

Numerical methods for strongly correlated systems

Thereza Paiva



SCHOOL ON RECENT ADVANCES IN STRONGLY CORRELATED QUANTUM MATERIALS

October 5-9, 2026 ICTP-SAIFR

Summary

- 1 – Classical Monte Carlo**
- 2 – Quantum Monte Carlo**
- 3 – Measurements in QMC – I**
- 4 – Measurements in QMC – II**
- 5 – The Sign problem**

Summary

- 1 – Classical Monte Carlo
- 2 – Quantum Monte Carlo
- 3 – Measurements in QMC – I
- 4 – Measurements in QMC – II
- 5 – The Sign problem

The Sign problem

Other unbiased numerical methods

Overview

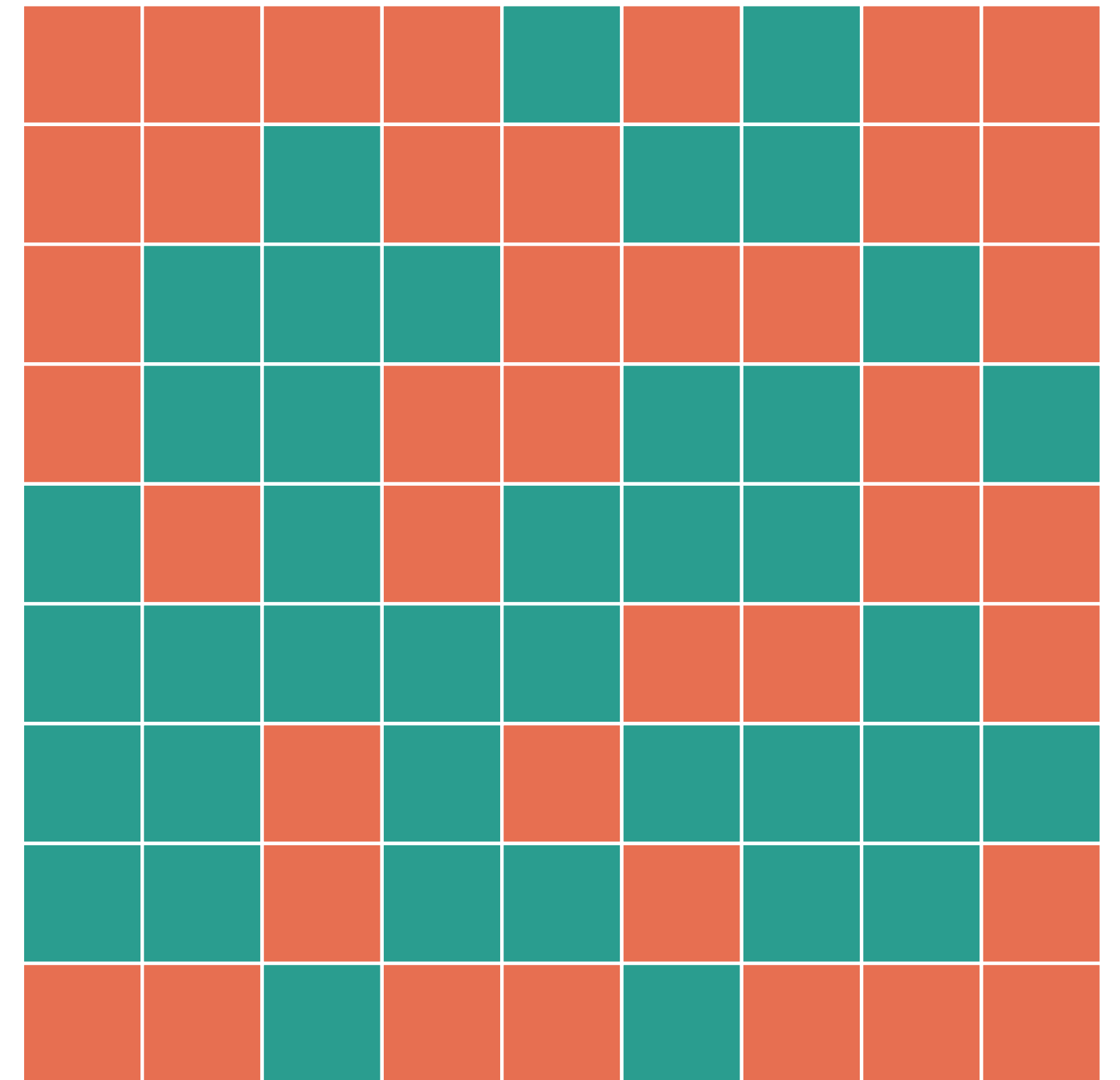
The Sign problem

What is the sign problem?

Can we fix it?

Is it always a bad thing?

The sign problem



Hubbard–Stratonovich field $s(i, \tau) = \pm 1$

Known since the beginning of QMC

PHYSICAL REVIEW B

VOLUME 41, NUMBER 13

1 MAY 1990

Sign problem in the numerical simulation of many-electron systems

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(Received 7 August 1989)

We discuss the problems that arise in the numerical simulation of many-electron systems when the measure of the functional integrals is not positive definite. We present theoretical arguments and numerical data which indicate that the expectation value of the sign of the measure decreases exponentially as the inverse temperature β increases, unless the measure is forced to be positive by an explicit symmetry. We therefore conclude that a recent proposal for dealing with the sign problem due to Sorella *et al.* leads to an uncontrolled approximation. In the cases we have studied it is a good approximation for the ground-state energy, and we present a method for calculating the correction needed to make it exact. However, for some physical quantities, such as the *d*-wave pair field susceptibility, the neglect of signs can yield misleading results.

Not only in Condensed Matter

Quantum chemistry

Diffusion MC

J. Chem. Phys. **131**, 054106 (2009)

High-energy physics and
nuclear physics

Green's function MC
Variational Quantum MC
Lattice QCD Methods

Rev. Mod. Phys. **87**, 1067 (2015)
Lattice methods for QCD, WS (2006)

Condensed Matter

World-line QMC
Stochastic Series Expansion
Auxiliary field QMC

Hirsch et al. Phys. Rev. B **26** 5033 (1982)
Sandvik, Kurkijarvi, Phys. Rev. B **43**, 5950 (1991)
BSS, Phys. Rev. D **24**, 2278 (1981)

NP-hard problem

Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations

[Matthias Troyer](#)¹ and [Uwe-Jens Wiese](#)²

Show more ▾

Phys. Rev. Lett. **94**, 170201 – Published 4 May, 2005

Quantum Monte Carlo simulations, while being efficient for bosons, suffer from the “negative sign problem” when applied to fermions—causing an exponential increase of the computing time with the number of particles. A polynomial time solution to the sign problem is highly desired since it would provide an unbiased and numerically exact method to simulate correlated quantum systems. Here we show that such a solution is almost certainly unattainable by proving that the sign problem is nondeterministic polynomial (NP) hard, implying that a generic solution of the sign problem would also solve all problems in the complexity class NP in polynomial time.

Back to the end of class 2

$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \text{Tr}_{\{s\}} \det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\})$$

Determinantal Quantum Monte Carlo

or

Auxiliary field Quantum Monte Carlo

Introducing the B matrices

$$\mathbf{B}_\ell^\sigma \equiv e^{-\Delta\tau\mathbf{K}} e^{-\Delta\tau V^\sigma(\ell)}$$

$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \text{Tr}_{\{s\}} \prod_{\sigma} \det [\mathbf{1} + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \dots \mathbf{B}_1^\sigma]$$

Introducing the O matrices

$$\mathbf{O}^\sigma(\{s\}) \equiv \mathbf{1} + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \dots \mathbf{B}_1^\sigma$$

Defining the A matrices

$$g^{\sigma}(\ell) \equiv [1 + A^{\sigma}(\ell)]^{-1}$$

$$A^{\sigma}(\ell) \equiv B_{\ell-1}^{\sigma} B_{\ell-2}^{\sigma} \dots B_1^{\sigma} B_M^{\sigma} \dots B_{\ell}^{\sigma}$$

Then

$$R_{\sigma} \equiv \frac{\det O^{\sigma}(\{s\}')} {\det O^{\sigma}(\{s\})} \quad \rightarrow \quad R_{\sigma} = \frac{\det [1 + A^{\sigma}(\ell) \Delta_{\ell}^{\sigma}(\mathbf{i})]} {\det [1 + A^{\sigma}(\ell)]}$$

What is the sign problem?

Negative matrix elements

Fermionic nature

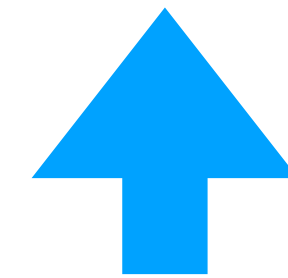
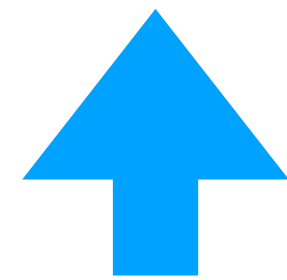
The product of fermionic determinants
is not positive definite

A counter example: repulsive Hubbard model at half-filling

Particle-hole transformation

$$c_{\mathbf{i}\sigma}^\dagger \rightarrow d_{\mathbf{i}\sigma} = (-1)^{\mathbf{i}} c_{\mathbf{i}\sigma}^\dagger, \quad c_{\mathbf{i}\sigma} \rightarrow d_{\mathbf{i}\sigma}^\dagger = (-1)^{\mathbf{i}} c_{\mathbf{i}\sigma}$$

$$n_{\mathbf{i}\sigma} \equiv c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i}\sigma} = 1 - d_{\mathbf{i}\sigma}^\dagger d_{\mathbf{i}\sigma} \equiv 1 - \tilde{n}_{\mathbf{i}\sigma}$$



Particle-hole symmetry

Determinant at symmetry point

$$n = 1$$

$$\mu = U/2$$

$$\begin{aligned}\det O^\uparrow &= \mathcal{T}_{\{n\}} r \prod_{\ell} e^{-\Delta\tau K_{\uparrow}} e^{\lambda \sum_i s_i(\ell) n_{\mathbf{i}\uparrow}} = \\ &= \mathcal{T}_{\{\tilde{n}\}} r \prod_{\ell} e^{-\Delta\tau \tilde{K}_{\uparrow}} e^{-\lambda \sum_i s_i(\ell) \tilde{n}_{\mathbf{i}\uparrow}} e^{-\lambda \sum_i s_i(\ell)} = \\ &= e^{-\lambda \sum_{i\ell} s_i(\ell)} \det O^\downarrow,\end{aligned}$$

Therefore

$$\det O^\uparrow \cdot \det O^\downarrow > 0, \text{ for } n = 1, U \geq 0.$$

Another counter example: attractive Hubbard model

Lack of spin dependence in HS transformations

$$O^{\uparrow}(\{s\}) \equiv O^{\downarrow}(\{s\})$$

Sign is positive for all fillings

Another counter example: attractive Hubbard model

Lack of spin dependence in HS transformations

$$O^{\uparrow}(\{s\}) \equiv O^{\downarrow}(\{s\})$$

Sign is positive for all fillings

Not true with spin imbalance

When symmetries protect the sign

MODEL	MECHANISM	RESULT
● Attractive Hubbard, any filling	charge-channel HS field: both spins see the same matrix	$P = (\det O)^2 \geq 0$
● Repulsive Hubbard, half filling, bipartite lattice	particle-hole transformation of one spin species	$\det O_{\downarrow} = (\text{positive}) \times \det O_{\uparrow}$
● Kane-Mele-Hubbard	time-reversal pairs the two spins	$\det O_{\downarrow} = (\det O_{\uparrow})^*$
● More general cases	Kramers positivity, Majorana reflection positivity	positive product of determinants
● Holstein model (electron-phonon)	the phonon field couples equally to both spins	$P = e^{-S_{\text{ph}}} (\det O)^2 \geq 0$

The sign depends on the basis

In the eigenbasis of H every weight $e^{-\Delta\tau E}$ is positive, but that basis is unknown.

Spinless fermions on the honeycomb lattice are sign-free in a Majorana formulation, yet the standard DQMC algorithm has an “unnecessary” sign problem.

What should we
do when the sign
isn't positive?

Partition function written as a sum over configurations

$$c \equiv \{s\}$$

"Boltzmann weight"

$$p(c) \equiv \det O^\uparrow(\{s\}) \det O^\downarrow(\{s\})$$

Keeping track of the sign:

$$p(c) = s(c)|p(c)| \quad \text{where} \quad s(c) = \pm 1$$

Average of a quantity A

$$\begin{aligned}\langle A \rangle_p &= \frac{\sum_c p(c) A(c)}{\sum_c p(c)} = \frac{\sum_c |p(c)| s(c) A(c)}{\sum_c |p(c)| s(c)} = \\&= \frac{[\sum_c |p(c)| s(c) A(c)] / \sum_c |p(c)|}{[\sum_c |p(c)| s(c)] / \sum_c |p(c)|} = \\&= \frac{\sum_c p'(c) [s(c) A(c)]}{\sum_c p'(c) [s(c)]} \equiv \frac{\langle sA \rangle_{p'}}{\langle s \rangle_{p'}},\end{aligned}$$

where $p'(c) \equiv |p(c)|$

Average of a quantity A

$$\begin{aligned}\langle A \rangle_p &= \frac{\sum_c p(c) A(c)}{\sum_c p(c)} = \frac{\sum_c |p(c)| s(c) A(c)}{\sum_c |p(c)| s(c)} = \\ &= \frac{[\sum_c |p(c)| s(c) A(c)] / \sum_c |p(c)|}{[\sum_c |p(c)| s(c)] / \sum_c |p(c)|} = \\ &= \frac{\sum_c p'(c) [s(c) A(c)]}{\sum_c p'(c) [s(c)]} \equiv \frac{\langle sA \rangle_{p'}}{\langle s \rangle_{p'}},\end{aligned}$$

Can be very small

where $p'(c) \equiv |p(c)|$

Sampling with IW moves the sign into the observables

Sample $|W(s)|$ and carry the sign along

$$\langle A \rangle = \langle A S \rangle / \langle S \rangle$$

Both numerator and denominator are averages over the positive weights $|w|$.

Average sign $\langle S \rangle$: the fraction of positive minus the fraction of negative configurations.

When $\langle S \rangle$ is small, two noisy numbers close to zero are divided: the error bars explode.

Contributions to Z

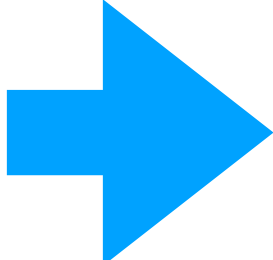


Large terms of both signs almost cancel: Z is a small difference of large numbers.

Average sign of the product of fermionic determinants

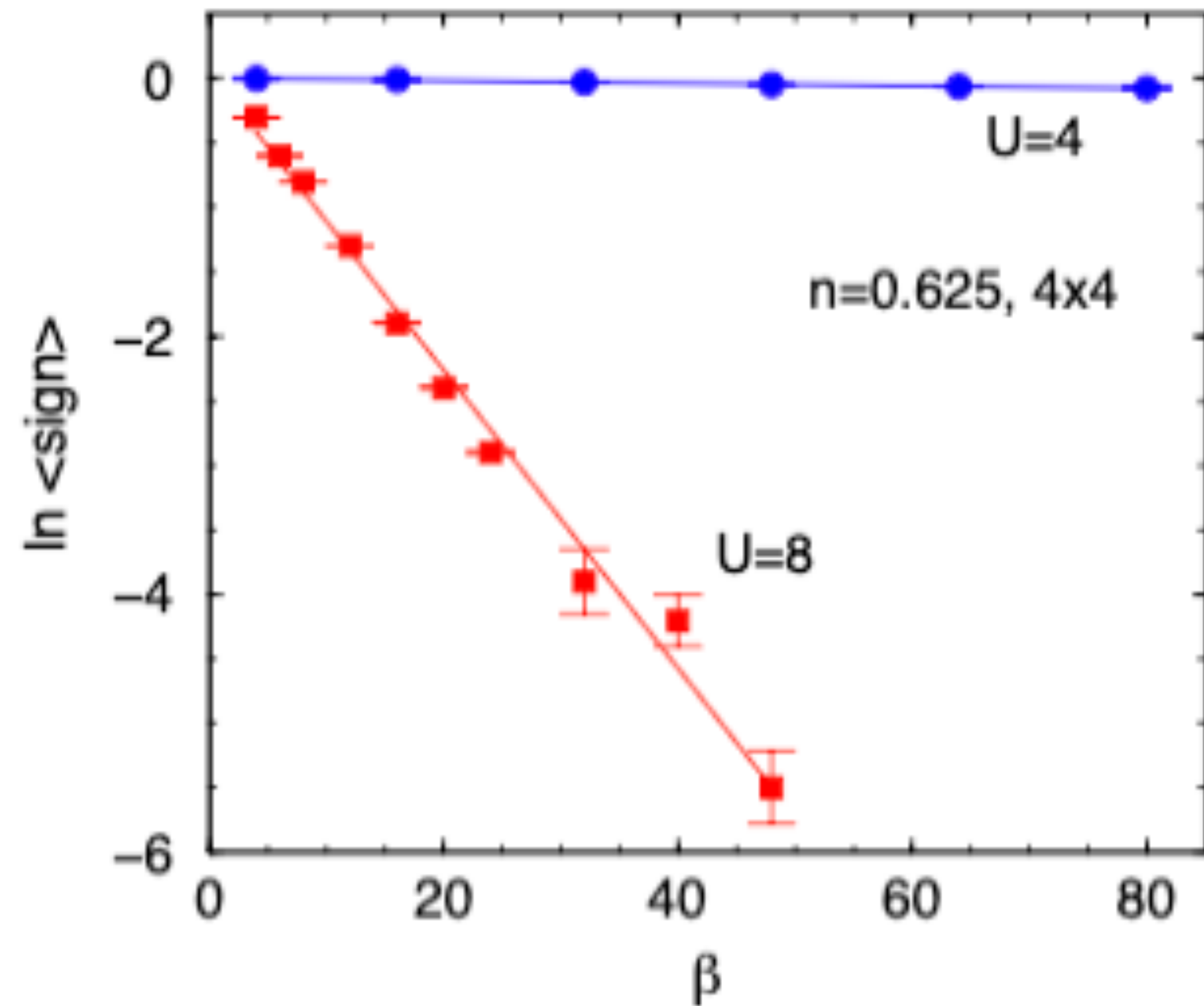
$$\langle sign \rangle \equiv \langle s \rangle_{p'}$$

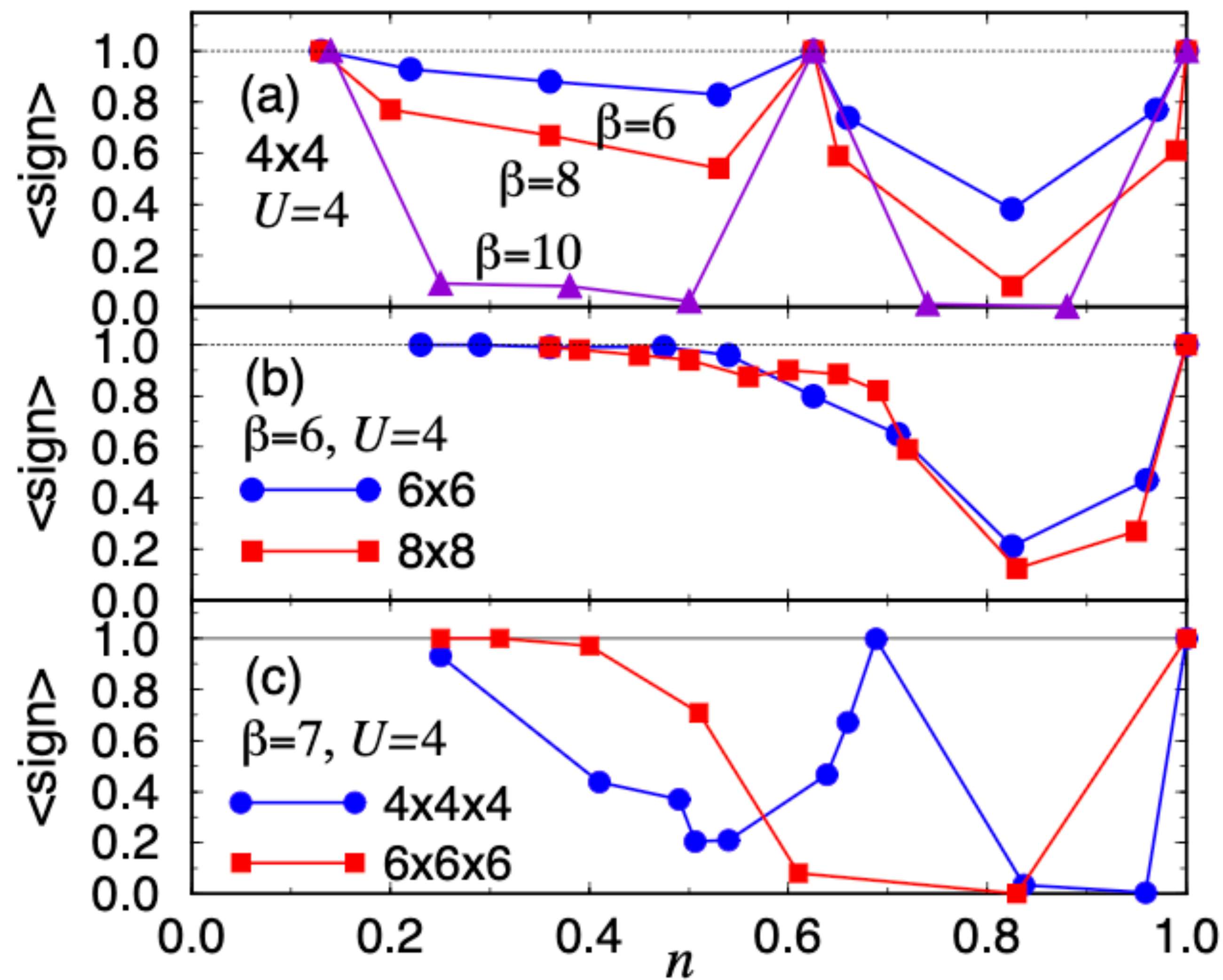
$$\langle sign \rangle \sim e^{-\beta N_s \gamma}$$

γ  Depends on U and n

Log scale

Square lattice

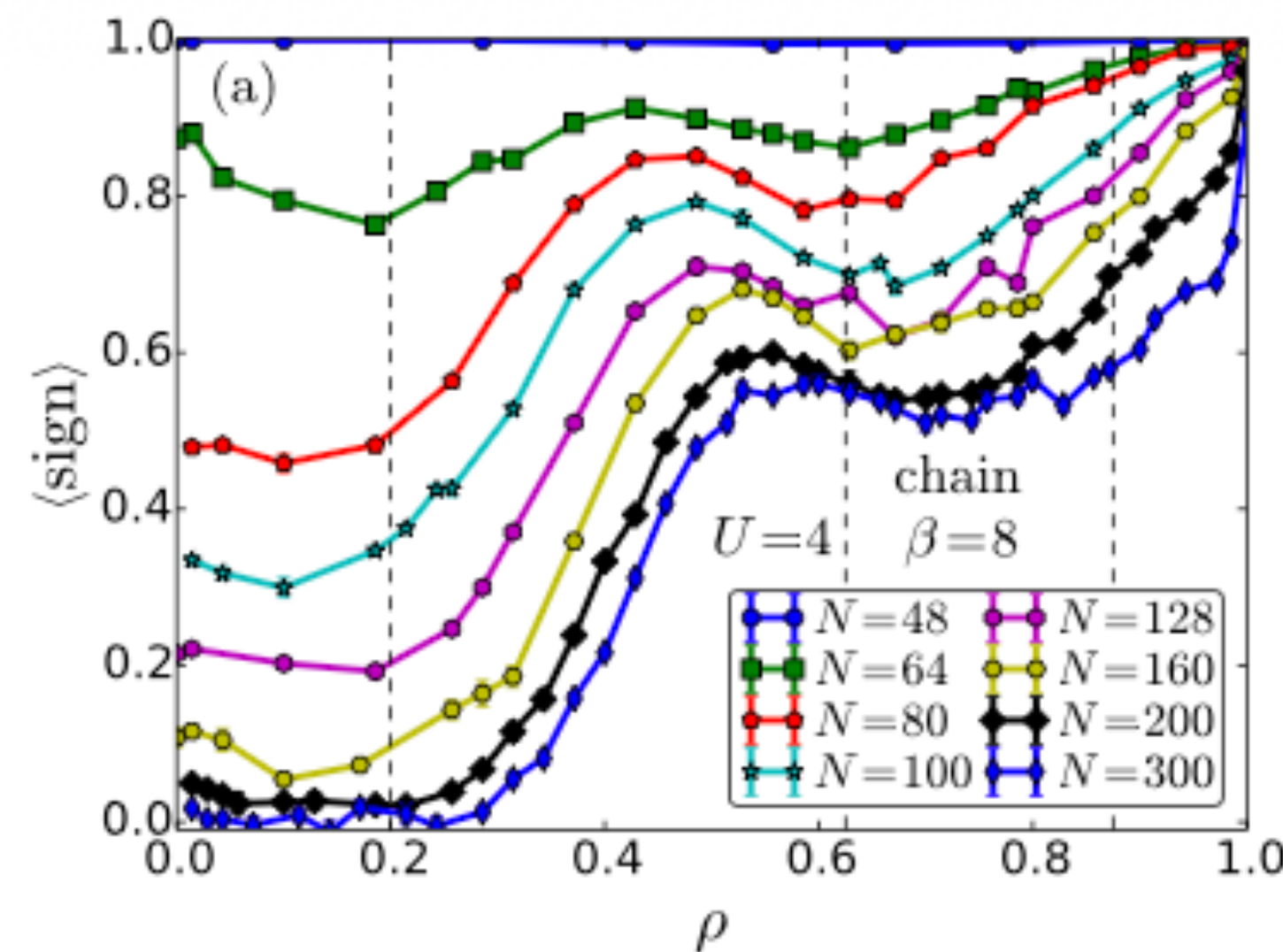




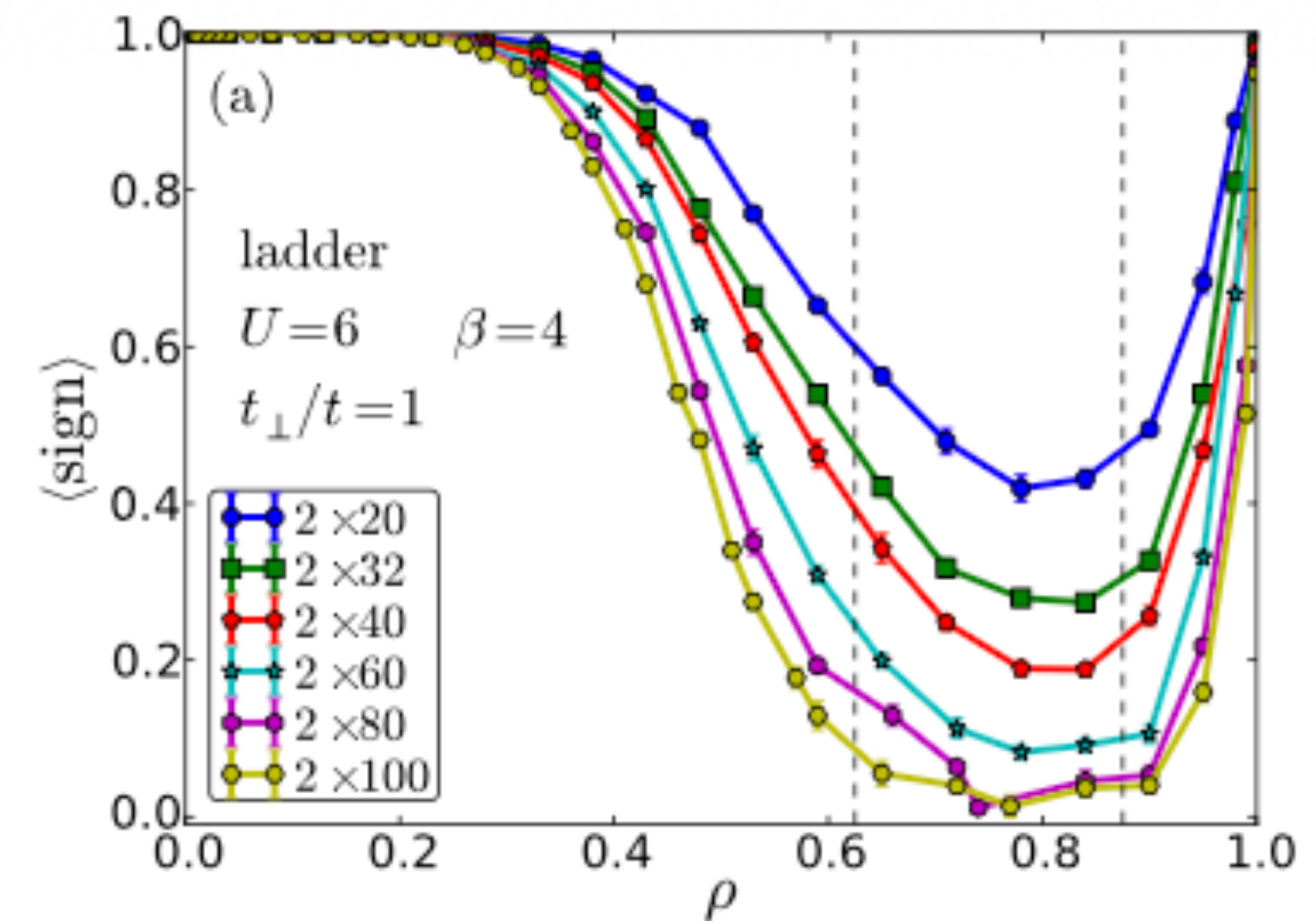
Square lattice

Geometry dependence of the sign problem in quantum Monte Carlo simulations

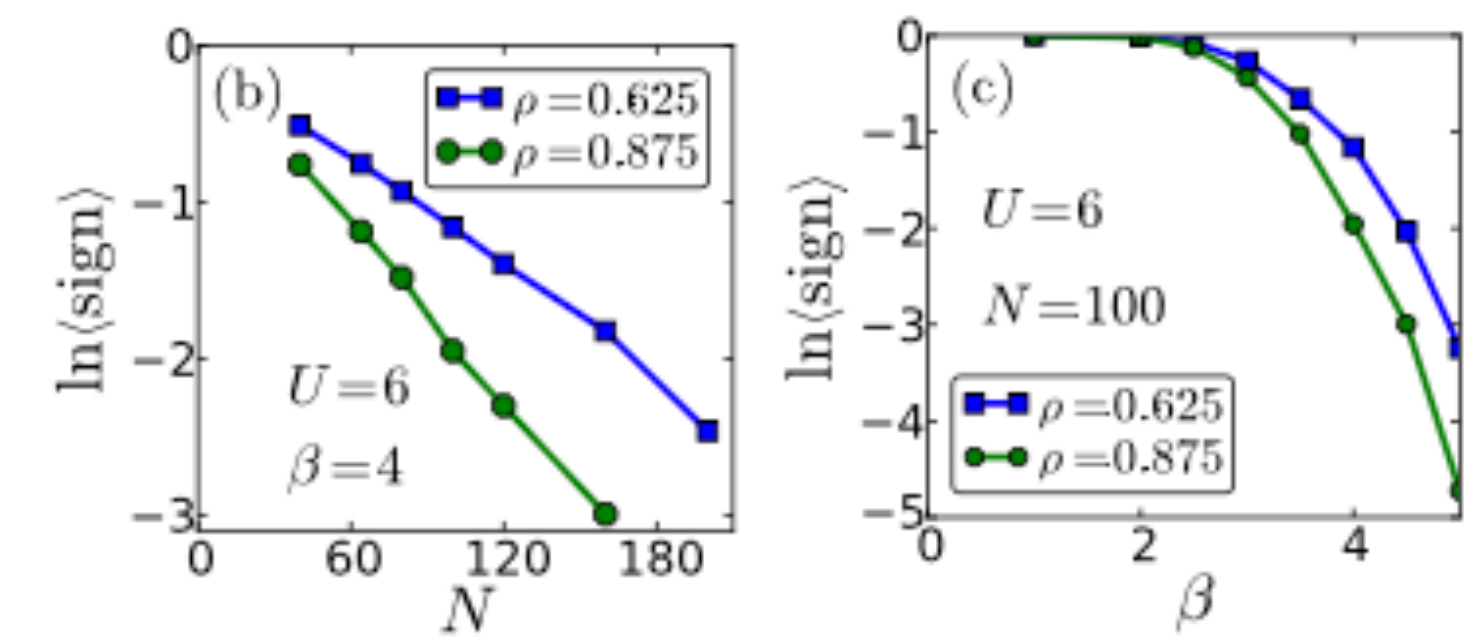
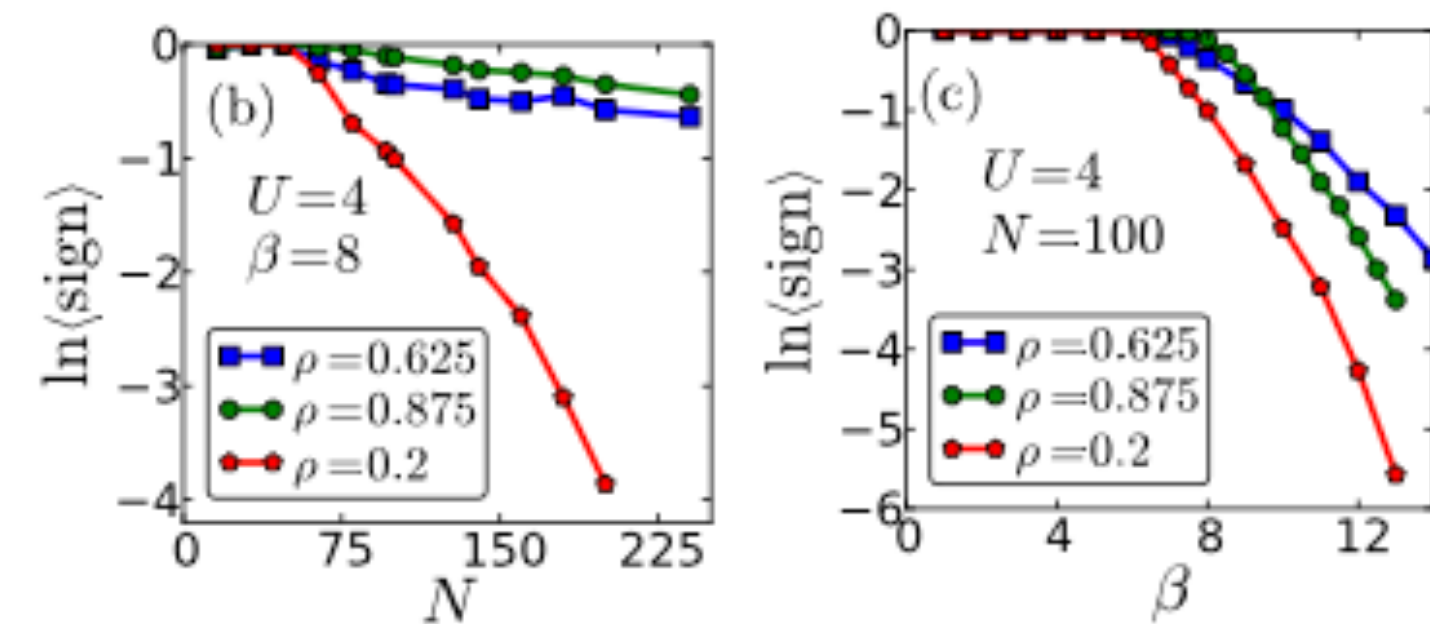
V. I. Iglovikov,¹ E. Khatami,² and R. T. Scalettar¹



Chain



Ladder



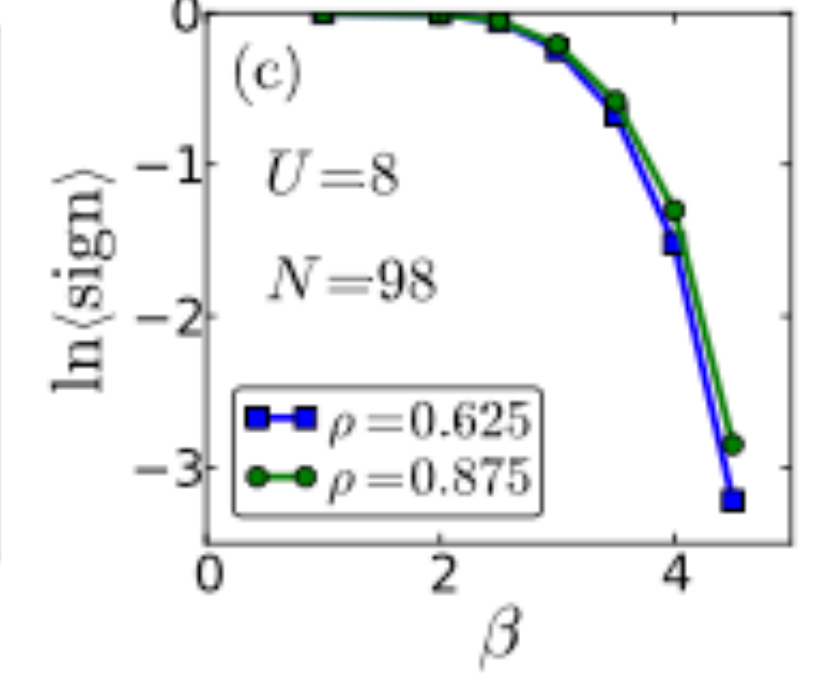
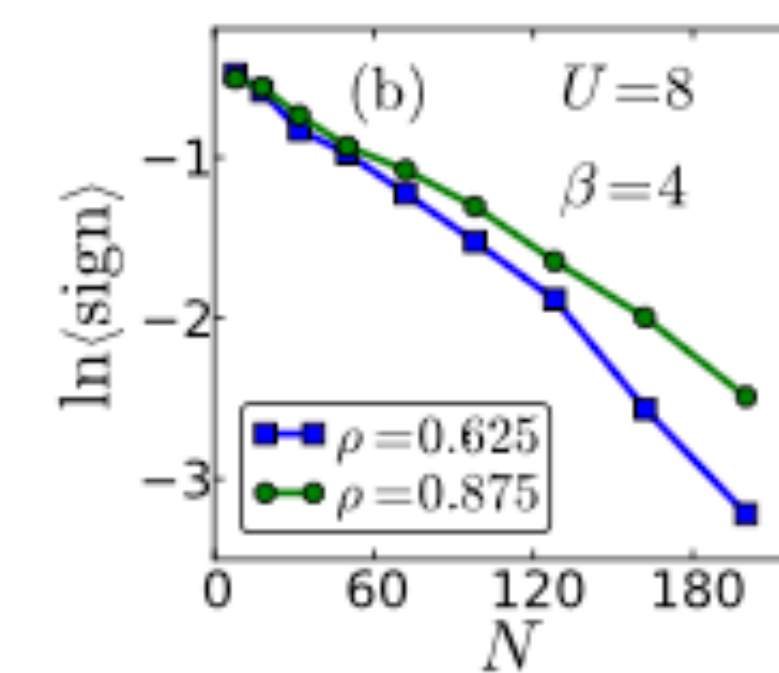
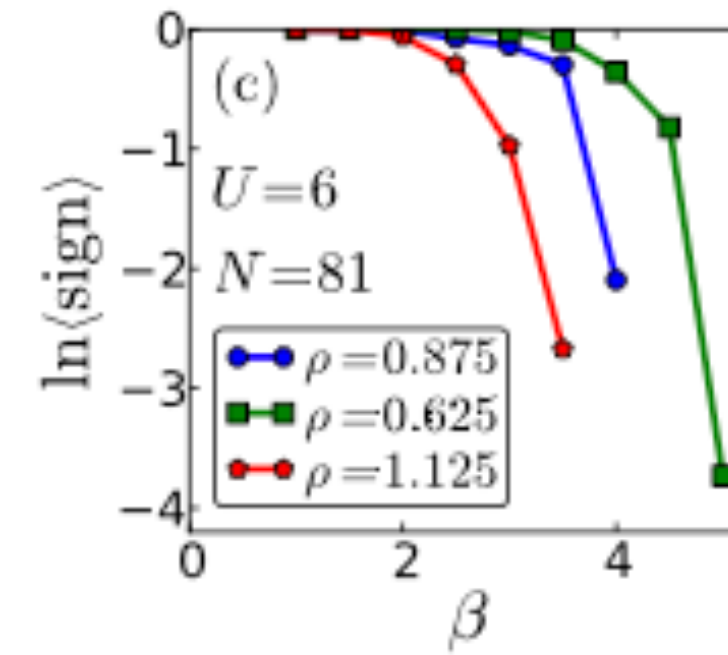
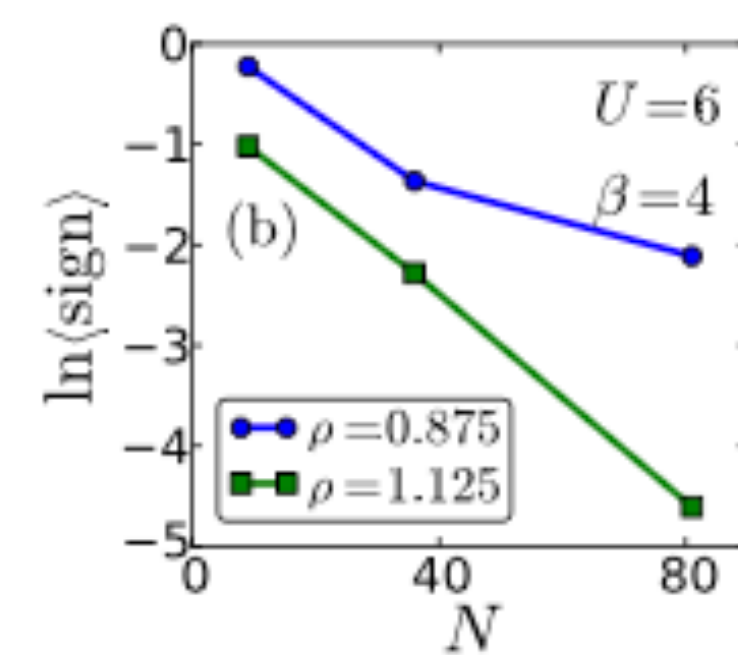
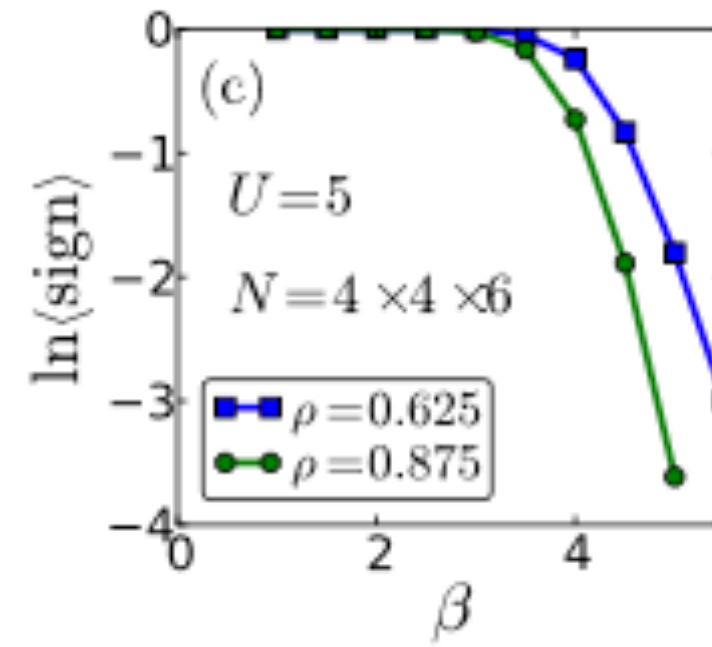
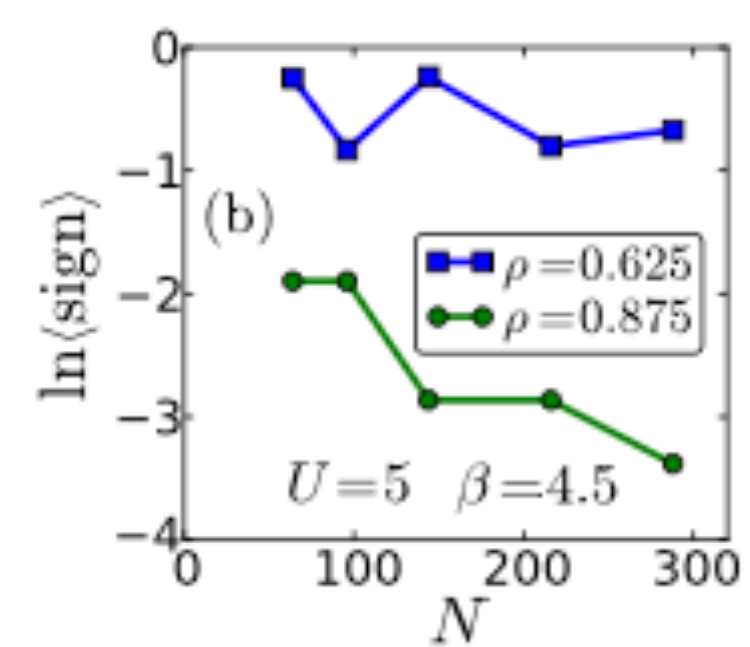
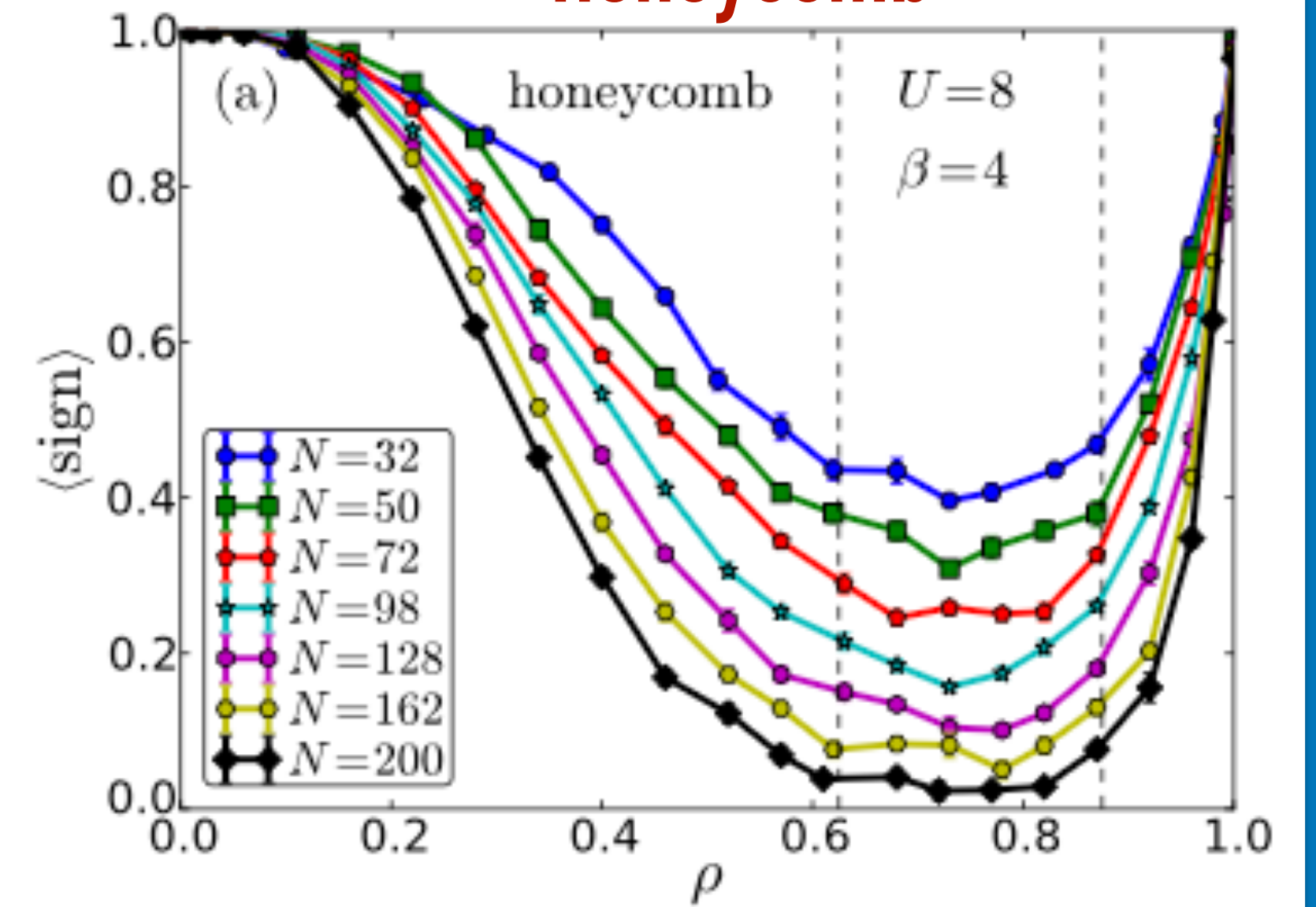
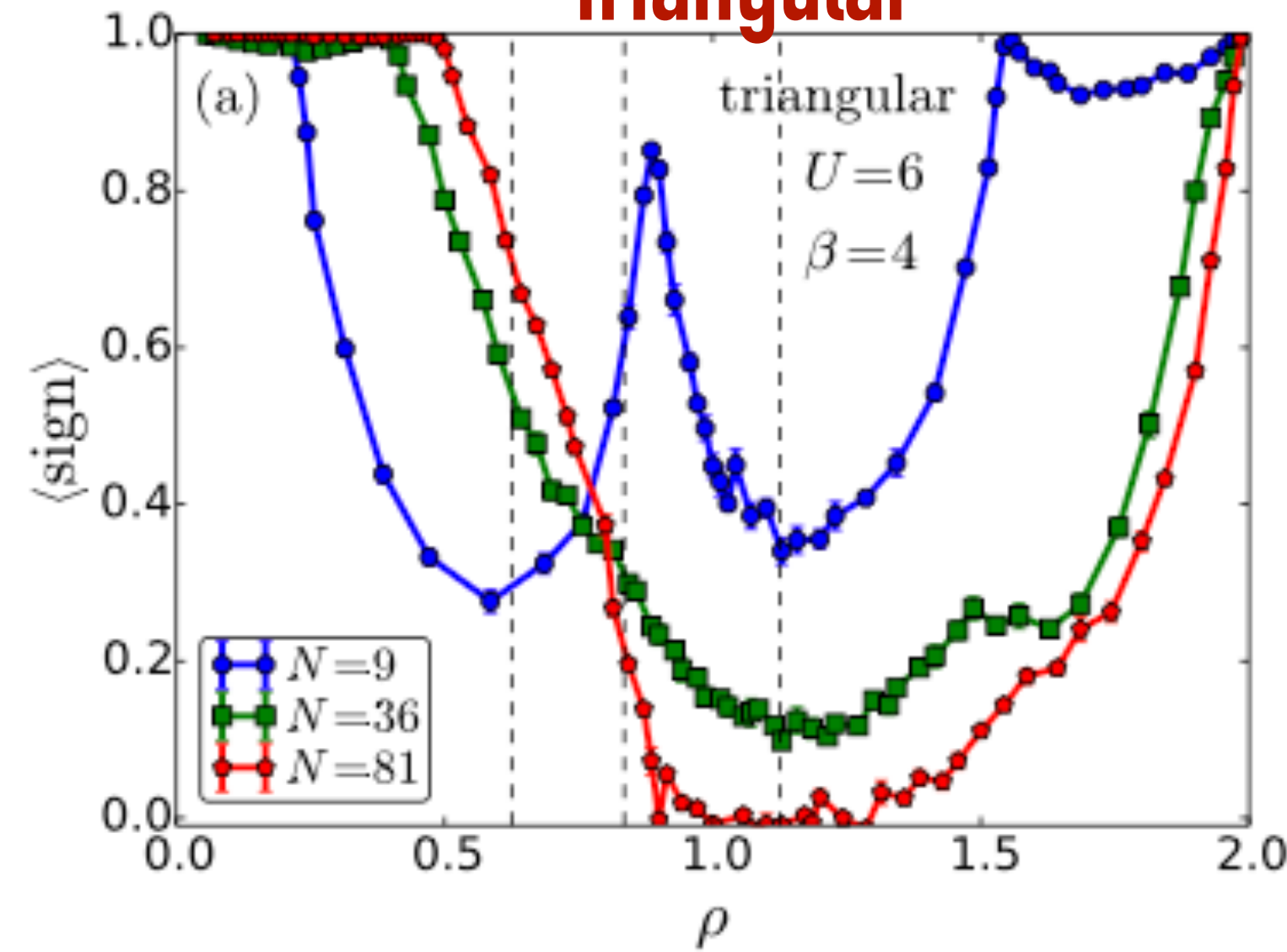
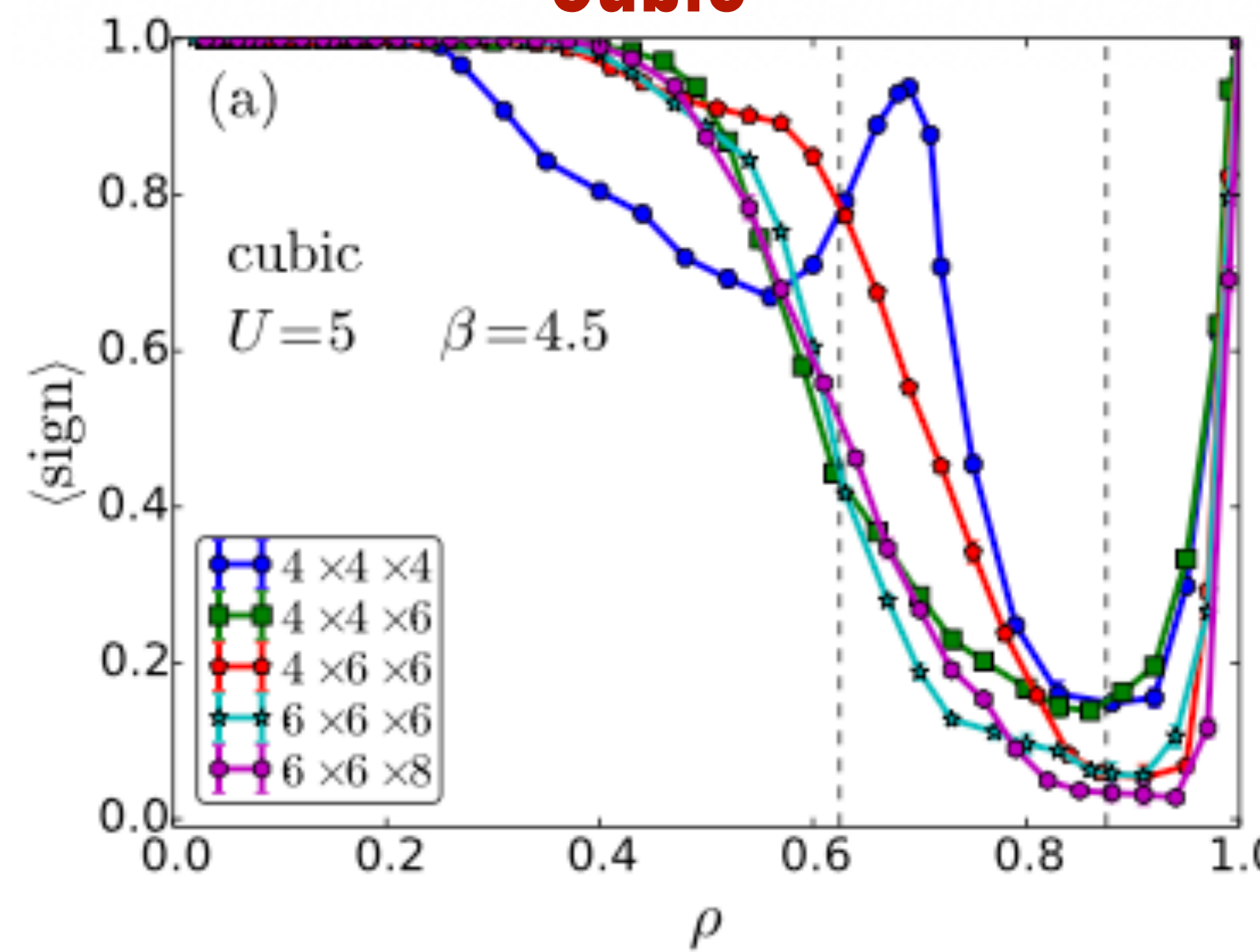
Geometry dependence of the sign problem in quantum Monte Carlo simulations

V. I. Iglovikov,¹ E. Khatami,² and R. T. Scalettar¹

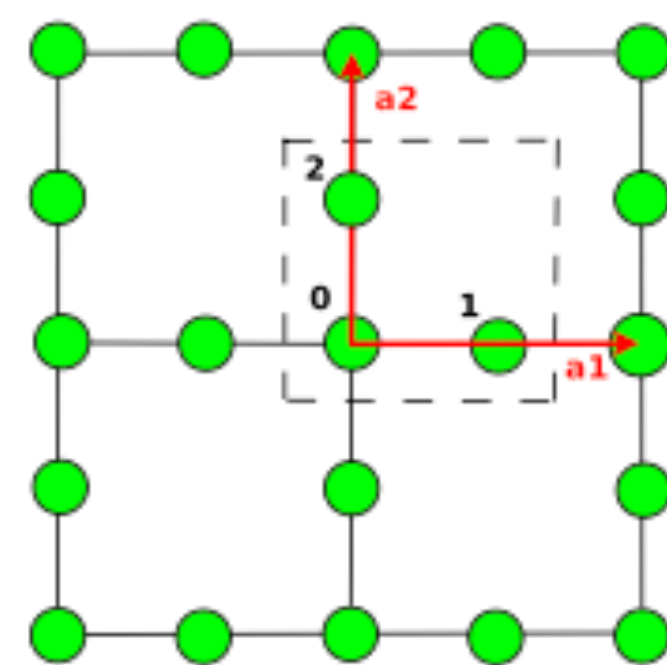
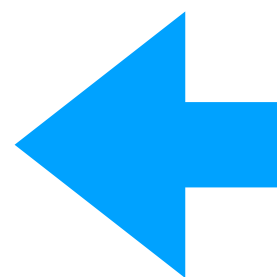
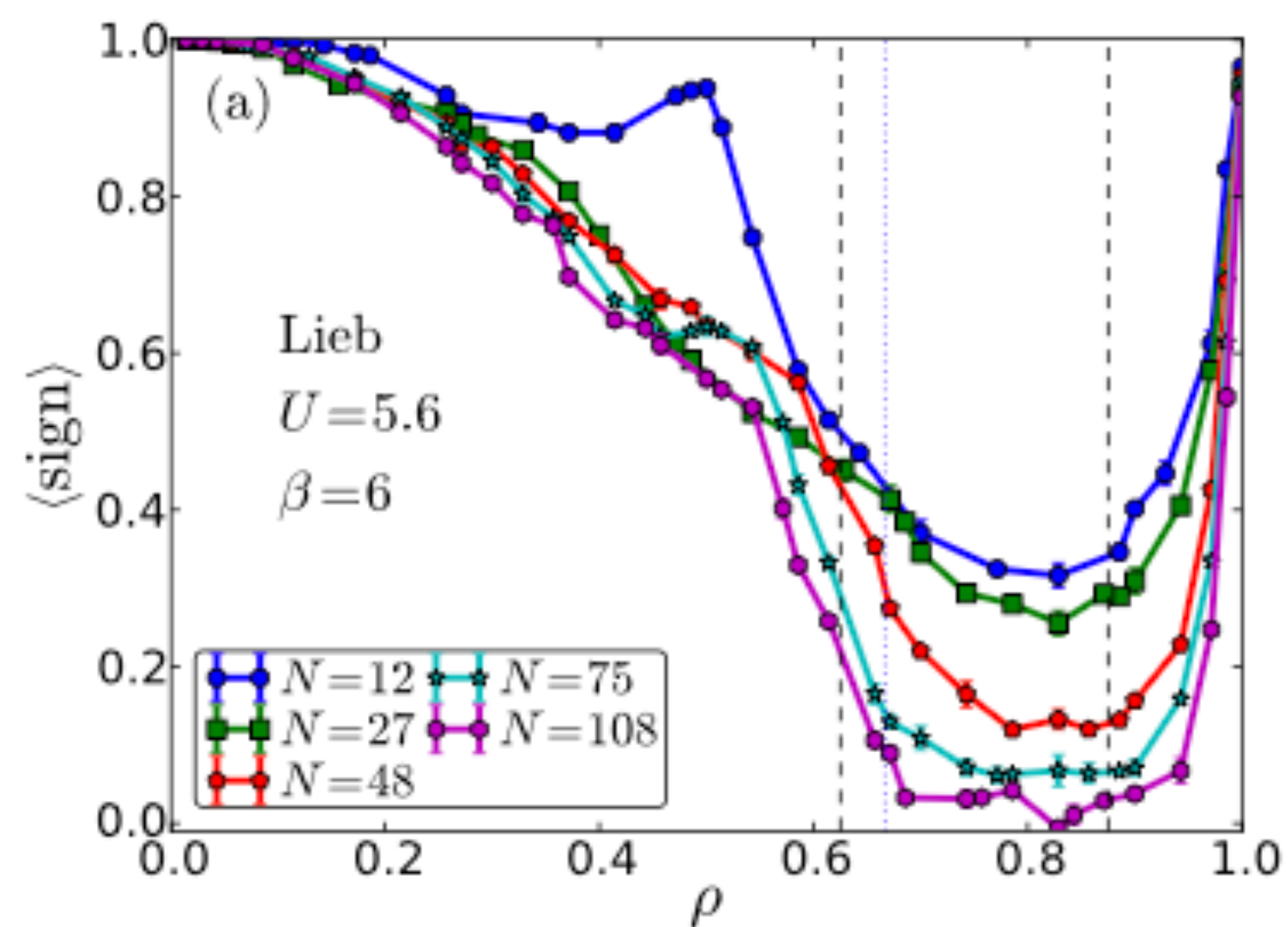
Cubic

Triangular

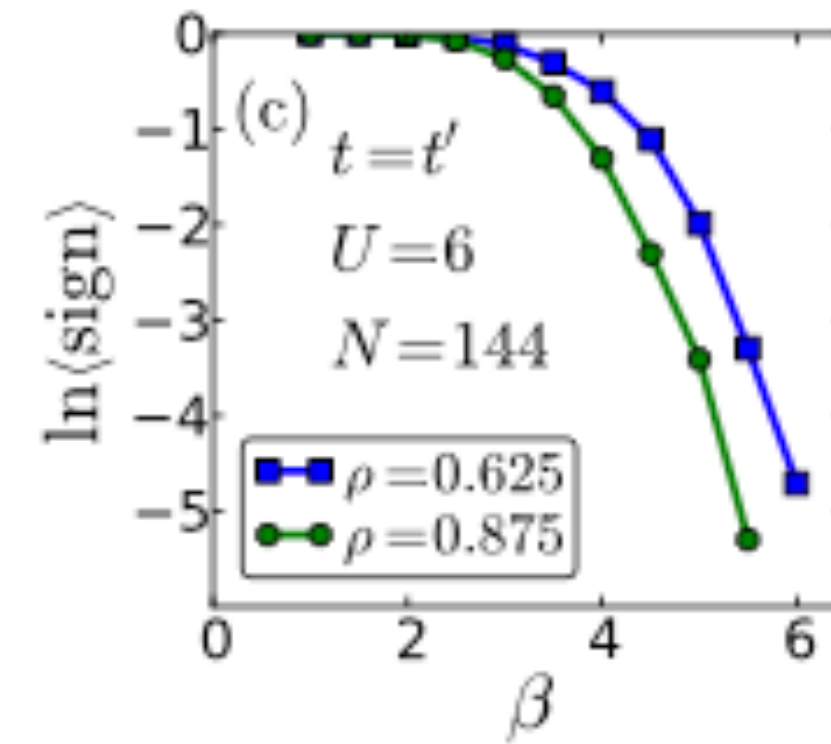
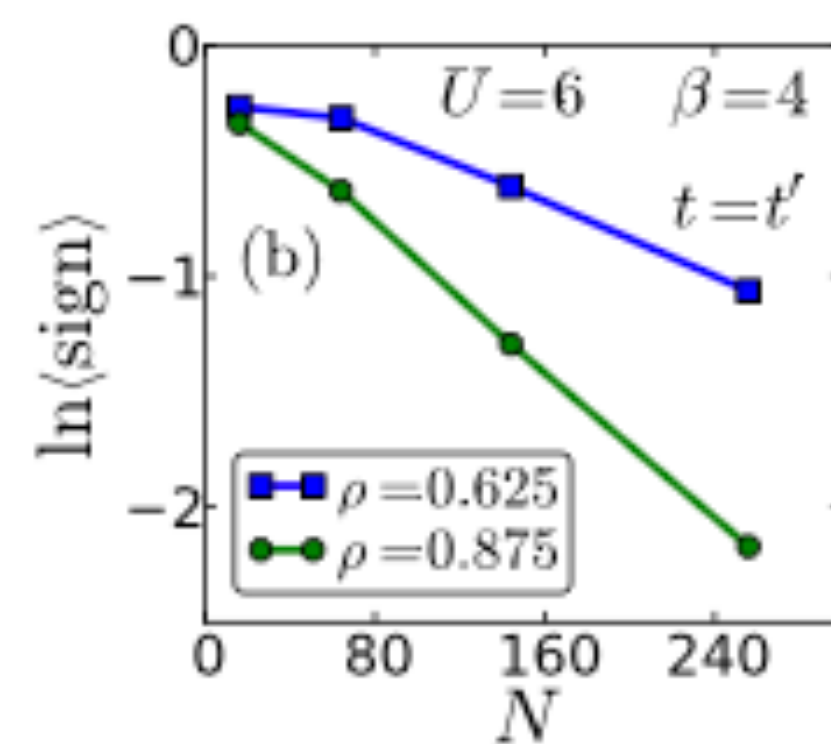
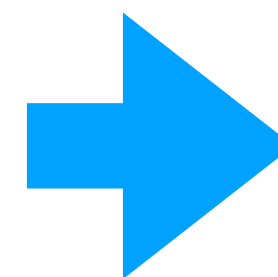
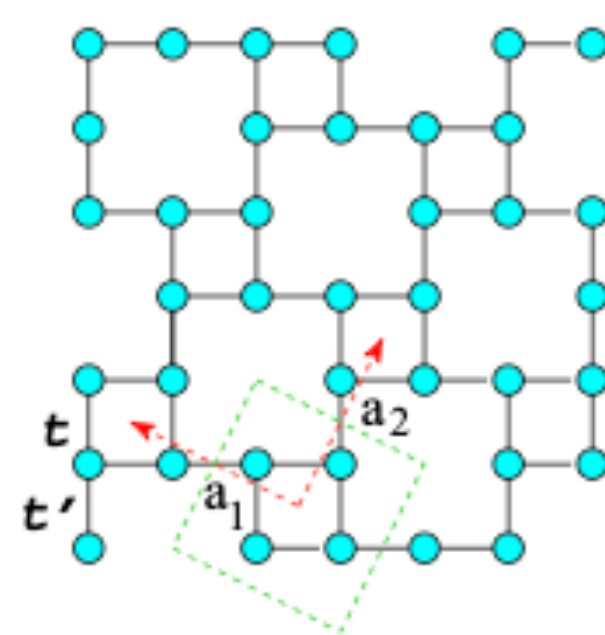
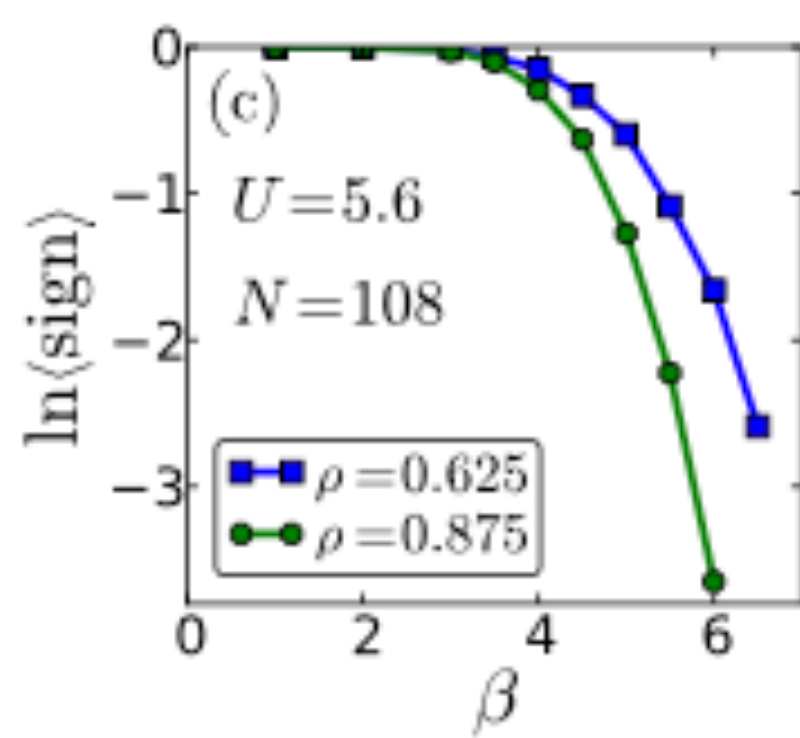
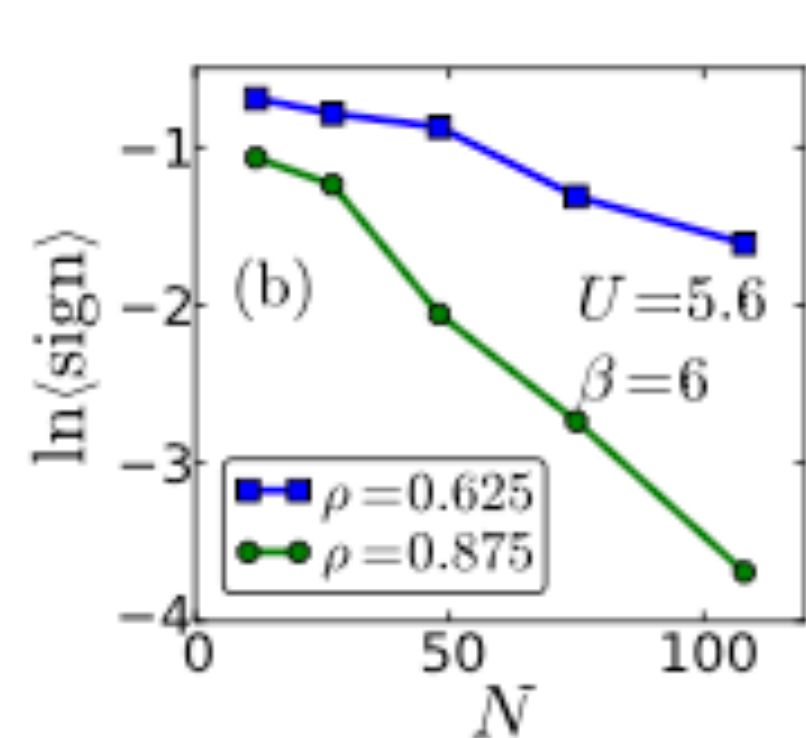
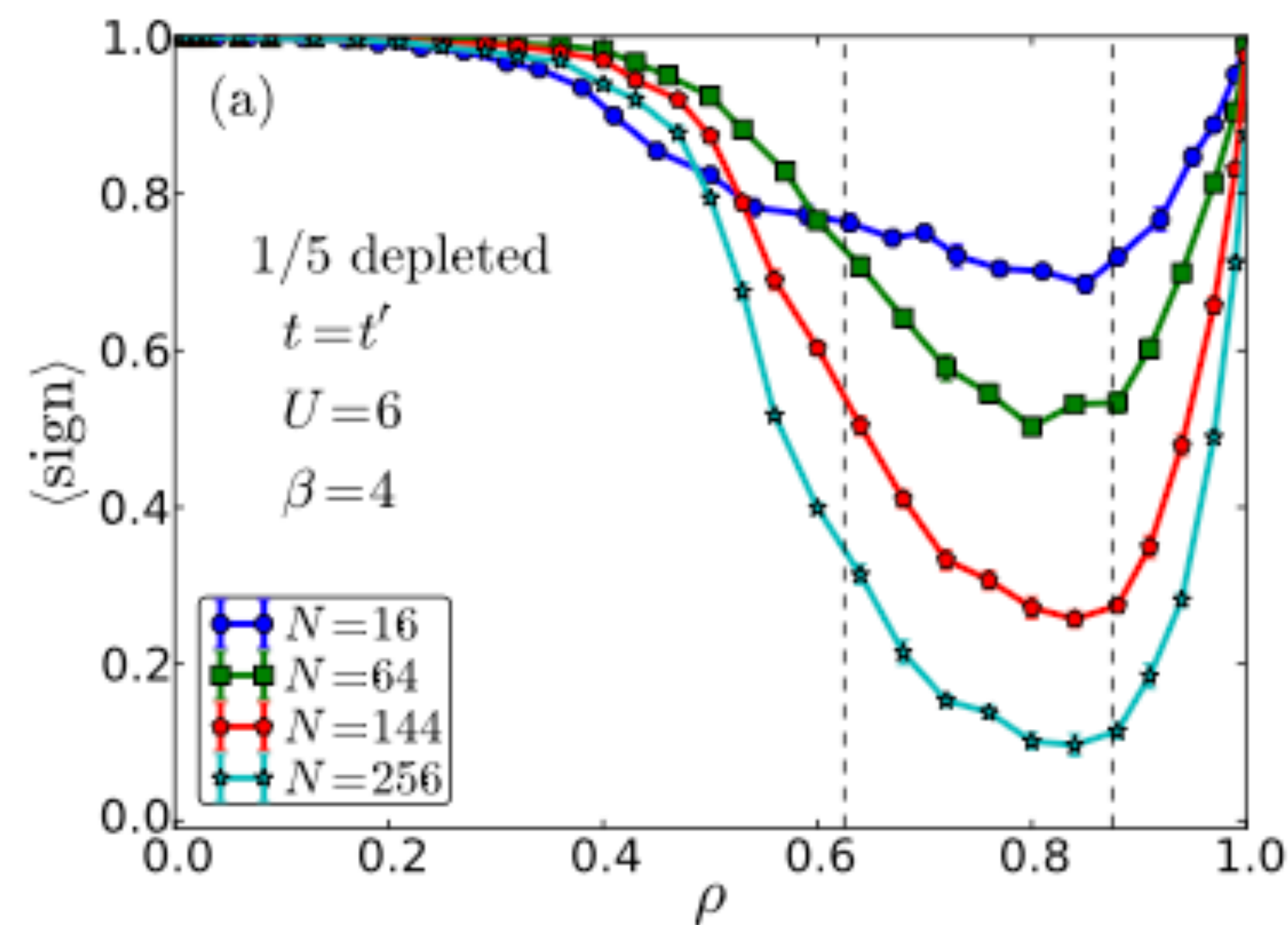
Honeycomb



Lieb



1/5 depleted



Can we understand it?

Change in notation

HS configuration of the $\ell - th$ time slice

$$S_\ell \equiv \{s_1(\ell), s_2(\ell), \cdots s_{N_s}(\ell)\}$$

Complete path in the space of the HS fields

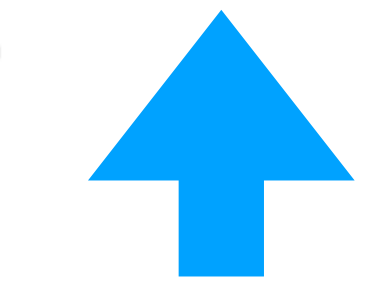
$$S \equiv \{S_1, S_2, \cdots S_M\}$$

$$\mathcal{Z} = \sum_S \mathcal{T}r \prod_{\sigma} B^{\sigma}(S_M) B^{\sigma}(S_{M-1}) \cdots B^{\sigma}(S_1)$$

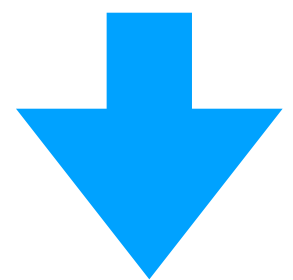
Partial path

The first ℓ slices

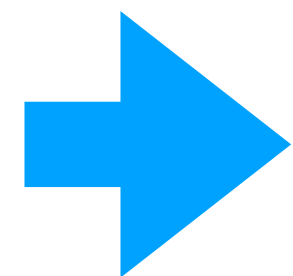
$$\mathcal{P}_\ell(\{S_1, S_2, \dots, S_\ell\}) \\ \equiv \text{Tr} \left[\mathcal{B} \mathcal{B} \dots \mathcal{B} \prod_{\sigma} \mathbf{B}^{\sigma}(S_\ell) \mathbf{B}^{\sigma}(S_{\ell-1}) \dots \mathbf{B}^{\sigma}(S_1) \right]$$



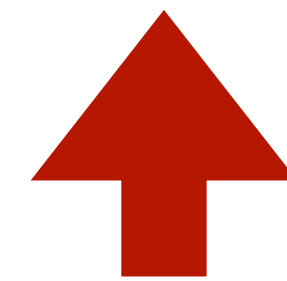
No HST



$$\mathcal{P}_0 \equiv \mathcal{Z}$$



Positive



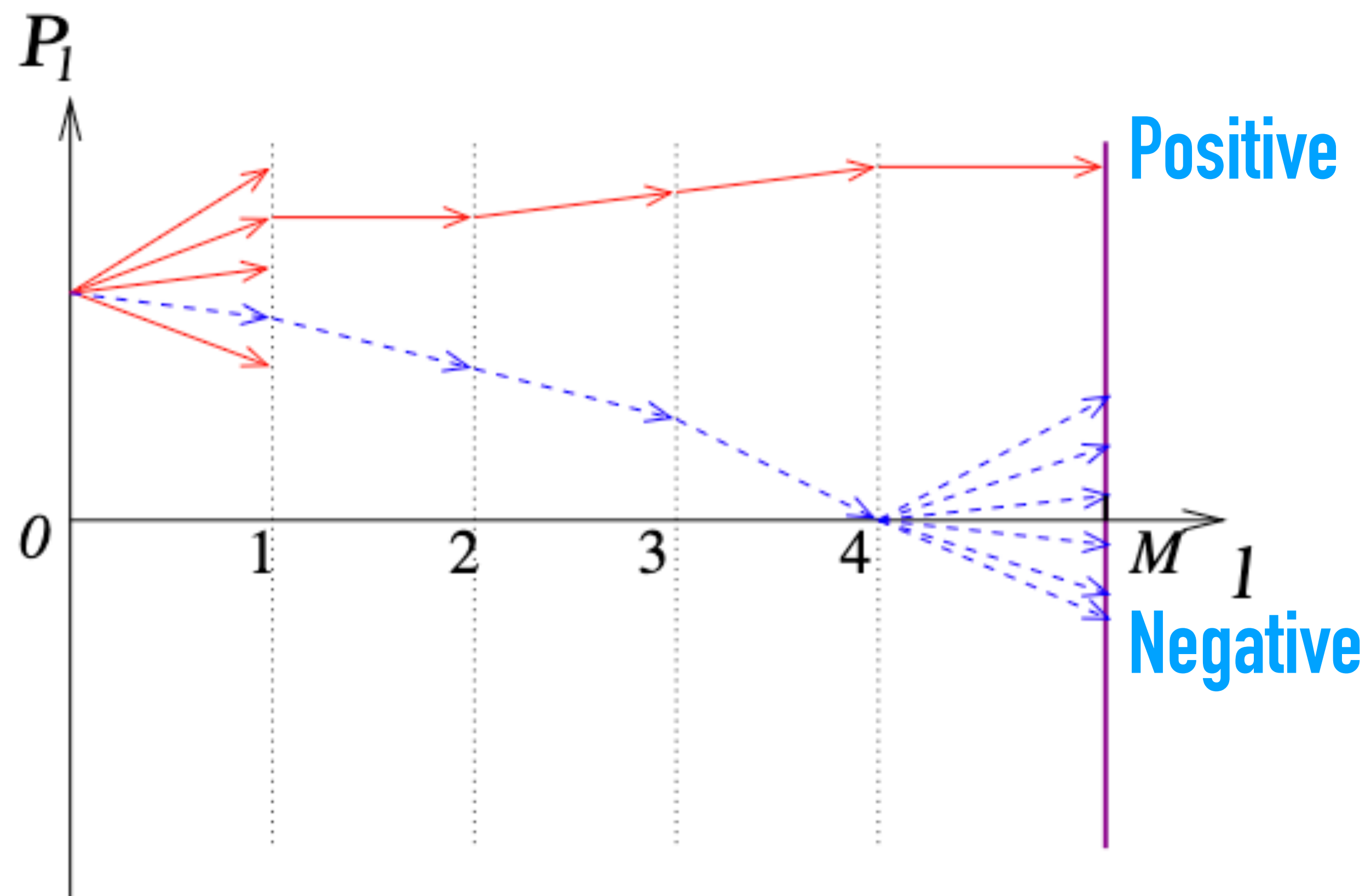
HST

$$\mathcal{P}_0 \equiv \mathcal{Z}$$

$\mathcal{P}_1 \rightarrow 2_s^N$ possibilities

$\mathcal{P}_\ell \rightarrow 2_s^N$ possibilities

From each $\mathcal{P}_{\ell-1}$



Can it be fixed?

Constrained Path Quantum Monte Carlo Method for Fermion Ground States

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J. Carlson and J. E. Gubernatis

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 28 December 1994)

We propose a new quantum Monte Carlo algorithm to compute fermion ground-state properties. The ground state is projected from an initial wave function by a branching random walk in an over-complete basis space of Slater determinants. By constraining the determinants according to a trial wave function $|\Psi_T\rangle$, we remove the exponential decay of signal-to-noise ratio characteristic of the sign problem. The method is variational and is exact if $|\Psi_T\rangle$ is exact. We report results on the two-dimensional Hubbard model up to size 16×16 , for various electron fillings and interaction strengths.

Problem: biased method

Who's afraid of the ~~big bad wolf~~ sign problem?



By Rubem Mondaini

QUANTUM CRITICALITY

Quantum critical points and the sign problem

Science 2022

R. Mondaini¹, S. Tarat¹, R. T. Scalettar²

Can the sign problem tell us something about the physics of the system?

QUANTUM CRITICALITY

Quantum critical points and the sign problem

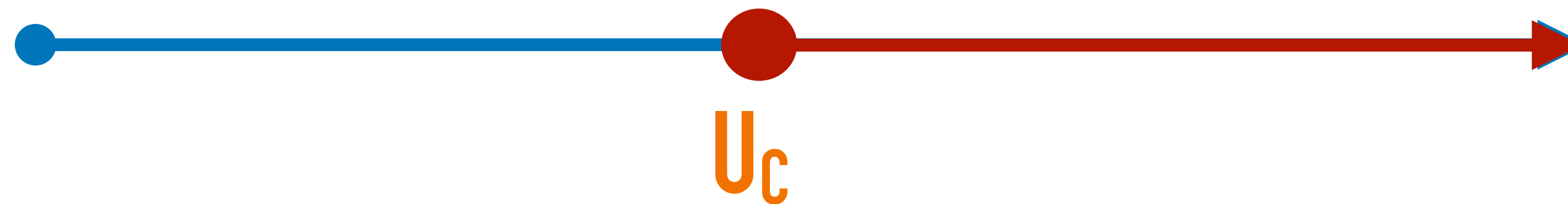
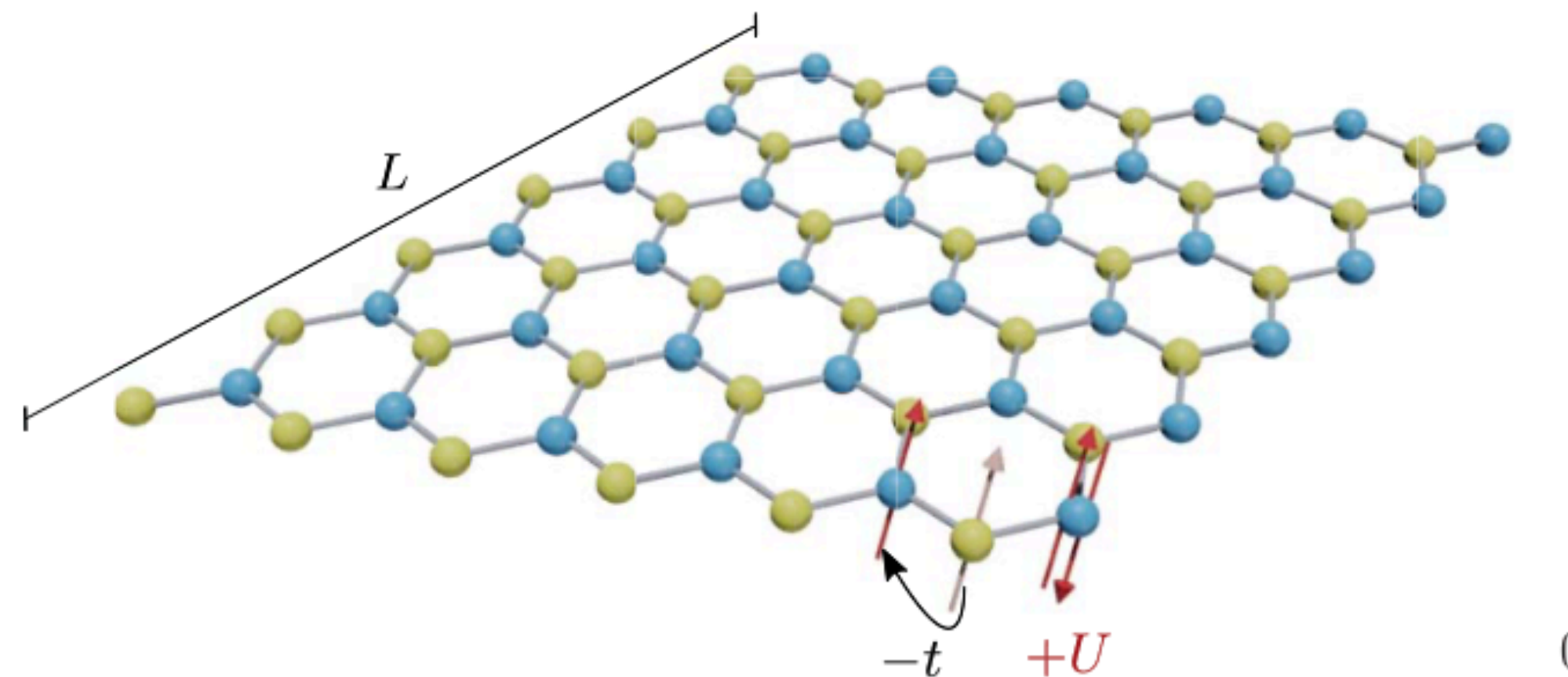
Science 2022

R. Mondaini¹, S. Tarat¹, R. T. Scalettar²

Can the sign problem tell us something about the physics of the system?

Yes, it is deeply connected to Quantum Phase Transitions

TEST 1: Hubbard model on a honeycomb lattice



Paramagnetic, (semi)metal

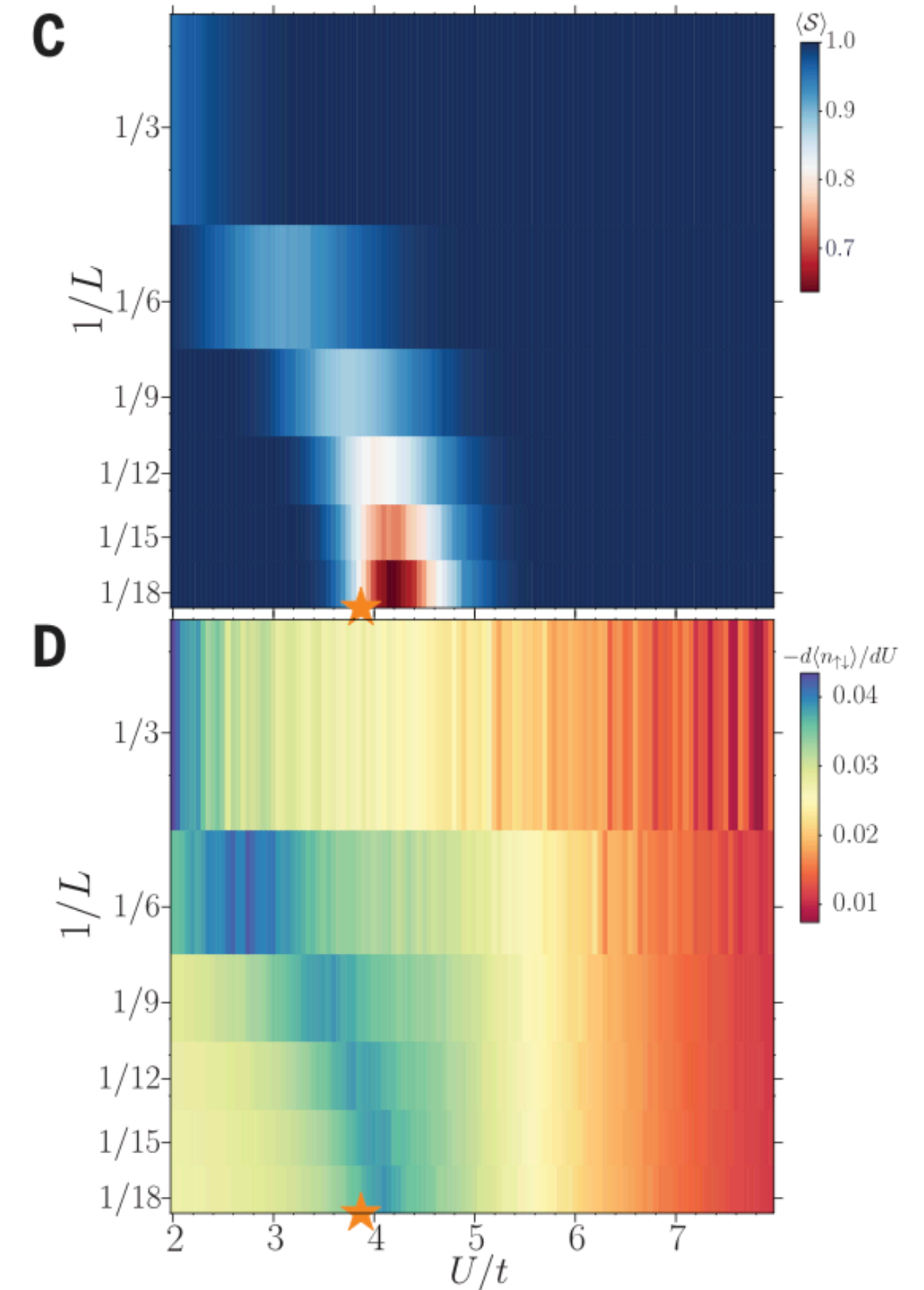
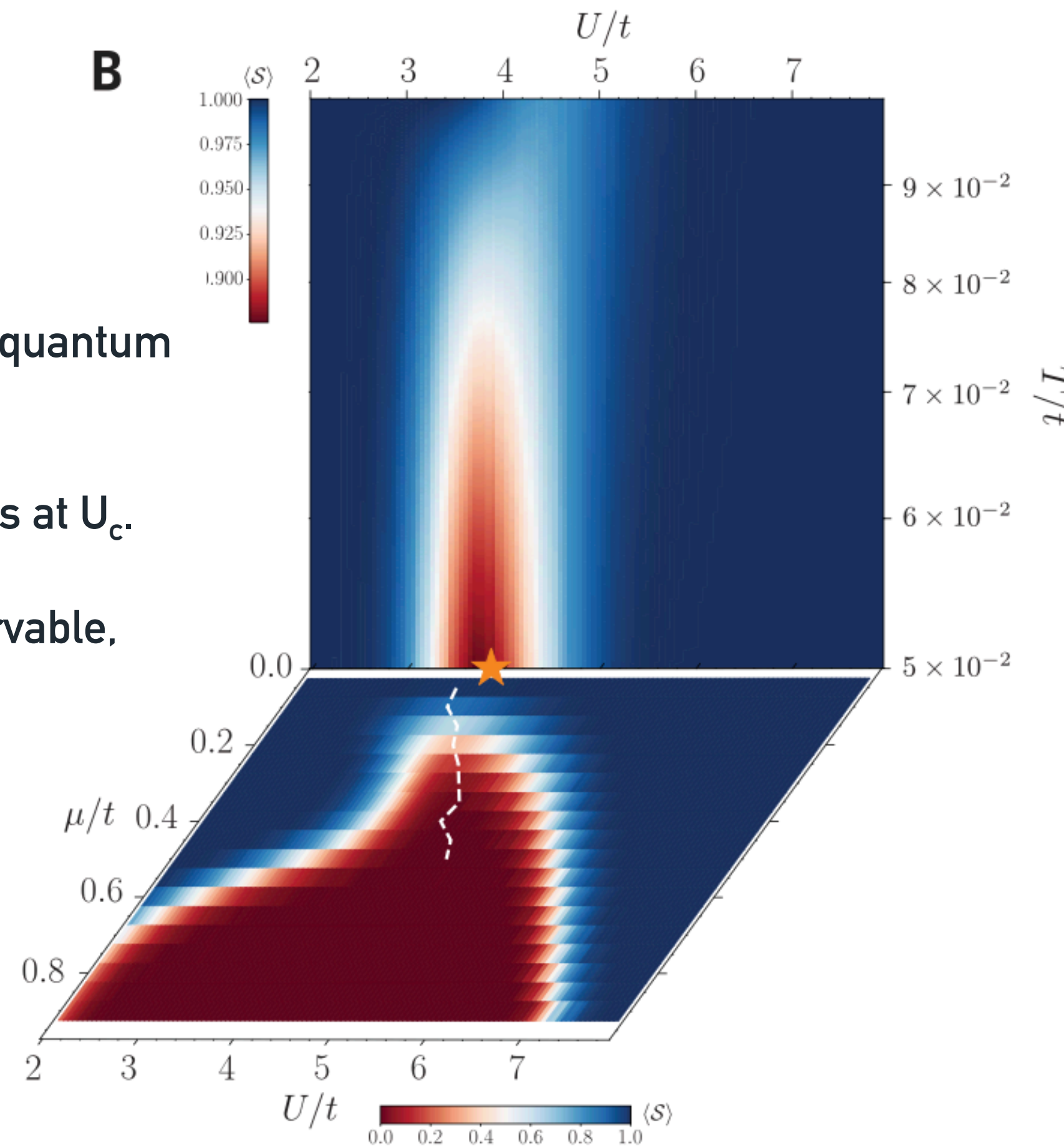
Antiferromagnetic, Mott insulator

Add $\mu/t = 0.1$ to switch the sign problem on.

B: as T drops, $\langle S \rangle$ dips only near U_c , tracing the quantum critical fan.

C: extrapolating in system size, the dip sharpens at U_c .

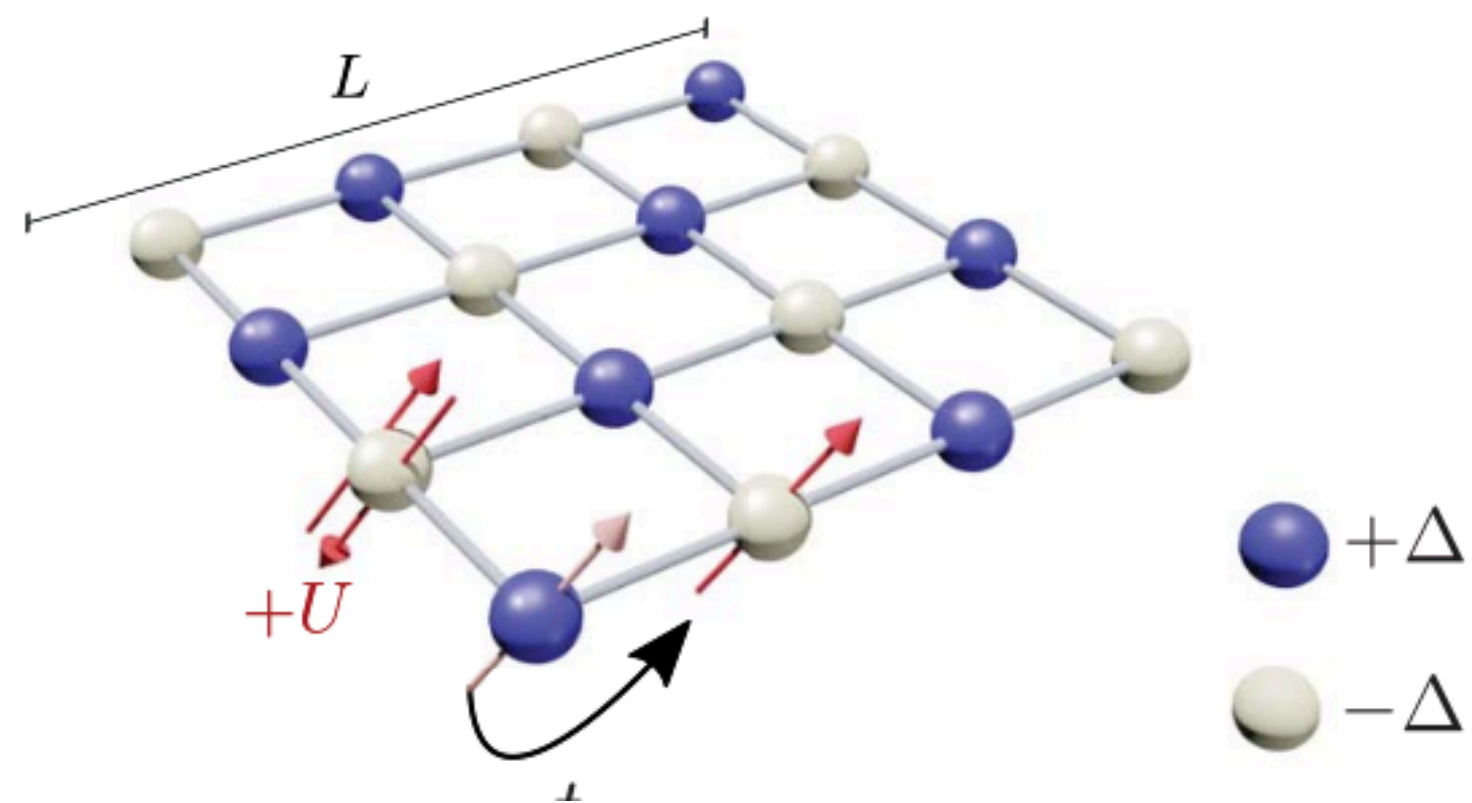
D: the same picture appears in a physical observable, $-d\langle n_\uparrow n_\downarrow \rangle/dU$.



Three limits pin the critical point:
 $\mu \rightarrow 0, T \rightarrow 0, L \rightarrow \infty$.

Mondaini, Tarat & Scalettar, Science 2022

TEST 2: Ionic Hubbard model



Band insulator

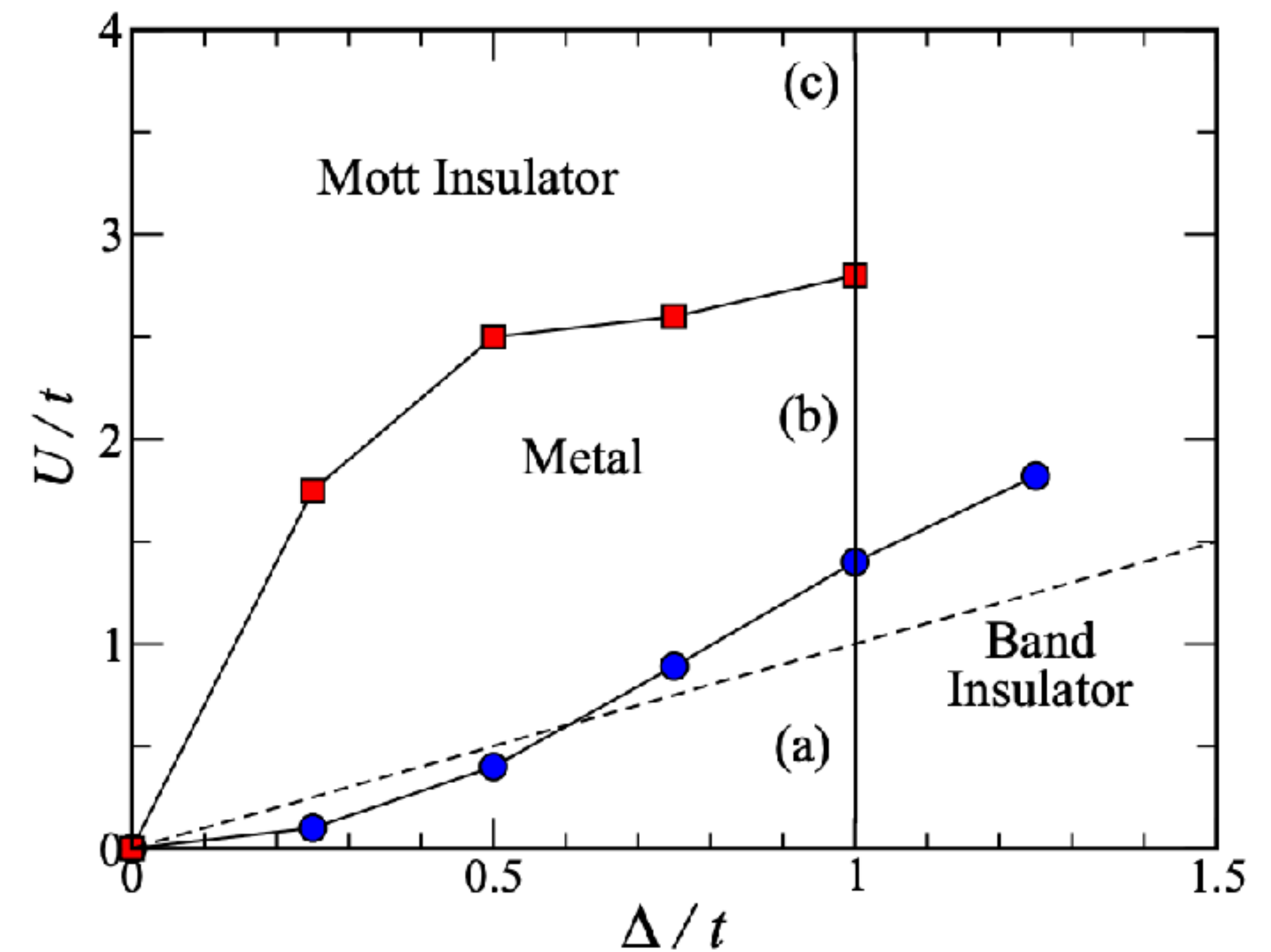


$$\Delta \gg U$$

Mott insulator

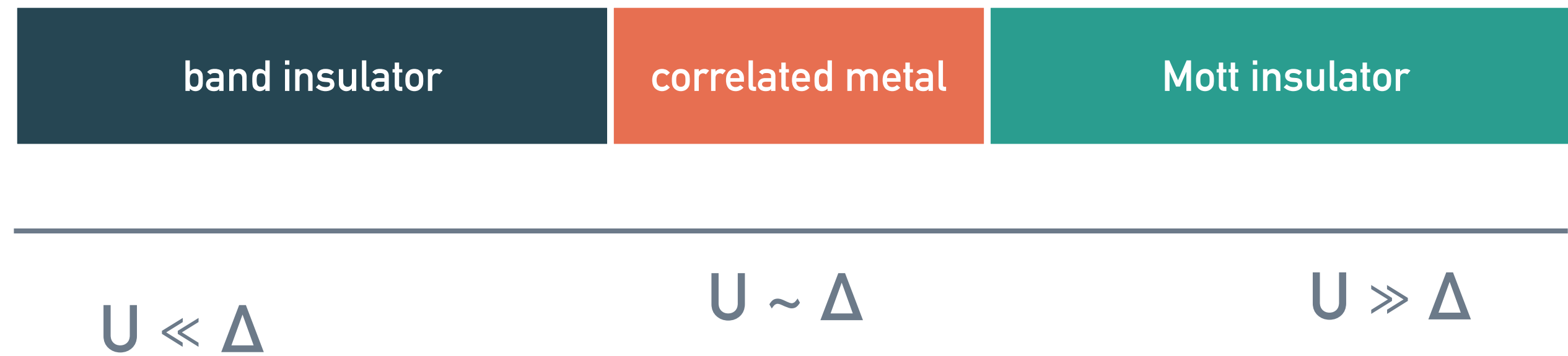


$$\Delta \ll U$$



Bouadim et al PRB 2007

Staggered potential $\pm\Delta$ against repulsion U , at half filling

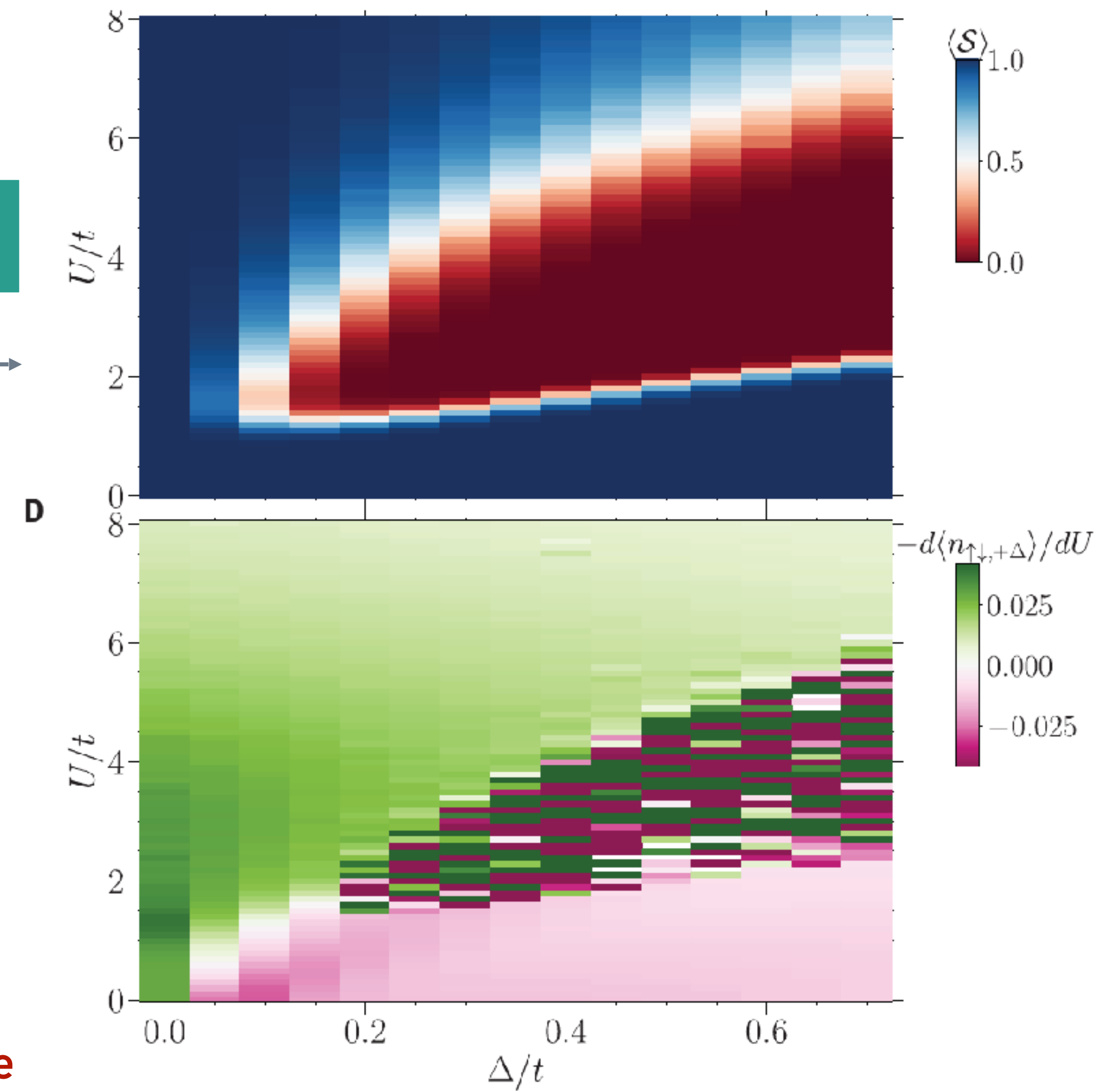


Here the sign problem exists even at half filling

at $T = t/24$, $\langle S \rangle$ is small in a window that matches the metallic region found earlier from the conductivity.

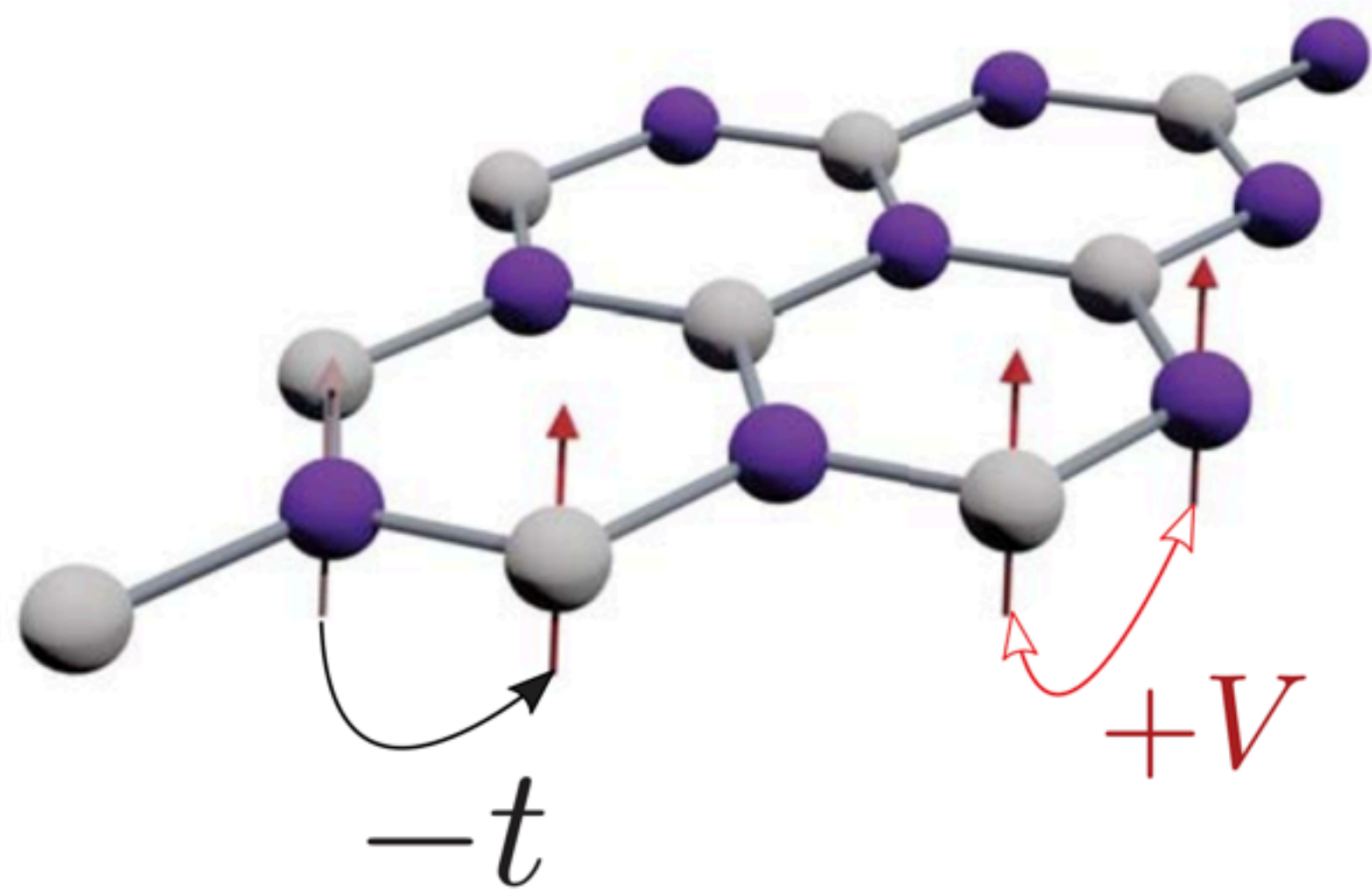
D: the double occupancy on the $+\Delta$ sites changes sign across the same boundaries.

Inside the metal, ordinary observables are noisy precisely because $\langle S \rangle$ vanishes: the sign itself becomes the cleanest signal.



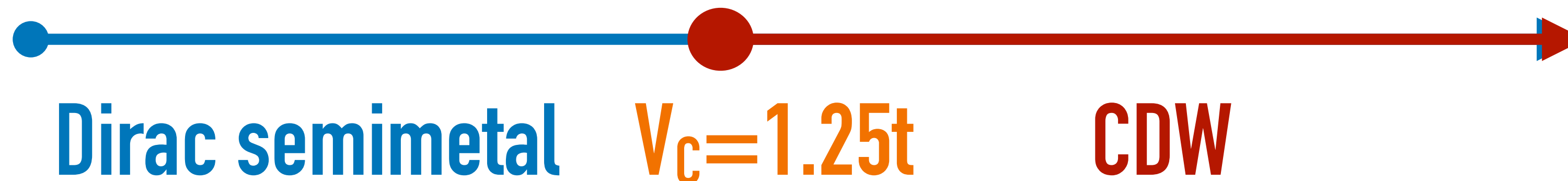
Mondaini, Tarat & Scalettar, Science 375, 418 (2022), Fig. 2

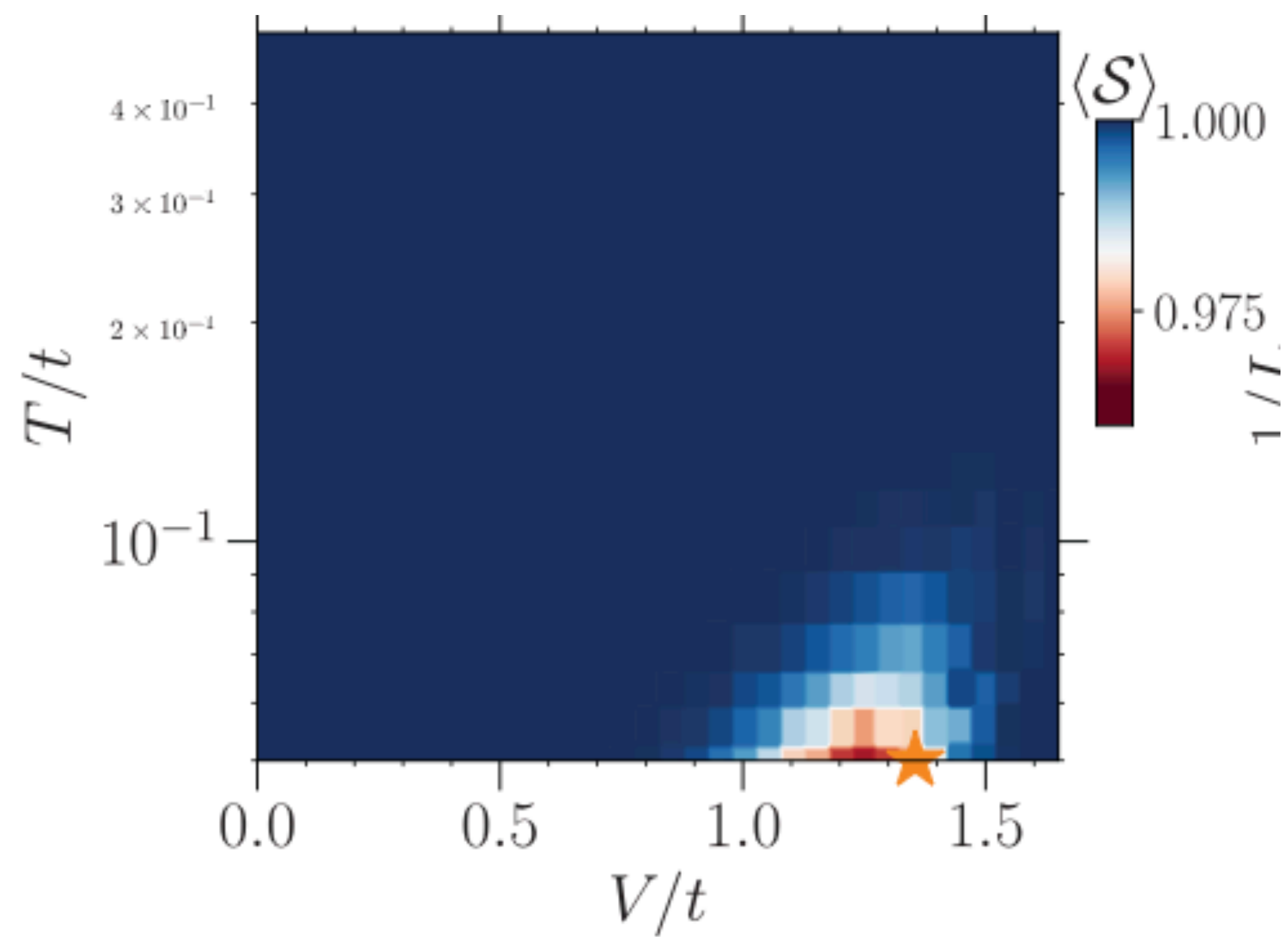
TEST 3: U(1) Hubbard model on a honeycomb lattice



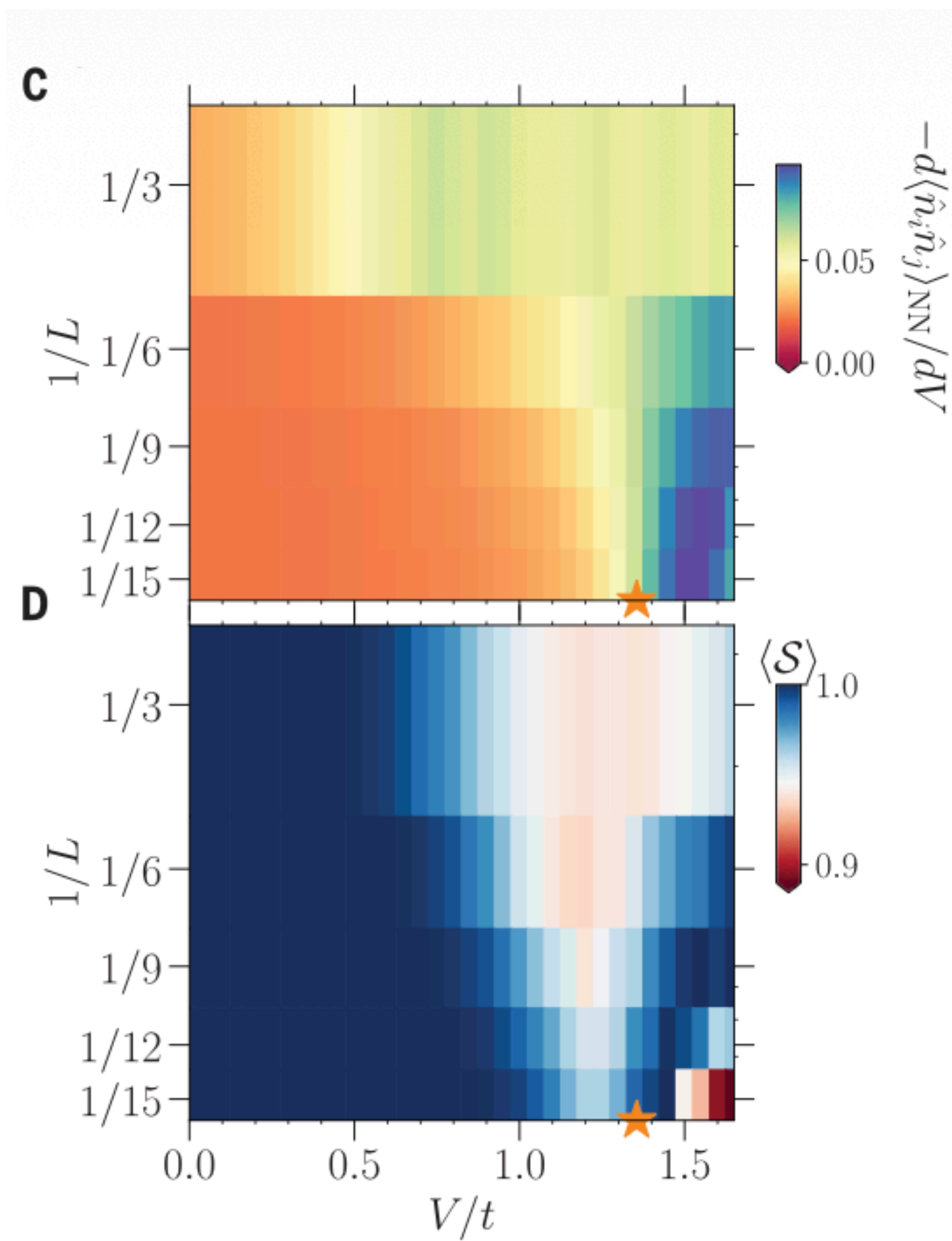
Fermionic sign problem avoidable with continuous time QMC or Majorana representation but present with usual BSS algorithm

$$\hat{H} = -t \sum_{\langle ij \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$



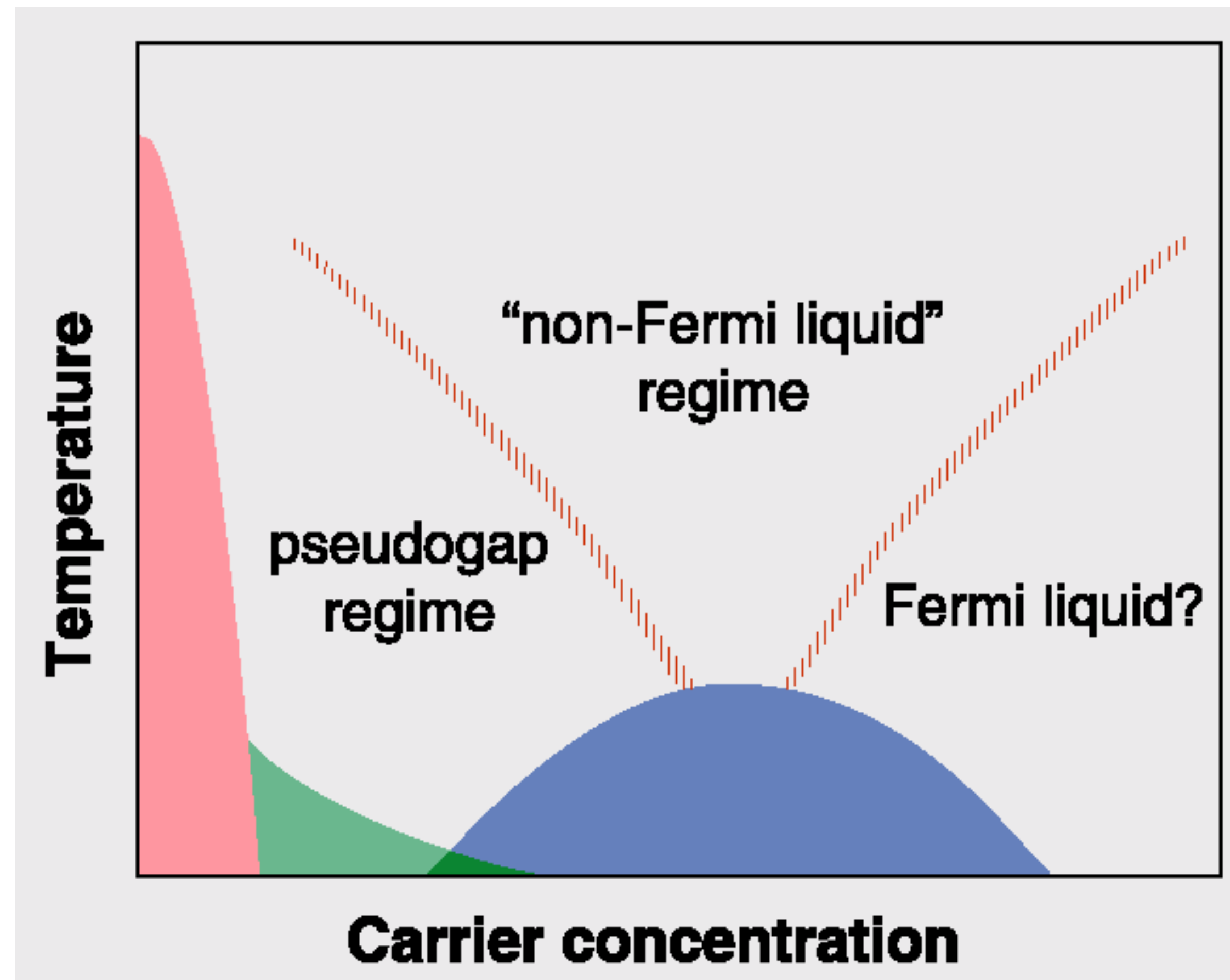
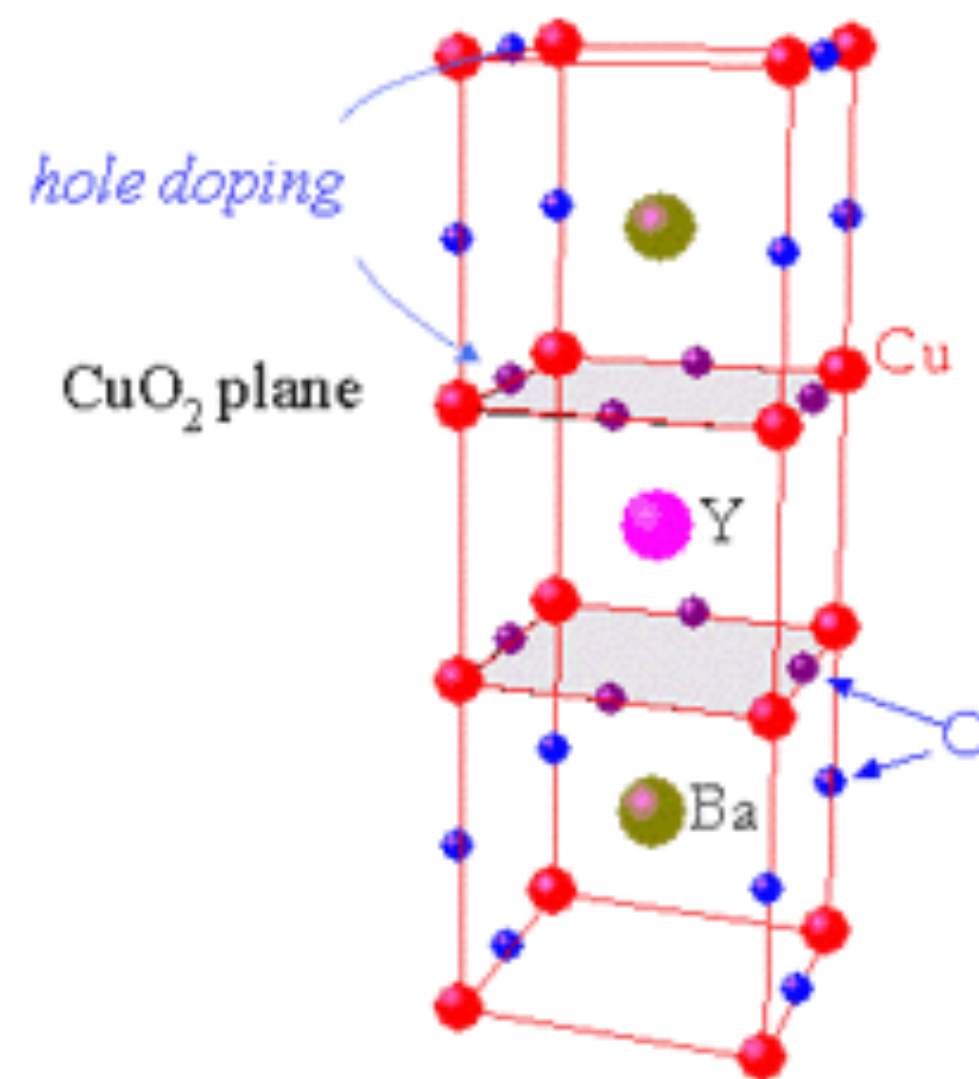


$L=3$

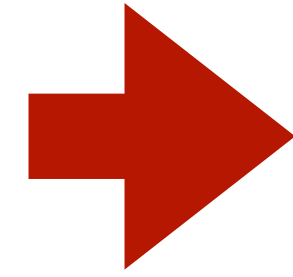


TEST 4: Square lattice Hubbard model

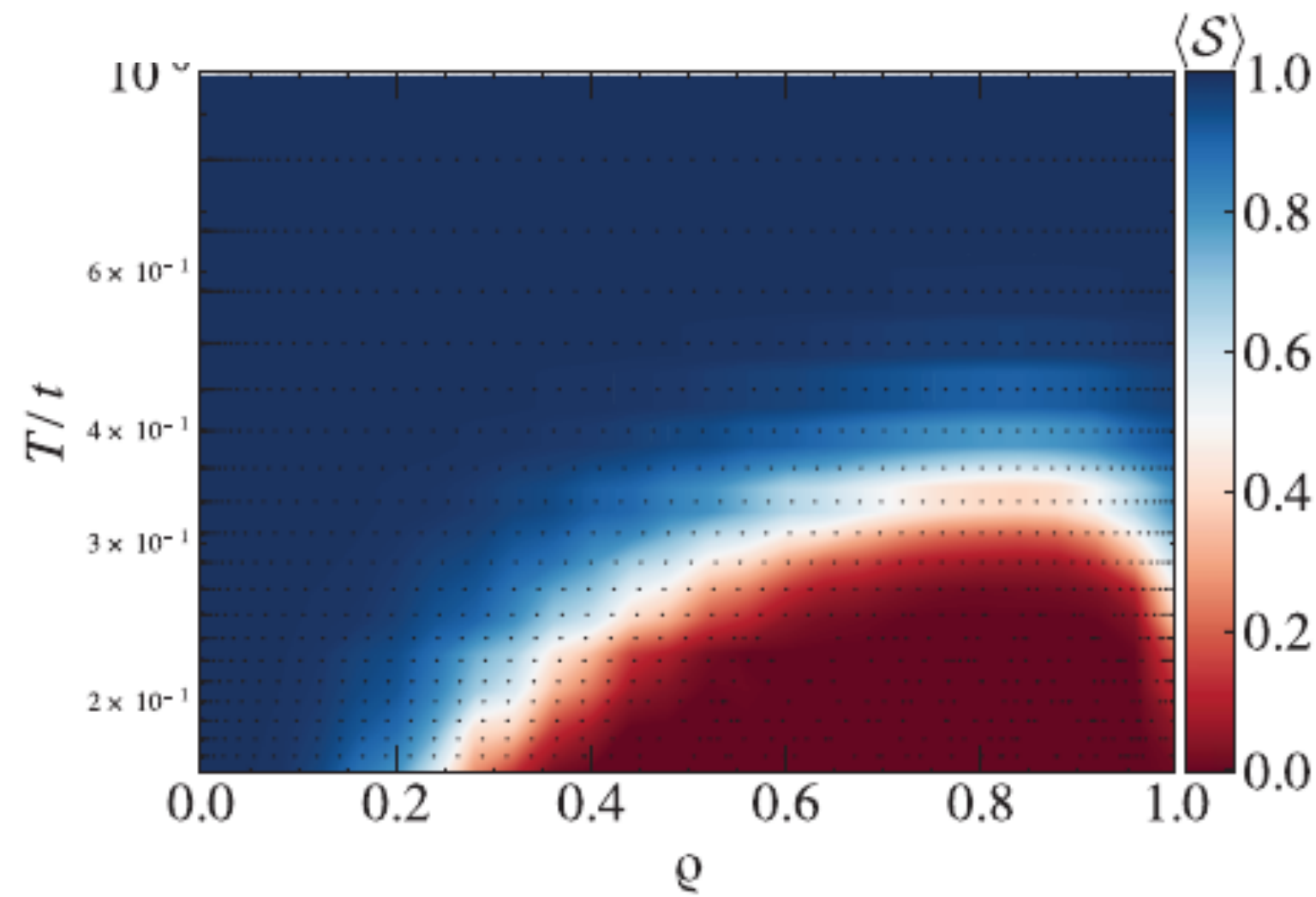
High TC superconductors



$L=16, U=6, t'/t=-0.2$

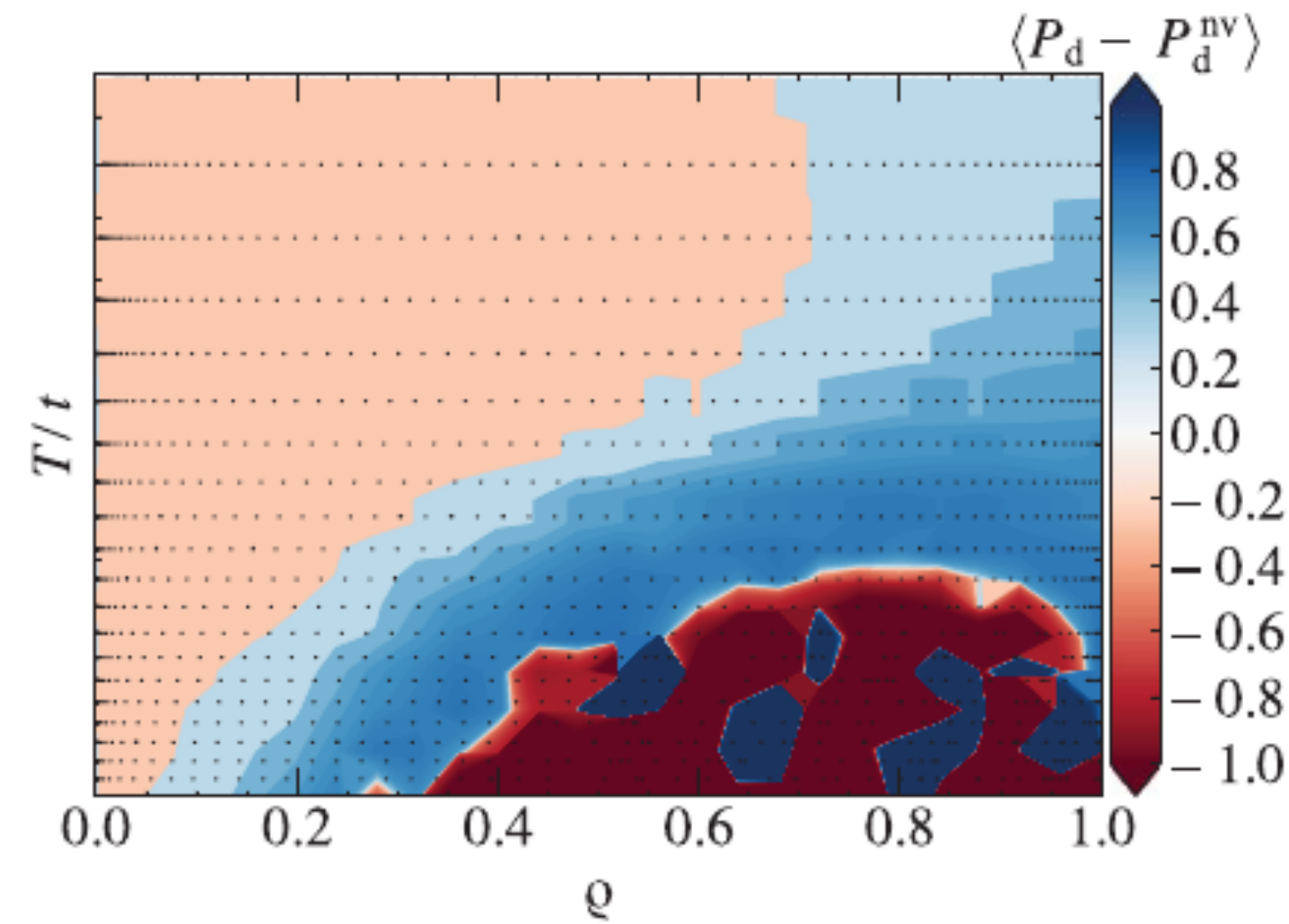


Next-near-neighbor hopping



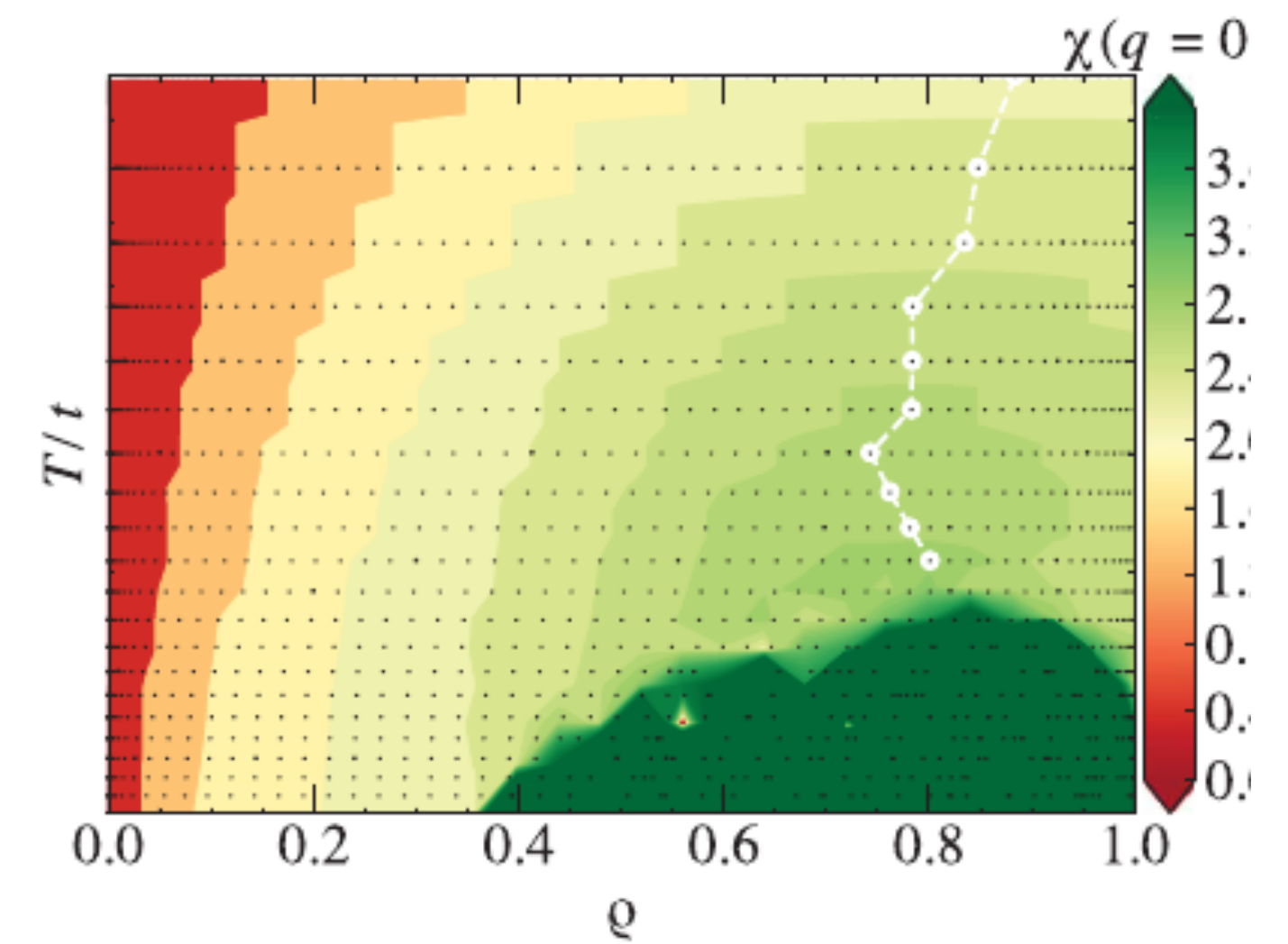
average sign

$\langle S \rangle$ vanishes in a dome, $0.4 \lesssim p \lesssim 1$, as T is lowered.



d-wave pairing

The d-wave pair susceptibility is enhanced around the dome.



spin susceptibility

The peak of $\chi(q=0)$, the pseudogap scale, ends at the top of the dome.

Non-analyticity of the sign problem

$$\langle s \rangle_{|W|} = \frac{\mathcal{Z}_W}{\mathcal{Z}_{|W|}} \quad \therefore \quad \mathcal{Z}_W = \langle s \rangle_{|W|} \cdot \mathcal{Z}_{|W|}$$

$\mathcal{Z}_W$: Partition function of the **original** model

$\mathcal{Z}_{|W|}$: Partition function of the **reference** model

$$\rightarrow \mathcal{Z} = \exp(-\beta \mathcal{F})$$

Non-analyticity of the sign problem

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$\mathcal{Z}_W$: Partition function of the **original** model

$$\rightarrow \mathcal{Z} = \exp(-\beta \mathcal{F})$$

$\mathcal{Z}_{|W|}$: Partition function of the **reference** model

At a phase transition, a control parameter x is changed such that at x_c , $\mathcal{F}$ exhibits non-analytic* behavior

If we know that $\mathcal{Z}_W$ is non-analytic at $x_c \rightarrow$ either $\begin{cases} \langle s \rangle \\ \mathcal{Z}_{|W|} \end{cases}$ is non-analytic at the same point

➡ Provided that $\mathcal{Z}_{|W|}$ is sufficiently analytic close to $x_c \rightarrow \langle s \rangle$ has to display non-analytic behavior at x_c

*Analytic function: Infinitely differentiable function over a variable x such that it can be Taylor expanded at every point in its domain

By Rubem Mondaini

➡ Provided that $\mathcal{Z}_{|W|}$ is sufficiently analytic close to $x_c \rightarrow \langle s \rangle$ has to display non-analytic behavior at x_c

If a problem has a phase transition  there has to be a sign problem (provided $\mathcal{Z}_{|W|} \neq \mathcal{Z}_W$)

➡ Provided that $\mathcal{Z}_{|W|}$ is sufficiently analytic close to $x_c \rightarrow \langle s \rangle$ has to display non-analytic behavior at x_c

If a problem has a phase transition  there has to be a sign problem (provided $\mathcal{Z}_{|W|} \neq \mathcal{Z}_W$)

The converse is not true! There can be sign problem but not a phase transition in $\mathcal{Z}_W$

Example: Free fermions in 2d for WLQMC

$E_{\mathbf{k}} = -2t (\cos k_x + \cos k_y)$ $\mathcal{Z}_W$ Is clearly analytic (there are no phase transitions for free fermions!)

$$\mathcal{Z}_W = \int dn_1 \langle n_1 | \hat{U}_{\Delta\tau}^{L\tau} | n_1 \rangle = \int dn_1 \dots dn_{L\tau} \prod_{\tau} \langle n_{\tau} | \hat{U}_{\Delta\tau} | n_{\tau+1} \rangle$$

- Negative signs are due to fermionic phases from hoppings
- Taking the absolute value is akin to studying a hard-core boson model

2d hardcore bosons can have a finite T (BKT) transition to a superfluid phase

→ $\mathcal{Z}_{|W|}$ is non-analytic → **sign problem**

By Rubem Mondaini

Take-away messages

1 A nuisance and a signal

The sign problem limits DQMC to high temperatures and small lattices, but where the sign collapses tells us where the physics changes.

2 Not gauge invariant

The average sign depends on the algorithm and on the Hubbard–Stratonovich choice.

3 Not a solution

Nothing here removes the sign problem, and a dip does not prove a transition.

In practice: a map of $\langle S \rangle$ is a free by-product of every DQMC run. Look at it before discarding a parameter region.

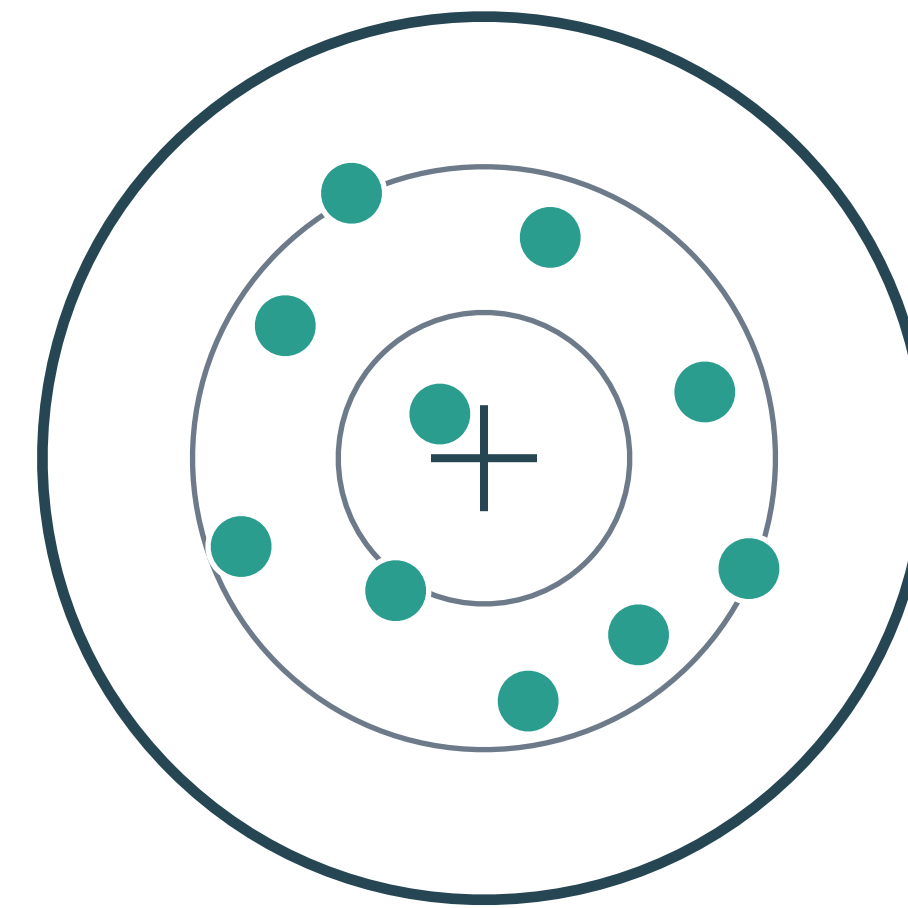
Other unbiased numerical methods

Exact diagonalization

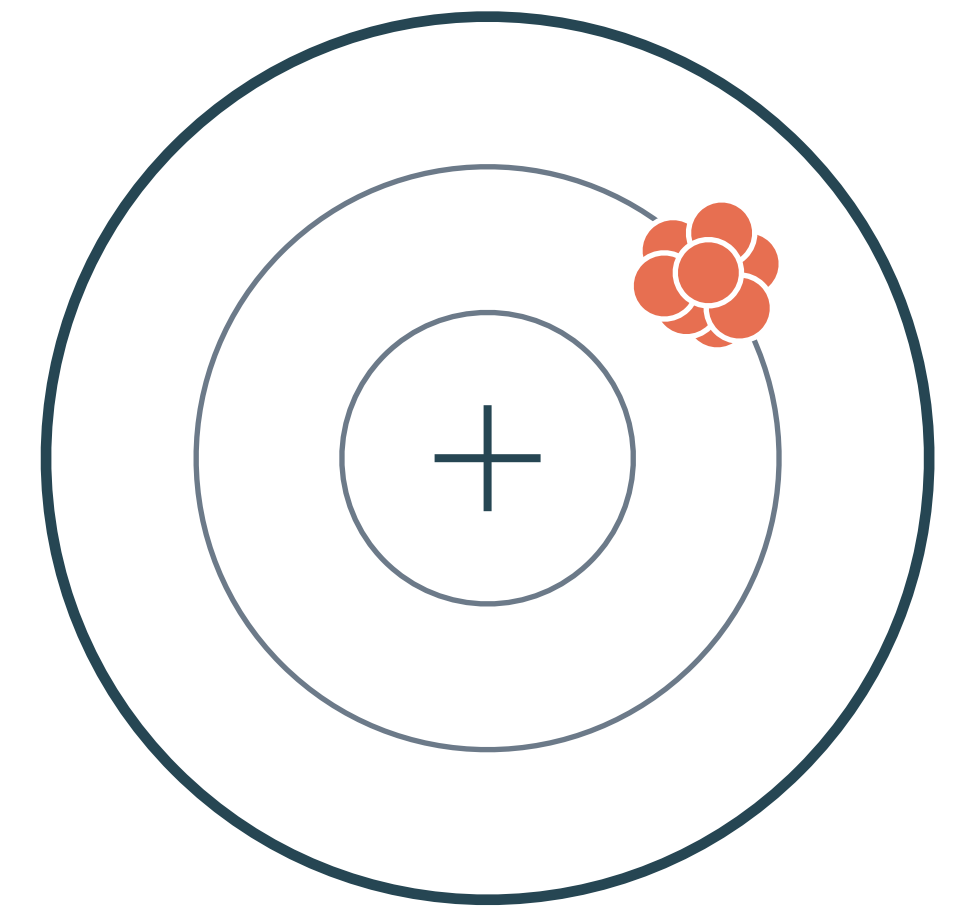
Lanczos method

Numerical Linked Cluster Expansion

Biases and unbiased methods



unbiased



biased

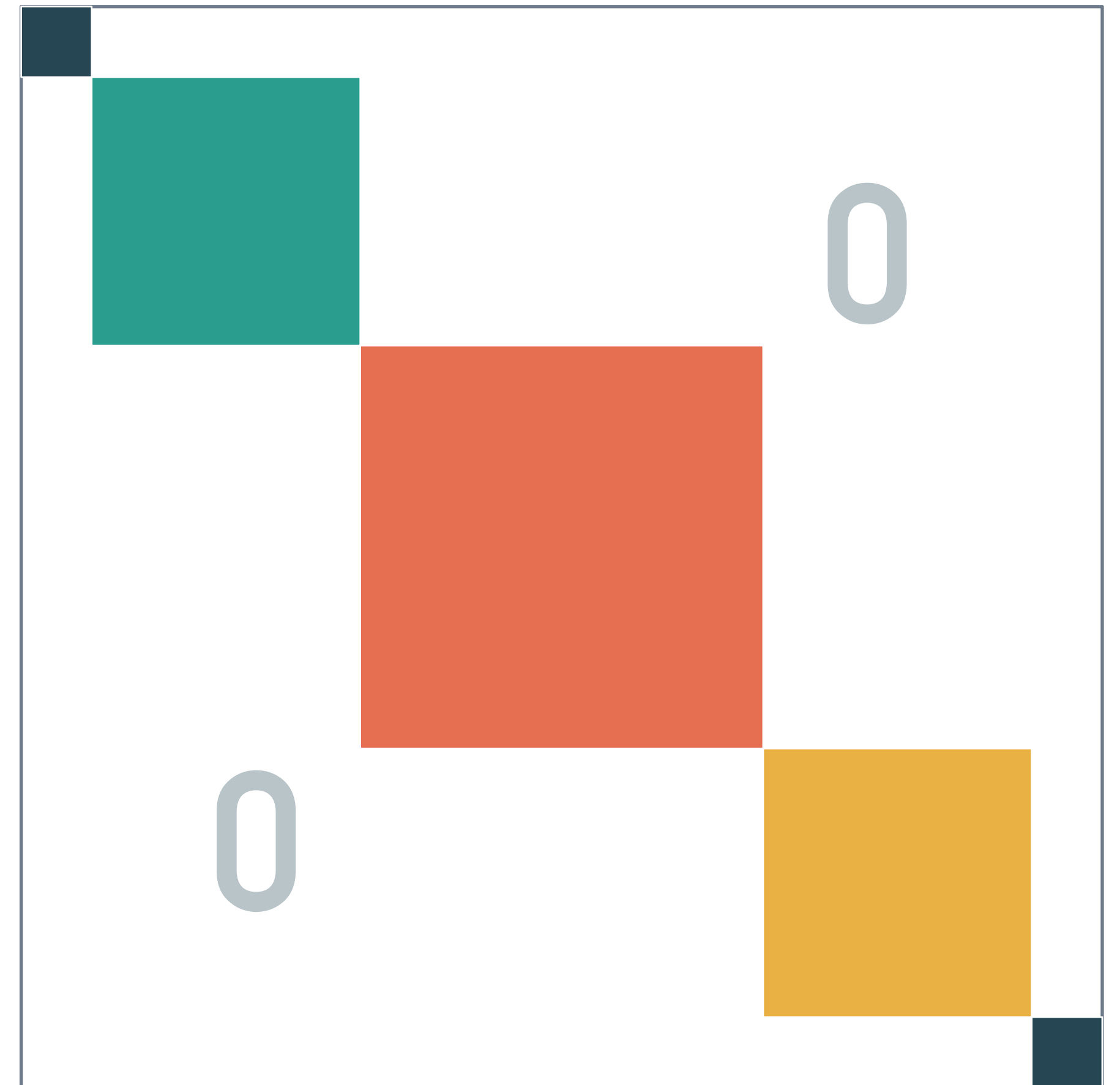
Unbiased methods and their error sources

METHOD	WHAT IS EXTRAPOLATED	KEEP IN MIND
● Exact diagonalization (full or Lanczos)	Cluster size	Small clusters only
● Quantum Monte Carlo: determinant, SSE, worm, path integral	Statistical error, system size, Trotter error	Sign problem
● Diagrammatic Monte Carlo	Statistical error, diagram order	Works directly in the thermodynamic limit
● DMRG and tensor networks (MPS, PEPS)	Bond dimension	Best in 1D and at low entanglement
● Series expansions: high temperature, numerical linked cluster expansion	Expansion order	Only where the series converges
● Numerical renormalization group	Discretization, states kept	Impurity models

Unbiased methods and their error sources

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Exact diagonalization



Exact Diagonalization

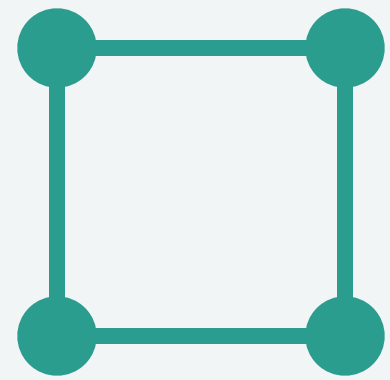
$$H |\psi\rangle = E |\psi\rangle$$

Choose a basis

Write the matrix in this basis

$$H |\psi\rangle = E |\psi\rangle$$

How to do it



1

Pick a cluster

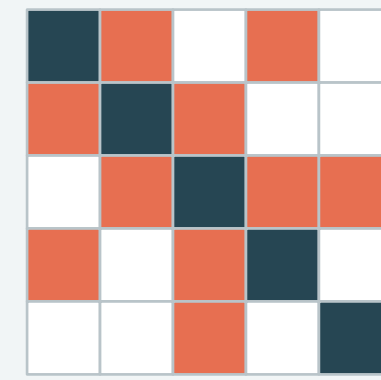
A few lattice sites, with open or periodic boundaries.

$|\uparrow\downarrow\uparrow\downarrow\rangle$
 $|\uparrow\uparrow\downarrow\downarrow\rangle$
 $|\downarrow\uparrow\uparrow\downarrow\rangle \dots$

2

Choose a basis

For example, all occupation or spin configurations.



3

Build the matrix

The elements of H between all pairs of basis states.



4

Diagonalize

All energies and eigenstates: any observable, at any temperature.

The price: the Hilbert space grows exponentially with the number of sites N

$$2^N$$

states for N spins $1/2$

$$4^N$$

states for the Hubbard model on N sites

$$4.3 \times 10^9$$

Hubbard states for $N = 16$ (65,536 for spins)

$$D^2 \text{ and } D^3$$

memory and time to fully diagonalize a matrix of dimension D

An observable that commutes with H makes the matrix block diagonal

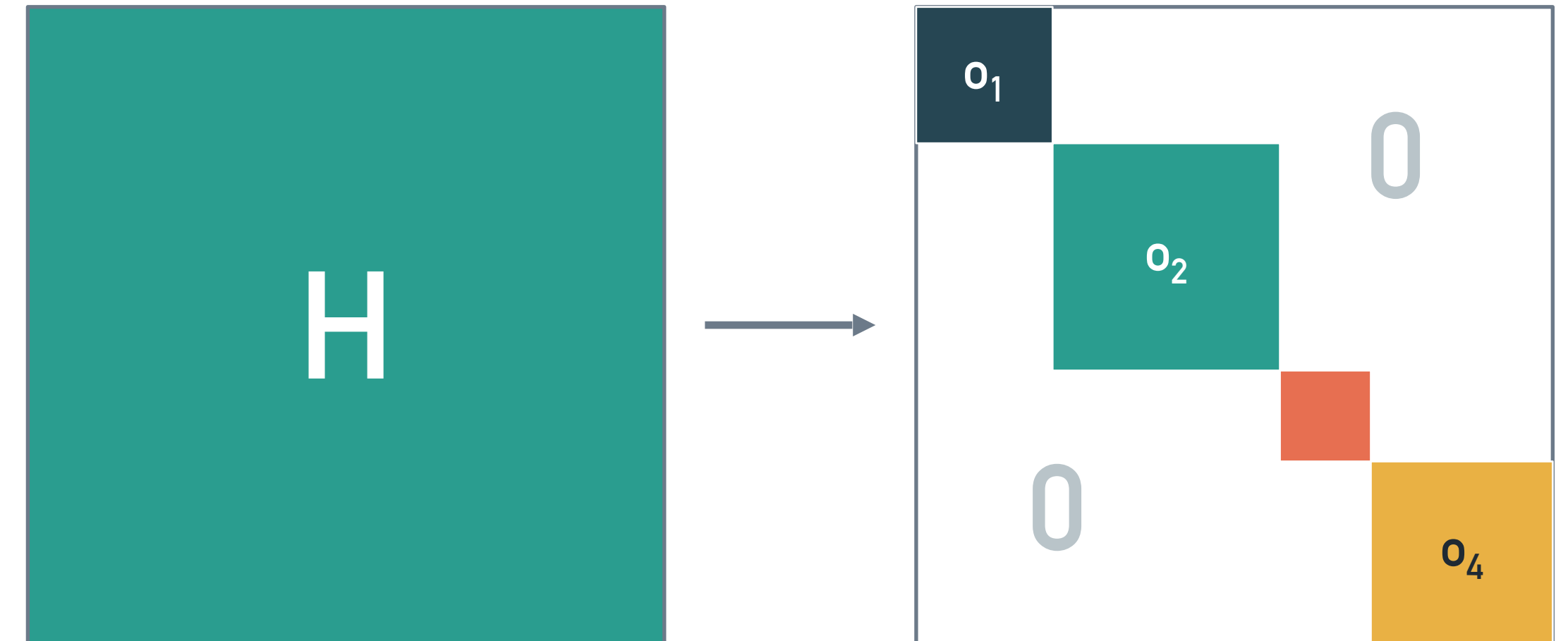
$$[H, O] = 0$$

Take two eigenstates of O, with eigenvalues o_a and o_b :

$$\langle a | [H, O] | b \rangle = (o_b - o_a) \langle a | H | b \rangle = 0$$

Whenever $o_a \neq o_b$ the matrix element $\langle a | H | b \rangle$ must vanish. H only connects states with the same quantum number.

- Order the basis by the eigenvalue of O and the zeros gather into off-diagonal blocks.
- Each block is a smaller, independent eigenvalue problem.
- Every eigenstate comes labelled by its quantum number.



H in an arbitrary basis

H in a basis of eigenstates of O

$$D^3 \rightarrow D_1^3 + D_2^3 + D_3^3 + \dots$$

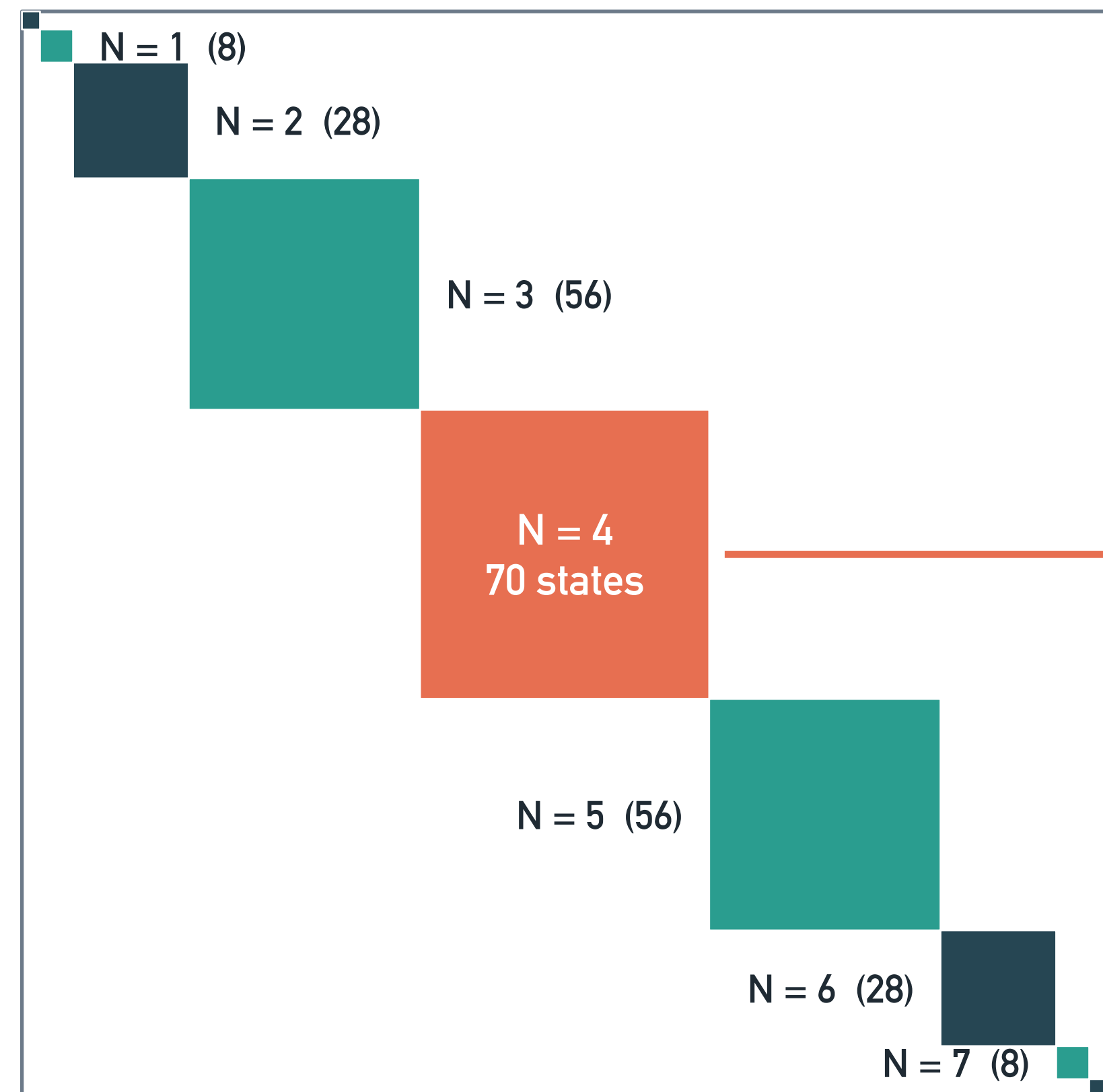
The cost of diagonalizing is set by the largest block, not by the full dimension.

Particle number and S^z : the Hubbard model on four sites

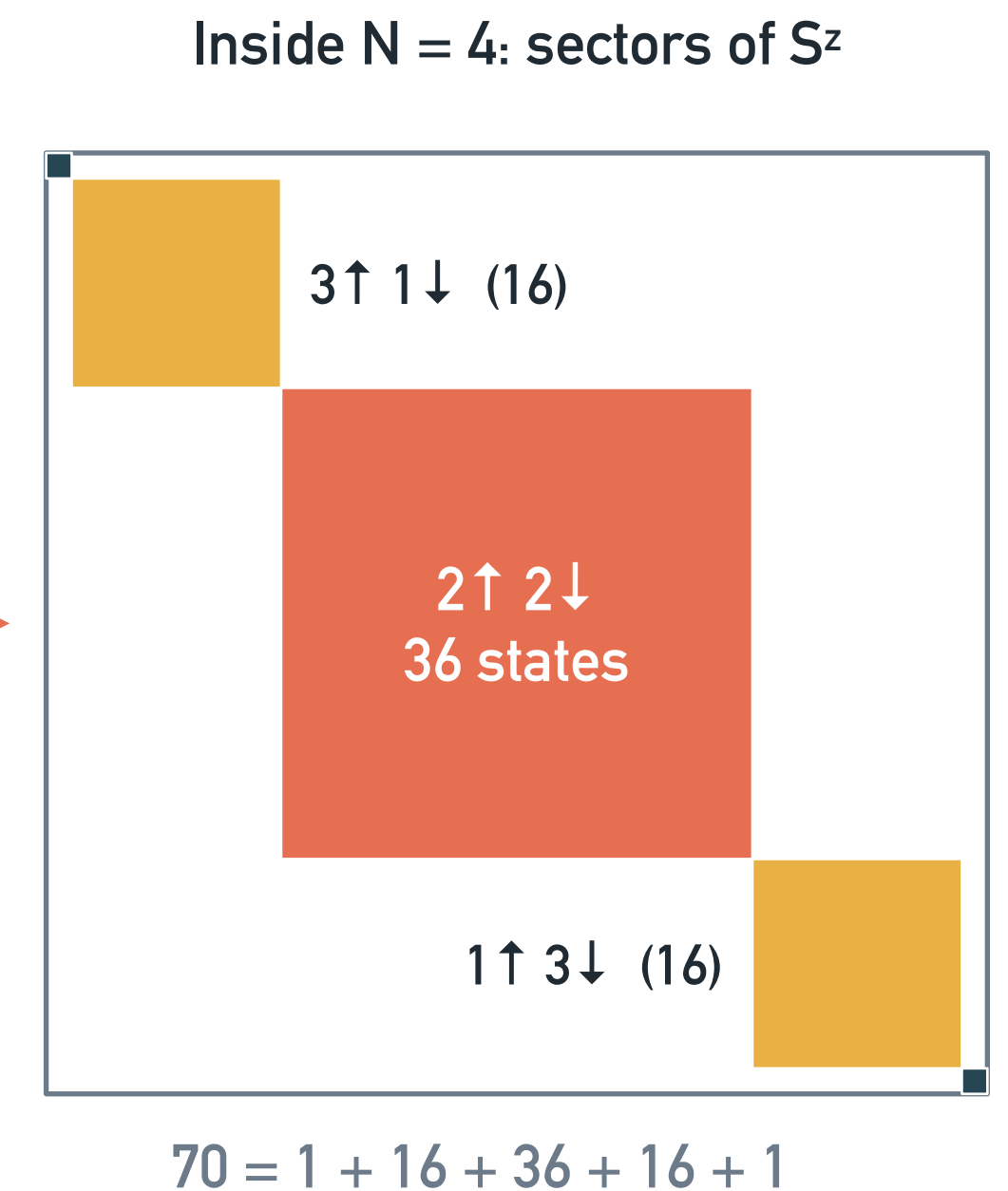
- Four states per site (empty, $\uparrow$, $\downarrow$, doubly occupied) give $4^4 = 256$ basis states.
- H conserves the particle number N : nine blocks, $N = 0$ to 8 , the largest with 70 states.
- H also conserves the spin projection: the $N = 4$ block splits into five, the largest with 36 states.

36 instead of 256

Largest block to diagonalize. With cost $\propto D^3$, about 360 times less work.



256 $\times$ 256 matrix, basis ordered by N . White areas are zeros.



Other symmetries also give blocks, but are harder to implement



N and S^z : just sort the basis

Every state of the occupation basis already has a definite N and S^z . Building the blocks only means grouping the basis states.

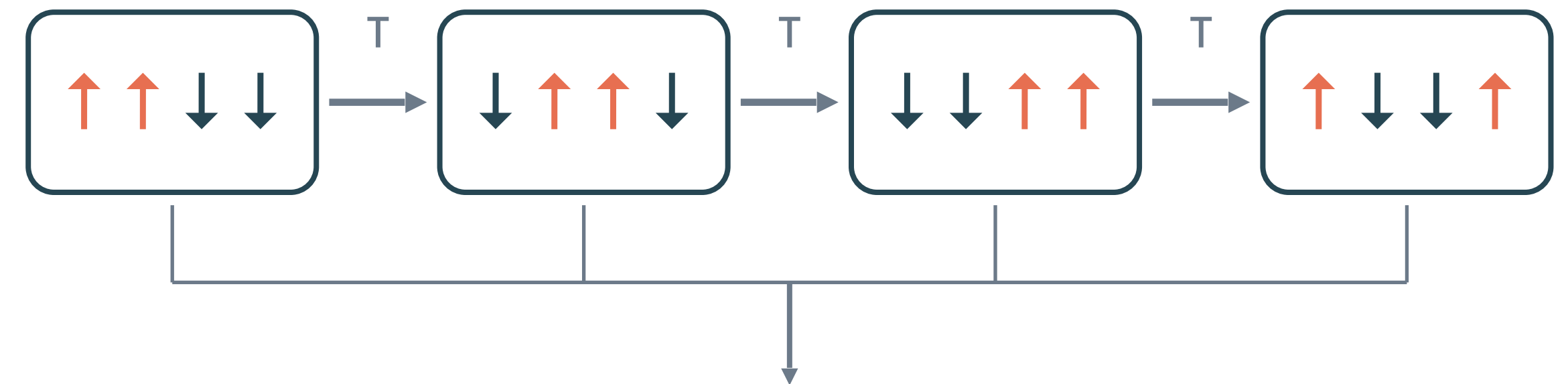


Translation, point group, time reversal or spin inversion

These operations turn one basis state into another. One has to build symmetry-adapted combinations and keep track of representatives, normalizations, phases and fermionic signs. Momentum blocks are complex matrices.

Translation on a 4-site ring

T shifts every spin by one site

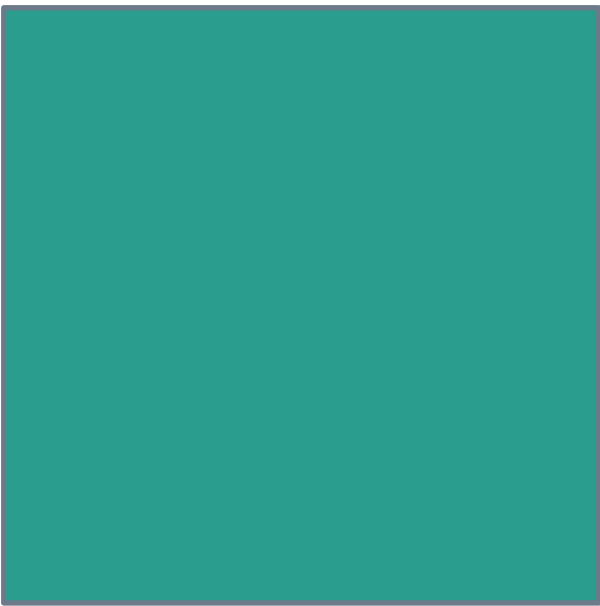


$$|a(k)\rangle = N_a^{-1/2} \sum_r e^{-ikr} T^r |a\rangle$$

Four basis states become one state per momentum k. Only one representative $|a\rangle$ is stored, and each block shrinks by roughly the number of sites.

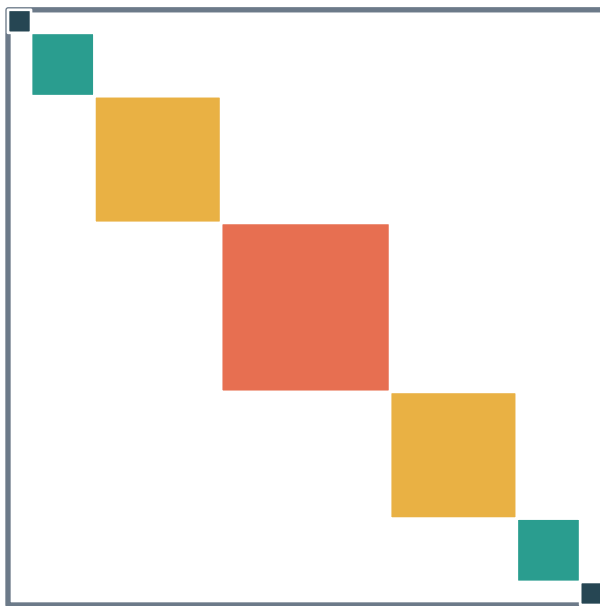
Each extra symmetry cuts the largest block again

Spin-1/2 Heisenberg ring with 16 sites: dimension of the largest matrix to diagonalize



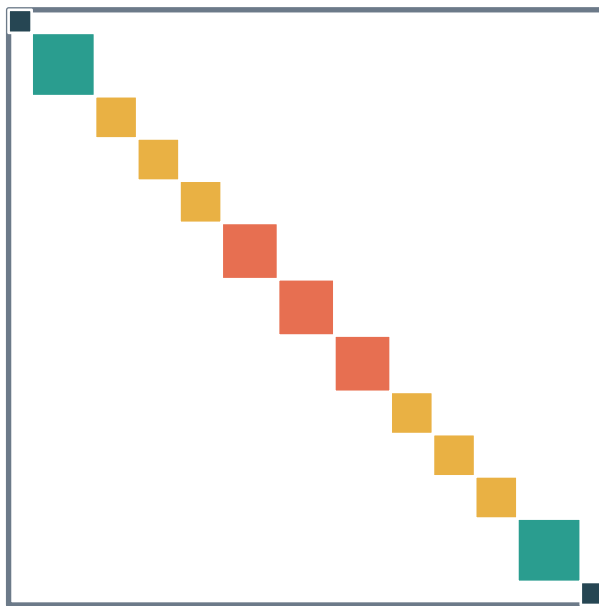
65,536

no symmetry used



12,870

$S^z = 0$ block



810

$S^z = 0, k = 0$ block

SYMMETRY	QUANTUM NUMBER	BLOCK SIZE	IMPLEMENTATION
Particle number, spin projection	N, S^z	strong reduction	● Easy: sort the basis
Translation	momentum k	$\div$ number of sites	● Representatives and phases
Point group: reflections, rotations	parity, irreps	$\div$ 2 to 8	● Only at special momenta
Time reversal or spin inversion	± 1 , at $S^z = 0$	$\div$ 2	● Extra phases to track
Total spin	S	sizeable	● Hard: no simple product basis

Exact diagonalization in practice

1

Encode the basis

Store each basis state as an integer whose bits are the occupations.

2

Sort into sectors

Group the states by N and S_z ; add momentum or parity if needed.

3

Build H block by block

Only a few non-zero elements per row: the blocks are sparse.

4

Diagonalize each block

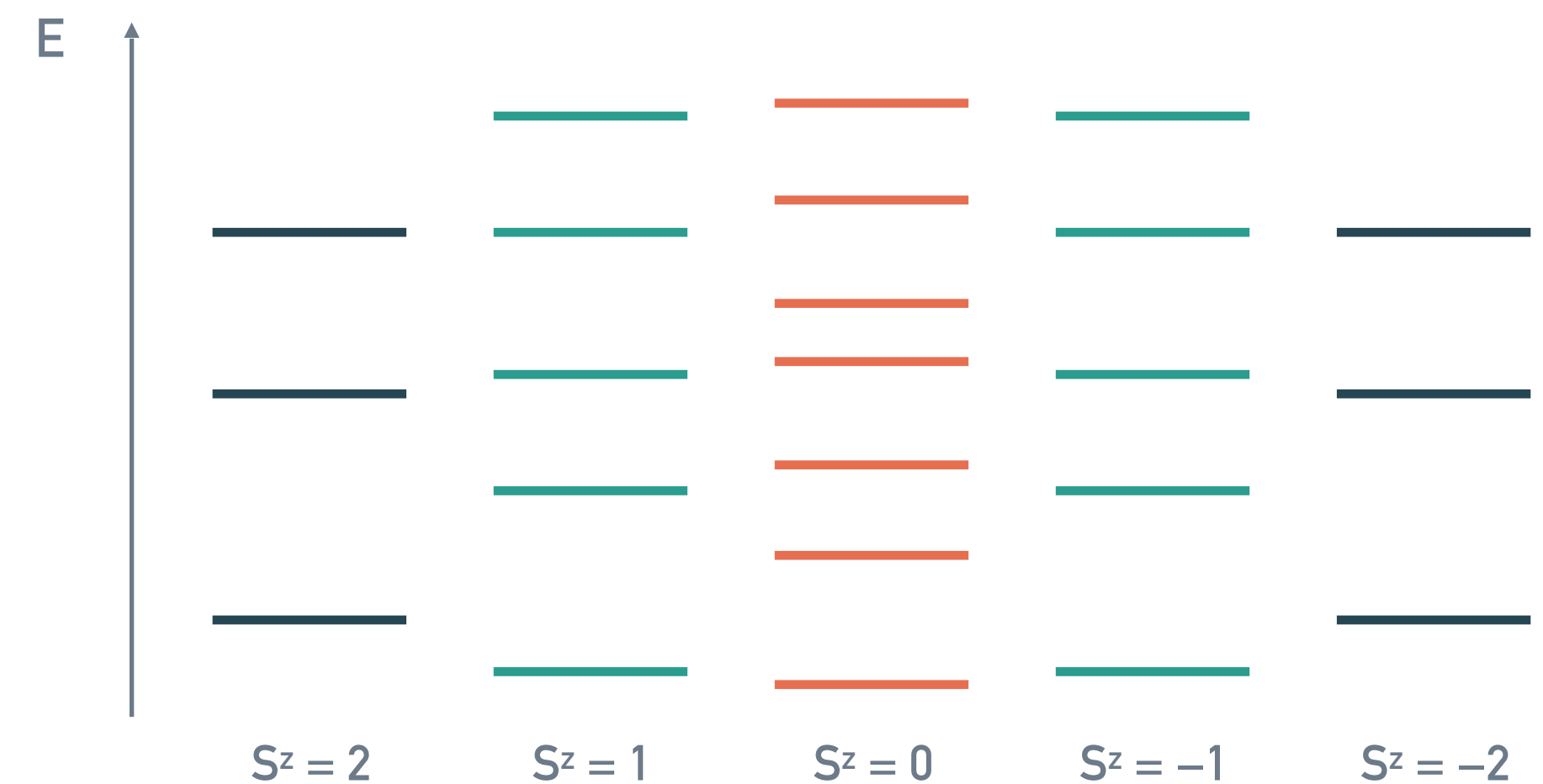
Full diagonalization for all temperatures; Lanczos for ground states of larger clusters.

5

Combine the sectors

Sum over all blocks to obtain thermal averages.

One spectrum per block



$$Z = \sum_{\text{blocks}} \sum_n e^{-\beta E}$$

The blocks are independent problems, but thermal averages need all of them.

Advantages

Exact

All eigenvalues and eigenstates

Can be easy to code

Limitations

Restricted to small system sizes

Can be hard to code if many symmetries are implemented to increase system sizes

Lanczos method

An Iteration Method for the Solution of the Eigenvalue Problem of Linear Differential and Integral Operators¹

By Cornelius Lanczos

The present investigation designs a systematic method for finding the latent roots and the principal axes of a matrix, without reducing the order of the matrix. It is characterized by a wide field of applicability and great accuracy, since the accumulation of rounding errors is avoided, through the process of "minimized iterations". Moreover, the method leads to a well convergent successive approximation procedure by which the solution of integral equations of the Fredholm type and the solution of the eigenvalue problem of linear differential and integral operators may be accomplished.

Lanczos method

Write the hamiltonian in a tridiagonal form

Diagonalize as it is built

$\left[\begin{array}{c} a_0 \end{array} \right]$

$\left[\begin{array}{c} \end{array} \right]$

$|\phi_0\rangle$

$$a_n = \frac{\langle \phi_n | \hat{H} | \phi_n \rangle}{\langle \phi_n | \phi_n \rangle},$$

$$b_0 = 0$$

$$\begin{bmatrix} a_0 & b_1 \\ b_1 & a_1 \end{bmatrix}$$

$$\begin{bmatrix} |\phi_1\rangle = \hat{H}|\phi_0\rangle - \frac{\langle\phi_0|\hat{H}|\phi_0\rangle}{\langle\phi_0|\phi_0\rangle}|\phi_0\rangle \\ a_n = \frac{\langle\phi_n|\hat{H}|\phi_n\rangle}{\langle\phi_n|\phi_n\rangle}, \quad b_n^2 = \frac{\langle\phi_n|\phi_n\rangle}{\langle\phi_{n-1}|\phi_{n-1}\rangle} \end{bmatrix}$$

$$\langle\phi_0|\phi_1\rangle = 0$$

$$\begin{bmatrix} a_0 & b_1 & 0 \\ b_1 & a_1 & b_2 \\ 0 & b_2 & a_2 \end{bmatrix}$$

$$\begin{bmatrix}$$

$$|\phi_2\rangle = \hat{H}|\phi_1\rangle - \frac{\langle\phi_1|\hat{H}|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle}|\phi_1\rangle - \frac{\langle\phi_1|\phi_1\rangle}{\langle\phi_0|\phi_0\rangle}|\phi_0\rangle$$

$$a_n = \frac{\langle\phi_n|\hat{H}|\phi_n\rangle}{\langle\phi_n|\phi_n\rangle}, \quad b_n^2 = \frac{\langle\phi_n|\phi_n\rangle}{\langle\phi_{n-1}|\phi_{n-1}\rangle}$$

$$\langle\phi_1|\phi_2\rangle = \langle\phi_0|\phi_2\rangle = 0$$

$$\begin{bmatrix} a_0 & b_1 & 0 & 0 \\ b_1 & a_1 & b_2 & 0 \\ 0 & b_2 & a_2 & b_3 \\ 0 & 0 & b_3 & a_3 \end{bmatrix}$$

$$\begin{bmatrix}$$

$$|\phi_{n+1}\rangle = \hat{H}|\phi_n\rangle - a_n|\phi_n\rangle - b_n^2|\phi_{n-1}\rangle$$

$$a_n = \frac{\langle \phi_n | \hat{H} | \phi_n \rangle}{\langle \phi_n | \phi_n \rangle}, \quad b_n^2 = \frac{\langle \phi_n | \phi_n \rangle}{\langle \phi_{n-1} | \phi_{n-1} \rangle}$$

$$\langle \phi_n | \phi_{n+1} \rangle = 0$$

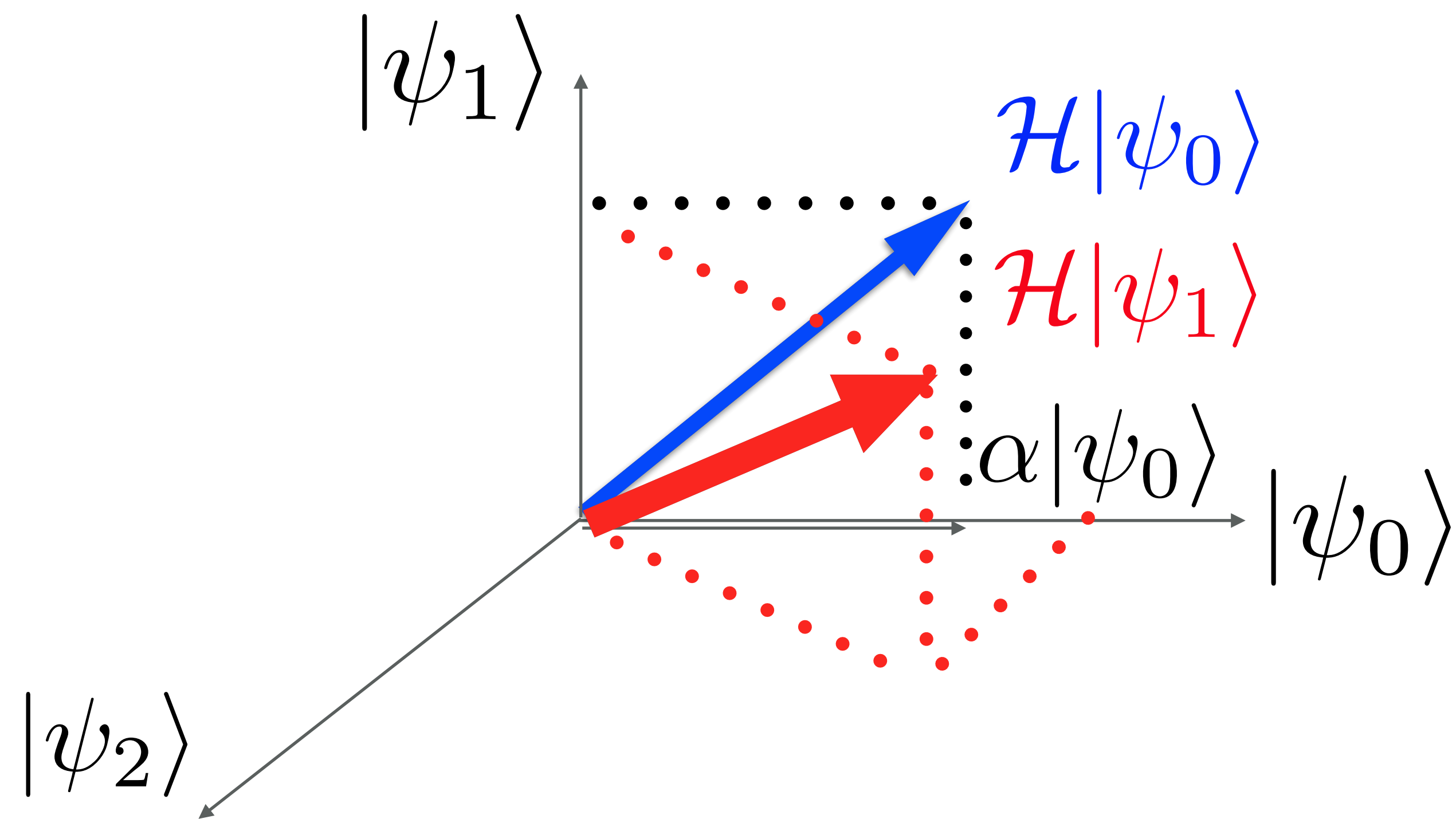
Lanczos method

Write the hamiltonian in a tridiagonal form

Diagonalize as it is built

Compare the energy at each step

Stop when $|\varepsilon^{n+1} - \varepsilon^n| < \epsilon$



An alternative implementation

PHYSICAL REVIEW B

VOLUME 34, NUMBER 3

1 AUGUST 1986

Correlation functions of the antiferromagnetic Heisenberg model using a modified Lanczos method

Eduardo R. Gagliano

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8400 San Carlos de Bariloche, Río Negro, Argentina*

Elbio Dagotto and Adriana Moreo

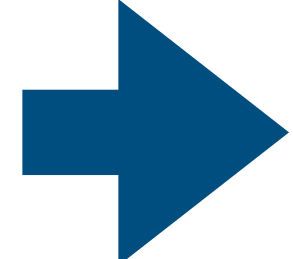
Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801

Francisco C. Alcaraz

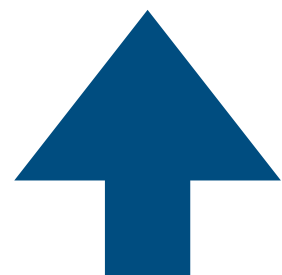
Departamento de Física da Universidade Federal de São Carlos, Caixa Postal 616, 13 560 São Carlos, São Paulo, Brazil

(Received 23 September 1985; revised manuscript received 30 January 1986)

An alternative implementation

ψ_0  Initial trial function

$$\langle \phi_0 | \psi_0 \rangle \neq 0$$


True ground state

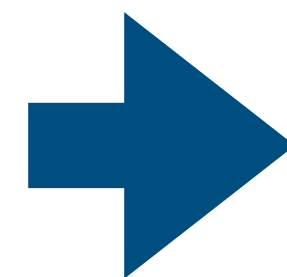
An alternative implementation

$\psi_0 \rightarrow$ Initial trial function

$\psi_1 \rightarrow \psi_1 = \frac{H\psi_0 - \langle H \rangle \psi_0}{(\langle H^2 \rangle - \langle H \rangle^2)^{1/2}} \rightarrow \langle \psi_0 | \psi_1 \rangle = 0$

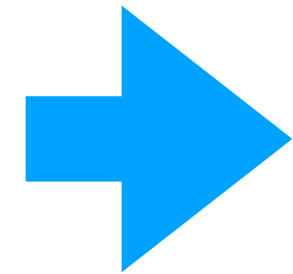
$\uparrow$
 $\langle \psi_0 | H^n | \psi_0 \rangle = \langle H^n \rangle$

2 x 2 space



**Easy to diagonalize
and to store**

Improved energy



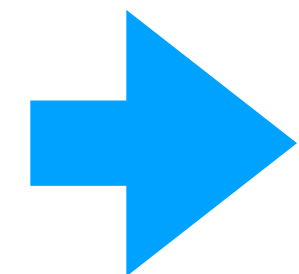
$$\varepsilon_1 = \langle H \rangle + b\alpha$$

$$b = (\langle H^2 \rangle - \langle H \rangle^2)^{1/2},$$

$$\alpha = f - (f^2 + 1)^{1/2}$$

$$f = \frac{\langle H^3 \rangle - 3\langle H \rangle \langle H^2 \rangle + 2\langle H \rangle^3}{2(\langle H^2 \rangle - \langle H \rangle^2)^{3/2}}$$

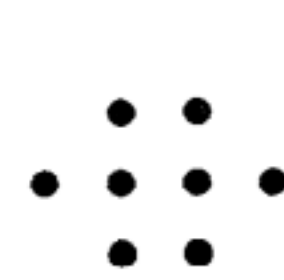
Improved state



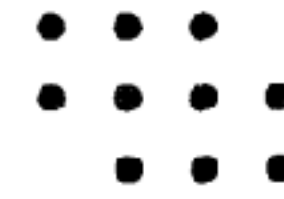
$$\tilde{\psi}_0 = \frac{\psi_0 + \alpha\psi_1}{(1 + \alpha^2)^{1/2}}$$

Stop when $|\varepsilon^{n+1} - \varepsilon^n| < \epsilon$

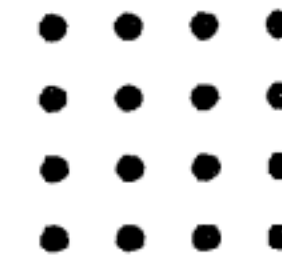
Popular tilted lattices for ED and Lanczos



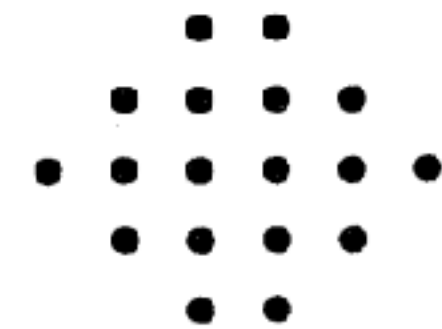
$N = 8$



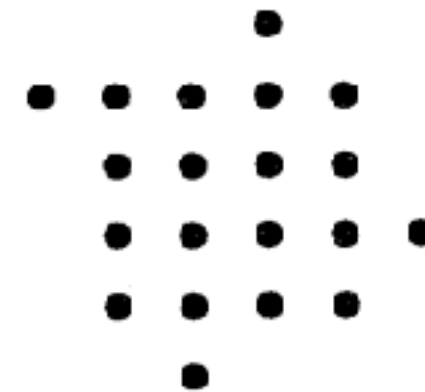
$N = 10$



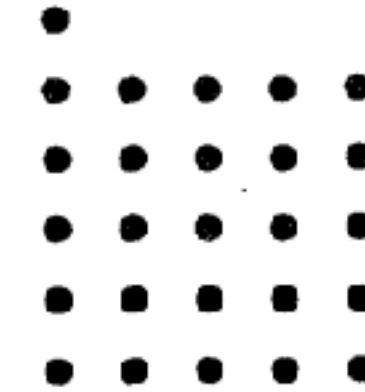
$N = 16$



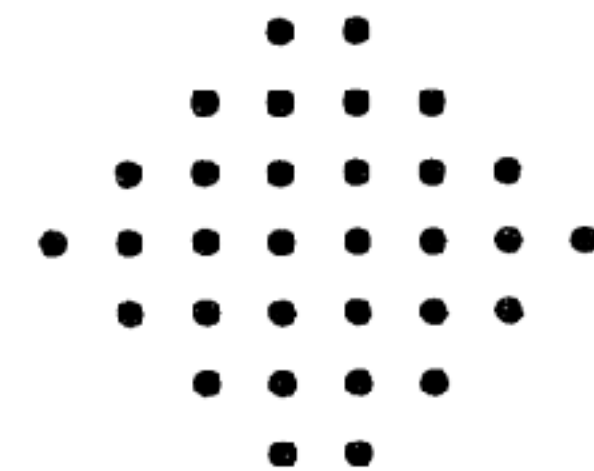
$N = 18$



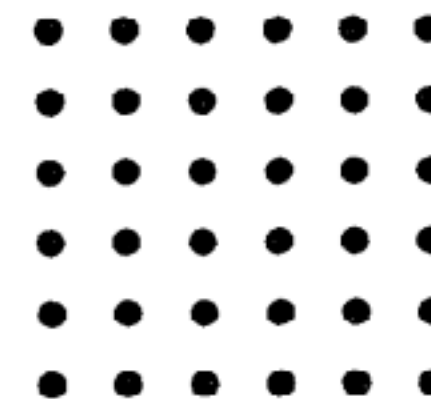
$N = 20$



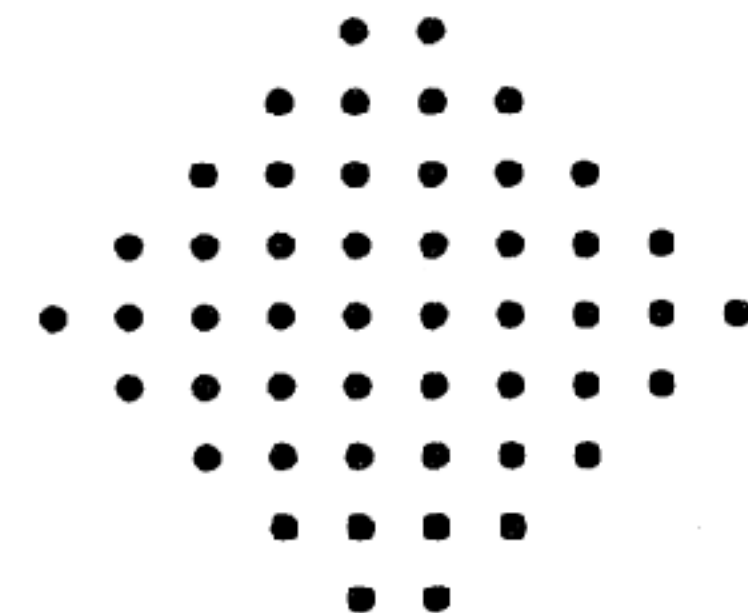
$N = 26$



$N = 32$



$N = 36$



$N = 50$



Advantages

Easy to code

Exact

System sizes larger than
direct ED



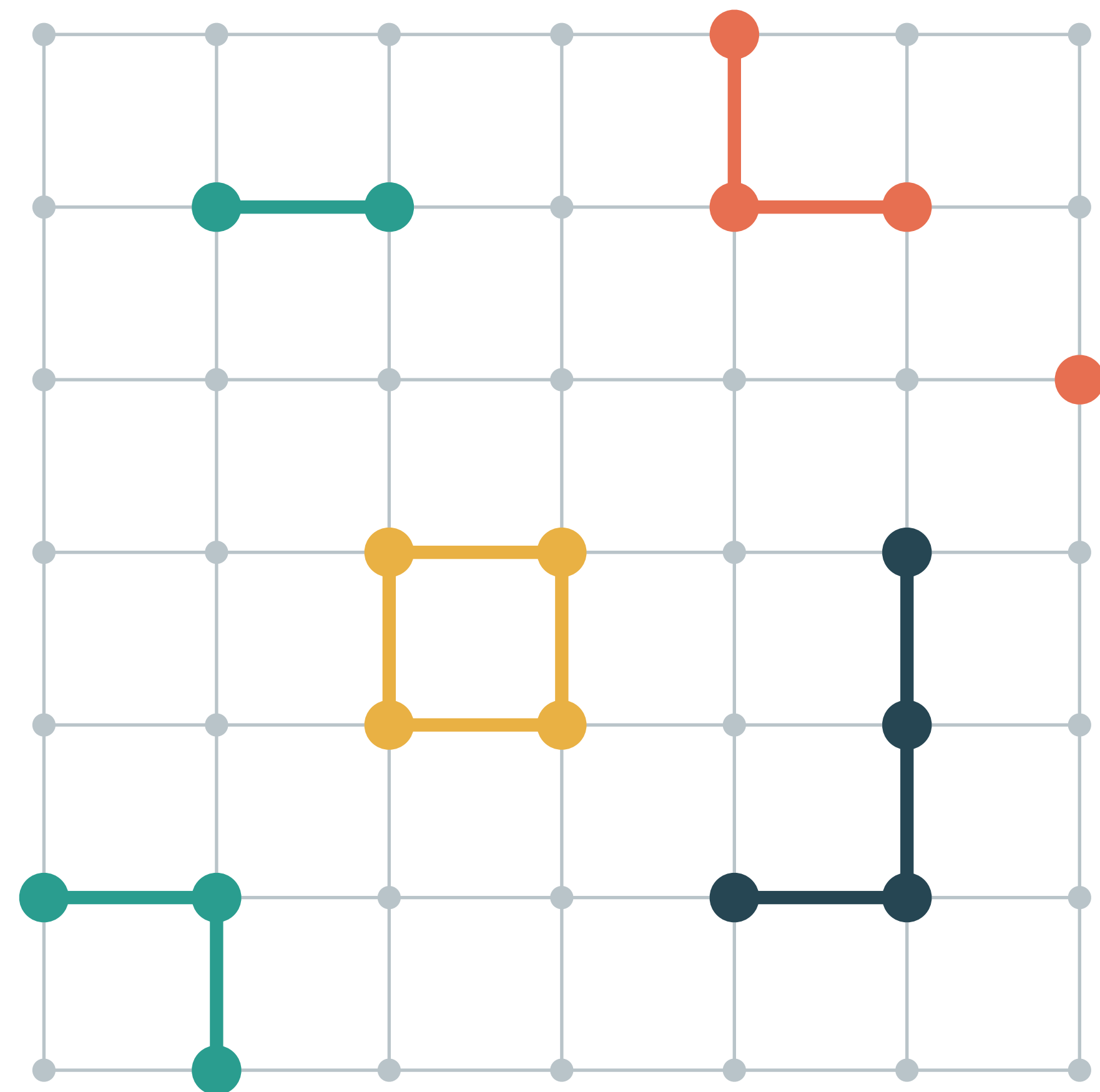
Limitations

Ground state and low energy
states

Restricted to small system sizes

Problem when the ground state is
degenerate

Numerical Linked Cluster Expansion



Numerical Linked-Cluster Approach to Quantum Lattice Models

Marcos Rigol, Tyler Bryant, and Rajiv R. P. Singh

Department of Physics, University of California, Davis, California 95616, USA

(Received 15 August 2006; published 3 November 2006)

We present a novel algorithm that allows one to obtain temperature dependent properties of quantum lattice models in the thermodynamic limit from exact diagonalization of small clusters. Our numerical linked-cluster approach provides a systematic framework to assess finite-size effects and is valid for any quantum lattice model. Unlike high temperature expansions, which have a finite radius of convergence in inverse temperature, these calculations are accurate at all temperatures provided the range of correlations is finite. We illustrate the power of our approach studying spin models on kagomé, triangular, and square lattices.

PHYSICAL REVIEW E **75**, 061118 (2007)

Numerical linked-cluster algorithms. I. Spin systems on square, triangular, and kagomé lattices

Marcos Rigol

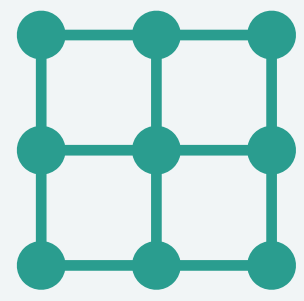
Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089, USA

Tyler Bryant and Rajiv R. P. Singh

Department of Physics, University of California, Davis, California 95616, USA

(Received 31 October 2006; published 21 June 2007)

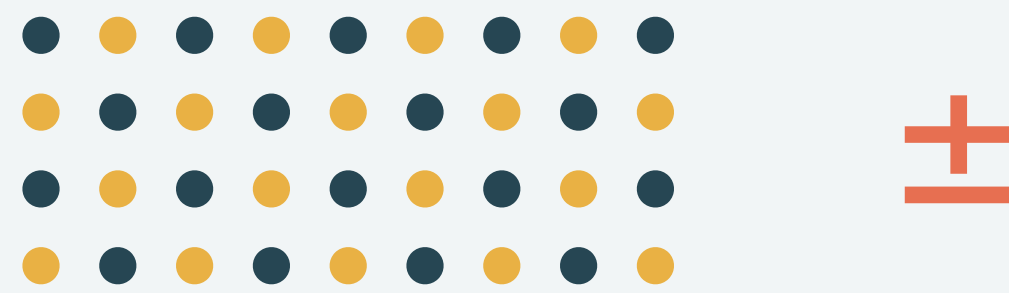
Three standard routes to finite-temperature properties, each with a blind spot



Exact diagonalization

finite clusters

Exact, any model. But only small clusters, and finite-size effects are hard to assess at $T > 0$ in more than one dimension.



Quantum Monte Carlo

finite, large lattices

Much larger systems. But the sign problem severely limits the models that can be studied (frustration, fermions).

$$1 + a_1\beta + a_2\beta^2 + a_3\beta^3 + \dots$$

High-temperature expansion

thermodynamic limit

No finite-size effects. But the series in $\beta = 1/T$ diverges below $T \sim J$, even when correlations are still short ranged.

NLCE

Keep the linked-cluster basis of the high-temperature expansion, but **replace the expansion in β by an exact diagonalization of every cluster**, valid at any temperature.

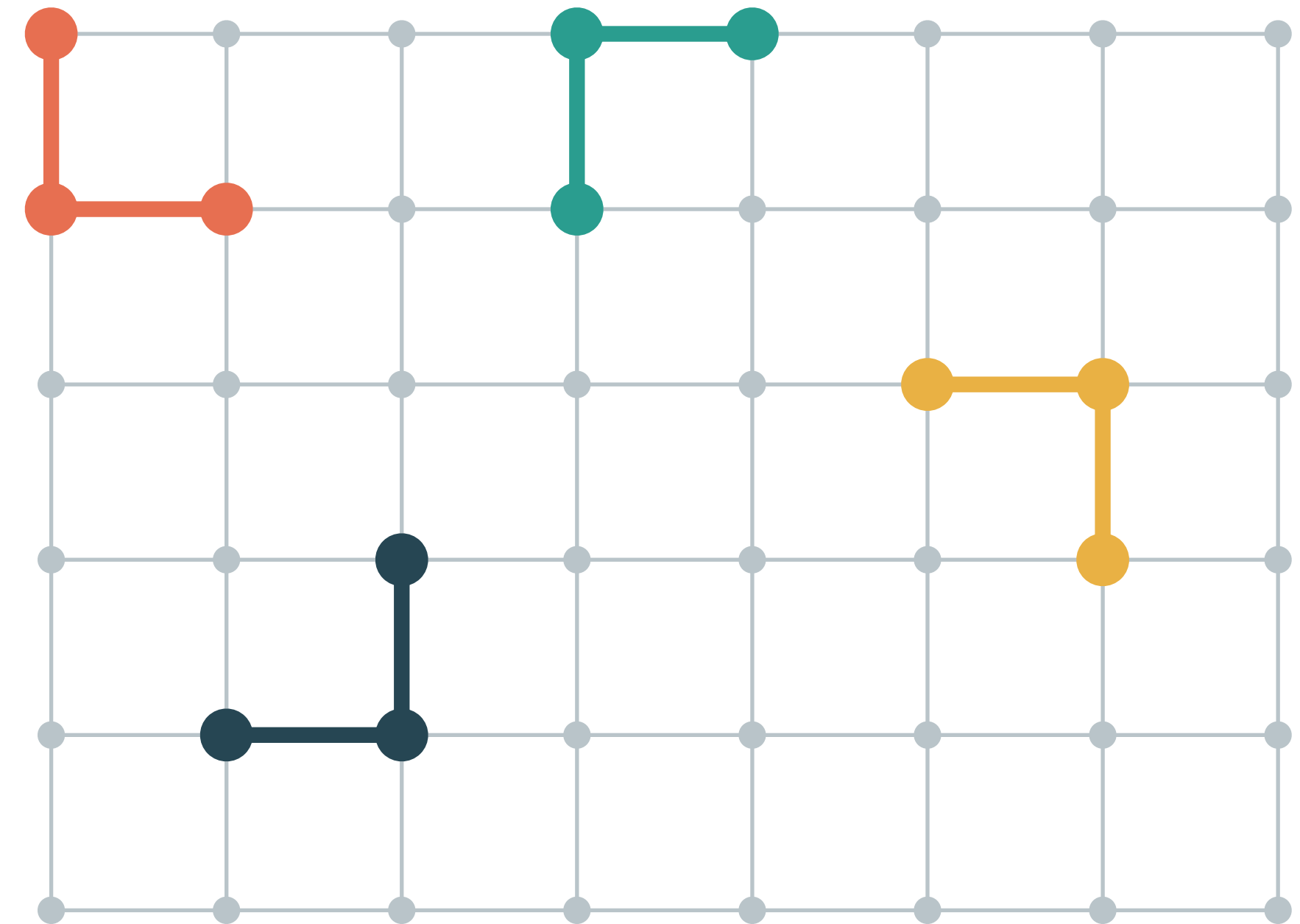
One sum over clusters, with weights fixed by inclusion–exclusion

$$P(L) / N = \sum_c L(c) \times W_p(c)$$

- P : extensive property of the infinite lattice (energy, entropy, specific heat, susceptibility)
- $L(c)$: lattice constant, the number of embeddings of cluster c per site
- $W(c)$: weight of cluster c

$$W_p(c) = P(c) - \sum_{s \subset c} W_p(s)$$

- $P(c)$: the property computed on the finite cluster c , with open boundaries
- The sum runs over all proper subclusters s of c
- HTE expands $P(c)$ in β and truncates; NLCE diagonalizes c exactly



Lattice constant, by example. The bent 3-site cluster fits the square lattice in 4 distinct orientations per site, so $L(c) = 4$.

The smallest clusters on the square lattice

CLUSTER

L(c)

WEIGHT



1

$$W_1 = P_1$$



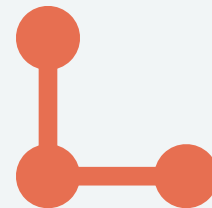
2

$$W_2 = P_2 - 2W_1$$



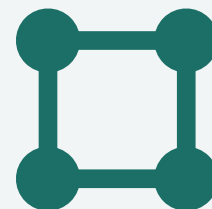
2

$$W_{3a} = P_{3a} - 2W_2 - 3W_1$$



4

$$W_{3b} = P_{3b} - 2W_2 - 3W_1$$



1

$$W_4 = P_4 - 4W_{3b} - 4W_2 - 4W_1$$

Reading the weights

- $W(c)$ is what cluster c adds beyond all of its parts.
- Check: for decoupled sites $P(c) = n P_1$, so every weight beyond the single site vanishes.
- Weights become negligible once clusters are larger than the correlation length. That is the convergence test.

$$P/N \approx W_1 + 2W_2 + 2W_{3a} + 4W_{3b} + \dots$$

each weight multiplied by its lattice constant

Square lattice

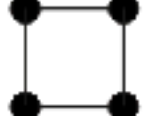
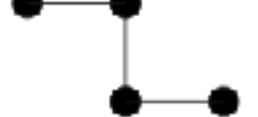
	c	$L(c)$
	1	1
	2	2
	3	2
	4	4
	5	4
	6	2
	7	1
	8	4
	9	8

TABLE II. Number of topological clusters and sum of lattice constants for clusters with up to 16 sites in the square lattice.

No. of sites	No. of topological clusters	$\Sigma L(c)$
1	1	1
2	1	2
3	1	6
4	3	19
5	4	63
6	10	216
7	19	760
8	51	2725
9	112	9910
10	300	36 446
11	746	135 268
12	2042	505 861
13	5450	1 903 890
14	15 197	7 204 874
15	42 192	27 394 666
16	119 561	104 592 937

The algorithm in six steps

1 Enumerate clusters

Generate all linked clusters up to order n for the chosen building block and count their embeddings per site, $L(c)$.



2 Group by topology

Clusters with the same connectivity share one Hamiltonian, so each topology is diagonalized only once.



3 Diagonalize exactly

Full diagonalization with open boundaries gives $P(c)$ at any temperature: energy, entropy, specific heat, susceptibility.

4 Subtract subclusters

Build the weights $W(c)$ by inclusion-exclusion, starting from the single site and moving up.



5 Sum order by order

Add $L(c) \times W(c)$ over all clusters of order n , and form the partial sums $P_1, P_2, \dots, P_n$.

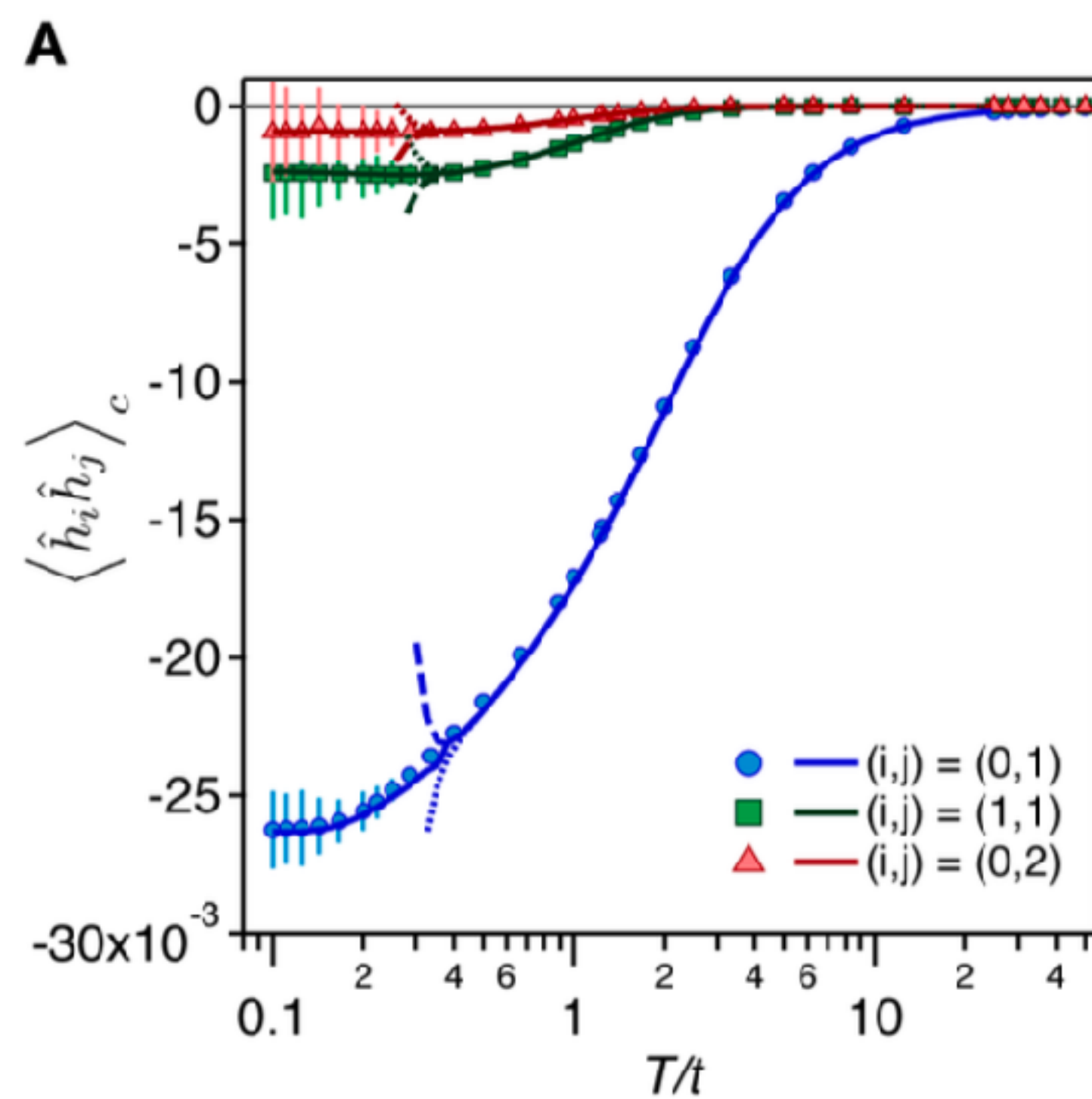


6 Test convergence

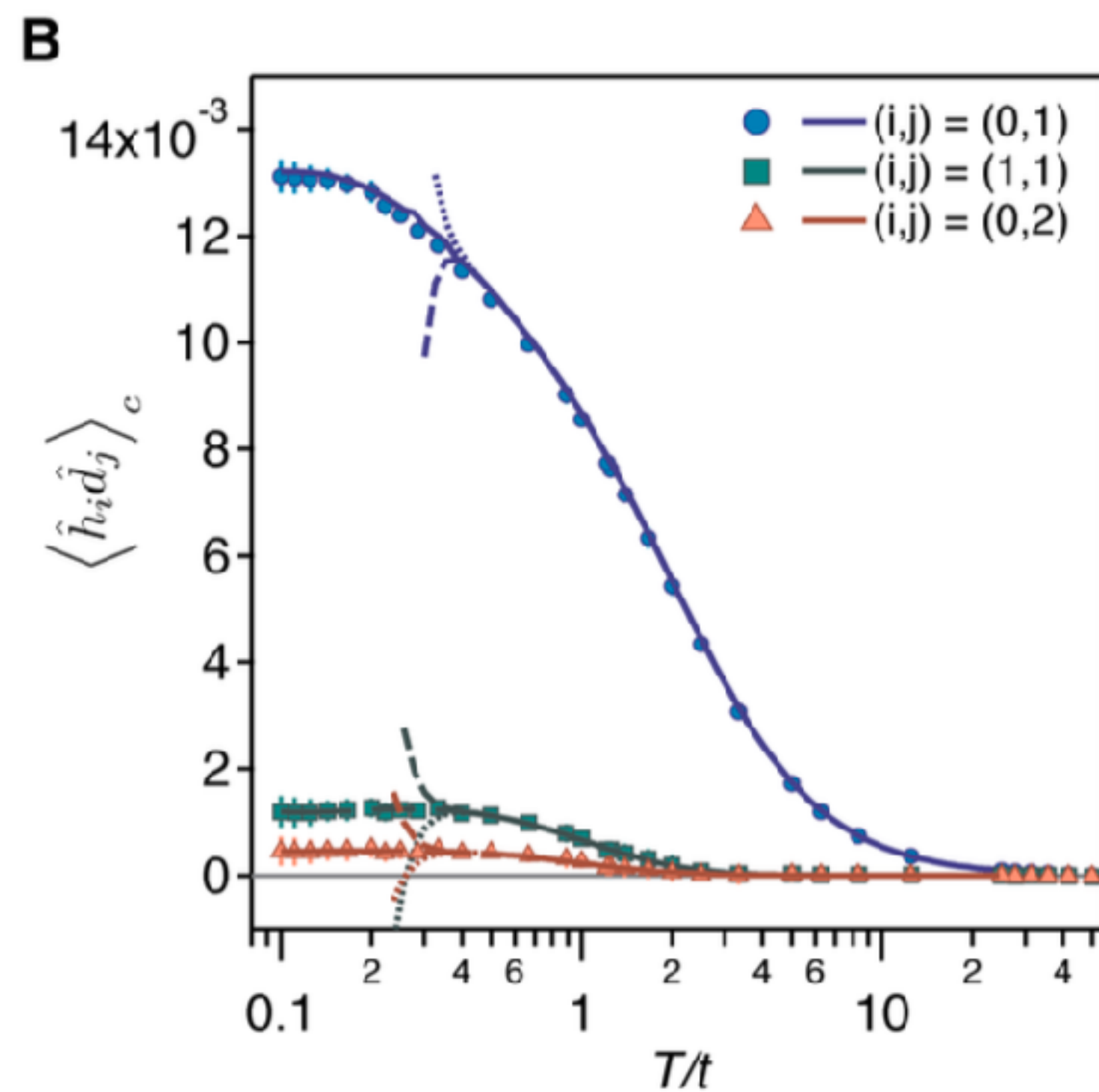
Compare the last two orders. Where they split, resum the sequence: Wynn, Brezinski or Euler.

In the original work the bottleneck was computing time, from the sheer number of clusters, and not memory: 16 to 60 hours on a 3.2 GHz desktop PC.

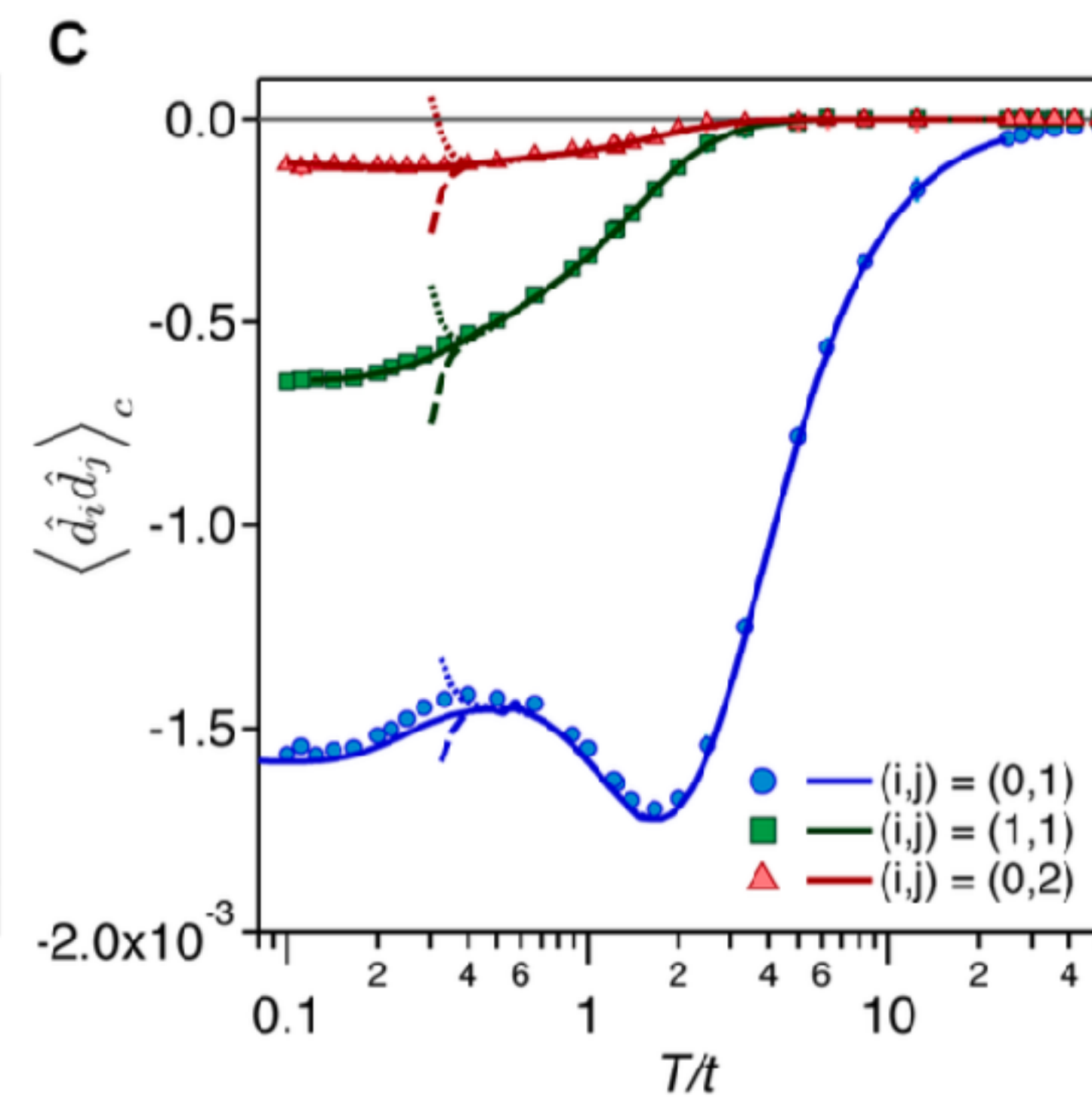
Hole-hole



Hole-doublon



Doublon-doublon



Advantages

- Thermodynamic limit directly. No finite-size extrapolation, unlike ED or QMC on finite lattices.
- Goes beyond HTE. Each cluster is exact at any T , and the convergence region grows with cluster size.
- No sign problem. Works for frustrated magnets and fermions, where QMC fails.
- Self-diagnosing. Where successive orders agree, the result is converged.
- Unbiased. Open clusters of every shape: no periodic box that favours one type of order.
- Flexible. Bonds, sites, squares or triangles; copes with widely separated energy scales.

Limitations

- Limited by the correlation length. Fails at low T in ordered or critical systems.
- Exponential cost. Both the number of clusters and the ED of each one: 13 to 17 sites in the original work.
- Resummation is uncontrolled. Wynn, Brezinski and Euler give no rigorous error bars, like Padé for HTE.
- No analytic structure in β . HTE remains the better tool for critical points and exponents.
- QMC wins where it applies. Without a sign problem it reaches far larger lattices and lower T .

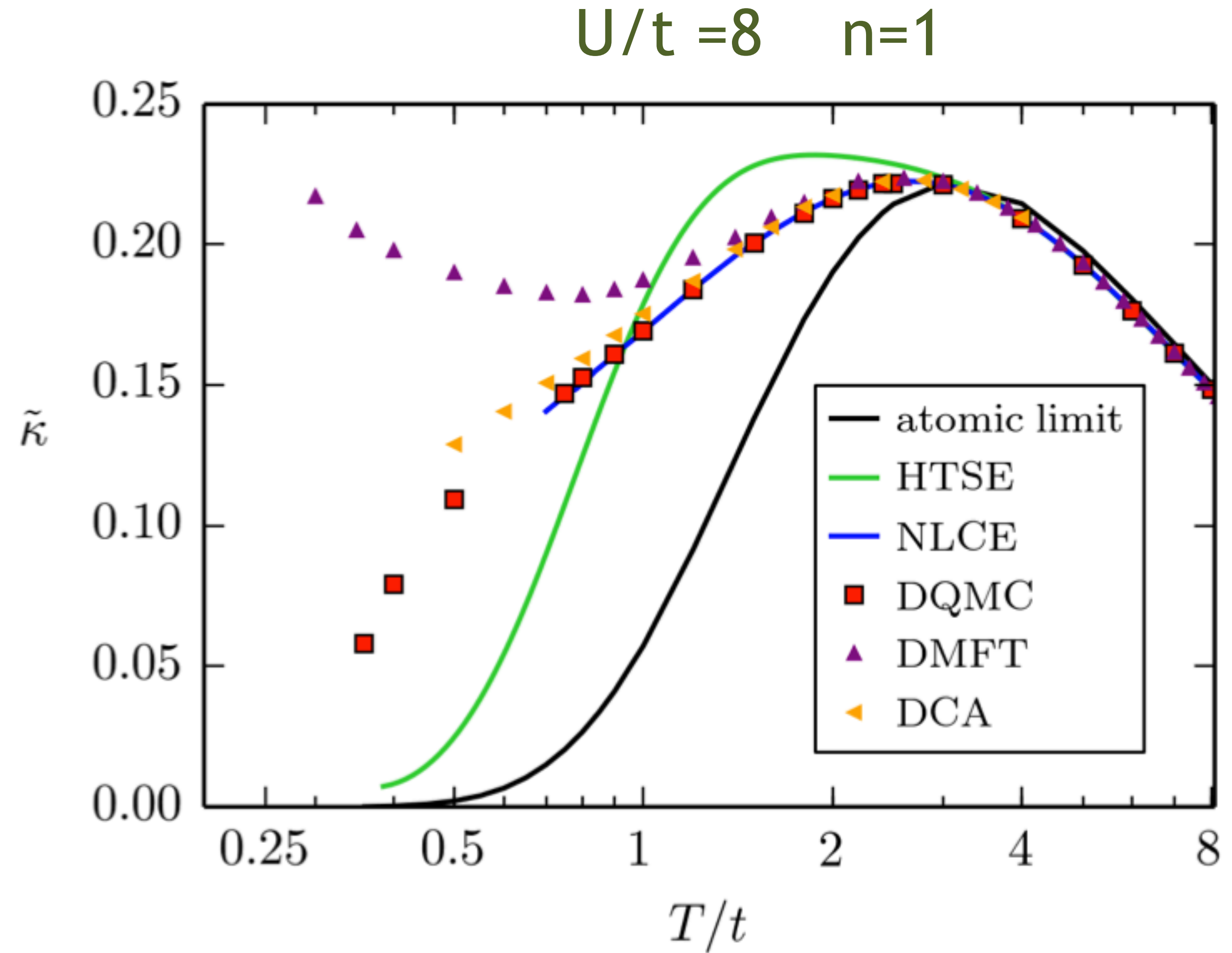
Comparing different methods

$T/t > 2$
Atomic limit, HTSE

$T/t \sim 1$
DMFT

$T/t \sim 0.5$
DQMC, DCA, NLCE

DCA - E. Gull
DMFT - J. Imriska and T. Schäfer



Summarizing what we discussed this
week

Monte Carlo Method

Importance sampling

Markovian processes

Ergodicity

Detailed balance

Monte Carlo Method

Measurements

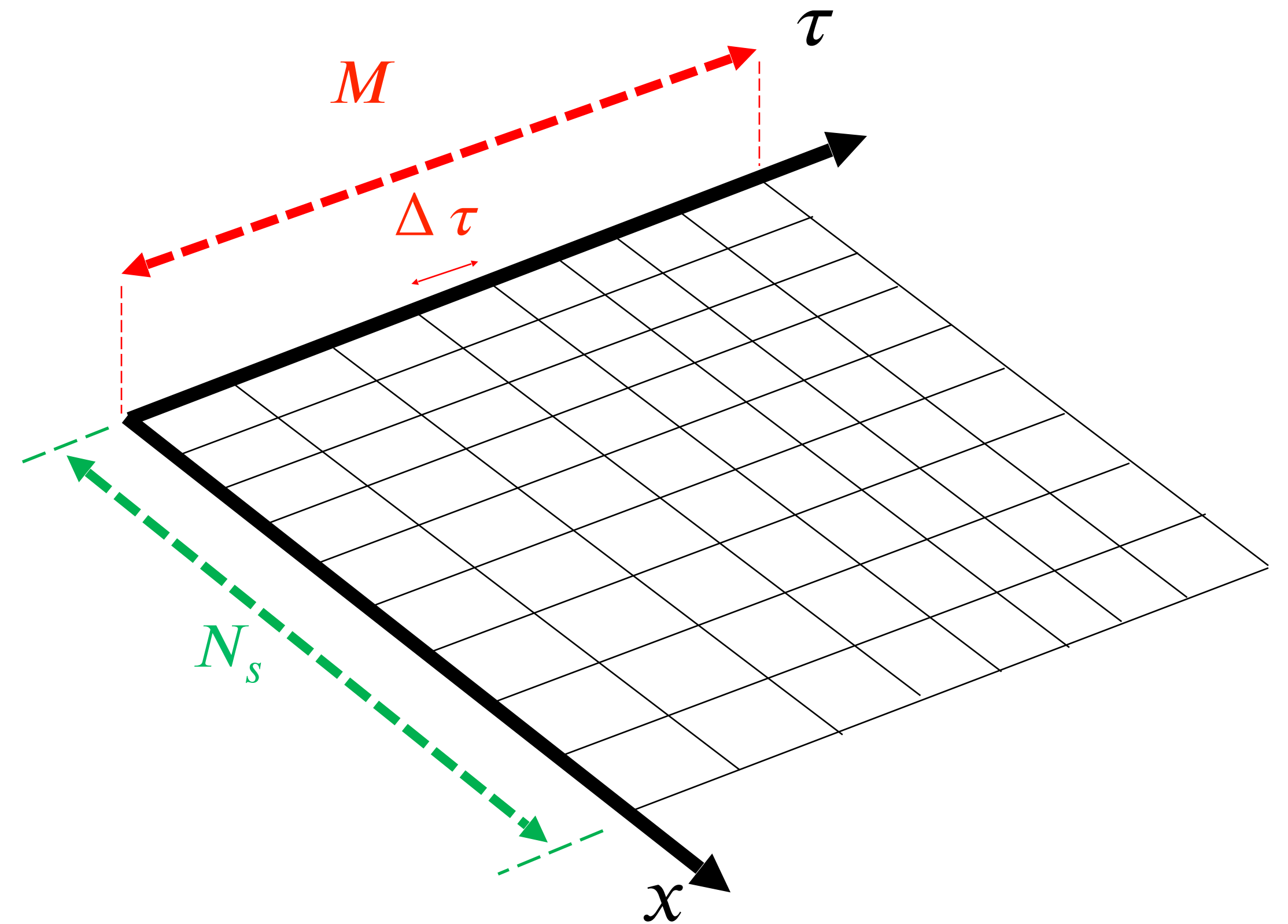
Finite size scaling

DQMC

$$e^{-\beta H} = \underbrace{e^{-\Delta\tau H} e^{-\Delta\tau H} \dots e^{-\Delta\tau H}}_{M \text{ factors}},$$

$$\Delta\tau = \beta/M$$

$$e^{-\Delta\tau(A+B)} = e^{-\Delta\tau A} e^{-\Delta\tau B} + \mathcal{O}(\Delta\tau^2)$$

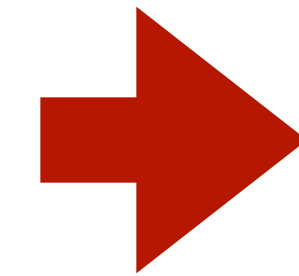


Maps a d-dimensional quantum problem in a d+1 dimensional classical problem

DQMC

Choose a basis

Do a Trotter–Suzuki decomposition

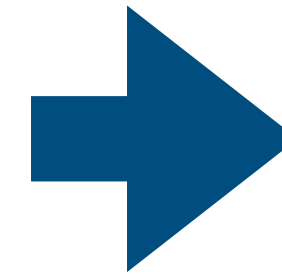


Imaginary time

Insert identities

PROBLEM

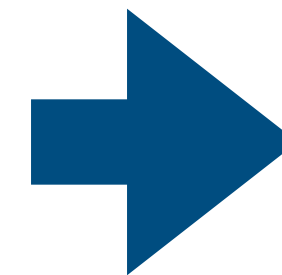
$$K = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$



Quadratic



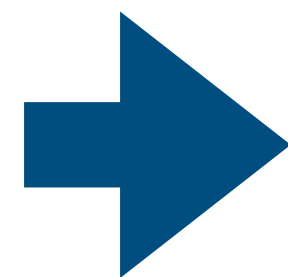
$$V = U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$$



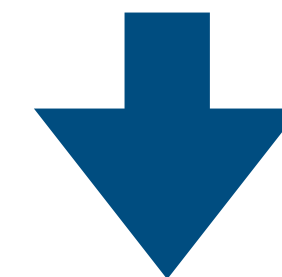
Quartic



SOLUTION



Hubbard-Stratonovich transformation



Introduce auxiliary field: $s = \pm 1$

$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \text{Tr}_{\{s\}} \mathcal{T} r \prod_{\ell=M}^1 \prod_{\sigma=\uparrow,\downarrow} e^{-\Delta\tau \sum_{i,j} c_{i\sigma}^\dagger K_{ij} c_{j\sigma}} e^{-\Delta\tau \sum_i c_{i\sigma}^\dagger V_i^\sigma(\ell) c_{i\sigma}}$$

$\ell = M, \dots, 1$ Earlier times to the right

$$V_i^\sigma(\ell) = \frac{1}{\Delta\tau} \lambda_\sigma s_i(\ell) + \left(\mu - \frac{U}{2} \right)$$

Trace over the $N \times M$
auxiliary variables:

Monte Carlo Sampling

Introducing the B matrices

$$\mathbf{B}_\ell^\sigma \equiv e^{-\Delta\tau\mathbf{K}} e^{-\Delta\tau V^\sigma(\ell)}$$

$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \text{Tr}_{\{s\}} \prod_{\sigma} \det [\mathbf{1} + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \dots \mathbf{B}_1^\sigma]$$

Introducing the O matrices

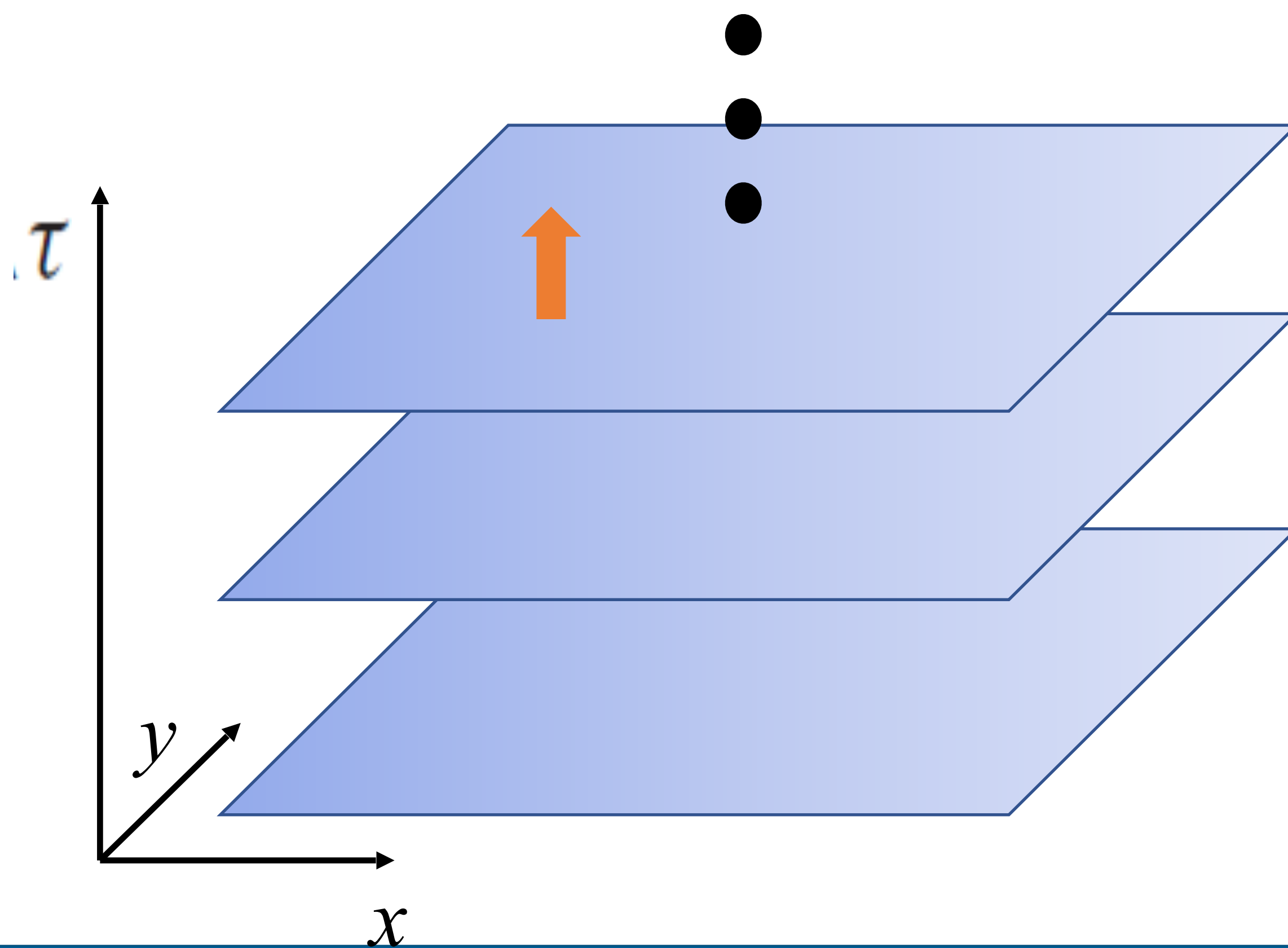
$$\mathbf{O}^\sigma(\{s\}) \equiv \mathbf{1} + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \dots \mathbf{B}_1^\sigma$$

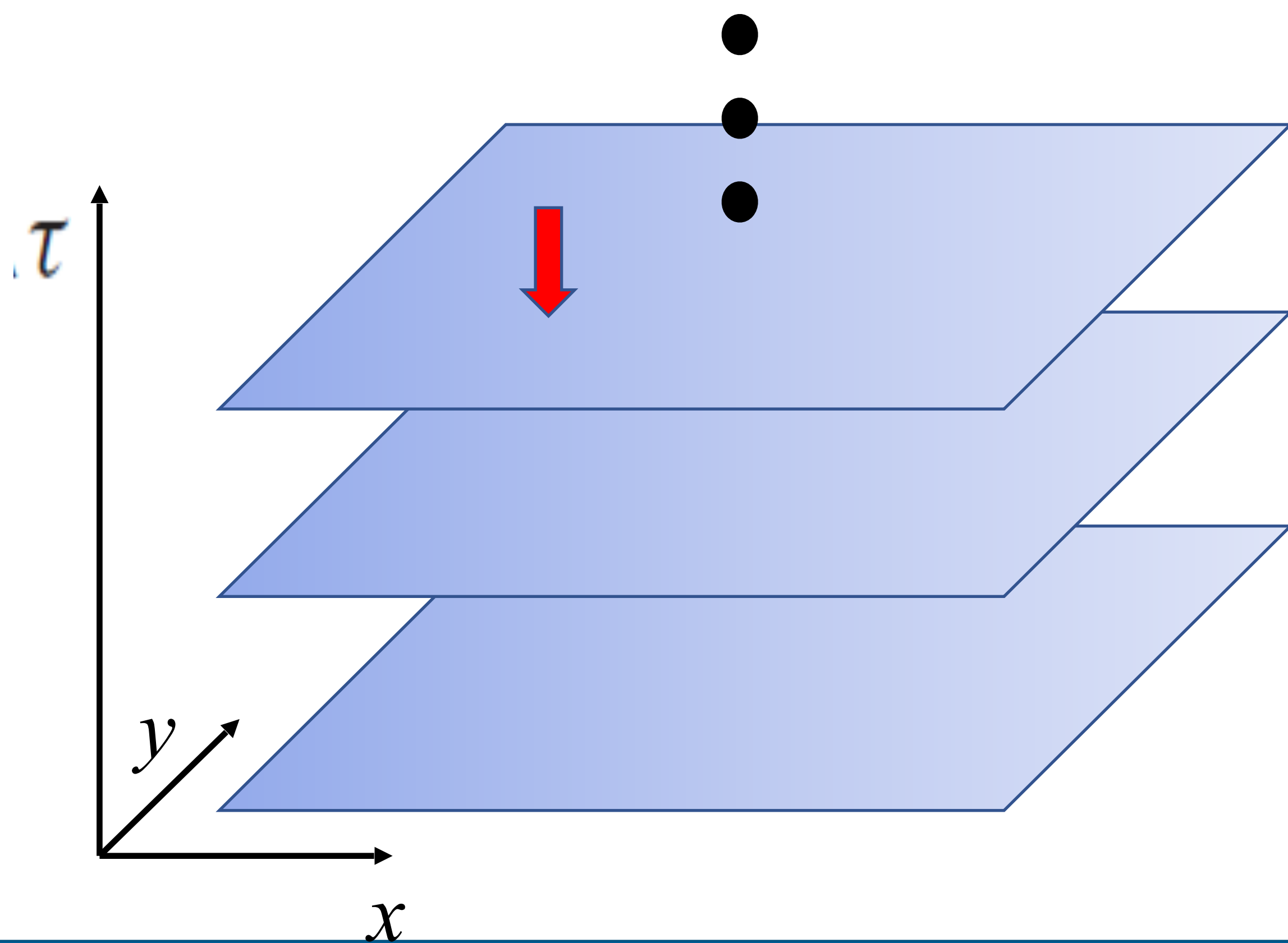
$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \text{Tr}_{\{s\}} \det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\})$$

Determinantal Quantum Monte Carlo

or

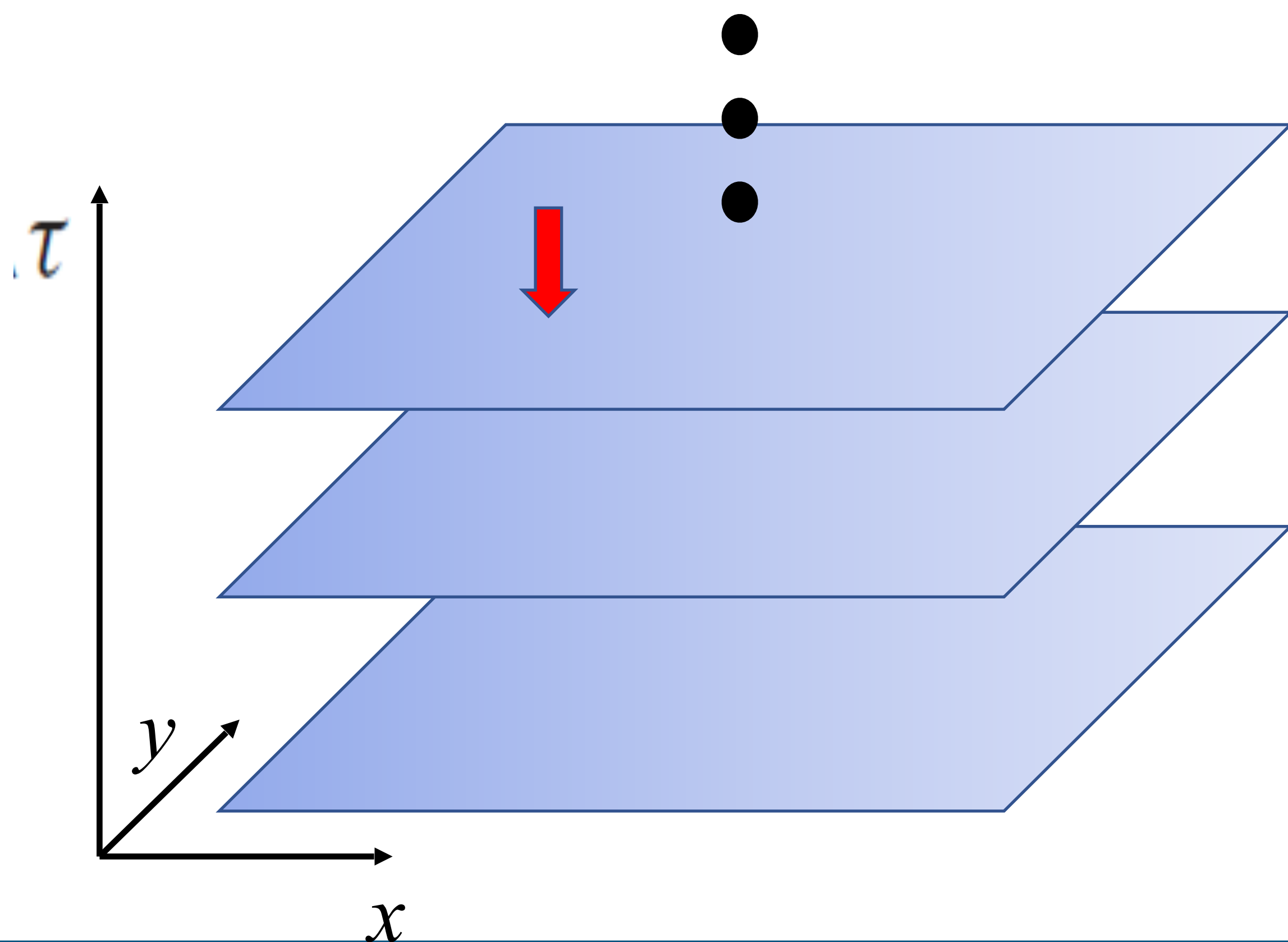
Auxiliary field Quantum Monte Carlo





$$\mathcal{R}^\sigma = \frac{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}'^\sigma(l+1, l) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}$$

$$\mathbf{B}^\sigma(l+1, l) \xrightarrow{x_{\mathbf{i}, l} \rightarrow -x_{\mathbf{i}, l}} \mathbf{B}'^\sigma(l+1, l)$$



$$\mathcal{R}^\sigma = \frac{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}'^\sigma(l+1, l) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}$$

$$\mathbf{B}^\sigma(l+1, l) \xrightarrow{x_{i,l} \rightarrow -x_{i,l}} \mathbf{B}'^\sigma(l+1, l)$$

$$r = \mathcal{R}^\uparrow \mathcal{R}^\downarrow \quad \text{Metropolis}$$

$$r = \frac{\mathcal{R}^\uparrow \mathcal{R}^\downarrow}{1 + \mathcal{R}^\uparrow \mathcal{R}^\downarrow} \quad \text{Heat-bath}$$

Thermalization and measurements

Start with thermalization sweeps

Then do measurement sweeps

Along this week

- Biased and Unbiased methods are different in what is assumed and how errors are dealt
- Numerical methods are a very useful tool to study strongly interacting fermionic systems
- DQMC is a powerful method where it works and can provide information about a wide variety of quantities for different systems

Thank you!