Were fermions born under a bad sign?

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ÉCOLE POLYTECHNIQUE

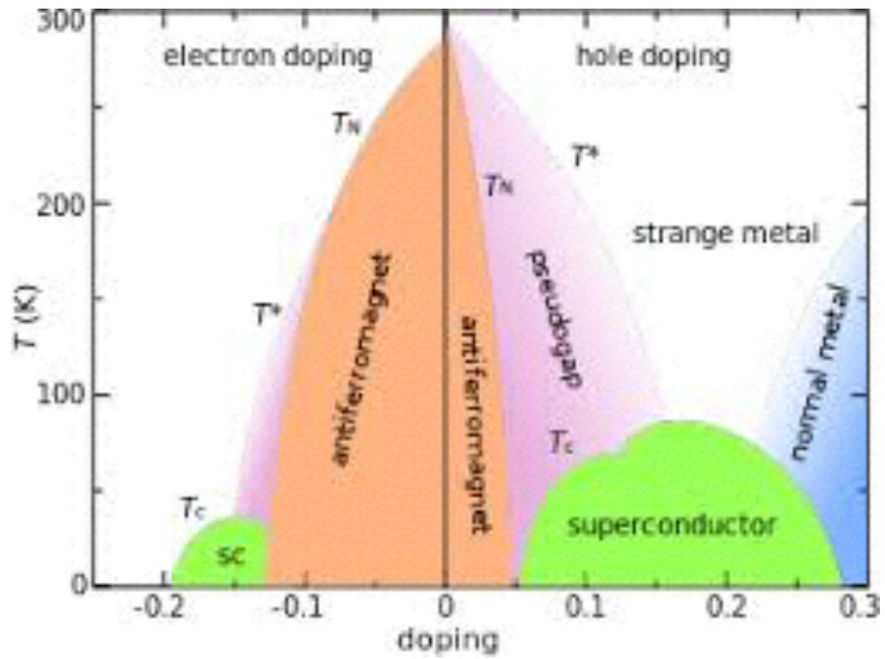
Outline

- Why are fermionic quantum systems difficult?
  - Hamiltonian approaches and Hilbert space size explosion
  - Action-based approaches and Monte Carlo methods
- A very quick introduction to Monte Carlo methods
  - How to compute integrals stochastically
  - The origin of the sign problem
- Continuous-time quantum Monte Carlo algorithms
  - The three flavors of algorithms and the fermionic sign problem
  - What have they allowed to do?
- Diagrammatic Monte Carlo algorithms
  - Addressing the infinite lattice directly
  - Applications to the two-dimensional Hubbard model

Strongly-correlated systems: The challenge

- Strongly-interacting quantum systems:
  - Exciting physics, rich phase diagrams
  - What can we actually solve?
- Let us take our favorite spherical ~~cow~~ sheep model, the Hubbard model:

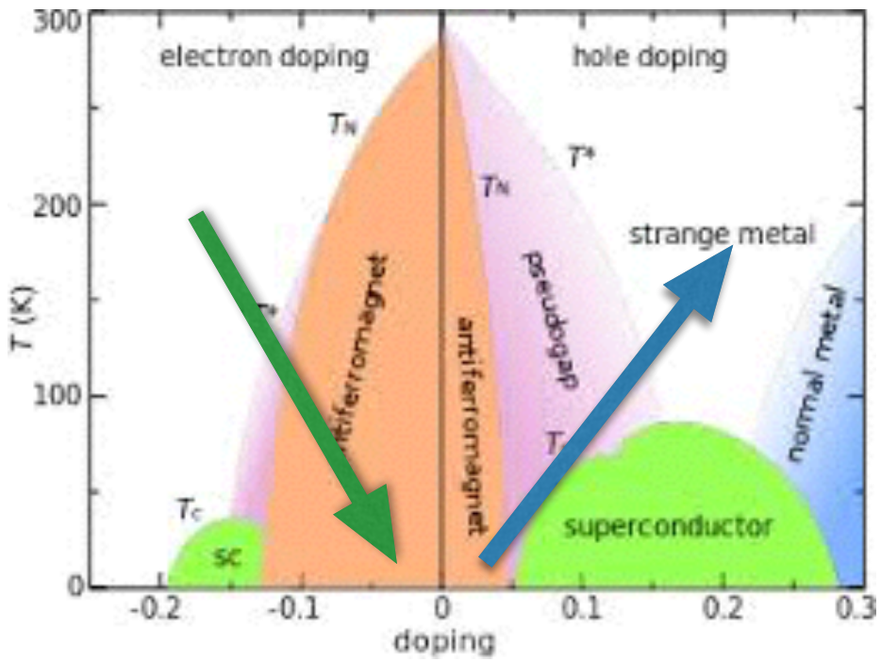
$$\mathcal{H} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



- Why is it so hard to solve?
  - No analytical solutions
  - It is a quantum problem
  - It involves many particles

Numerical approaches to strongly-correlated systems

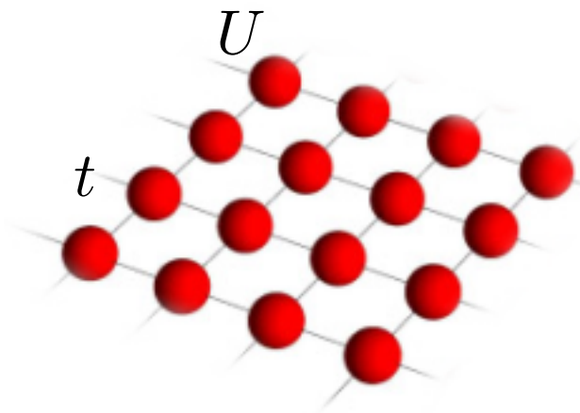
- Can roughly be divided into two categories:
- Bottom to top (often Hamiltonian-based methods)
  - Exact diagonalization, density-matrix renormalization group, tensor networks, …
  - Exponential size of the Hilbert space: 4^N
    Quantum entanglement of ground state
  - Approximation by some clever truncation
- Top to bottom (often action / path integral-based methods)
  - Continuous-time quantum Monte Carlo, auxiliary-field quantum Monte Carlo, diagrammatic Monte Carlo, …
  - They are usually based on a stochastic algorithm
  - Suffer from the fermionic sign problem
  - Limited by interaction strength, temperature, system size

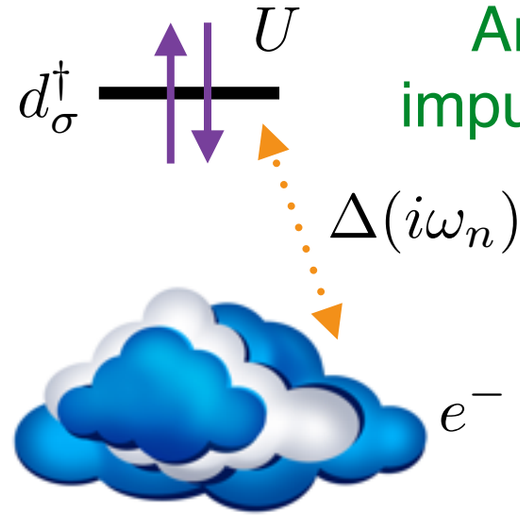


Dynamical mean-field theory equations

- The critical part of the dynamical mean-field theory equations is to find the solution of an Anderson impurity model

Hubbard model





Anderson impurity model

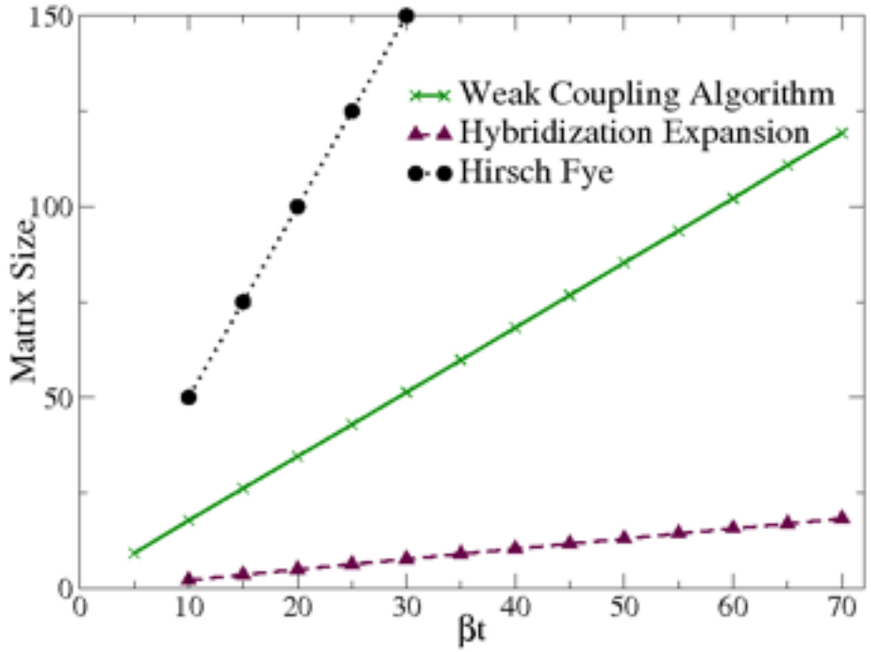
$$\Sigma_{\text{lattice}}(k, i\omega_n) \simeq \Sigma_{\text{impurity}}(i\omega_n)$$

A. Georges et al., RMP (1996)

- Wishlist for the impurity solver:
  - Sensitive to bath structure at all energy scales
  - Generic Hamiltonians (multiband, clusters, …)
  - Different temperature regimes
  - Numerically exact
- Is this really easier than the original problem? Well yes, easier… But still not easy!

Continuous-time quantum Monte Carlo algorithms

- The Anderson impurity is still a very difficult problem
  - Infinite number of degrees of freedom
  - But essentially one dimensional
- Hamiltonian approaches:
  - Finite-temperature is not very easy
  - But mainly: does not scale well with increasing number of orbitals



- The continuous-time quantum Monte Carlo algorithms
  - They have been a bit of a revolution
  - They come in three different flavors
  - Can address multiorbital strongly-correlated materials or clusters (e.g. DCA)
  - They are based on a stochastic Monte Carlo algorithm
  - Their limitation is the fermionic sign problem

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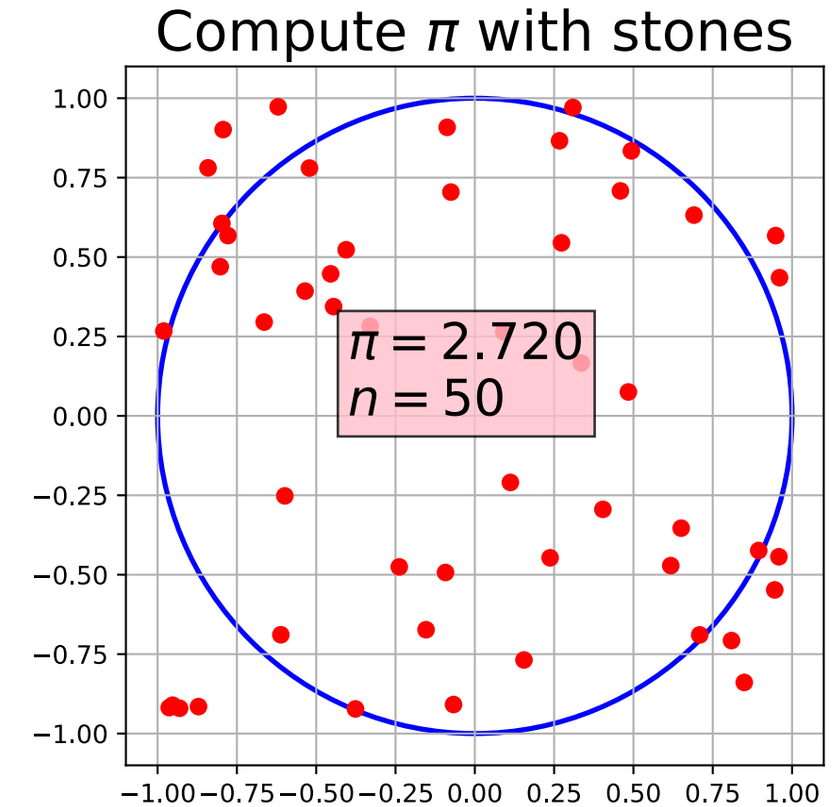
Compute π by throwing stones

- Let us try to compute π by throwing stones
- N stones uniformly thrown in a 2x2 square
- We count the fraction that falls inside a radius 1 circle

$$\pi \simeq 4 \cdot \frac{\#\,\mathrm{inside}}{\#\,\mathrm{total}}$$

- Let us make this more formal and let us call X_i the random variable associated to a single throw

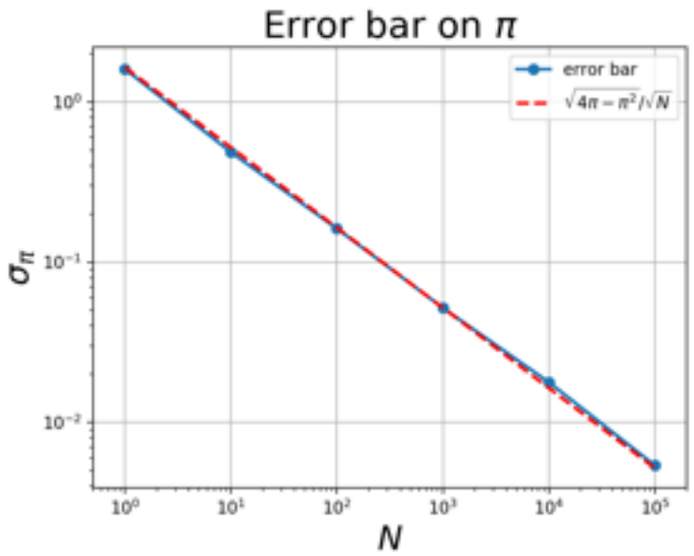


$$\langle X_i \rangle = \frac{\pi}{4} \cdot 4 + \frac{4-\pi}{4} \cdot 0 = \pi \qquad \langle X_i^2 \rangle = 4\pi \qquad \sigma_{X_i} = \sqrt{4\pi - \pi^2}$$

$$\langle X_i \rangle = \pi \pm 1.64$$

- But if I throw many stones, the error bar decreases

$$X = \frac{1}{N} \sum_{i=1}^{N} X_i \qquad \langle X \rangle = \pi \qquad \sigma_X = \frac{\sigma_{X_i}}{\sqrt{N}} \propto \frac{1}{\sqrt{N}}$$



Using Monte Carlo to compute integrals

- More generally Monte Carlo methods allow to stochastically compute integrals

$$I = \int f(x)\,dx = \int \rho(x)\frac{f(x)}{\rho(x)}\,dx \simeq \frac{1}{N}\sum_{x}^{\mathrm{MC}} g(x)$$

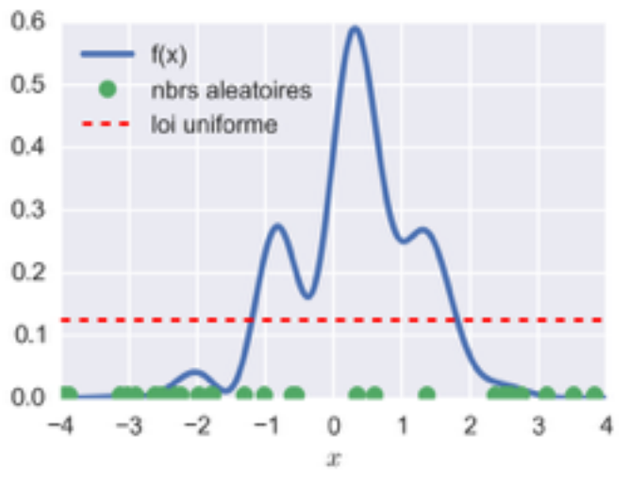
$$g(x) = \frac{f(x)}{\rho(x)} \qquad \int \rho(x)\,dx = 1 \qquad \rho(x) > 0$$

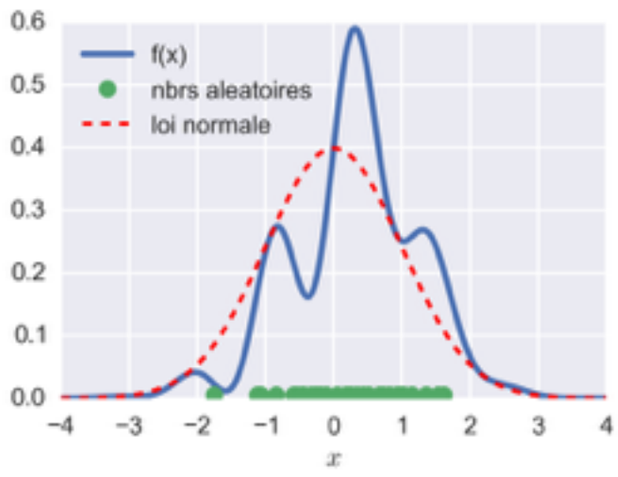
- The idea is to generate a Markov chain $\{x_1, x_2, x_3, \ldots\}$ such that the x_i are distributed according to the probability law $\rho(x)$

- In practice this can be achieved in different ways, e.g. using the Metropolis-Hastings algorithm
- Stone example:

$$\pi = \int_{\mathrm{square}} \frac{1}{4}\,g(x)\,dx \qquad g(x) = \frac{f(x)}{\rho(x)} = \begin{cases} 4 & x \in \text{circle} \\ 0 & x \notin \text{circle} \end{cases}$$

- A more general function $f(x)$
- Choosing a good $\rho(x)$ Importance sampling





Metropolis-Hastings (1953)

- The Metropolis-Hastings algorithms allows to sample a chosen distribution $\rho(x)$
- Achieve this through a Markov chain

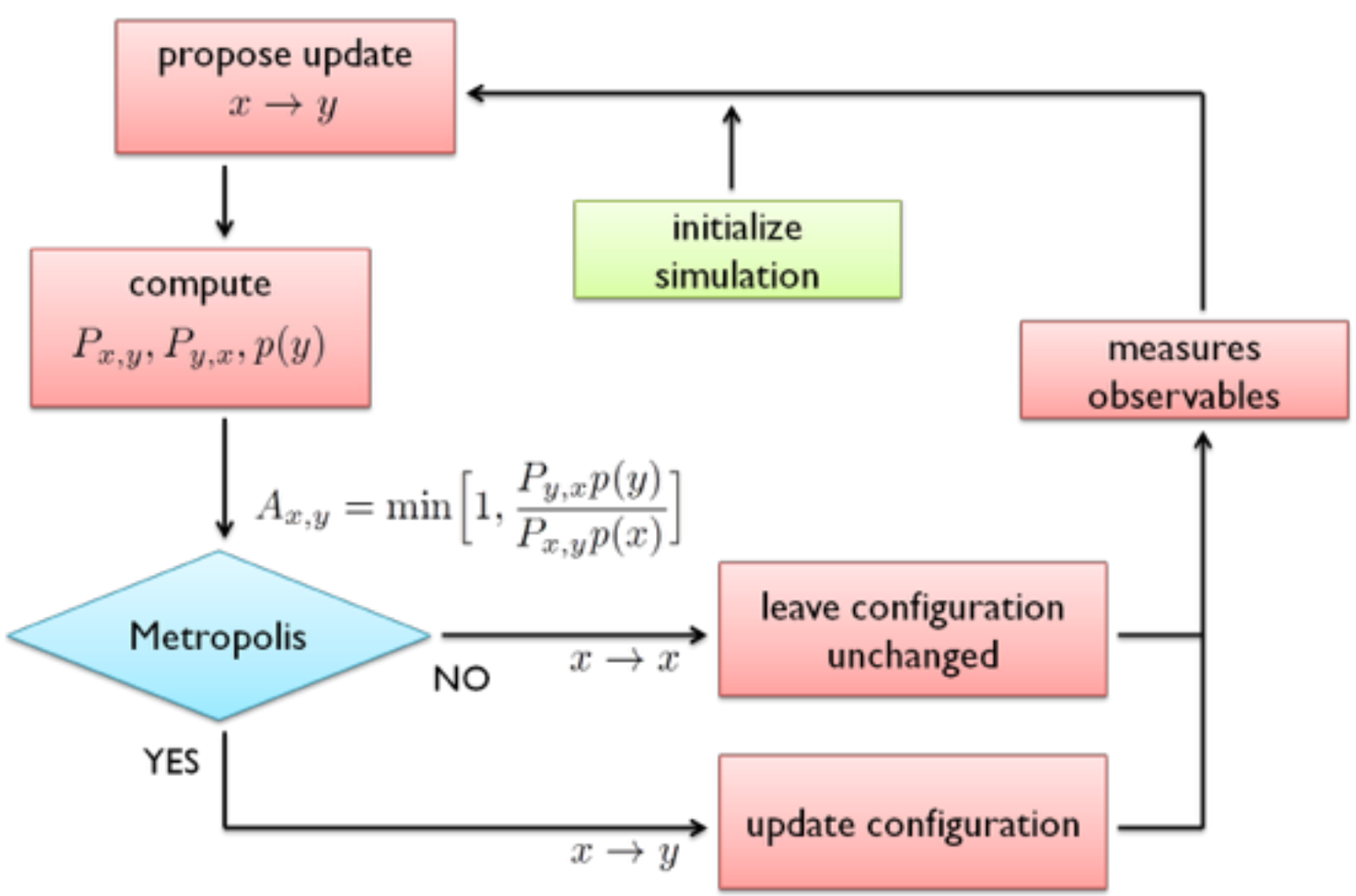
$$x_1 \to x_2 \to x_3 \to x_4 \to \dots$$

- Start from random x_1
- Propose a new y with some chosen probability $P_{x_1,y}$
- Accept or reject this proposal with probability

$$A_{x_1 y} = \min\left(1, \frac{\rho(y) P_{y,x_1}}{\rho(x_1) P_{x_1,y}}\right)$$

$$x_2 = \begin{cases} y & \text{if proposal accepted} \\ x_1 & \text{otherwise} \end{cases}$$

- Continue with $x_3, \dots$
- This generates the desired $\rho(x)$



Monte Carlo and classical systems

- Monte Carlo methods can be very powerful in classical statistical physics
- Let consider the Ising model $H_{\text{Ising}} = J \sum_{\langle i,j \rangle} \sigma_i \cdot \sigma_j - h \sum_i \sigma_i \qquad \sigma_i = \pm 1$
- The average magnetization

$$\langle m \rangle = \frac{1}{Z} \sum_{\mathcal{C}} e^{-\beta H_{\text{Ising}}(\mathcal{C})} \, m(\mathcal{C}) \qquad \mathcal{C} = \{\sigma_1, \sigma_2, \sigma_3, \ldots\}$$

- The sum over all configurations is exponential! 2^N
- Monte Carlo: This can be written as

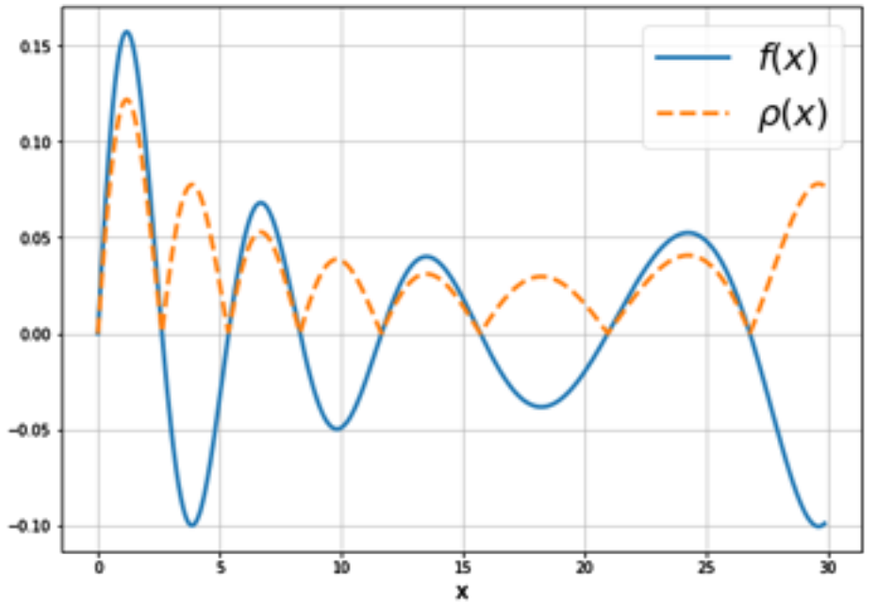
$$\langle m \rangle = \frac{\sum_{\mathcal{C}} \rho(\mathcal{C}) \, m(\mathcal{C})}{\sum_{\mathcal{C}} \rho(\mathcal{C})} \qquad \rho(\mathcal{C}) = e^{-\beta H_{\text{Ising}}(\mathcal{C})} \qquad g(\mathcal{C}) = m(\mathcal{C})$$

- There is a very natural choice for $\rho(\mathcal{C})$ which has the nice property $\rho(\mathcal{C}) > 0$
- With quantum systems: no such nice choice for $\rho(\mathcal{C})$
- In particular it is hard to find a positive probability distribution

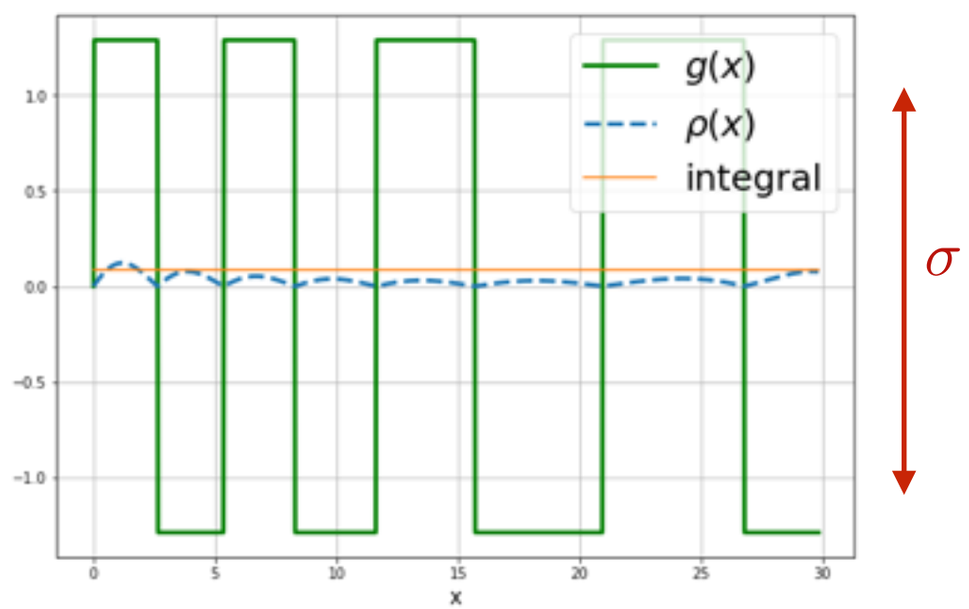
The sign problem in Monte Carlo methods

- What if the function that we try to integrate is alternating in sign?
- What probability density should we take?
- Let us try $\rho(x) = \gamma\,|f(x)|$
- Then the function to sample is

$$I \simeq \frac{1}{N}\sum_{x}^{\mathrm{MC}} g(x) \qquad g(x) = \frac{f(x)}{\rho(x)} = \frac{1}{\gamma}\mathrm{sign} f(x)$$



- But $g(x)$ has big oscillations around the result
- This leads to a larger variance $\dfrac{\sigma}{\sqrt{N}}$
- This is known as the sign problem
- Algorithms that simulate fermionic systems generally have a sign problem where σ grows exponentially with temperature, system size, etc.



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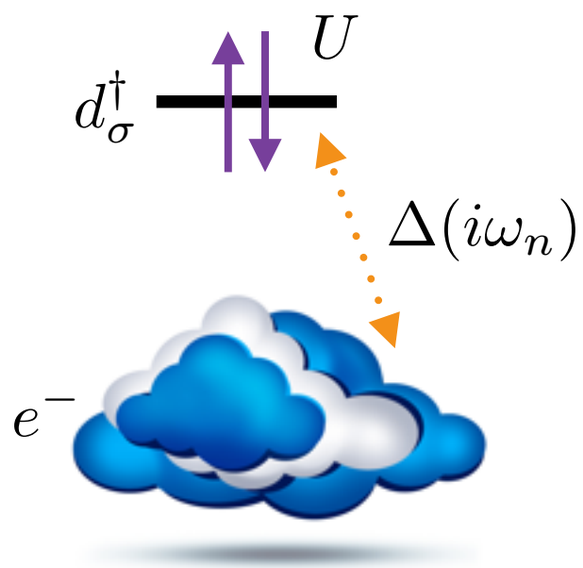
Continuous-time quantum Monte Carlo algorithms

- They allow to find the solution of an Anderson impurity model



$$Z = \int \mathcal{D}[d^\dagger, d]\, e^{-S} \qquad \langle A \rangle = \frac{1}{Z} \int \mathcal{D}[d^\dagger, d]\, e^{-S}\, A$$

$$S = -\sum_\sigma \int_0^\beta d\tau d\tau' d^\dagger_\sigma(\tau) G^{-1}_{0\sigma}(\tau - \tau') d_\sigma(\tau')$$

$$+ \int_0^\beta d\tau\, U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \qquad \beta = 1/T$$

$$G^{-1}_{0\sigma}(i\omega_n) = i\omega_n - \epsilon_0 - \Delta_\sigma(i\omega_n)$$

Describes the structure of the bath (self-consistently determined)

- They come in three flavors:
  - CT-INT: Interaction expansion Rubtsov and Lichtenstein, JETP Lett. (2004)
  - CT-HYB: Hybridization expansion Werner and Millis, PRB (2006)
  - CT-AUX: Auxiliary-field formulation Gull et al., EPL (2008)
- All are based on different perturbative expansions of the partition function
- The terms of the perturbation series are computed stochastically

Interaction expansion algorithm

- We start from $Z = \int \mathcal{D}[d^\dagger, d]\, e^{-S} \qquad \langle A \rangle = \frac{1}{Z} \int \mathcal{D}[d^\dagger, d]\, e^{-S}\, A$

$$S = S_0 + S_U = -\sum_\sigma \int_0^\beta d\tau d\tau'\, d^\dagger_\sigma(\tau) G^{-1}_{0\sigma}(\tau - \tau') d_\sigma(\tau') + \int_0^\beta d\tau\, U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$

Treat this term perturbatively

- The partition function becomes

$$Z = \int \mathcal{D}[d^\dagger, d]\, e^{-S_0} e^{-S_U} = Z_0 \left\langle T_\tau e^{-S_U} \right\rangle_0$$

- Writing the Taylor series in the interaction for the exponential

$$Z = Z_0 \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \ldots d\tau_n \left\langle T_\tau n_{d\uparrow}(\tau_1) \ldots n_{d\uparrow}(\tau_n) n_{d\downarrow}(\tau_1) \ldots n_{d\downarrow}(\tau_n) \right\rangle_0$$

$$Z = Z_0 \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \ldots d\tau_n \, \frac{(-U)^n}{n!} \det D(\tau_1, \ldots, \tau_n)$$

$D(\tau_1, \ldots, \tau_n)$ is an n x n matrix

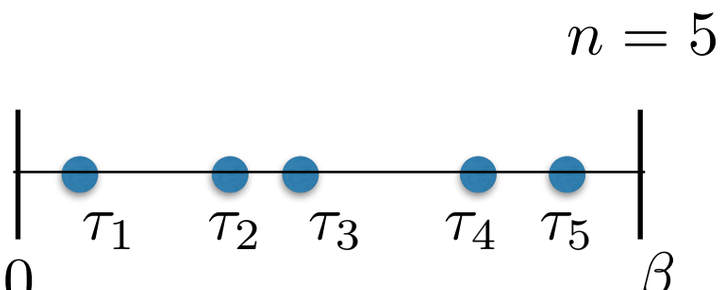
- This is a large sum: Let us try to compute it by Monte Carlo!

Monte Carlo sampling

- Monte Carlo sampling of the partition function

$$Z = Z_0 \underbrace{\sum_{n=0}^{\infty} \int_0^{\beta} d\tau_1 \dots d\tau_n}_{\sum_{\mathcal{C}}} \underbrace{\frac{(-U)^n}{n!} \det D(\tau_1, \dots, \tau_n)}_{\omega(\mathcal{C})} = Z_0 \sum_{\mathcal{C}} \omega(\mathcal{C})$$

- Monte Carlo configurations: $\mathcal{C} = \{n, \tau_1, \dots, \tau_n\}$ ⟶



- Some observable:

$$\langle n_\uparrow \rangle = \frac{\sum_{\mathcal{C}} \omega(\mathcal{C}) \frac{\det \tilde{D}(\mathcal{C})}{\det D(\mathcal{C})}}{\sum_{\mathcal{C}} \omega(\mathcal{C})}$$

- We could use $\omega(\mathcal{C})$ as a Monte Carlo weight. Warning: it can be negative! So we must use the absolute value

$$\langle n_\uparrow \rangle = \frac{\sum_{\mathcal{C}} \left|\omega(\mathcal{C})\right| \frac{\det \tilde{D}(\mathcal{C})}{\det D(\mathcal{C})} \cdot \mathrm{sign}(\omega)}{\sum_{\mathcal{C}} \left|\omega(\mathcal{C})\right| \cdot \mathrm{sign}(\omega)} \simeq \frac{\sum_{\mathcal{C}}^{\mathrm{MC}} \frac{\det \tilde{D}(\mathcal{C})}{\det D(\mathcal{C})} \cdot \mathrm{sign}(\omega)}{\sum_{\mathcal{C}}^{\mathrm{MC}} \mathrm{sign}(\omega)}$$

Induces a very large variance $\sigma \propto \exp(n)$

- The variance of $\omega(\mathcal{C})$ leads to an exponential sign problem

The fermionic sign problem

- What is the typical amplitude of a <u>sampled</u> contribution?

$$Z = Z_0 \sum_{n=0}^{\infty} \int_0^\beta d\tau_1 \dots d\tau_n \underbrace{\frac{(-U)^n}{n!} \det D(\tau_1, \dots, \tau_n)}_{\omega(\mathcal{C})}$$

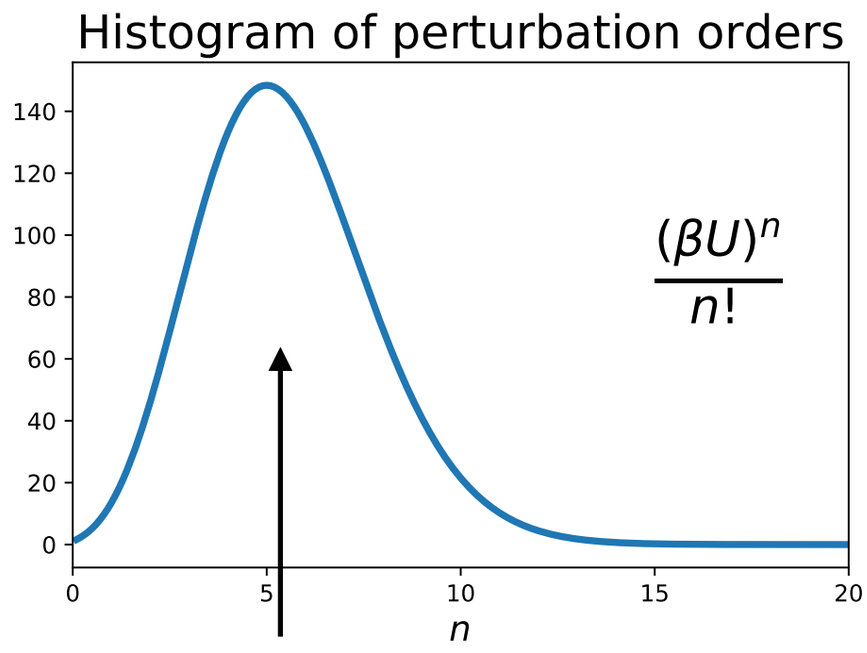
- The contributions go as $\omega(\mathcal{C}) \sim \frac{(U\beta)^n}{n!}$

- Therefore the orders that contribute most are found around $n_{\max} \simeq \beta U$

- The main contributions have alternating signs with a typical variance

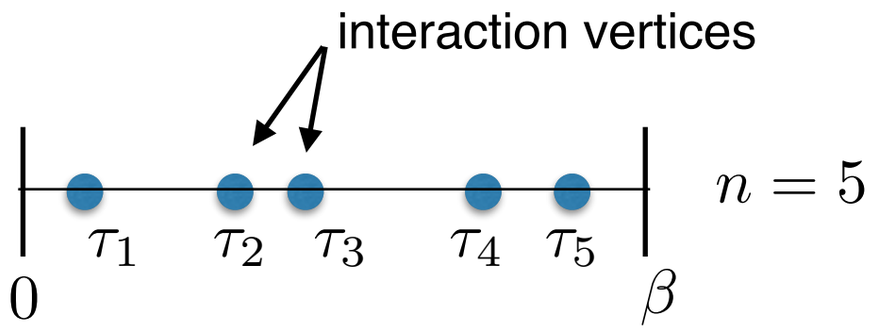
$$\sigma \sim \frac{(\beta U)^{\beta U}}{(\beta U)!} \sim \exp(\beta U)$$

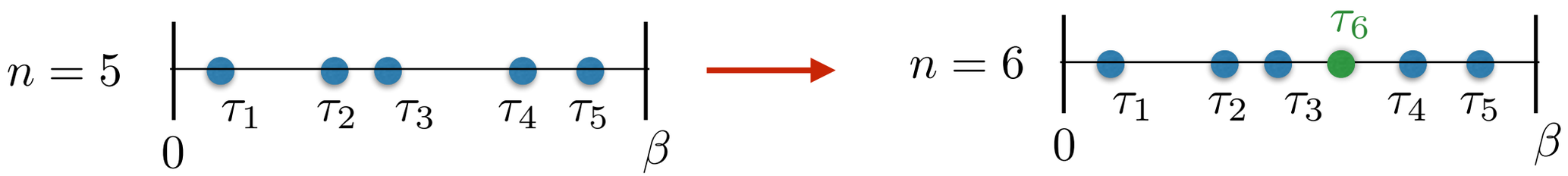
- This is the exponential fermionic sign problem



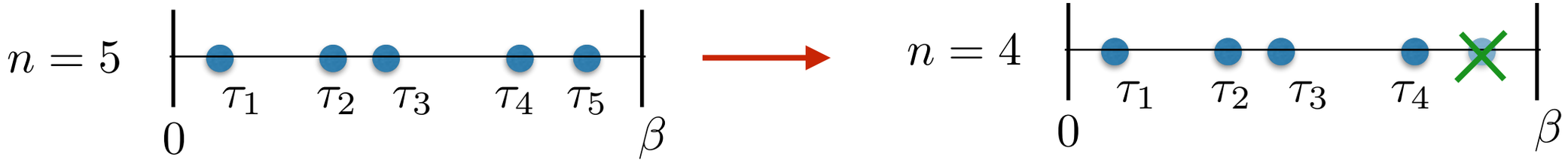
The algorithm in practice

- We use a Metropolis-Hastings scheme
- Start from some configuration
- Propose new configurations
  - Add a vertex:





  - Remove a vertex:



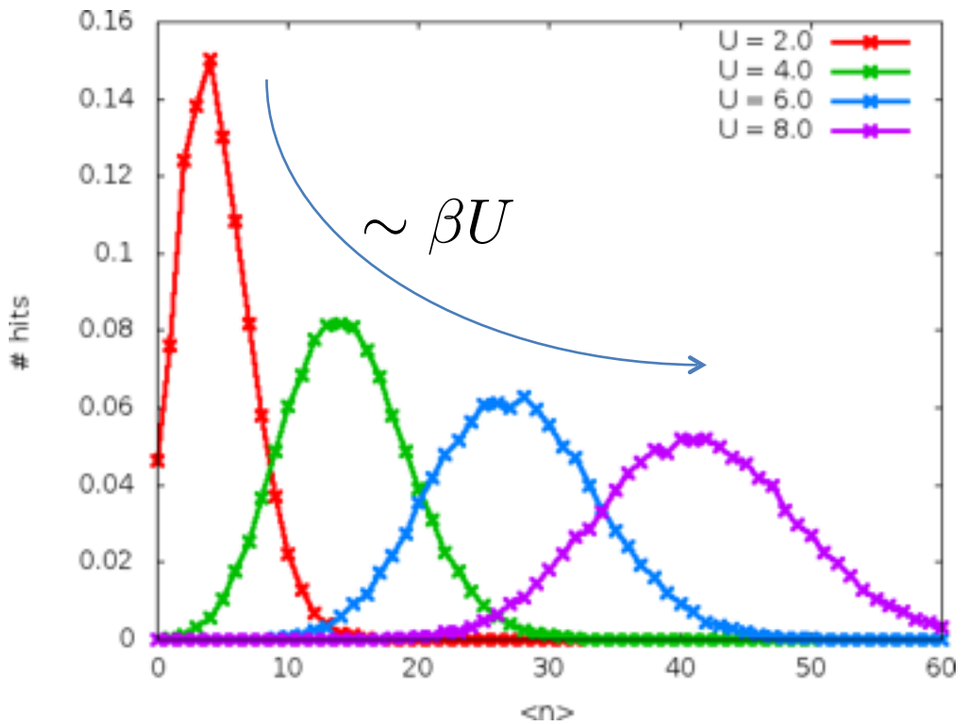
- Accept or reject the proposed configurations with relevant probability

Is all hope lost?

- Extra freedom in the theory:

$$\mathcal{H}_{\text{int}} = U n_\uparrow n_\downarrow = U(n_\uparrow - \alpha)(n_\downarrow - \alpha) + U\alpha(n_\uparrow + n_\downarrow) + \text{const}$$

- This additional α changes the non-interacting starting point (different chemical potential)
- A clever choice for α can completely suppress the sign problem in the single-orbital Anderson impurity model!
- For multiorbital models there is a sign problem that gets worse and low temperatures or high interaction
- Complexity: $\mathcal{O}(n^3)$
- Average perturbation order $n \sim \beta U$
- Sign problem $\sigma \sim \exp(\beta U)$



Hybridization-expansion algorithm

- Very similar in spirit

$$S = -\sum_{\sigma} \int_0^{\beta} d\tau d\tau'\, d_\sigma^\dagger(\tau) G_{0\sigma}^{-1}(\tau - \tau') d_\sigma(\tau') + \int_0^{\beta} d\tau\, U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$

- We treat the hybridization to the bath as a perturbation

$$S = S_{\rm loc} + \sum_{\sigma} S_\Delta^\sigma$$

$$= \int_0^{\beta} d\tau \left[\sum_{\sigma} d_\sigma^\dagger(\tau)(-\partial_\tau + \epsilon_0) d_\sigma(\tau) + U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \right] \longleftarrow \text{atomic limit}$$

$$+ \sum_{\sigma} \int_0^{\beta} d\tau d\tau'\, d_\sigma^\dagger(\tau) \Delta_\sigma(\tau - \tau') d_\sigma(\tau') \longleftarrow \text{perturbation}$$

- Writing the Taylor expansion for e^{-S_Δ}

$$Z = \int \mathcal{D}[d^\dagger, d] e^{-S_{\rm loc}} \prod_{\sigma} \Big[\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(S_\Delta^\sigma\right)^n \Big] = \Big\langle \prod_{\sigma} \Big[\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(S_\Delta^\sigma\right)^n \Big] \Big\rangle_{\rm loc}$$

average value to be computed in the isolated impurity

Monte Carlo sampling

- Now configuration are given by a set of pairs of times

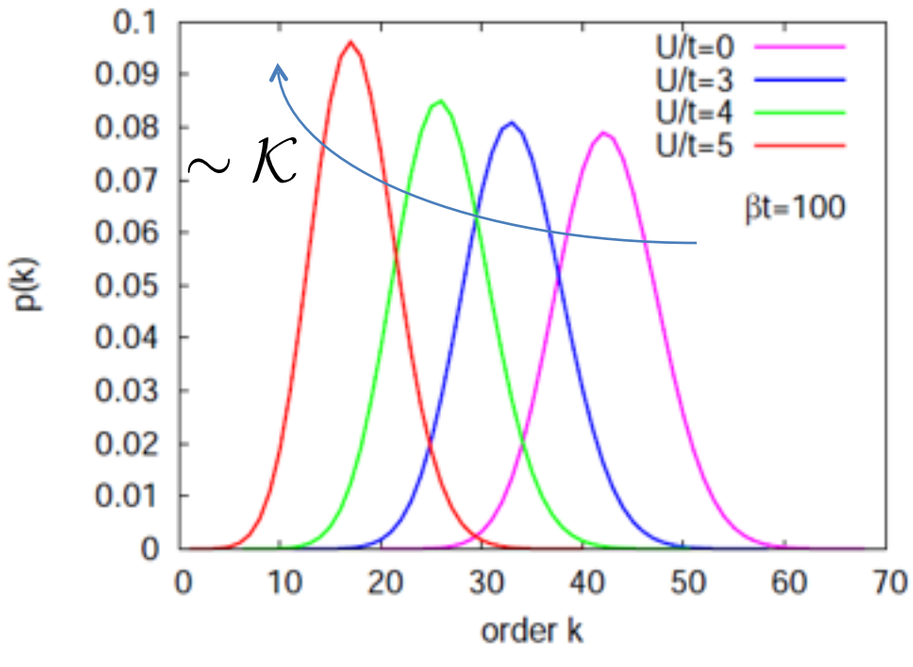
$$\mathcal{C} = \{n, \tau_i^\sigma, \tau_i^{'\sigma}\}$$

n insertions of hybridization lines

$$Z = \sum_{\mathcal{C}} \underbrace{(-1)^n \det \Delta(\mathcal{C}) \cdot \mathrm{Tr}\, \mathcal{C}}_{\omega(\mathcal{C})}$$

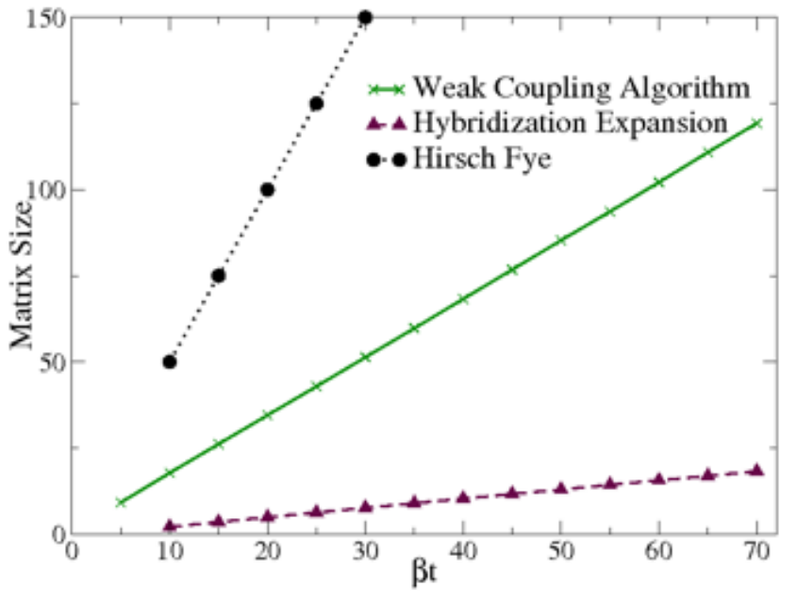
- The contributions to the partition function do not need to be positive
- But: in single-orbital models there is no sign problem

- For multiorbital models there is a sign problem that gets worse at low temperatures
- Complexity: $\mathcal{O}(n^3)$
- Average perturbation order $\sim \mathcal{K}$
- For multiorbital systems, the local impurity Hilbert space grows exponentially
- The trace calculation becomes the bottleneck



Summary: continuous-time QMC algorithms

- Their development has been very important within DMFT
- CT-INT & CT-AUX: series in the interaction
  - Many orbitals, weak coupling, high temperatures
  - Low temperatures, generic Hamiltonians are difficult
- CT-HYB: series in the hybridization
  - Generic Hamiltonians, low temperatures
  - Bad scaling with number of orbitals
- Many models have been investigated
  - Hubbard model, Holstein-Hubbard, Kondo lattice
  - Extensions of DMFT: DCA, CDMFT, dual-fermions, DΓA
  - Within DFT + DMFT realistic structure calculations
  - Out-of-equilibrium generalization



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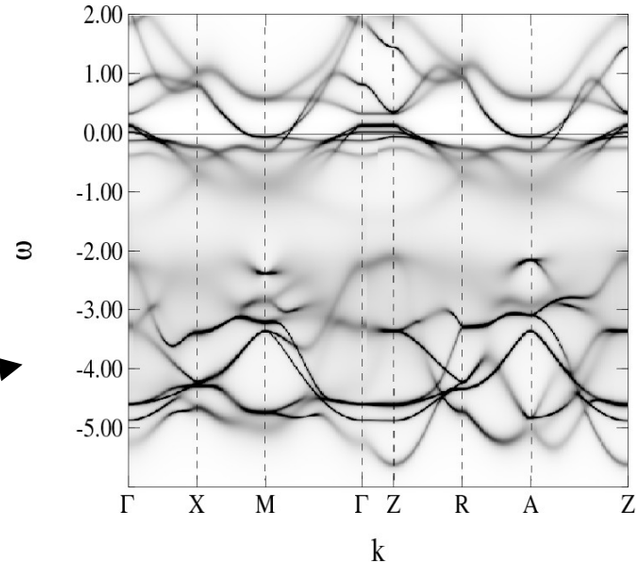
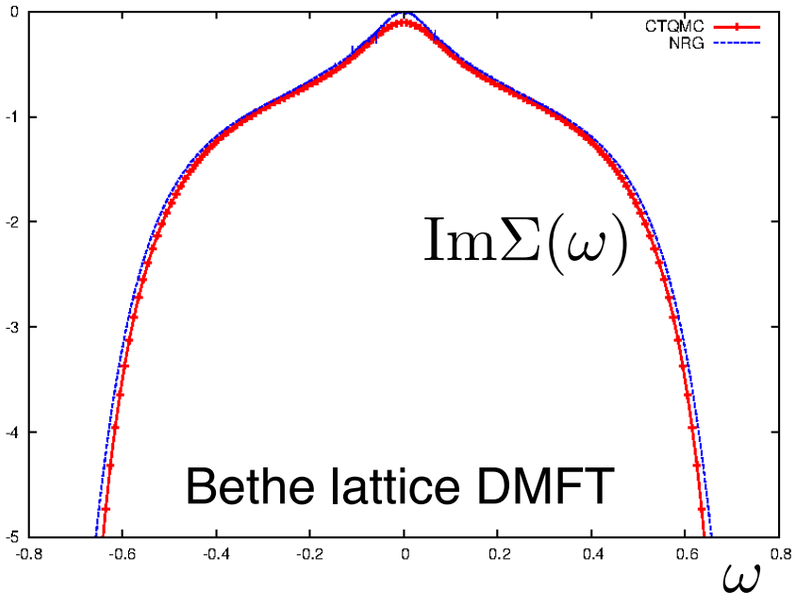
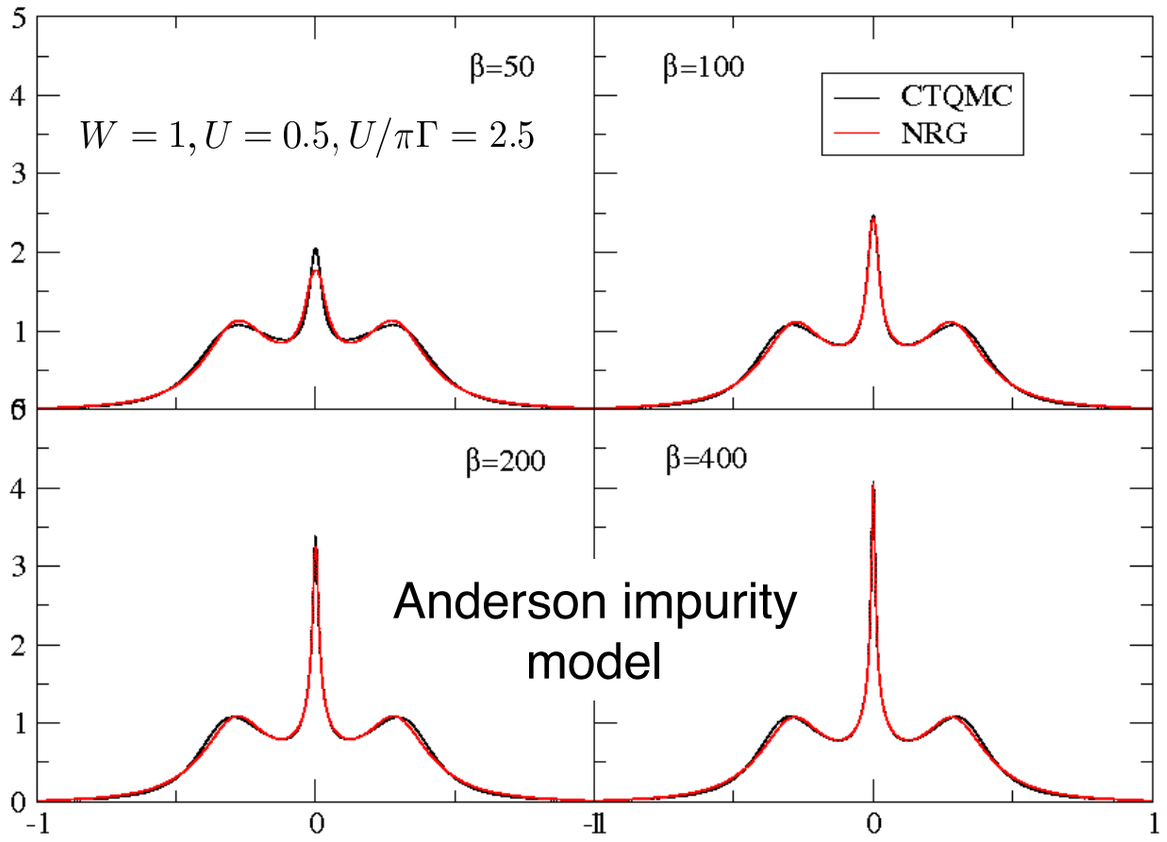


M. Aichhorn et al., PRB (2009)

Two applications of CT-QMC solvers

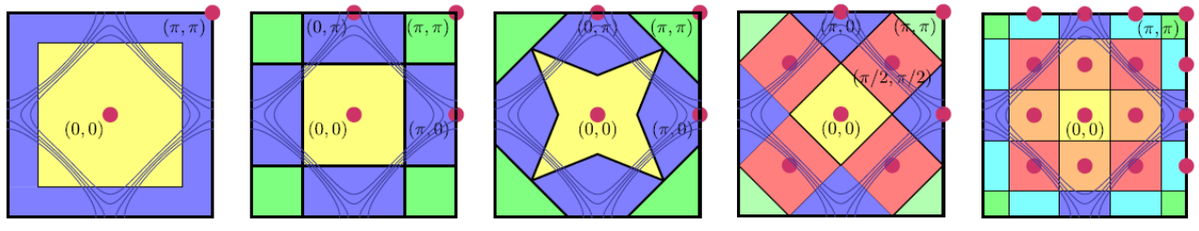
- CT-QMC (with Padé) and numerical renormalization group comparison





NRG: Rok Zitko
CTQMC: Jernej Mravlje

- Dynamical cluster extension of DMFT

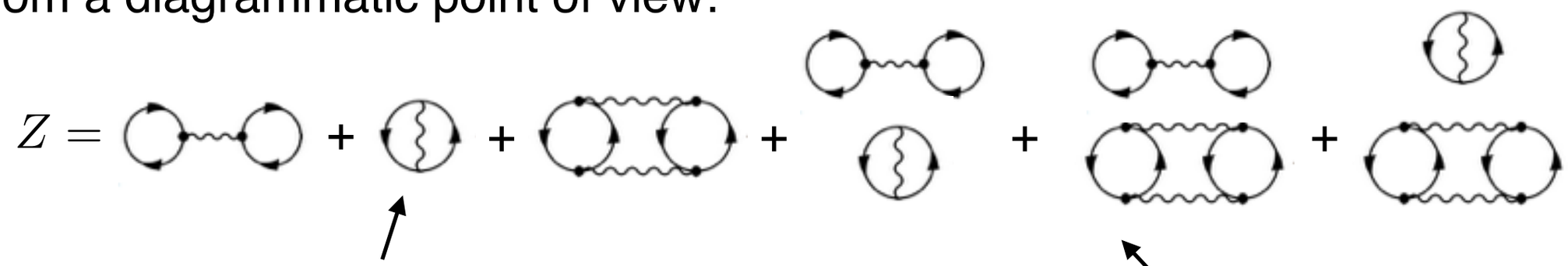


E. Gull et al., PRB (2010)

- The approach to the Mott insulator is characterized by successive Mott transition in reciprocal space
- Region close to the antinode get insulating first while regions close to the node remain metallic down to the Mott insulating state

Continuous-time algorithms for the lattice?

- CT-QMC are very efficient for impurity models. Can they be extended to the lattice?
- The hybridization algorithm suffers from exponential increase of local Hilbert space
- The interaction expansion algorithm
  - The perturbation order increases rapidly with the number of sites and the sign problem becomes very severe
  - The reason is that we sample the partition function which is extensive
  - From a diagrammatic point of view:



- At large orders the contribution from connected diagrams is only a small fraction of the total sum of diagrams. A relatively small error bar on the total sum can be large for the connected diagrams contribution!

Outline

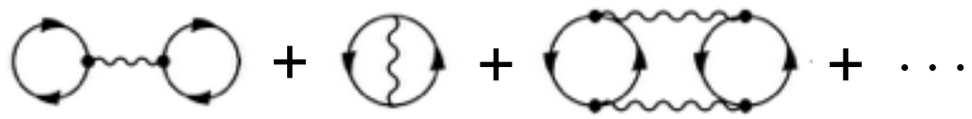
- Why are fermionic quantum systems difficult?
  - Hamiltonian approaches and Hilbert space size explosion
  - Action-based approaches and Monte Carlo methods
- A very quick introduction to Monte Carlo methods
  - How to compute integrals stochastically
  - The origin of the sign problem
- Continuous-time quantum Monte Carlo algorithms
  - The three flavors of algorithms and the fermionic sign problem
  - What have they allowed to do?
- Diagrammatic Monte Carlo algorithms
  - Addressing the infinite lattice directly
  - Applications to the two-dimensional Hubbard model

Diagrammatic Monte Carlo

- We consider a model on an infinite lattice (thermodynamic limit)
- The idea is to write a perturbation series in U for the physical quantity of interest

$$\mathcal{A} = \sum_{n=0}^{\infty} a_n U^n$$ ← e.g. density, double occupation, Green function, …

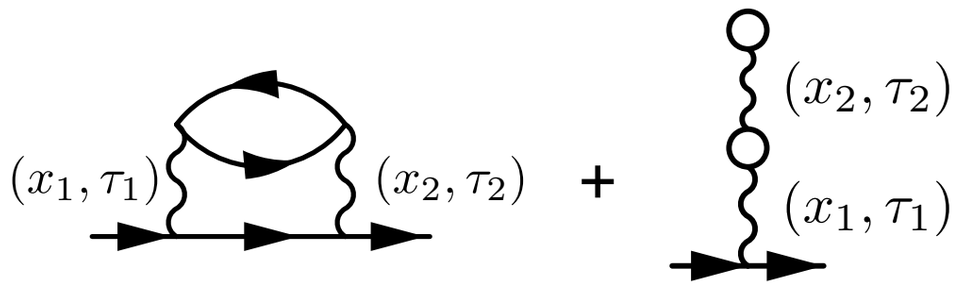
- From a diagrammatic point of view, e.g.

$$\mathcal{A} = \ln Z =$$  ← Only connected diagrams contribute to physical intensive quantities

- The two challenges:
  1. Fermionic sign problem → difficult to get many coefficients a_n
  2. Resum the series → analytical structure in complex U plane?
- The partition function $Z(U)$ is an entire function in the complex Uplane
- Physical observables $\mathcal{A}(U)$ usually have poles in the complex plane
- Therefore the series for $\mathcal{A}$ generally has a finite convergence radius!

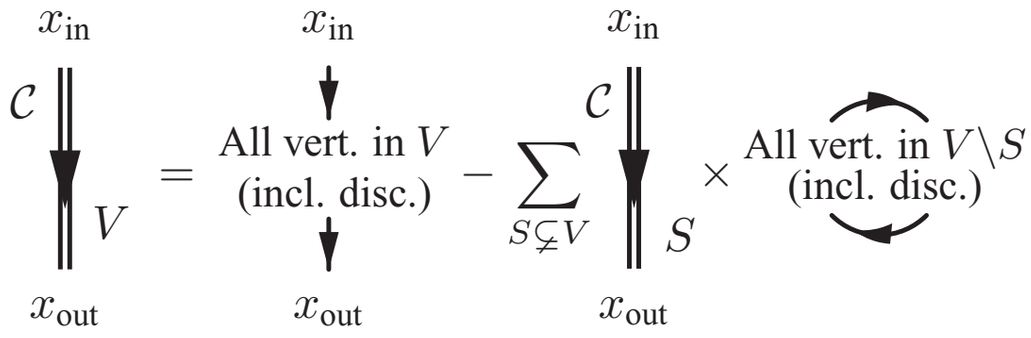
Challenge 1: Compute series coefficents

- No simple formula for the coefficients of physical observables (unlike Z)
- They are best represented diagrammatically (e.g. connected diagrams)
- Original algorithm (DiagMC): stochastically sample all topologies (≈ 6-7 orders)
- Sign problem has two origins:
  - Integration over internal variables
  - Alternating sign between different topologies



N.V. Prokofiev and B.V. Svistunov, PRL (2007)

- Reduce sign problem: Sum topologies with the same set of internal vertices *V*
- Huge computational effort: there is a factorial number of diagrams!
- CDet: Can be done in exponential time 3^n using determinants (disconnected diagrams removed recursively)

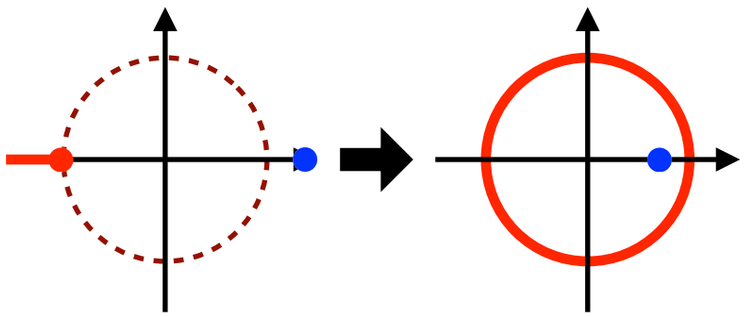


- Up to ≈ 10-12 orders for Hubbard model

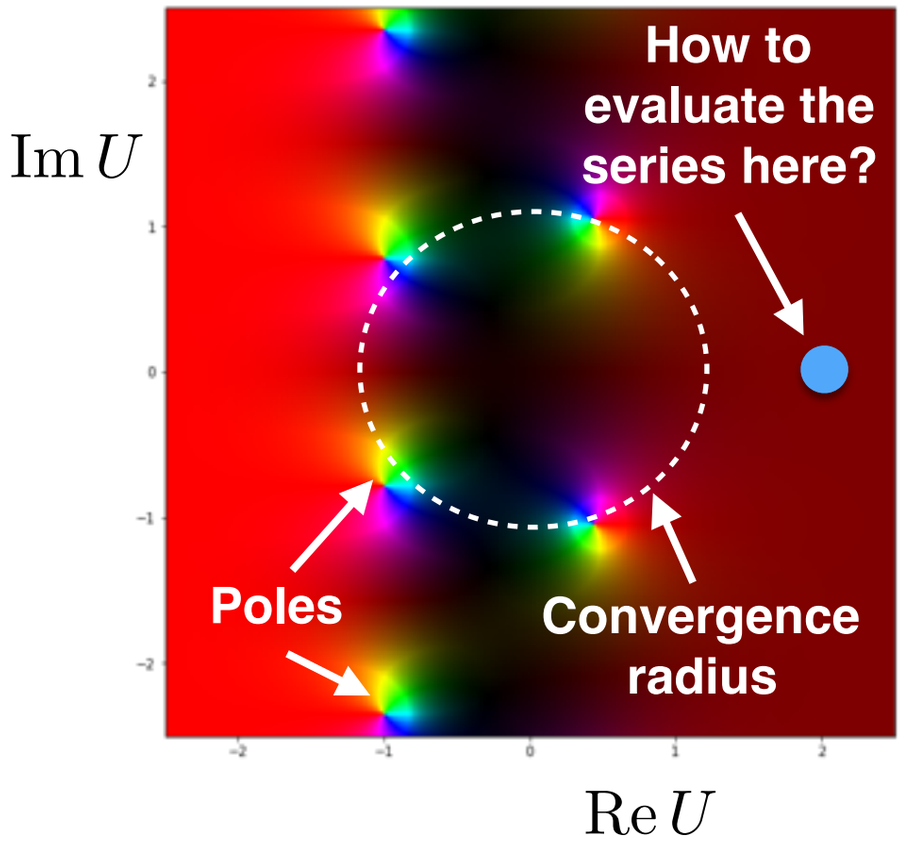
Rossi, PRL (2016)
Moutenet et al., PRB (2018); Simkovic and Kozik, arXiv (2017)

Challenge 2: Resummation of the series

- Series convergence controlled by structure in complex plane
- How do we evaluate the series beyond its convergence radius?
- Conformal maps, integral approximants, Padé approximants, …



$n(U)$ in the Hubbard atom



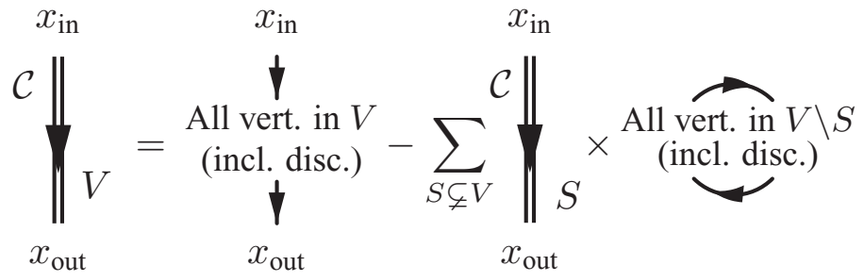
- Generate new series with freedom in the starting point of the perturbation theory

$$G_0 = \frac{1}{i\omega_n + \mu - \epsilon_k} \rightarrow \tilde{G}_0 = \frac{1}{i\omega_n + \mu - \epsilon_k - \alpha}$$

- A proper choice of α can increase radius and accelerate convergence

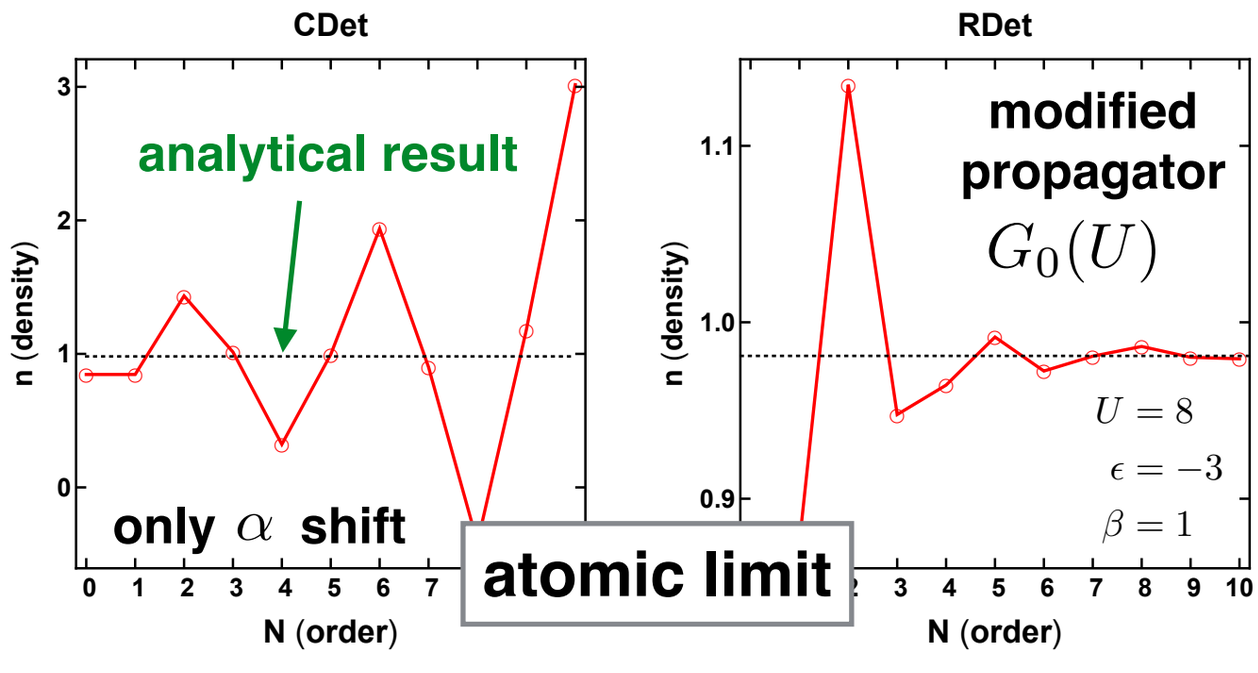
Summary: diagrammatic Monte Carlo

- Stochastically sample contributions to intensive physical observable
- Can directly address infinite lattice size
- Exponential complexity with orders $\sim 3^n$
- In practice: 10-12 orders for Hubbard model
- The series generally have finite convergence radius
- Ongoing efforts



- Generalize to different models, different perturbation series
- Find better starting points (why not DMFT!)
- In particular can we generalize the formalism to start from a propagator that would be a well-defined function of U

$$G_0 \;\rightarrow\; G_0(U)$$

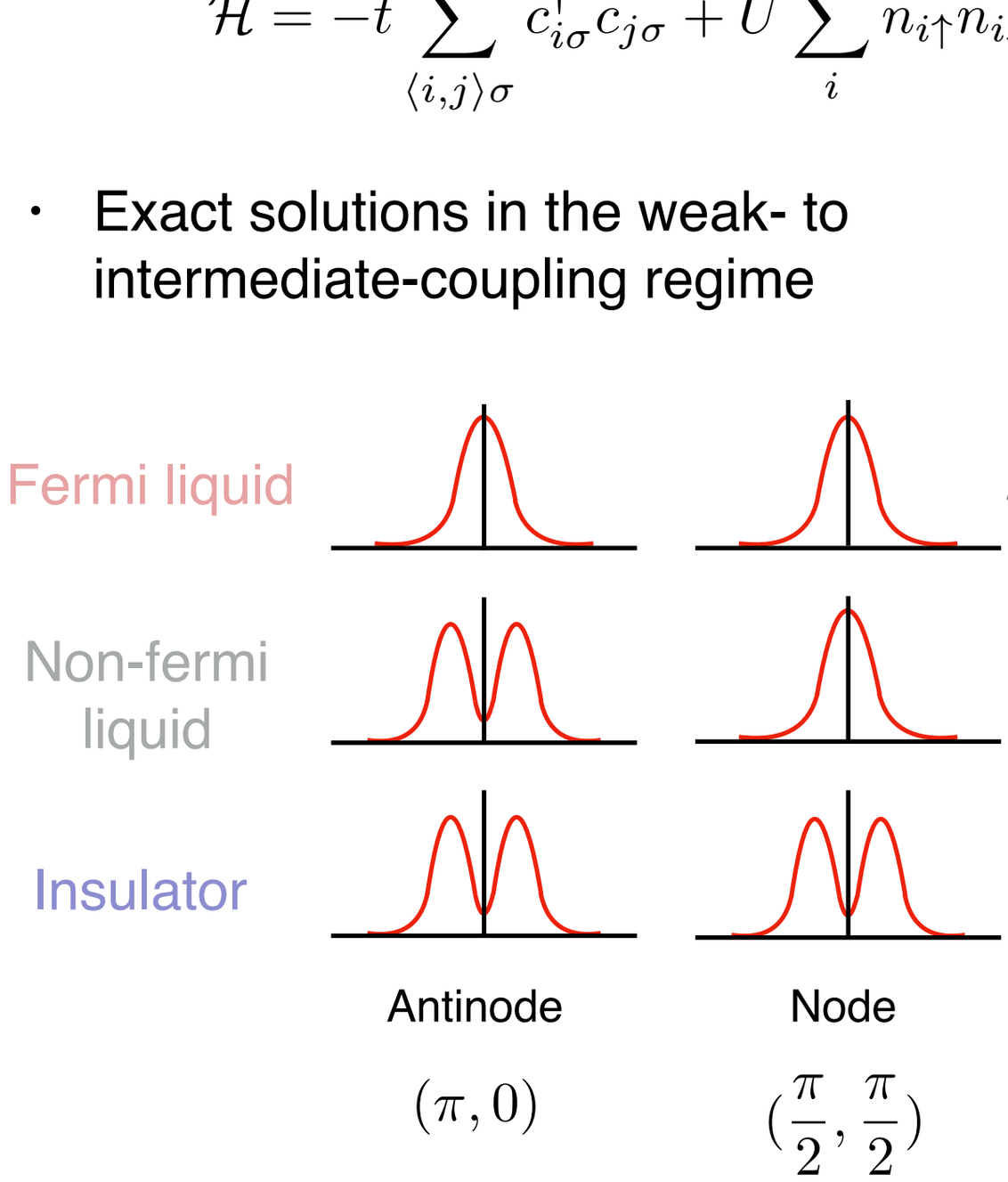


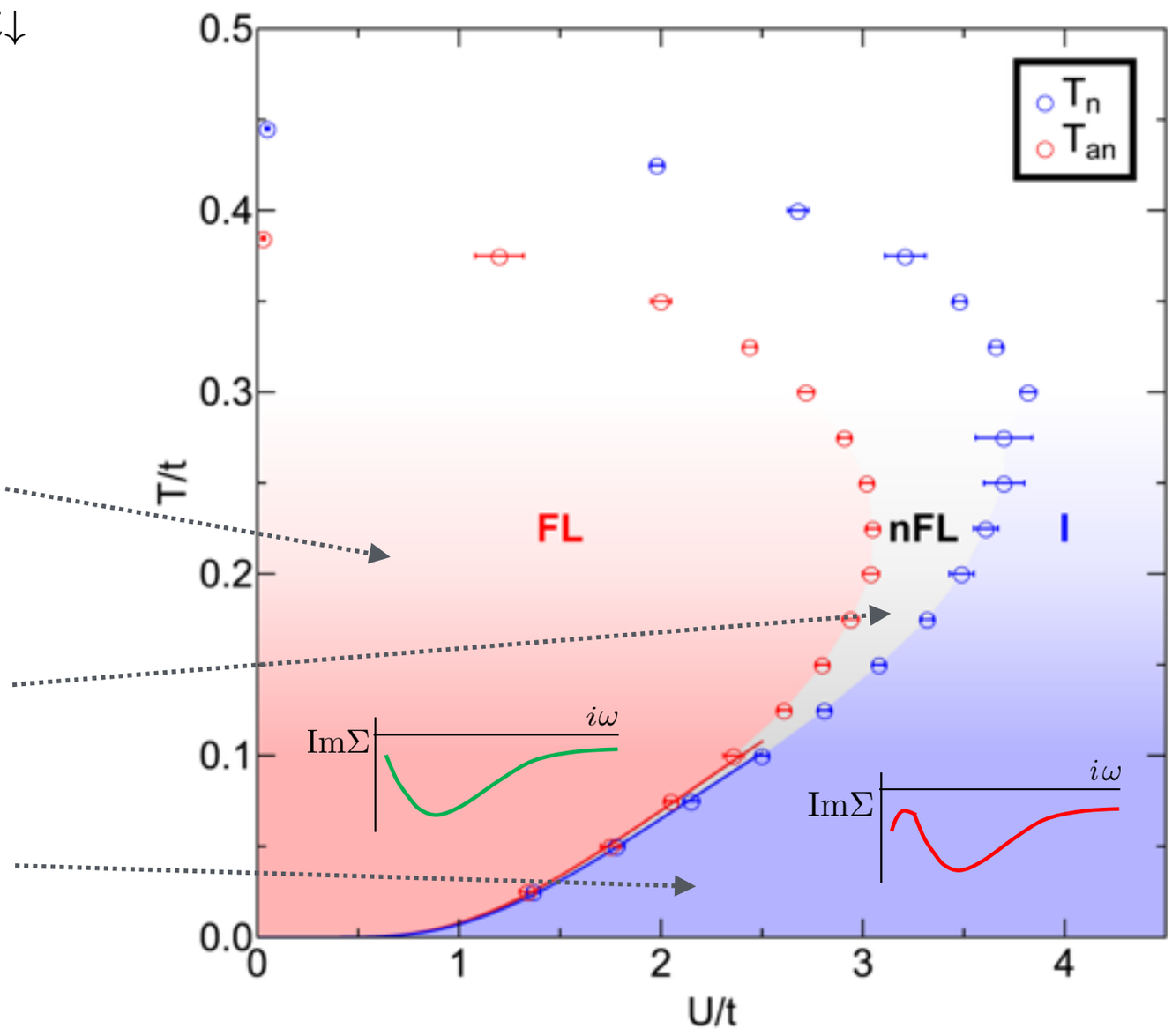
Application: Half-filled Hubbard model

- The half-filled Hubbard model is a good testbed for diagrammatic Monte Carlo, where it is expected to work best

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

- Exact solutions in the weak- to intermediate-coupling regime

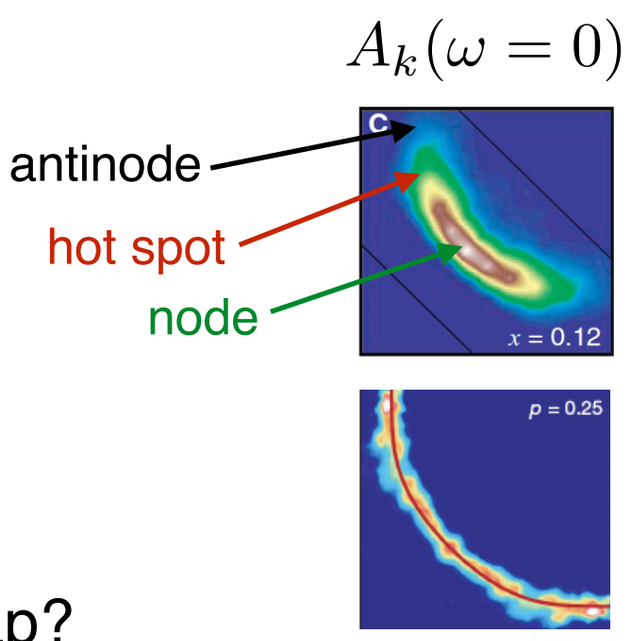


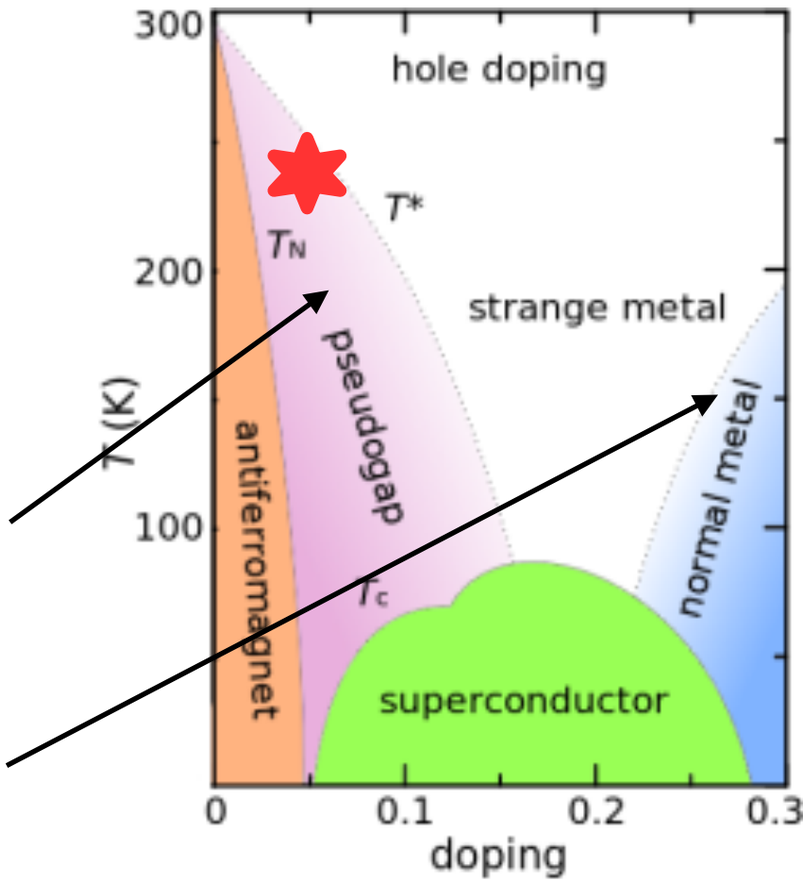


F. Simkovic et al., arXiv (2018)
T. Schäfer et al. (in preparation)

Application: Pseudogap physics in Hubbard model

- Investigate doped 2D Hubbard model
- Relevant to cuprate superconductors
- The pseudogap region:
  - Nodal / antinodal differentiation
  - Loss of spectral weight at the antinode
- Open questions:
  - Mechanism of the pseudogap?
  - Role of Mott insulator?
  - Ordered phase?
  - Good or bad for superconductivity?



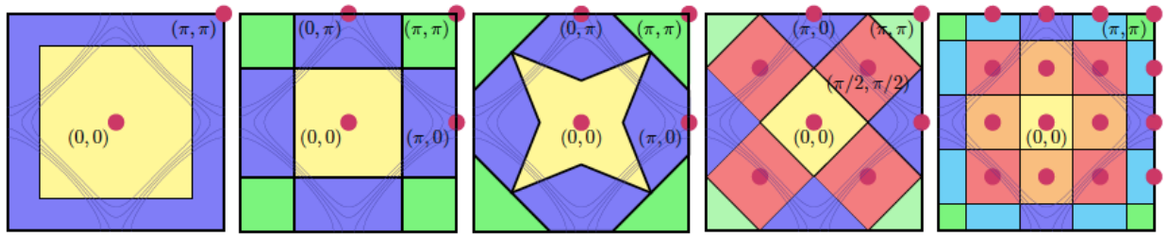


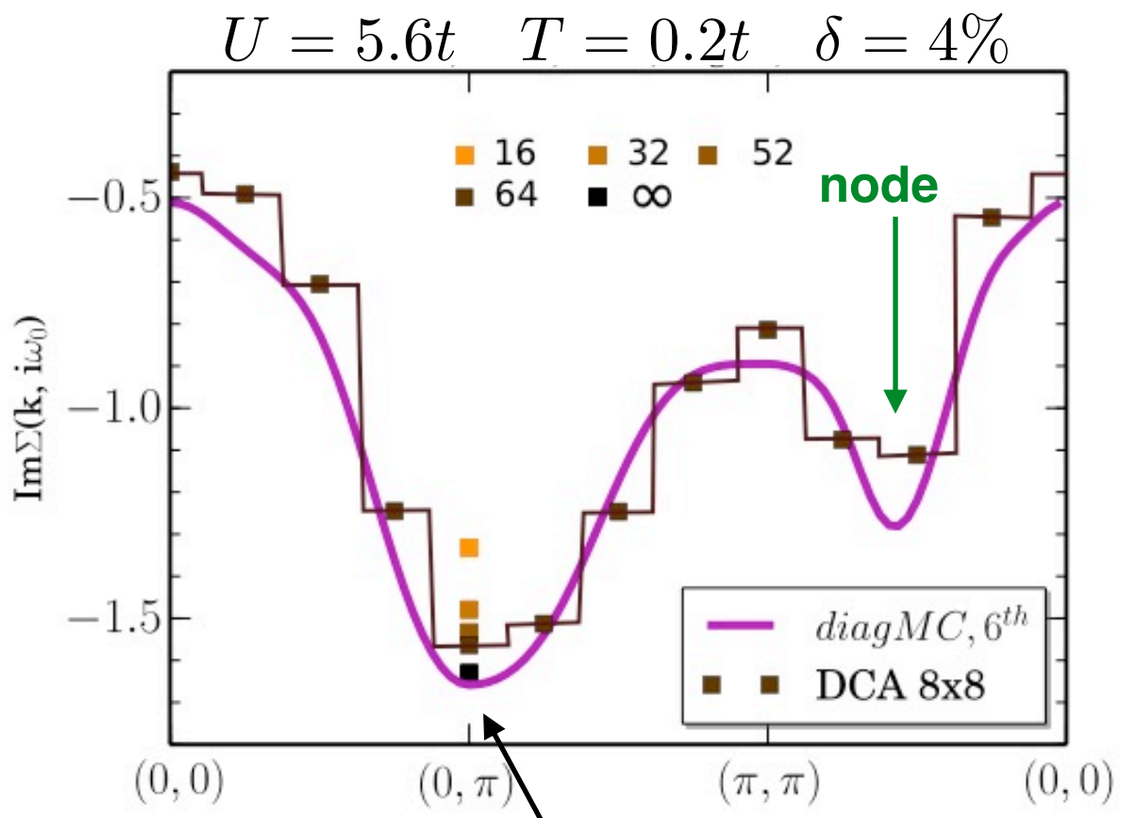
$$\mathcal{H} = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Both nearest-neighbor t
and next-nearest neighbor $t' = -0.3t$

Complementary numerical approaches

- Cluster extensions of DMFT such as the dynamical cluster calculations (DCA)





- Diagrammatic Monte Carlo

- There is a non-trivial regime where both me agree at a quantitative level
- Confirm there is a pseudogap in Hubbard model
- An important addition of diagrammatic Monte Carlo is its infinite momentum resolution
- Allows to address question that are difficult with other approaches

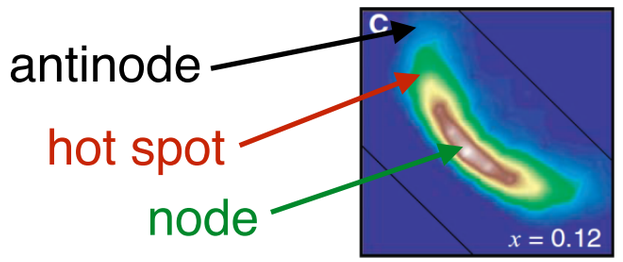
W.Wu, MF, A. Georges, E. Kozik, PRB (2017)

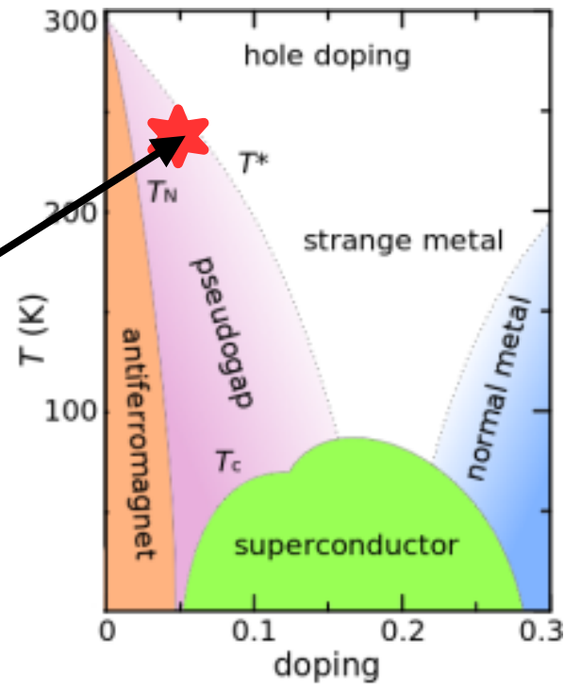
Entering the pseudogap region

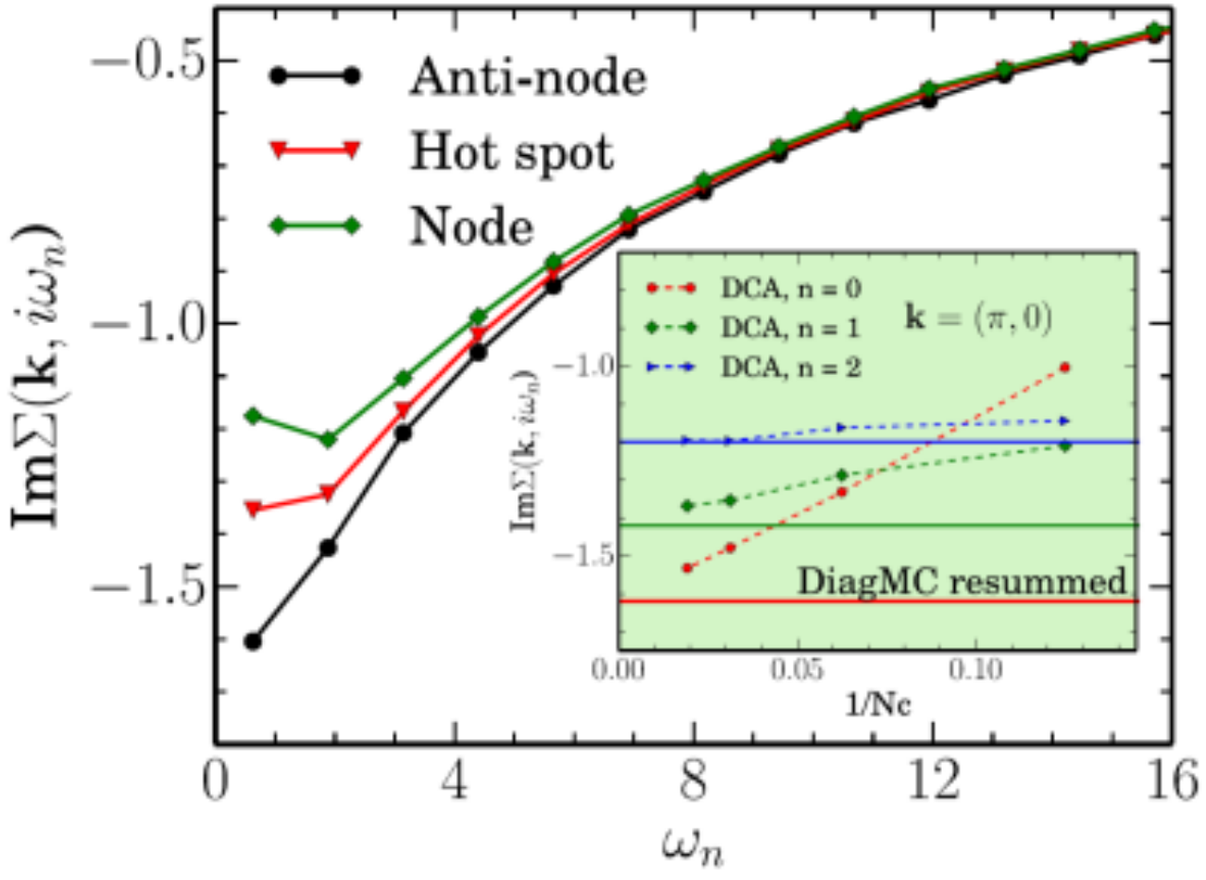
- Converged results for

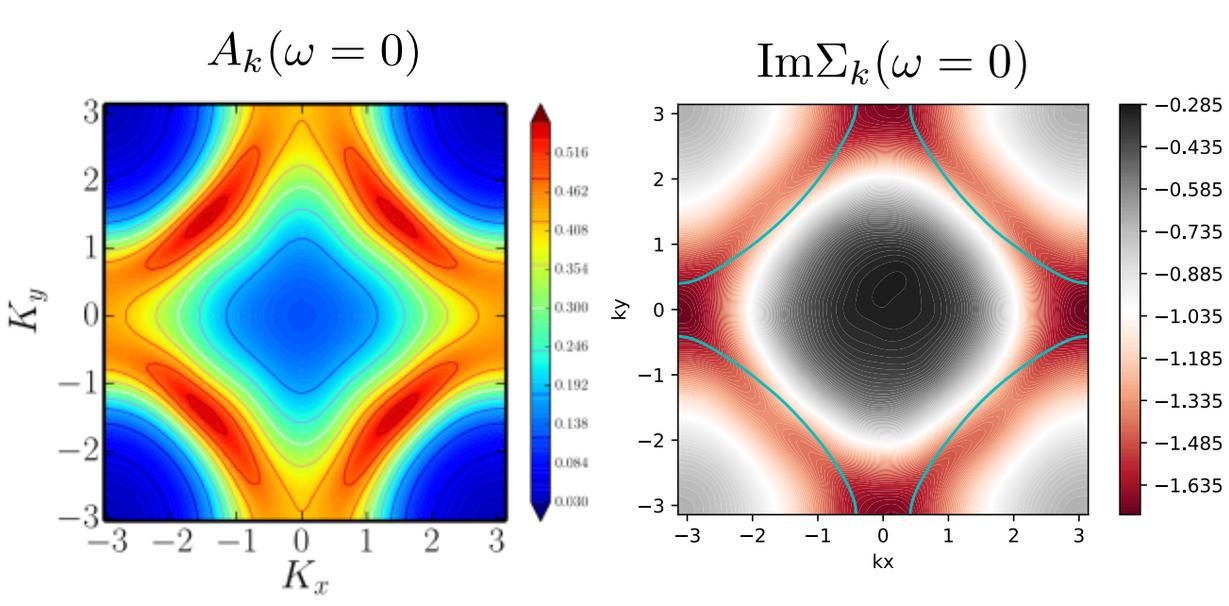
$$U = 5.6t \quad T = 0.2t \quad \delta = 4\%$$

- Top of pseudogap region
- Clear nodal / antinodal differentiation
- Antinode hotter than hotspot ≠ weak-coupling









obtained from diagrammatic Monte Carlo

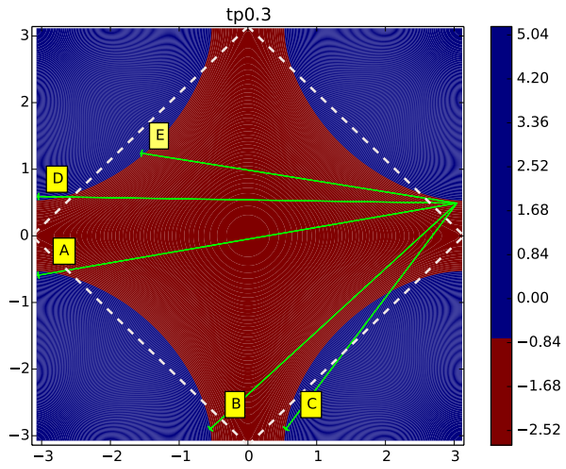
(*Note: also recent results at* $U = 7t \quad T = 0.2t \quad \delta = 5\%$)

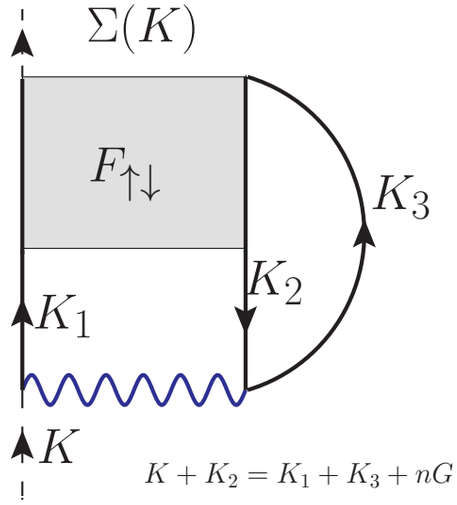
Origin of the pseudogap: fluctuation diagnostics

O. Gunnarson, T. Schäfer, et al., PRL (2015)

- Fluctuation analysis

$$\Sigma(K) = \sum_q \Sigma_X^q(K) + \frac{Un}{2}$$



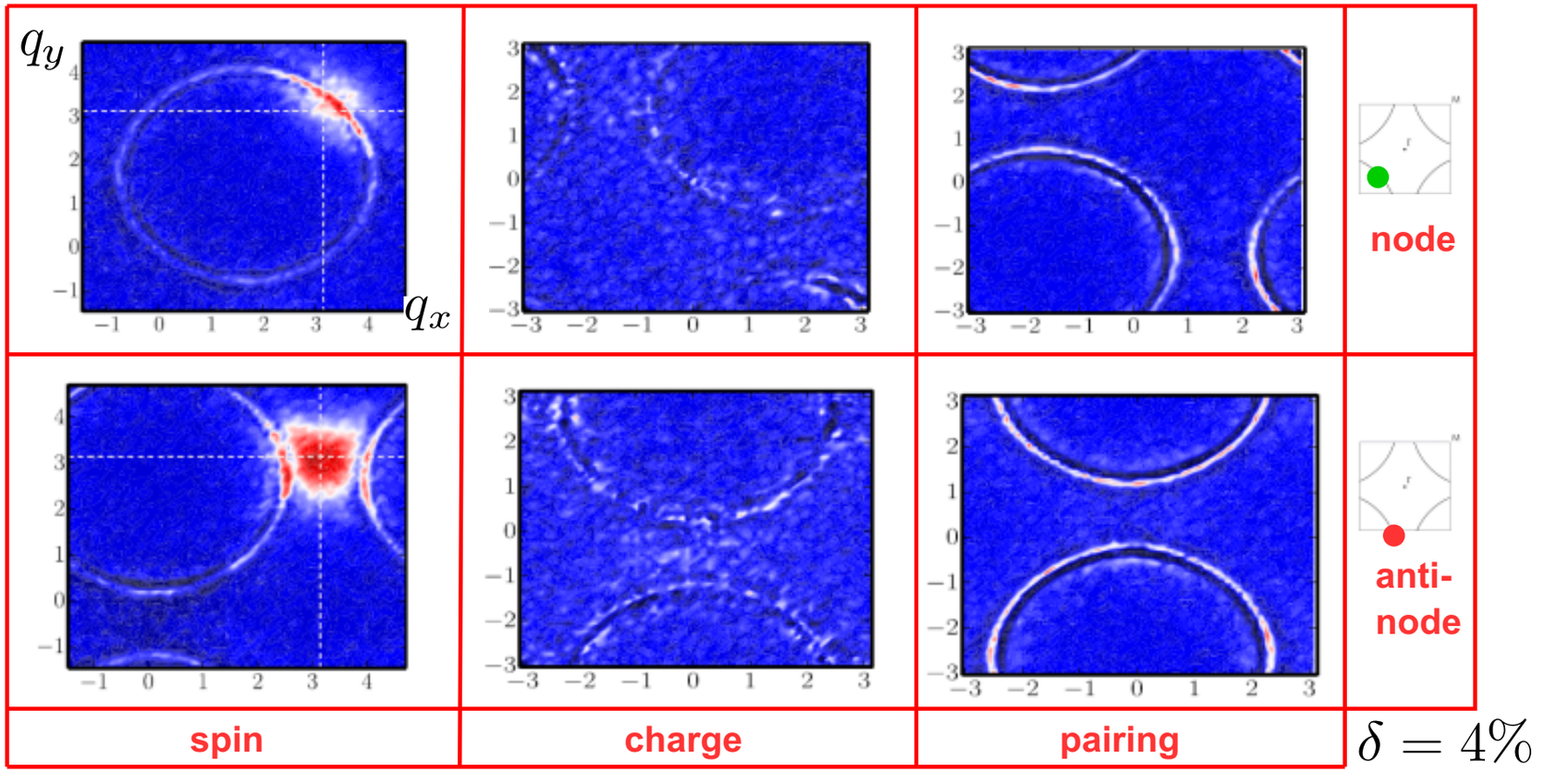


- Gives info about nature of scattering
- Spin, charge and pairing representations
- Spin: Fermi surface scattering at node, commensurate at antinode
- From spin susceptibility

$$\xi \simeq 1.5$$

- Pseudogap due to short-range, antiferromagnetic correlations

W.Wu, MF, A. Georges, E. Kozik, PRB (2017)



Conclusion ?

Hard luck and trouble is my only friend…
If it wasn't for bad luck, I wouldn't have no luck at all…

Conclusion: on a more positive note ♪

- Fermionic problems are very challenging!
- There has nevertheless been great progress in the development of modern numerical algorithms
- Among those Monte Carlo approaches play an important role
- They are always limited by the sign problem but their boundaries are always pushed further
- Within dynamical-mean field theory:
  - Continuous-time algorithms opened new avenues for the method
  - Different models, extensions of DMFT, realistic structure calculations
- Addressing the infinite lattice is possible within diagrammatic Monte Carlo
  - Non-trivial regimes can be addressed (e.g. pseudogap)
  - Many ideas remain to be explored

Acknowledgements










Thank you for your attention!

SIMONS FOUNDATION