\left[e^{-(\beta-\tau_n)H_1}(-H_2)\ldots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1}\right],$$

Configuration space

$$Z = \sum_c w_c, \qquad w_c = Tr\left[e^{-(\beta-\tau_n)H_1}(-H_2)\ldots e^{-(\tau_2-\tau_1)H_1}(-H_2)e^{-\tau_1 H_1}\right] d\tau^n.$$

$$c = \{\tau_1, \ldots, \tau_n\},\ n = 0, 1, \ldots,\ \tau_i \in [0, \beta)$$

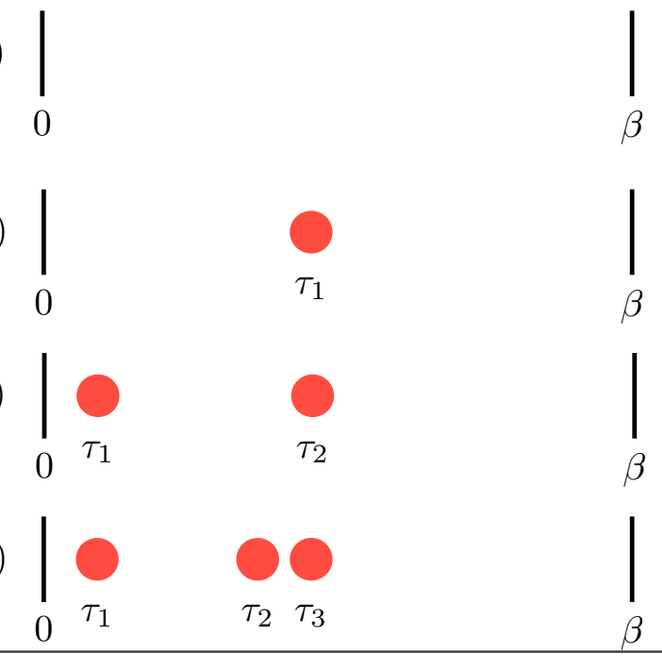
Graphical representation of terms of the integral at different orders:

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

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

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

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



Excerpts of a derivation

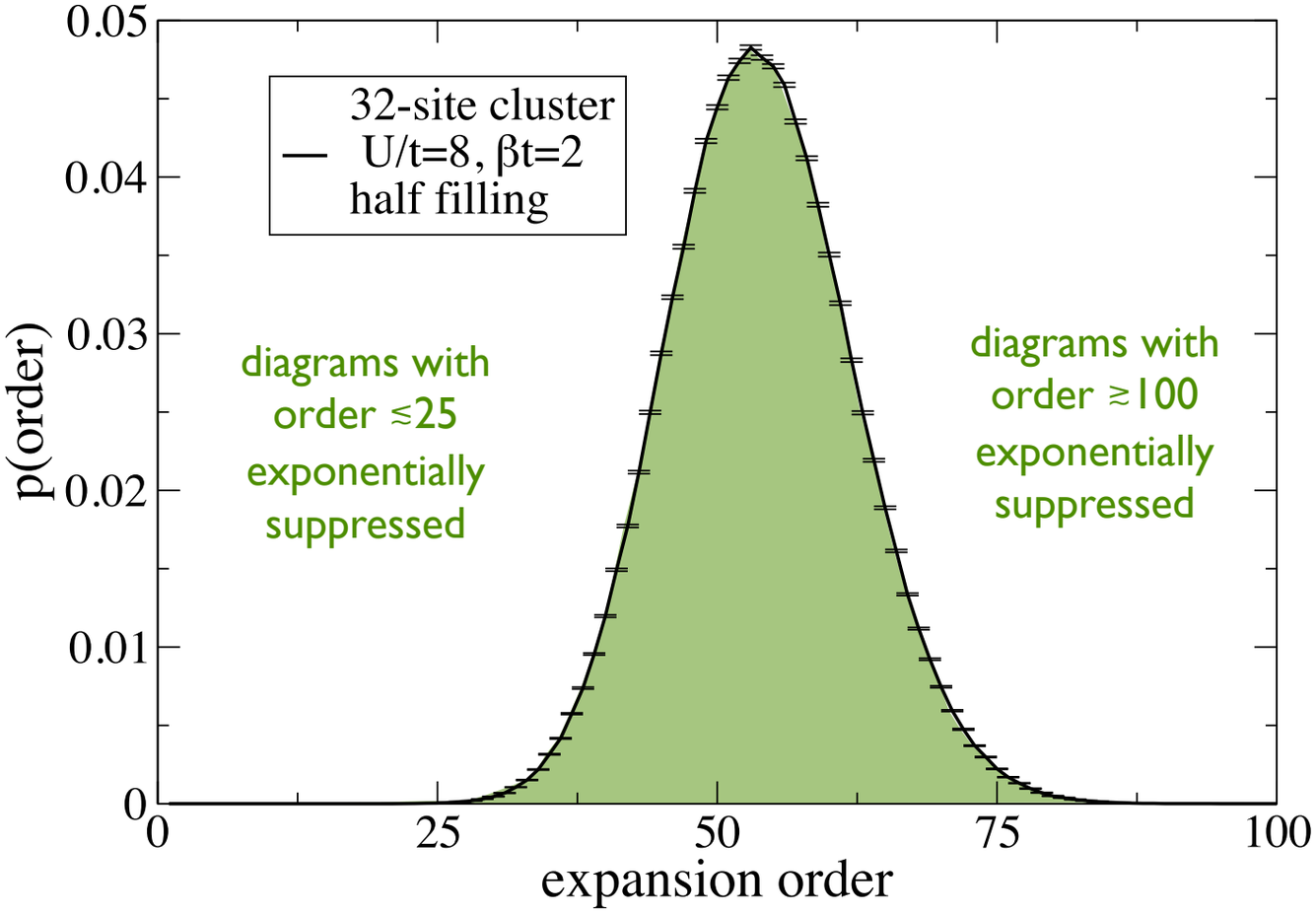
Monte Carlo integration

$$Z = \sum_c w_c,$$

Metropolis random walk in diagram space, importance sampling of diagrams

Space is infinite dimensional (no explicit truncation at diagram order)

Walk through diagram space by changing diagrams, typically inserting and removing diagram vertices



…configurations better be positive and normalizable or we have a problem!

Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner, Continuous-time Monte Carlo methods for quantum impurity models, Rev. Mod. Phys. 83, 349 (2011)

Excerpts of a derivation

Interaction Expansion

$$H = H_0 + H_U + H_{\text{bath}} + H_{\text{mix}}$$

$$H_0 = -(\mu - U/2)(n_\uparrow + n_\downarrow),$$

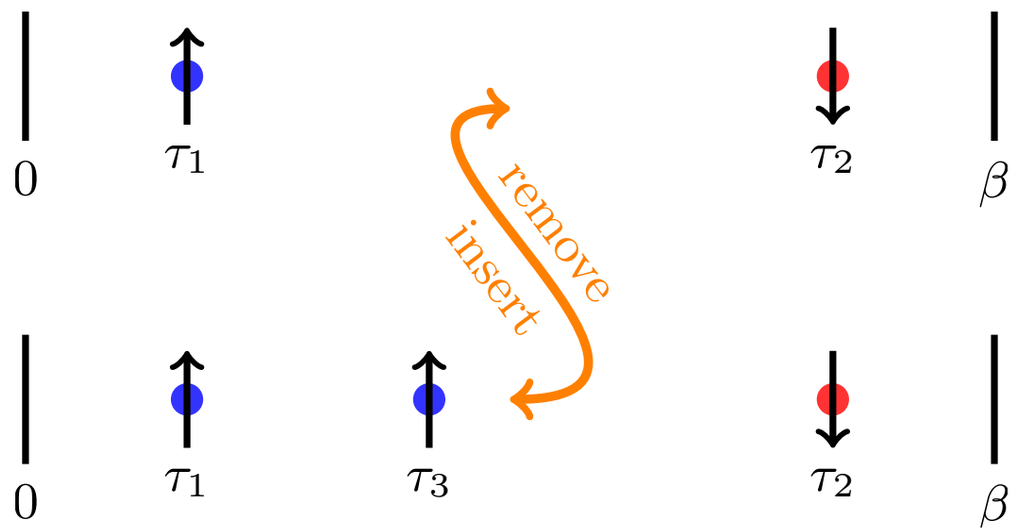
$$H_U = U(n_\uparrow n_\downarrow - (n_\uparrow + n_\downarrow)/2$$

$$H_{\text{bath}} = \sum_{\sigma,p} \epsilon_p a^\dagger_{p,\sigma} a_{p,\sigma},$$

$$H_{\text{mix}} = \sum_{\sigma,p} (V^\sigma_p d^\dagger_\sigma a_{p,\sigma} + h.c.).$$

$$H_1 = H_0 + H_{\text{bath}} + H_{\text{mix}}$$

$$H_2 = H_U$$



- Numerical effort grows cubically with increasing U and beta
- Requires additional ‘decoupling’ (leading to auxiliary variables, e.g. spins)
- In practice works very well for clusters, single orbital models. ‘Default’ algorithm for large cluster problems.
- Works less well for general electronic structure Hamiltonians

- Rubtsov, Savkin, and Lichtenstein, Continuous-time quantum Monte Carlo method for fermions, Phys. Rev. B 72, 035122 (2005)
- Gull, Werner, Parcollet, and Troyer, Continuous-time auxiliary-field Monte Carlo for quantum impurity models, EPL 82, 57003 (2008)

Excerpts of a derivation

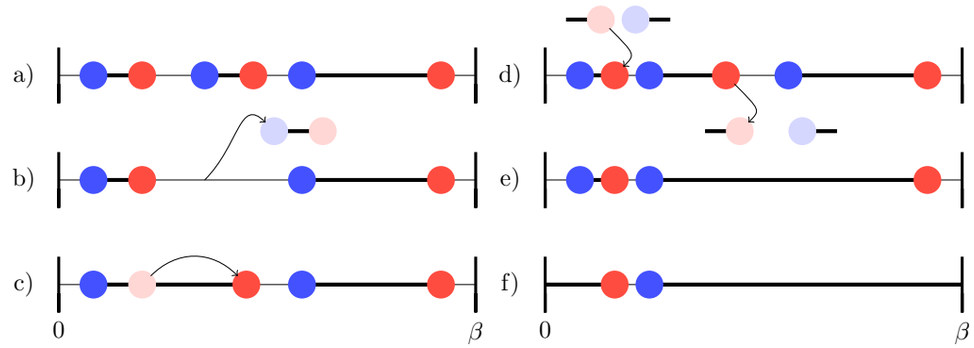
Hybridization Expansion

$$
\begin{aligned}
H_0 &= -(\mu - U/2)(n_\uparrow + n_\downarrow), \\
H_U &= U(n_\uparrow n_\downarrow - (n_\uparrow + n_\downarrow)/2) \\
H_{\text{bath}} &= \sum_{\sigma,p} \epsilon_p a^\dagger_{p,\sigma} a_{p,\sigma}, \\
H_{\text{mix}} &= \sum_{\sigma,p} (V^\sigma_p d^\dagger_\sigma a_{p,\sigma} + h.c.).
\end{aligned}
$$

$$H = H_0 + H_U + H_{\text{bath}} + H_{\text{mix}}$$

$$H_1 = H_0 + H_U + H_{\text{bath}}$$

$$H_2 = H_{\text{mix}}$$

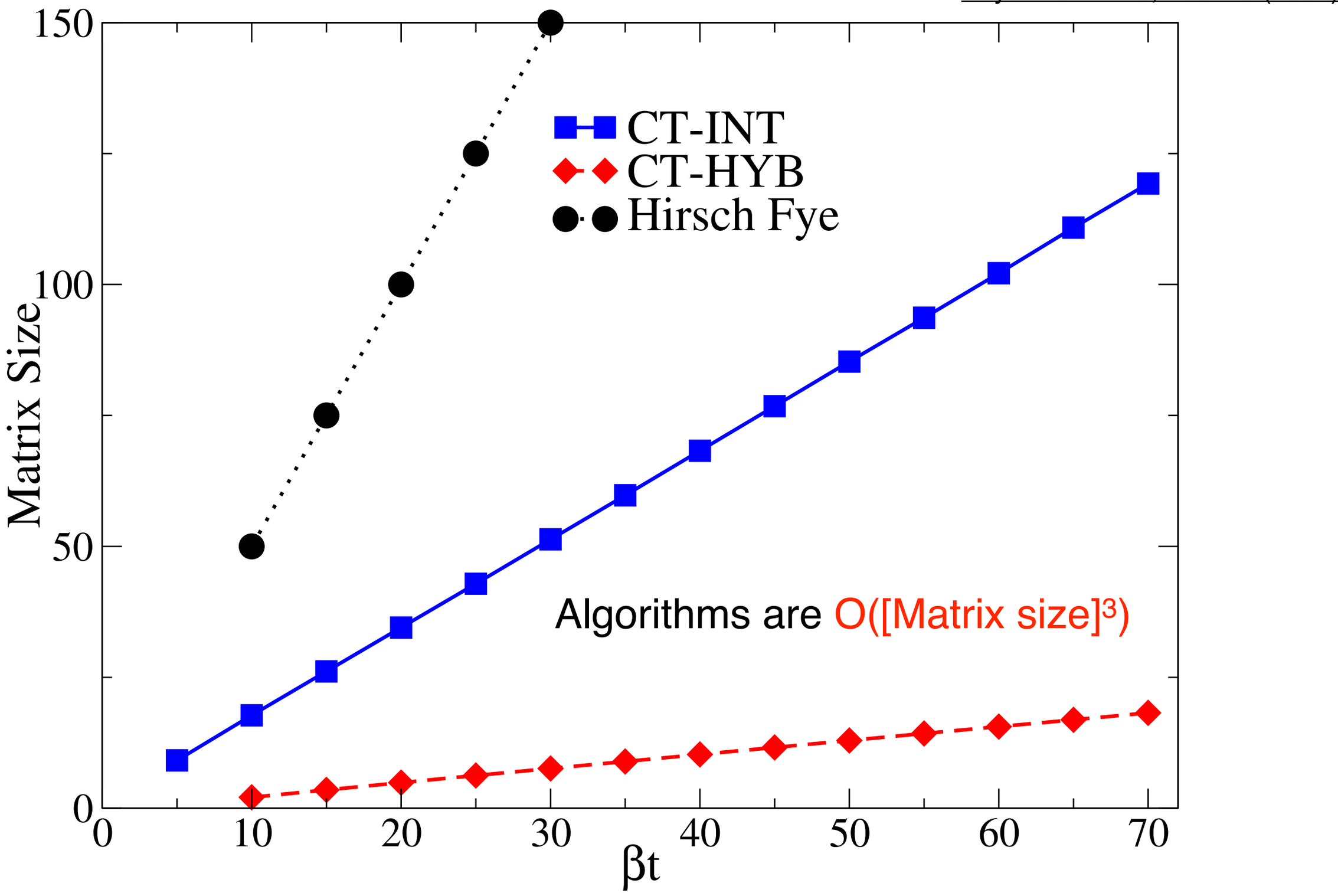


- Numerical effort grows with increasing ‘mixing’, but mostly independent of U
- Requires treatment of local Hamiltonian: easy for density-density interactions, harder for general interactions
- In practice works very well for multi-orbital systems, not too well for clusters.

- Werner, Comonac, de Medici, Troyer, Millis, Continuous-Time Solver for Quantum Impurity Models, Phys. Rev. Lett. 97, 076405 (2006)
- Werner and Millis, Hybridization expansion impurity solver: General formulation and application to Kondo lattice and two-orbital models, Phys. Rev. B 74, 155107 (2006)
- Läuchli and Werner, Krylov implementation of the hybridization expansion impurity solver and application to 5-orbital models, Phys. Rev. B 80, 235117 (2009)

Advantages of CT-QMC

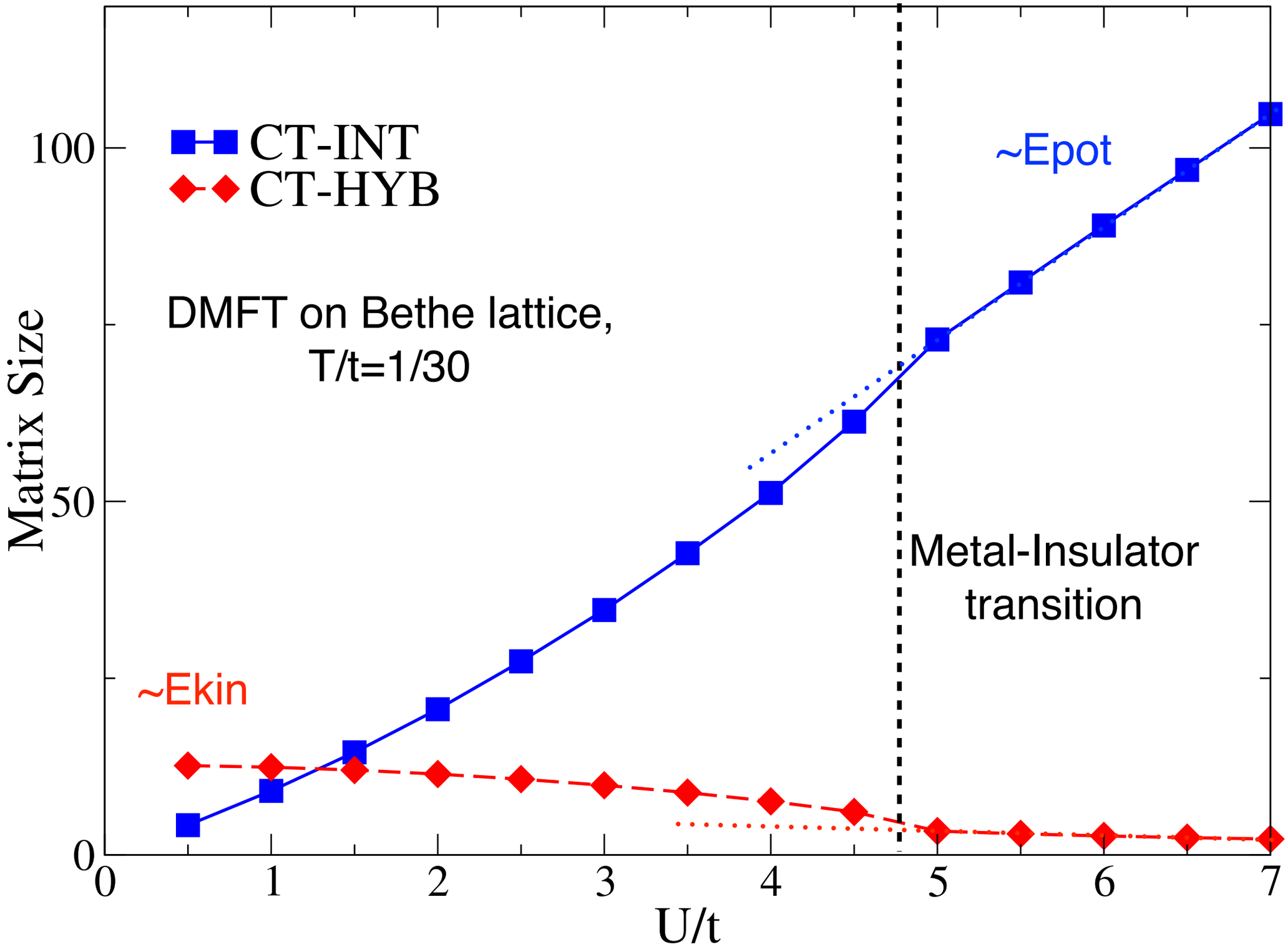
Gull, Werner, Troyer, Millis,
Phys. Rev. B 76, 235123 (2007)



Expansion orders and energies

Expansion gives physical insight: <order> ~ **Epot**, **Ekin**

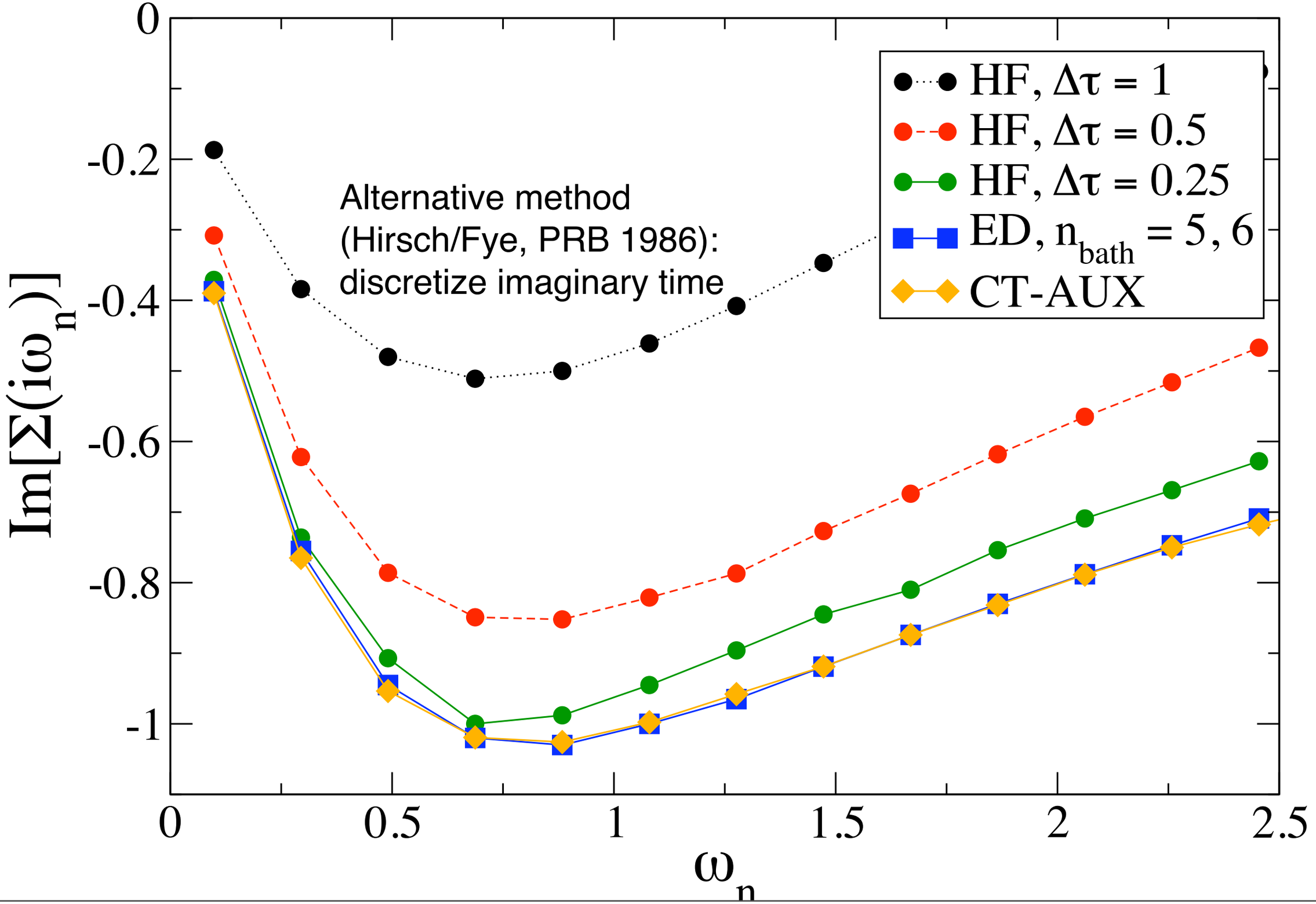
Gull, Werner, Troyer, Millis,
Phys. Rev. B 76, 235123 (2007)



Discretization / Trotter errors

No Trotter error / **Numerically exact** results

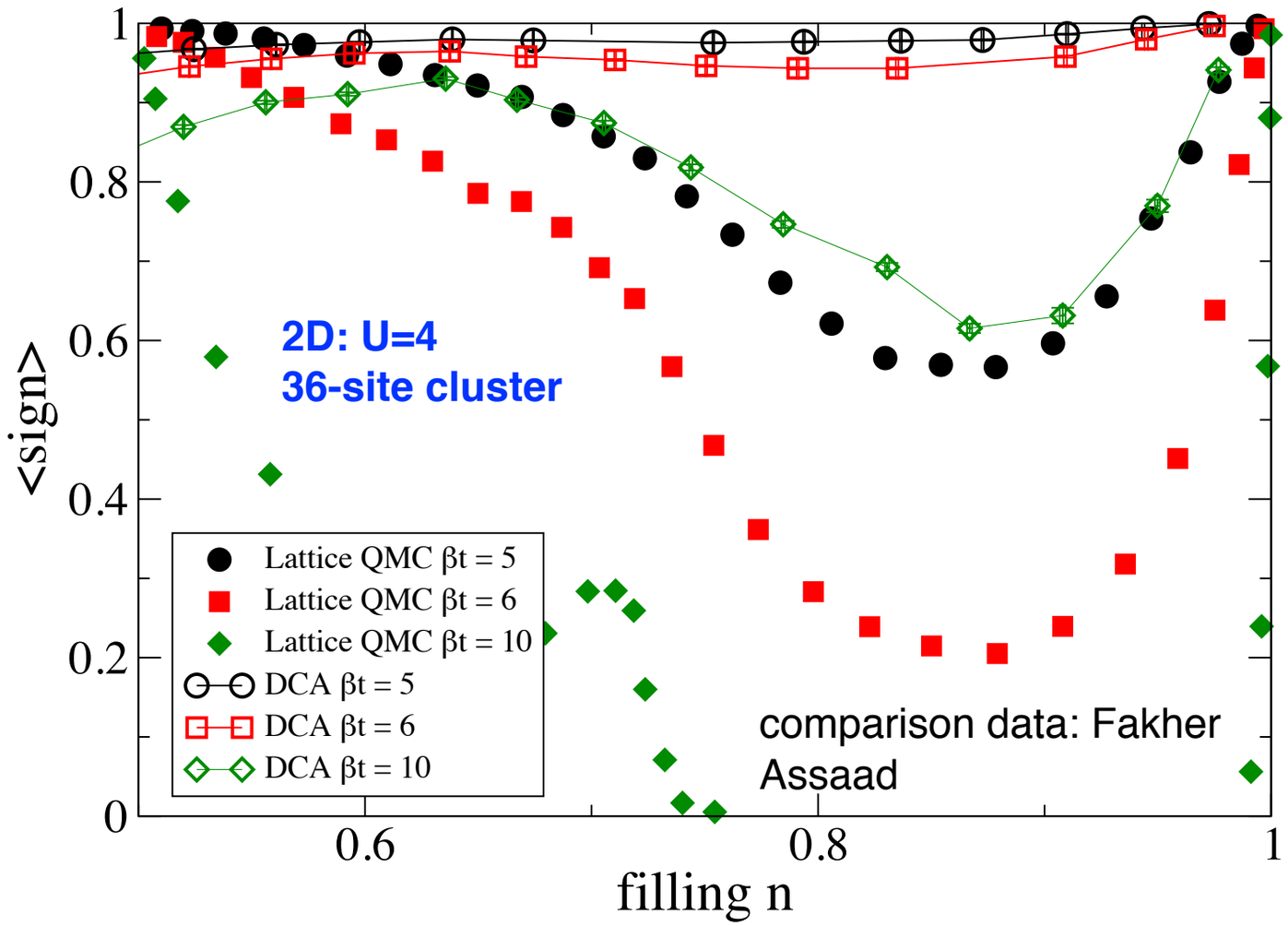
Gull, Werner, Parcollet, Millis,
EPL 82 57003 (2008)



Sign Problems

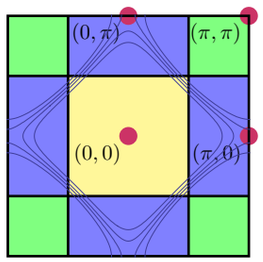
In practice: only hard limitation given by the **fermionic sign problem**.

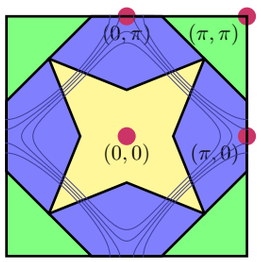
Dynamical mean field bath helps to increase <sign>: larger parameter space available even though scaling is cubic, not linear, in βt



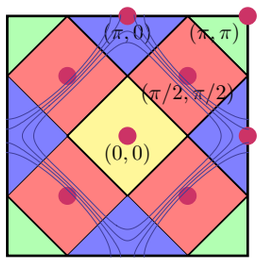
‘Ultimate’ limitation: For U/t = 7-8

Sign problem not severe.

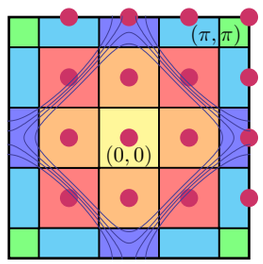




no t’: βt ~ 60. with t’~ -0.15t: βt ~ 20



no t’: βt ~ 40-60 t’~ -0.15t: βt ~ 10



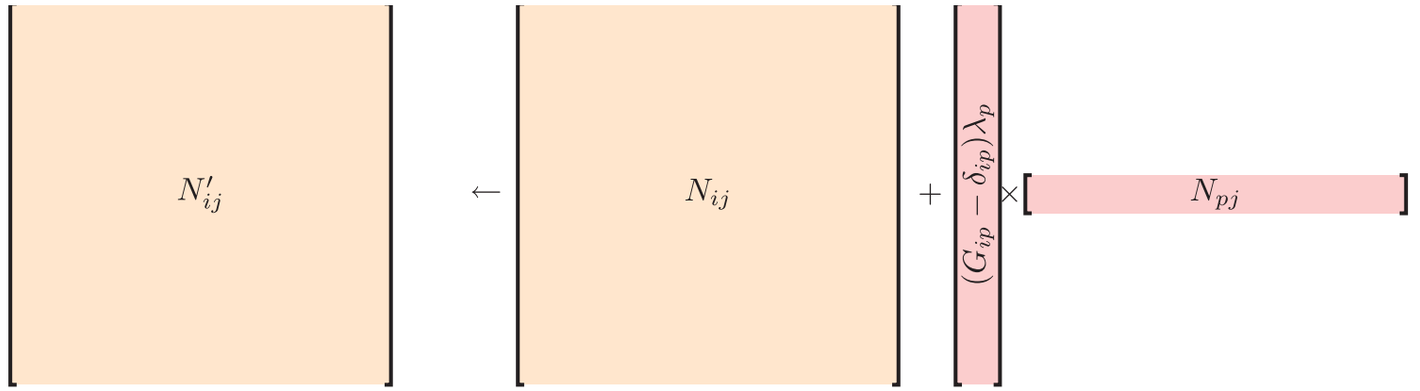
Strongly dependent on details: doping, phase, quality of data and error bars required (analytic continuation), etc.

Numerics

Numerical methods: **Submatrix updates** replace data intensive vector-vector and matrix-vector operations (O(N2) data for O(N2) operations) by compute-intensive matrix-matrix operations and some (cheap) redundant operations (O(N3) operations on O(N2) data):

Order of magnitude faster:

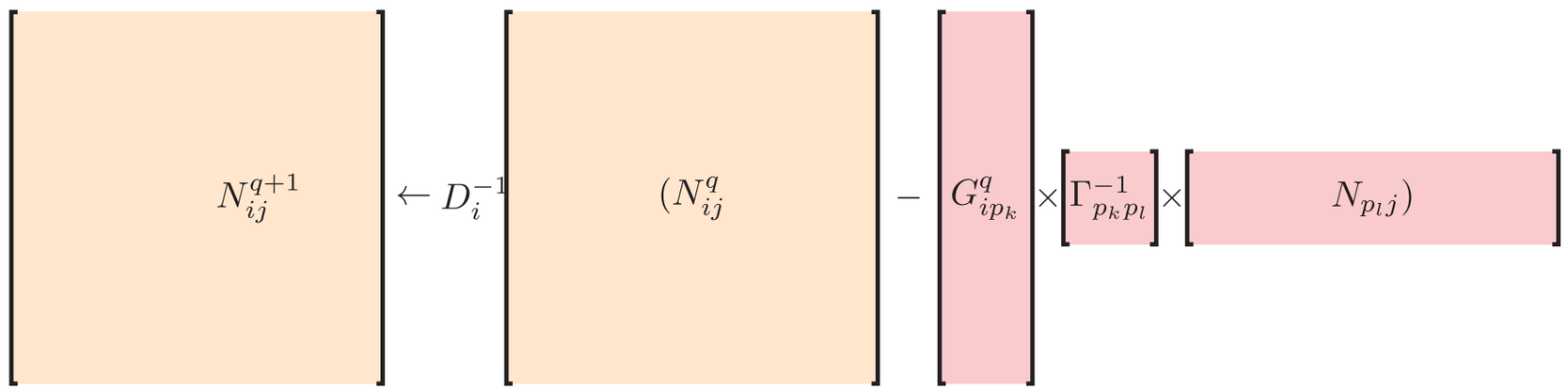
Replace dger



(a)

E. Gull et al., Phys. Rev. B 83, 075122 (2011)

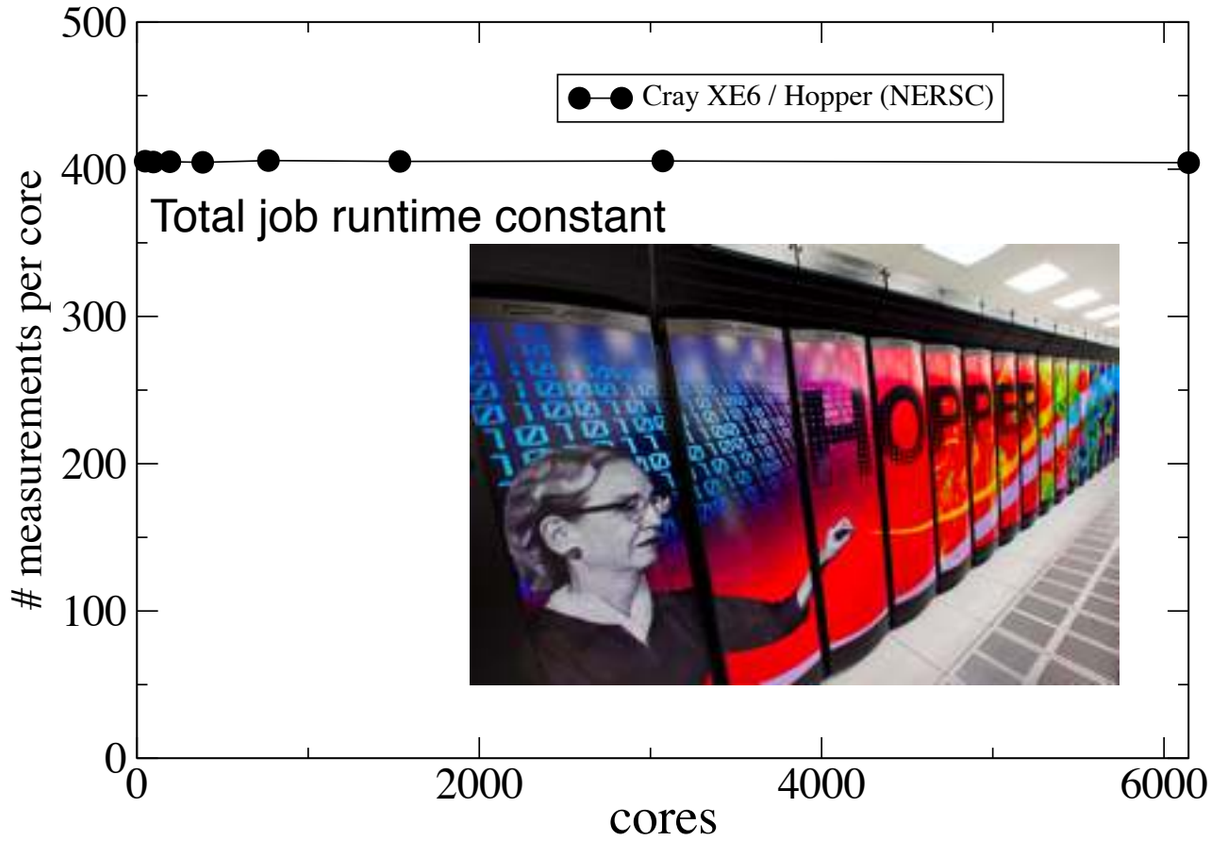
by dgemm



Parallelization

Reducing the **prefactor**:

Monte Carlo simulations of this type are **trivially parallel**: Scale to a very large (>10000) number of cores. Measurements are comparatively expensive; thermalization time small, Amdahl's law relevant only at very large #cores



ALPS NGS scheduler: Monte Carlo simulations with correct binning and error analysis using only collective communications: **Proper error analysis**, error propagation possible on very large machines!

Types of CT-QMC algorithms

Ernest Rutherford,
1871-1937

There are two types of science: Physics and Stamp collecting

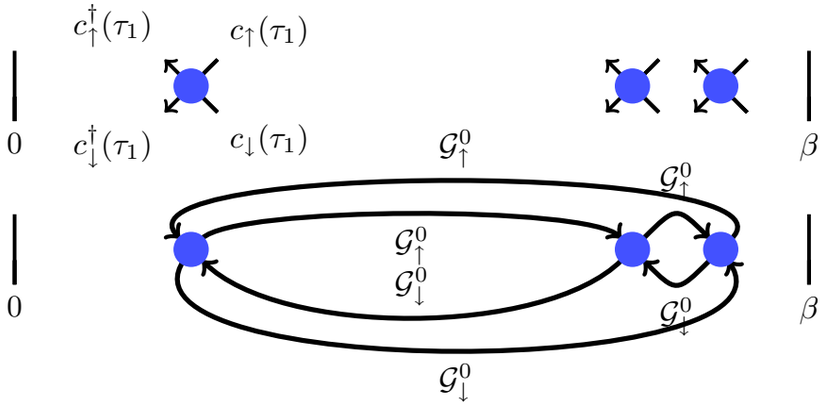
From now on: stamp collecting.

CT-INT formulation

Weak coupling partition function expansion (SIAM):

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

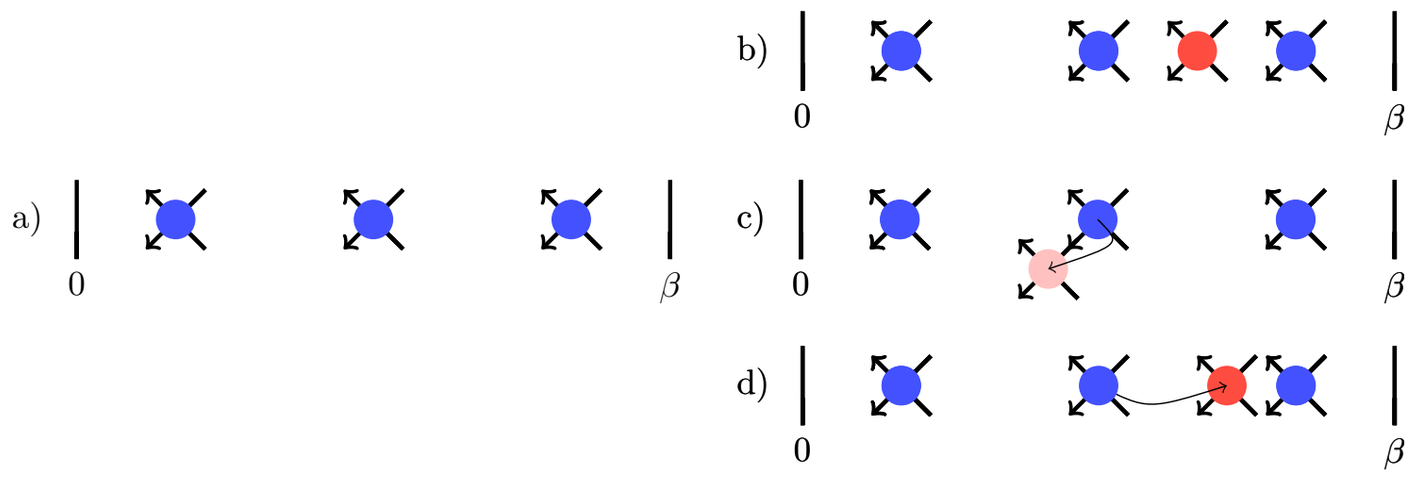
$$= \sum_{k=0}^{\infty} \frac{(-U)^k}{k!} \iiint_0^\beta d\tau_1 \cdots d\tau_k \sum_{s_1 \cdots s_k} \prod_{\sigma} \det D_k^\sigma$$



Location of interaction vertices

Green's function lines

Monte Carlo sampling process:



Vertex insertion.

Vertex removal.

Vertex shift.

- Rubtsov and Lichtenstein, Continuous-time quantum Monte Carlo method for fermions: Beyond auxiliary field framework, JETP Lett 80, 61 (2004)
- Rubtsov, Savkin, and Lichtenstein, Continuous-time quantum Monte Carlo method for fermions, Phys. Rev. B 72, 035122 (2005)

(CT-INT) worms

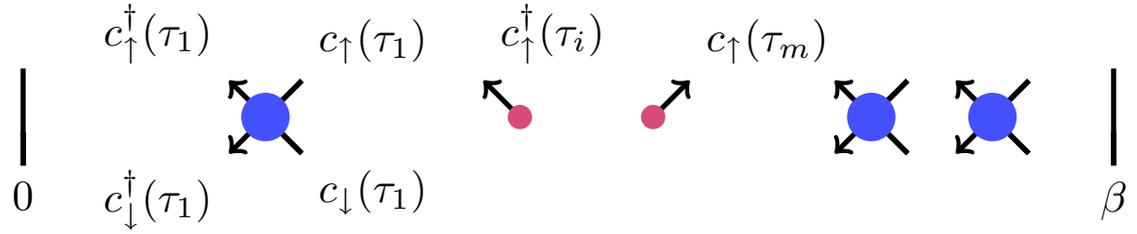
Weak coupling: Sample partition function series:

$$Z = \sum_k \frac{(-U)^k}{k!} \sum_{s,\sigma} \int dx_1 \cdots \int dx_k \langle c^\dagger_{s_1,\sigma_1}(\tau_1) c_{s_1,\sigma_1}(\tau_1) \cdots \rangle_{S_0}$$

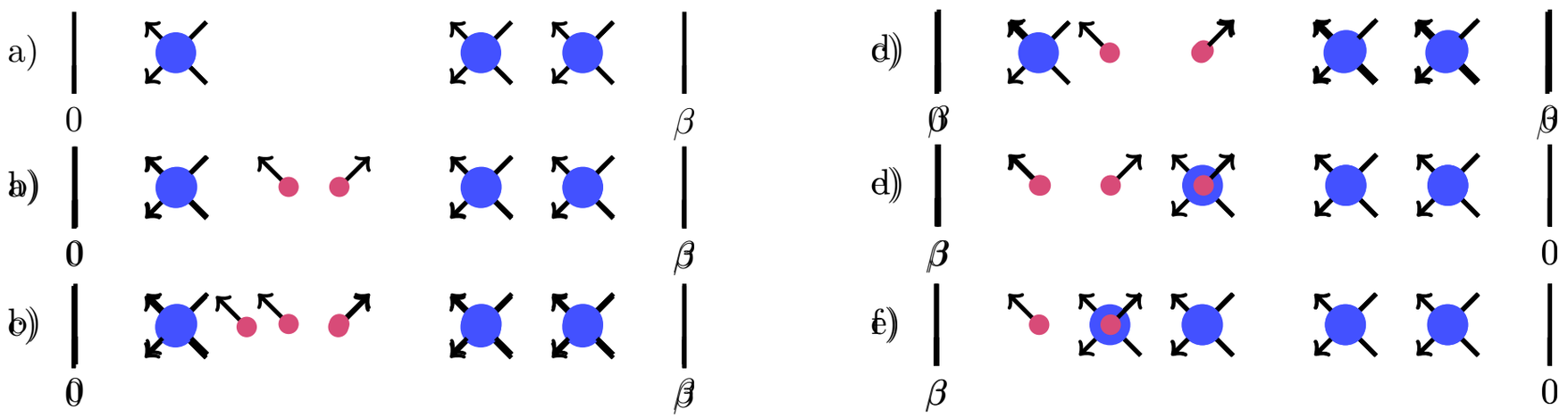
Worm algorithm: Sample Green's function series:

$$G_{\sigma,s_i,s_m}(\tau_i,\tau_m) = \sum_k (-U)^k/k! \sum_{s,\sigma} \int dx_1 \cdots \int dx_k$$
$$\langle c^\dagger_{s_i\sigma}(\tau_i) c_{s_m\sigma}(\tau_m) c^\dagger_{s_1,\sigma_1}(\tau_1) c_{s_1,\sigma_1}(\tau_1) \cdots \rangle.$$

Green's function diagrams:



Sampling of Green's functions and partition function diagrams



Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner, Continuous-time Monte Carlo methods for quantum impurity models, Rev. Mod. Phys. 83, 349 (2011)

CT-AUX formulation

Decoupling of the interaction with an auxiliary field:

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

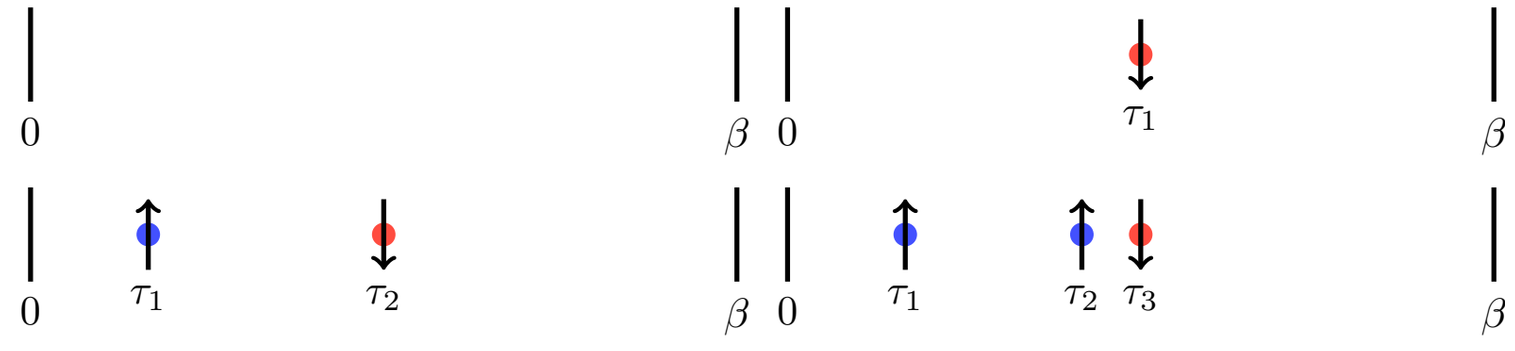
$$\cosh(\gamma) = 1 + \frac{U\beta}{2K}.$$

Partition function expansion in the interaction representation:

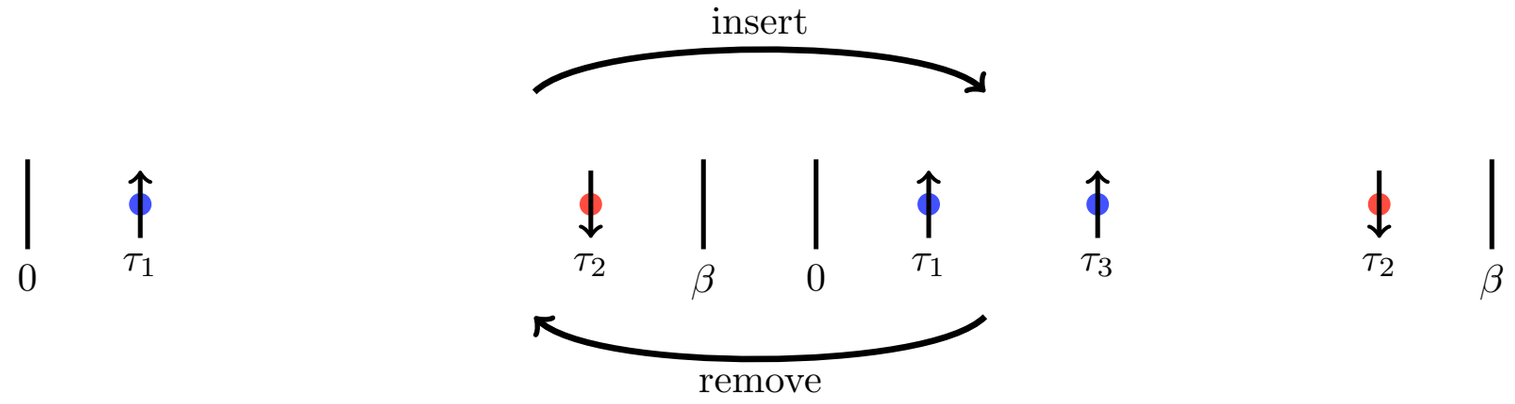
$$Z = \sum_{k=0}^{\infty}\sum_{s_1,\cdots s_k=\pm 1}\int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \left(\frac{K}{2\beta}\right)^k Z_k(\{s_k,\tau_k\}),$$

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

Diagrams of the partition function:



Monte Carlo Sampling:



- Gull, Werner, Parcollet, and Troyer, Continuous-time auxiliary-field Monte Carlo for quantum impurity models, EPL 82, 57003 (2008)

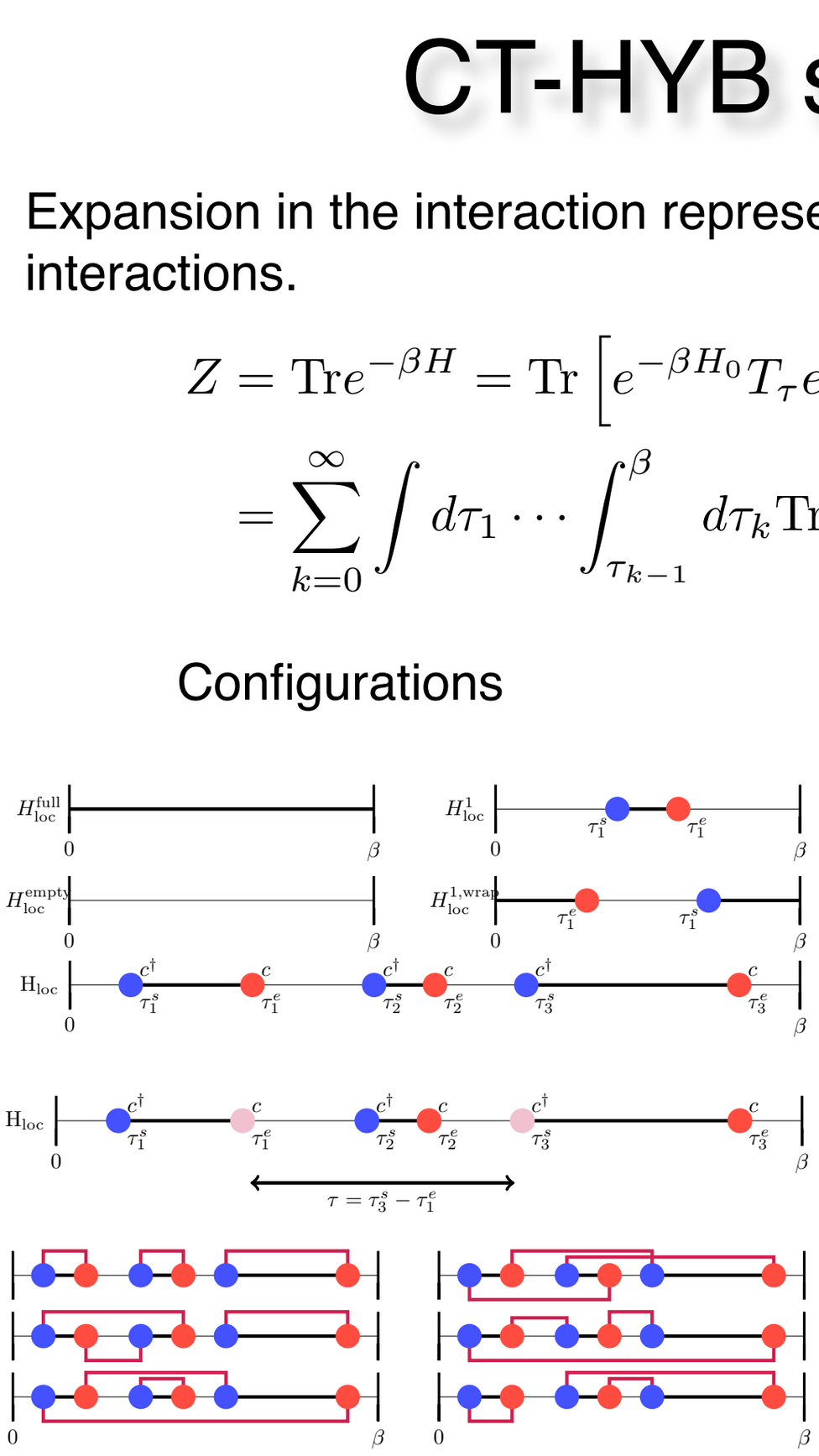
CT-HYB segment formulation

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

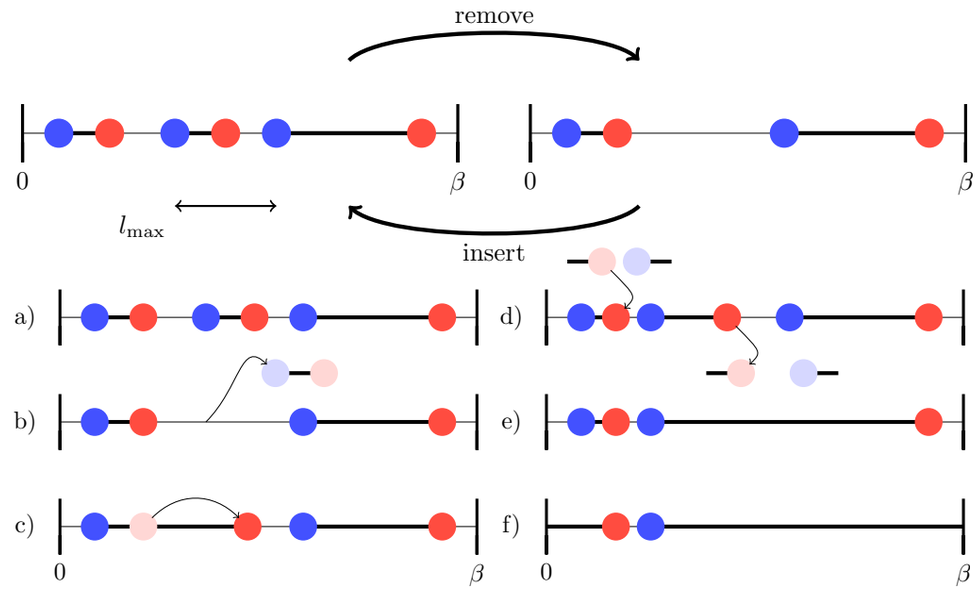
$$Z = \mathrm{Tr} e^{-\beta H} = \mathrm{Tr}\left[e^{-\beta H_0} T_\tau e^{-\int_0^\beta d\tau H_{\mathrm{mix}}(\tau)}\right]$$

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

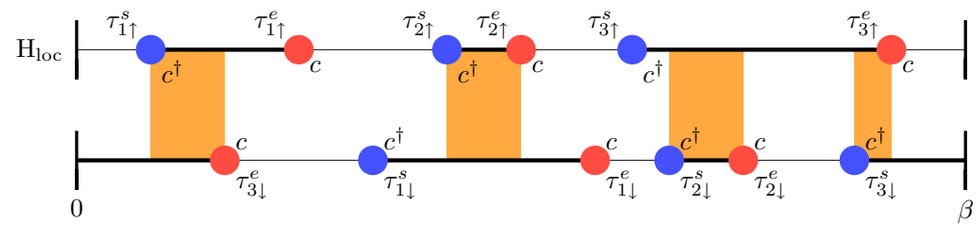
Configurations



Sampling Process



Interactions (density density)



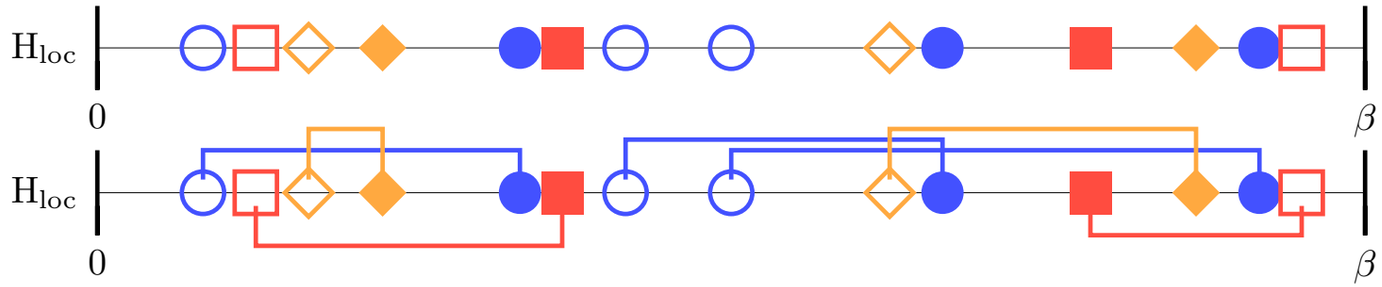
- Werner, Comonac, de Medici, Troyer, Millis, Continuous-Time Solver for Quantum Impurity Models, Phys. Rev. Lett. 97, 076405 (2006)

CT-HYB matrix formulation

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

Configuration of H_{loc}

Configuration of V

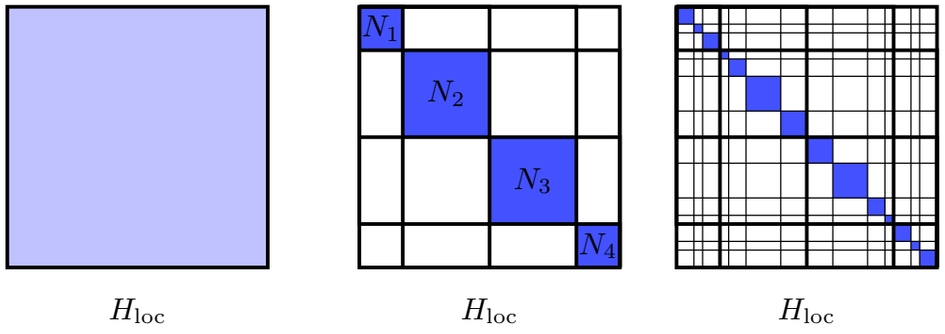


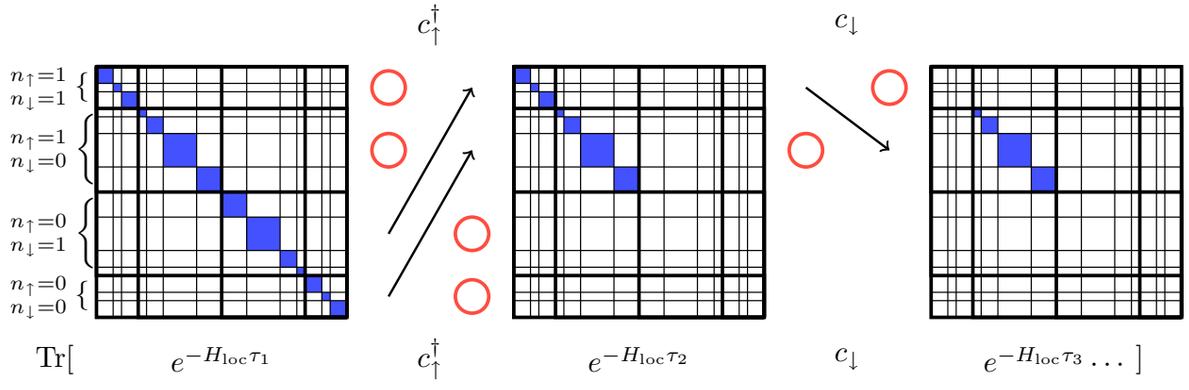
Matrix exponentials

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

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

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

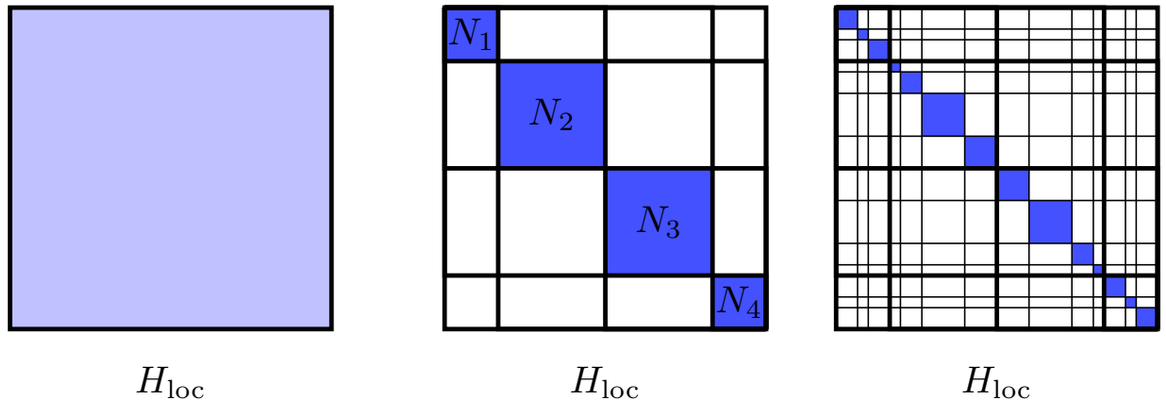




Werner and Millis, Hybridization expansion impurity solver: General formulation and application to Kondo lattice and two-orbital models, Phys. Rev. B 74, 155107 (2006)

CT-HYB Krylov formulation

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



H_{loc} H_{loc} H_{loc}

What to do if these blocks are still too large?

Use Krylov subspace methods -> next talk by Giorgio Sangiovanni

…avoid full diagonalization of symmetry blocks…

Still exponential in the dimension of the local Hilbert space, but prefactor is much better!

CT-J formulation

$$H_{\mathrm{CS}} = H_{\mathrm{bath}} + H_{\mathrm{spin}} + H_J$$

large U situations: model spins instead of electrons, do spinflips directly

'Schrieffer Wolf' transformation

$$H_{\mathrm{bath}} = \sum_{kb} \varepsilon_k c^\dagger_{kb} c_{kb},$$

$$H_{\mathrm{spin}} = \sum_{\alpha} E_\alpha X_{\alpha\alpha},$$

$$H_{\mathrm{J}} = -\sum_{\substack{\alpha\alpha',bb' \\ kk'}} J^{kk',bb'}_{\alpha\alpha'} X_{\alpha\alpha'} c_{kb} c^\dagger_{k'b'}.$$

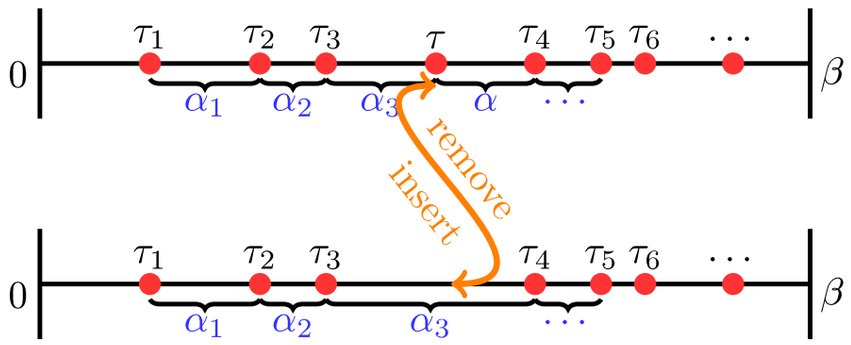
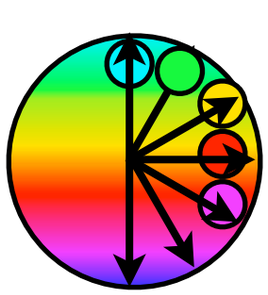


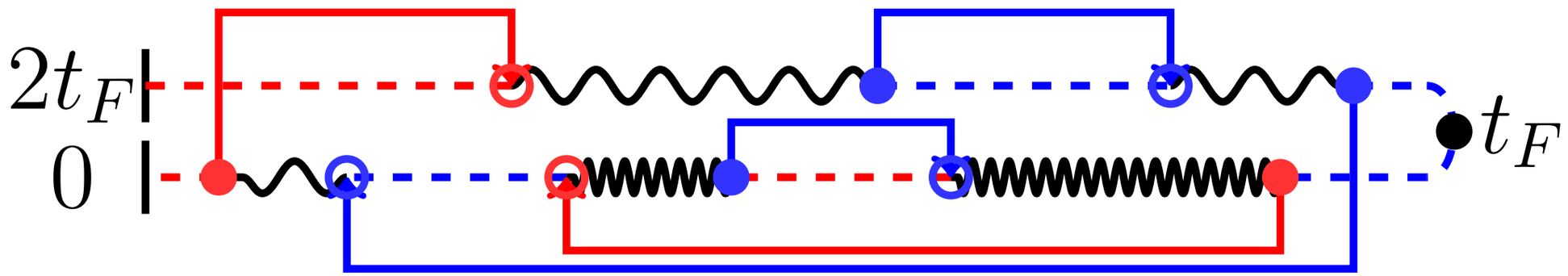
FIG. 13 Illustration of an insertion of a segment. The diagrams represent the configurations of $\{\tau_i\}$ and $\{\alpha_i\}$.



Updates work by inserting J processes that change the local state

- J. Otsuki, H. Kusunose, P. Werner, and Y. Kuramoto, Continuous-Time Quantum Monte Carlo Method for the Coqblin–Schrieffer Model, J. Phys. Soc. Jpn. 76 (11), 114707 (2007).

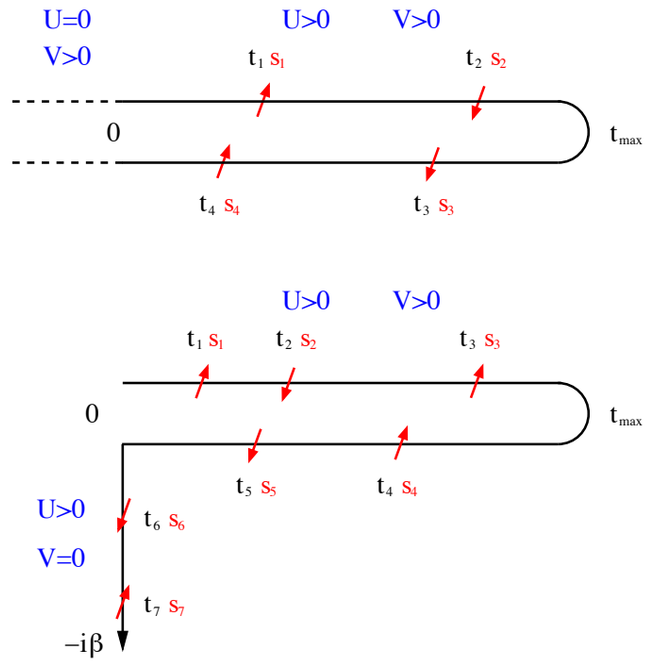
Real Time formulation



$$\langle \hat{O}(t_F) \rangle = \mathrm{Tr}\left[\hat{O}\hat{\rho}(t_F)\right] = \mathrm{Tr}\left[\hat{O}e^{-iHt_F}\,\hat{\rho}_0 e^{iHt_F}\right].$$

Typical **Observables**: **current**, **dot density matrix**.

- **Initial transient** (short-time behavior)
- **Steady state**
  - Steady state observables? (current, occupancy, …)
  - Relaxation to steady state?



Diagrammatic expansion on the Keldysh contour. Contour-ordered operators, double contours, etc

Hybridization expansion & interaction expansion possible

Mühlbacher, Rabani, Phys. Rev. Lett. 100, 176403 (2008)

Real Time formulation

Limiting factor with CT-QMC out of equilibrium: Complex sign (phase) problem!

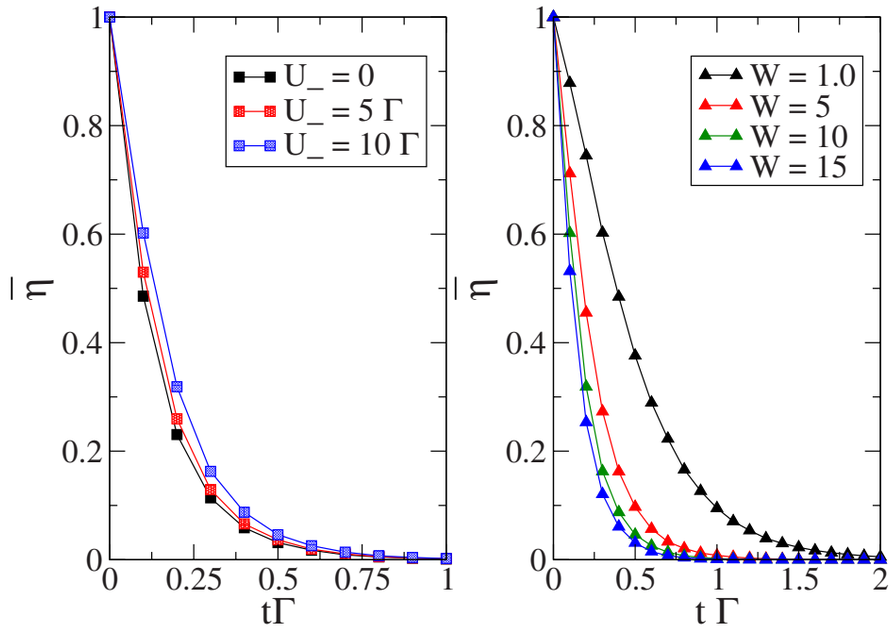


FIG. 5. (Color online) Average sign as a function of time t for different initial preparations. We clearly see an exponential decay on a very short-time scale. Left panel shows data obtained fixing the final value of the interaction $U_+=0$ and tuning the initial value $U=0,5,10$. We see a slight increase in the average sign. Right panel shows the dependence of $\bar{\eta}$ from the bandwidth of conduction electrons and suggest that much longer time scales can be reached in the regime $W\sim\Gamma$.

Schiro et al.,
Phys. Rev. B 81, 085126 (2010)

Dynamic sign problem:
direct consequence of oscillation
of real time propagation

'bare' CT-QMC: average sign decays exponentially as a function of real time.

Hard cutoff in times that can be reached, exponential cost for longer times

Mühlbacher, Rabani, Phys. Rev. Lett. 100, 176403 (2008)

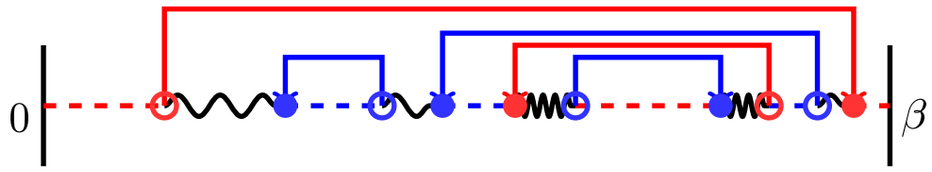
Werner, Oka, Millis, Phys. Rev. B 79, 035320 (2009)

…to boldly go where no man…

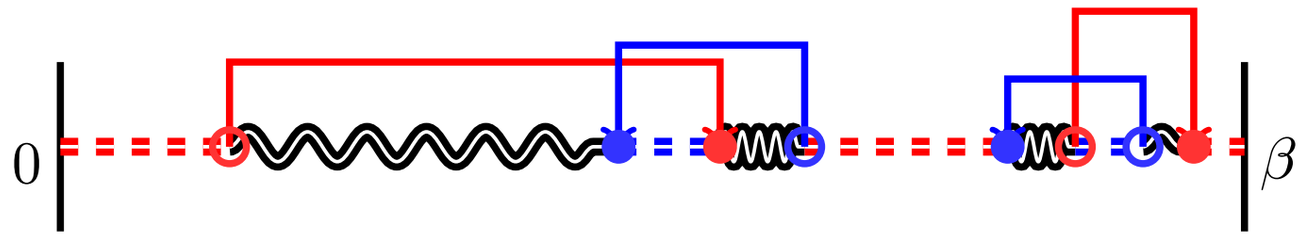
1.Use the partial summation to sum up **important class of diagrams,** typically using coupled integral equations)

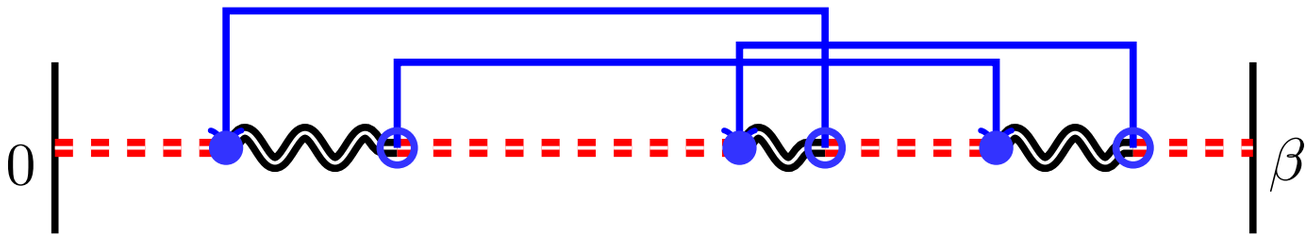
$$\Sigma_{|0\rangle}(\tau) = G_{|\uparrow\rangle}(\tau)\Delta_{\uparrow}(\tau) + G_{|\downarrow\rangle}(\tau)\Delta_{\downarrow}(\tau),$$
$$\Sigma_{|\sigma\rangle}(\tau) = G_{|0\rangle}(\tau)\Delta_{\sigma}(-\tau) + G_{|\uparrow\downarrow\rangle}(\tau)\Delta_{-\sigma}(\tau),$$
$$\Sigma_{|\uparrow\downarrow\rangle}(\tau) = G_{|\uparrow\rangle}(\tau)\Delta_{\downarrow}(-\tau) + G_{|\downarrow\rangle}(\tau)\Delta_{\uparrow}(\tau).$$
$$G_{|j\rangle} = G^0_{|j\rangle} + G^0_{|j\rangle}\Sigma_{|j\rangle}G_{|j\rangle}$$

Obtain dressed propagators and self-energies



2.Use a continuous-time quantum Monte Carlo algorithm to sum all correction terms to the partial summation



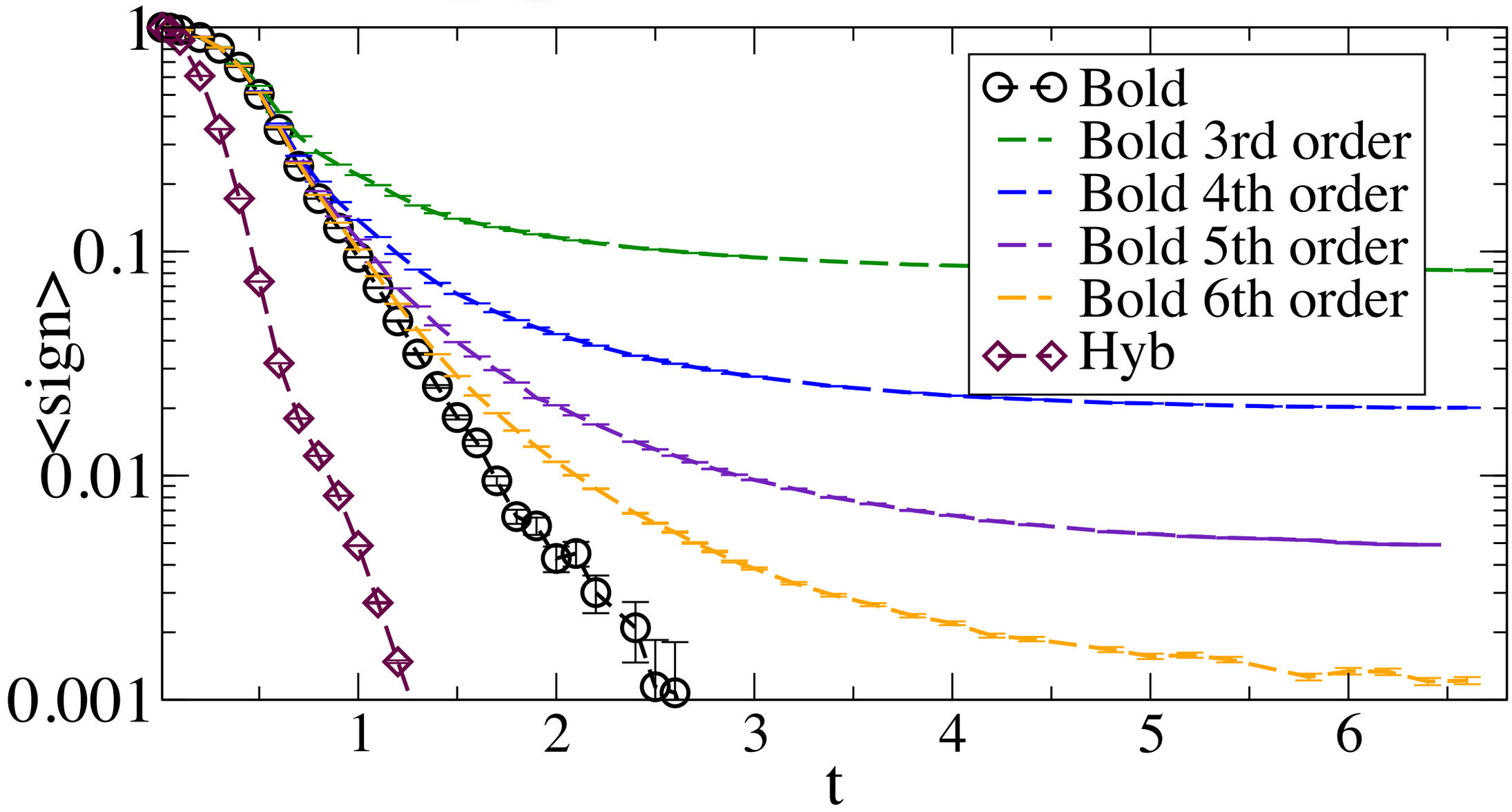


Typically loses antisymmetric structure of determinant, typically exponential scaling

Advantageous where all else fails...

- E. Gull, D. R. Reichman, and A. J. Millis, Bold Line Diagrammatic Monte Carlo Method: General formulation and application to expansion around the Non-Crossing Approximation, Phys. Rev. B 82, 075109 (2010)

…to boldly go where no man: Real Time



Twice as long times accessible with bold.

If bold expansion is truncated at a fixed order (3rd, 4th, 5th, 6th order), sign problem plateaus, arbitrarily long times accessible.

E. Gull, D. R. Reichman, and A. J. Millis, Numerically Exact Long Time Behavior of Nonequilibrium Quantum Impurity Models, Phys. Rev. B 84, 085134 (2011)

Nambu formulation

E. Gull, O. Parcollet, and A. J. Millis, Superconductivity and the Pseudogap in the 2d Hubbard model, Phys. Rev. Lett. 110, 216405 (2013)

Introduce general spinors

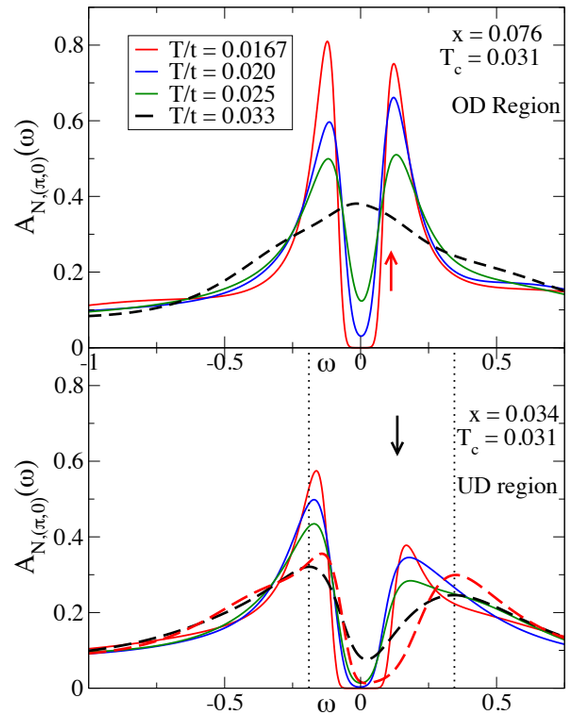
$$\Psi_i^+(\tau) \equiv (\psi_{1i}^+, \psi_{2i}^+, \psi_{3i}^+, \psi_{4i}^+) = \left(c_{i\uparrow}^+, c_{i\downarrow}^+, c_{i\uparrow}, c_{i\downarrow}\right)$$

(or, in typical cases, only)

$$\Psi_i^\dagger = \left(c_{i\uparrow}^\dagger, c_{i\downarrow}\right)$$

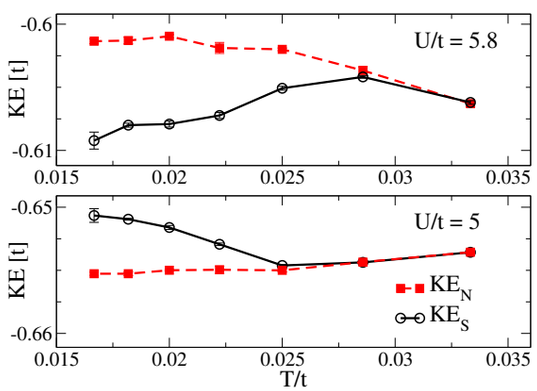
Allow for correlation functions that contain 'offdiagonal' terms:

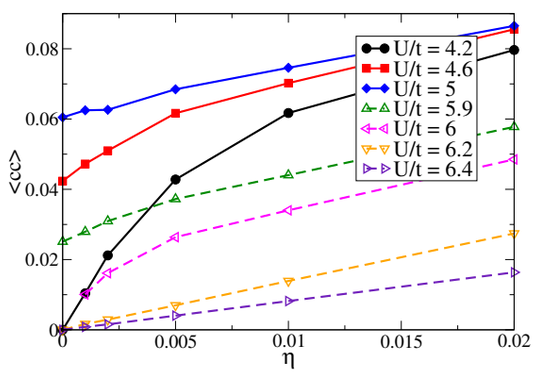
$$G(\mathbf{k},\tau,\tau') = \begin{pmatrix} G(\mathbf{k},\tau,\tau') & F(\mathbf{k},\tau,\tau') \\ F^+(\mathbf{k},\tau,\tau') & -G(-\mathbf{k},\tau',\tau) \end{pmatrix}$$

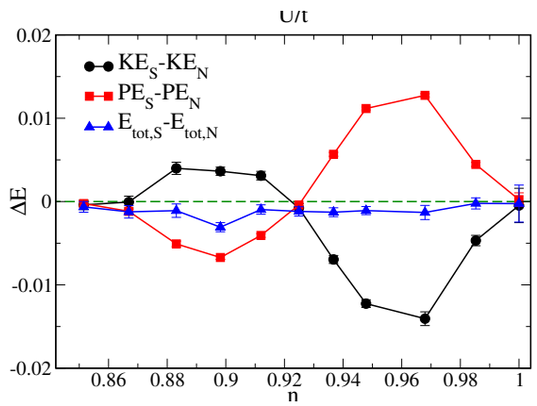


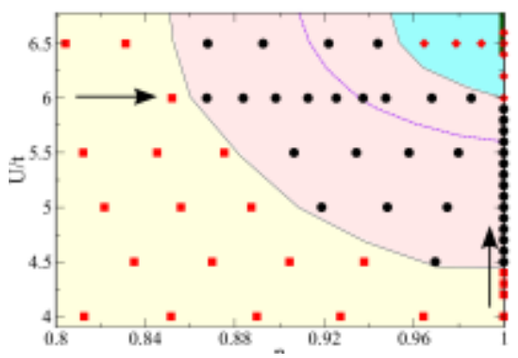
Perform partition function expansion. In Hybridization case: Delta matrix gets bigger. In Interaction expansion case: contractions now have to go over all possible operators.

Superconductivity ('cooper pairs') in attractive and repulsive Hubbard model, …





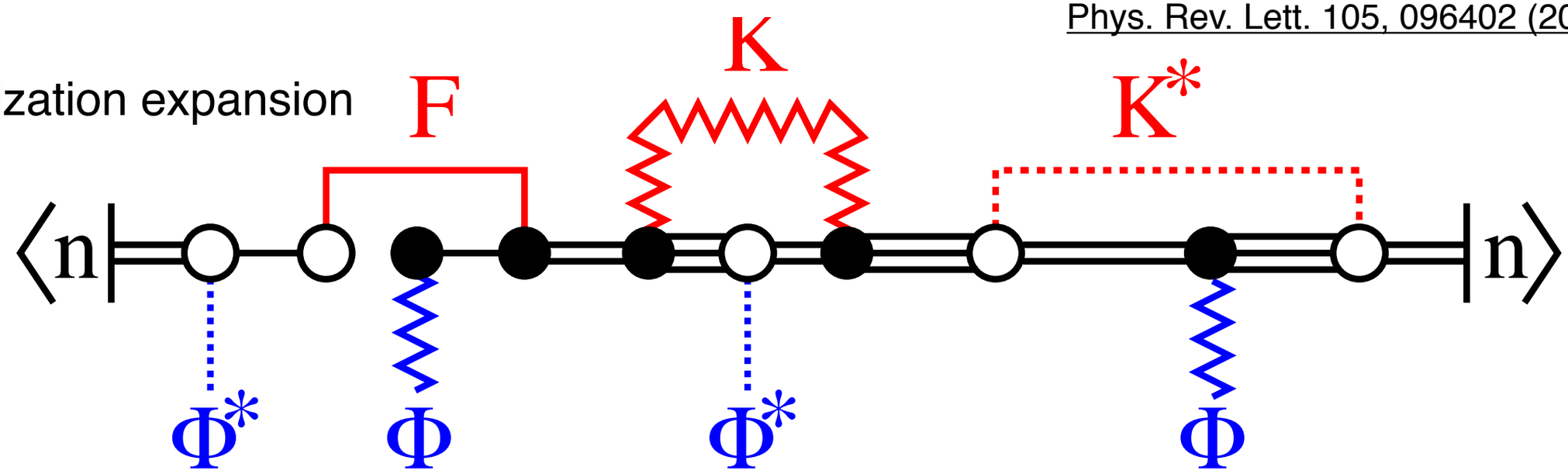




Bosons

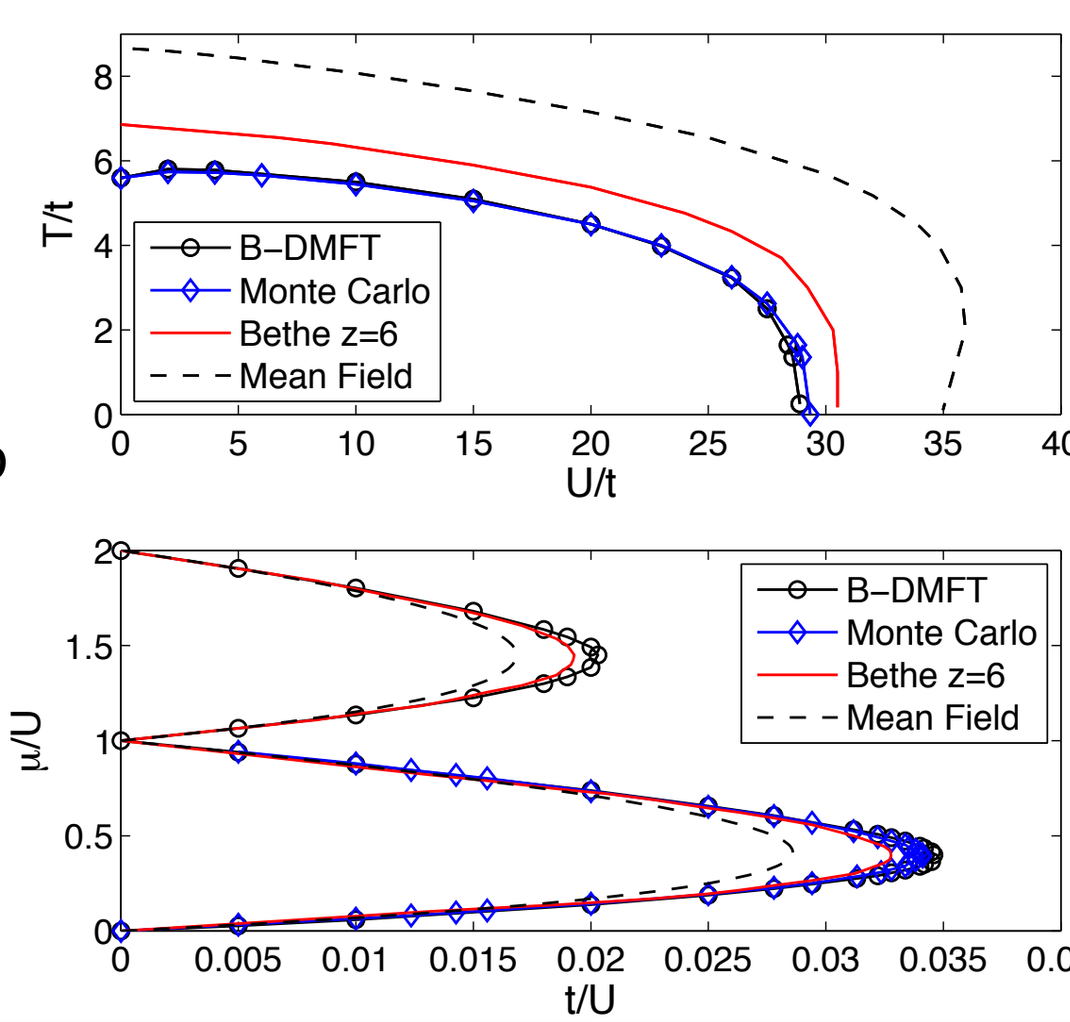
Anders, Gull, Pollet, Troyer, Werner, Dynamical Mean Field Solution of the Bose-Hubbard Model, Phys. Rev. Lett. 105, 096402 (2010)

Hybridization expansion



Bosons are very different!

- Permanents, not determinants
- No Pauli
- Like to condense in ground state (...all fall into the same state...): Nambu always needed
- Unbounded number of energy levels per site
- Essentially classical! Instead of doing something interesting/correlated they just condense.



Adding Phonons to the interaction expansion

For effective models with frequency dependent interactions
Next step in real materials simulations?

F. Assaad and T. Lang, Diagrammatic Determinantal methods: projective schemes and applications to the Hubbard-Holstein model, Phys. Rev. B 76, 035116 (2007)

Supplement Hamiltonian by bosons and coupling Hamiltonian

$$H_{\mathrm{B}} + H_{\text{el-B}} = \sum_{\nu a} g_{\nu}^{a} \mathcal{O}^{a} (b_{\nu}^{\dagger} + b_{\lambda}) + \sum_{\nu} \omega_{\nu} b_{\nu}^{\dagger} b_{\nu}.$$

O^a denotes a bilinear fermion operator

Then expand in fermion and boson degrees of freedom

$$\sum_{V(\tau)} = \sum_{i,\sigma,\sigma',s,\nu} \int_{0}^{\beta} \mathrm{d}\tau',$$

$$w\left[V(\tau)\right] = \delta_{\nu,0} \frac{\tilde{U}}{2} \delta(\tau - \tau') + \delta_{\nu,1} W(\tau - \tau').$$

$$V\left(\tau'\right) = \left\{i, \tau, \sigma, \tau', \sigma', s, \nu\right\},$$

vertex number

vertex spin and time locations

aux spin

vertex type (binary: boson or fermion)

vertex weight

$$w\left[V(\tau)\right] = \delta_{\nu,0} \frac{\tilde{U}}{2} \delta(\tau - \tau') + \delta_{\nu,1} W(\tau - \tau').$$

Advantage: completely general, any type of bosonic Hamiltonian.

Disadvantage: multi-dimensional Taylor is expensive, multi-variable expansion.

Adding Phonons to the hybridization expansion

Special ‘trick’ in the where phonons are simple oscillators at a fixed frequency and the coupling is linear, e.g. Hubbard Holstein model.

$$H_{\rm loc} = -\mu(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$$
$$+\sqrt{2}\lambda(n_\uparrow + n_\downarrow - 1)X + \frac{\omega_0}{2}\left(X^2 + P^2\right).$$

boson fermion coupling

boson coordinate

boson momentum

First step: apply unitary transform to operators (‘Lang Firsov transform’)

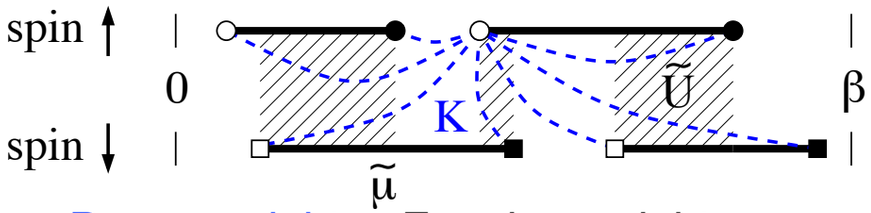
$$X_0 = (\sqrt{2}\lambda/\omega_0)(n_\uparrow + n_\downarrow - 1). \qquad \tilde{H}_{\rm loc} = e^{iPX_0} H_{\rm loc} e^{-iPX_0}$$

$$\tilde{\mu} = \mu - \lambda^2/\omega_0,$$
$$\tilde{U} = U - 2\lambda^2/\omega_0.$$

$$\tilde{H}_{\rm loc} = -\tilde{\mu}(\tilde{n}_\uparrow + \tilde{n}_\downarrow) + \tilde{U}\tilde{n}_\uparrow\tilde{n}_\downarrow + \frac{\omega_0}{2}(X^2 + P^2)$$

$$\tilde{d}^\dagger_\sigma = e^{iPX_0} d^\dagger_\sigma e^{-iPX_0} = e^{\frac{\lambda}{\omega_0}(b^\dagger - b)} d^\dagger_\sigma,$$
$$\tilde{d}_\sigma = e^{iPX_0} d_\sigma e^{-iPX_0} = e^{-\frac{\lambda}{\omega_0}(b^\dagger - b)} d_\sigma,$$

Second step: compute weights as products of boson and fermion weights



Boson weights Fermion weights

Advantage: no computational overhead.
Disadvantage: only works for this special case...

Acknowledgments

UNIVERSITY OF MICHIGAN

Non-equilibrium Collaborators: A.J. **Millis**, D. **Reichman**, G. **Cohen**, and Qiaoyuan **Dong**

Main Equilibrium Collaborators (over the years): A. **Antipov**, J. **Le Blanc**, Xi **Chen**, A.J. **Millis**, Joe **Paki**, O. **Parcollet**, M. **Troyer**, P. **Werner**

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