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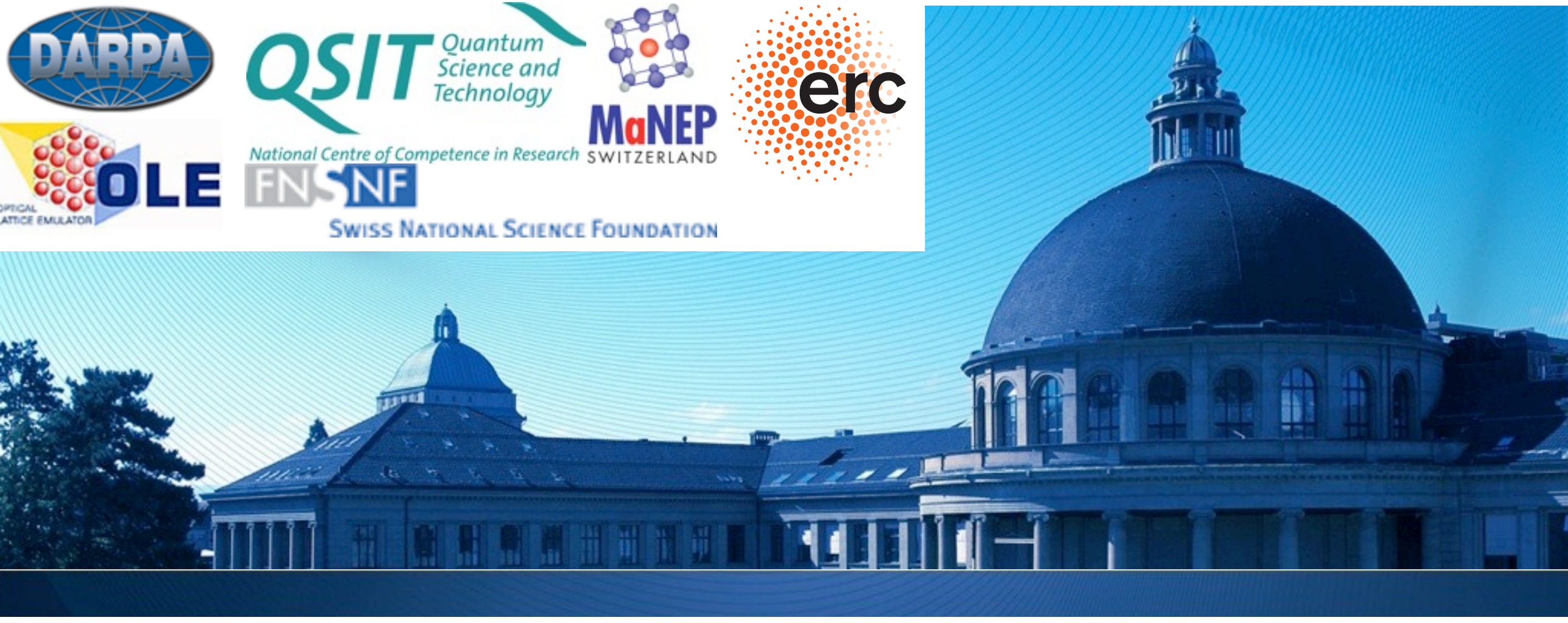
Institute for Theoretical Physics

CT-QMC solvers for quantum impurity problems and the equation of state of the 3D Hubbard model

Matthias Troyer (ETH Zurich)

E. Gull *et al*., Rev. Mod. Phys. **83**, 349 (2011)

DARPA
QSIT Quantum Science and Technology
MaNEP SWITZERLAND
National Centre of Competence in Research
FNSNF
Swiss National Science Foundation
erc
OLE
OPTICAL LATTICE EMULATOR



“Optical lattice emulators” as quantum simulators

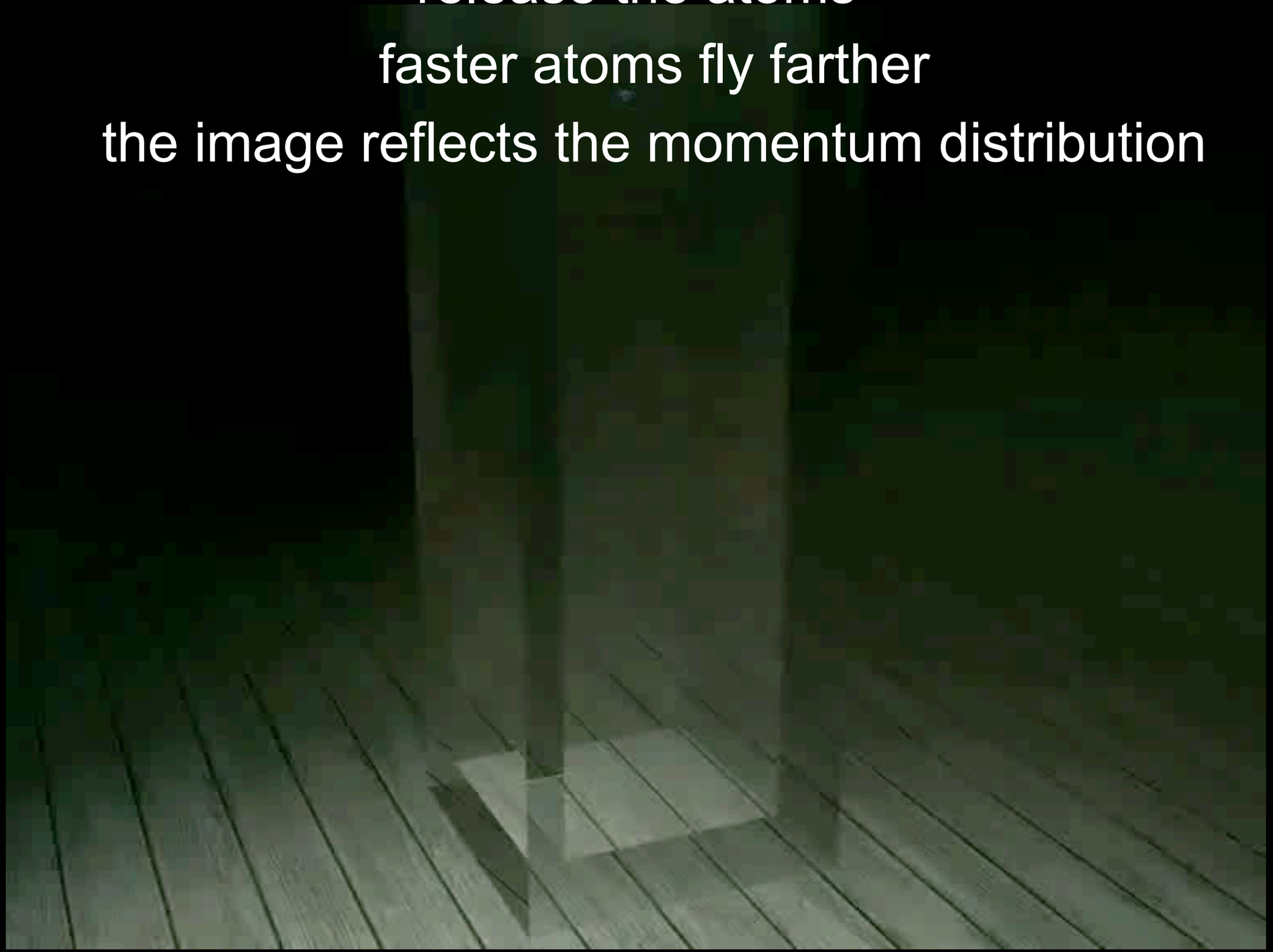
- Ask experimentalists to use cold atomic gases in an optical lattice to “solve” the Hamiltonian that we cannot solve.

How do we detect these quantum gases ?

release the atoms

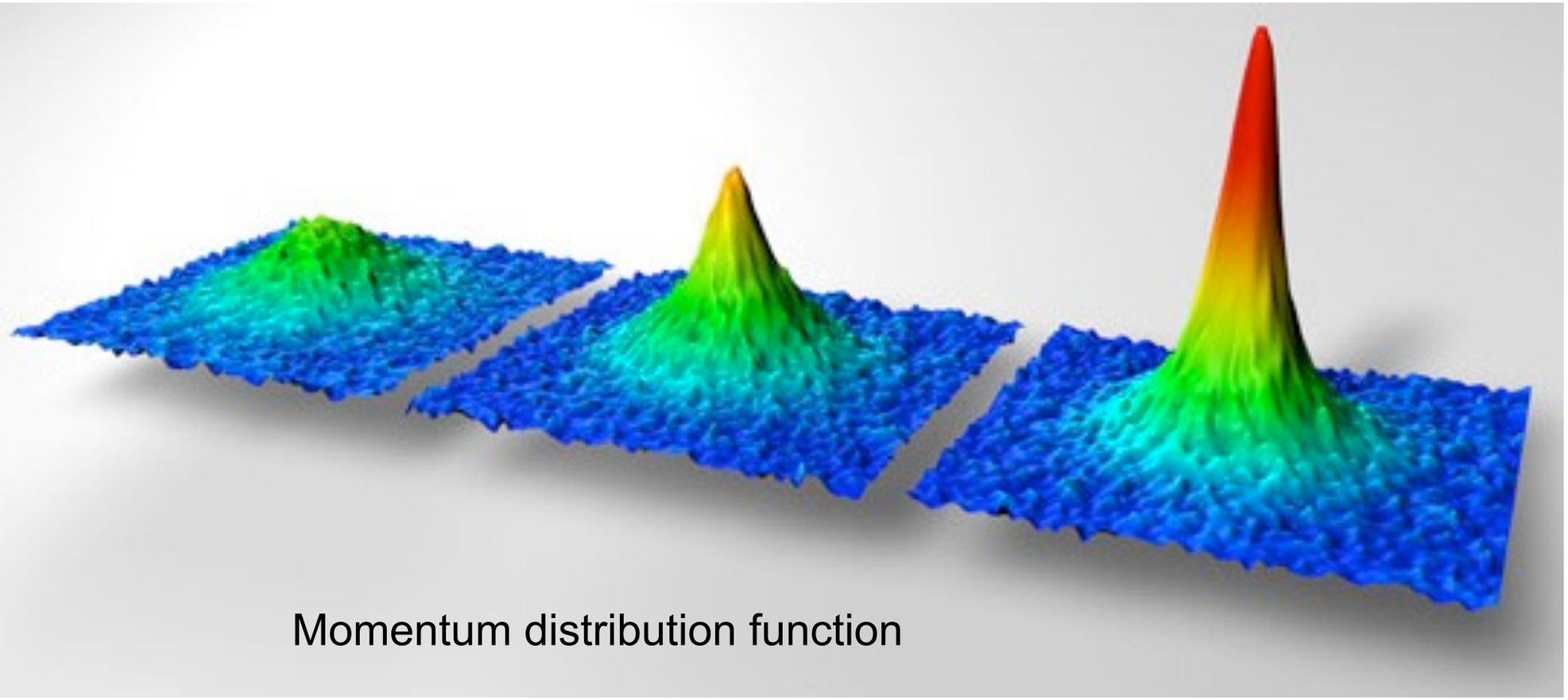
faster atoms fly farther

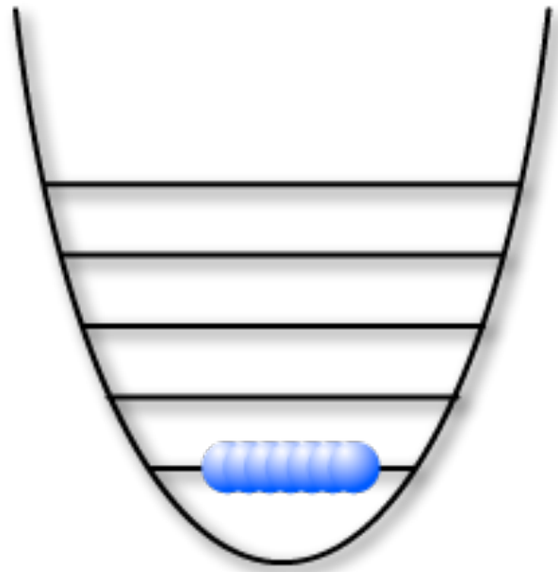
the image reflects the momentum distribution



Bose-Einstein condensation in cold atomic gases

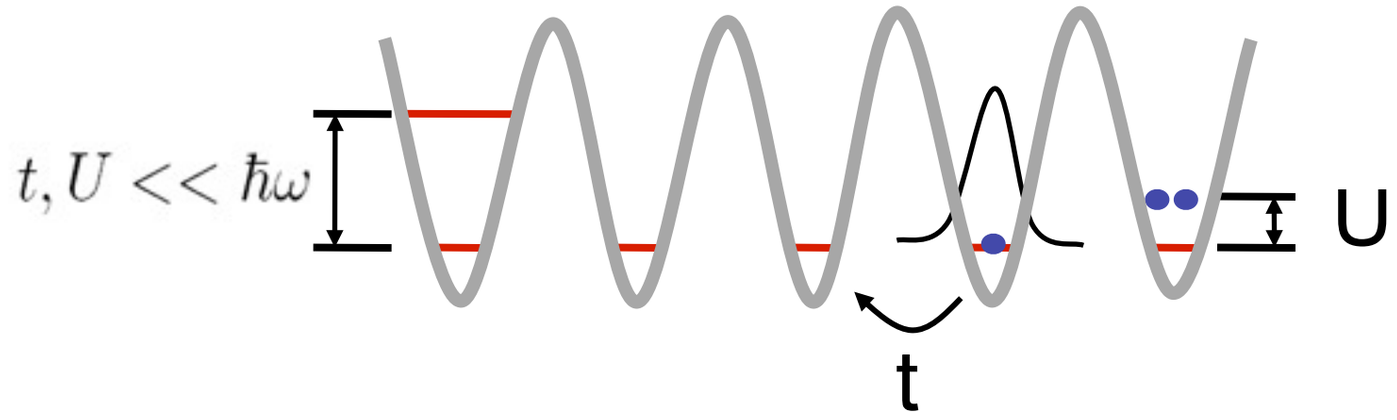
- At close to zero temperatures, a macroscopic fraction of all atoms in a Bose gas occupy the same quantum state
- A diverging occupation of the zero momentum state

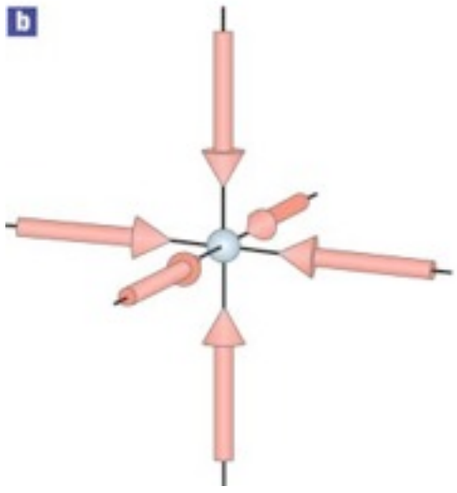


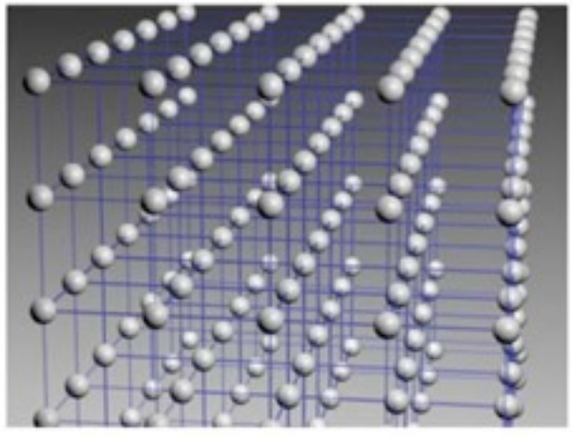


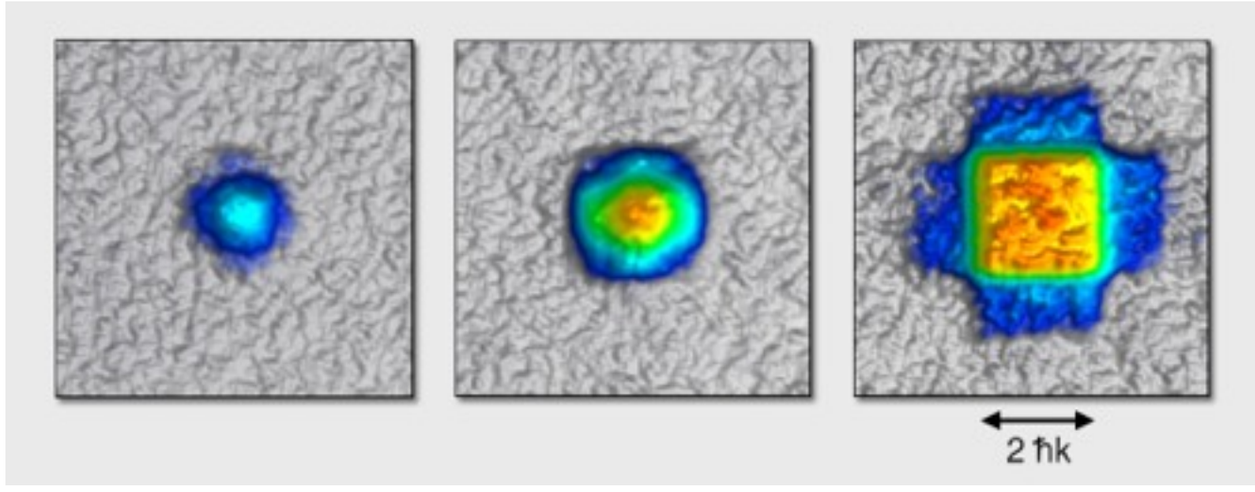
Ultracold atoms in optical lattices

- Take a dilute gas of fermions at nK temperatures
- Add a standing wave optical lattice
- Obtain a controlled, clean and tunable Hubbard model









fermionic momentum distribution function (Esslinger group)

Does it work for bosonic models that we can solve?

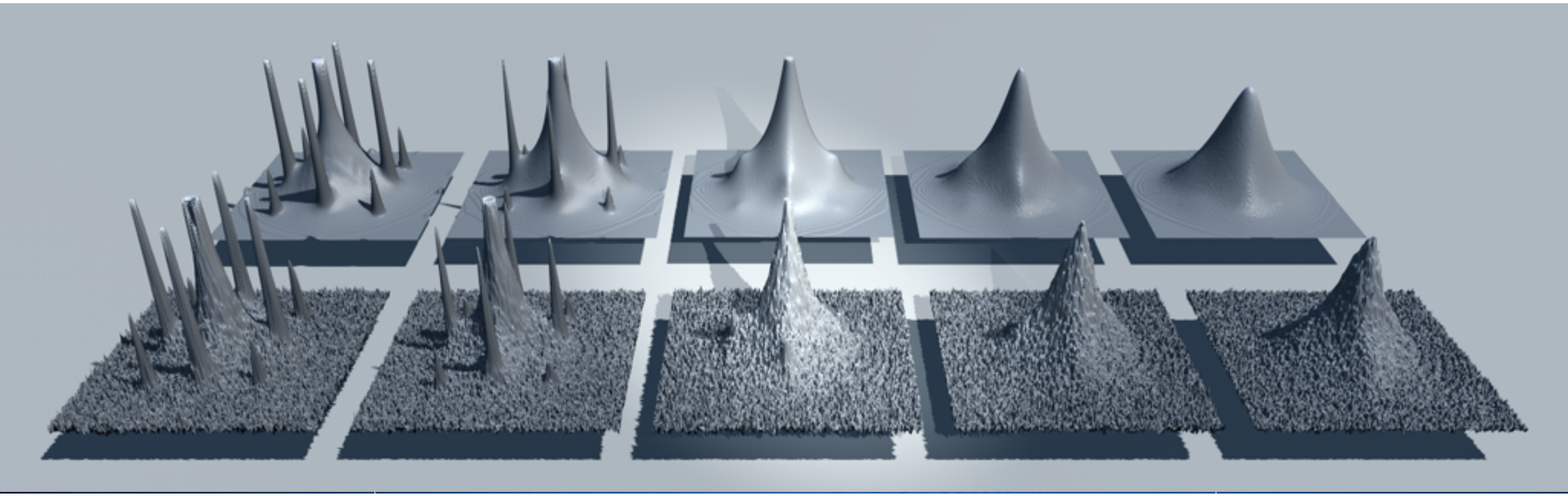
- We model all important details of the experiment
- The experiment should better reproduce what we get!
- and it does: Trotzky, Pollet *et al*, Nature Phys. **6**, 998 (2010).

SCIENCE VOL 330 17 DECEMBER 2010

BREAKTHROUGH OF THE YEAR

THE RUNNERS-UP

Quantum Simulators Pass First Key Test



Simulating fermions

- There is no “black box” solution for all fermion problems
  - Fermionic sign problem prevents large-scale simulations
  - We need to think hard and find good (approximate) methods
- We can still simulate fermions in some regimes:
  - High-temperature expansions: valid down to T ≈1.4 t
  - Dynamical mean field theory (DMFT) approximation and cluster extensions to lower temperatures
  - Diagrammatic QMC methods for intermediate interactions
- We might not be able to reach the ground state, but we can simulate the relevant regime for cold atoms
- I will discuss CT-QMC solvers for cluster versions of DMFT

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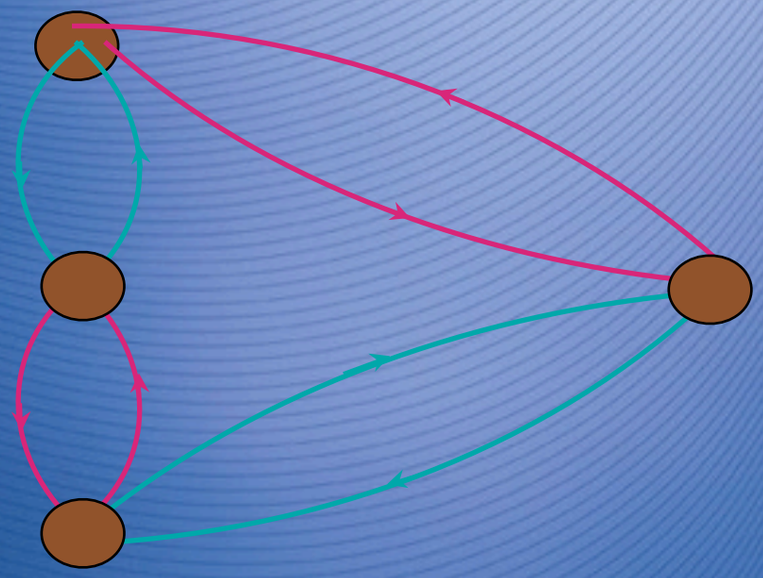
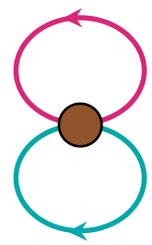
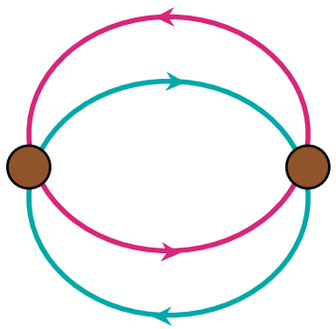
CT-QMC for the Hubbard model

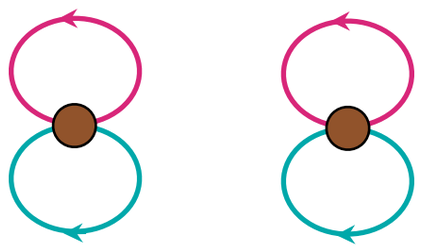


Diagrammatic expansion in interaction

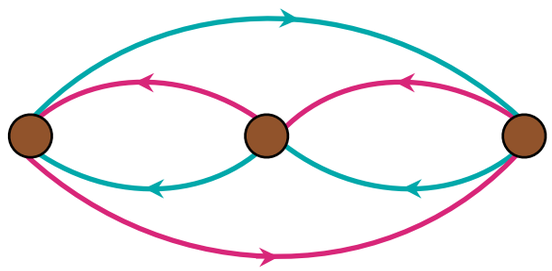


$-U$



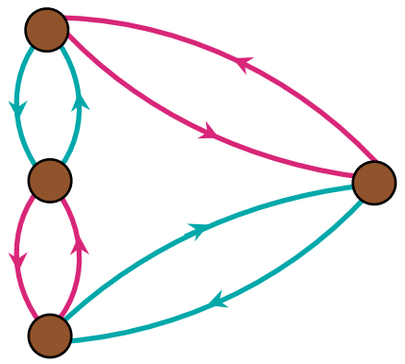


$G_{\uparrow}(r_i - r_j, \tau_i - \tau_j)$

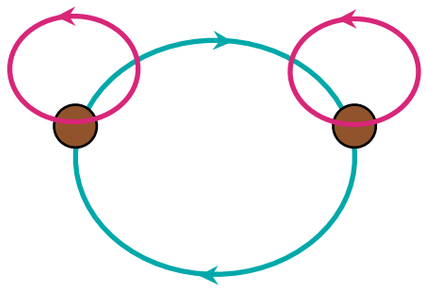


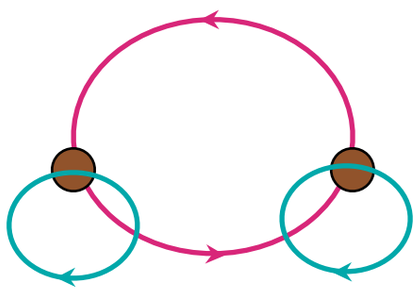
$G_{\uparrow}(r_i - r_j, \tau_i - \tau_j)$

$(-U)^3$



$(-U)^4$





$(-U)^2$

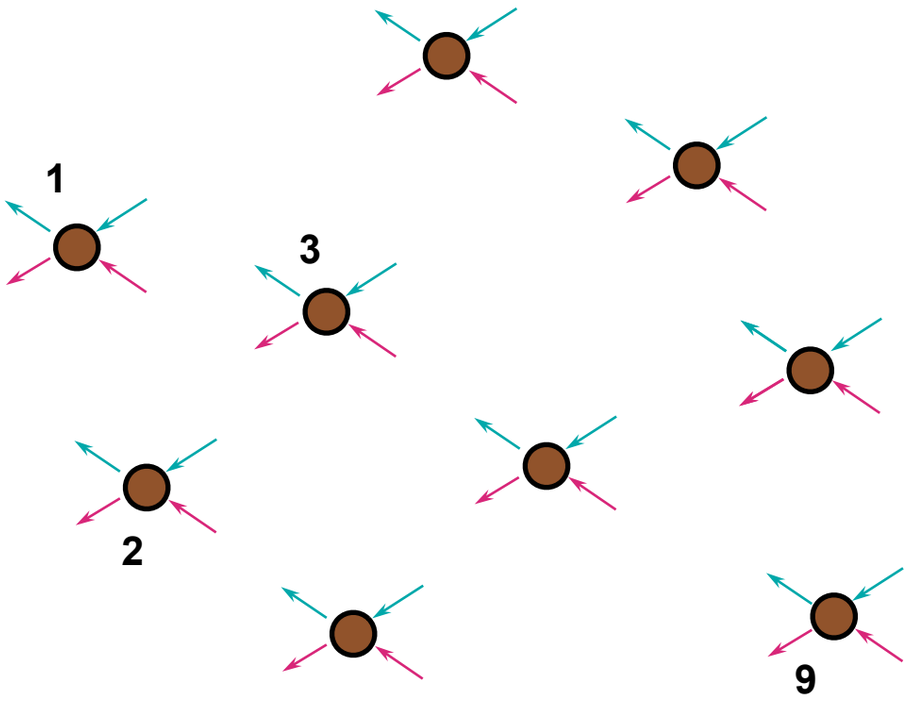
too many to draw all p!^{2} possible topologies …

but easy to sum all of them into a determinant

Diagrammatic expansion in interaction

A.N. Rubtsov & A.I. Lichtenstein, Pis'ma v JETP 80, 67 (2004)

A.N. Rubtsov, V.V. Savkin, A.I. Lichtenstein, Phys. Rev. B 72, 035122 (2005)



The sum of all $p!^2$ diagrams for a given vertex configuration $(\mathbf{r}_1,\tau_1;\mathbf{r}_2,\tau_2;\ldots;\mathbf{r}_p,\tau_p)$ is a determinant squared

$$\det G_{ij} = \begin{vmatrix} G_{11} & G_{12} & \ldots & G_{1p} \\ G_{21} & G_{22} & \ldots & G_{2p} \\ \ldots & \ldots & \ldots & \ldots \\ G_{p1} & G_{p2} & \ldots & G_{pp} \end{vmatrix}$$

$$Z = \sum_{\xi} D_n(\xi) = \sum_{p} \int \ldots \int (d\vec{r}d\tau)^p (-U)^p \det{}^2 G_{\uparrow}(\vec{x}_i, \vec{x}_j)$$

Sign-problem free for attractive interactions U<0 and balanced population of up and down spins

Repulsive interactions

- Repulsive interactions: U>0
- $(-U)^n$ can be negative: sign problem
- Perform particle-hole transformation on one spin-species
  - U changes sign

$$Un_{i,\uparrow}n_{i,\downarrow} \rightarrow Un_{i,\uparrow}(1-n_{i,\downarrow}) = Un_{i,\uparrow} - Un_{i,\uparrow}n_{i,\downarrow}$$

  - Equal population condition changes to a half-band filling condition

$$n_{i,\downarrow} = n_{i,\downarrow} \rightarrow n_{i,\downarrow} = 1 - n_{i,\downarrow} \Rightarrow n_{i,\downarrow} + n_{i,\downarrow} = 1$$

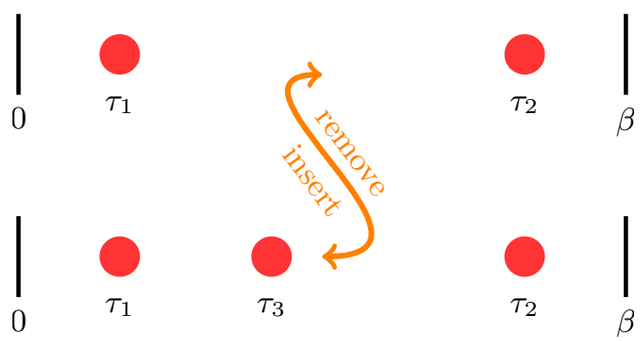
- We can simulate repulsive fermions (only) at half filling

How can we do updates in continuous time?

- Simplified example:

$$Z = \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \cdots \int_0^\beta d\tau_k \, \frac{w(k)}{k!},$$

- CT-QMC updates consist of insertion and removal of interaction vertices.



- Acceptance probabilities are not infinitesimal if done right

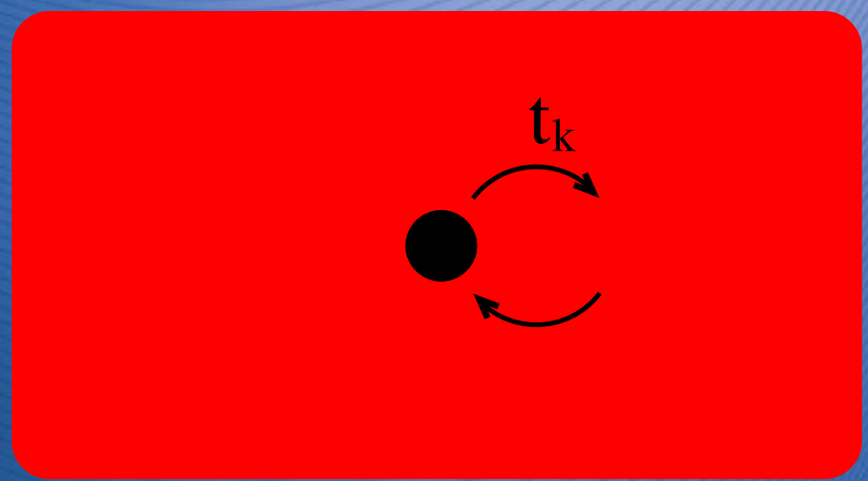
Advantages of continuous time

- No need to extrapolate in time step
  - a single simulation is sufficient
  - no additional errors from extrapolation

- Less memory and CPU time required
  - Instead of a time step $\Delta\tau << t$ we only have to store changes in the configuration happening at mean distances $\approx t$

- Conceptual advantage
  - we directly sample a diagrammatic perturbation expansion

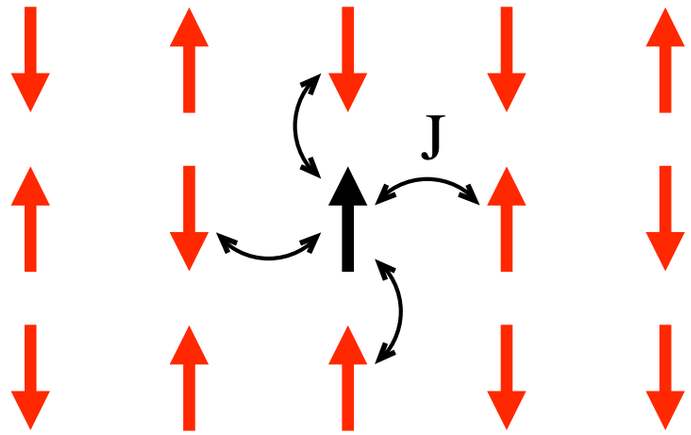
Dynamical mean field theory



Mean-field theory for Ising Model

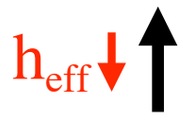
- Lattice model (nearest neighbor coupling J, coordination number z)

  $H_{\text{latt}} = -J \sum_{i,j} S_i S_j$



- Single site model ($m_i = \langle S_i \rangle$, $h_{\text{eff}} = J \sum_{0,i} m_i = zJm$)

  $H_0 = -h_{\text{eff}} S_0$



- Self-consistency condition

  $m = \langle m_0 \rangle_{H_0}$ ($= \tanh(\beta h_{\text{eff}}) = \tanh(\beta z J m)$)

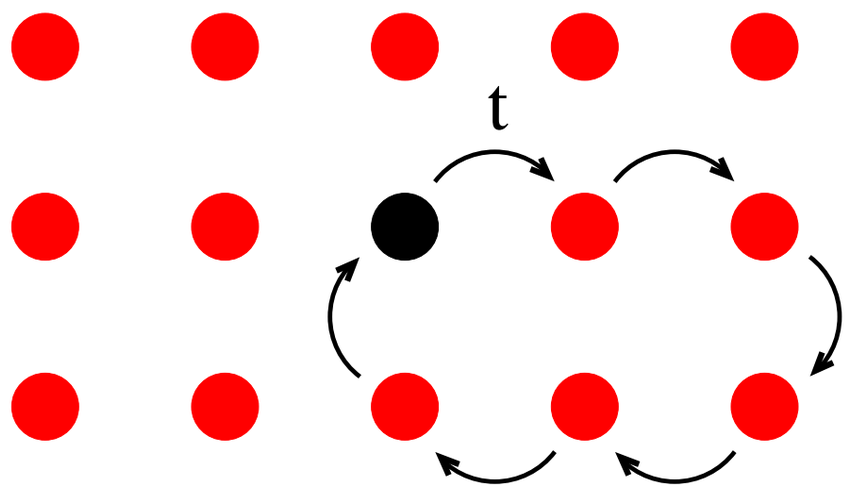
Dynamical mean field theory

- Lattice model

Metzner & Vollhardt, PRL (1989)

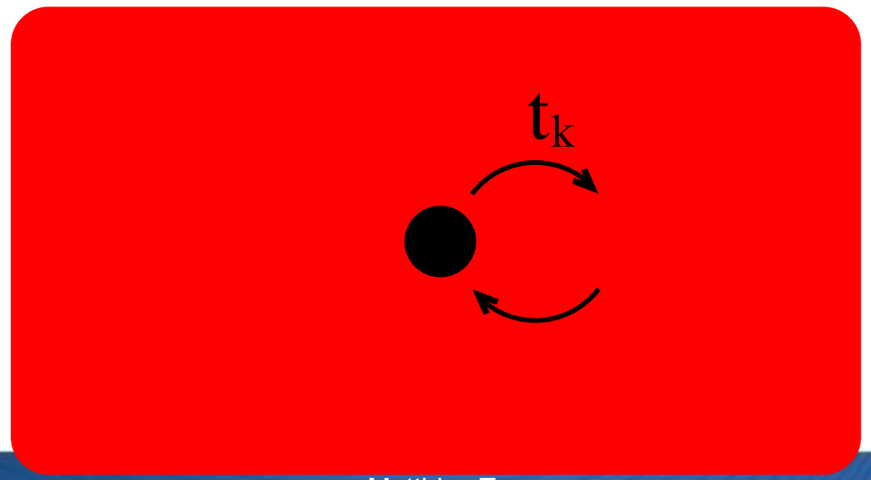
Georges & Kotliar, PRB (1992)

$$H_{latt} = U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma}$$



- Quantum impurity model

$$H_{imp} = U n_\uparrow n_\downarrow - \sum_{k,\sigma} (t_k c^\dagger_\sigma a^{bath}_{k,\sigma} + h.c.) + H_{bath}$$

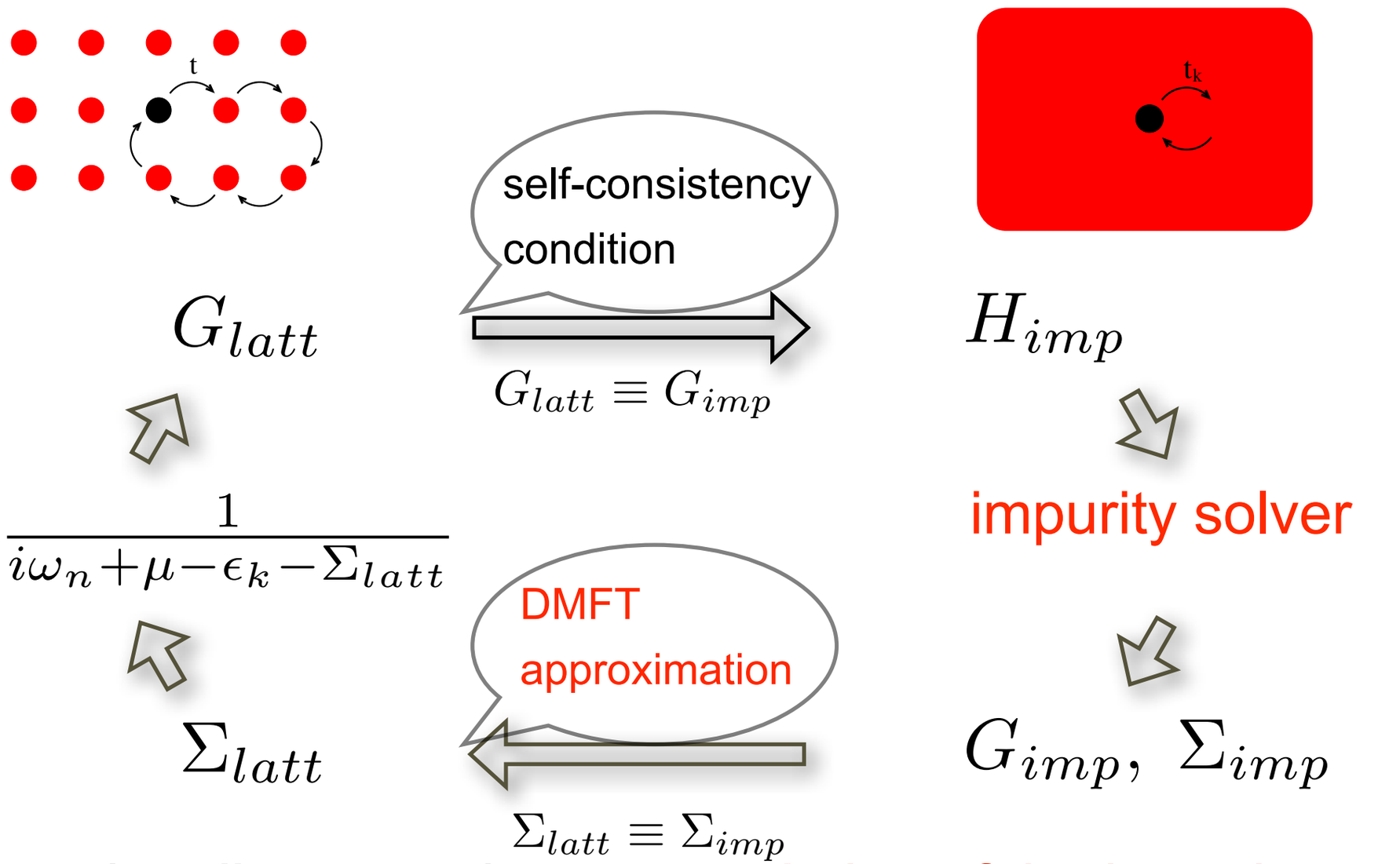


Dynamical mean field theory

- Self-consistency loop

Metzner & Vollhardt, PRL (1989)

Georges & Kotliar, PRB (1992)



- Computationally expensive step: solution of the impurity model

Hirsch-Fye QMC solver

J.E. Hirsch & R.M. Fye, Phys. Rev. Lett. 56, 2521 (1986)

- Uses M discrete time steps $\Delta\tau = \beta/M$
- Decouples quartic interaction using Hubbard-Stratonovich transformation and auxiliary fields *s*

$$e^{-\Delta\tau U(n_\uparrow n_\downarrow + 1/2(n_\uparrow + n_\downarrow))} = \frac{1}{2}\sum_{s=\pm 1} e^{\lambda(U,\Delta\tau)s(n_\uparrow + n_\downarrow)}$$

- Integration over fermionic Gaussian integrals gives determinants

$$Z = \sum_{s_i} \det G^{-1}_{0,\uparrow}(s_1, ..., s_N) G^{-1}_{0,\downarrow}(s_1, ..., s_N)$$

- Monte Carlo sampling of auxiliary fields s_i
- Was the standard QMC solver for two decades

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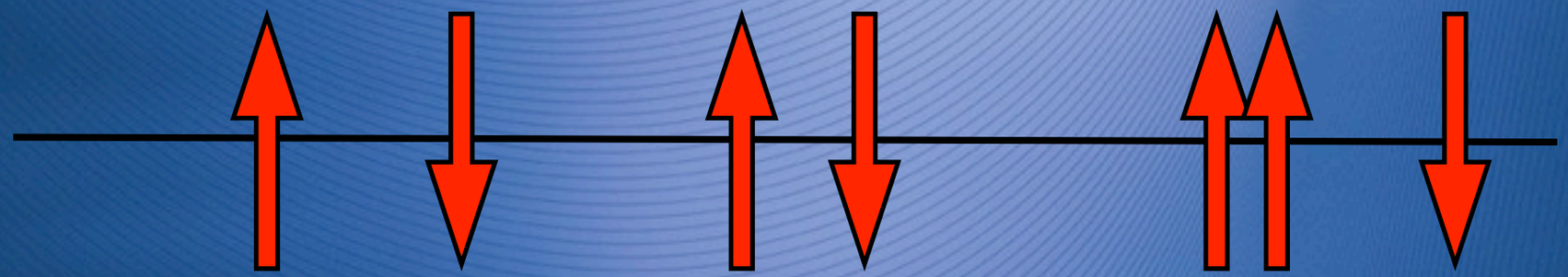
CT-QMC:
Continuous time diagrammatic QMC solvers



Diagrammatic (continuous time) QMC

- General recipe:

1. Split Hamiltonian into two parts: $H = H_1 + H_2$

2. Use interaction representation in which $O(\tau) = e^{\tau H_1} O e^{-\tau H_1}$

3. Write partition function as time-ordered exponential and expand in powers of H_2

$$
\begin{aligned}
Z &= Tr\left[e^{-\beta H_1} T e^{-\int_0^\beta d\tau H_2(\tau)}\right] \\
&= \sum_k \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k \frac{(-1)^k}{k!} Tr\left[e^{-\beta H_1} T H_2(\tau_1) \ldots H_2(\tau_k)\right]
\end{aligned}
$$

CT-QMC algorithms differ by choice of H_1 and H_2

- For a review see Gull *et al,* Rev. Mod. Phys. 83, 349 (2011)
- Interaction expansion CT-INT
  - Rubtsov et al. (2005)
  - Expand in **interactions**, treat quadratic terms exactly
- Auxiliary field method CT-AUX
  - Rombouts et al., (1999), Gull et al. (2008)
  - Decouple interactions using **auxiliary** fields
- Hybridization expansion CT-HYB
  - Werner et al., (2006), Werner & Millis (2006), Haule (2007)
  - Expand in **hybridizations**, treat local terms exactly

CT-AUX

Rombouts et al., PRL (1999)

Gull et al., EPL (2008)

- Impurity model given by

$$\begin{aligned} H &= H_0 + H_U \\ H_0 &= K/\beta - (\mu - U/2)(n_\uparrow + n_\downarrow) + H_{hyb} + H_{bath} \\ H_U &= U(n_\uparrow n_\downarrow - (n_\uparrow + n_\downarrow)/2) - K/\beta \end{aligned}$$

- Expand partition function into powers of the interaction term

$$Z = \sum_k \frac{(-1)^k}{k!} \int d\tau_1 \ldots \int d\tau_k Tr\left[Te^{-\beta H_0} H_U(\tau_1) \ldots H_U(\tau_k)\right]$$

- Decouple the interaction terms using

$$-H_U = \frac{K}{2\beta} \sum_{s=\pm 1} e^{\gamma s(n_\uparrow - n_\downarrow)}, \qquad \cosh(\gamma) = 1 + \frac{\beta U}{2K}$$

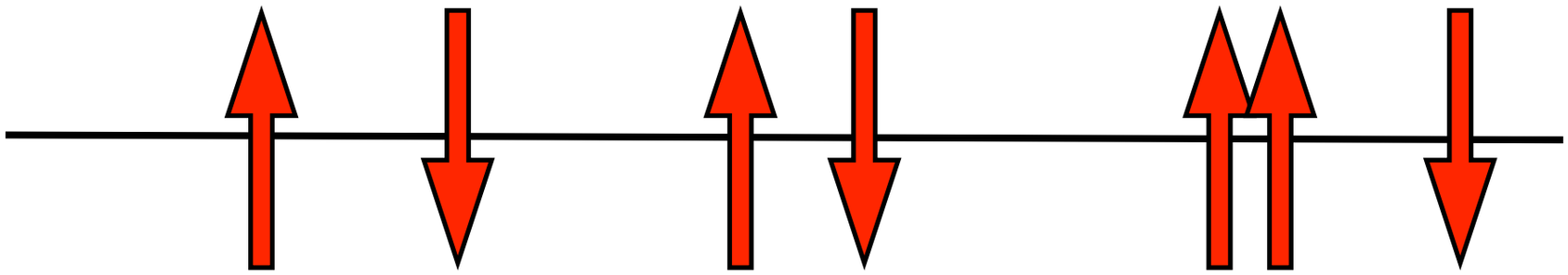
- then integrate over fermionic Gaussian integrals

CT-auxiliary field QMC (CT-AUX)

Rombouts et al., PRL (1999)

Gull et al., EPL (2008)

- Configuration space: all possible time-ordered spin configurations



- Weight: $w(\tau_1, s_1; \ldots; \tau_k, s_k) = \left(\frac{K d\tau}{2\beta}\right)^k \prod_\sigma \det N_\sigma^{-1}(\{\tau_i, s_i\})$

$$N_\sigma^{-1} = e^{\Gamma_\sigma} - G_{0\sigma}\left(e^{\Gamma_\sigma} - 1\right)$$

$$e^{\Gamma_\sigma} = \mathrm{diag}(e^{\gamma\sigma s_1}, \ldots, e^{\gamma\sigma s_k})$$

- Monte Carlo updates: random insertion/removal of a spin
- Formally similar to discrete-time Hirsch-Fye method

Interaction expansion CT-INT

Rubtsov et al., PRB (2005)

- Impurity model given by

$$\begin{aligned} H &= H_0 + H_U \\ H_0 &= -\mu(n_\uparrow + n_\downarrow) + \alpha_\uparrow n_\downarrow + \alpha_\downarrow n_\uparrow + H_{hyb} + H_{\mathrm{bath}} \\ H_U &= U(n_\uparrow - \alpha_\uparrow)(n_\downarrow - \alpha_\downarrow) \end{aligned}$$

- Expand partition function into powers of the interaction term

$$Z = \sum_k \frac{(-1)^k}{k!} \int d\tau_1 \ldots \int d\tau_k Tr\left[Te^{-\beta H_0} H_U(\tau_1) \ldots H_U(\tau_k)\right]$$

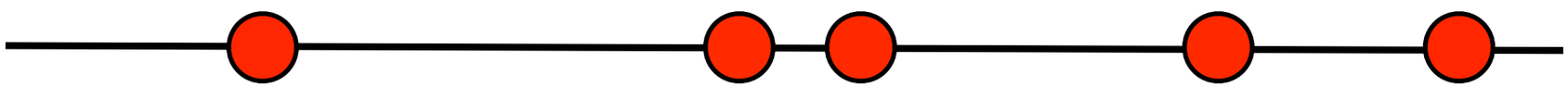
- Wick's theorem yields weight of vertex configurations

- alpha-terms necessary to avoid sign problem

Interaction expansion CT-INT

Rubtsov et al., PRB (2005)

- Configuration space: all possible time-ordered vertex configurations



- Weight: $$w(\tau_1, \ldots, \tau_k) = (-U d\tau)^k \prod_{\sigma} \det G_{0\sigma}^{(\alpha_\uparrow, \alpha_\downarrow)}(\{\tau_i\})$$

- Monte Carlo updates: random insertion/removal of a vertex

Hybridization expansion (CT-HYB)

Werner et al., PRL (2006)
Werner & Millis, PRB (2006)
Haule, PRB (2007)

- Impurity model given by

$$\begin{aligned} H &= H_{loc} + H_{bath} + H_{hyb} \\ H_{loc} &= U n_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow) \\ H_{hyb} &= \sum_{p,\sigma} t_p^\sigma c_\sigma^\dagger a_{p,\sigma} + h.c. \end{aligned}$$

- Expand partition function into powers of the hybridization term

$$Z = \sum_k \frac{1}{2k!} \int d\tau_1 \ldots \int d\tau_{2k} Tr\left[T e^{-\beta(H_{loc}+H_{bath})} H_{hyb}(\tau_1) \ldots H_{hyb}(\tau_{2k}) \right]$$

- Trace over bath degrees of freedom yields determinant of hybridization functions *F*

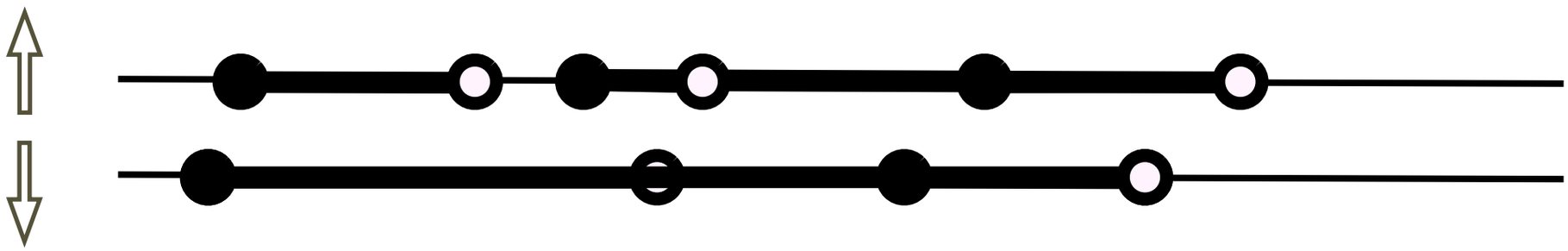
$$Tr_{bath}[\ldots] = \prod_\sigma \det M_\sigma^{-1}, \qquad M_\sigma^{-1}(i,j) = F_\sigma(\tau_i^{(c)} - \tau_j^{(c^\dagger)})$$

$$F_\sigma(-i\omega_n) = \sum_p \frac{|t_p^\sigma|^2}{i\omega_n - \epsilon_p}$$

Werner et al., PRL (2006)
Werner & Millis, PRB (2006)
Haule, PRB (2007)

Hybridization expansion

- Monte Carlo configurations consist of segments for spin up and down



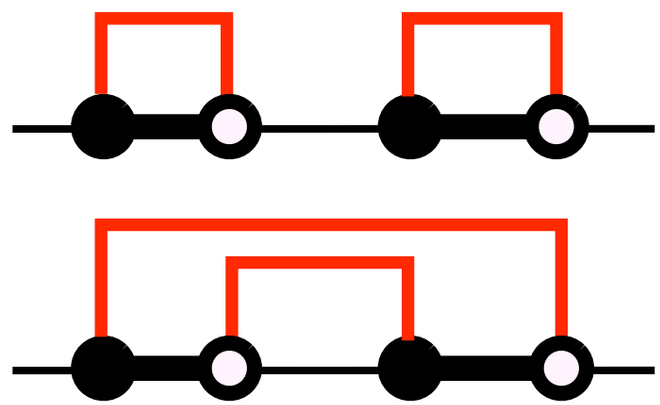
- Monte Carlo updates: random insertion/removal of (anti-)segments

- Weight of a segment configuration:

$$w\left(\tau_1^{\sigma(c)}, \tau_1^{\sigma(c^\dagger)}; \ldots; \tau_{k_\sigma}^{\sigma(c)}, \tau_{k_\sigma}^{\sigma(c^\dagger)}\right) = \underbrace{e^{-U l_{overlap} + \mu(l_\uparrow + l_\downarrow)}}_{Tr_{imp}[\ldots]} \prod_\sigma \underbrace{\det M_\sigma^{-1}}_{Tr_{bath}[\ldots]} d\tau^{2k_\sigma}$$

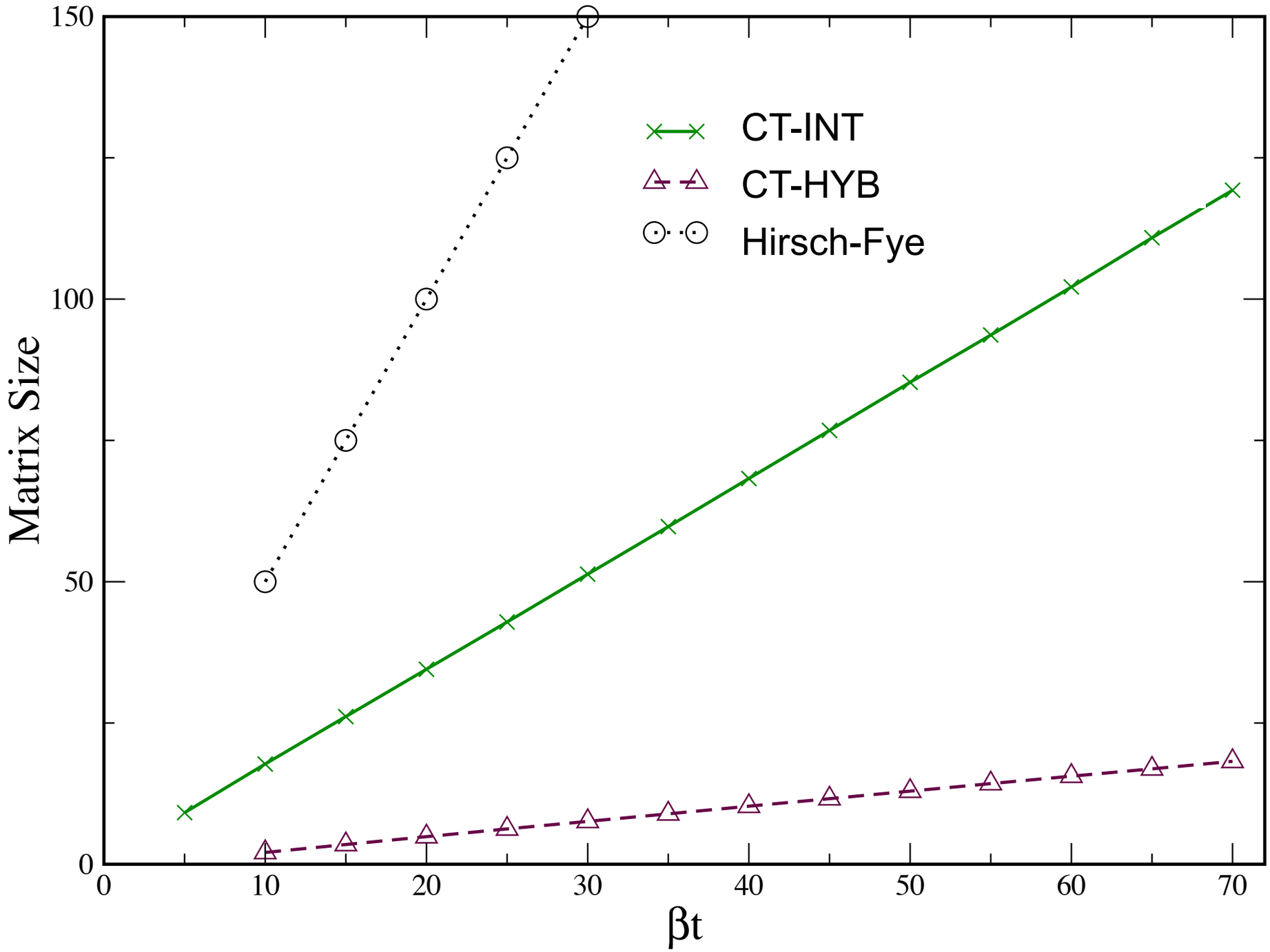
- Determinant of a *k x k* matrix resums *k!* diagrams

$$\det \begin{pmatrix} F_\sigma(\tau_1^{(c)} - \tau_1^{(c^\dagger)}) & F_\sigma(\tau_1^{(c)} - \tau_2^{(c^\dagger)}) \\ F_\sigma(\tau_2^{(c)} - \tau_1^{(c^\dagger)}) & F_\sigma(\tau_2^{(c)} - \tau_2^{(c^\dagger)}) \end{pmatrix}$$



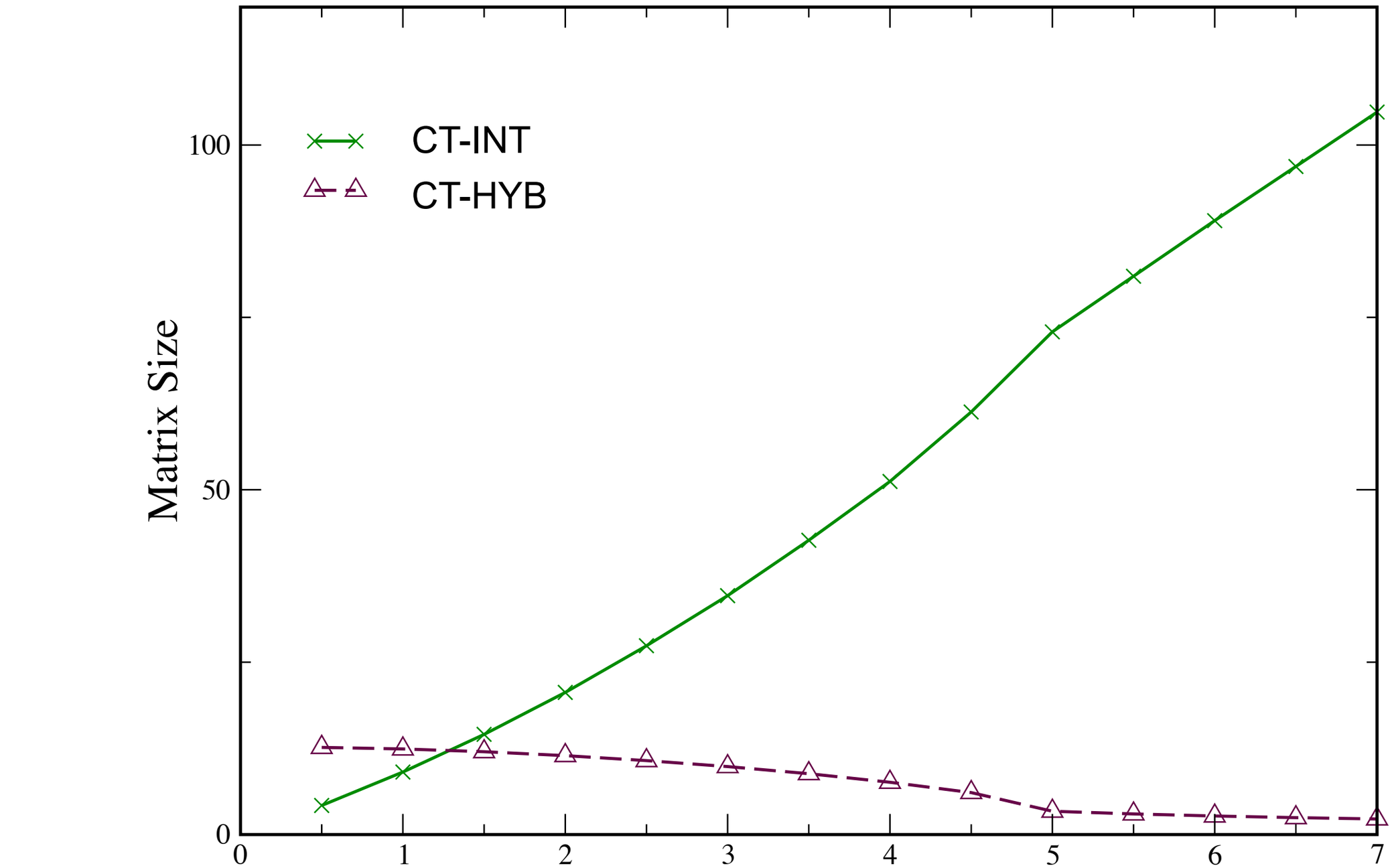
- Eliminates sign problem

Solver Comparison - Matrix Sizes



U/t=4

Matrix Sizes - coupling dependence



Typical region of interest:

βt=30

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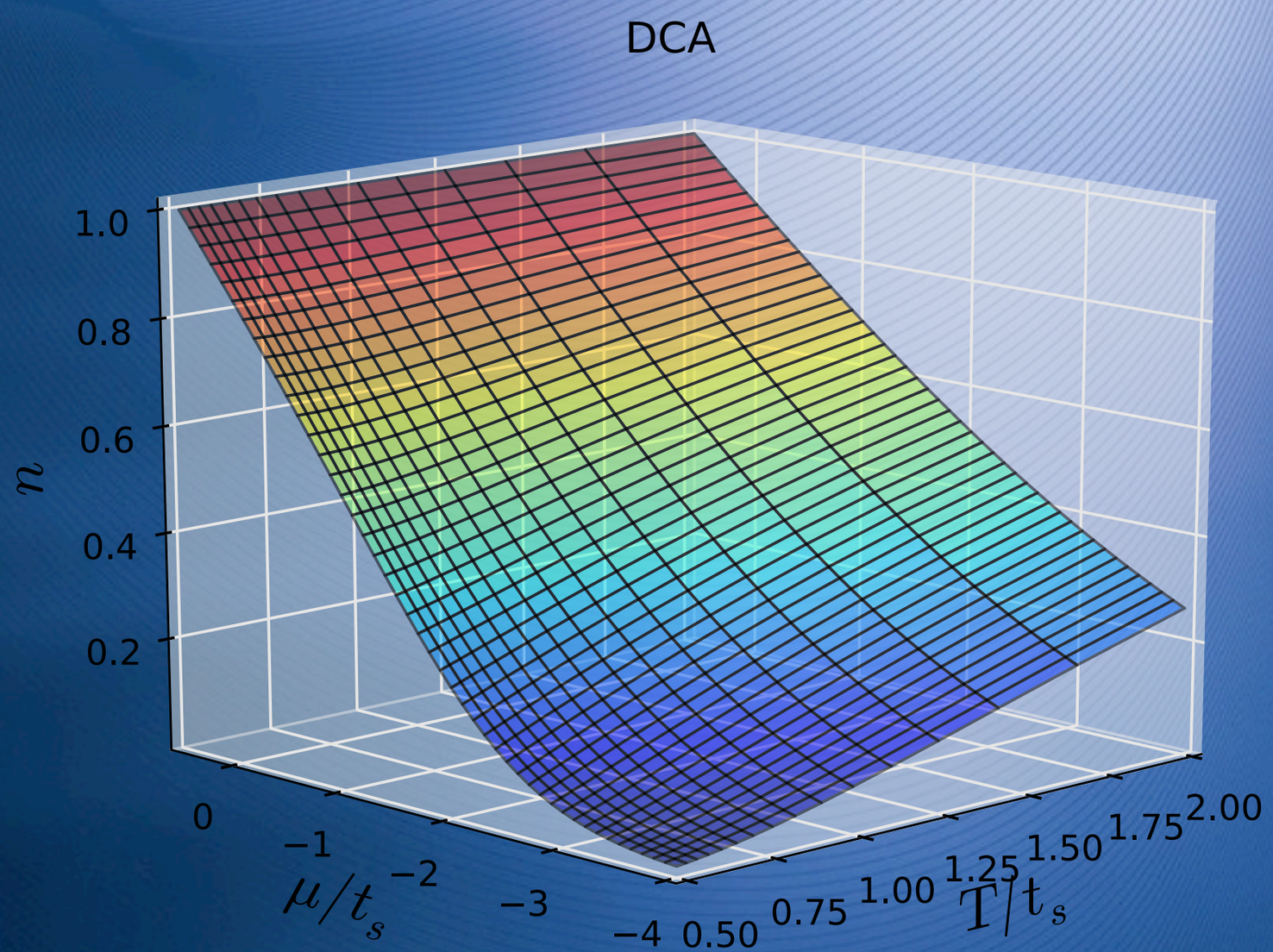
Equation of state of the 3D Hubbard model



What do we want to know about the Hubbard model?

- Quantities of interest
  - equation of state: density, energy, entropy, free energy
  - double occupancy, density and spin correlations
  - momentum distribution function
- Experimentally relevant questions
  - How much does one need to cool to see antiferromagnetic ordering at the Néel temperature?
  - Reference data for thermometry and validation of experiments
  - Finally, use experiments to check simulations and approximations
- Note: these are isolated systems at (ideally) constant entropy and not constant temperature

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Cluster Dynamical Mean Field Theory

Maier et al., Rev. Mod. Phys. 77, 1027

$$\Sigma(k,\omega) = \sum_n \Sigma_n(\omega)\phi_n(k) \approx \sum_n^{N_c} \Sigma_n(\omega)\phi_n(k)$$

Approximation:
Systematic truncation by cluster sites N_c

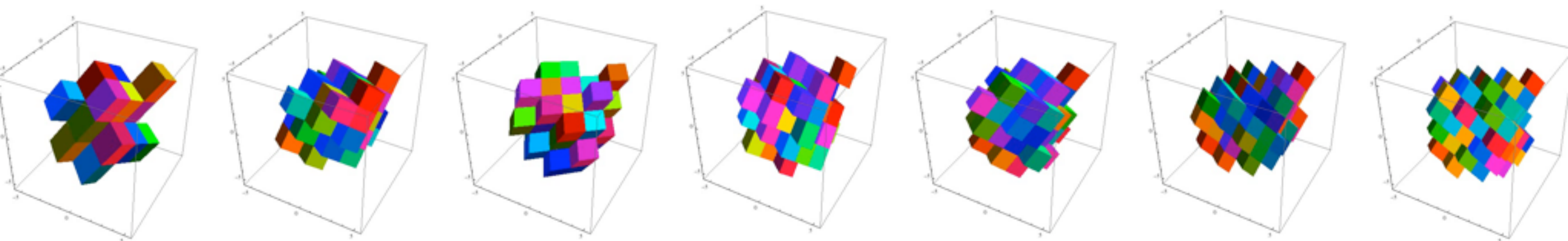
$\phi_n(k)$ Basis functions

$\Sigma_n(\omega)$ Energy dependent, k-independent self-energy

'Machinery' for obtaining approximated self energy: Cluster DMFT.

Cluster DMFT is a controlled approximation.

Variants of cluster DMFT: Dynamical Cluster Approximation (used here) and Cellular Dynamical Mean Field Theory: Differ in types of basis functions $\phi_n(k)$
Within DCA: $\phi_n(k)$ chosen to be constant on patches in momentum space.



18 36 48 56 64 84 100

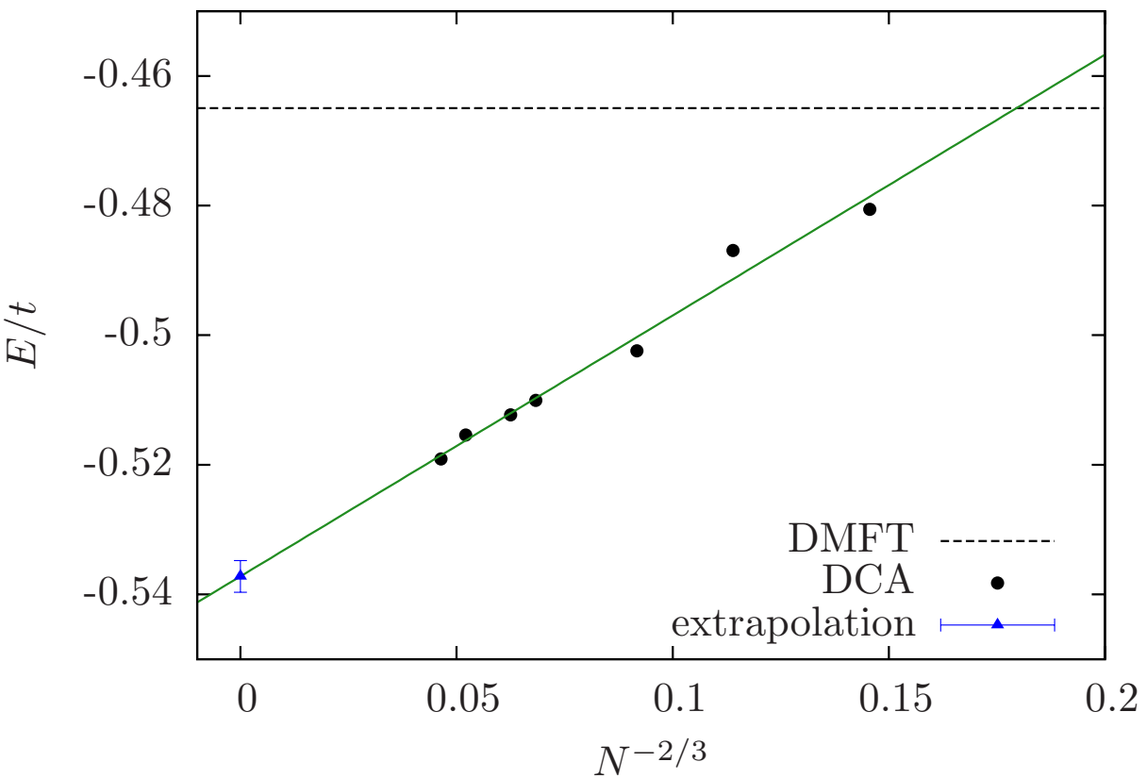
Going to larger impurity systems

- CT-AUX and CT-INT
  - effort is polynomial (cubic) in impurity cluster size
  - sign problem returns when impurity is bigger than one site
  - restricted to Hubbard-like models
  - used for up to 100 orbitals

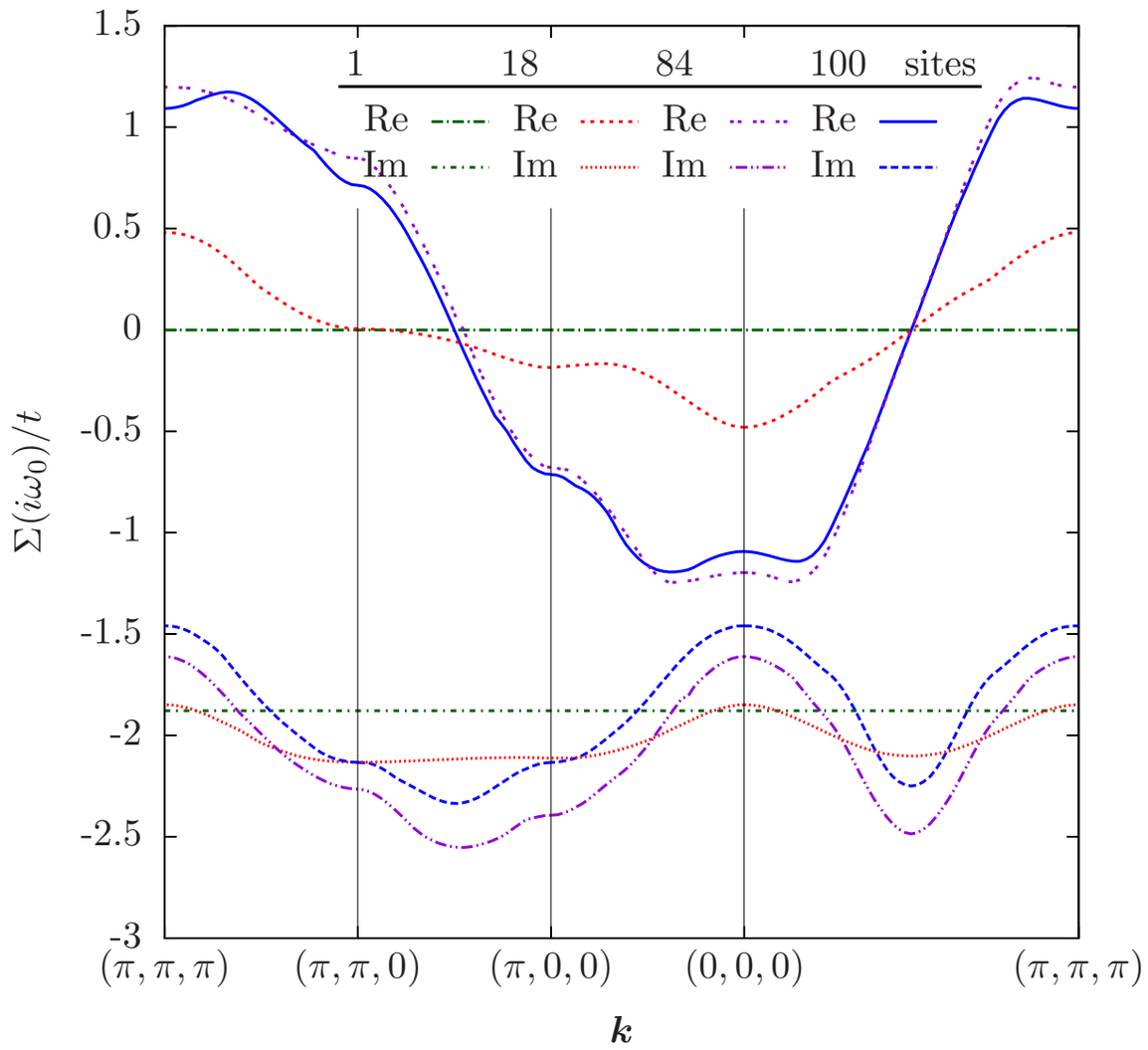
- CT-HYB
  - effort is exponential in impurity cluster size since we need to diagonalize the local Hamiltonian
  - can do arbitrary interactions, e.g. full Coulomb
  - used for up to 5-7 orbitals in LDA+DMFT simulations

Extrapolation of DCA results

- Extrapolation of DCA results to infinite cluster size is crucial
  - Large clusters are needed since there is structure in momentum space!



S. Fuchs *et al,.* PRL (2011)

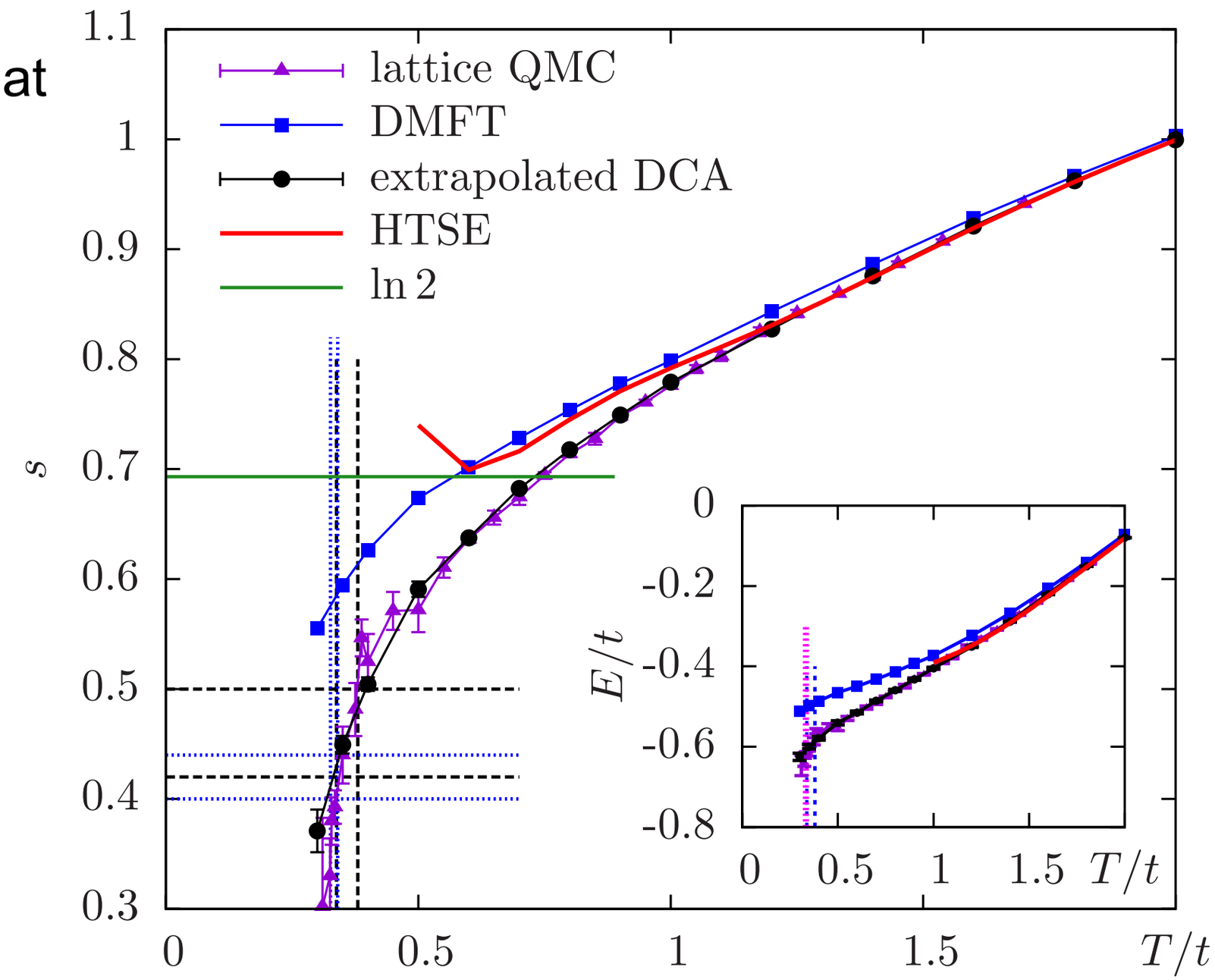


E. Gull *et al,.* PRB (2011)

Comparison of DCA to high-T series and lattice QMC

Perfect agreement with lattice QMC calculations at half filling at all temperatures

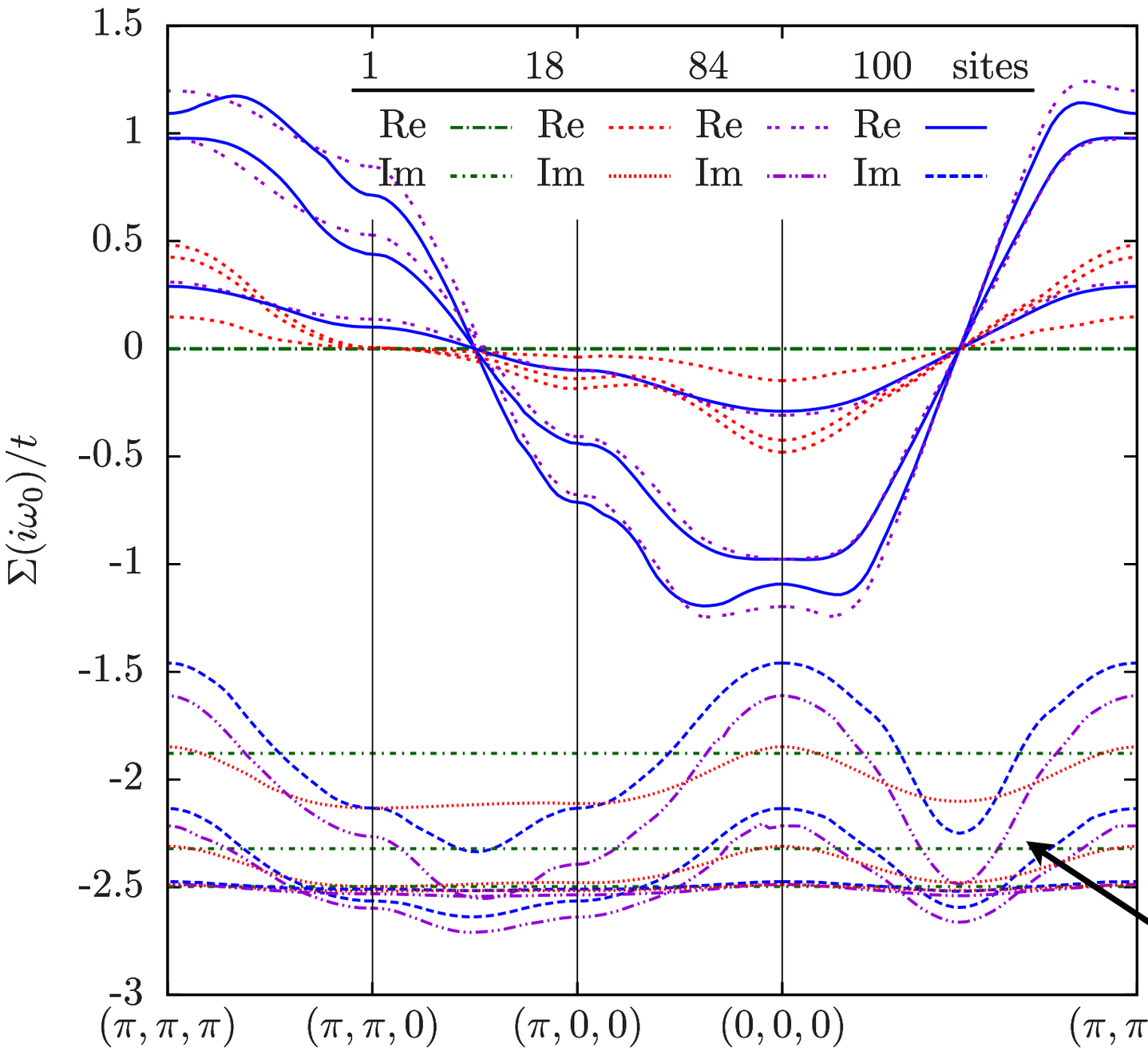
10-th order high-T series works down to T/t ≈ 1.4



Cluster size dependence

S. Fuchs, E. Gull, L. Pollet, E. Burovski, E. Kozik, T. Pruschke, M. Troyer, PRB (2011)

Non-local (momentum dependent) physics beyond DMFT is important for many quantities!



High temperature T/t = 1: Exact convergence of the self energy as a function of cluster size.

Intermediate temperature T/t = 0.5: Convergence visible, extrapolation needed.

Low temperature T/t = 0.35: Convergence not obvious, critical regime with diverging correlation length not well captured.

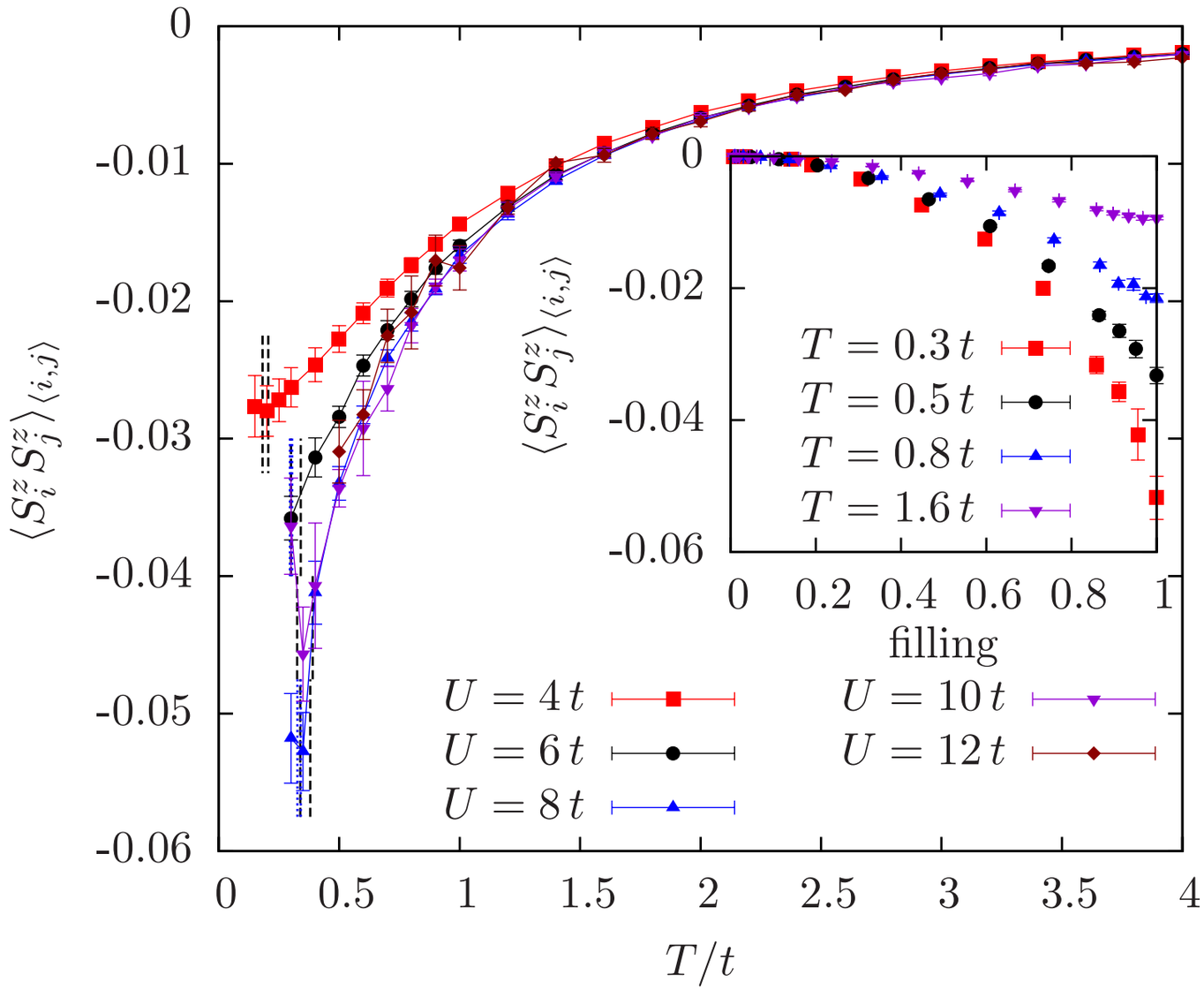
Non-trivial momentum dependence!

DCA results

- Full thermodynamic data available for $U/t \leq 12$, $T \geq T_N$, all fillings
  - energy
  - entropy
  - density
  - free energy
  - double occupancy
  - nearest neighbor spin correlation
- Can be used for validation and thermometry of fermionic experiments down to lower temperature

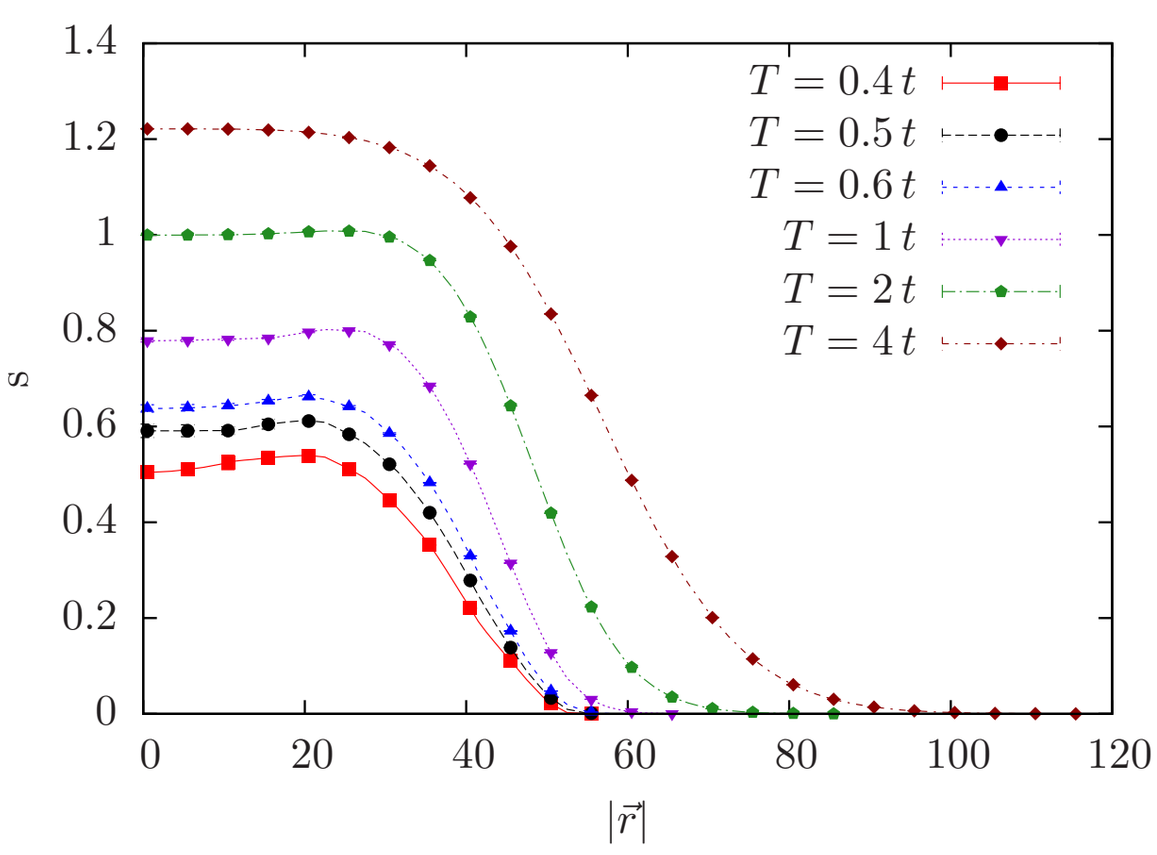
Spin correlation thermometry

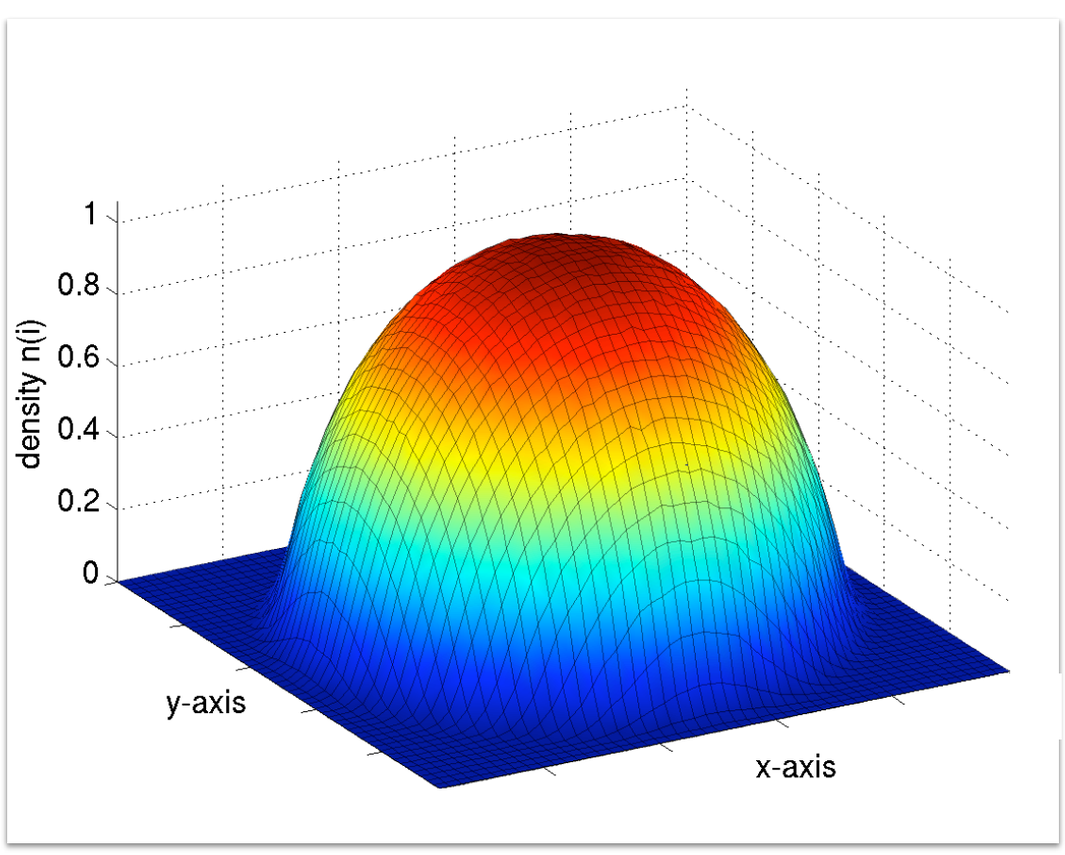
- The nearest neighbor spin correlation is very sensitive to temperature close to T_N and an ideal thermometer



Entropy in a trap (using a local density approximation)

- Current experiments: $s \approx 1.2$
- Homogeneous system: $s_N \approx 0.41(3)$
- Trap captures entropy in metallic shell: $s_N \approx 0.65(6)$ is sufficient!
- It will be a bit easier to reach the Néel state in a trap!



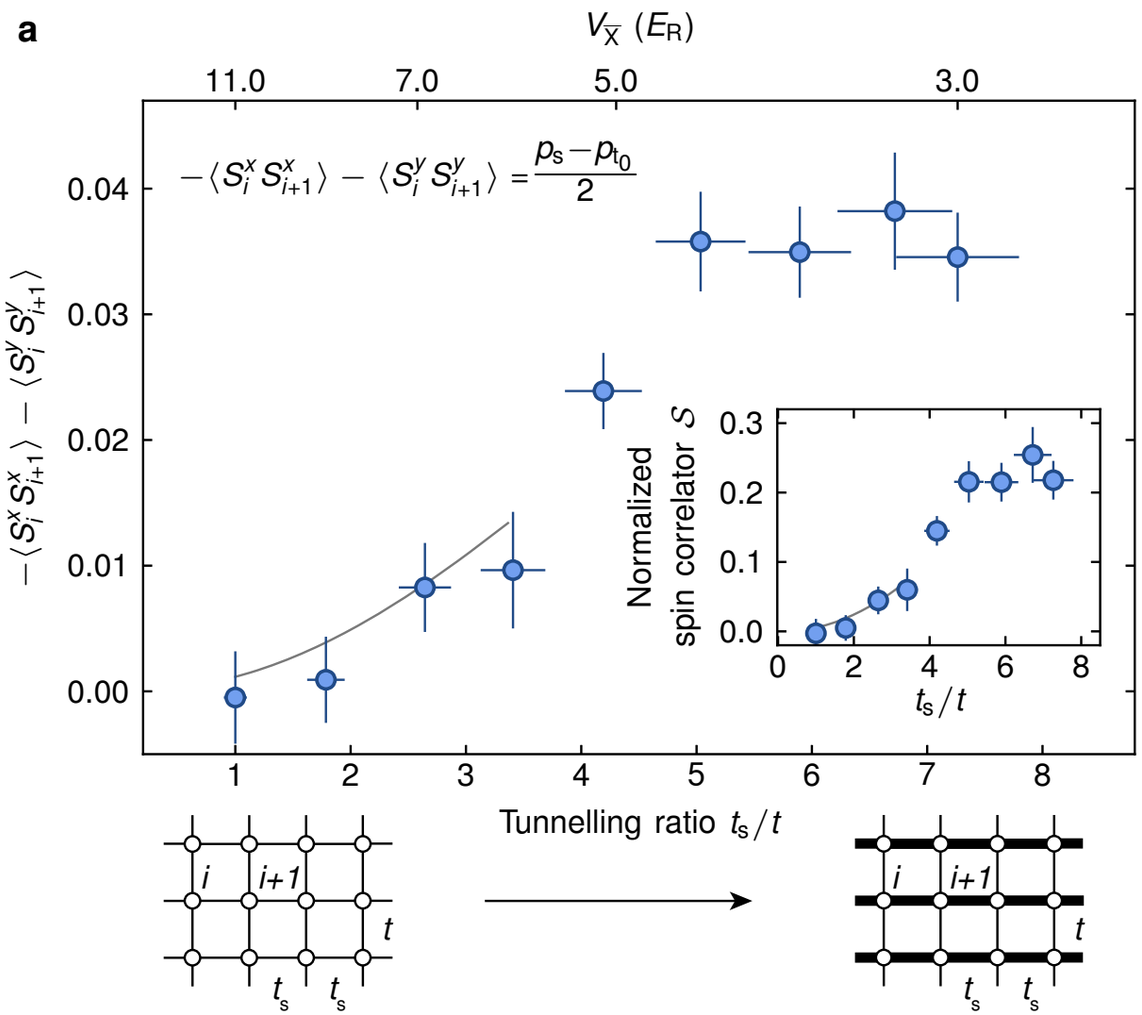


Recent experiments by the Esslinger group

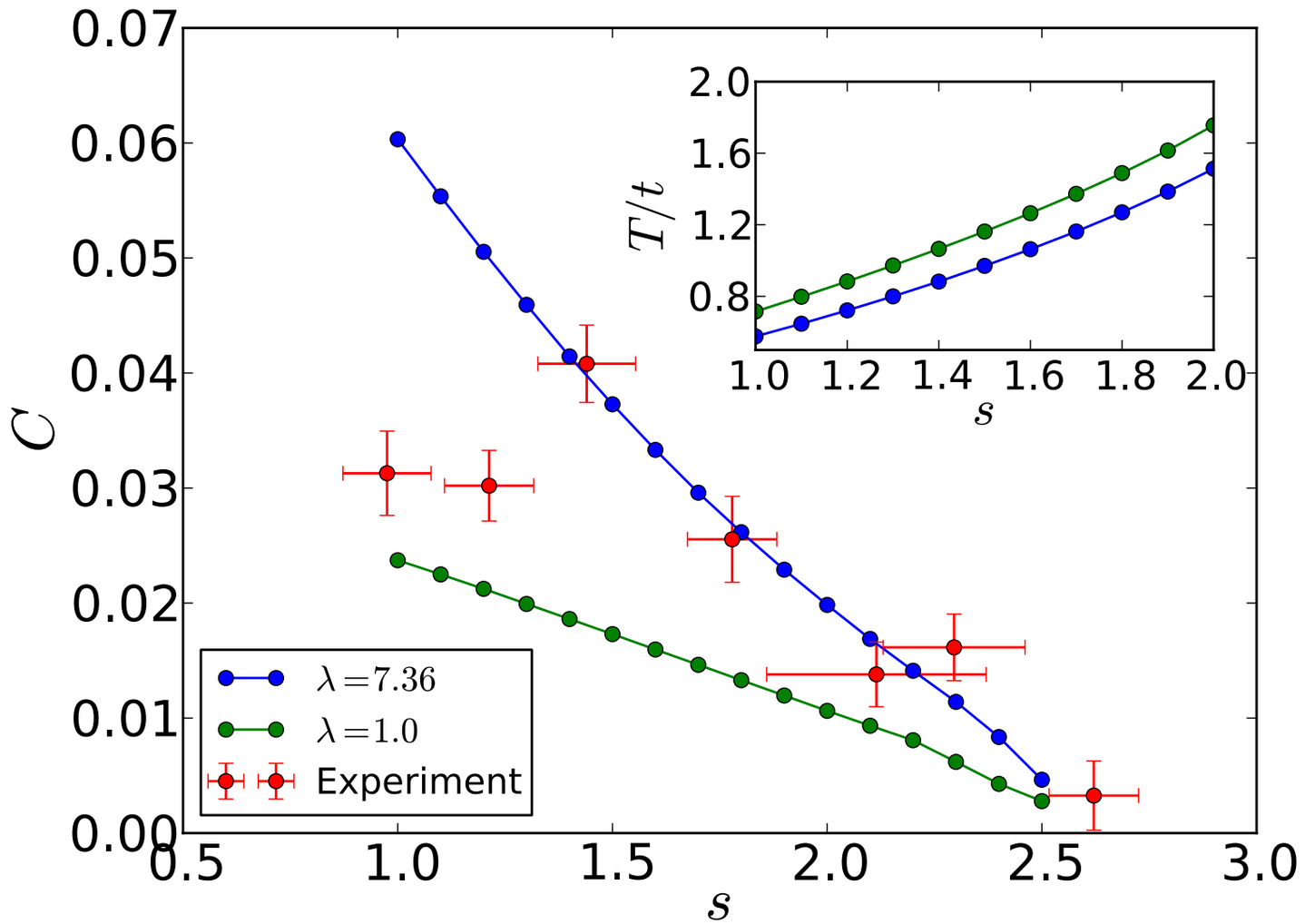
D. Greif *et al*, Science (in press), arXiv 1212.2634

- Measurements of nearest neighbor spin correlations on anisotropic cubic lattices
- Stronger correlations in anisotropic lattice: closer to Néel order?

Anisotropic cubic lattice



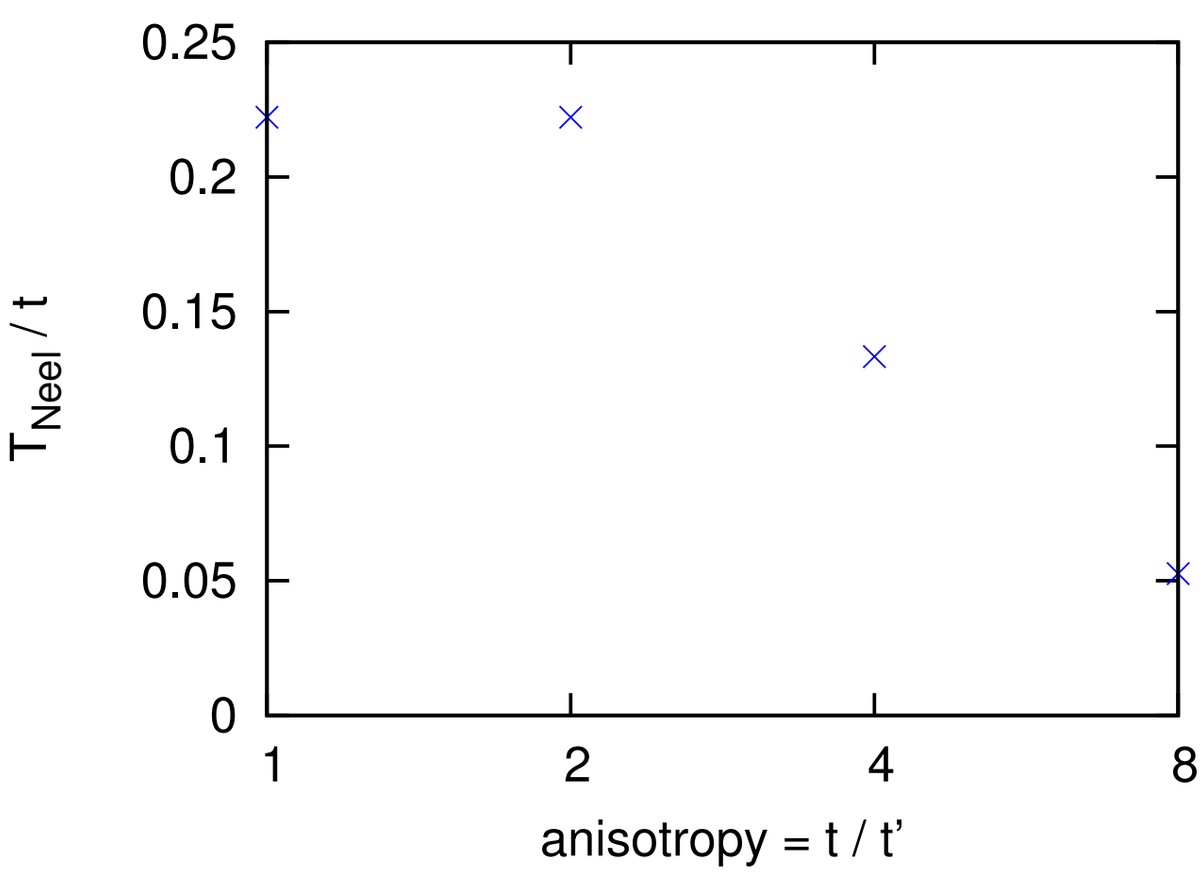
Comparison against QMC simulations

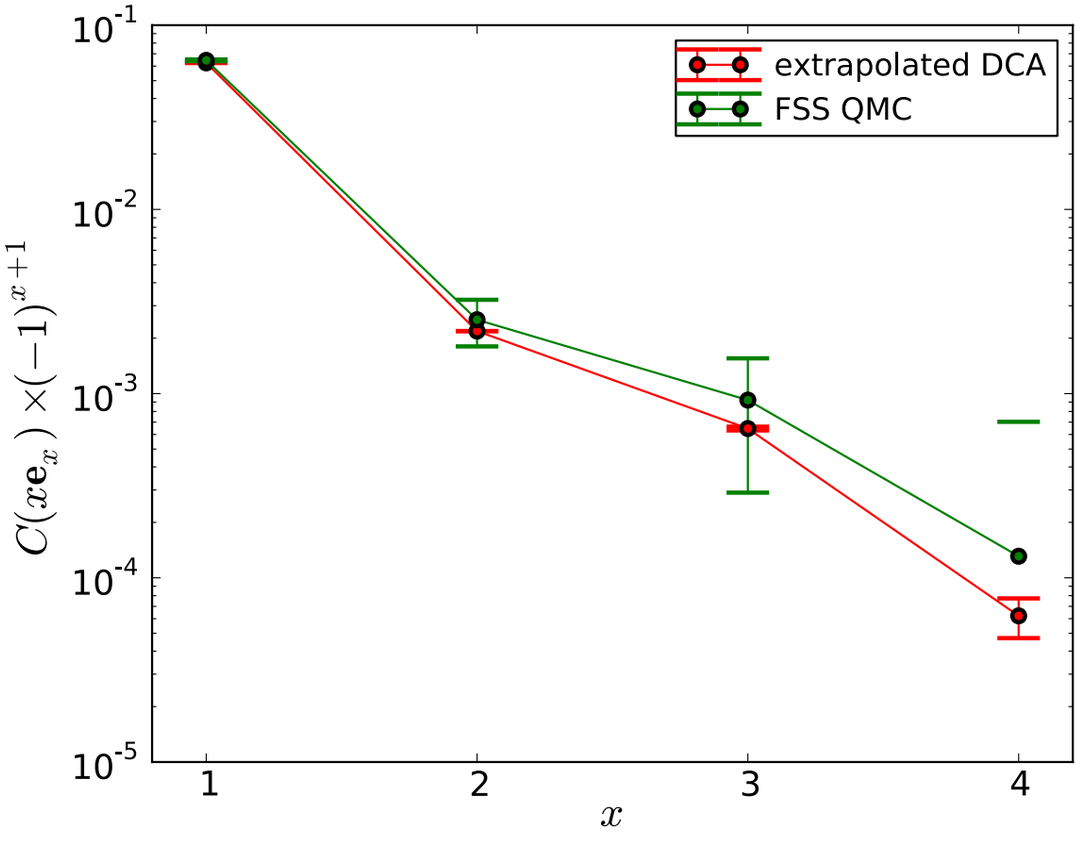


- Good agreement at higher temperatures
- Smaller than expected spin correlations at lower temperature
  - heating during loading?
  - insufficient time to equilibrate?

We are not closer to the Néel temperature

- Temperature is slightly lower in the anisotropic case but the Néel temperature is even lower
- QMC simulations show very short range magnetic correlations





Summary

- CT-QMC algorithms for quantum impurity problems have become the new state of the art
  - faster
  - higher accuracy
  - more flexible

- The Hubbard model can be solved accurately down to $T \approx 0.3t$,
  - much lower than accessible in cold atom experiments
  - provides quantitative validation and interpretation to experiments

- Extensions of existing solvers are of importance in materials simulations
  - frequency-dependent interactions
  - phonons, ...