Introduction to diagrammatic Monte Carlo

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Diagrammatic Monte Carlo

- Diagrammatic Monte Carlo is a stochastic method that samples the connected diagrams of a perturbation expansion
- Concrete example: Hubbard model on infinite lattice (thermodynamic limit) and at equilibrium

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

- Start from $U = 0$ and construct perturbation series in U for an observable A:

$$\mathrm{A} = \sum_{n=0}^{\infty} a_n U^n \quad \longleftarrow$$

e.g. density, double occupation, Green's function, …

- It is similar to the CT-INT but note that we have not written A as a fraction
- First goal: compute the series coefficients a_n
- Second goal: resum the series

Introduction to diagrammatic Monte Carlo

- **Overview of diagrammatic Monte Carlo**

  The idea of diagrammatic Monte Carlo, differences with respect to CT-INT / DDMC

- **The connected determinant algorithm (CDet)**

  How to efficiently compute the sum of all connected diagrams describing an observable

- **Resummation of the series**

  Resummation techniques and freedom to choose the starting point of the perturbation expansion

- **An illustration of CDet**

  Self-energies and pseudogap in the doped Hubbard model

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Reminder about CT-INT (also called DDMC)

- The CT-INT algorithm is computing physical properties from the ratio $\mathsf{A} = \dfrac{\mathrm{Tr} e^{-\beta H} \hat{\mathsf{A}}}{Z}$
- Both the numerator and the denominator are written as a series in U
- For the partition function we have

$$Z = \mathrm{Tr} e^{-\beta H} = \int \mathscr{D}[\bar{c}, c] e^{-S[\bar{c},c]}$$

- We write the action of the system as $S = S_0 + S_U$ where

$$S_0 = \sum_{ij} \int_0^\beta \int_0^\beta \bar{c}_i(\tau) \, [G_0^{-1}]_{ij}(\tau - \tau') \, c_j(\tau') \, d\tau d\tau' \qquad\qquad S_U = U \sum_i \int_0^\beta n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) d\tau$$

and the Fourier transform of $[G_0]_{ij}(\tau - \tau')$ is the non-interacting propagator

$$G_0(k, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_k}$$

Reminder about CT-INT (also called DDMC)

- Expanding the exponential we find

$$Z = \int \mathscr{D}[\bar{c}, c] e^{-S_0[\bar{c},c]} \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \sum_{i_1,\ldots,i_n} \int_0^\beta d\tau_1 \ldots d\tau_n \, n_{i_1\uparrow}(\tau_1) n_{i_1\downarrow}(\tau_1) \ldots n_{i_n\uparrow}(\tau_n) n_{i_n\downarrow}(\tau_n)$$

$$= Z_0 \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \sum_{i_1,\ldots,i_n} \int_0^\beta d\tau_1 \ldots d\tau_n \left\langle n_{i_1\uparrow}(\tau_1) n_{i_1\downarrow}(\tau_1) \ldots n_{i_n\uparrow}(\tau_n) n_{i_n\downarrow}(\tau_n) \right\rangle_0$$

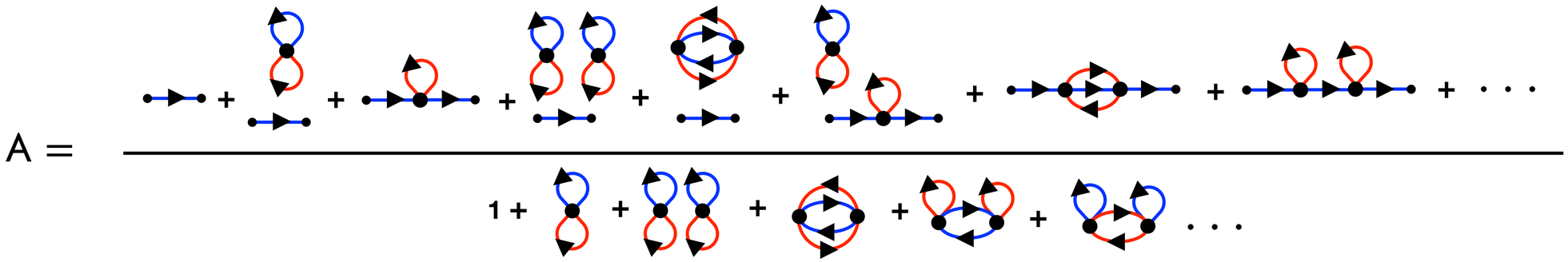
$$= Z_0 \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \sum_{i_1,\ldots,i_n} \int_0^\beta d\tau_1 \ldots d\tau_n \, \det D_n^\uparrow \, \det D_n^\downarrow$$

- We have used Wick's theorem in the last line and $D_n^\sigma = \left\{ [G_0]_{ij}(\tau_i - \tau_j) \right\}$ is an $n \times n$ matrix
- One can find a similar expression for the numerator and eventually obtain

$$\mathsf{A} = \frac{\mathrm{Tr} e^{-\beta H} \hat{\mathsf{A}}}{Z} = \frac{\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{\mathscr{C}} \det D_n^\uparrow D_n^\downarrow \, \mathscr{A}_n(\mathscr{C}) \, U^n}{\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{\mathscr{C}} \det D_n^\uparrow D_n^\downarrow \, U^n} \qquad \mathscr{C} = \{(r_1, \tau_1), \ldots, (r_n, \tau_n)\}$$

Diagrammatic interpretation of CT-INT

- In CT-INT, the numerator and denominator are both sampled and the ratio is taken in the end
- The average perturbation order $\sim \beta UN$, where N is the number of sites
- This makes it very difficult to address large systems (increasing perturbation order → worse sign)
- Why is the perturbation order $\sim \beta UN$?
- From a Feynman diagrammatic point of view (taking the example $\mathrm{A} = G$ the Green function):

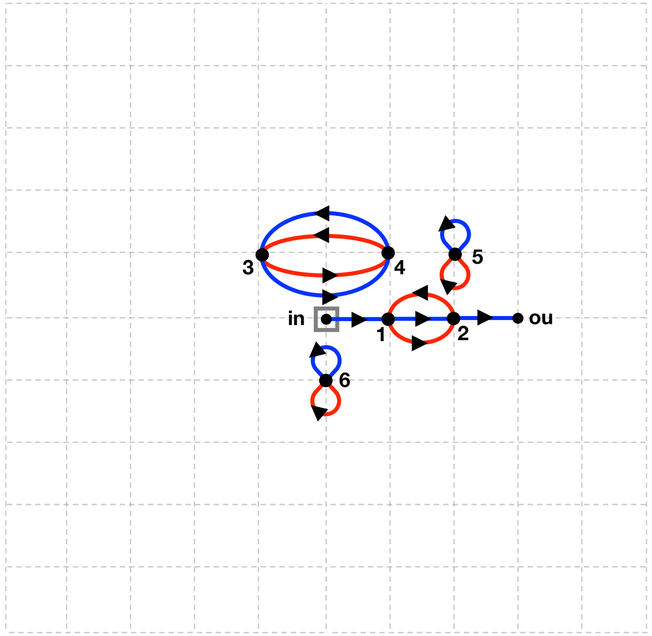


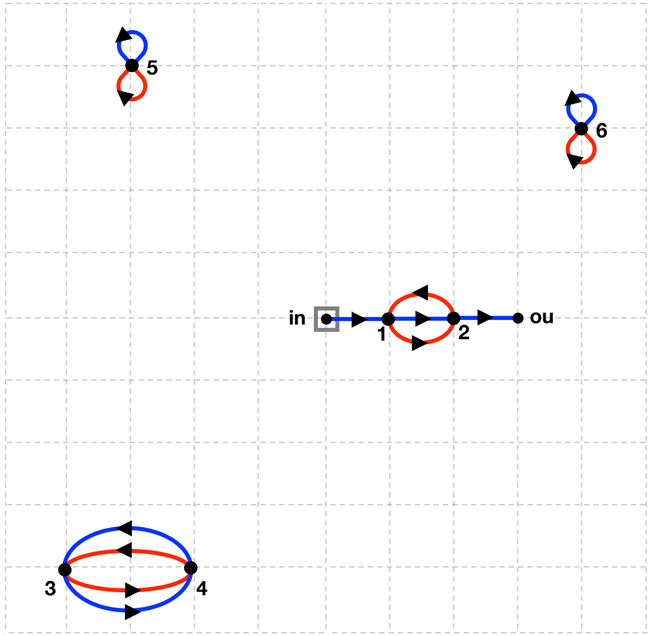
- The observable is a ratio of two sums involving all Feynman diagrams connecting the interaction vertices

Disconnected diagrams and perturbation order

- The Monte Carlo weight of a configuration with n vertices is given by its contributions to the partition function
- It corresponds to the sum of all connected + disconnected diagrams living on the n vertices
- Let us take two examples at order 6
- These two diagrams have the same weight
- This means that the disconnected pieces will be integrated over the entire lattice
- At order k, the dominant contribution will be the diagram with k pieces:

$$= U\langle n_\uparrow\rangle\langle n_\downarrow\rangle$$

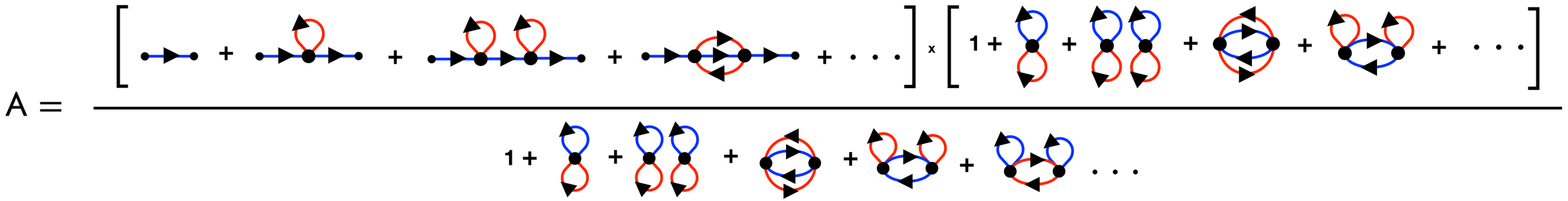




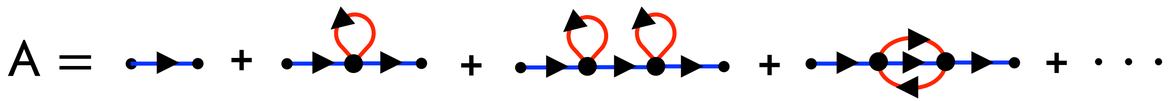
- Therefore the largest weight $\simeq \dfrac{(UN\beta)^k}{k!}$ which is consistent with a maximum at $k \simeq \beta UN$

Linked cluster theorem and diagrammatic Monte Carlo

- It seems clear that there is redundant information with disconnected diagrams
- From the linked cluster theorem we know that the fraction



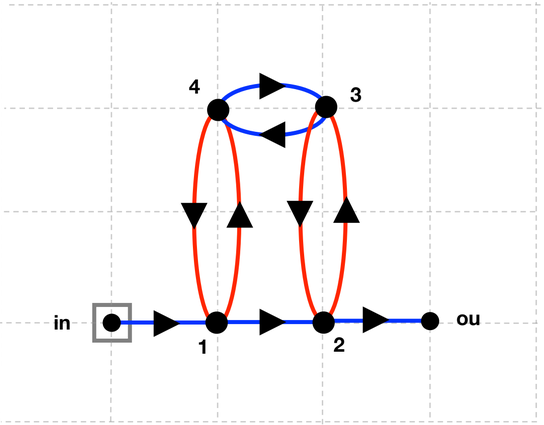
eliminates the disconnected diagrams so that we can rewrite A as a sum of connected diagrams only



- Instead of sampling both terms of a fraction, we can also sample the series of connected diagrams
- This is the essence of the diagrammatic Monte Carlo methods

Pros and cons of diagrammatic Monte Carlo

- Sampling only connected diagrams can have several advantages:
  - Less redundancy, only the “physical” diagrams are sampled
  - The weight of a connected diagram depends on its extent
  - Therefore the diagrams that contribute have vertices that remain close to each other
  - This allows to treat infinite lattices directly (thermodynamic limit)



- But there is no free lunch:
  - In CT-INT, the sum of a factorial number of diagrams is computed with a single determinant
  - Can something like this be done for connected diagrams? Yes, but exponential cost
  - In CT-INT, the numerator and denominator are both entire functions of U. The corresponding series therefore have infinite convergence radius
  - What about the series of the ratio? They have finite convergence radius in general

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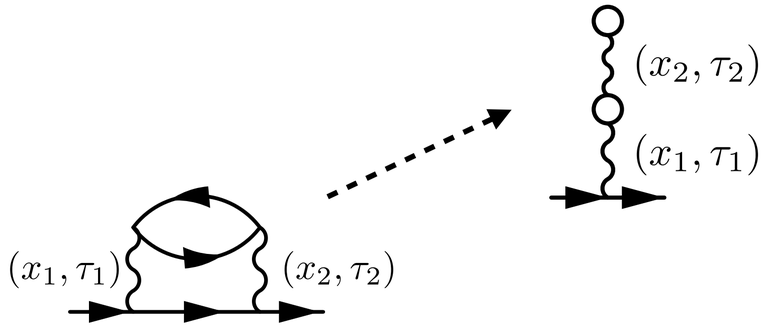
Sampling connected diagrams



- How do we sample only connected diagrams?
- A possibility is to do create a Markov chain of individual topologies
  - This is the original DiagMC approach
  - Drawback: two diagrams on the same vertices may have different signs
  - This leads to a sign problem and only about 6-7 orders can be computed

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

- We can explicitly sum all connected diagrams for a given set of vertices
  - Drawback: this comes with a huge computational cost as it requires a factorial number of operations
- It would be nice to use determinants as in the CT-INT
- This is the idea of the CDet algorithm: it computes the sum of all connected diagrams with an exponential effort

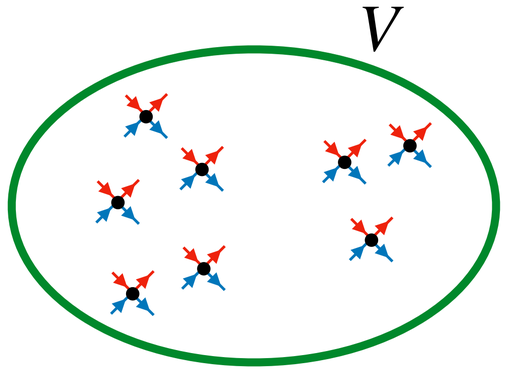
R. Rossi, PRL (2017)
A. Moutenet et al., PRB (2018); Šimkovic and Kozik, PRB (2019)

Other approaches:

R. Profumo et al, PRB (2015)
K. Chen and K. Haule, Nat. Comm. (2019)
A. Taheridehkordi et al., PRB (2019, 2020)
J. Vucicevic et al., PRB (2020), PRR (2021)
M. Maček et al., PRL (2020)

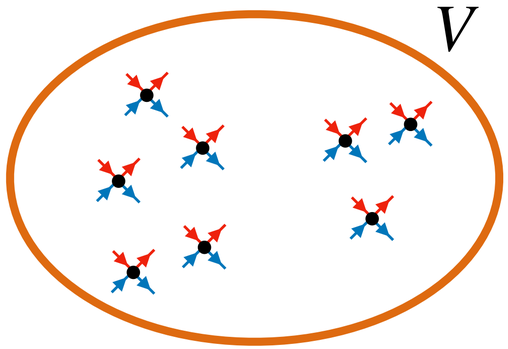
Connected determinant algorithm (CDet)

- Let us consider a set $V = \{(x_1, \tau_1), \ldots, (x_n, \tau_n)\}$ with n interaction vertices
- We want to compute the sum $\mathbf{C}(V)$ of all connected diagrams living on these vertices

$\mathbf{C}(V) =$ 

Sum of all connected diagrams

- We start from the product of determinants $\det D_n^{\uparrow} \det D_n^{\downarrow}$
- The elements of D_n^{σ} are Green functions connecting the vertices in V
- The product of the determinants yields the sum of all connected and disconnected diagrams living on V. We will denote it as $\mathbf{D}(V)$.

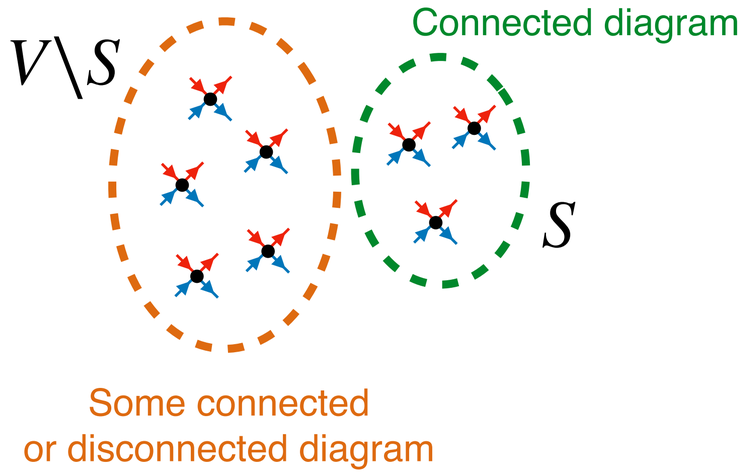
$\mathbf{D}(V) = \det D_n^{\uparrow} \det D_n^{\downarrow} =$ 

Sum of all diagrams, including disconnected

- We now need to remove the disconnected diagrams

Connected determinant algorithm (CDet)

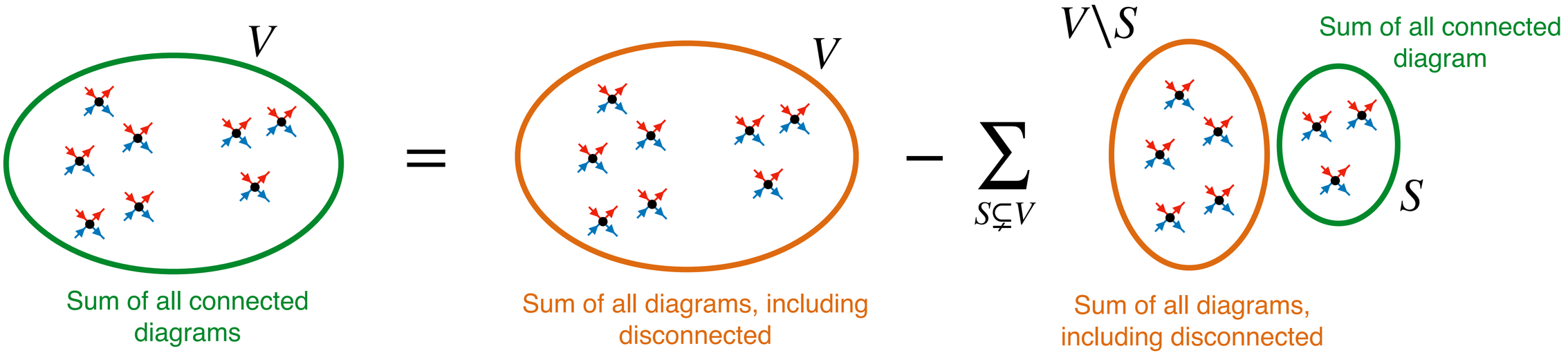
- The trick is to note that any disconnected diagram is composed of:
  - A connected part involving some subset $S \subsetneq V$
  - Another part with connected and/or disconnected diagrams involving the remaining $V \backslash S$



- To generate all disconnected diagrams, it is enough to consider all subsets $S \subsetneq V$ and take the product of
  - The sum $\mathbf{C}(S)$ of all connected diagrams living on the vertices in S
  - The sum $\mathbf{D}(V \backslash S)$ of all connected and disconnected diagrams living on the vertices in $V \backslash S$

Connected determinant algorithm (CDet)

- We eventually obtain the formula



$$\mathbf{C}(V) = \mathbf{D}(V) - \sum_{S \subsetneq V} \mathbf{D}(V \backslash S)\, \mathbf{C}(S)$$

R. Rossi, PRL (2016)

- One starts by computing $\mathbf{D}(S)$ for all subsets S. This can be done in $\mathcal{O}(2^n)$ operations.
- Then the recursion is computed and all $\mathbf{C}(S)$ are obtained. This is done in $\mathcal{O}(3^n)$ operations.
- Similar formulas allow one to filter out self-energy diagrams

A. Moutenet et al., PRB (2018); Šimkovic and Kozik, PRB (2019)

CDet Monte Carlo

- The Monte Carlo algorithm samples the coefficients a_n of the series for A

$$\mathsf{A} = \sum_n a_n U^n \quad \rightarrow \quad a_n = \sum_{V \in \Omega_n} \mathbf{C}(V) = \sum_{V \in \Omega_n} |\mathbf{C}(V)| \operatorname{sign}(\mathbf{C}(V)) \simeq \sum_{V \in \mathrm{Markov}} \operatorname{sign}(\mathbf{C}(V))$$

  where Ω_n contains all the sets of n vertices

- The sampling is implemented with a Metropolis-Hastings algorithm
  - The weight of a configuration V of vertices is $|\mathbf{C}(V)|$
  - New configurations are proposed and then accepted or rejected as usual
  - The coefficient a_n are estimated from the average sign
  - Unlike most quantum Monte Carlo algorithms, a single step is quite expensive
  - We do not have a ratio → we need to normalize the Markov chain. This is typically achieved by also sampling another quantity (like a_0) that we know analytically.
- There are different variants, e.g. some allow one to compute all a_n's in the same run

F. Šimkovic, R. Rossi, arXiv (2021)

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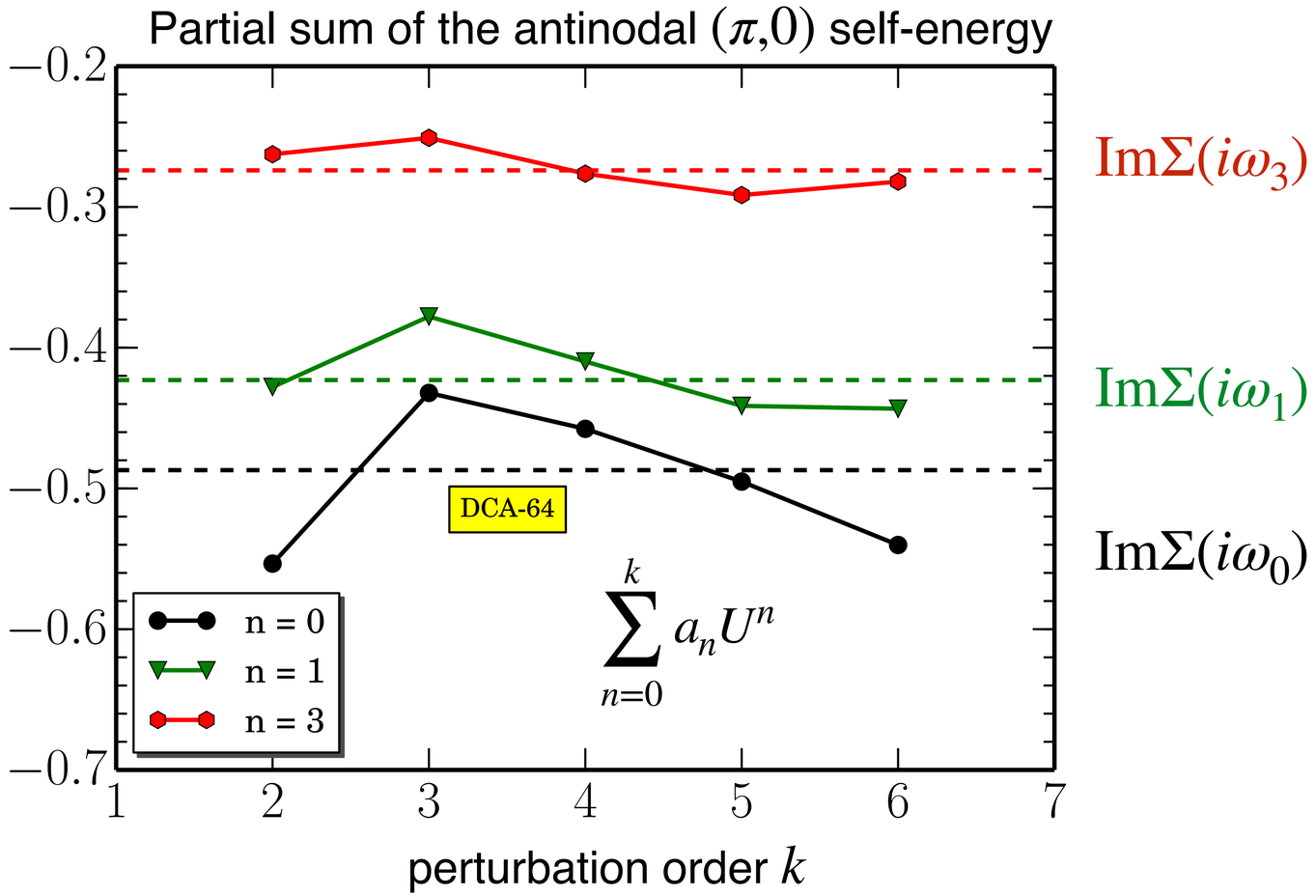
Resummation of the series

- We have a way to compute the coefficients. In practice, one can compute $\sim$ 10-13 coefficients
- Typical example for Hubbard model with $U = 4t \quad t' = 0.3 \quad \mu = 0 \quad T = 0.5$

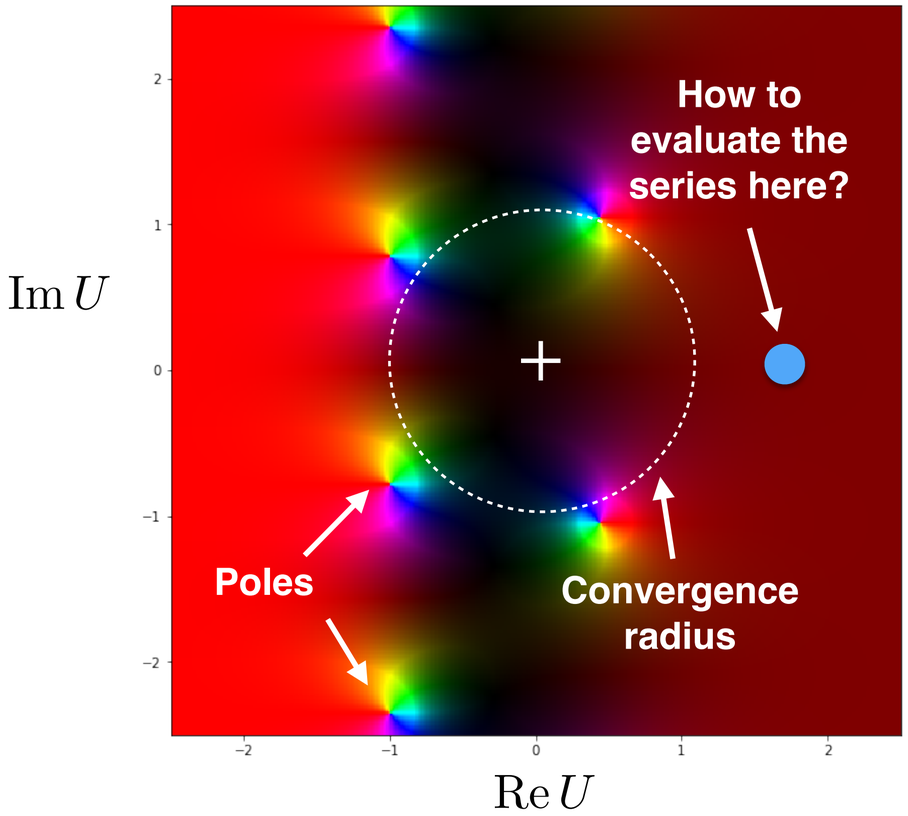


Resummation of the series

- The partial series do not always nicely converge!
- Unlike CT-INT, the function $\mathrm{A}(U)$ may have poles in the complex-U plane
- One needs to be able to evaluate the function beyond its radius of convergence
- How does one resum the series?
- Option 1: Conformal maps, Padé approximants, integral approximants, …
- Option 2: Generate new series with the freedom to choose the starting point of the series expansion

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

$n(U)$ in the Hubbard atom

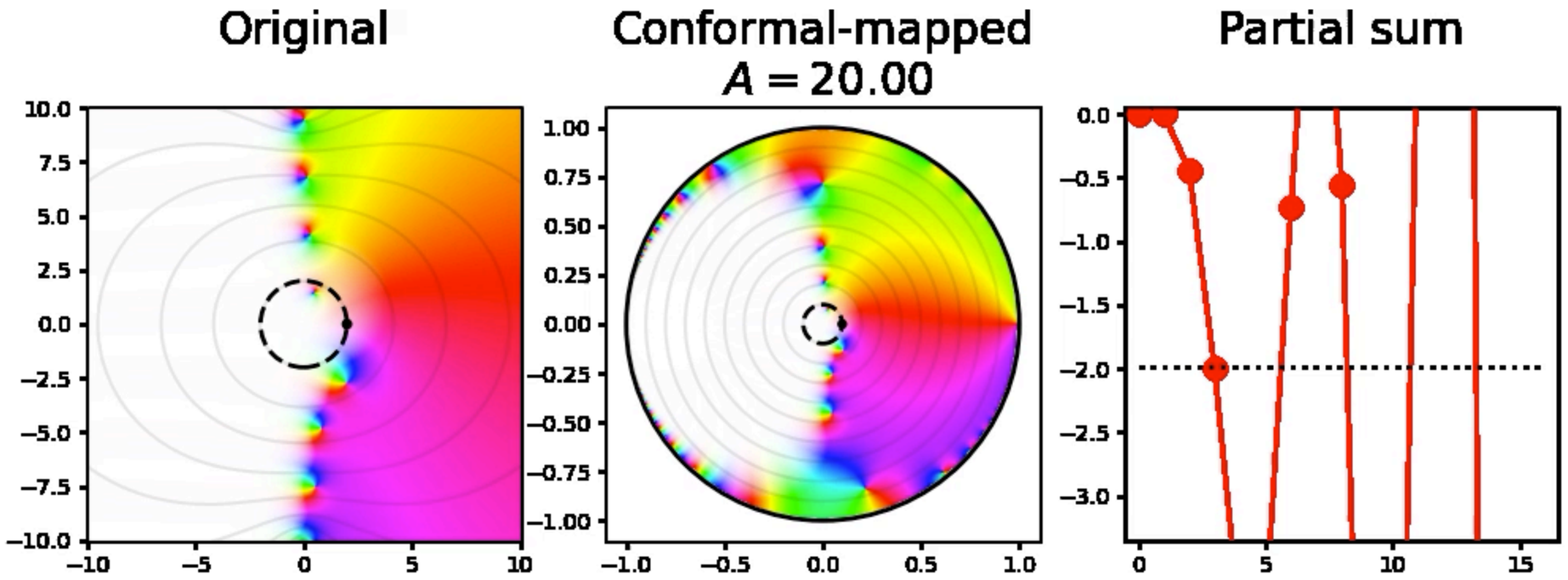


Example: standard resummation tools

- Conformal maps: new series is obtained from a change of variable

$$\sum_n a_n \left(U(\omega)^n\right) = \sum_n b_n \omega^n$$

$$U(\omega) = \frac{A\omega}{(1-\omega)(1+\omega)}$$



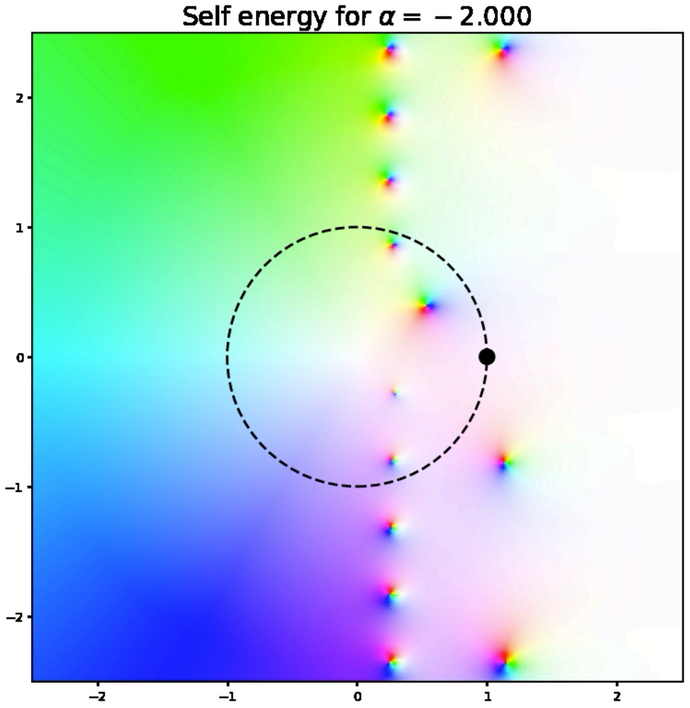
Freedom in the starting point of the perturbation series

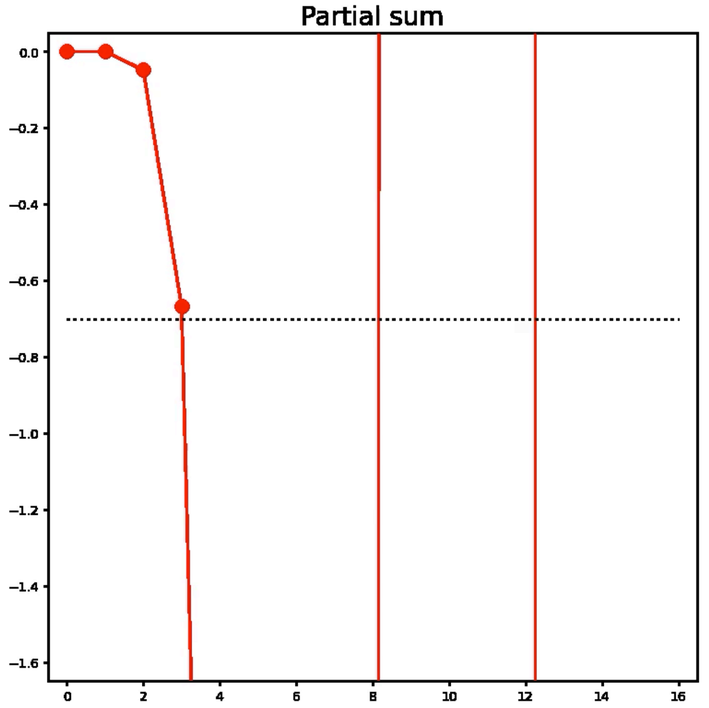
- Optimize series convergence with modified bare propagator

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

- The series must be changed to compensate for the α shift. This turns out to be easy.

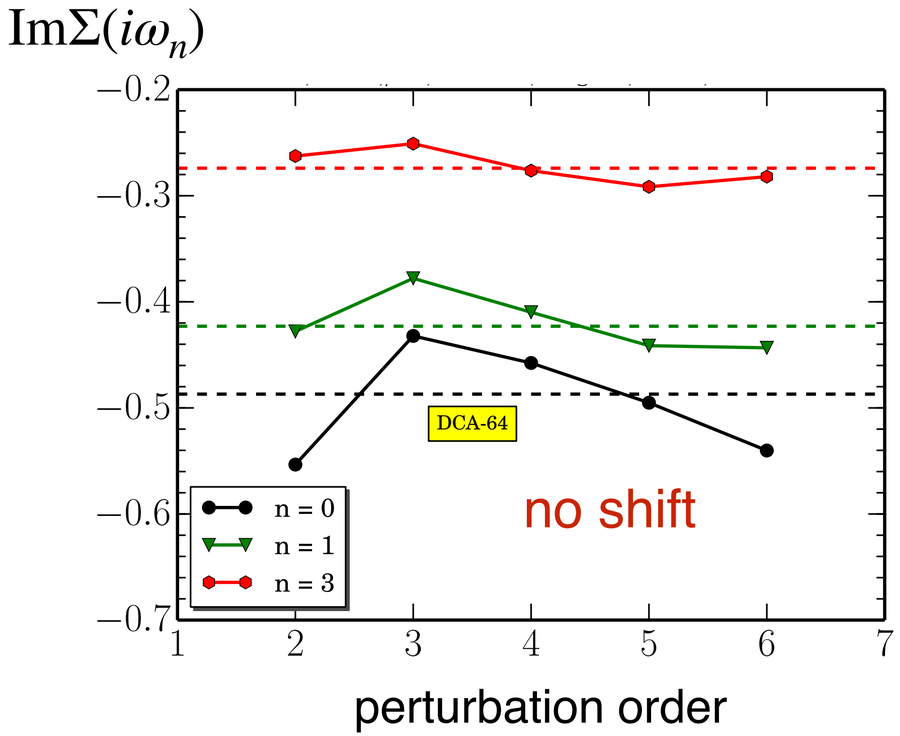
$\mathrm{Im}\Sigma(i\omega_0)$
Hubbard atom

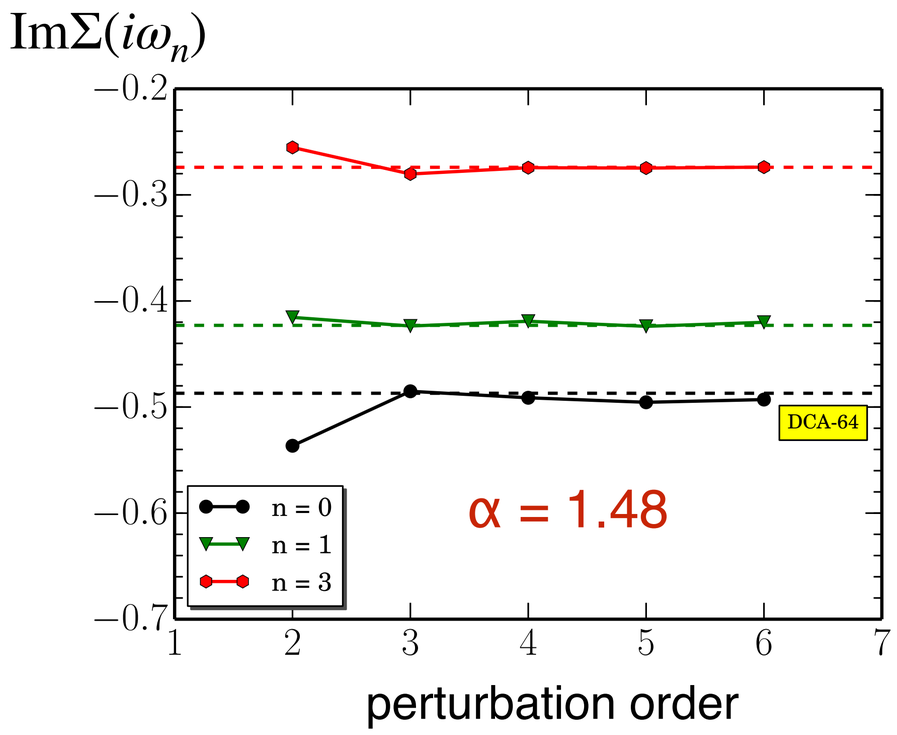




Freedom in the starting point of the perturbation series

- For the previous example on the Hubbard model





- A good choice for α helps a lot. Often mean-field is a good starting point
- There are many other choices that have been explored

Profumo et al., PRB (2015)
W.Wu et al., PRB (2017)

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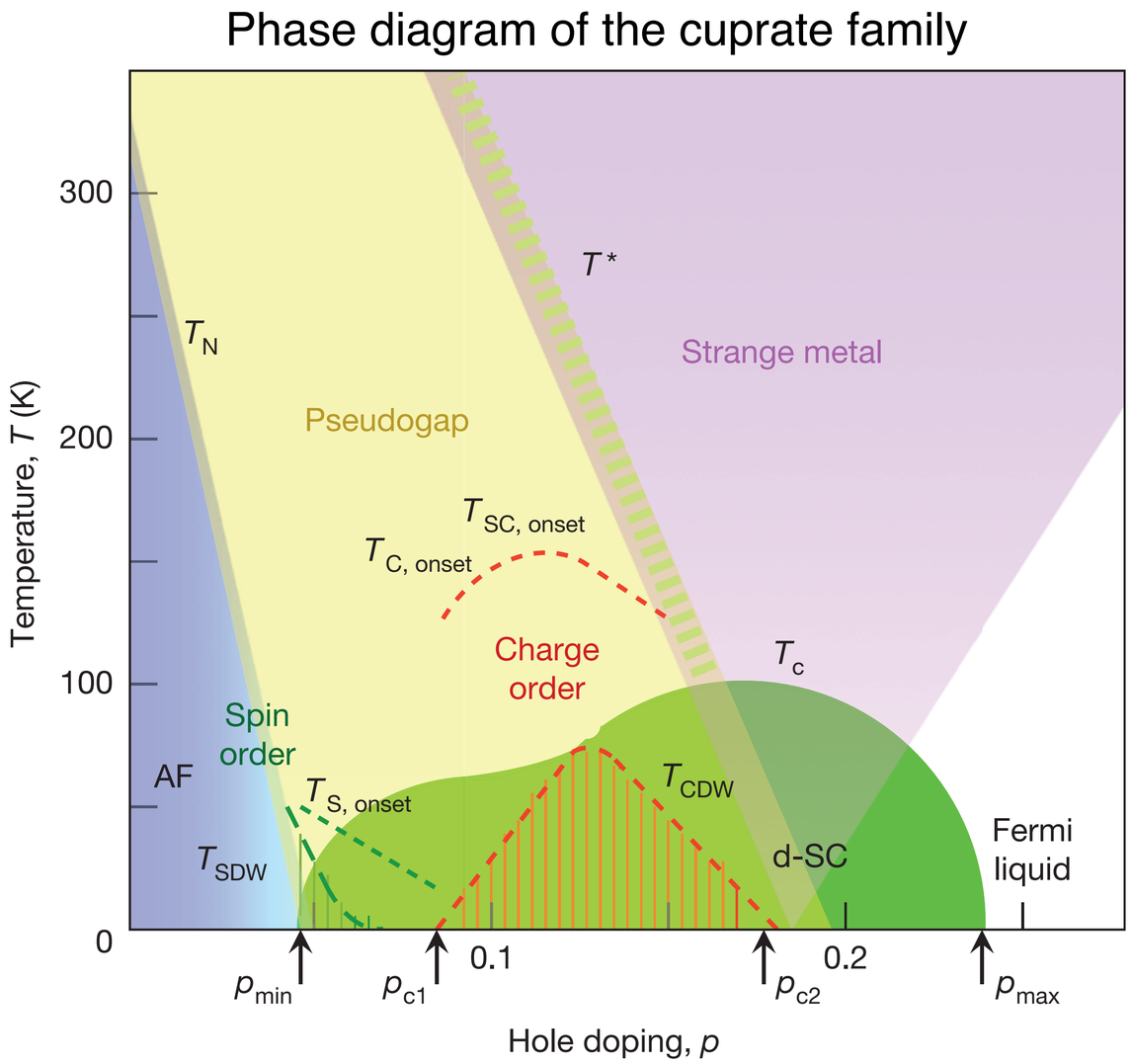
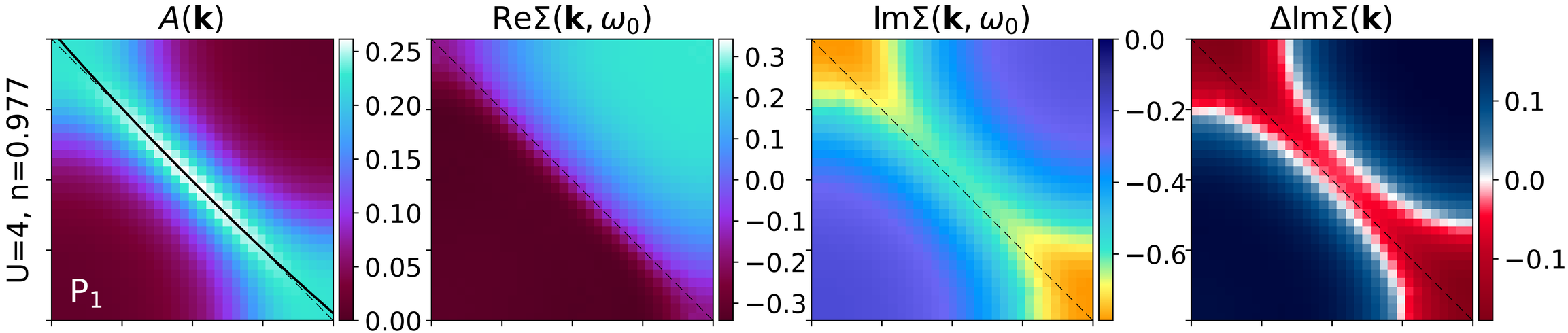
Pseudogap physics and the doped Hubbard model

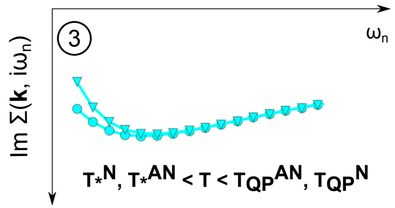


- Very rich phase diagram
- Can the single band Hubbard model reproduce some of the features in the phase diagram?
- In particular, pseudogap region very intriguing, seen in several families of strongly correlated materials
- What is its relation with superconductivity?
- Is there something like a zero temperature pseudogap state?

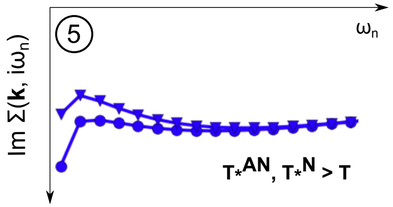
Spectral properties from CDet in the doped Hubbard model

$$T = 0.2, U = 4, n = 0.977, t' = 0$$





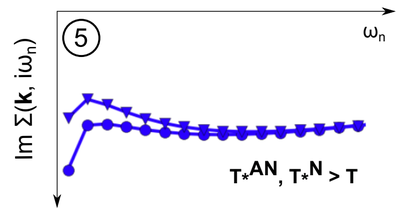
$\Delta \mathrm{Im}\Sigma > 0$

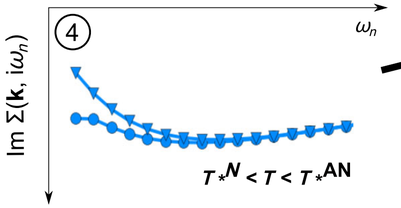


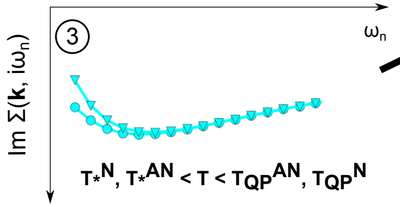
$\Delta \mathrm{Im}\Sigma < 0$

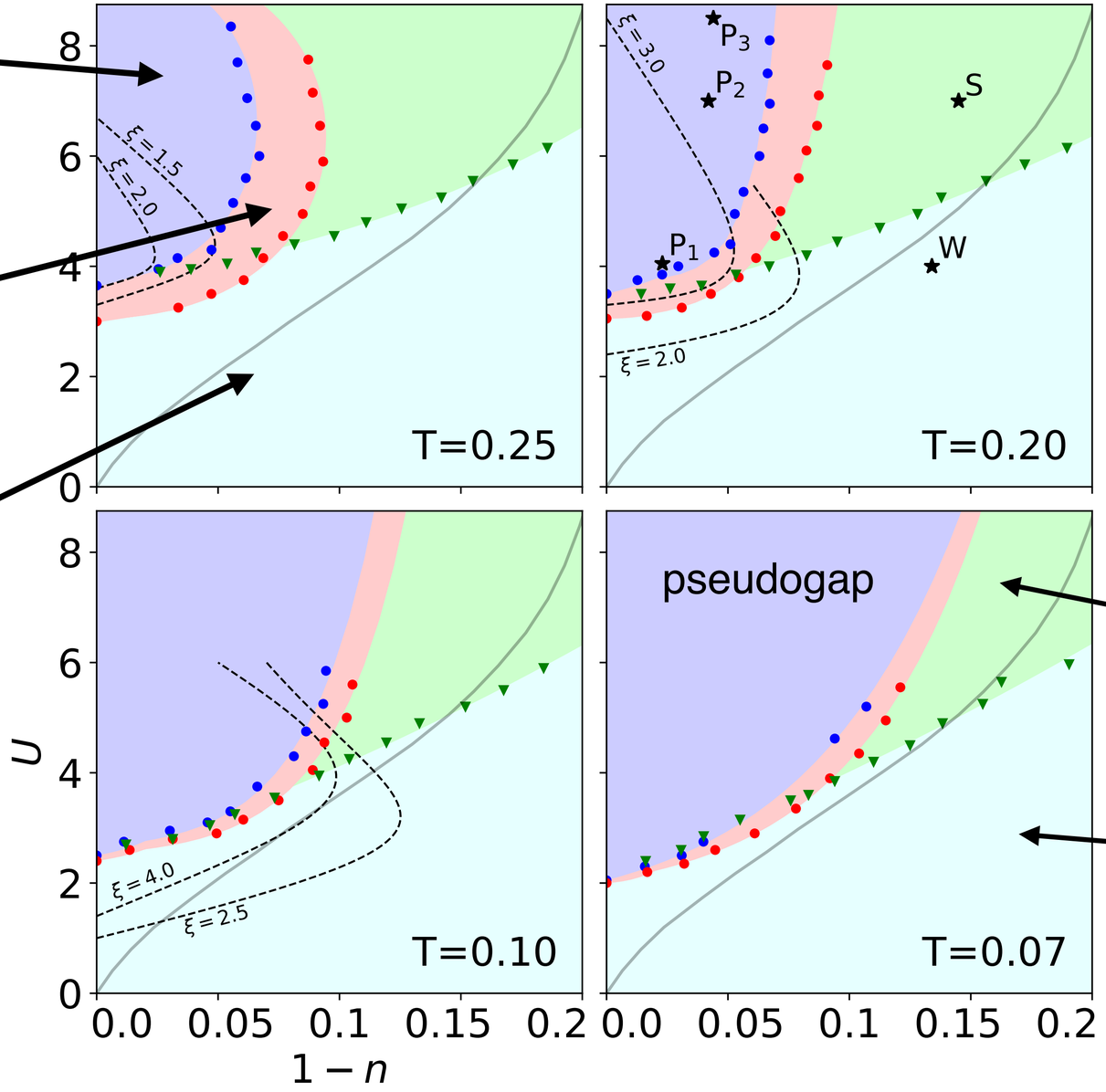
slope of the self-energy at low imaginary frequencies

Pseudogap region, weak and strong coupling





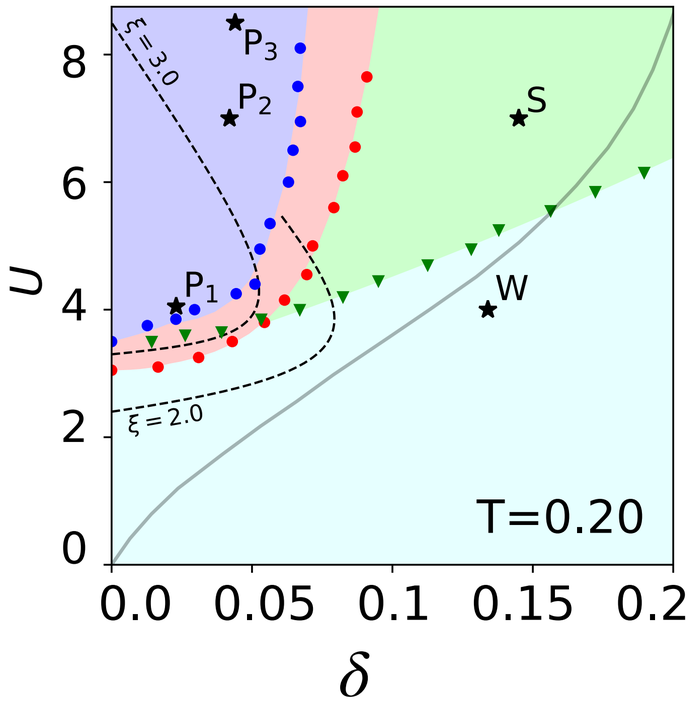


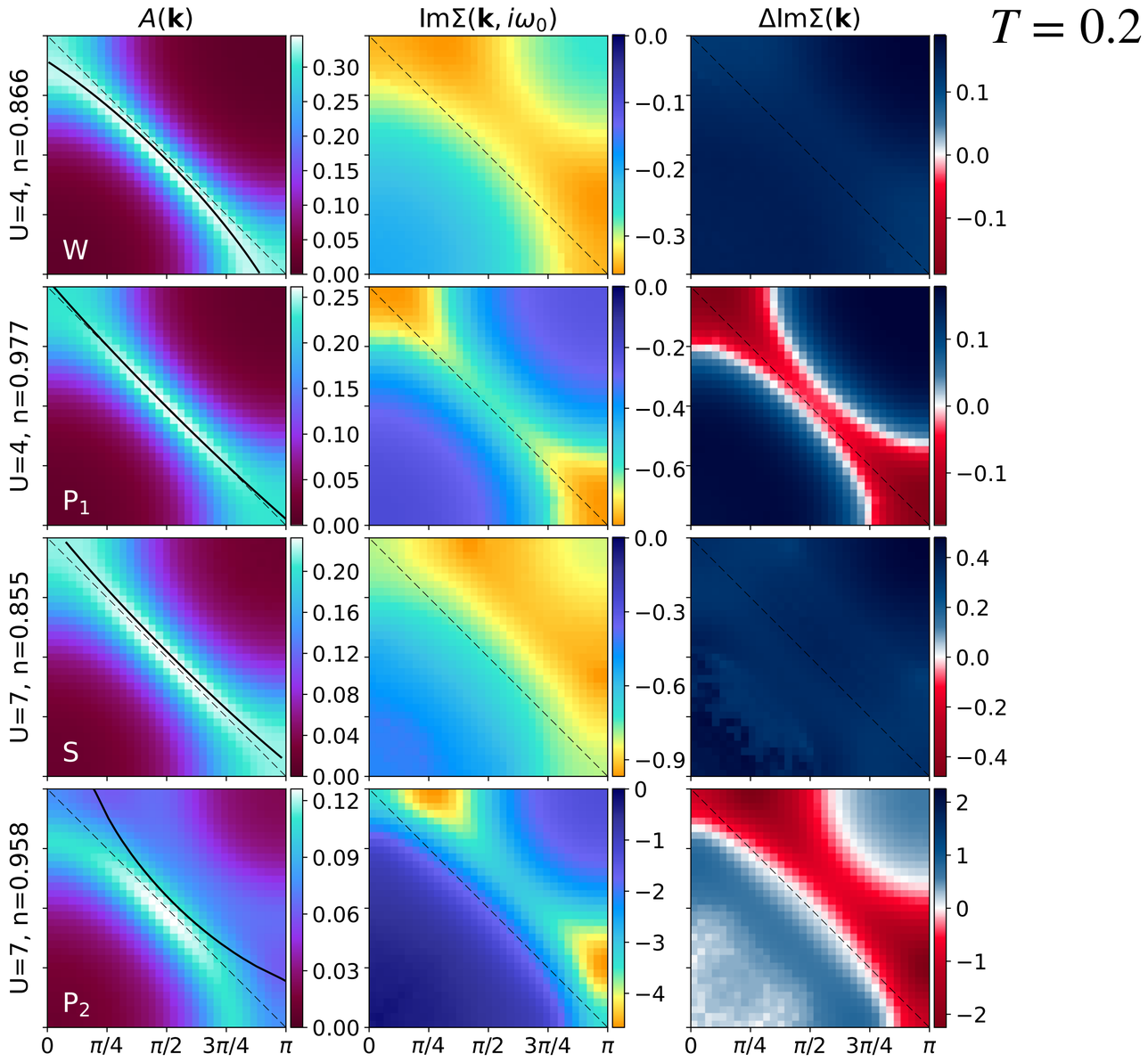


hole-like FS

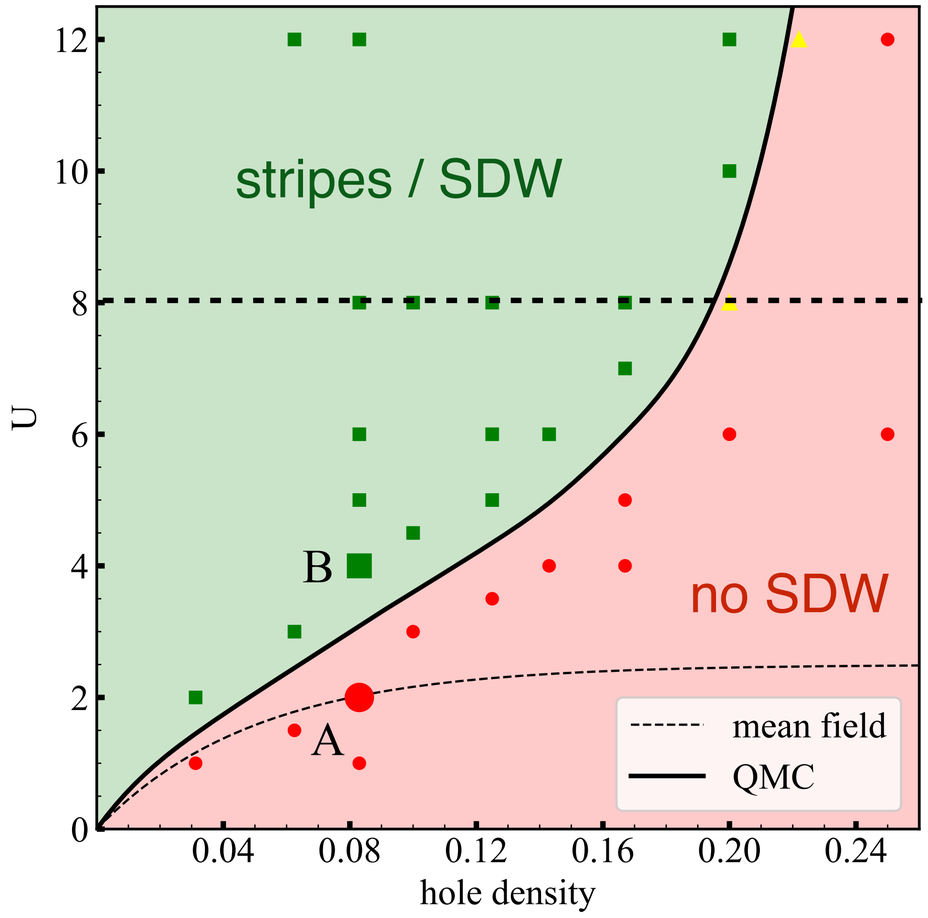
electron-like FS

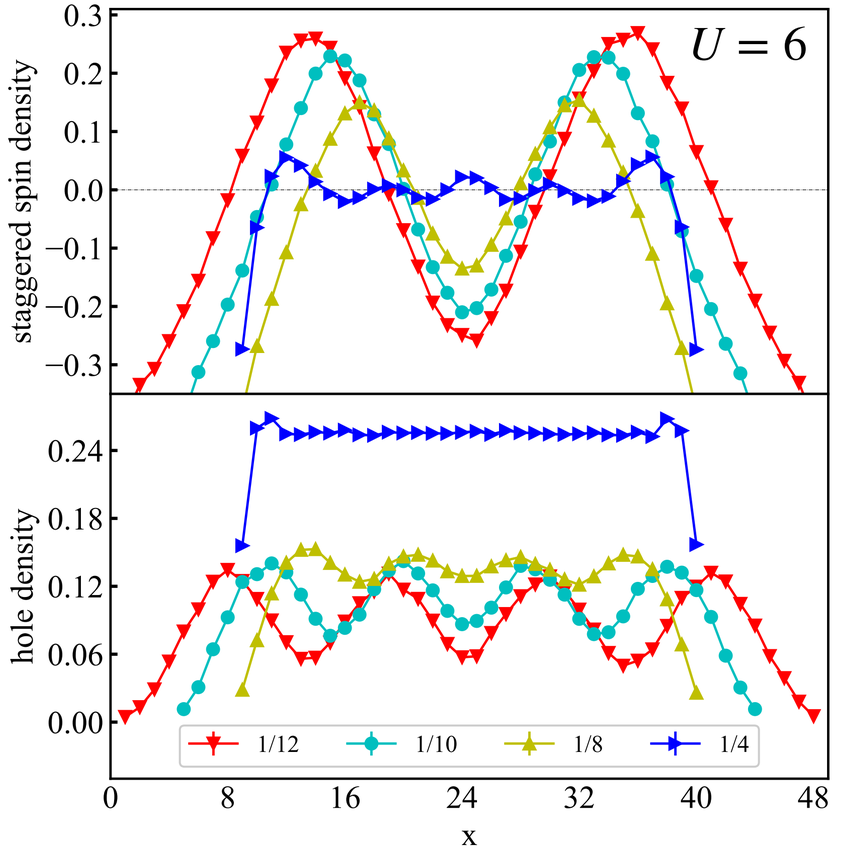
Characterization of the different regimes

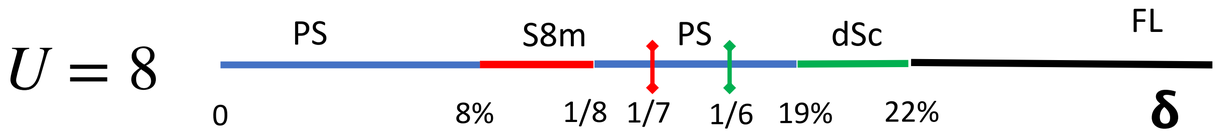




Pseudogap and connection with stripe-ordered ground state

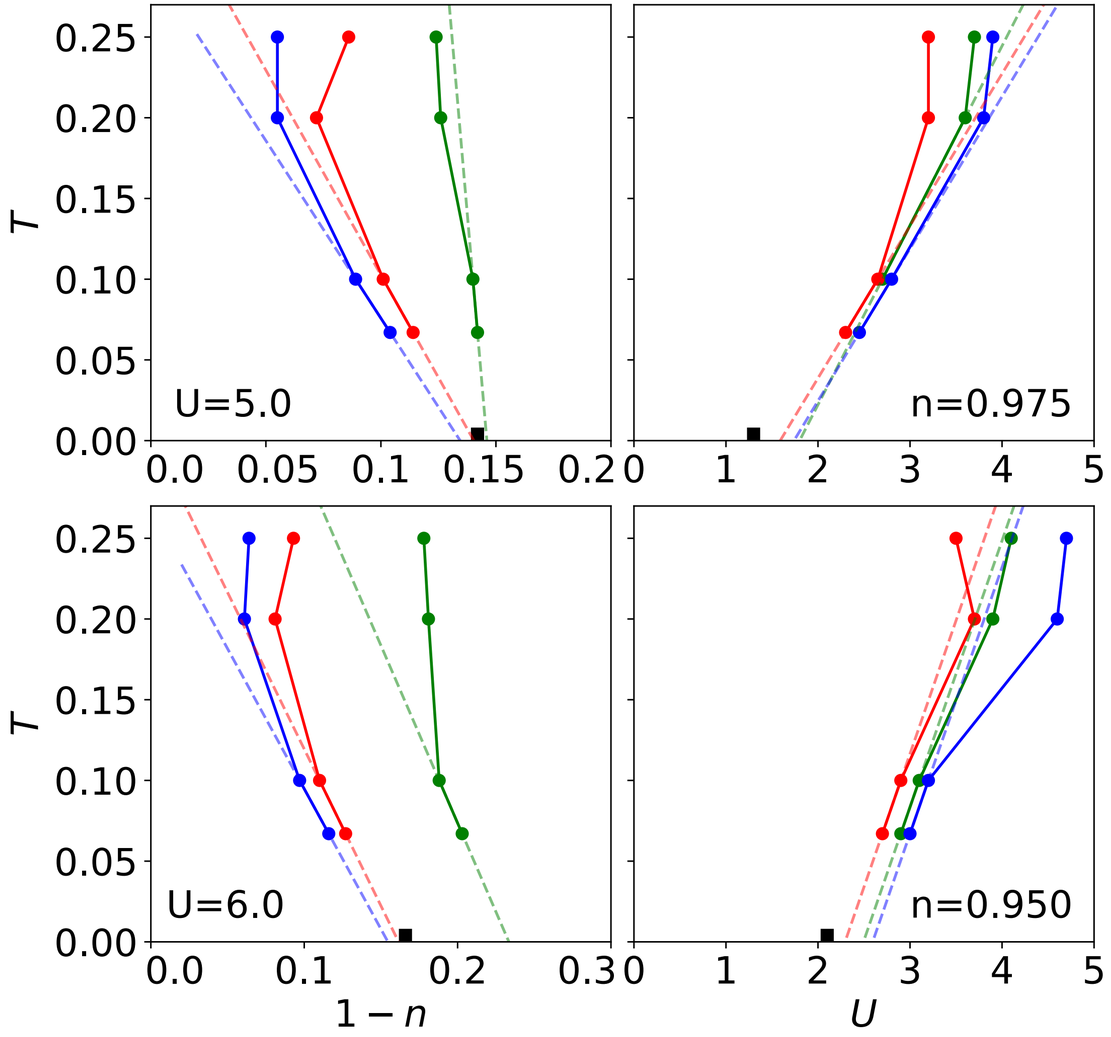






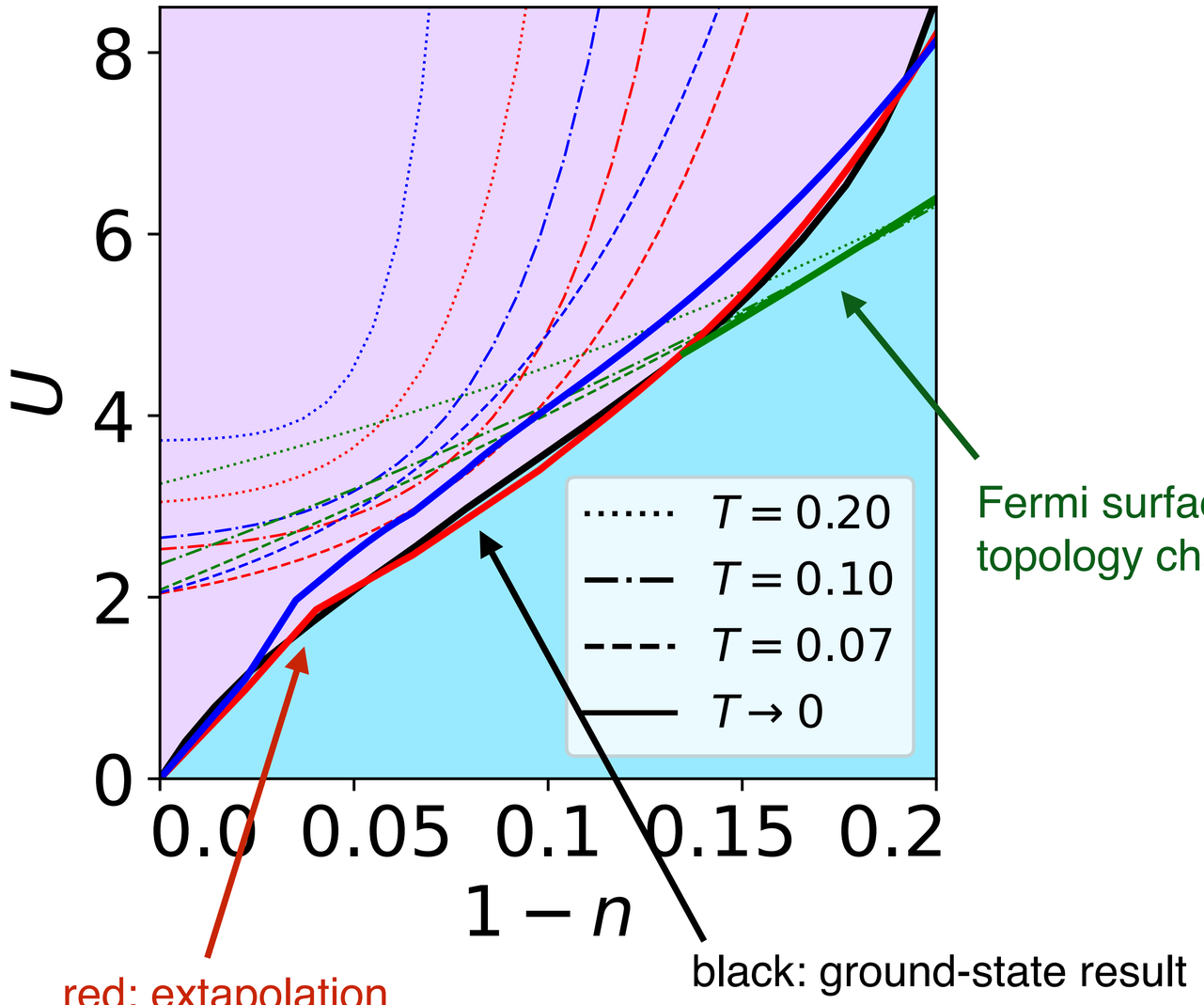
M. Qin et al, PRX (2020)
S. Sorella, arXiv (2021)
Hao Xu et al., arXiv (2021)

Handshake with ground-state approaches



Extrapolation of the pseudogap region to zero temperature

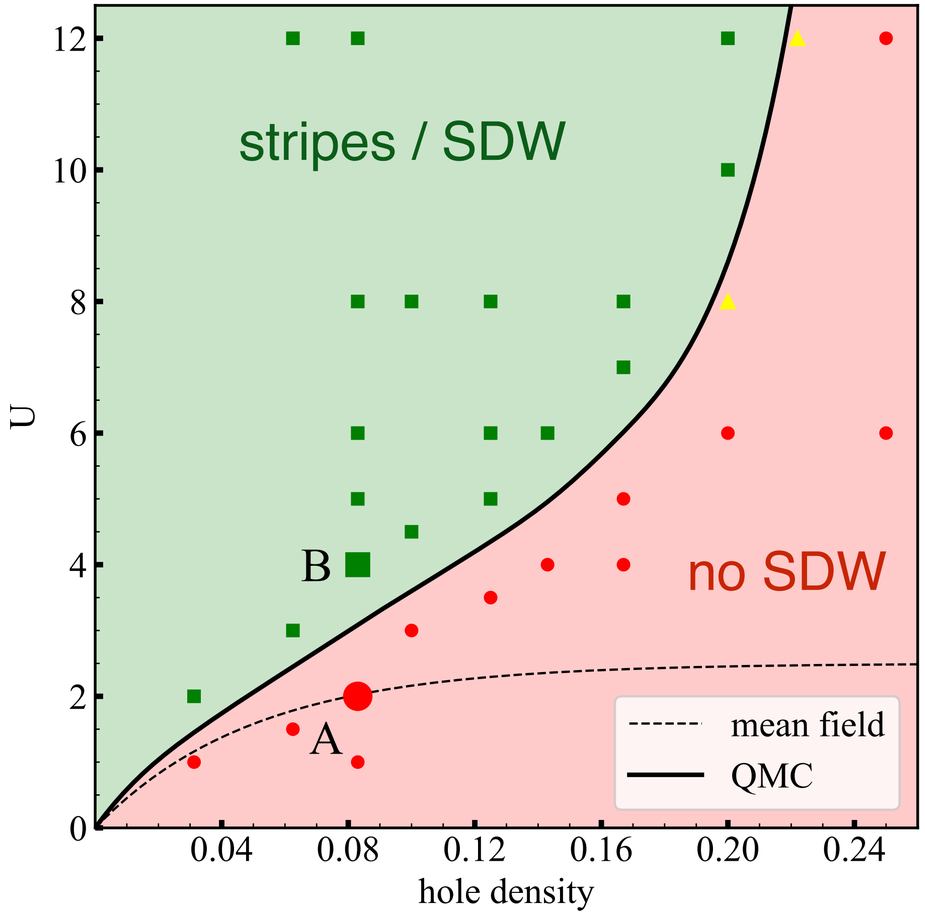
Handshake with ground-state approaches



Fermi surface topology change

red: extapolation

black: ground-state result



The fate of the pseudogap at zero temperature seems to be a stripe-ordered state when there is no next-nearest neighbor hopping $t' = 0$

Summary

- Diagrammatic Monte Carlo algorithms directly sample the connected diagrams describing an observable
- They can be used directly in the thermodynamic limit (infinite lattice)
- The CDet algorithm computes the sum of all connected diagrams at a cost $\mathcal{O}(n^3)$ at order n
- In practice about 10-13 orders can be computed
- Resumming the series can be challenging because of the presence of poles in the complex-U plane
- Results have been obtained in the intermediate to strong coupling regime of the Hubbard model
  - Pseudogap physics
  - Spin and charge susceptibilities
  - Magnetic phase transitions, etc.
- But more work is needed to be able to compute more coefficients and especially to find robust ways to do the resummation of the series