The Monte Carlo sign problem – a diagrammatic Monte Carlo perspective

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Boston, May 2014

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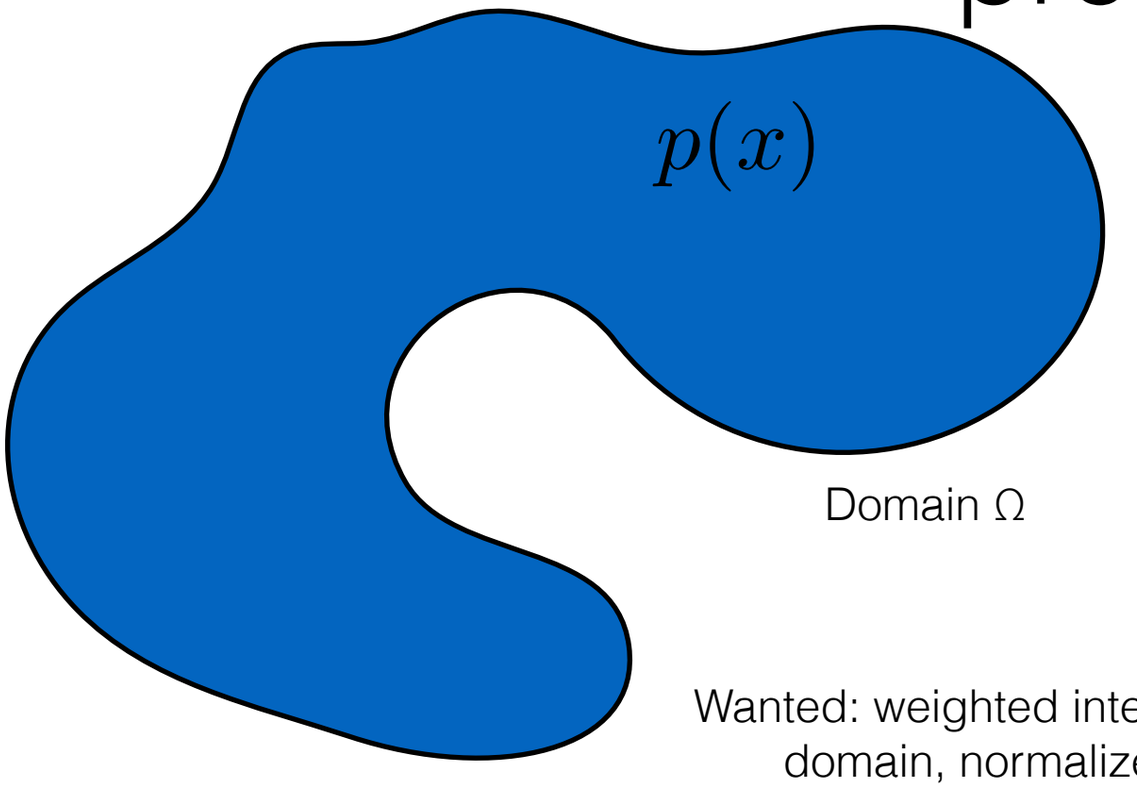
Poor man's introduction to the sign problem



Domain Ω

Given: general positive weight function on domain $p(x)$

$$Z = \int_\Omega p(x)dx$$

Wanted: weighted integral on domain, normalized.

$$\langle A \rangle_p = \frac{1}{Z} \int_\Omega \mathcal{A}(x)p(x)dx$$

We have a practical way of computing this integral: use a MC process

generate p-distributed random numbers (select M points x_i with probability p(x)/Z) and compute

$$\langle A \rangle_p \sim \langle A \rangle_{\mathrm{MC}} = \frac{1}{M} \sum_{i=1}^{M} \mathcal{A}(x_i)$$

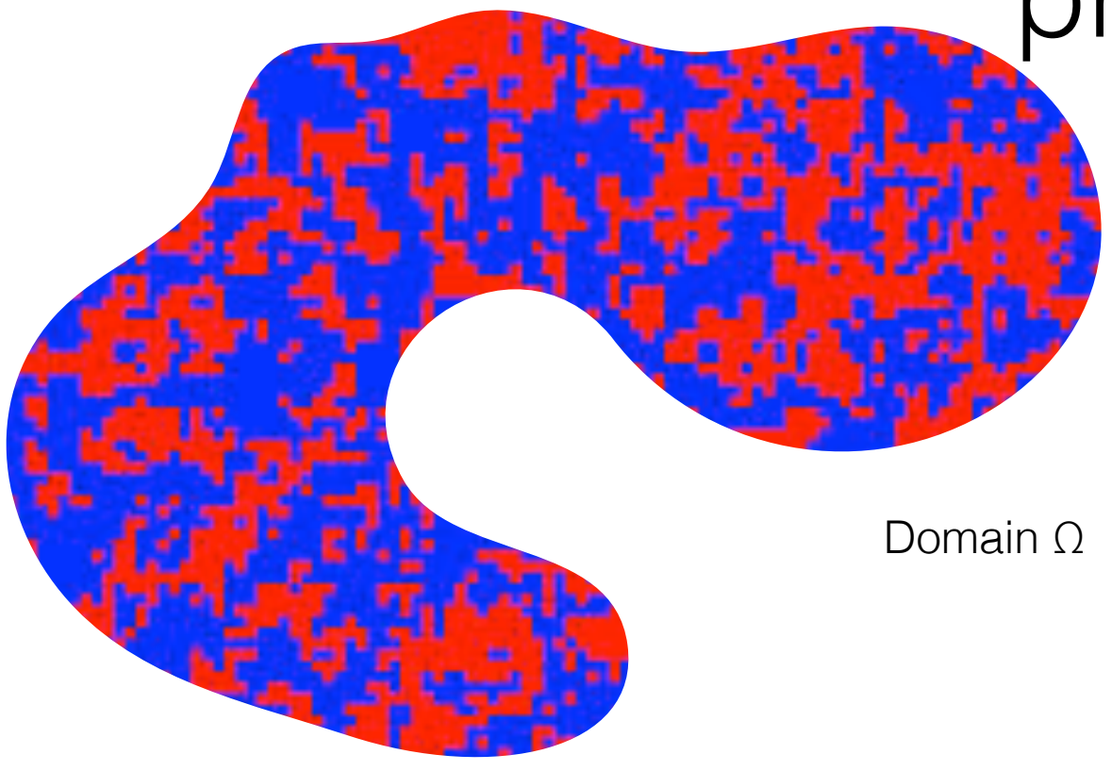
CLT will make this converge with variance

$$(\Delta A)^2 = (\langle A_{\mathrm{MC}} - A_p)^2 \rangle = \frac{\mathrm{var}(A)}{M}$$

If the variance is small (A is large where p is large), this will be a good method.

Usage scenario: Stat mech distribution functions, typically strongly peaked in a small part of phase space.

Poor man's introduction to the sign problem



Domain Ω

Given: general non-positive weight function on domain $p(x)$

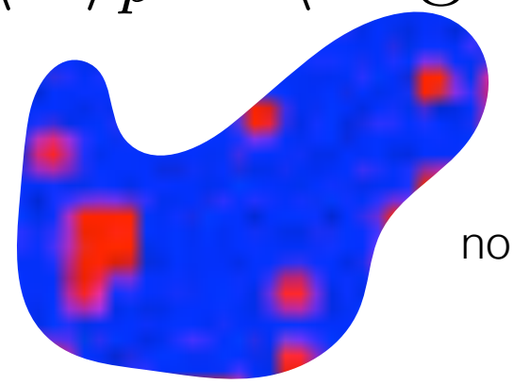
$$Z = \int_\Omega p(x)dx$$

$$\langle A \rangle_p = \frac{1}{Z} \int_\Omega \mathcal{A}(x)p(x)dx$$

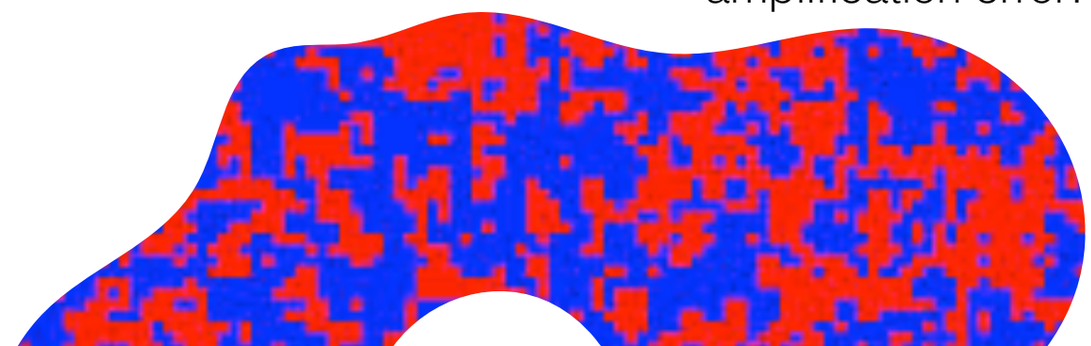
$$\langle A \rangle_p = \frac{1}{Z_p} \int_\Omega \mathcal{A}(x)p(x)dx = \left[\frac{1}{Z_{|p|}} \int_\Omega \mathcal{A}(x)\mathrm{sgn}(x)|p(x)|dx \right] / \left[\frac{1}{Z_{|p|}} \int_\Omega \mathrm{sgn}(x)|p(x)|dx \right]$$

$$\langle A \rangle_p = \langle A\mathrm{sgn} \rangle_{|p|} / \langle \mathrm{sgn} \rangle_{|p|}$$

This works well if the average sign is close to one.
Does not work well if average sign goes to zero: noise amplification error!



no pb, average sign large

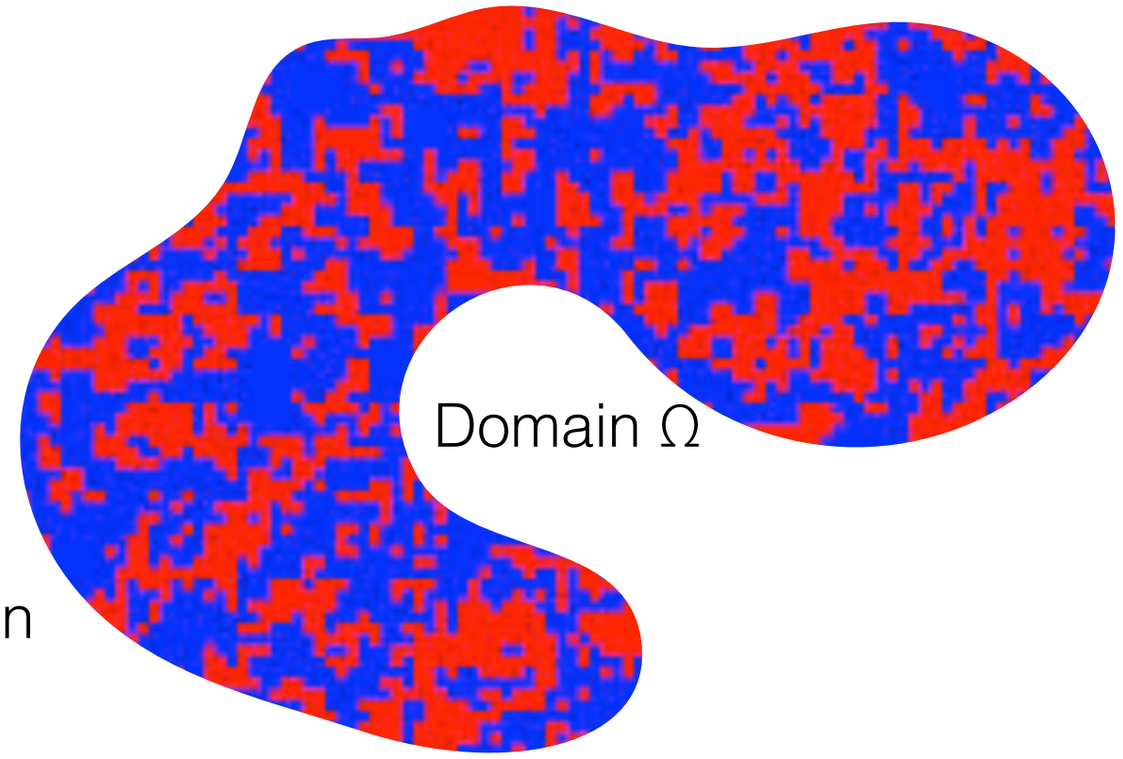


problem, average sign close to zero

configurations and domains

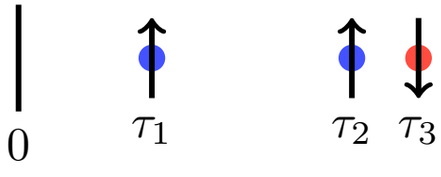
What we have seen so far:

- Configurations are discretized path integrals in imaginary time.
- Domain consists of all possible paths.

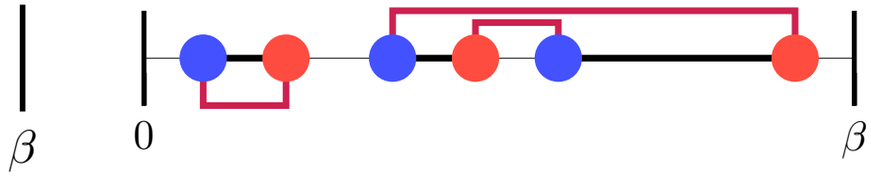


Most of what I'll talk about:

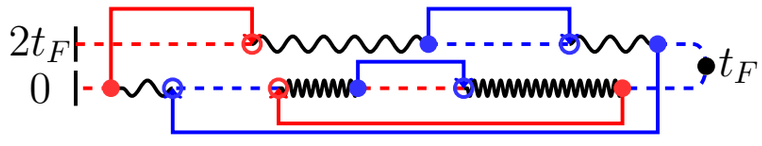
- Configuration space is space of all Feynman diagrams.
- Configurations are diagrams.
- Random walk consists of sampling diagrams by adding and removing parts of it.



In an interaction expansion on a lattice



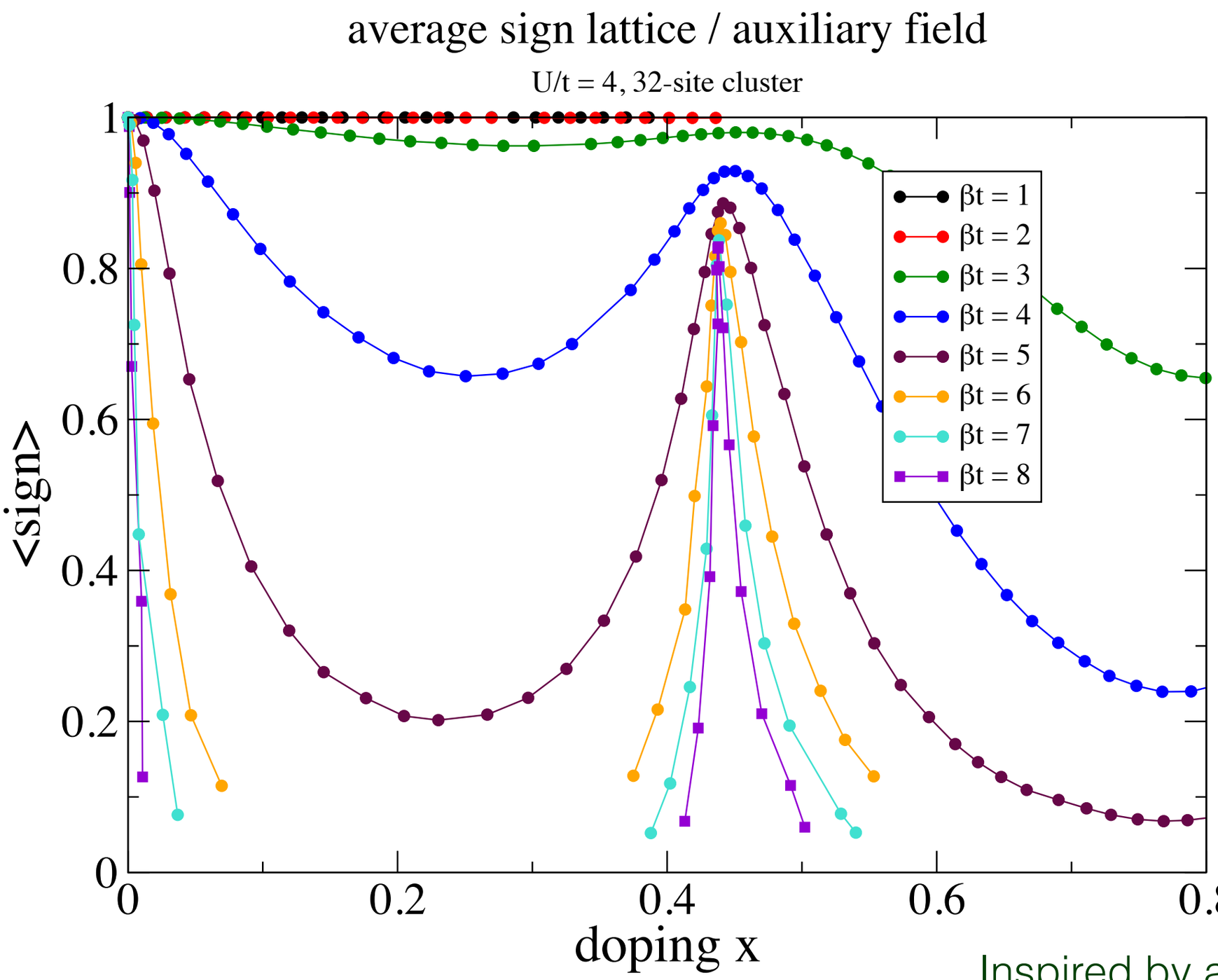
In a hybridization ('hopping') expansion of a quantum impurity



For a real-time 'Keldysh' problem

Feynman diagrams are Taylor expansion coefficient – no a priori reason for them to be positive (but sometimes we can find representations where they are).

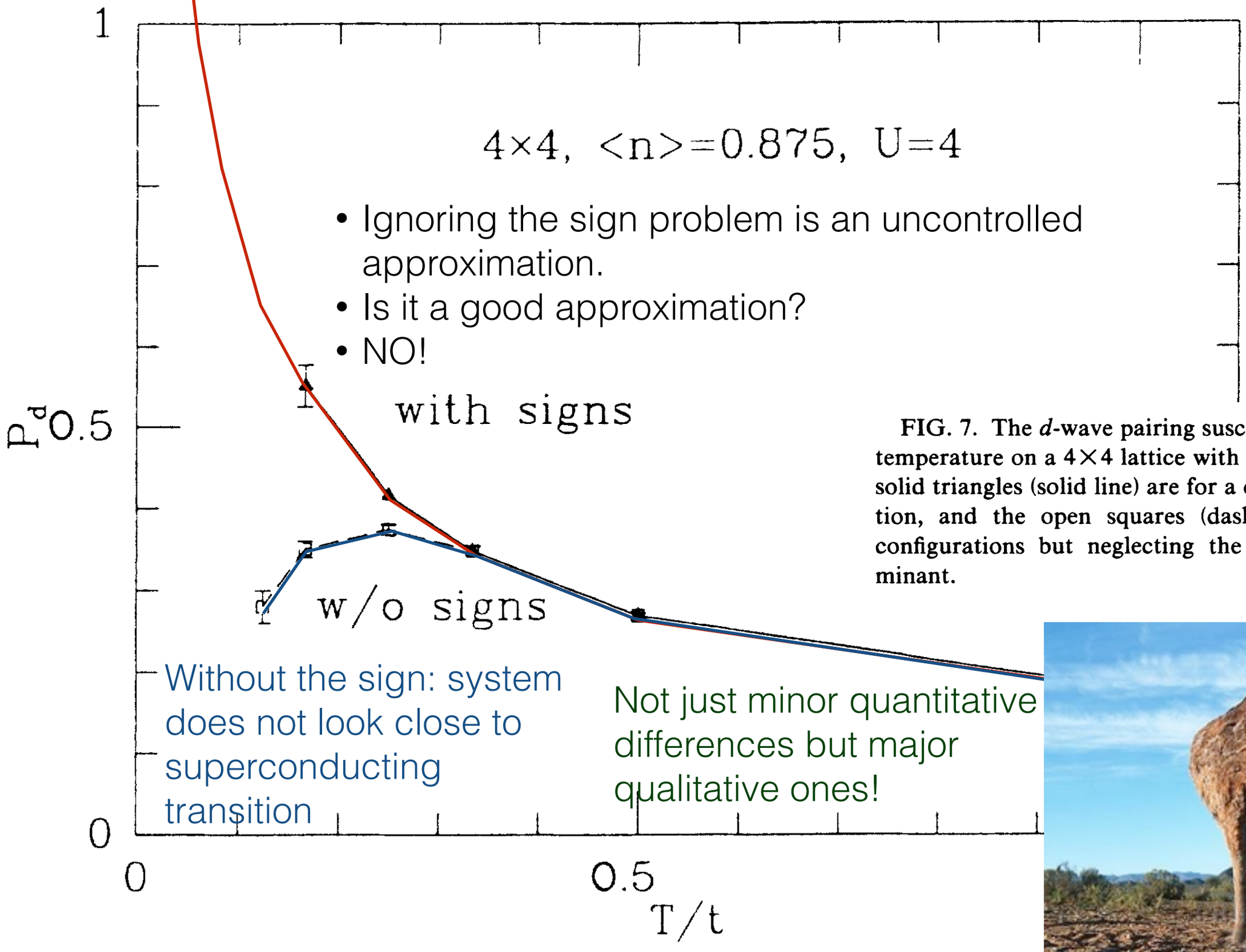
Sign problem: Lattice QMC



Inspired by a plot of F. Assaad, Würzburg

With the sign: system close to superconducting transition?

Let's ignore the sign problem!

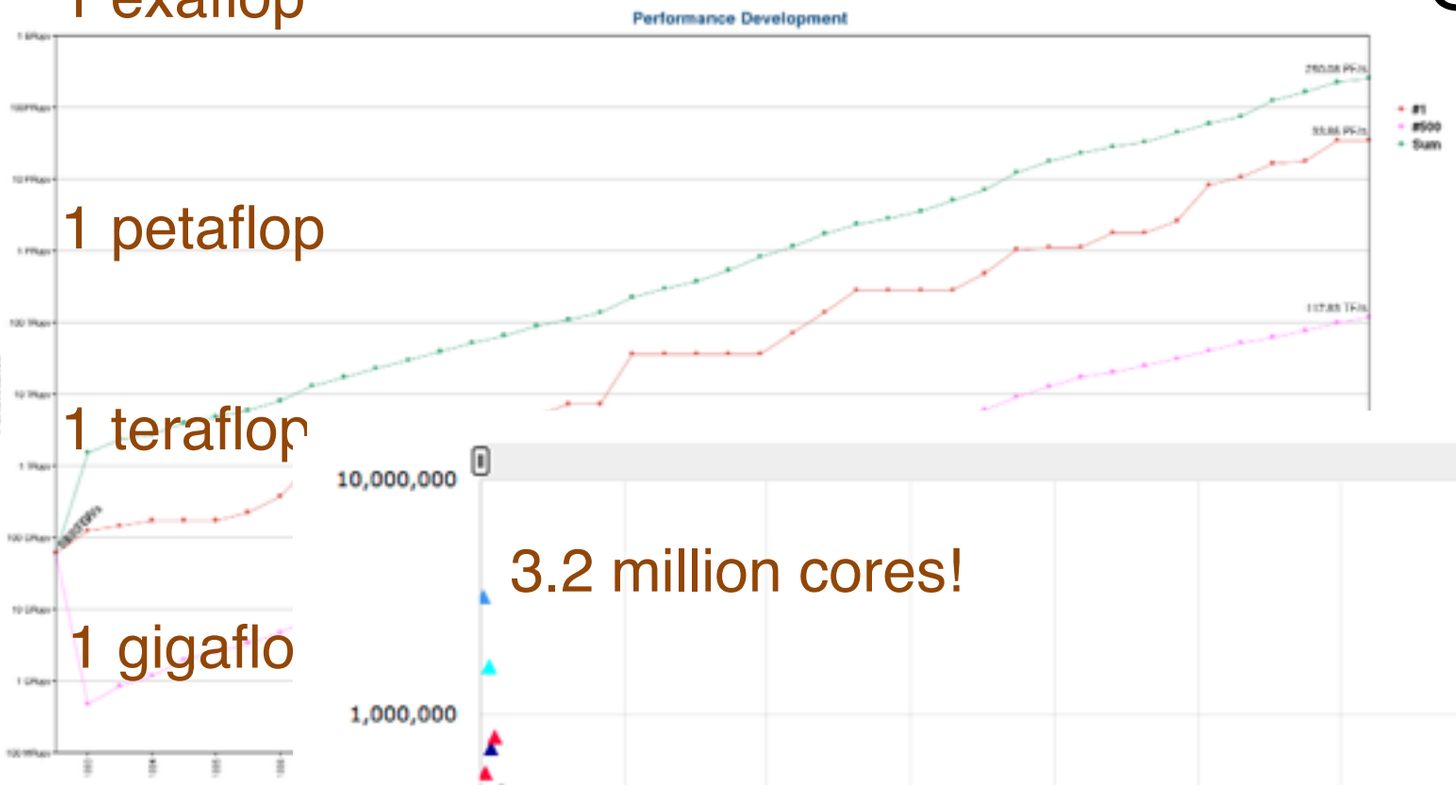


Sign problem in the numerical simulation of many-electron systems, **Phys. Rev. B 41, 9301 (1990),** E. Y. Loh, Jr., J. E. Gubernatis, **R. T. Scalettar, S. R. White**, D. J. Scalapino, and R. L. Sugar

FIG. 7. The *d*-wave pairing susceptibility, P_d as a function of temperature on a 4×4 lattice with $U=4$ and $\langle n \rangle = 0.875$. The solid triangles (solid line) are for a correct Monte Carlo calculation, and the open squares (dashed line) are for the same configurations but neglecting the sign of the fermion determinant.

Let's beat the sign problem!

1 exaflop



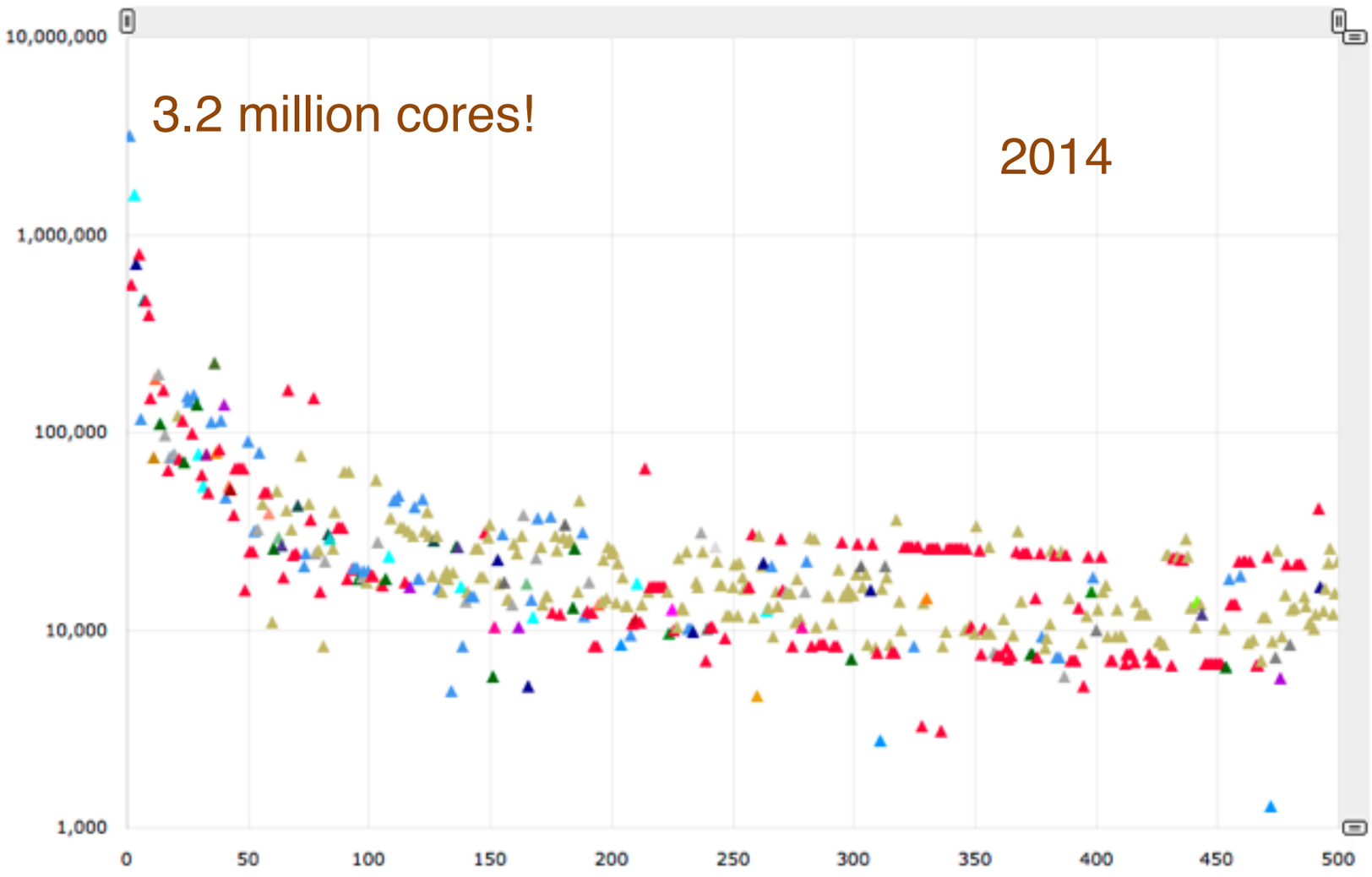
1 petaflop

1 teraflop

1 gigaflo

1993

#cores



3.2 million cores!

2014

top 500 machines

top machine

machine #500

Moore's law: performance grows exponentially.

With it:

- complexity
- number of cores
- power consumption

also for lower end / commodity machines!

Remember Amdahl's law!

More physics for a small system: Self-energy approximation, Dyson

Lattice QMC:
Controlled approximation
Finite lattice, finite size errors,
exact for number of sites $N_c \to \infty$

Cluster DMFT:
Controlled approximation, Inifinite lattice with approximated self energy, approximation errors,
exact for number of sites $N_c \to \infty$

Resulting lattice system mapped onto **impurity model** & **self-consistency**

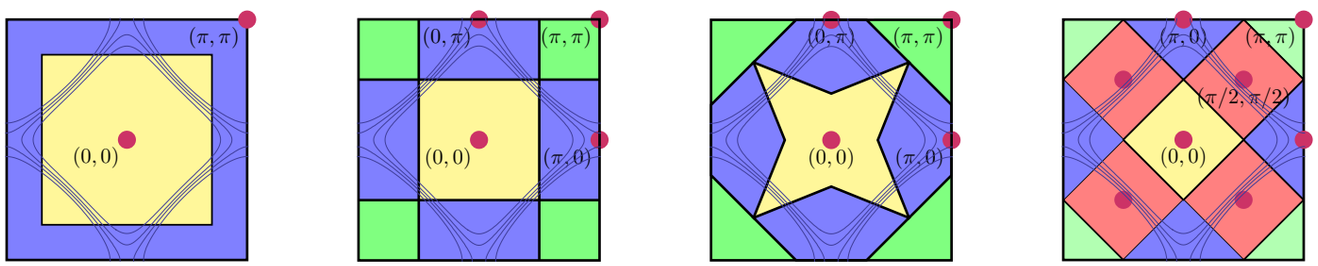
Approximation to self energy:

Systematic truncation with cluster size N_c

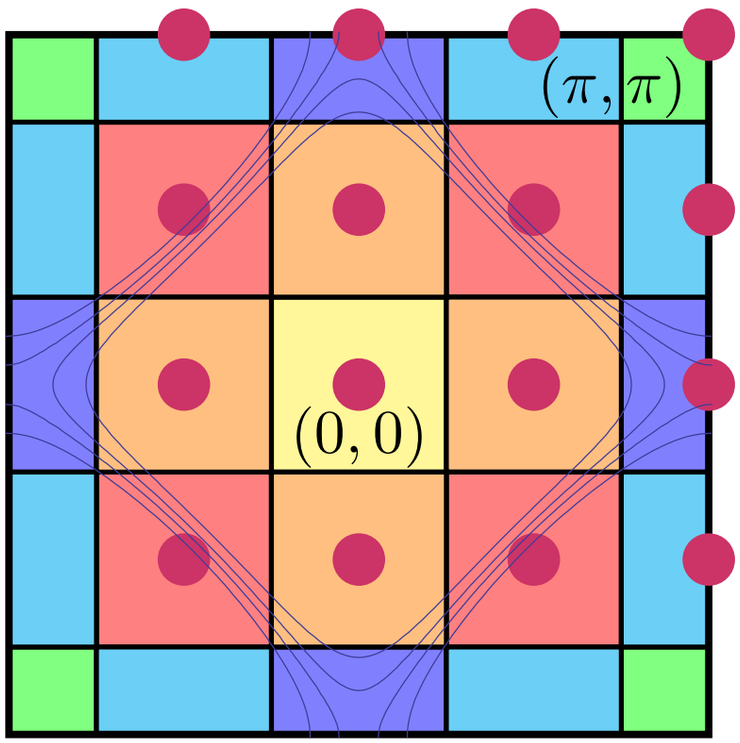
$$\Sigma(k,\omega) = \sum_n \Sigma_n(\omega)\phi_n(k) \approx \sum_n^{N_c} \Sigma_n(\omega)\phi_n(k)$$

Basis functions

Example tiling of the BZ: 2d, N_c = 2, 4, 4, 8



Example tiling of the BZ: 2d, N_c = 16



Metzner, Vollhardt, Georges, Kotliar, Jarrell, Lichtenstein, Katsnelson, Maier, etc. See e.g. Rev. Mod. Phys. 77, 1027 (2005).

Quantum Monte Carlo continuous-time impurity solvers (Fakher Assaad's talk)

$$H = H_1 + H_2$$

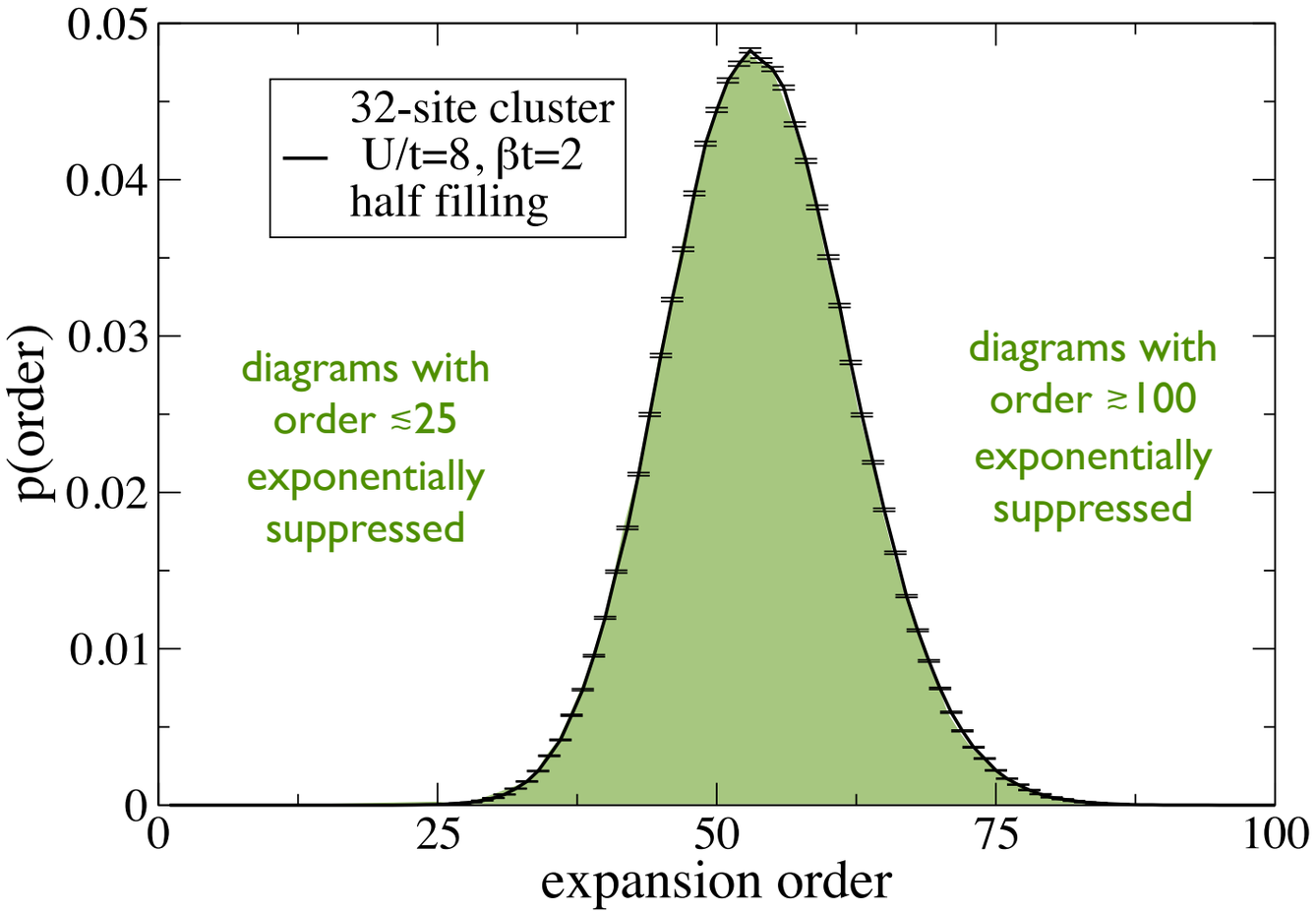
$$A(\beta) = e^{\beta H_1} e^{-\beta H}$$

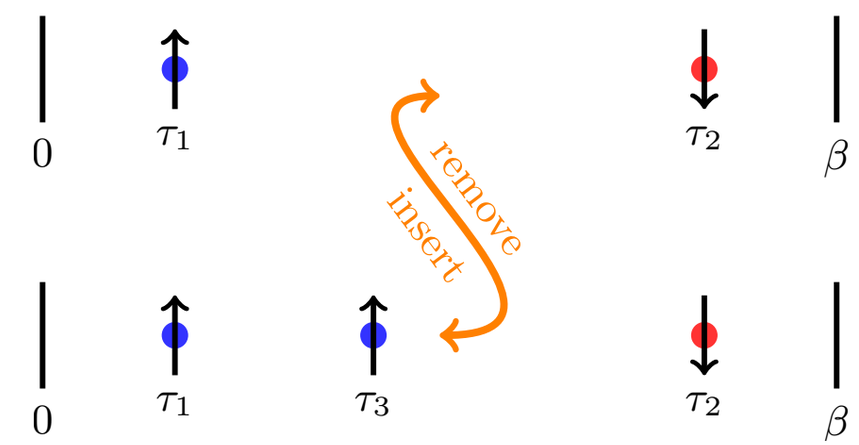
$$A(\beta) = T \exp[-\int_0^\beta d\tau H_2(\tau)]$$

$$Z = Tr[e^{-\beta H_1} A(\beta)].$$

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

Use Wick's theorem to write Trace of operators as determinant of matrix, then use importance sampling for sampling the diagram series.





- 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)

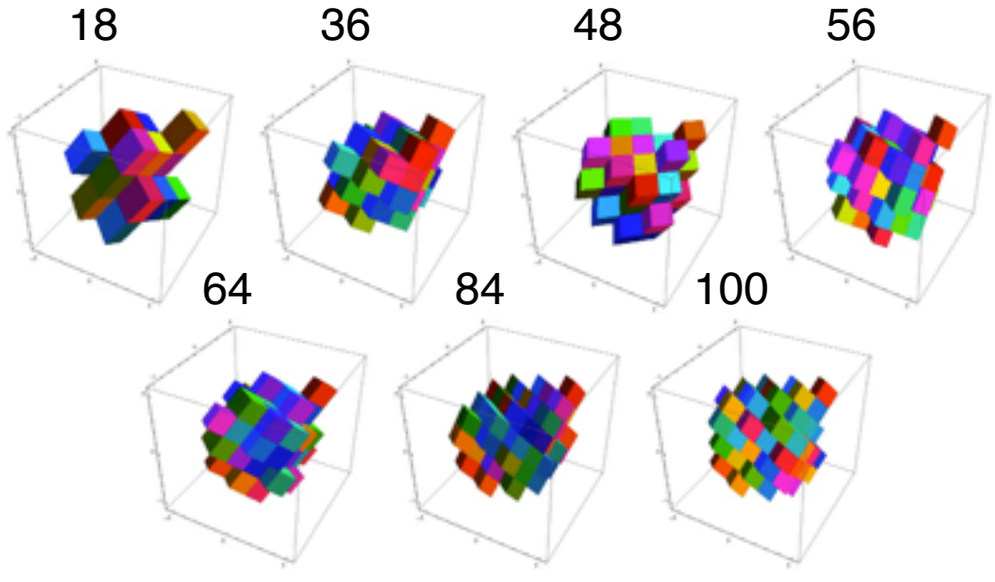
Cluster DMFT in the TD limit

Solve a correlated quantum impurity system self-consistently for a range of system sizes. Then extrapolate in system size.

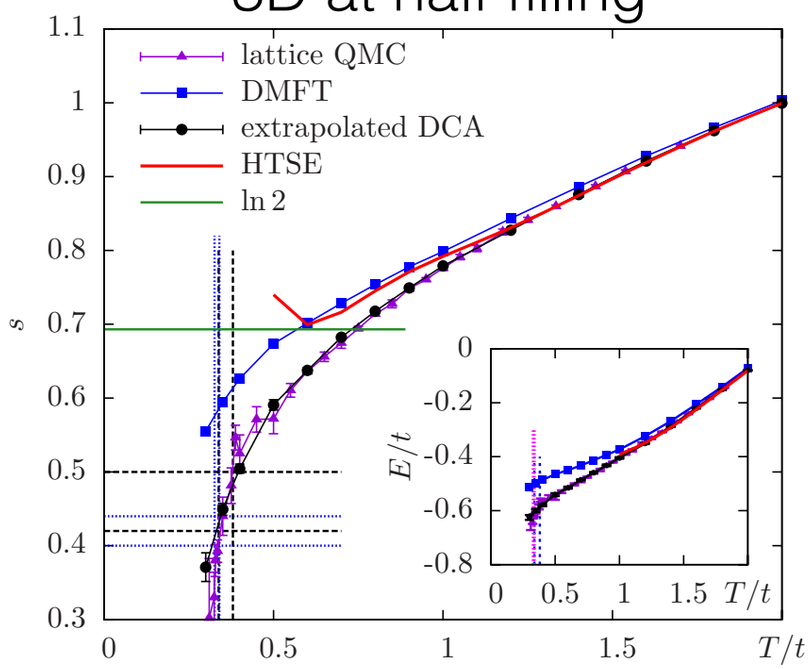
$$\Sigma(k,\omega) = \sum_n \Sigma_n(\omega)\phi_n(k) \approx \sum_n^{N_c} \Sigma_n(\omega)\phi_n(k)$$

Basis function expansion

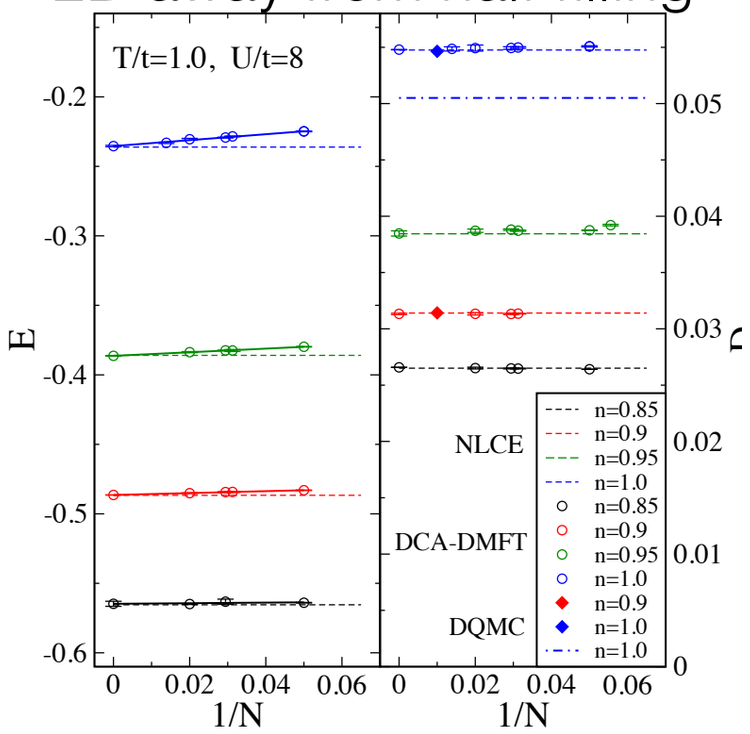
Truncation



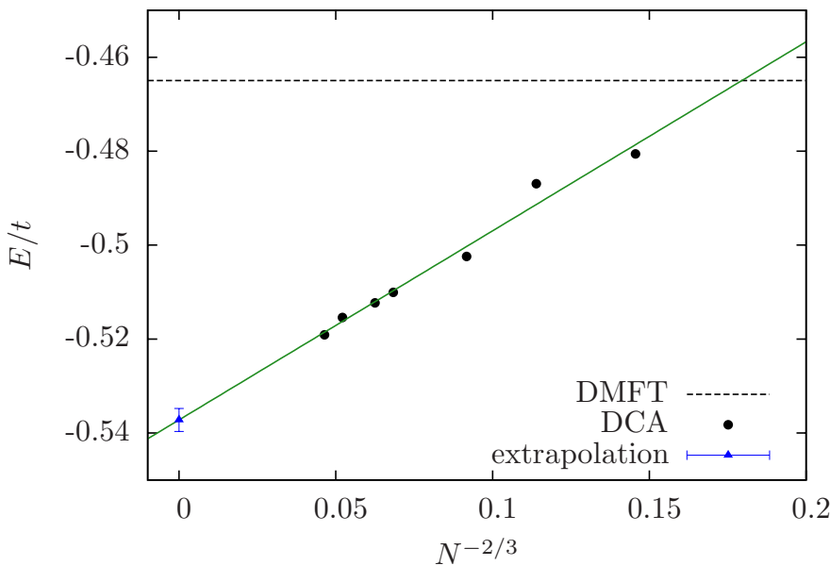
3D at half filling



2D away from half filling



Finite size extrapolation



validation against other methods

Convergence to TD Limit

A Cluster DMFT perspective

Plot: Gull *et al.*, Phys. Rev. B 82, 155101 (2010)

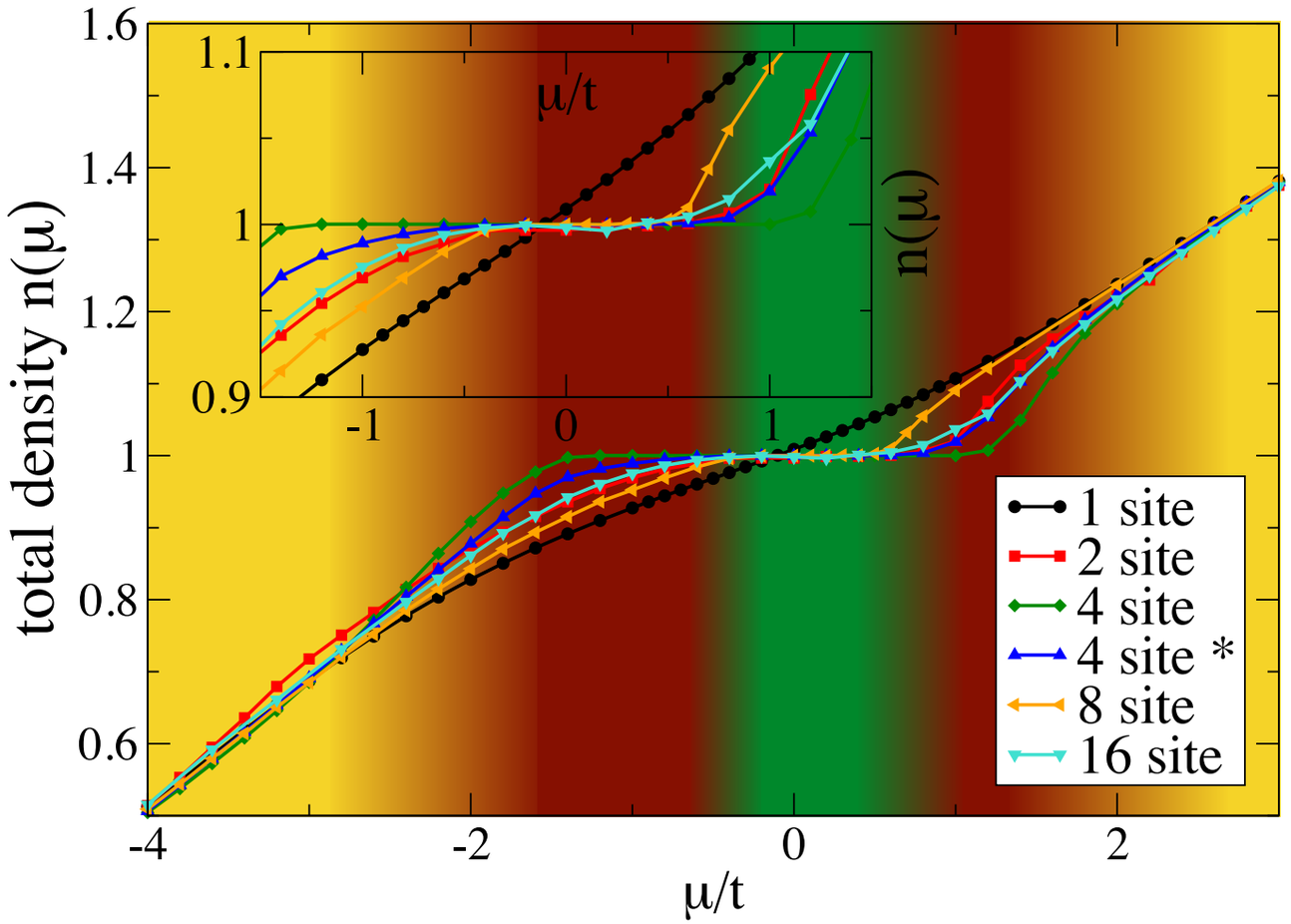


FIG. 3: Main panel: total electron density n as a function of chemical potential μ for clusters considered in this paper at inverse temperature $\beta t = 20$ for all clusters except 16, where $\beta t = 7.5$ is shown. Inset: expanded view of small chemical-potential region, highlighting region of Mott gap where $n = 1$ independent of μ.

The easiest part of phase space: accurate without a sign problem using the simplest single site DMFT method.

Some of the 'uncorrelated' 'easy' systems, e.g. good Fermi liquids or Mott insulators with a large gap, are accessible without a sign problem: convergence within the system size accessible.

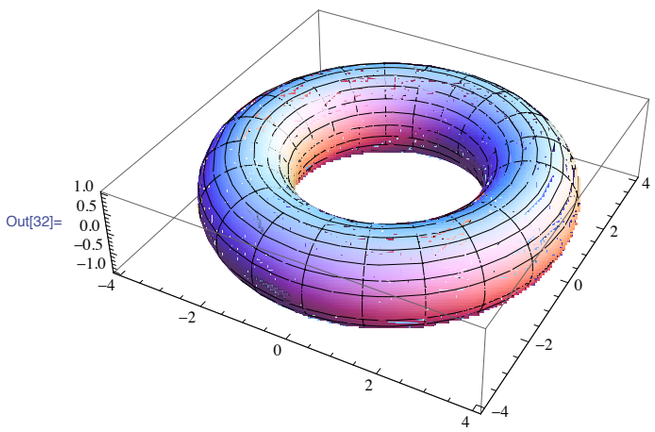
Some of the more interesting parameter regimes are not accessible: larger systems (prohibited by sign problem) would be needed to simulate them.

More physics for a small system: vertex functions, vertex approximation

in the spirit of getting more out of a small system:

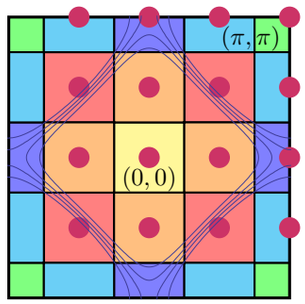
Lattice

Green's function discretized



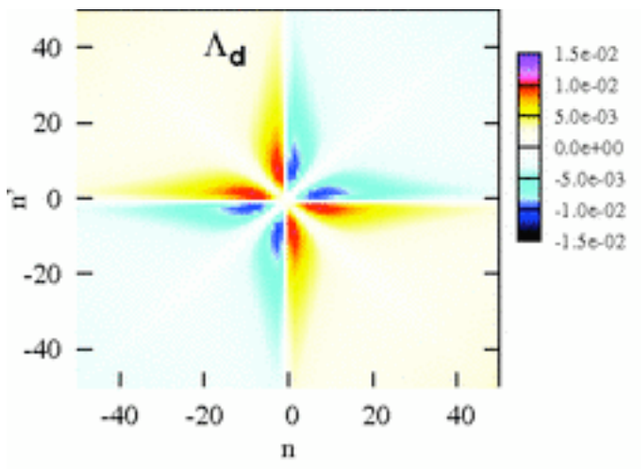
Cluster DMFT

Self energy discretized and approximated



DGammaA (and related methods)

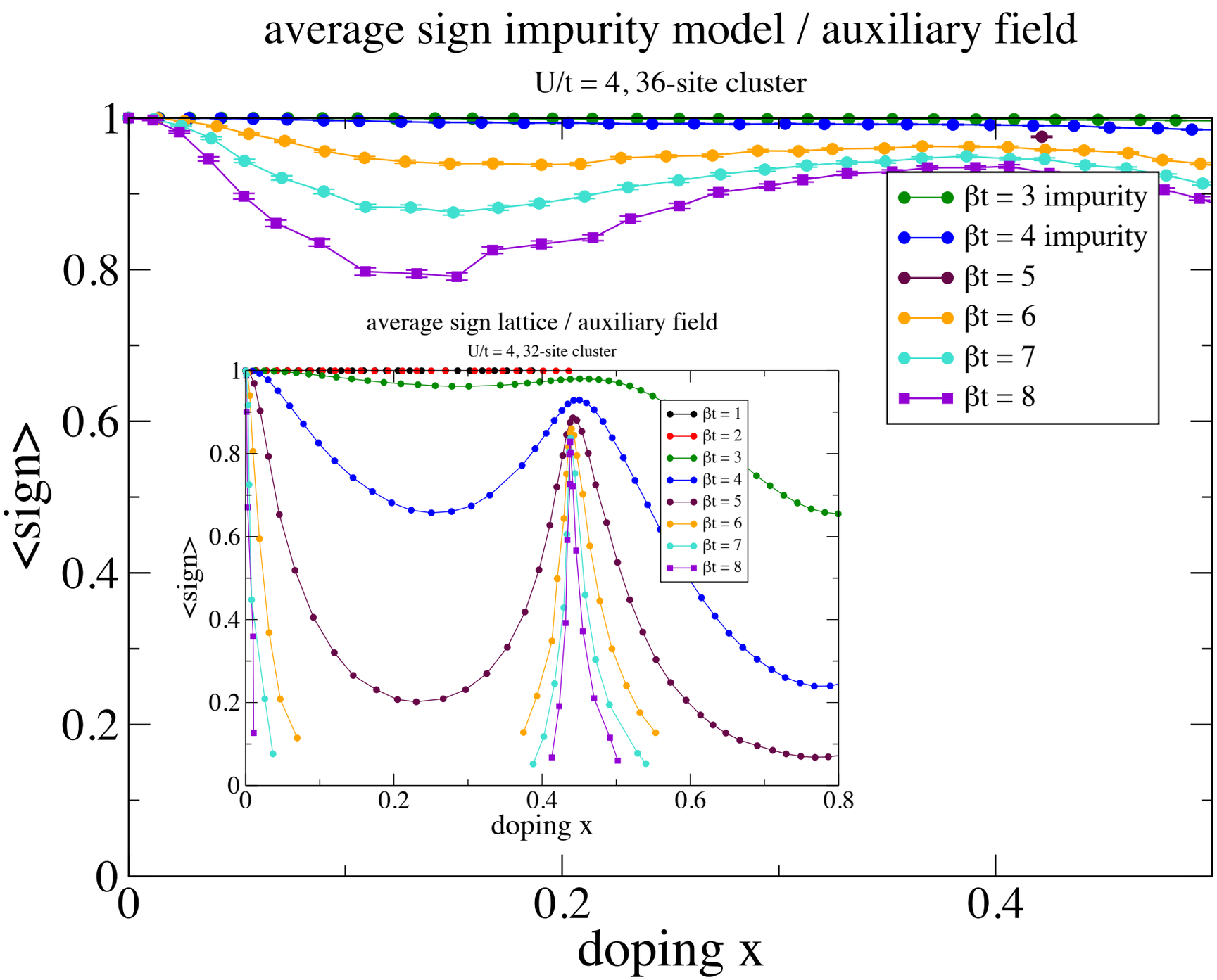
vertex discretized and approximated



See also: Dual Fermions / Cluster Dual Fermions

Methods seem to suffer from instabilities, require self-consistent solution of Dyson, Bethe-Salpeter, Parquet equations. Methods still under investigation! (Held, Toschi, Rubtsov, …)

Sign problem: quantum impurity model

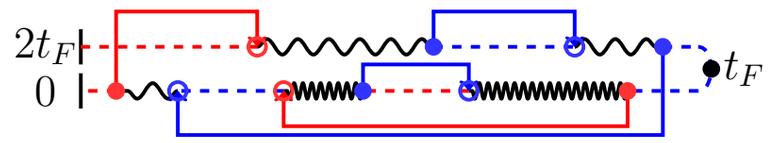


A look on the sign problem from a real-time / dynamics point of view

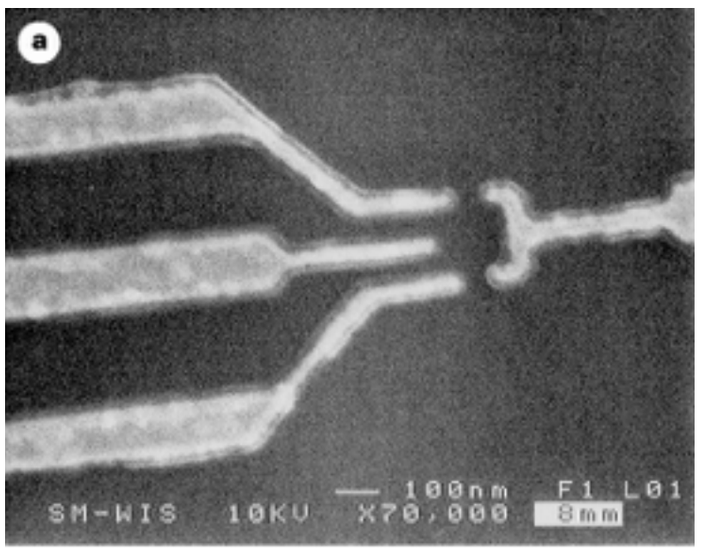
Expand observables into Feynman diagrams, sample them in a Monte Carlo process.

$$\langle A \rangle = \mathrm{Tr} e^{iHt} A e^{-iHt}$$

Obtain estimates for currents, occupations, Green's functions, etc as a function of (real) time

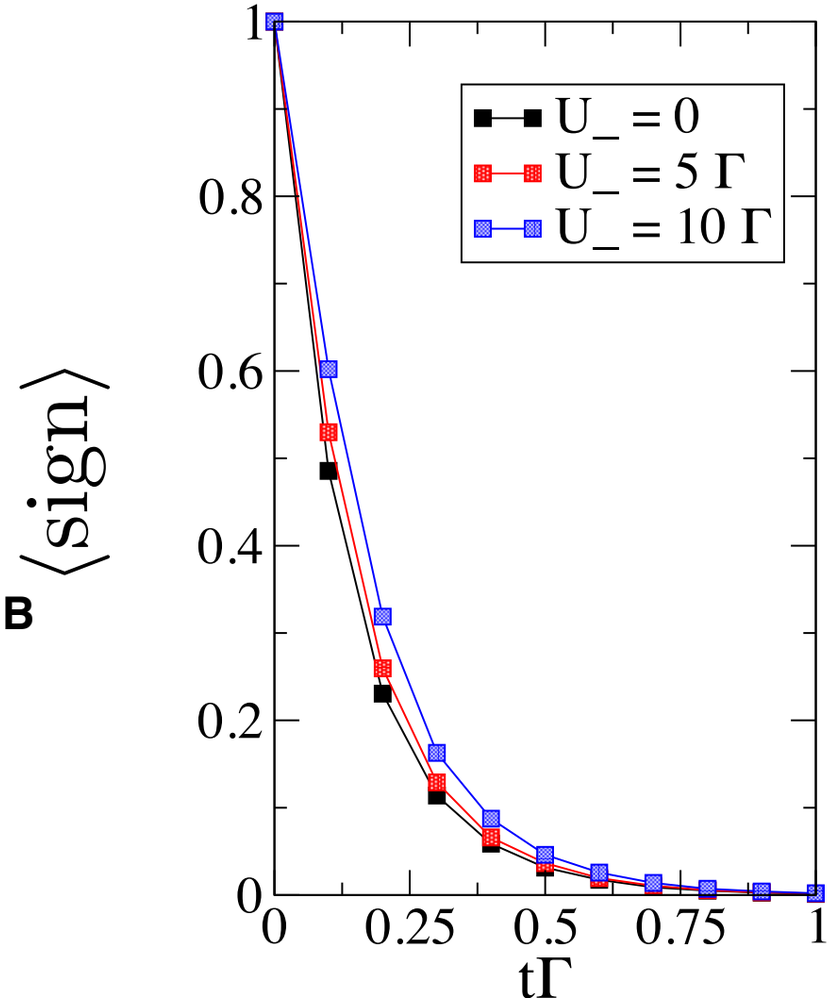


Everything is exponential!
Everything oscillates – severe sign problem
Lost cause?



Marco Schiró, Real-time dynamics in quantum impurity models with diagrammatic Monte Carlo, **Phys. Rev. B 81, 085126 (2010)**

D. Goldhaber-Gordon et al., Kondo effect in a single-electron transistor, **Nature 391, 156-159 (1998)**



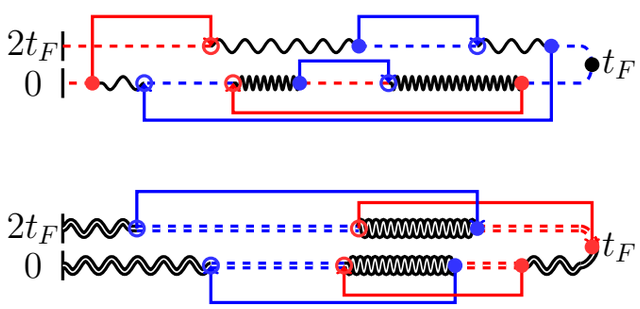
Bold: Combine MC and analytical methods!

1. start from **uncontrolled partial summation techniques (think RPA):**

obtain propagators that contain an infinite subset of diagrams.

2. use **Bold Diagrammatic MC procedure** to sum up **ALL** remaining diagrams:

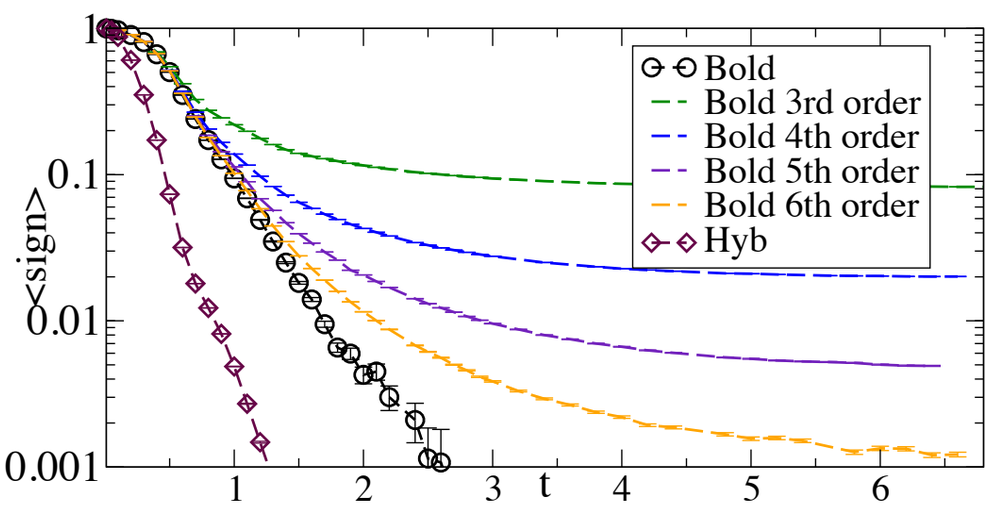
obtain propagators with all diagrams, compute observables. Numerically exact.

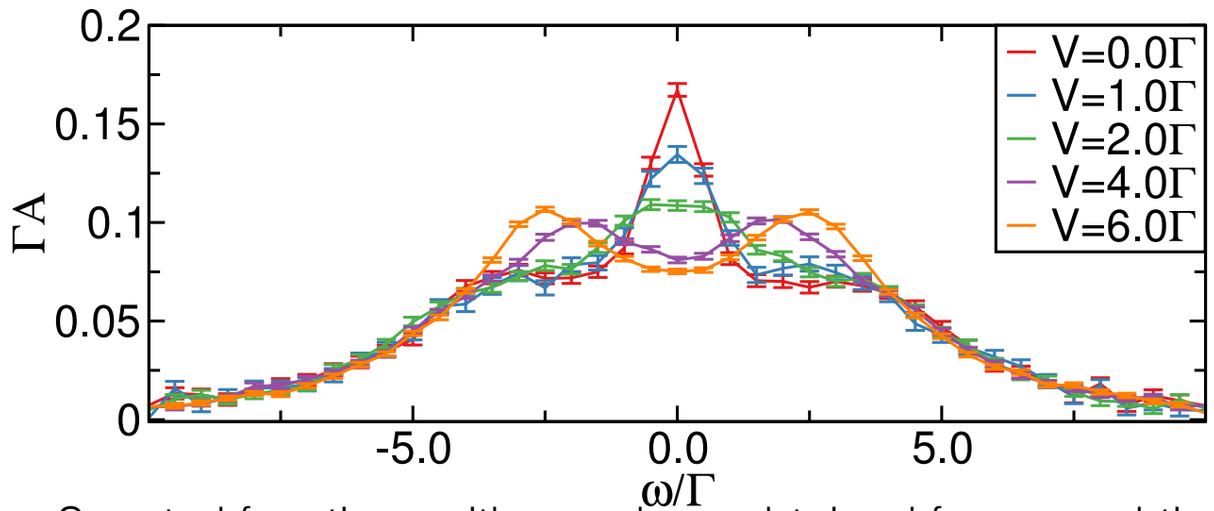


e.g. 1. integral equations for diagrams without crossing lines,

followed by 2. a procedure to sample all remaining diagrams.

Delegating diagrams to the integral equations decreases the sampling space, **increases the sign by an order of magnitude**!

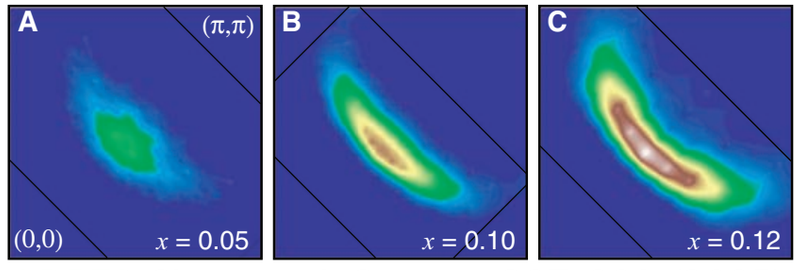




Spectral functions with error bars obtained from a real-time evolution of a quantum dot (AIM) with a voltage applied.

Analytic Continuation: Sign problem is not the only exponential barrier

- **Statics** can only tell us so much…
- Experiment cares about **dynamics**: spectral functions, optical response functions (Raman, optical conductivities, …), self energies!



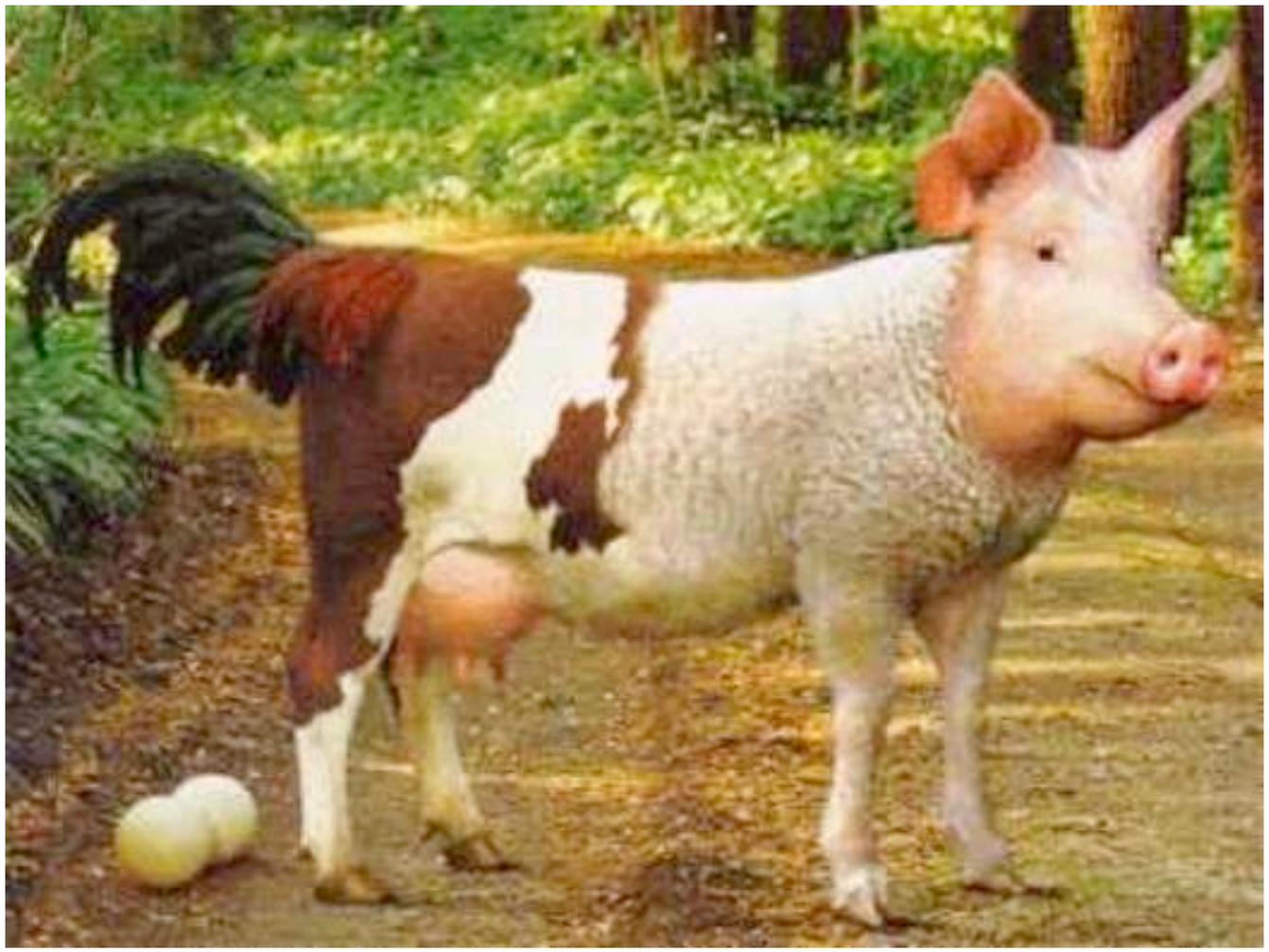
ARPES: Shen *et al.*, Science 307, 901 (2005)

- Equilibrium quantum statistical mechanics / imaginary time formulation of algorithm has a ‘bug’: small fluctuations in our simulation data cause large variations in the experimentally relevant quantities: Analytic continuation!

- Maximum entropy method, Padé, stochastic analytic continuation, etc use additional assumptions to generate appealing plots.

- **Do we have to give up the Matsubara formulation** to obtain unbiased estimates of response functions? What can replace it?

Does a generic solution to the sign problem exist?



Die Eierlegende Wollmilchsau
(egg laying wool milk pig)

Troyer and Wiese, Phys. Rev. Lett. 94, 170201 (2005)

Some sign problems are NP hard, i.e. a **general** solution of **all sign problems** implies P=NP. The sign problems that are NP hard are not necessarily the ones we care about. **Is there a large enough subset of sign problems for which we can find a practical polynomial-in-time solution?**

Thank you!

Many thanks to my collaborators, in particular

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