

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

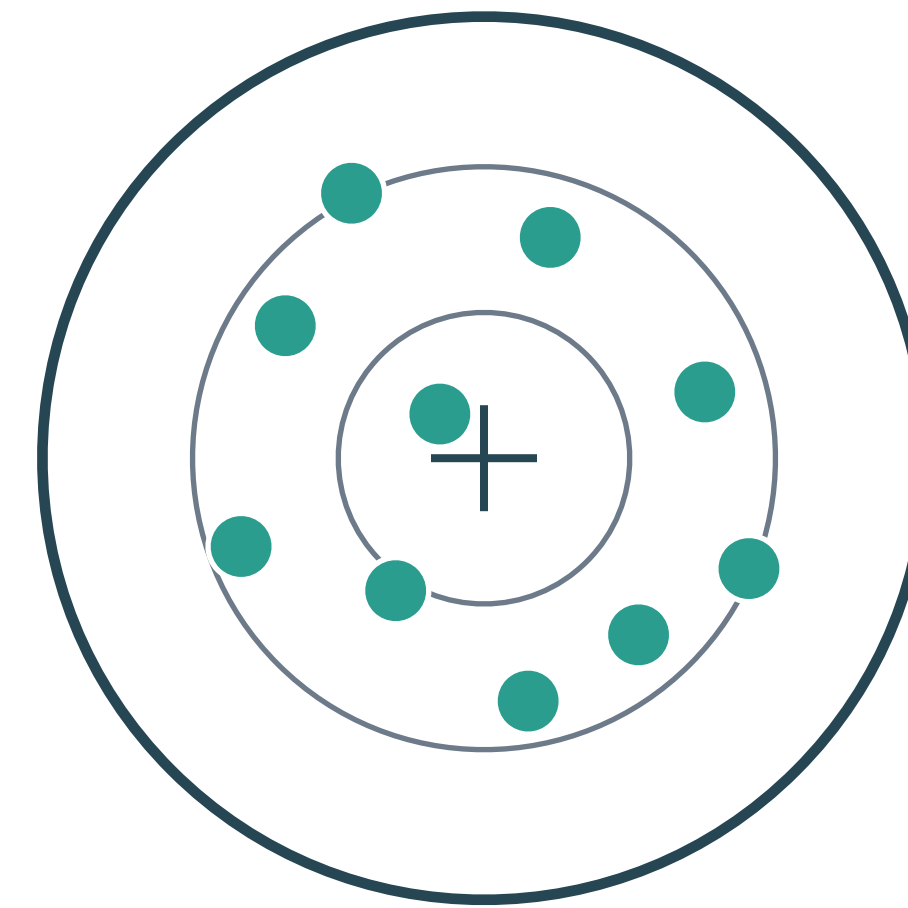
5 – The Sign problem

Before discussing the QMC method

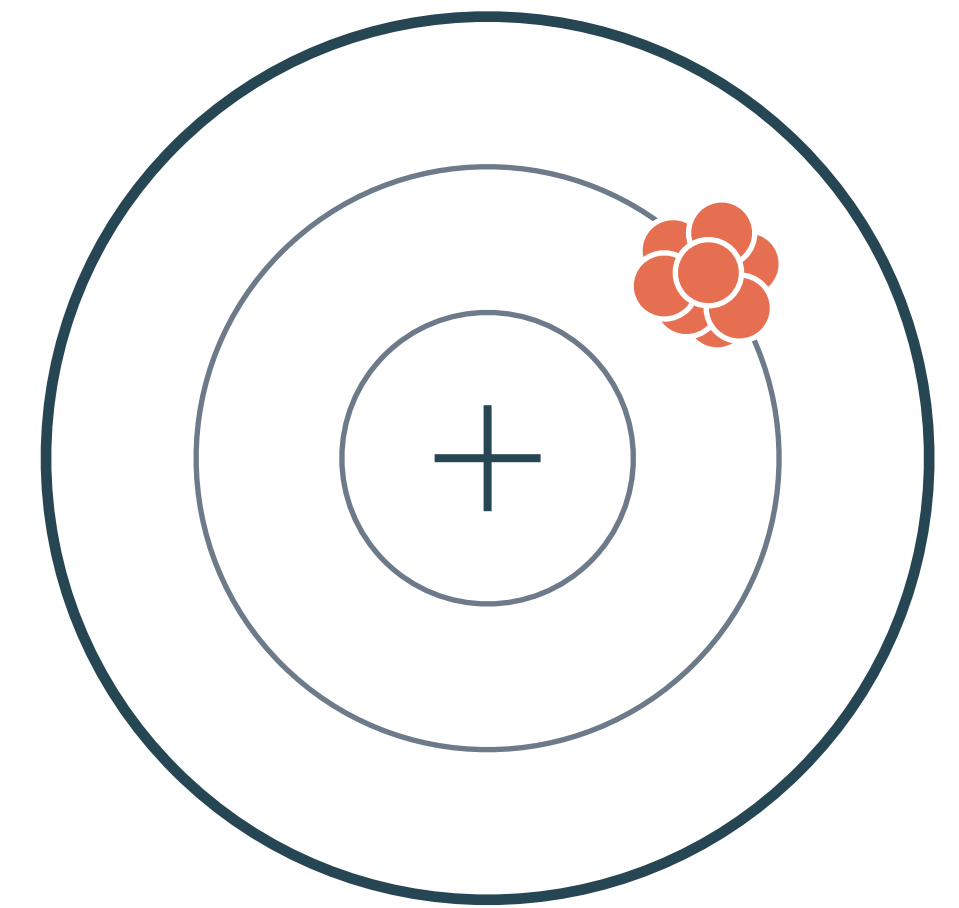
Before discussing the QMC method

QMC is an unbiased method

Biases and unbiased methods

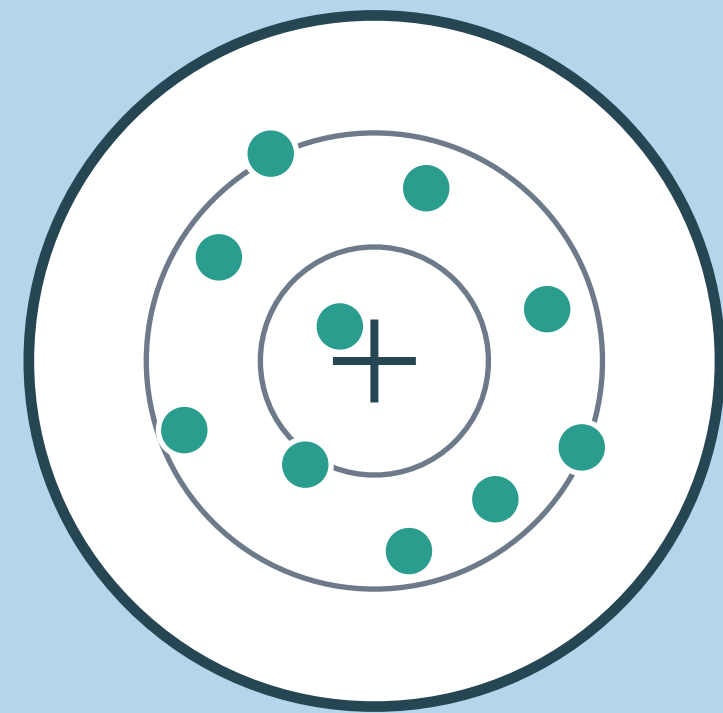


unbiased



biased

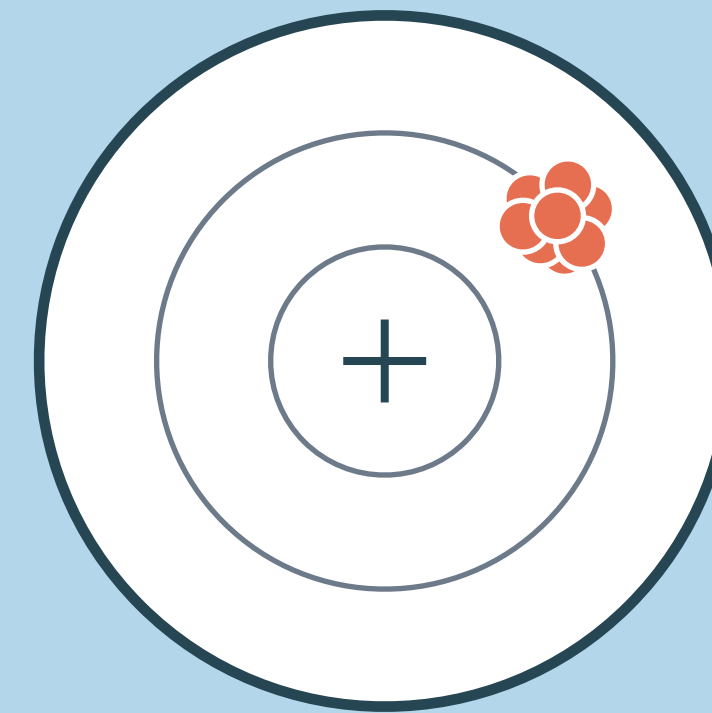
An unbiased method has only controlled errors



Unbiased

Assumes nothing about the answer.
Every error can be estimated and systematically reduced.

- Errors come with a knob: more samples, larger clusters, more states kept
- As the knob is turned, the result converges to the exact answer of the model
- The error bar is part of the result



Biased

Builds an assumption about the answer into the calculation: an uncontrolled approximation.

- Trial wave function, mean field, truncation without a control parameter
- The result depends on that choice
- The size of the error cannot be known from within the method

Precision is not accuracy. A biased result can carry a tiny error bar and still miss the exact answer.

Unbiased methods and their error sources

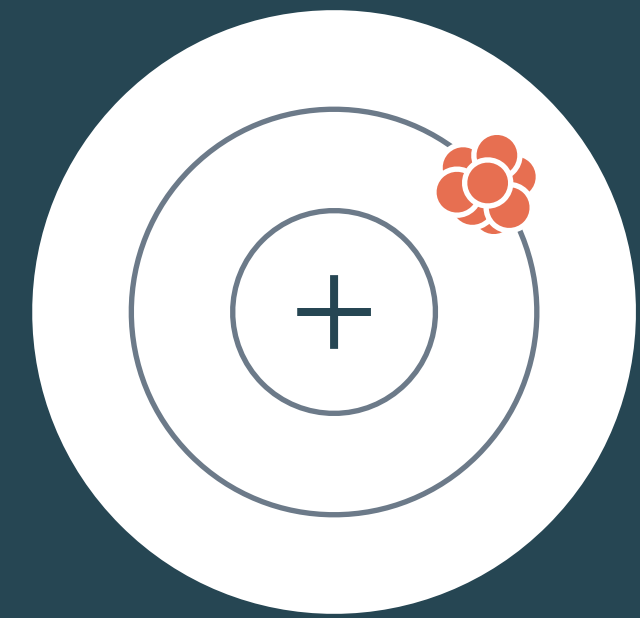
METHOD	WHAT IS EXTRAPOLATED	KEEP IN MIND
● Exact diagonalization (full or Lanczos)	Cluster size	Small clusters only
● Quantum Monte Carlo: determinant, SSE, worm, path integral	Statistical error, system size, Trotter error	Sign problem
● Diagrammatic Monte Carlo	Statistical error, diagram order	Works 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

METHOD	WHAT IS EXTRAPOLATED	KEEP IN MIND
● Exact diagonalization (full or Lanczos)	Cluster size	Small clusters only
● Quantum Monte Carlo without a sign problem: determinant, SSE, worm, path integral	Statistical error, system size, Trotter error	Sign problem
● Diagrammatic Monte Carlo	More about unbiased methods in another class	Works directly in the thermodynamic limit
● DMRG and tensor networks (MPS, PEPS)		Best in 1D and at low entanglement
● Series expansions: high temperature, numerical linked cluster expansion		Only where the series converges
● Numerical renormalization group	Discretization, states kept	Impurity models

Biased methods and their assumptions

METHOD	BUILT-IN ASSUMPTION
● Mean field, Hartree–Fock	The state is a single product state or Slater determinant
● Variational Monte Carlo	The form of the trial wave function
● Fixed-node and constrained-path QMC	The nodes or phases of a trial state
● DFT with approximate functionals	The exchange-correlation functional
● Single-site DMFT	A purely local self-energy
● RPA, FLEX, truncated diagrammatics	A chosen class of diagrams



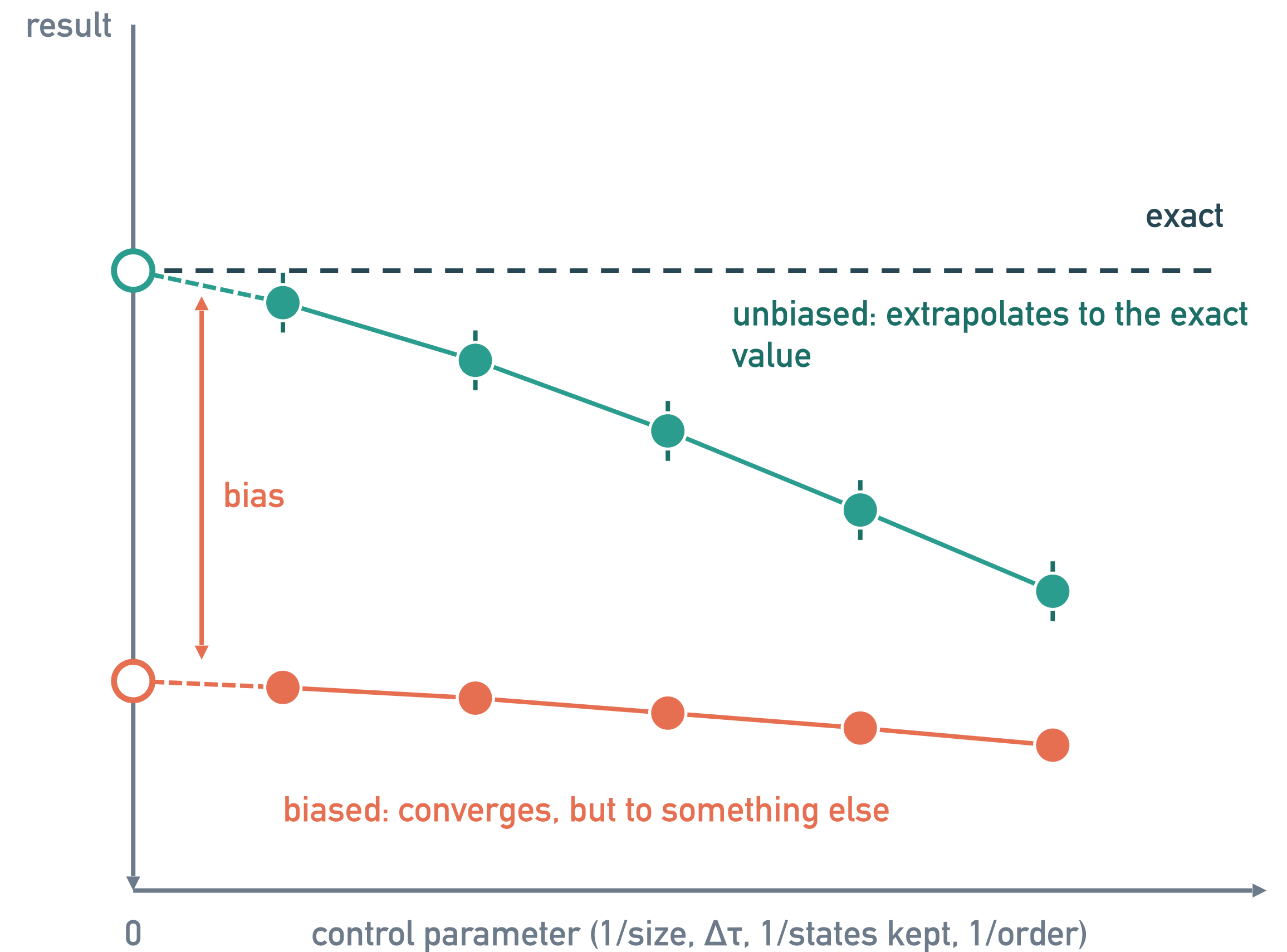
Biased does not mean useless

These methods reach sizes, temperatures and models that unbiased methods cannot. Their results need a benchmark against an unbiased method or experiment.

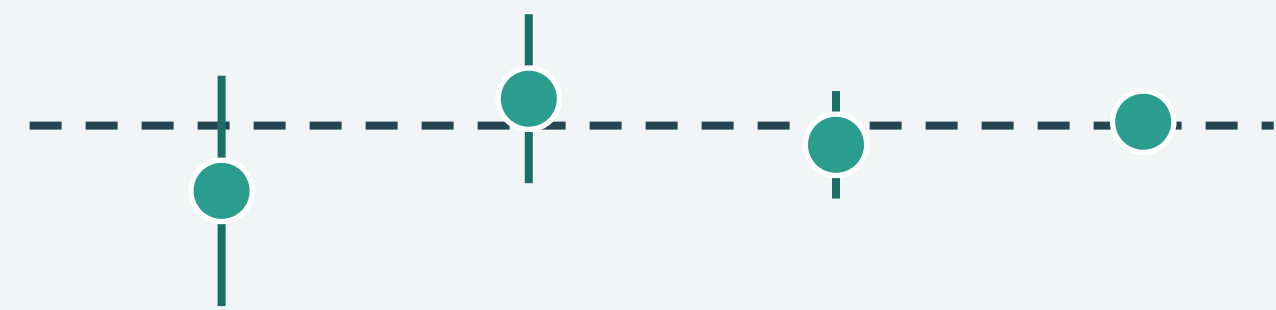
Controlled methods

What is controlled

- Statistical error: more Monte Carlo samples
- Finite size: larger lattices or clusters
- Time discretization: smaller Trotter step $\Delta\tau$
- Truncation: more states kept, larger bond dimension
- Expansion order: more terms in the series



Three caveats before putting a method in either box



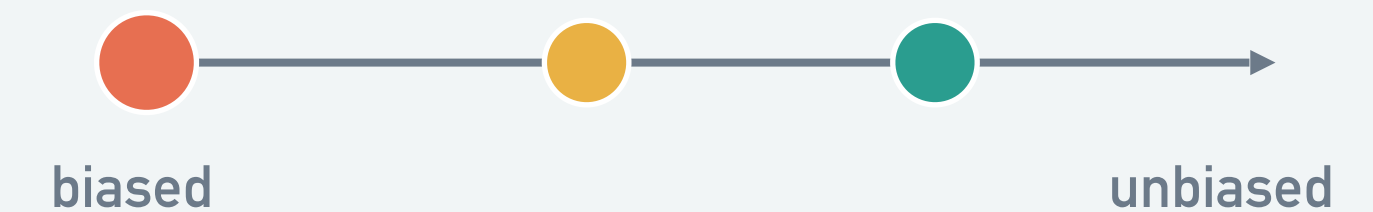
1 Unbiased is not without error

The result still has an error bar. The difference is that the error bar is known and can be made smaller.



2 Only inside the regime of convergence

DMRG in two dimensions, linked-cluster expansions at low temperature or QMC with a severe sign problem stay formally unbiased, but stop being practical.



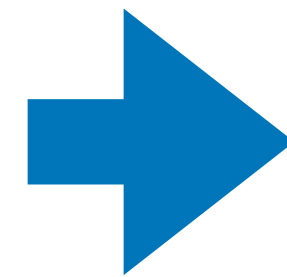
3 The frontier is not rigid

Cluster extensions of DMFT and constraint release in auxiliary-field DMRG is variational, yet counts as unbiased: its truncation error is monitored and extrapolated.

The question to ask of any method: which error is controlled, and by which parameter?

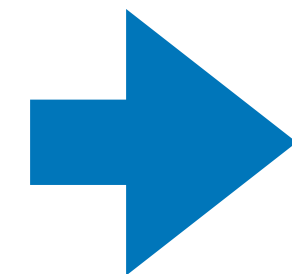
The auxiliary field QMC Method

Ising Model once again



**Ising model in a transverse field
Imaginary time
Feynman's path integrals**

Hubbard Model



**Trotter decomposition
The Hubbard–Stratonovich transformation
Determinantal weights
Simulations**

Suggested bibliography

Original articles

PHYSICAL REVIEW D

VOLUME 24, NUMBER 8

15 OCTOBER 1981

Monte Carlo calculations of coupled boson-fermion systems. I

R. Blankenbecler*

Laboratoire de Physique Théorique et Hautes Energies, University of Paris XI, 91405, Orsay, France

D. J. Scalapino and R. L. Sugar

Institute for Theoretical Physics and Department of Physics, University of California, Santa Barbara, California 93106

(Received 15 June 1981)

We present a formalism for carrying out Monte Carlo calculations of field theories with both boson and fermion degrees of freedom. The basic approach is to integrate out the fermion degrees of freedom and obtain an effective action for the boson fields to which standard Monte Carlo techniques can be applied. We study the structure of the effective action for a wide class of theories. We develop a procedure for making rapid calculations of the variation in the effective action due to local changes in the boson fields, which is essential for practical numerical calculations.

BSS algorithm

Original articles

PHYSICAL REVIEW B

VOLUME 26, NUMBER 9

1 NOVEMBER 1982

Monte Carlo simulations of one-dimensional fermion systems

J. E. Hirsch and R. L. Sugar

Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

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*Department of Physics and Institute for Theoretical Physics, University of California,
Santa Barbara, California 93106*

R. Blankenbecler

Stanford Linear Accelerator Center, Stanford University, Stanford, California 94305

(Received 27 May 1982)

RAPID COMMUNICATIONS

PHYSICAL REVIEW B

VOLUME 28, NUMBER 7

1 OCTOBER 1983

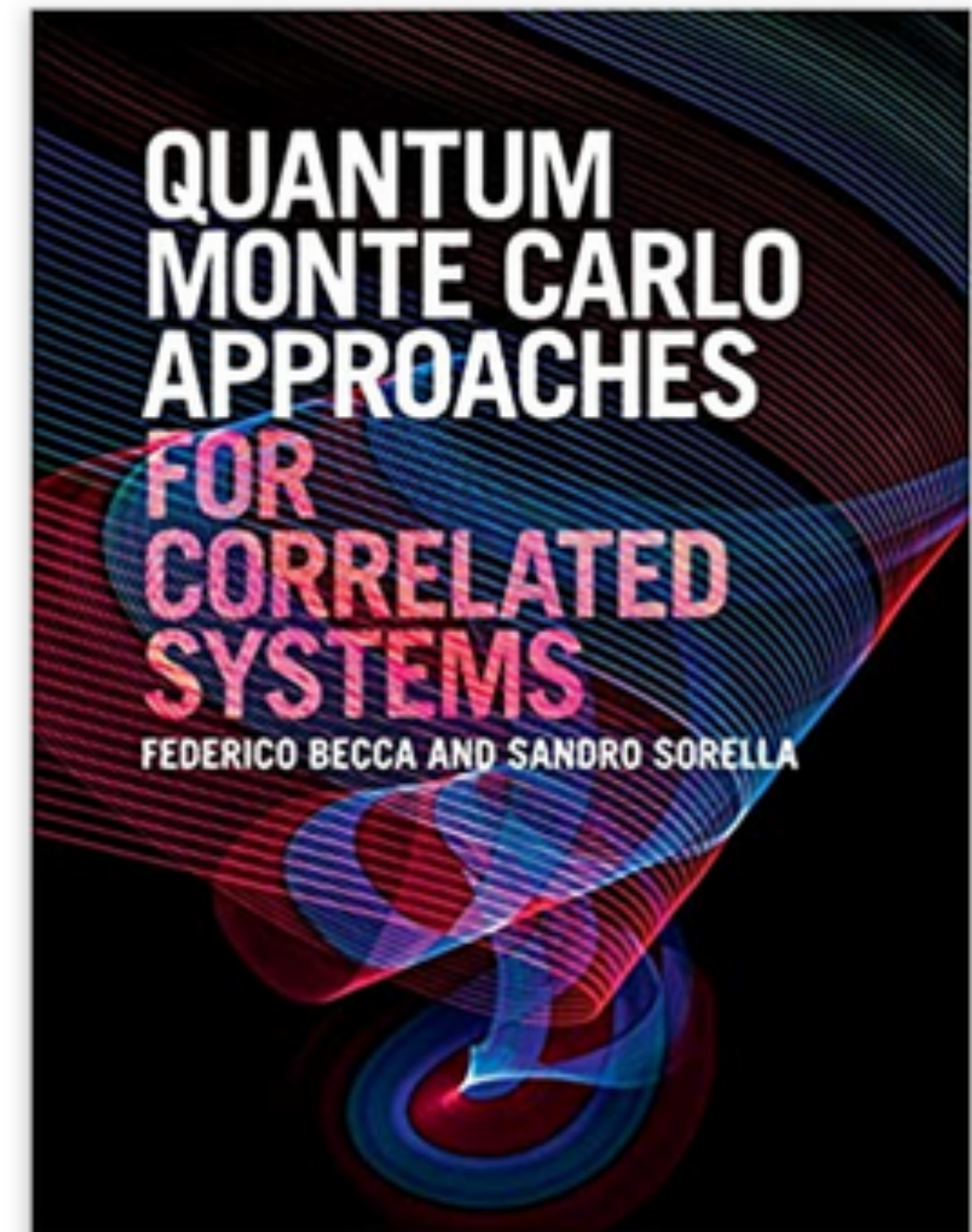
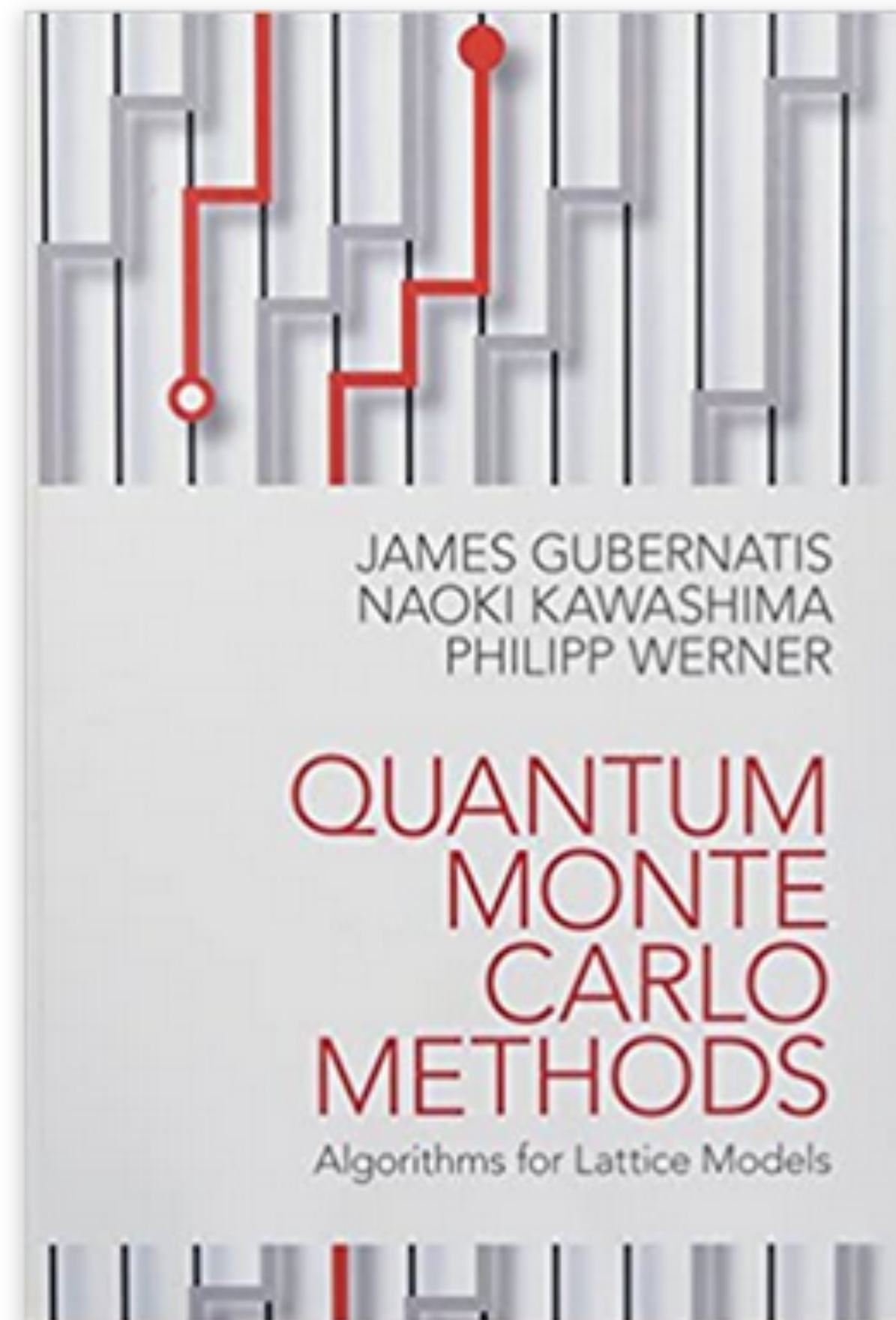
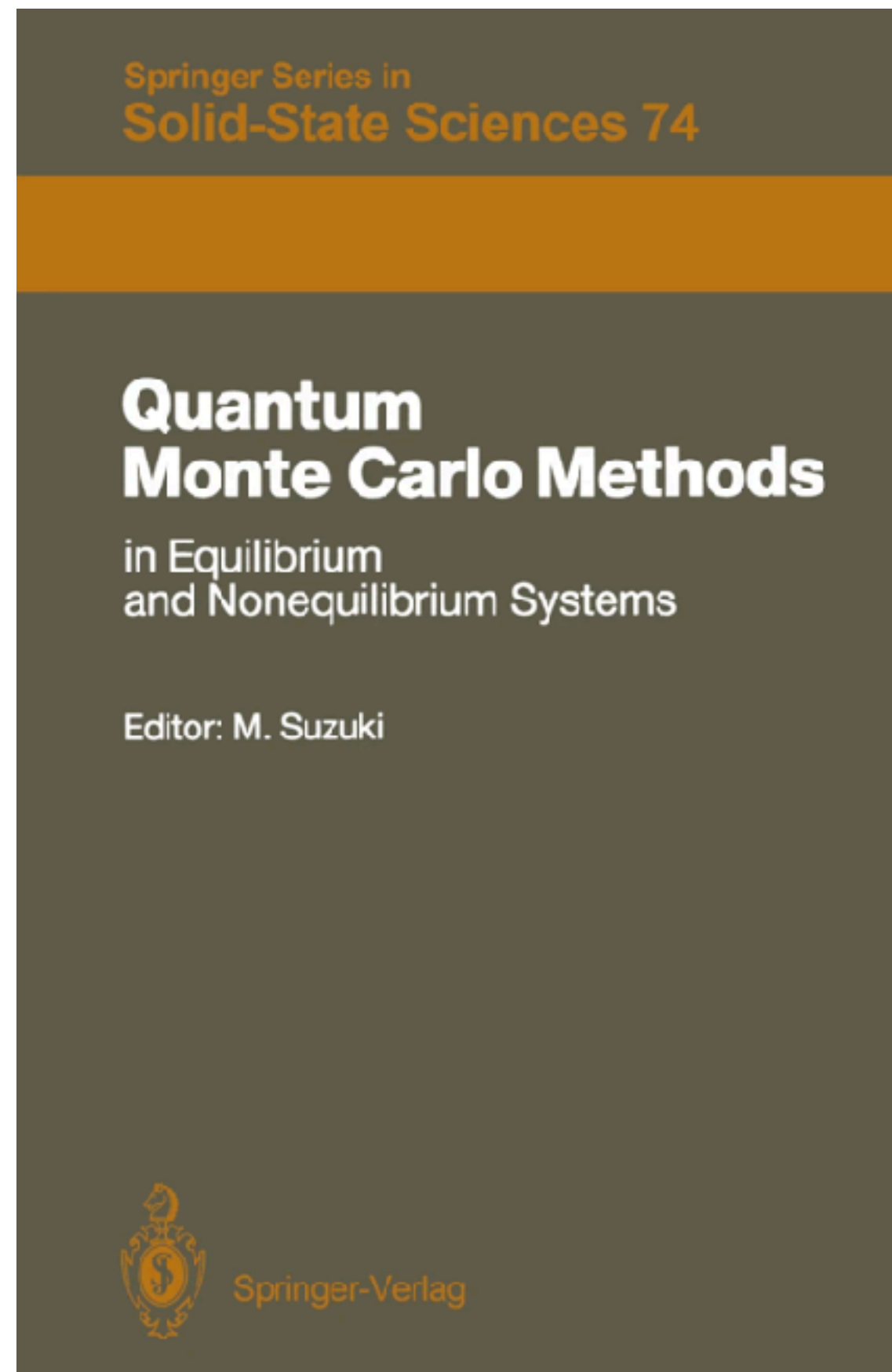
Discrete Hubbard-Stratonovich transformation for fermion lattice models

J. E. Hirsch

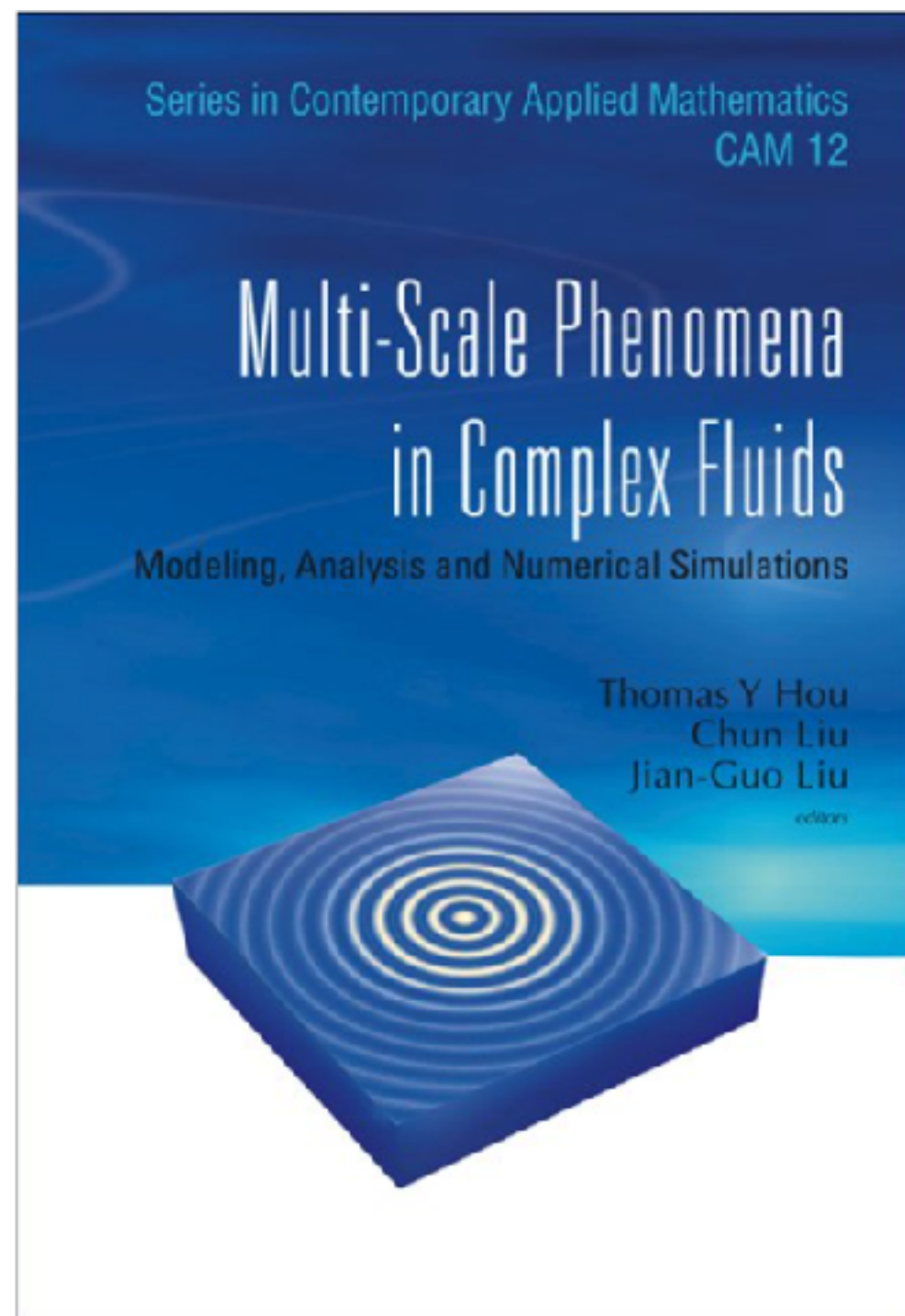
Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 16 June 1983)

Books



Book chapters



10 World-line and Determinantal Quantum Monte Carlo Methods for Spins, Phonons and Electrons

F.F. Assaad¹ and H.G. Evertz²

¹ Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

² Institut für Theoretische Physik und Computational Physics, Technische Universität Graz, A-8010 Graz, Austria

Numerical Methods for Quantum Monte Carlo Simulations of the Hubbard Model*

Zhaojun Bai

*Department of Computer Science and
Department of Mathematics
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Davis, CA 95616, USA
E-mail: bai@cs.ucdavis.edu*

Wenbin Chen

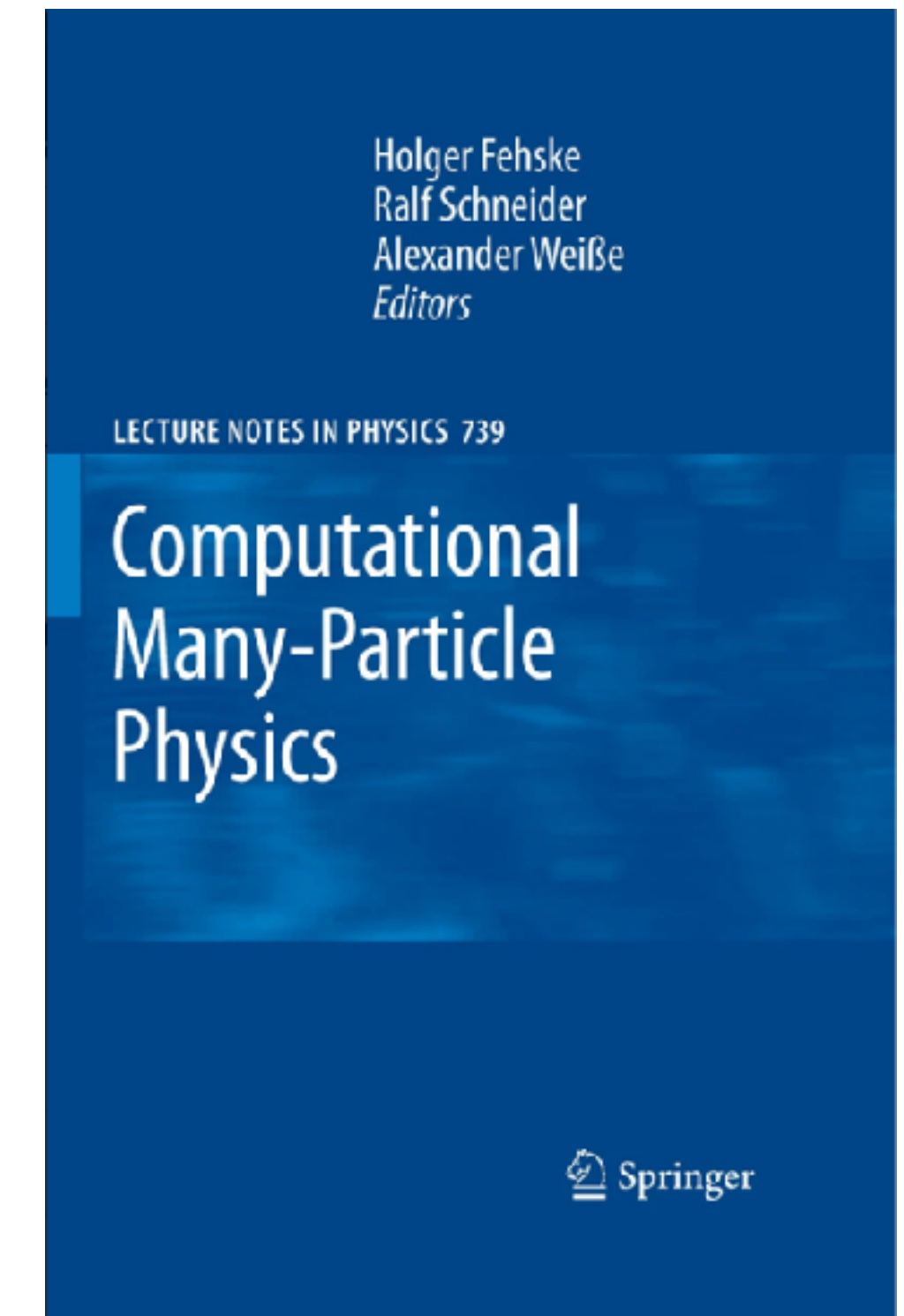
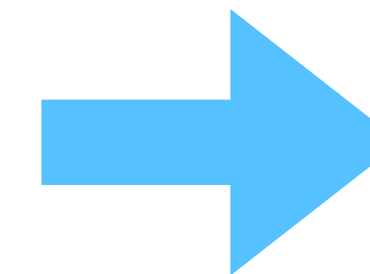
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Review article

36

Brazilian Journal of Physics, vol. 33, no. 1, March, 2003

Introduction to Quantum Monte Carlo Simulations for Fermionic Systems

Raimundo R. dos Santos

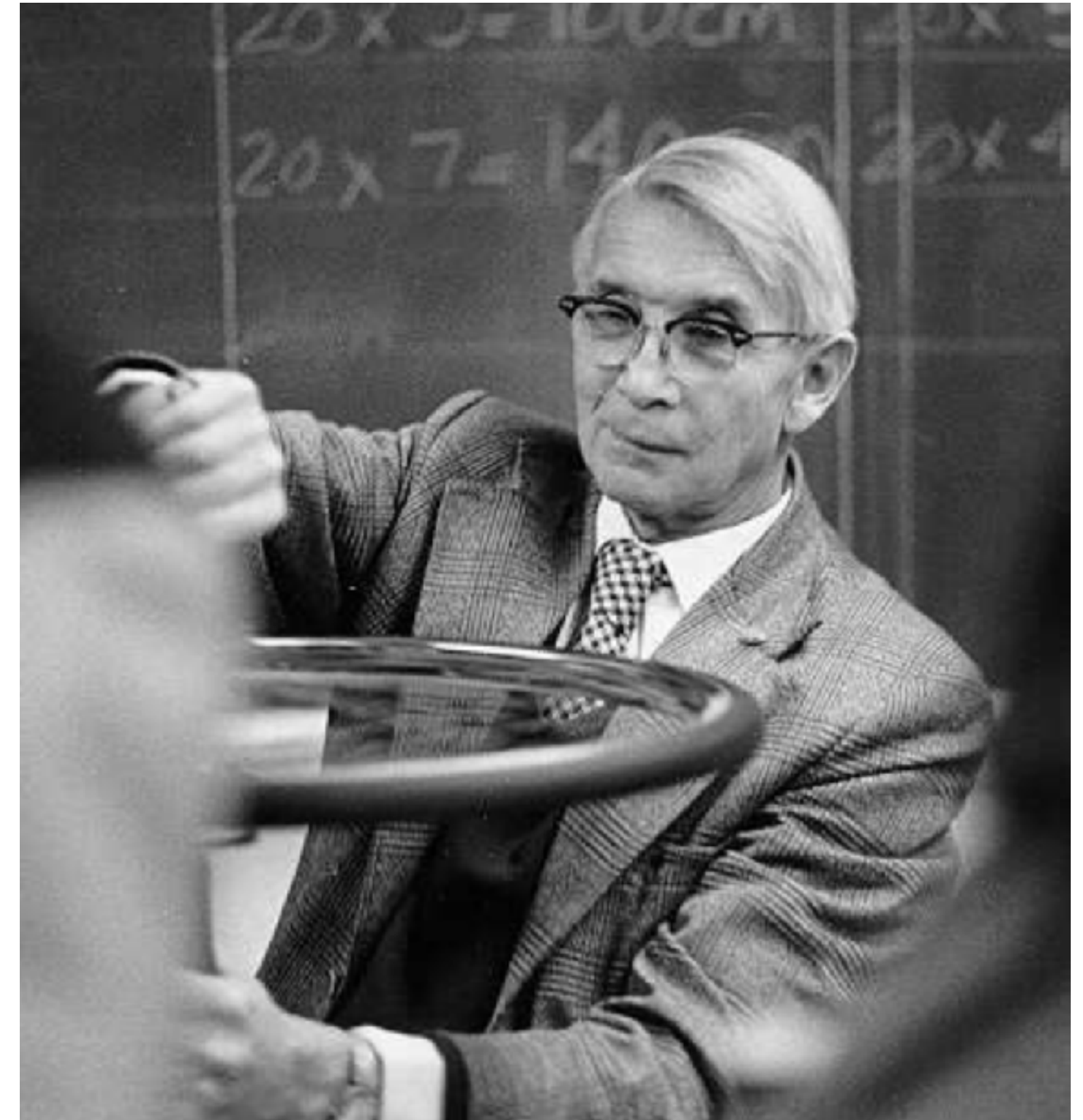
rrds@if.ufrj.br

*Instituto de Física, Universidade Federal do Rio de Janeiro,
Caixa Postal 68528, 21945-970, Rio de Janeiro, RJ, Brazil*

Received on 27 August, 2002

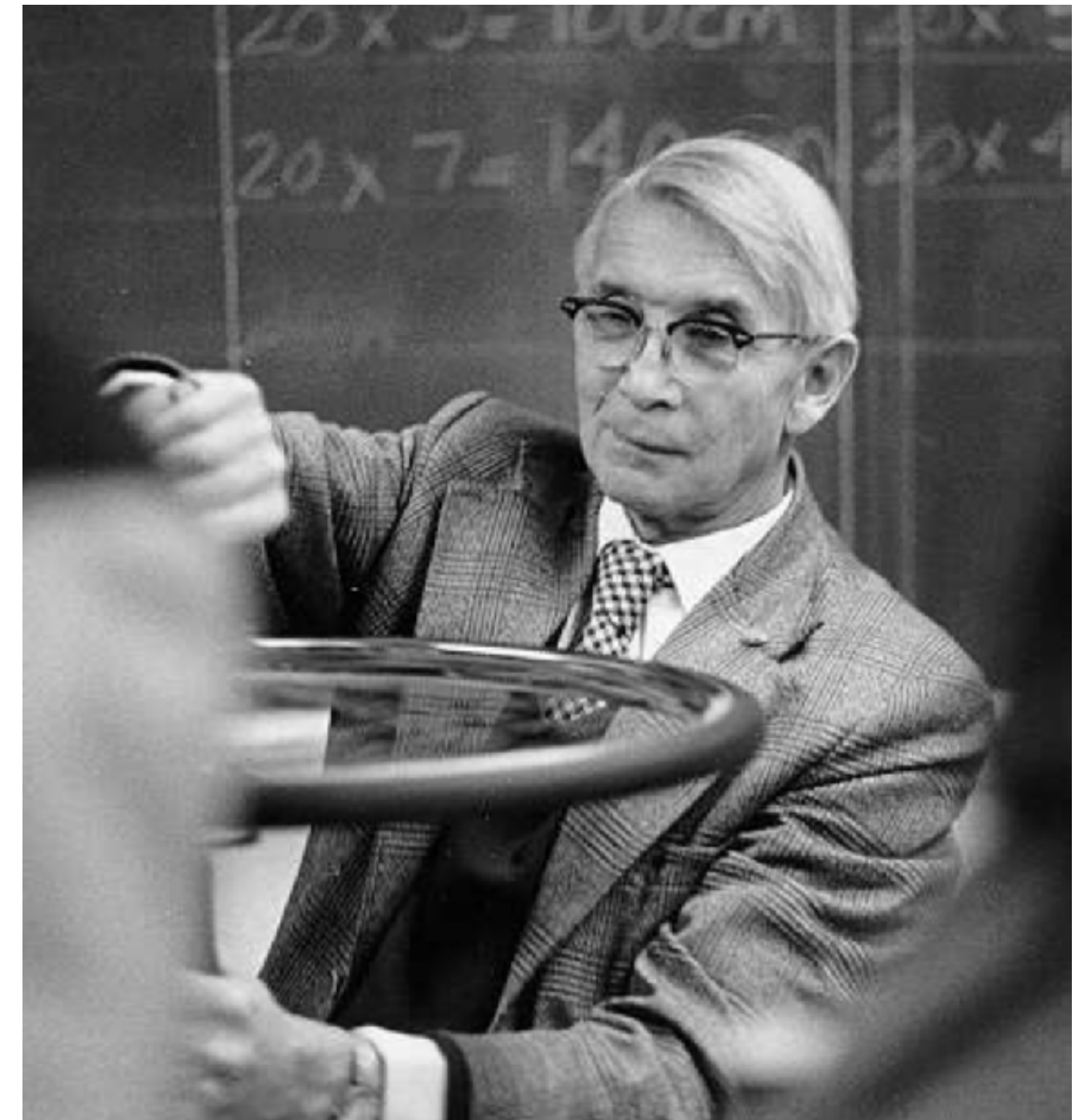
We tutorially review the determinantal Quantum Monte Carlo method for fermionic systems, using the Hubbard model as a case study. Starting with the basic ingredients of Monte Carlo simulations for classical systems, we introduce aspects such as importance sampling, sources of errors, and finite-size scaling analyses. We then set up the preliminary steps to prepare for the simulations, showing that they are actually carried out by sampling discrete Hubbard-Stratonovich auxiliary fields. In this process the Green's function emerges as a fundamental tool, since it is used in the updating process, and, at the same time, it is directly related to the quantities probing magnetic, charge, metallic, and superconducting behaviours. We also discuss the as yet unresolved 'minus-sign problem', and two ways to stabilize the algorithm at low temperatures.

The Ising Model



The Ising Model

Once again, but not quite
the same



Ising model with a magnetic field

$$H = -J_z \sum_i S_i^z S_{i+1}^z - H_z \sum_i S_i^z$$

$$S^\alpha = \frac{\hbar}{2} \sigma^\alpha \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$[S_i^z S_{i+1}^z, S_j^z S_{j+1}^z] = [S_i^z S_{i+1}^z, S_j^z] = [S_i^z, S_j^z] = 0 \quad i \neq j$$

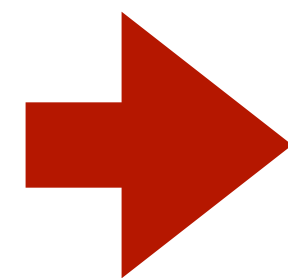
Back to Ising model with a magnetic field

$$H = -J_z \sum_i S_i^z S_{i+1}^z - H_z \sum_i S_i^z$$

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As we have seen last class: there is a basis that diagonalizes each spin operator simultaneously



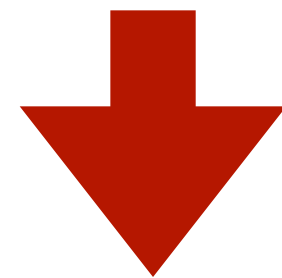
$$|C\rangle = |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle = |s_1 s_2 \cdots s_N\rangle,$$

Ising model with a magnetic field

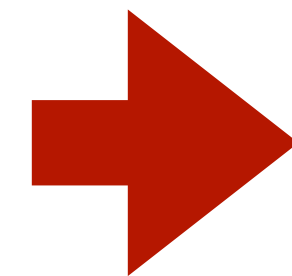
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$$Z = \text{Tr} [e^{-\beta H}] = \sum_C \langle C | e^{-\beta H} | C \rangle$$



$$\langle C | e^{-\beta H} | C \rangle = e^{-\beta E(C)}$$



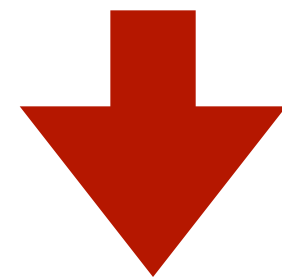
$$E(C) = -J \sum_i s_i s_{i+1} - H^z \sum_i s_i$$

Ising model with a magnetic field

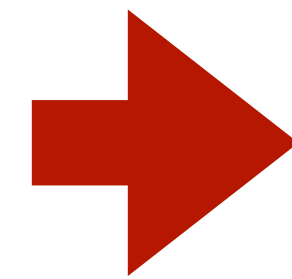
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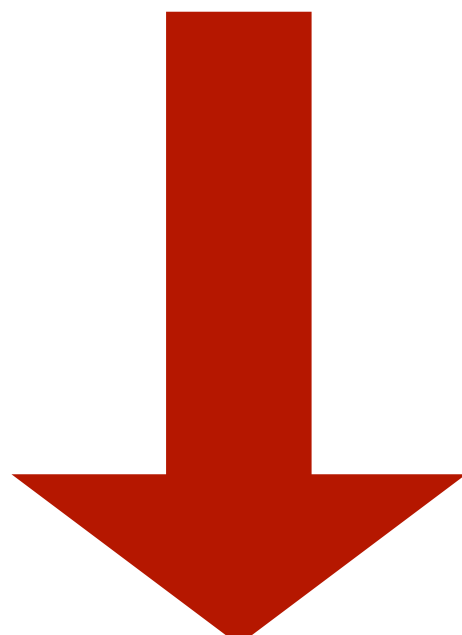
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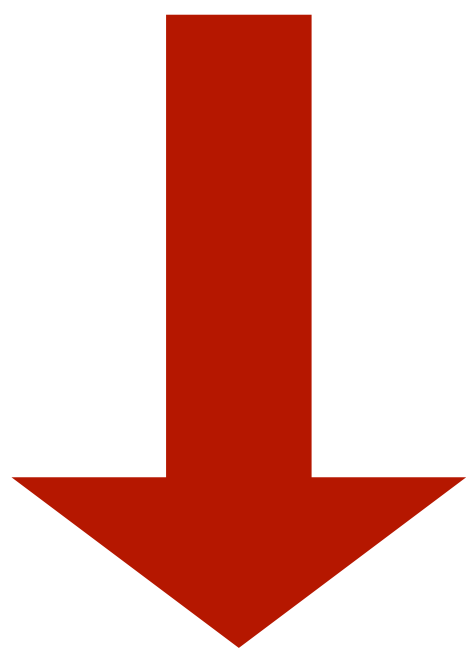

$$Z = \sum_C e^{-\beta E(C)}$$

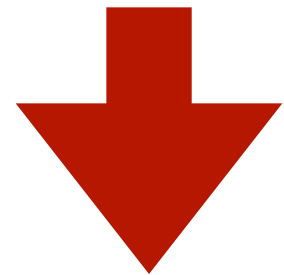
Ising model with a magnetic field

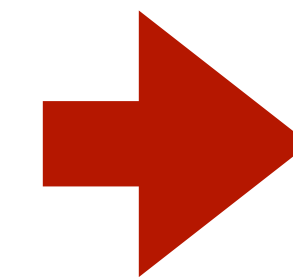
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$$S^\alpha = \frac{\hbar}{2} \sigma^\alpha$$

$$Z = \text{Tr} [e^{-\beta H}] = \sum_C \langle C | e^{-\beta H} | C \rangle$$



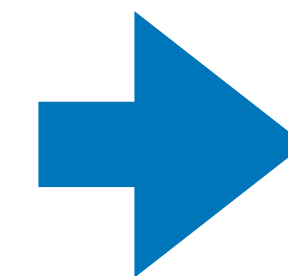

$$\langle C | e^{-\beta H} | C \rangle = e^{-\beta E(C)}$$



$$E(C) = -J \sum_i s_i s_{i+1} - H^z \sum_i s_i$$

$$Z = \sum_C e^{-\beta E(C)}$$

$$e^{-\beta E(C)}$$



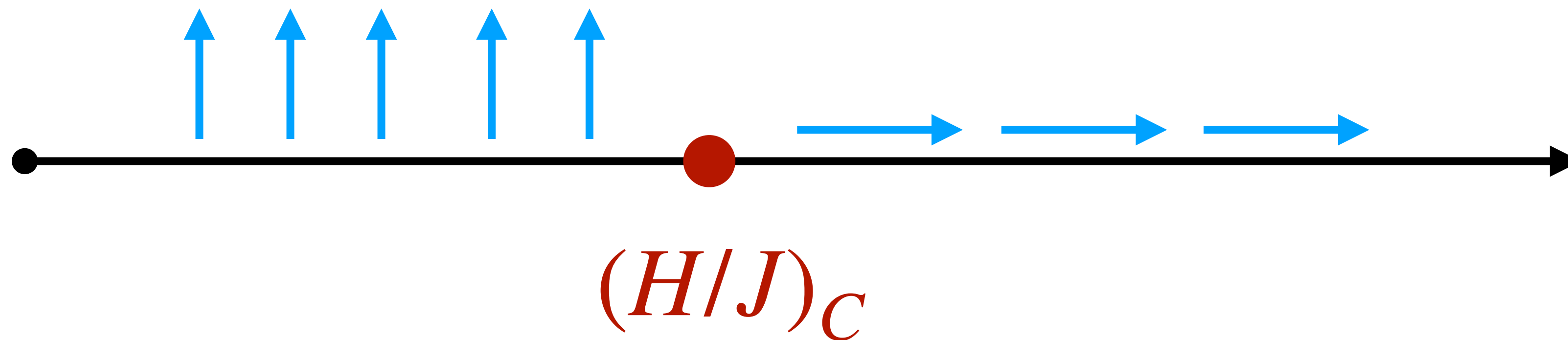
Statistical weight for configurations
for Monte Carlo simulations

**What happens when the two terms
on the Hamiltonian don't commute?**

Ising model with a transverse magnetic field

Ising model with a transverse magnetic field

$$H = -J \sum_i S_i^z S_{i+1}^z - H_x \sum_i S_i^x \quad S^\alpha = \frac{\hbar}{2} \sigma^\alpha$$



Ising model with a transverse magnetic field

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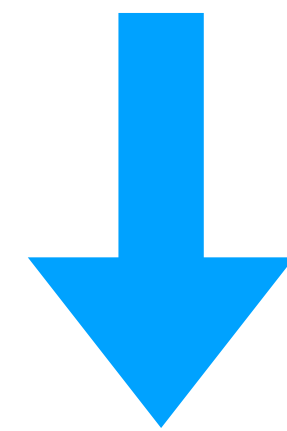
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad [\sigma_i^x, \sigma_i^y] = 2i\delta_{i,j}\sigma_i^z$$

$$H = H_0 + H_1 \quad H_0 = -J \sum_i S_i^z S_{i+1}^z \quad H_1 = -H_x \sum_i S_i^x$$

$$[H_0, H_1] \neq 0$$

$$Z = \text{Tr}[e^{-\beta H}] = \text{Tr}[e^{-\beta(H_0+H_1)}]$$

$$Z = \text{Tr}[e^{-\beta H}] = \text{Tr}[e^{-\beta(H_0+H_1)}] \neq \text{Tr}[e^{-\beta H_0}e^{-\beta H_1}]$$



$$[H_0, H_1] \neq 0$$

Baker–Campbell–Hausdroff formula

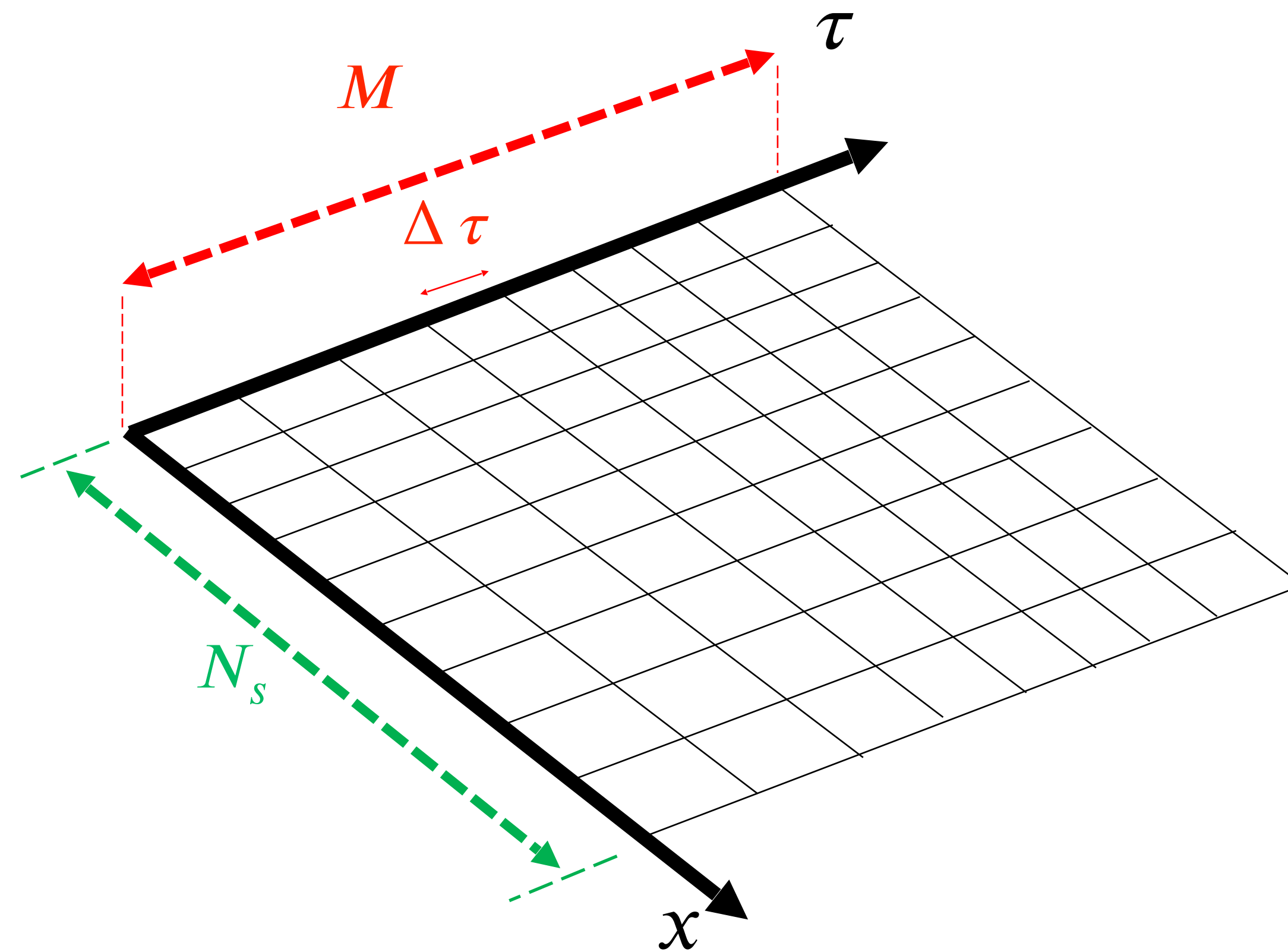
$$e^A e^B = \exp\left(A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] + \frac{1}{12}[B, [B, A]] + \dots\right)$$

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

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

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

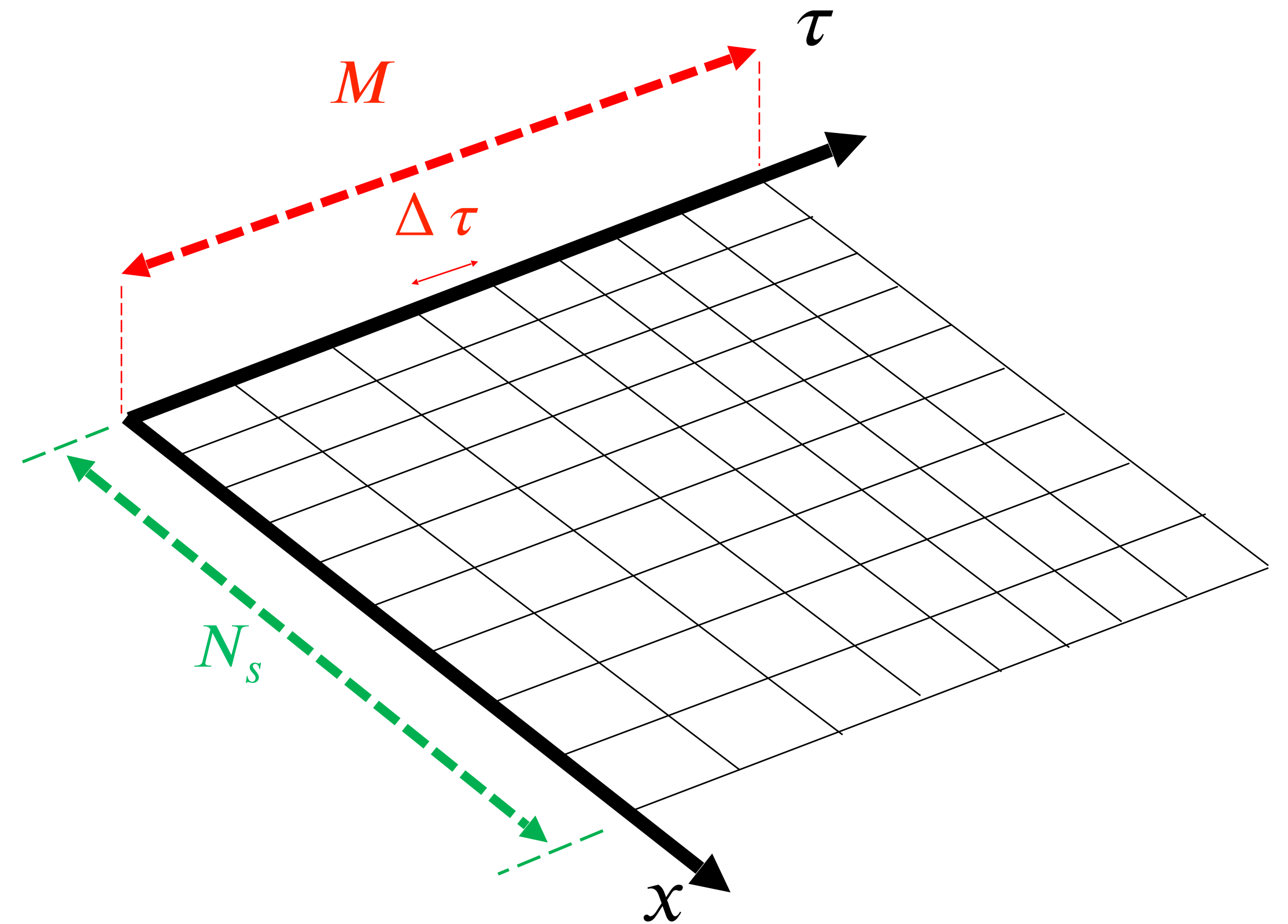
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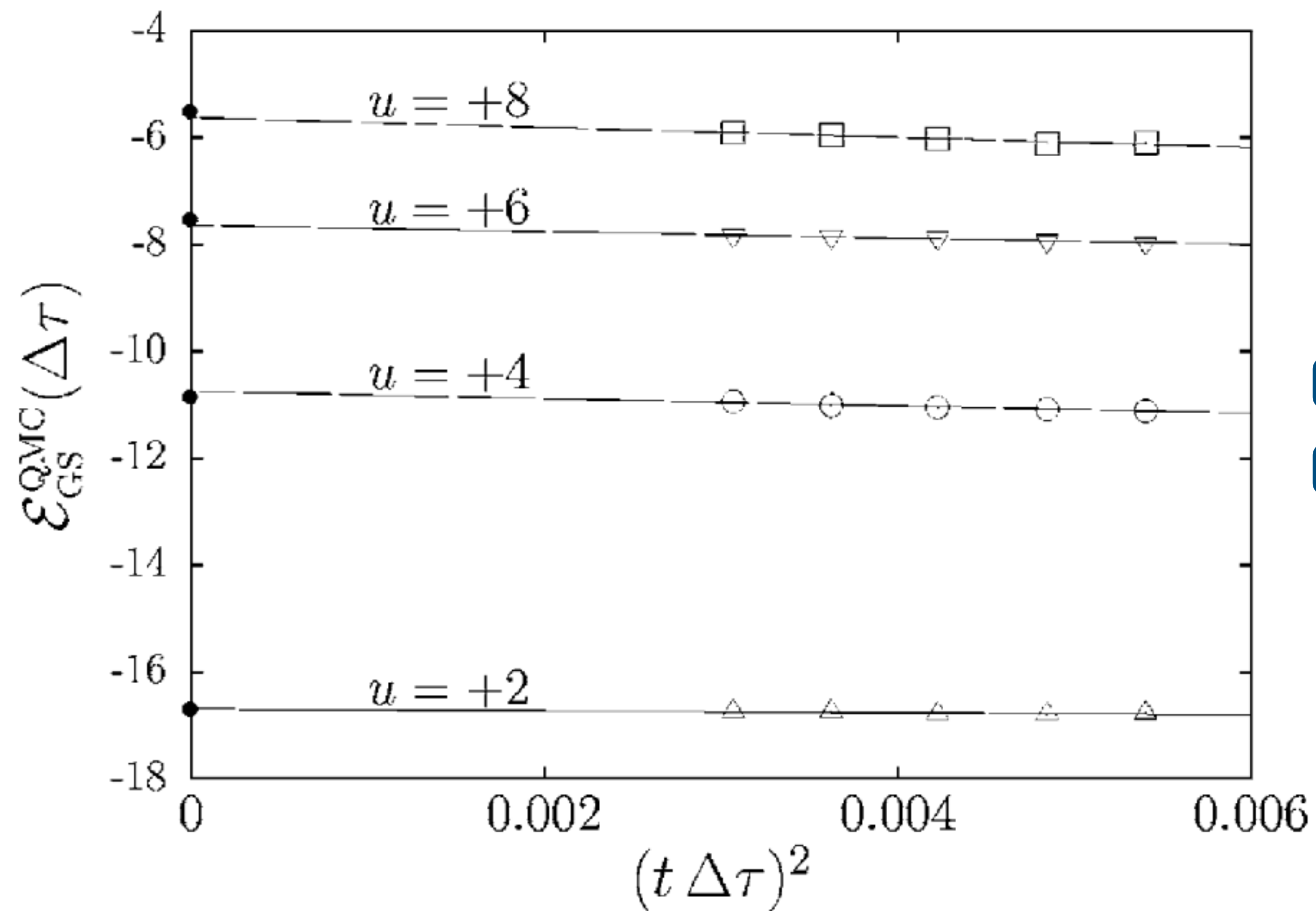
$$e^{-\Delta\tau(A+B)} = e^{-\Delta\tau A} e^{-\Delta\tau B} + \mathcal{O}(\Delta\tau^2)$$



**Very important: This is “the” approximation
in Quantum Monte Carlo Methods**

Does it work?

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



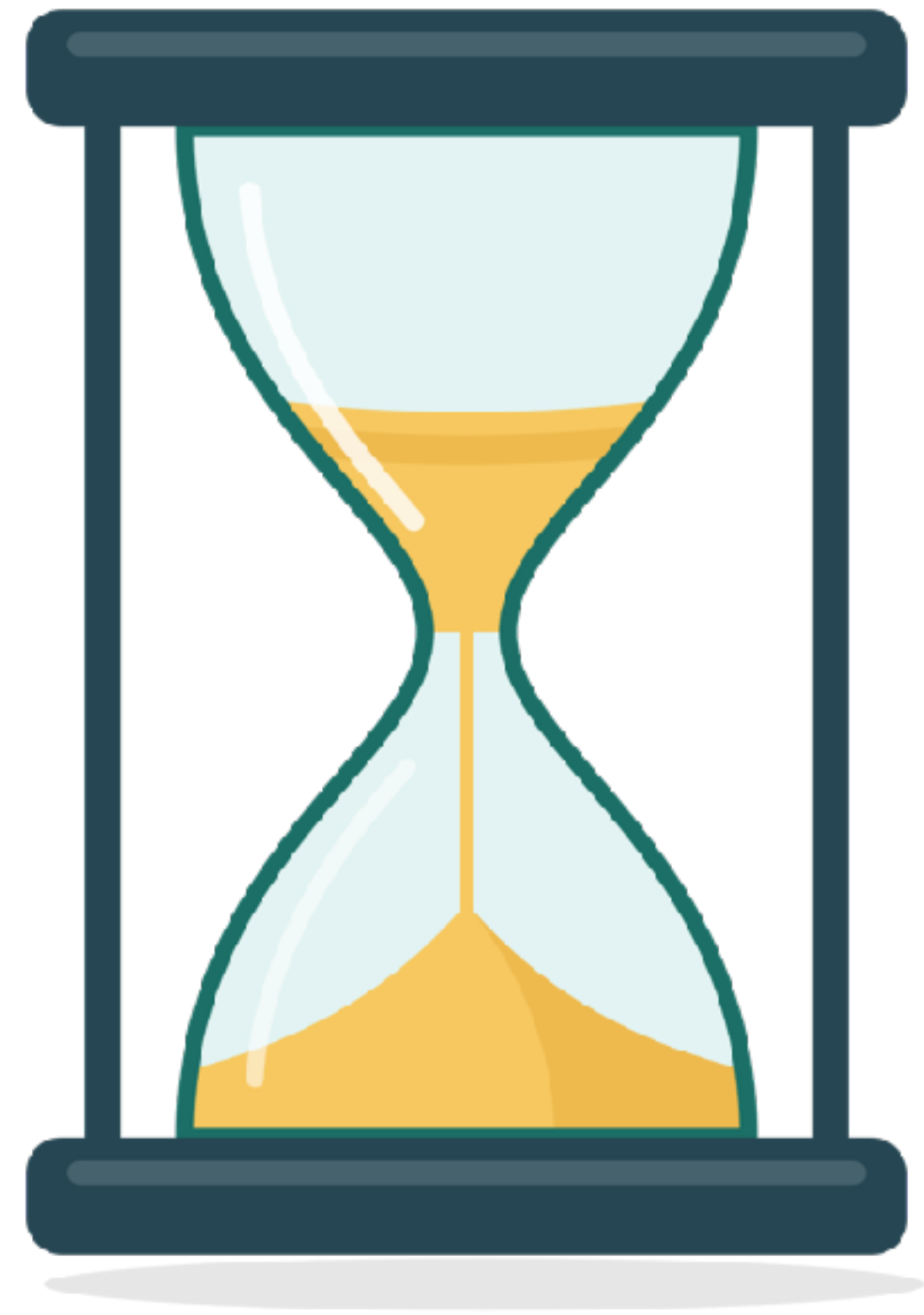
PRB 73, 165120 (06)

G. Xianlong et al.

Ground state energy: from Bethe Ansatz +LDA
Open symbols: QMC

Not for the Transverse Field Ising model

Imaginary time



Imaginary time

Monte Carlo time again,
but not quite the same



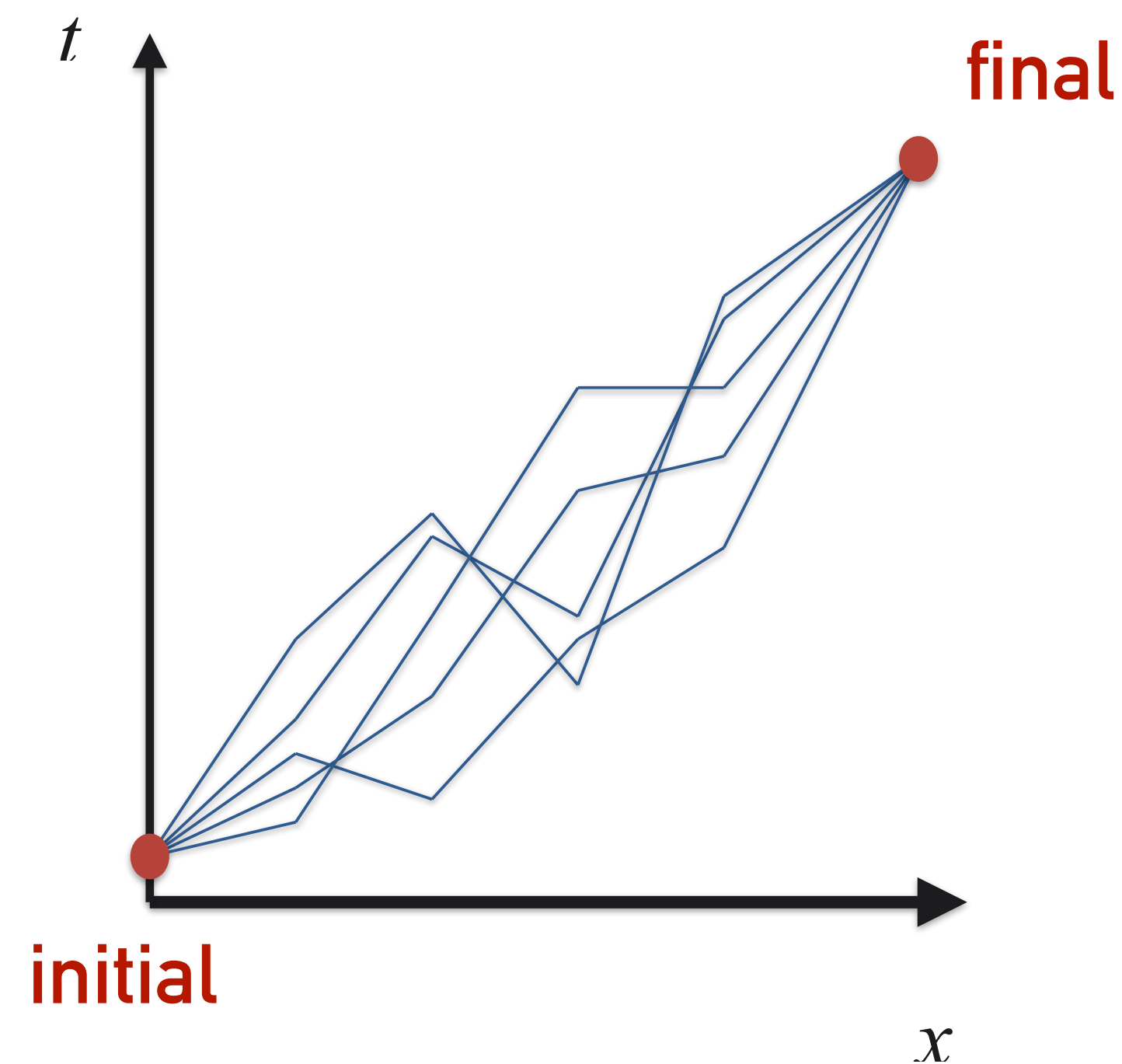
Time evolution operator in Quantum Mechanics

$$U = e^{-iHt/\hbar}$$

Imaginary time evolution operator in QMC

$$U_{\Delta\tau} = e^{-\Delta\tau H}$$

Feynman's path integrals

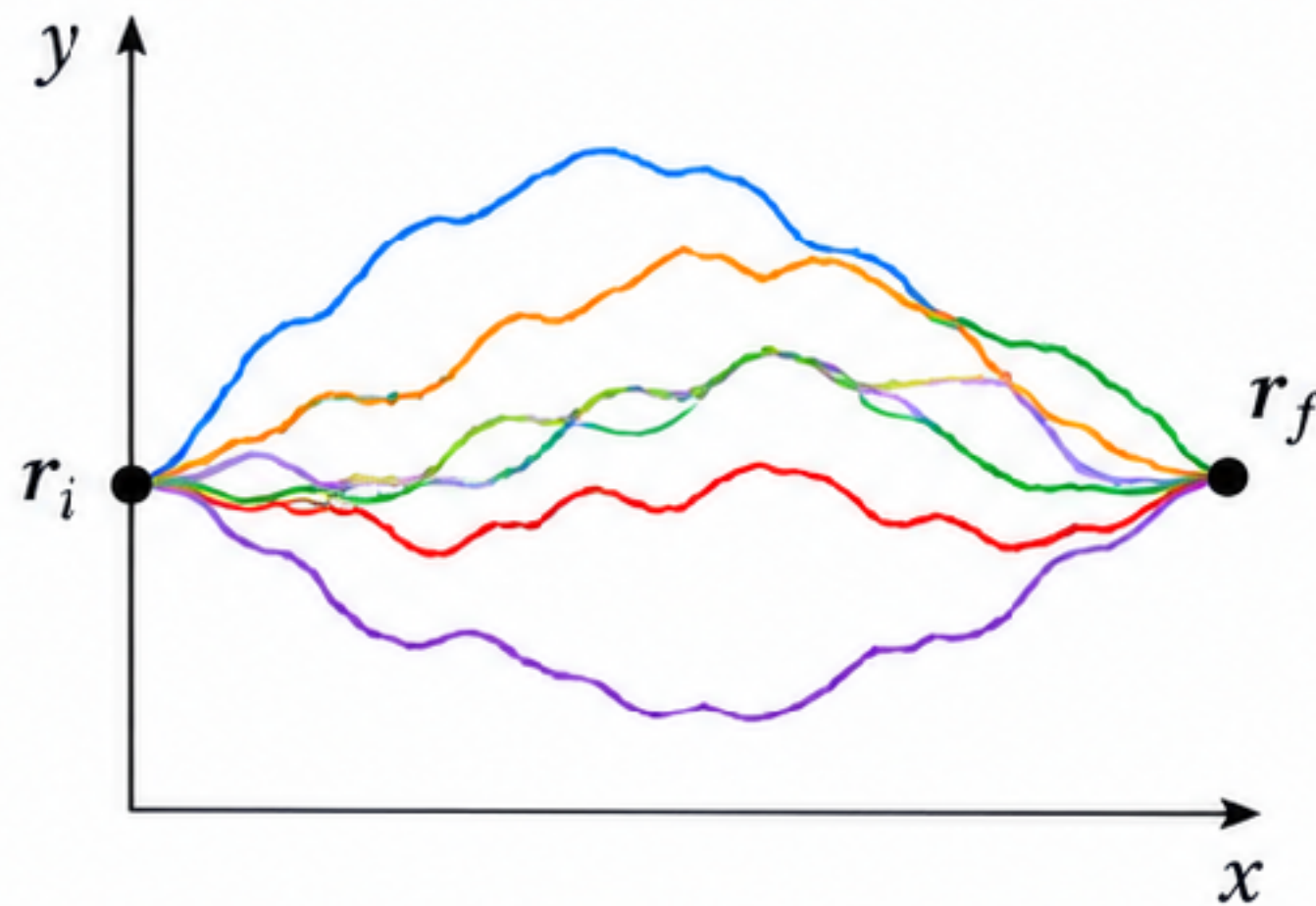


Instead of following one quantum trajectory, sum over all possible paths.

$$\langle \mathbf{x}_f | e^{-i\hat{H}t/\hbar} | \mathbf{x}_i \rangle = \int \mathcal{D}\mathbf{x}(t) e^{iS[\mathbf{x}]/\hbar}$$

Feynman's path integrals

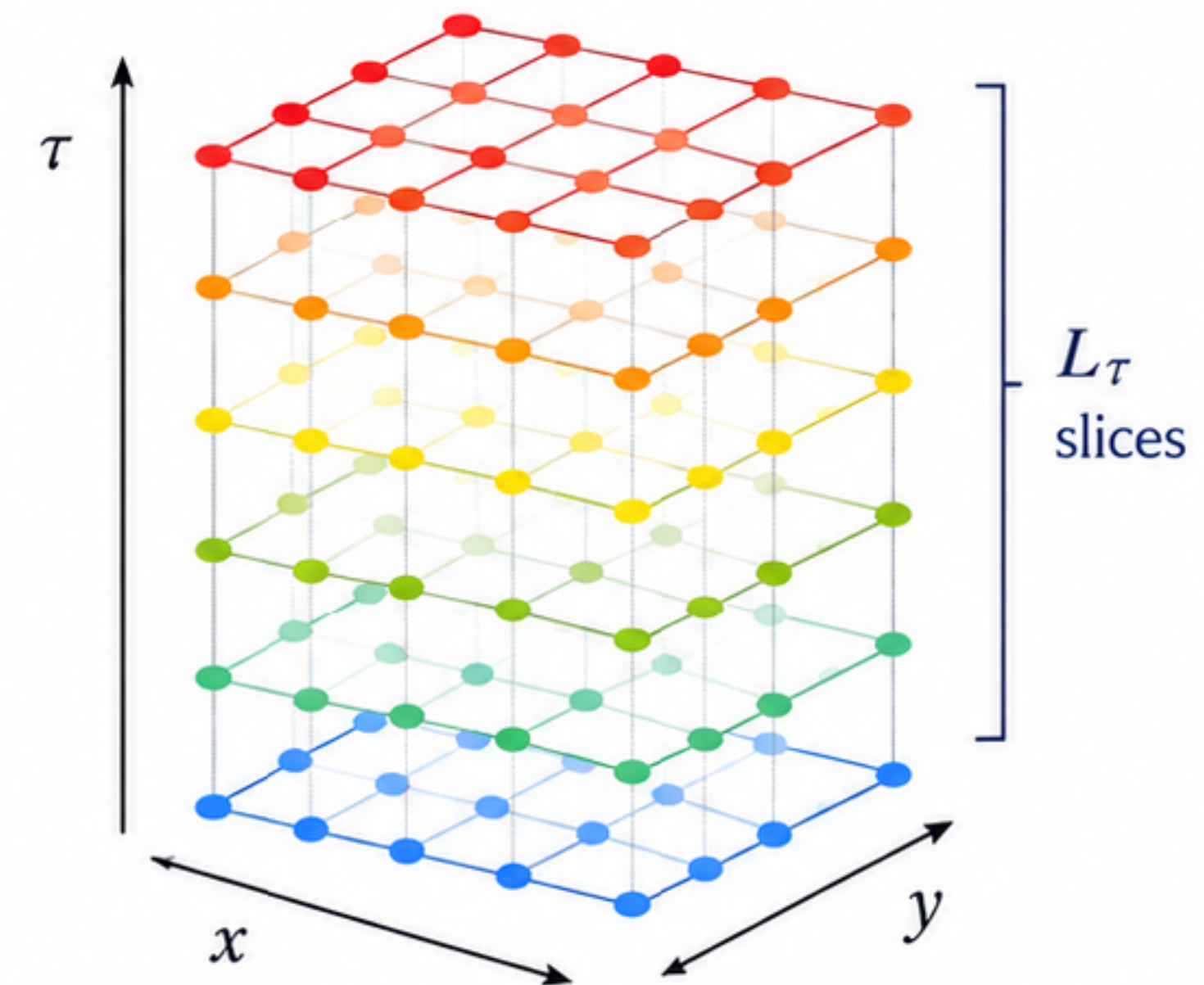
Quantum system in D dimensions
(spatial coordinates)



Feynman mapping
 $D \rightarrow D + 1$



Classical system in $D+1$ dimensions
(spatial coordinates + imaginary time)



The propagator is a sum over all paths connecting r_i and r_f in D dimensions.

$$K(r_f, r_i; \beta) = \int_{r_i}^{r_f} \mathcal{D}[r(\tau)] e^{-S_E[r(\tau)]/\hbar}$$

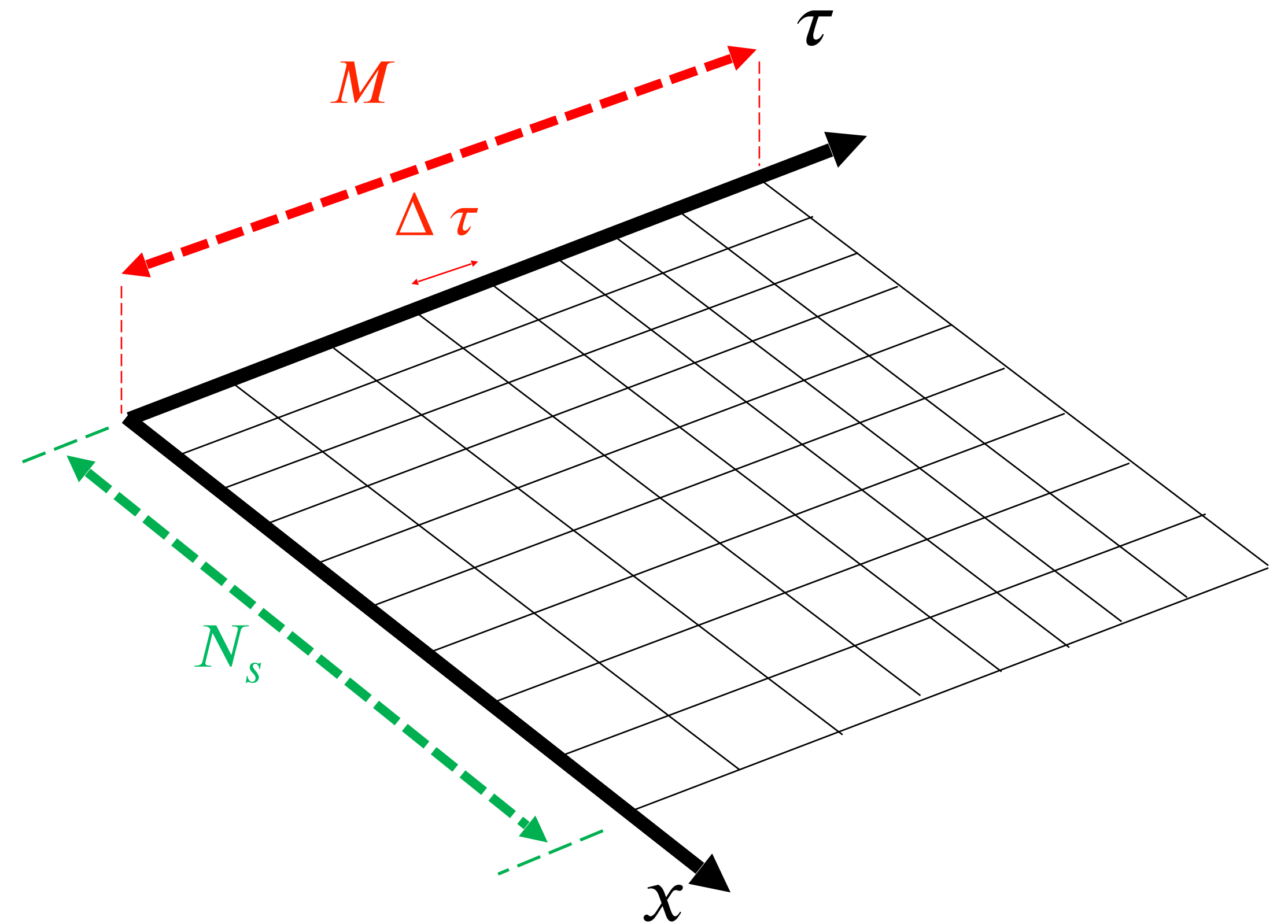
(integration over paths in D dimensions)

The D -dimensional quantum problem is equivalent to a $(D + 1)$ -dimensional classical statistical model.

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

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

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



$$Z = \sum_{C_1, C_2, \dots, C_M} \langle C_1 | e^{-\Delta\tau H} | C_M \rangle \underbrace{\langle C_M | e^{-\Delta\tau H} | C_{M-1} \rangle \dots \langle C_2 | e^{-\Delta\tau H} | C_1 \rangle}_{\sum_C |C\rangle \langle C| = I}.$$

$$\sum_C |C\rangle \langle C| = I$$

Ising model with a transverse magnetic field

$$H_0 = -J \sum_i S_i^z S_{i+1}^z \quad H_1 = -H_x \sum_i S_i^x$$

$$H_0 |C_k\rangle = E_0(C_k) |C_k\rangle$$

$$\langle C_{k+1} | e^{-\Delta\tau H} | C_k \rangle \approx e^{-\Delta\tau E_0(C_{k+1})} \underbrace{\langle C_{k+1} | e^{-\Delta\tau H_1} | C_k \rangle}$$

$$\langle C_{k+1} | e^{-\Delta\tau H_1} | C_k \rangle = \prod_i \langle S_{i,k+1}^z | e^{-\Delta\tau H_x S_i^x} | S_{i,k}^z \rangle$$

$$\langle S_{i,k+1}^z | e^{-\Delta\tau H^x S_i^x} | S_{i,k}^z \rangle = \sqrt{\sinh(\Delta\tau H^x) \cosh(\Delta\tau H^x)} \times e^{-K^\tau s_{i,k+1} s_{i,k}}$$

$$K^\tau = \frac{1}{2} \ln [\tanh(\Delta\tau H^x)]$$

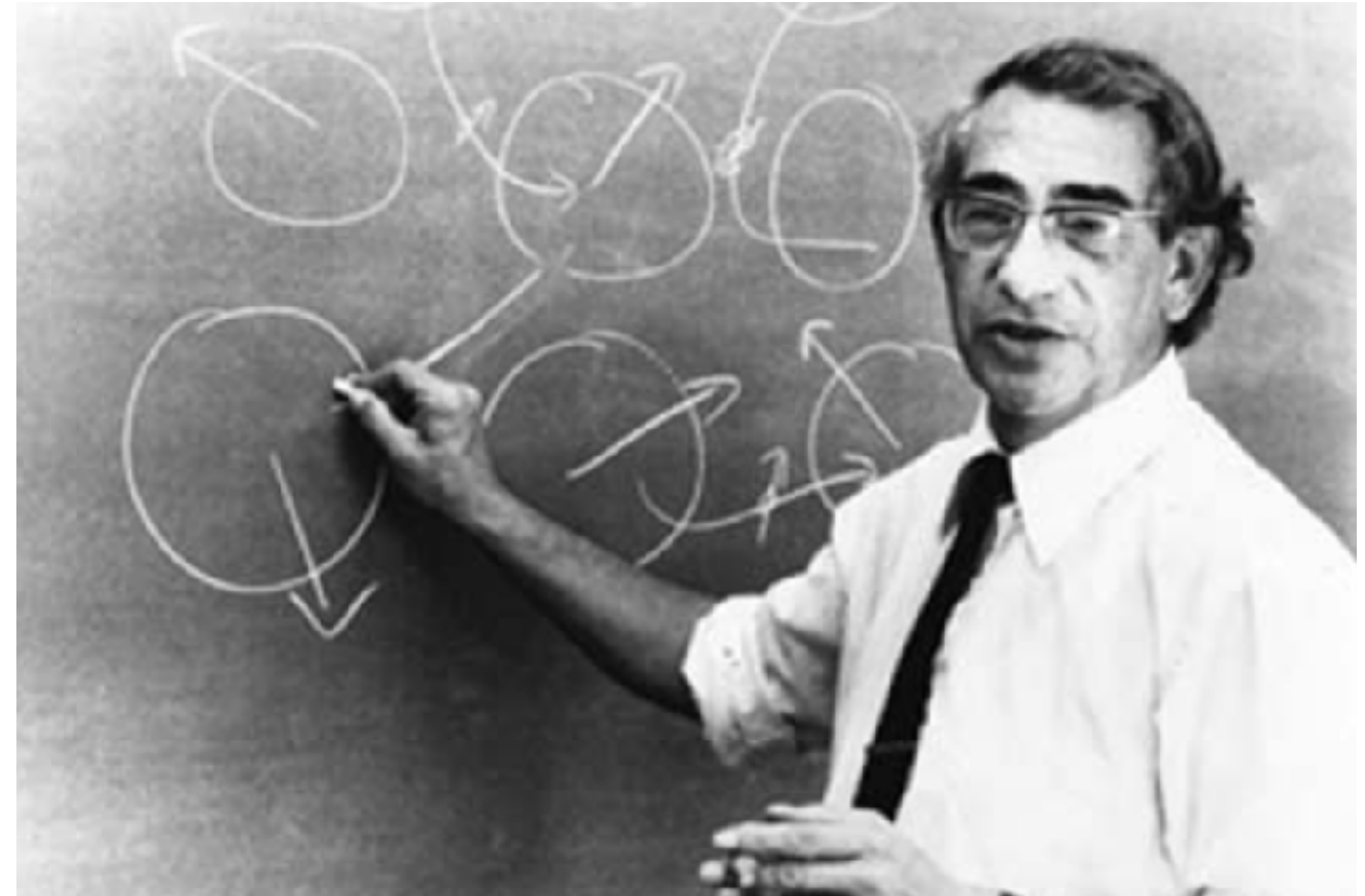
Show this!

$$Z \propto \sum_{C_1, C_2, \dots, C_M} \exp \left(\Delta\tau J^z \sum_{i,k} s_{i,k} s_{i+1,k} + K^\tau \sum_{i,k} s_{i,k} s_{i,k+1} \right).$$

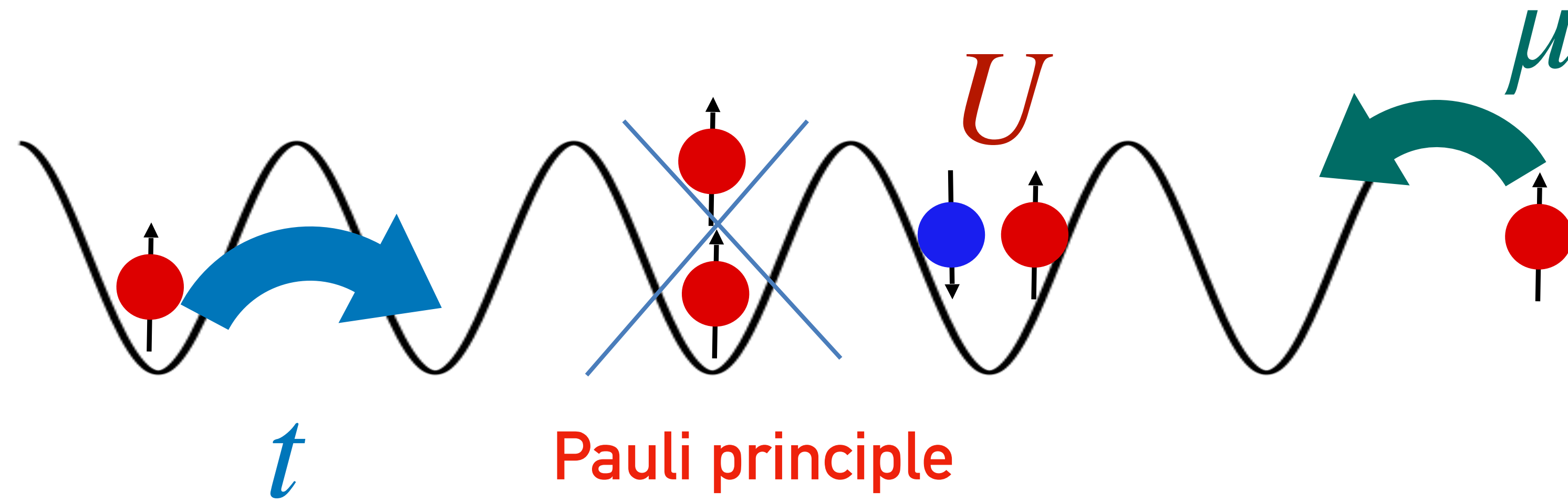
$$K^x = \Delta\tau J^z \quad K^\tau = \frac{1}{2} \ln [\tanh(\Delta\tau H^x)]$$

$$H_{\text{classical}} = -K^x \sum_{i,k} s_{i,k} s_{i+1,k} - K^\tau \sum_{i,k} s_{i,k} s_{i,k+1}$$

The Hubbard Model



Hubbard model



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

Physics of the Hubbard Model

Localization

X

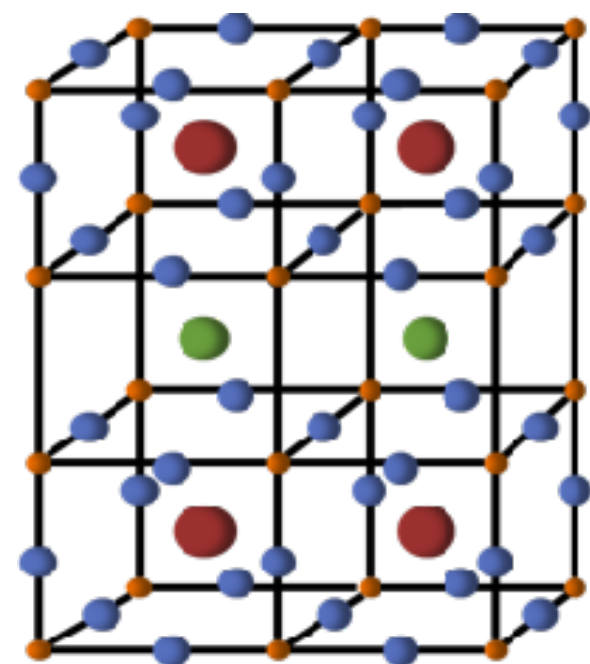
Itineracy

U

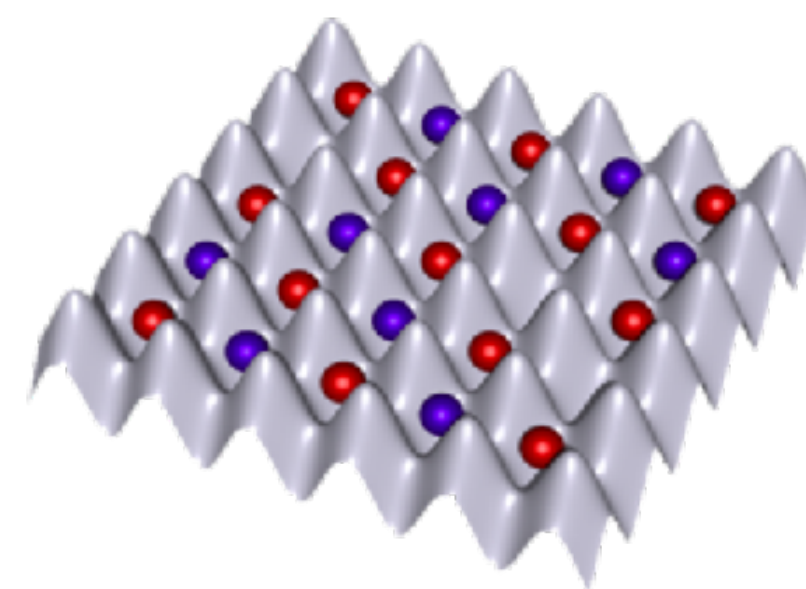
t

Metal- insulator transition
Magnetic ordering

Same physics

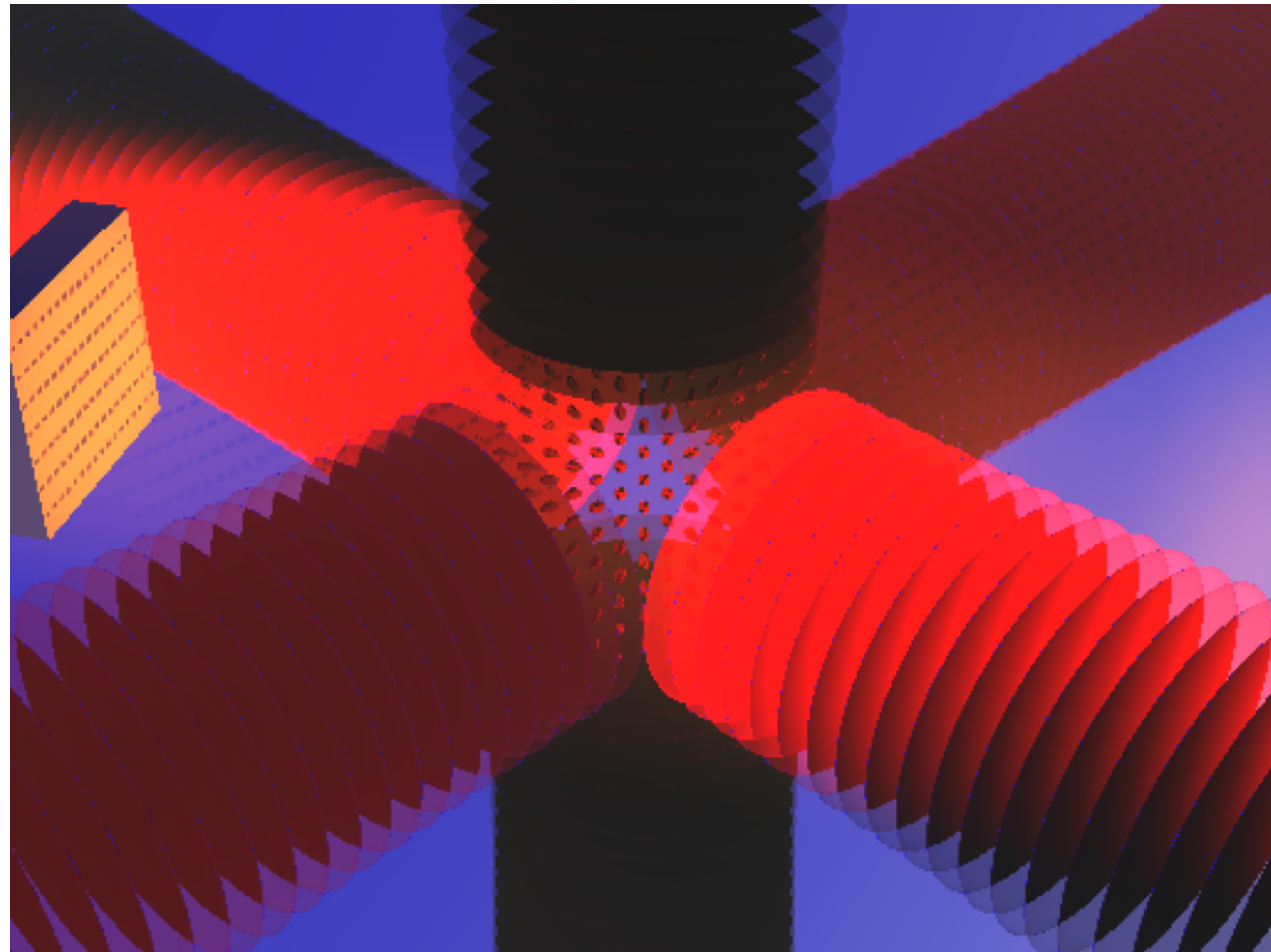


Strongly
correlated
materials



Ultracold
fermionic atoms
in optical lattices

Optical lattices

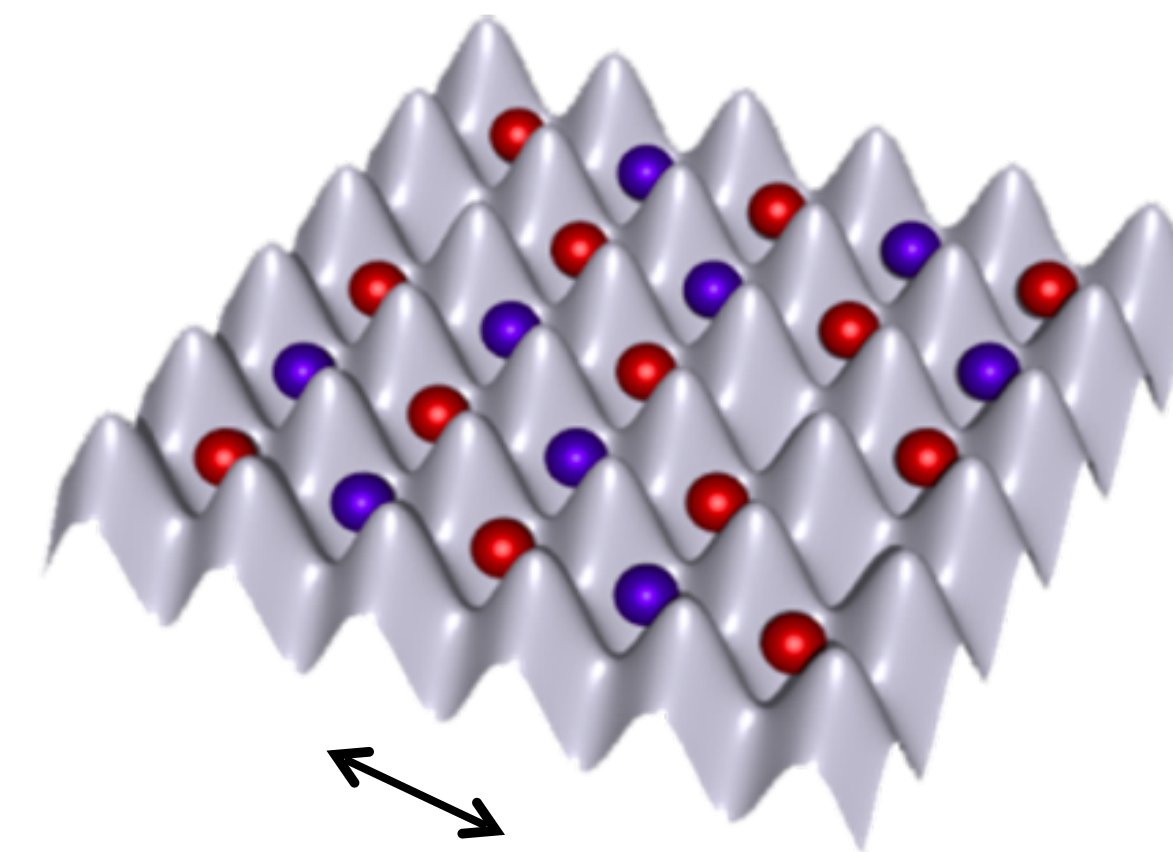
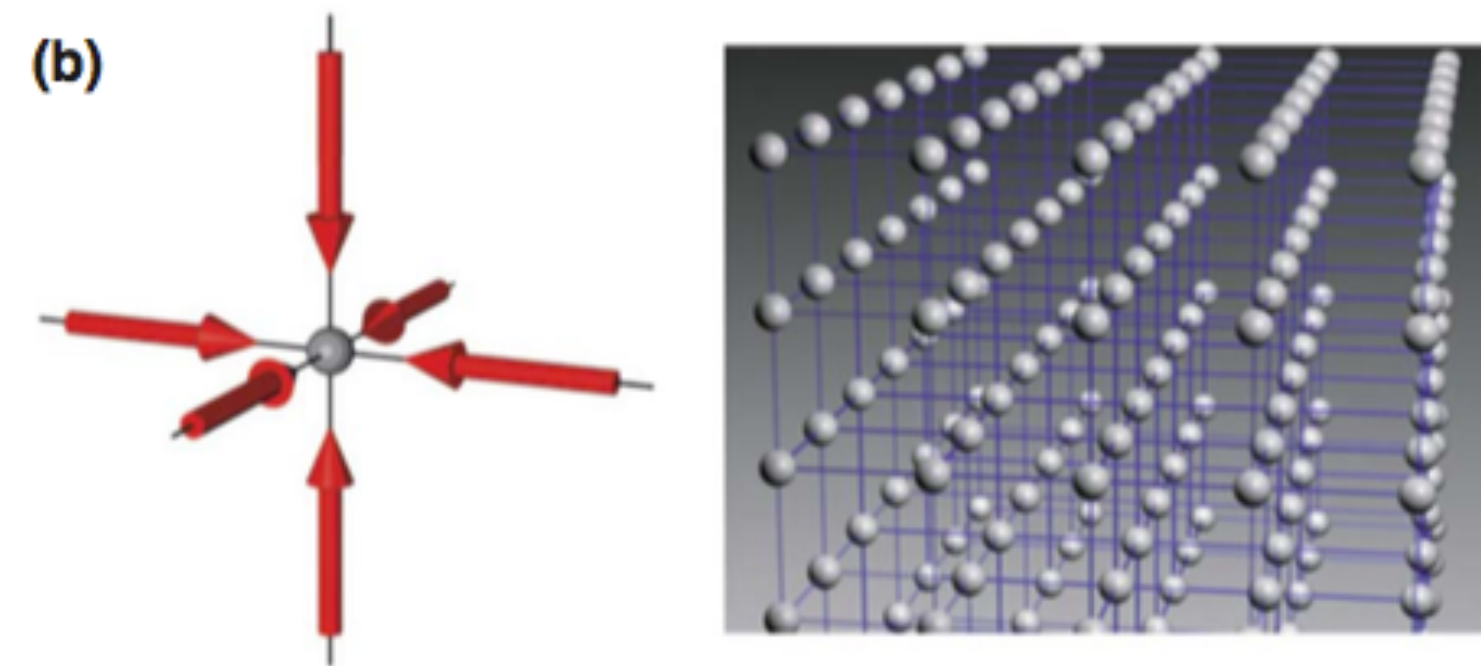
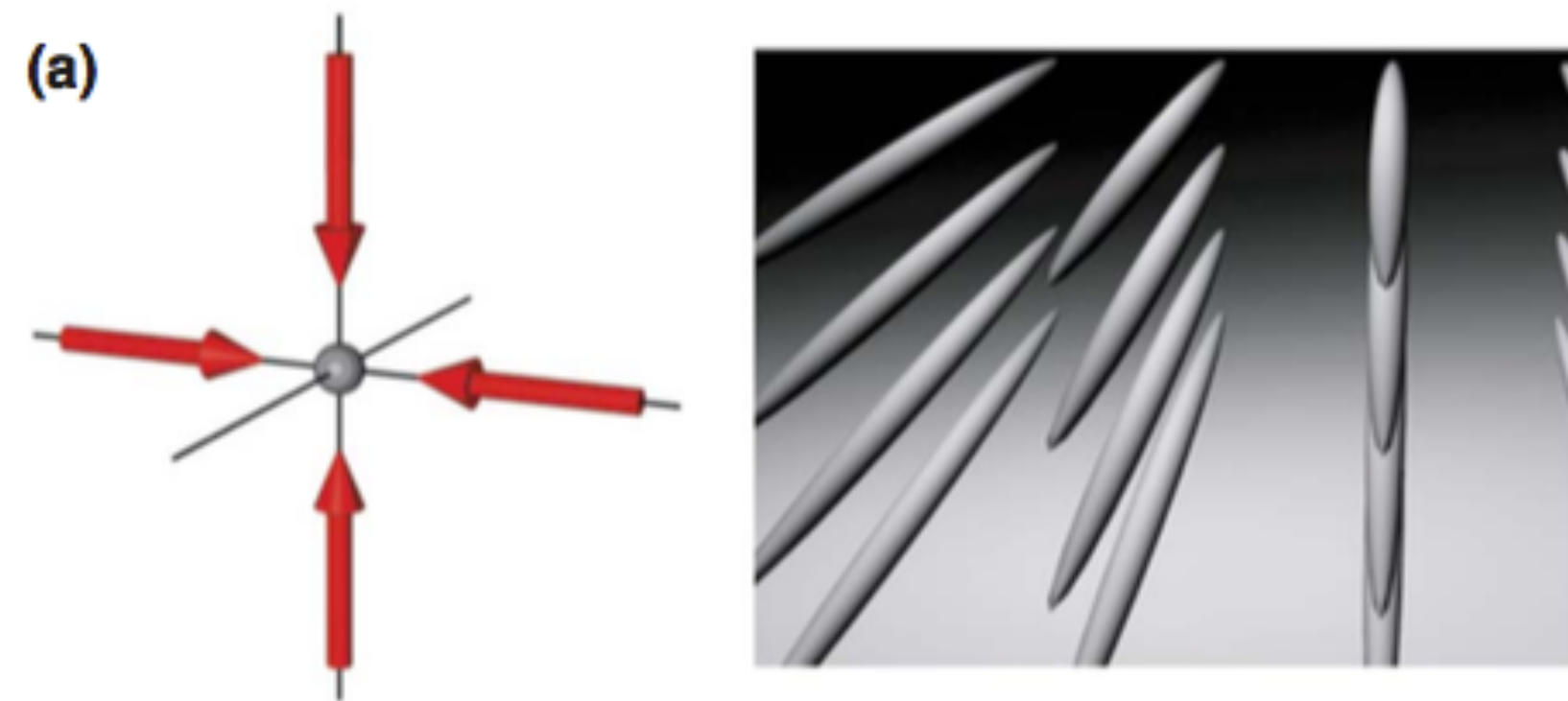
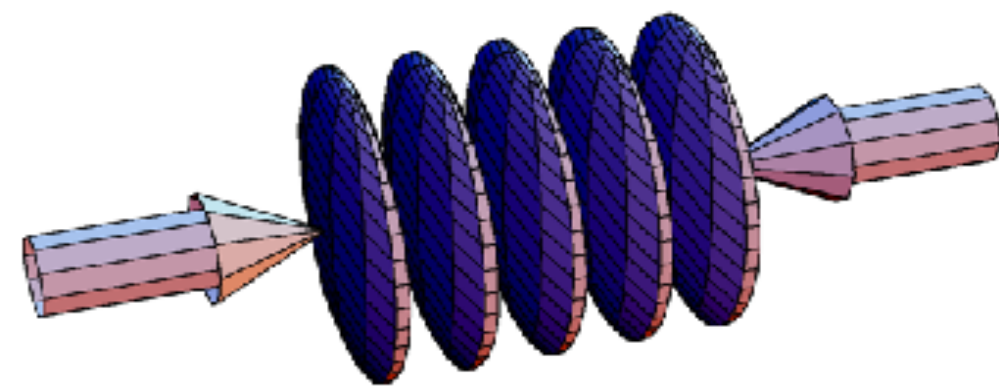


Confining potential

+

Periodic potential

Dimensionality



$d = 532 \text{ nm}$

Advantages of optical lattices

Control

- interaction strength (U)
- lattice hopping (t)
- dimensionality
- density (n)
- spin imbalance
- disorder
- spin-orbit interaction
- ...

Physics of the Attractive Hubbard Model

Pair formation

X

Itineracy

$-U$

t

Pair coherence
Superfluidity
BCS, BEC

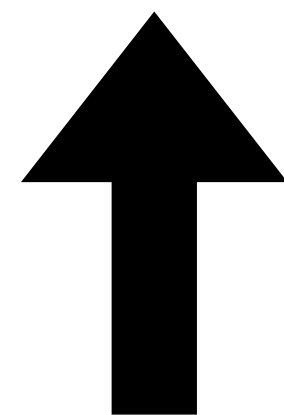
Physics of the Attractive Hubbard Model

Pair formation

X

Itineracy

$-U$

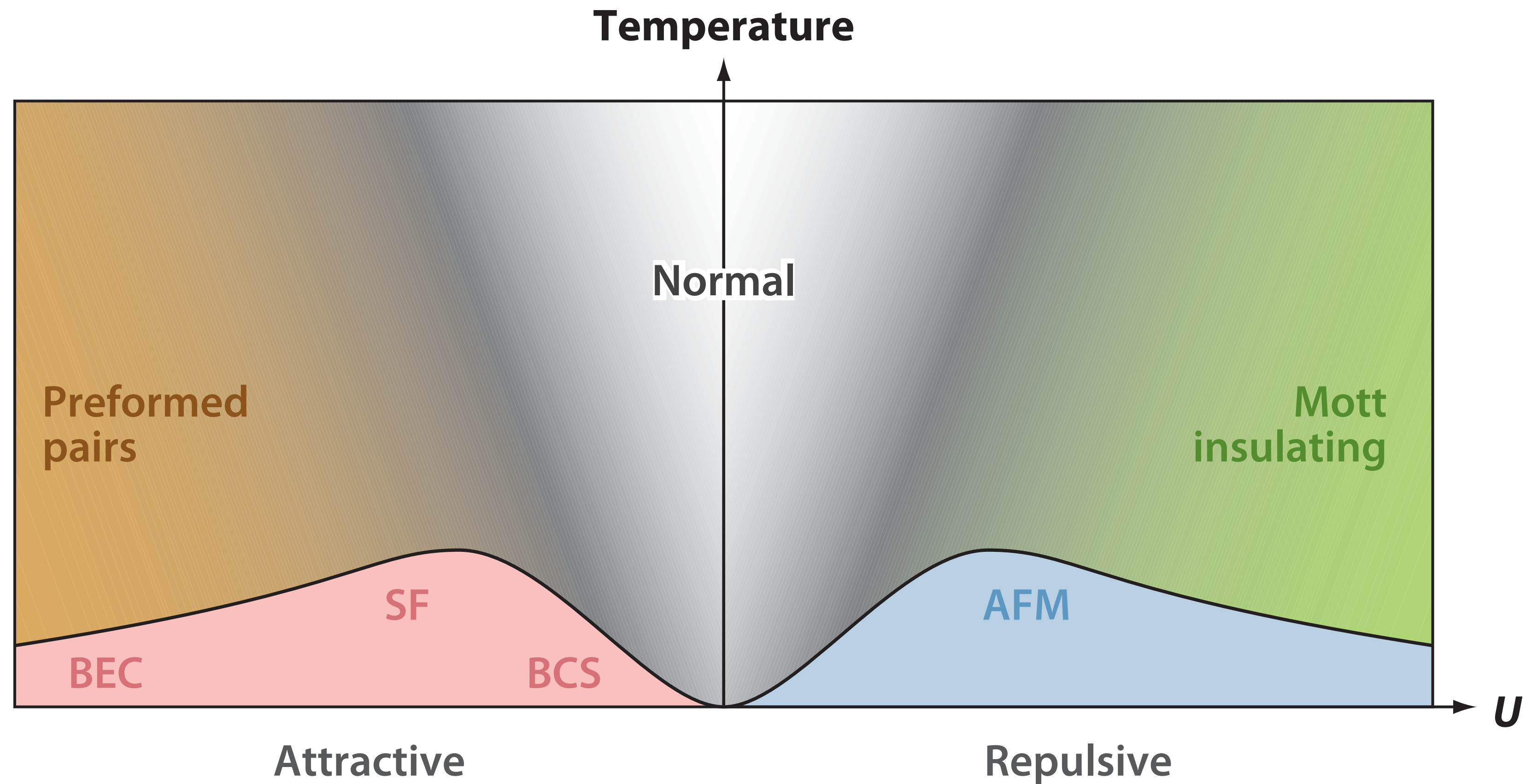


Pair coherence
Superfluidity
BCS, BEC

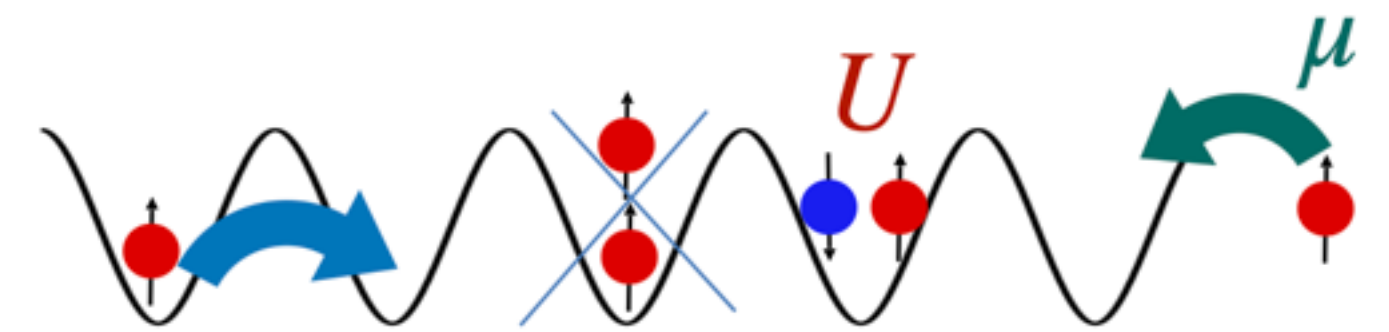
t

Phenomenological in early days
Realistic in cold atoms

Relation between repulsive and attractive models



QMC for the Hubbard Model



Hubbard model

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j,\sigma} + h.c.) - \mu \sum_i (n_{i\uparrow} + n_{i,\downarrow}) + U \sum_i (n_{i\uparrow} - 1/2)(n_{i,\downarrow} - 1/2)$$

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

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

$$\mathcal{H} = K + V \quad [K, V] \neq 0$$

Similar to the TFIM

Choose a basis

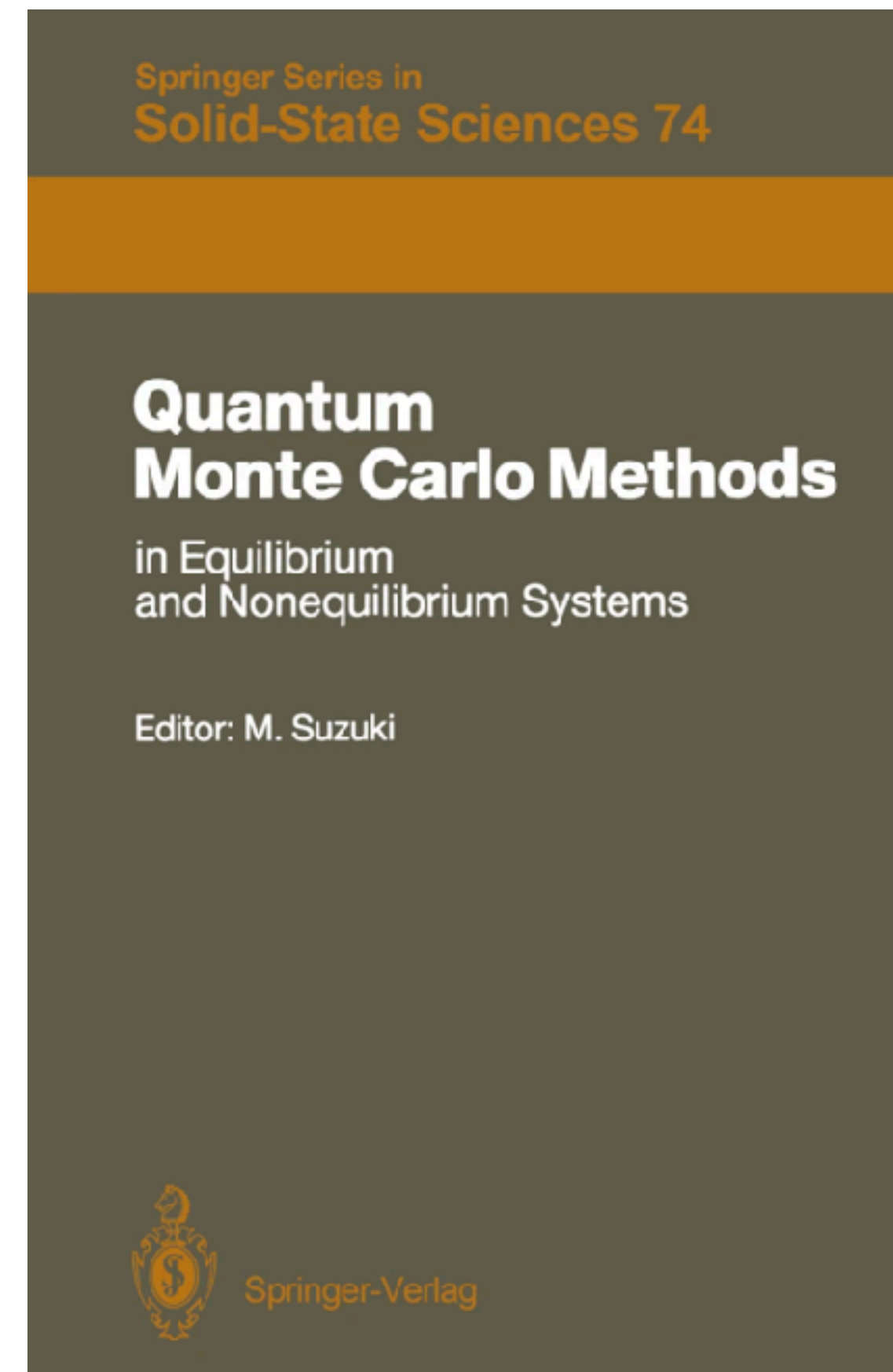
Do a Trotter–Suzuki decomposition

Insert identities

Choose a basis

$$|\psi_{N_\sigma}\rangle = |n_{1\sigma}, n_{2\sigma}, \dots, n_{N_\sigma}\rangle = c_{i_{N_\sigma}}^\dagger \cdots c_{i_2}^\dagger c_{i_1}^\dagger |0\rangle$$

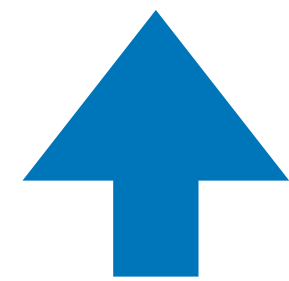
Suzuki–Trotter decomposition



Trotter-Susuki decomposition

$$Z = \text{Tr} e^{-\beta \mathcal{H}}$$

$$e^{-\beta(K+V)} = (e^{-\Delta\tau(K+V)})^M = (e^{-\Delta\tau K})^M (e^{-\Delta\tau V})^M + \mathcal{O}(\Delta\tau^2 U)$$

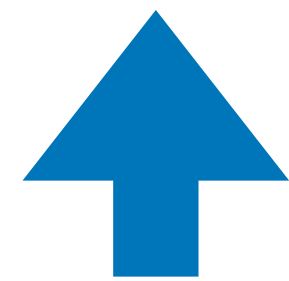


$$\Delta\tau = \beta / M$$

Trotter-Susuki decomposition

$$Z = \text{Tr} e^{-\beta \mathcal{H}}$$

$$e^{-\beta(K+V)} = (e^{-\Delta\tau(K+V)})^M = (e^{-\Delta\tau K})^M (e^{-\Delta\tau V})^M + \mathcal{O}(\Delta\tau^2 U)$$

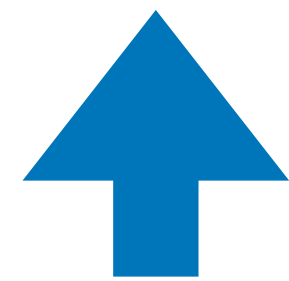


$$\Delta\tau = \beta / M$$

Trotter-Susuki decomposition

$$Z = \text{Tr} e^{-\beta \mathcal{H}}$$

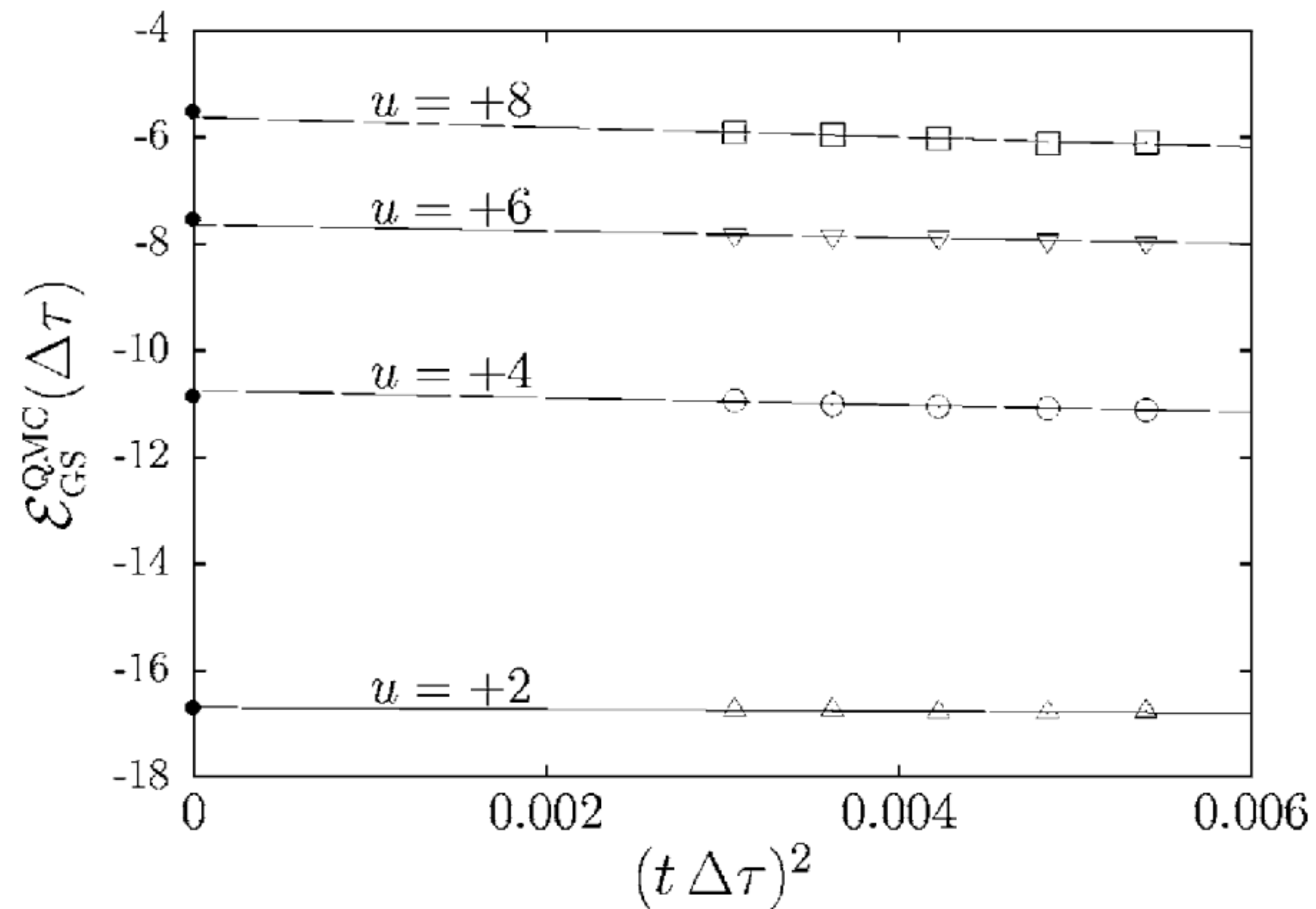
$$e^{-\beta(K+V)} = (e^{-\Delta\tau(K+V)})^M = (e^{-\Delta\tau K})^M (e^{-\Delta\tau V})^M + \mathcal{O}(\Delta\tau^2 U)$$



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

Once again: this is the approximation done in DQMC

How careful we have to be with the choice of $\Delta\tau$



PRB 73, 165120 (06)

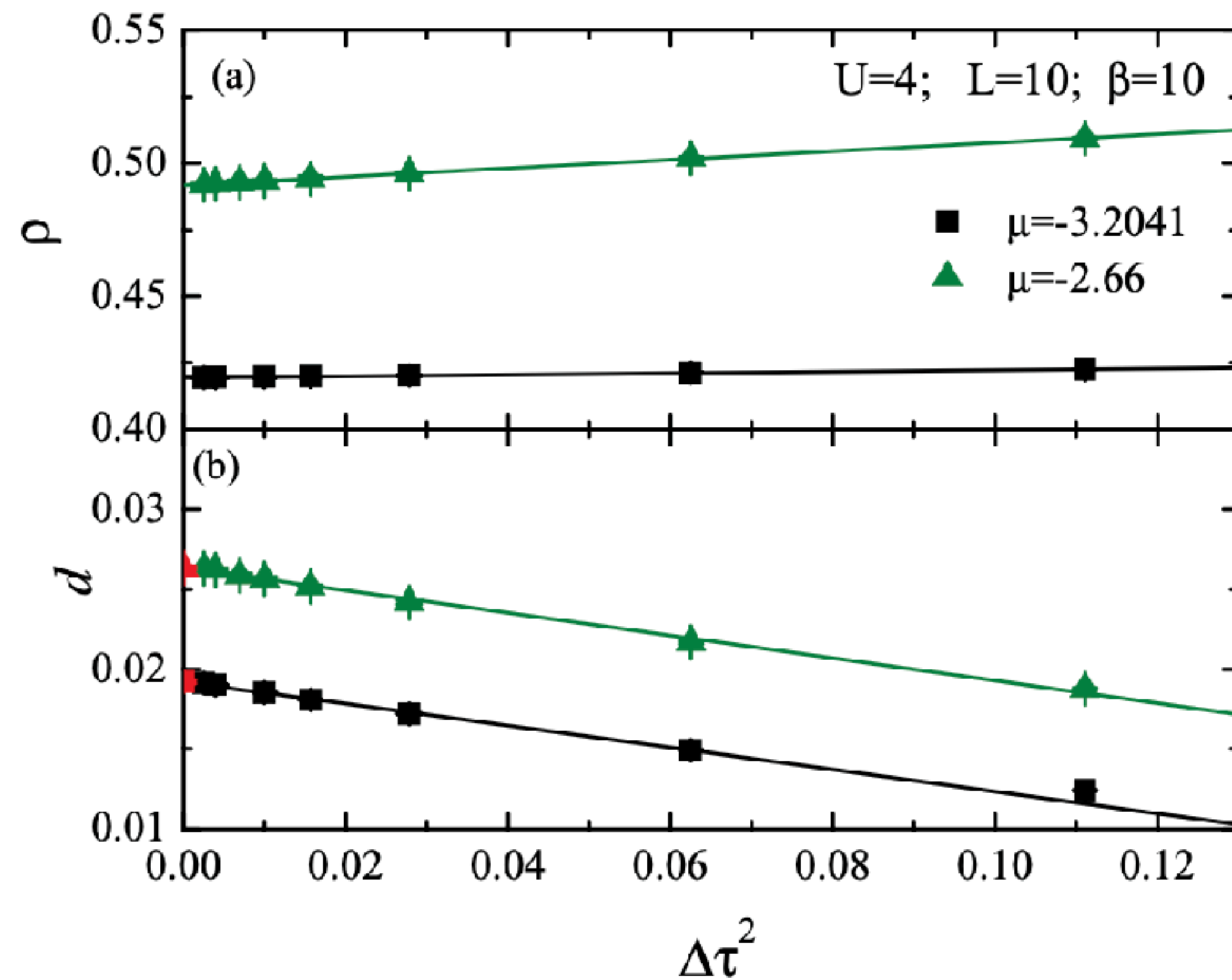
G. Xianlong et al.

Energy

Ground state energy: from
Bethe Ansatz +LDA

Open symbols: QMC

How careful we have to be with the choice of $\Delta\tau$



Density and double occupation

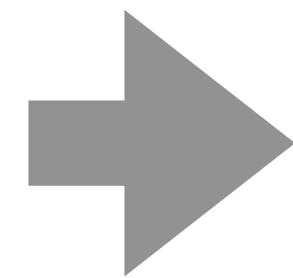
Mondaini et al PRB 2012

How careful we have to be with the choice of $\Delta\tau$

Early 80's $\rightarrow t\Delta\tau = 1/8$

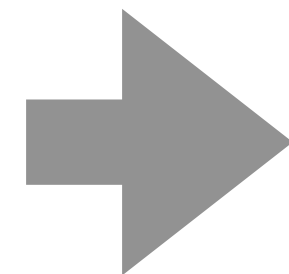
How careful we have to be with the choice of $\Delta\tau$

Early 80's



$$t\Delta\tau = 1/8$$

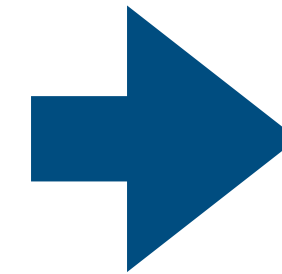
Comparison with
optical lattices
experiments



$$t\Delta\tau = 1/20$$

PROBLEM

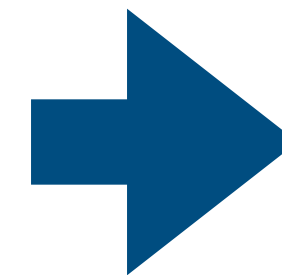
$$K = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j,\sigma} + h.c.) - \mu \sum_i (n_{i\uparrow} + n_{i,\downarrow})$$



Quadratic



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

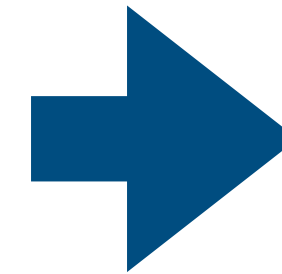


Quartic



PROBLEM

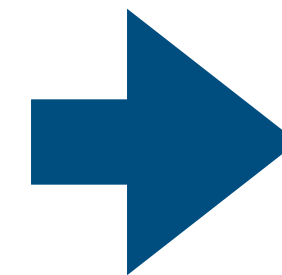
$$K = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$



Quadratic



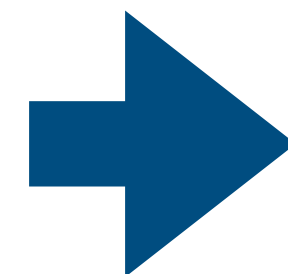
$$V = U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$$



Quartic



Solution



Hubbard-Stratonovich transformation

Hubbard–Stratonovich transformation

- R. L. Stratonovich, "On a method of calculating quantum distribution functions", Doklady Akad. Nauk SSSR 115, 1097 (1957); English translation in Soviet Physics Doklady 2, 416 (1958).
- J. Hubbard, "Calculation of partition functions", Phys. Rev. Lett. 3, 77 (1959), DOI: 10.1103/PhysRevLett.3.77.

Hubbard-Stratonovich transformation

PHYSICAL REVIEW B

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RAPID COMMUNICATIONS

1 OCTOBER 1983

Discrete Hubbard-Stratonovich transformation for fermion lattice models

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(Received 16 June 1983)

We discuss a new functional-integral formulation of interacting fermion systems on a lattice such as the Anderson or Hubbard models: the fermion-fermion interaction is eliminated by introducing auxiliary Ising variables. The resulting model for a d -dimensional quantum system is a $(d + 1)$ -dimensional Ising model with complicated interactions. The new transformation is particularly useful for performing numerical studies of these models using Monte Carlo techniques. We study its convergence properties and compare it with the usual Gaussian formulation for the case of the Hubbard model.

Hubbard-Stratonovich transformation

$$e^{\frac{1}{2}\hat{A}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 - x\hat{A}}$$

Hubbard-Stratonovich transformation

$$e^{\frac{1}{2}\hat{A}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 - x\hat{A}}$$

$$V = U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \quad \left\{ \begin{array}{l} (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - 1)^2 - \frac{1}{4}, \\ (n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2}) = -\frac{1}{2}(n_{\uparrow} - n_{\downarrow})^2 + \frac{1}{4} \end{array} \right.$$

Hubbard-Stratonovich transformation

$$e^{\frac{1}{2}\hat{A}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 - x\hat{A}}$$

$$V = U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \quad \left\{ \begin{array}{l} (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - 1)^2 - \frac{1}{4}, \\ (n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2}) = -\frac{1}{2}(n_{\uparrow} - n_{\downarrow})^2 + \frac{1}{4} \end{array} \right.$$

$$e^{-\Delta\tau U \left(n_{\uparrow} - \frac{1}{2}\right) \left(n_{\downarrow} - \frac{1}{2}\right)} = \left\{ \begin{array}{l} e^{-\frac{1}{4}\Delta\tau U} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 + x\sqrt{\Delta\tau U}(n_{\uparrow} - n_{\downarrow})}, \\ e^{+\frac{1}{4}\Delta\tau U} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 + x\sqrt{\Delta\tau |U|}(n_{\uparrow} + n_{\downarrow} - 1)} \end{array} \right.$$

Hubbard-Stratonovich transformation

$$e^{\frac{1}{2}\hat{A}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 - x\hat{A}}$$

New auxiliary variable x

$$V = U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \quad \left\{ \begin{array}{l} (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - 1)^2 - \frac{1}{4}, \\ (n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2}) = -\frac{1}{2}(n_{\uparrow} + n_{\downarrow})^2 + \frac{1}{4} \end{array} \right.$$

$$e^{-\Delta\tau U \left(n_{\uparrow} - \frac{1}{2}\right) \left(n_{\downarrow} - \frac{1}{2}\right)} = \left\{ \begin{array}{l} e^{-\frac{1}{4}\Delta\tau U} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 + x\sqrt{\Delta\tau U}(n_{\uparrow} - n_{\downarrow})}, \\ e^{+\frac{1}{4}\Delta\tau U} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 - x\sqrt{\Delta\tau |U|}(n_{\uparrow} + n_{\downarrow} - 1)} \end{array} \right.$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \quad \rightarrow \quad \sum_{x=\pm 1}$$

Auxiliary variable x :

Discrete and takes values +1 and -1

Ising like

$N \cdot M$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \quad \rightarrow \quad \sum_{x=\pm 1}$$

$$e^{-U\Delta\tau n_{\uparrow}n_{\downarrow}} = \frac{1}{2} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} e^{-\left(\sigma s\lambda + \frac{U\Delta\tau}{2}\right)n_{\sigma}}, \quad U > 0,$$

Repulsive

$$e^{|U|\Delta\tau n_{\uparrow}n_{\downarrow}} = \frac{1}{2} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} e^{\left(s\lambda + \frac{|U|\Delta\tau}{2}\right)\left(n_{\sigma} - \frac{1}{2}\right)}, \quad U < 0,$$

Attractive

$$\cosh \lambda = e^{|U|\Delta\tau/2}.$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \quad \rightarrow \quad \sum_{x=\pm 1}$$

$$e^{-U\Delta\tau n_{\uparrow}n_{\downarrow}} = \frac{1}{2} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} e^{-\left(\sigma s\lambda + \frac{U\Delta\tau}{2}\right)n_{\sigma}}, \quad U > 0,$$

Repulsive

$$e^{|U|\Delta\tau n_{\uparrow}n_{\downarrow}} = \frac{1}{2} \sum_{s=\pm 1} \prod_{\sigma=\uparrow,\downarrow} e^{\left(s\lambda + \frac{|U|\Delta\tau}{2}\right)\left(n_{\sigma} - \frac{1}{2}\right)}, \quad U < 0,$$

Attractive

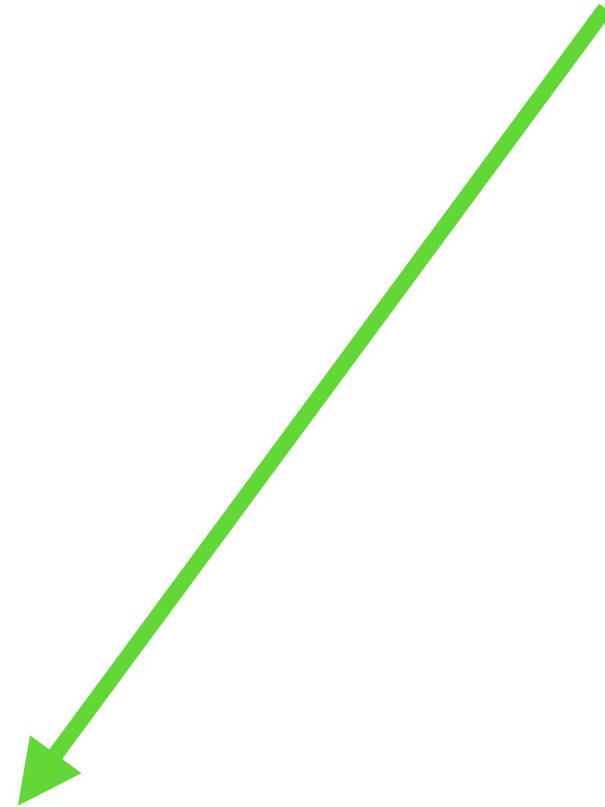
$$\cosh \lambda = e^{|U|\Delta\tau/2}.$$

Now we can write the partition function

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

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

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



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

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

Monte Carlo Sampling

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

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

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

Monte Carlo Sampling

Fermionic trace

??

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

$\ell = M, \dots, 1$ 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

Fermionic trace

??

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

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

Ns x Ns diagonal matrix

Kinetic energy

$$K_{ij} = \begin{cases} -t & \text{if } i \text{ and } j \text{ are nearest neighbours,} \\ 0 & \text{otherwise} \end{cases}$$

For a 1D system with periodic boundary conditions $N_s \times N_s$ matrix

$$K = \begin{pmatrix} 0 & -t & 0 & \dots & 0 & -t \\ -t & 0 & -t & \dots & 0 & 0 \\ 0 & -t & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -t & 0 & \dots & 0 & -t & 0 \end{pmatrix}$$

Kinetic energy contribution: checkerboard break-up

$$K = K_x^{(a)} + K_x^{(b)}$$

K^a – hopping between sites 1 and 2, 3 and 4, 5 and 6...



K^b – hopping between sites 2 and 3, 4 and 5, 6 and 7...

Suzuki-Trotter decomposition

$$e^{-\Delta\tau K} = e^{-\Delta\tau K_x^{(a)}} e^{-\Delta\tau K_x^{(b)}} + \mathcal{O}[(\Delta\tau)^2] \quad \Rightarrow \quad \text{Even powers of } K_x^{(\alpha)} \text{ become the identity} \quad \alpha = a, b$$

$$e^{-\Delta\tau K_x^{(\alpha)}} = K_x^{(\alpha)} \sinh(\Delta\tau t) + 1 \cosh(\Delta\tau t)$$

Convenient for numerical implementation

Some implementations of DQMC don't use checkerboard decomposition and exponentiate the full hopping matrix

Numerical cost



X

$U=0$ results are exact



Introducing the B matrices

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

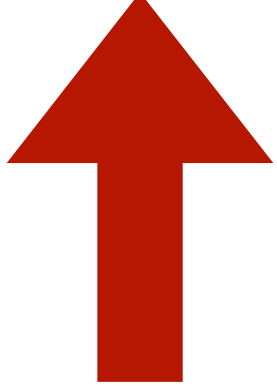
$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \text{Tr}_{\{s\}} \prod_{\sigma} \det [\mathbf{1} + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \dots \mathbf{B}_1^\sigma]$$

Introducing the O matrices

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

$$\begin{aligned}\mathcal{Z} &= \left(\frac{1}{2}\right)^{L^d M} \mathbf{Tr}_{\{s\}} \det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\}) = \\ &= \mathbf{Tr}_{\{s\}} \rho(\{s\}), \quad \rightarrow \text{Effective density matrix}\end{aligned}$$

Sum over Ising spins of a product of determinants


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

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

Determinantal Quantum Monte Carlo

or

Auxiliary field Quantum Monte Carlo

Determinant weights

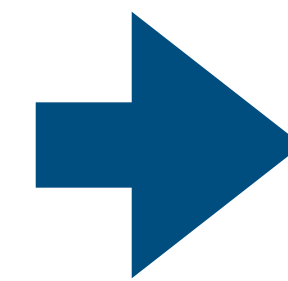


Determinantal weight

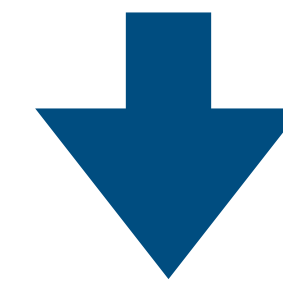
$$r' = \frac{\rho(\{s\}')}{\rho(\{s\})} = \frac{\det \mathbf{O}^\uparrow(\{s\}') \cdot \det \mathbf{O}^\downarrow(\{s\}')}{\det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\})} \Rightarrow \text{Statistical weight}$$

Determinantal weight

$$r' = \frac{\rho(\{s\}')}{\rho(\{s\})} = \frac{\det \mathbf{O}^\uparrow(\{s\}') \cdot \det \mathbf{O}^\downarrow(\{s\}')}{\det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\})}$$



Statistical weight



NOT ALWAYS POSITIVE

Determinantal weight

$$r' = \frac{\rho(\{s\}')}{\rho(\{s\})} = \frac{\det \mathbf{O}^\uparrow(\{s\}') \cdot \det \mathbf{O}^\downarrow(\{s\}')}{\det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\})} \Rightarrow \text{Statistical weight}$$



MINUS SIGN PROBLEM

NOT ALWAYS POSITIVE

MINUS SIGN PROBLEM

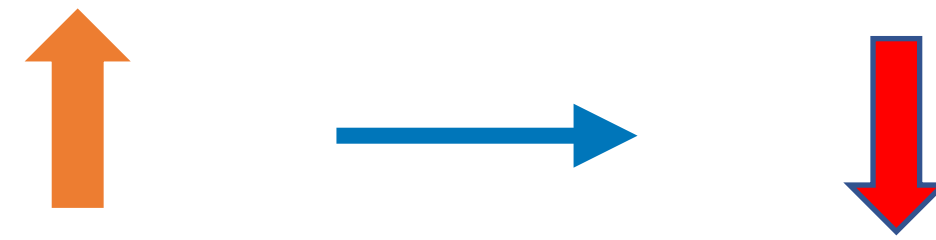
Later...

Simulations

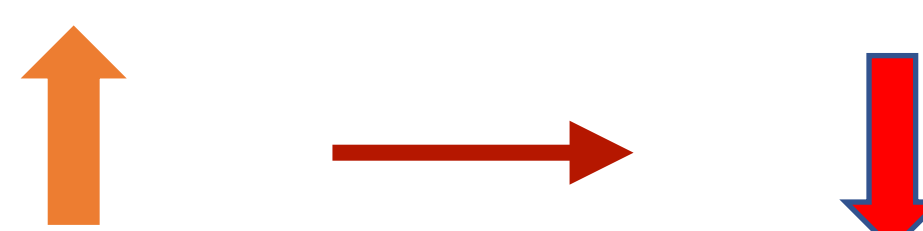


Propose a flip in an Ising spin

$$s_{\mathbf{i}}(\ell) \rightarrow -s_{\mathbf{i}}(\ell)$$



Propose a flip in an Ising spin

$$s_{\mathbf{i}}(\ell) \rightarrow -s_{\mathbf{i}}(\ell)$$


Change in V matrices

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

Propose a flip in an Ising spin

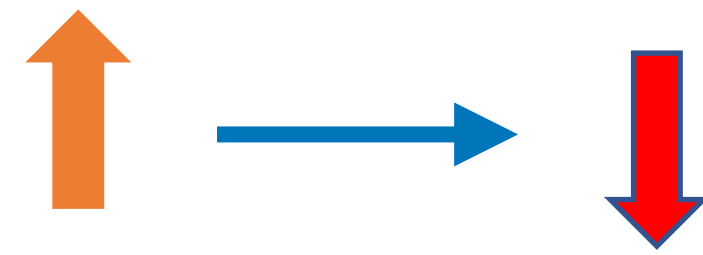
$$s_{\mathbf{i}}(\ell) \rightarrow -s_{\mathbf{i}}(\ell)$$


Change in V matrices

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

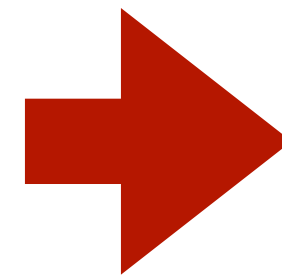
$$\delta V_{\mathbf{ij}}^\sigma(\ell) \equiv V_{\mathbf{ij}}^\sigma(\ell, -s) - V_{\mathbf{ij}}^\sigma(\ell, s) = -2\lambda\sigma s_{\mathbf{i}}(\ell) \delta_{\mathbf{ij}}$$

Propose a flip in an Ising spin



$$s_{\mathbf{i}}(\ell) \rightarrow -s_{\mathbf{i}}(\ell)$$

Changes in V matrices



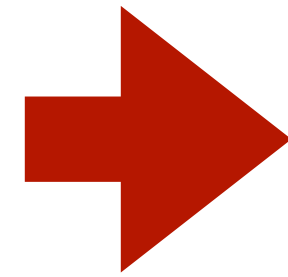
Changes in B matrices

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

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

Propose a flip in an Ising spin

Change in V matrices



Change in B matrices

$$\mathbf{B}_\ell^\sigma \rightarrow [\mathbf{B}_\ell^\sigma]' = \mathbf{B}_\ell^\sigma \Delta_\ell^\sigma(\mathbf{i})$$

$$[\Delta_\ell^\sigma(\mathbf{i})]_{\mathbf{j}\mathbf{k}} = \begin{cases} 0 & \text{if } \mathbf{j} \neq \mathbf{k}, \\ 1 & \text{if } \mathbf{j} = \mathbf{k} \neq \mathbf{i}, \\ e^{-2\lambda\sigma s_{\mathbf{i}}(\ell)} & \text{if } \mathbf{j} = \mathbf{k} = \mathbf{i}. \end{cases}$$

$$\{s\} \rightarrow \{s'\}$$

Configurations that differ by an Ising spin flipped on site $(\mathbf{i}, \ell)$

“Boltzmann weight”

$$r' = \frac{\rho(\{s'\})}{\rho(\{s\})} = \frac{\det \mathbf{O}^\uparrow(\{s'\}) \cdot \det \mathbf{O}^\downarrow(\{s'\})}{\det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\})} = R_\uparrow R_\downarrow,$$

With

$$R_\sigma \equiv \frac{\det \mathbf{O}^\sigma(\{s'\})}{\det \mathbf{O}^\sigma(\{s\})}$$

Update

We don't need to calculate determinants at every step

That would be very time consuming!

Update

We don't need to calculate determinants at every step

That would be very time consuming!

R_σ can be expressed in terms of the Green's functions

Operator a in the Heisenberg picture

$$a(\ell) \equiv a(\tau) = e^{\tau \mathcal{H}} a e^{-\tau \mathcal{H}}$$

$$\tau = \ell \Delta\tau$$

Initial time: $\Delta\tau$

Green's functions

$$\tilde{g}_{\mathbf{ij}}^\sigma \equiv [1 - g]_{\mathbf{ij}} \quad \tilde{G}_{\mathbf{ij}}^\sigma \equiv [1 - G]_{\mathbf{ij}}.$$

$$g^\sigma(\ell) \equiv \langle c_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma}^\dagger \rangle_{\{s\}} = \left[(1 + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \dots \mathbf{B}_1^\sigma)^{-1} \right]_{\mathbf{ij}}$$

$$G_{\mathbf{ij}}^\sigma(\ell_1; \ell_2) \equiv \langle c_{\mathbf{i}\sigma}(\ell_1) c_{\mathbf{j}\sigma}^\dagger(\ell_2) \rangle_{\{s\}} = [\mathbf{B}_{\ell_1}^\sigma \mathbf{B}_{\ell_1-1}^\sigma \dots \mathbf{B}_{\ell_2+1}^\sigma g^\sigma(\ell_2 + 1)]_{\mathbf{ij}}.$$

Green's functions

We'll see this in detail next class

$$G_{ij}^{\sigma}(\mathbf{r}, \mathbf{r}', \omega)$$

$$+ 1)]_{ij}$$

Defining the A matrices

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

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

Defining the A matrices

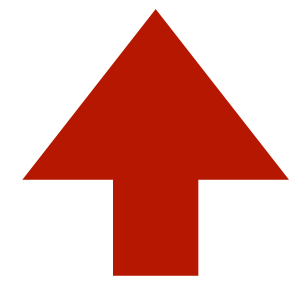
$$g^\sigma(\ell) \equiv [1 + A^\sigma(\ell)]^{-1}$$

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

Then

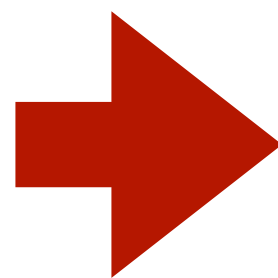
$$R_\sigma \equiv \frac{\det O^\sigma(\{s\}')}{\det O^\sigma(\{s\})} \quad \rightarrow \quad R_\sigma = \frac{\det [1 + A^\sigma(\ell) \Delta_\ell^\sigma(\mathbf{i})]}{\det [1 + A^\sigma(\ell)]}$$

$$\begin{aligned}
R_\sigma &= \frac{\det [\mathbf{1} + A^\sigma(\ell) \Delta_\ell^\sigma(\mathbf{i})]}{\det [\mathbf{1} + A^\sigma(\ell)]} \\
&= \det [(\mathbf{1} + A^\sigma(\ell) \Delta_\ell^\sigma(\mathbf{i})) g^\sigma(\ell)] = \\
&= \det [\mathbf{1} + (1 - g^\sigma(\ell)) (\Delta_\ell^\sigma(\mathbf{i}) - \mathbf{1})] = \\
&= 1 + (1 - g_{\mathbf{i}\mathbf{i}}^\sigma(\ell)) \left(e^{-2\lambda\sigma s_{\mathbf{i}}(\ell)} - 1 \right).
\end{aligned}$$



$$\Gamma_\ell^\sigma(\mathbf{i}) \equiv \Delta_\ell^\sigma(\mathbf{i}) - \mathbf{1}$$

A matrix where all elements
are zero except the $\mathbf{i}$ -th position
on the diagonal



$$\gamma_\ell^\sigma(\mathbf{i}) \equiv e^{-2\lambda\sigma s_{\mathbf{i}}(\ell)} - 1$$

Updates

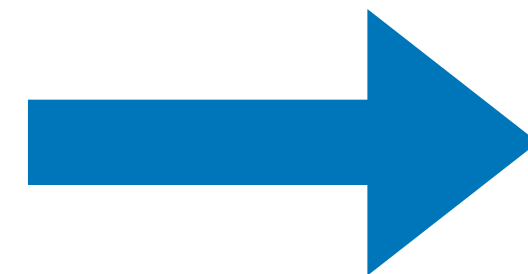
Two possibilities

From scratch

Iterating the Green's function

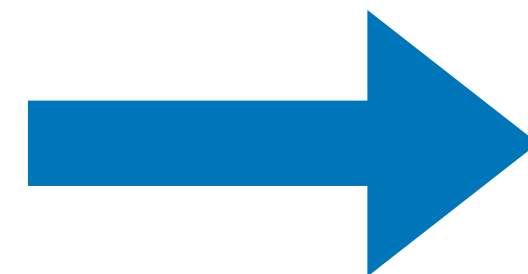
Two possibilities

From scratch



Time consuming: $\mathcal{O}(N_s^3)$

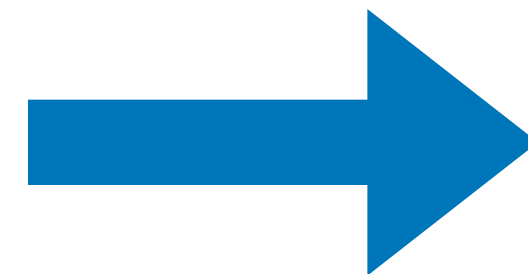
Iterating the Green's function



Faster: $\mathcal{O}(N_s^2)$

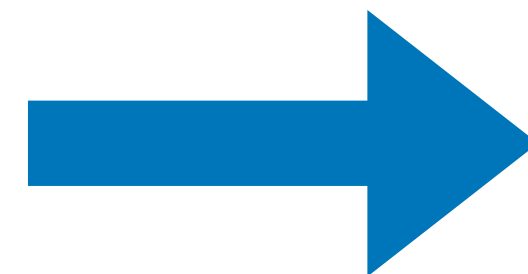
Two possibilities

From scratch



Time consuming: $\mathcal{O}(N_s^3)$
Rounding errors

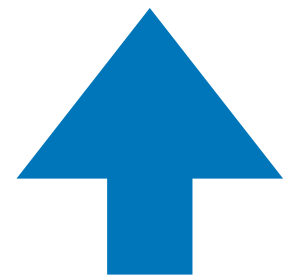
Iterating the Green's function



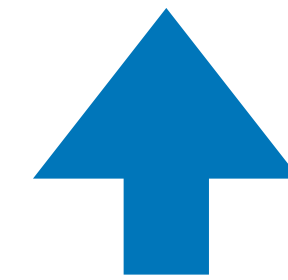
Faster: $\mathcal{O}(N_s^2)$

Iterating the Green's function

$$\bar{g}^{\sigma}(\ell) = \left[1 + (1 - g^{\sigma}(\ell))\Gamma_{\ell}^{\sigma}(\mathbf{i})\right]^{-1} g^{\sigma}(\ell).$$



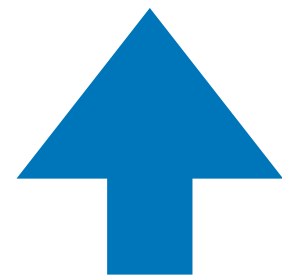
New



Old

Iterating the Green's function

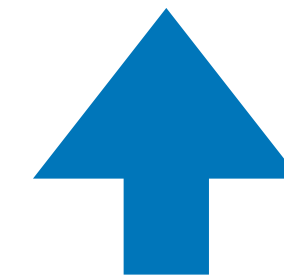
$$\bar{g}^{\sigma}(\ell) = \left[1 + (1 - g^{\sigma}(\ell))\Gamma_{\ell}^{\sigma}(\mathbf{i})\right]^{-1} g^{\sigma}(\ell).$$



New



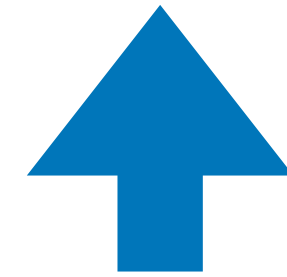
Calculate an inverse



Old

Calculate an inverse

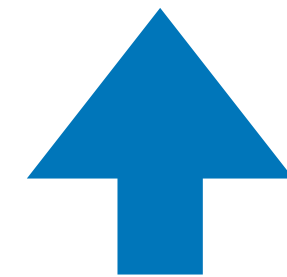
$$\left[1 + (1 - g^\sigma(\ell))\Gamma_\ell^\sigma(\mathbf{i})\right]^{-1} = 1 + x(1 - g^\sigma(\ell))\Gamma_\ell^\sigma(\mathbf{i})$$



To be determined

Calculate an inverse

$$\left[1 + (1 - g^\sigma(\ell)) \Gamma_\ell^\sigma(\mathbf{i})\right]^{-1} = 1 + x(1 - g^\sigma(\ell)) \Gamma_\ell^\sigma(\mathbf{i})$$



To be determined

Using the fact that $\Gamma_\ell^\sigma(\mathbf{i})$ is very sparse

$$x = -\frac{1}{R_\sigma}$$

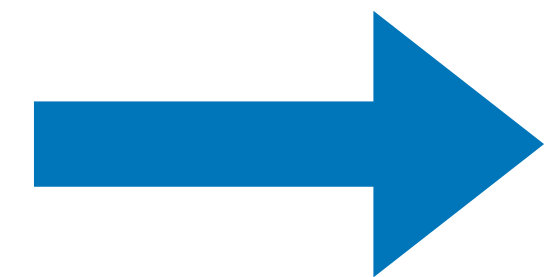
Elements of the Green's function

$$\bar{g}_{\mathbf{j}\mathbf{k}}^{\sigma}(\ell) = g_{\mathbf{j}\mathbf{k}}^{\sigma}(\ell) - \frac{\left[\delta_{\mathbf{j}\mathbf{i}} - g_{\mathbf{j}\mathbf{i}}^{\sigma}(\ell) \right] \gamma_{\ell}^{\sigma}(\mathbf{i}) g_{\mathbf{i}\mathbf{k}}^{\sigma}(\ell)}{1 + \left[1 - g_{\mathbf{i}\mathbf{i}}^{\sigma}(\ell) \right] \gamma_{\ell}^{\sigma}(\mathbf{i})}$$

The same result can be obtained by solving a Dyson's equation

Next slice

After the walker tries to flip the spin on the last site of ℓ – th time-slice

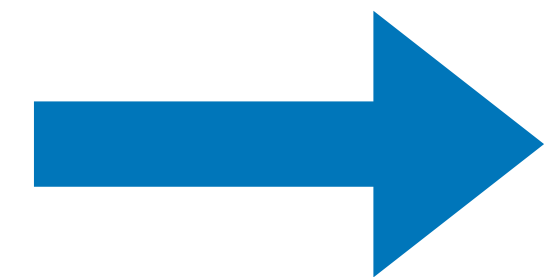


Green's function for the $(\ell + 1)$ – th time-slice

$$g^{\sigma}(\ell + 1) = \mathbf{B}_{\ell}^{\sigma} g^{\sigma}(\ell) [\mathbf{B}_{\ell}^{\sigma}]^{-1}$$

Next slice

After the walker tries to flip the spin on the last site of ℓ – th time-slice



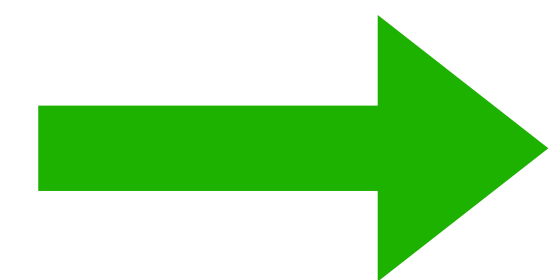
Green's function for the $(\ell + 1)$ – th time-slice

$$g^{\sigma}(\ell + 1) = B_{\ell}^{\sigma} g^{\sigma}(\ell) [B_{\ell}^{\sigma}]^{-1}$$

Repeat until the walker goes through all sites of time-slices

Summarizing

Determinantal Quantum Monte Carlo
or
Auxiliary field Quantum Monte Carlo



Green's functions

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

$$\left\{ \begin{array}{l} \mathbf{B}_{\ell}^{\sigma} \equiv e^{-\Delta\tau \mathbf{K}} e^{-\Delta\tau V^{\sigma}(\ell)} \\ O^{\sigma}(\{s\}) \equiv 1 + \mathbf{B}_M^{\sigma} \mathbf{B}_{M-1}^{\sigma} \dots \mathbf{B}_1^{\sigma} \end{array} \right.$$

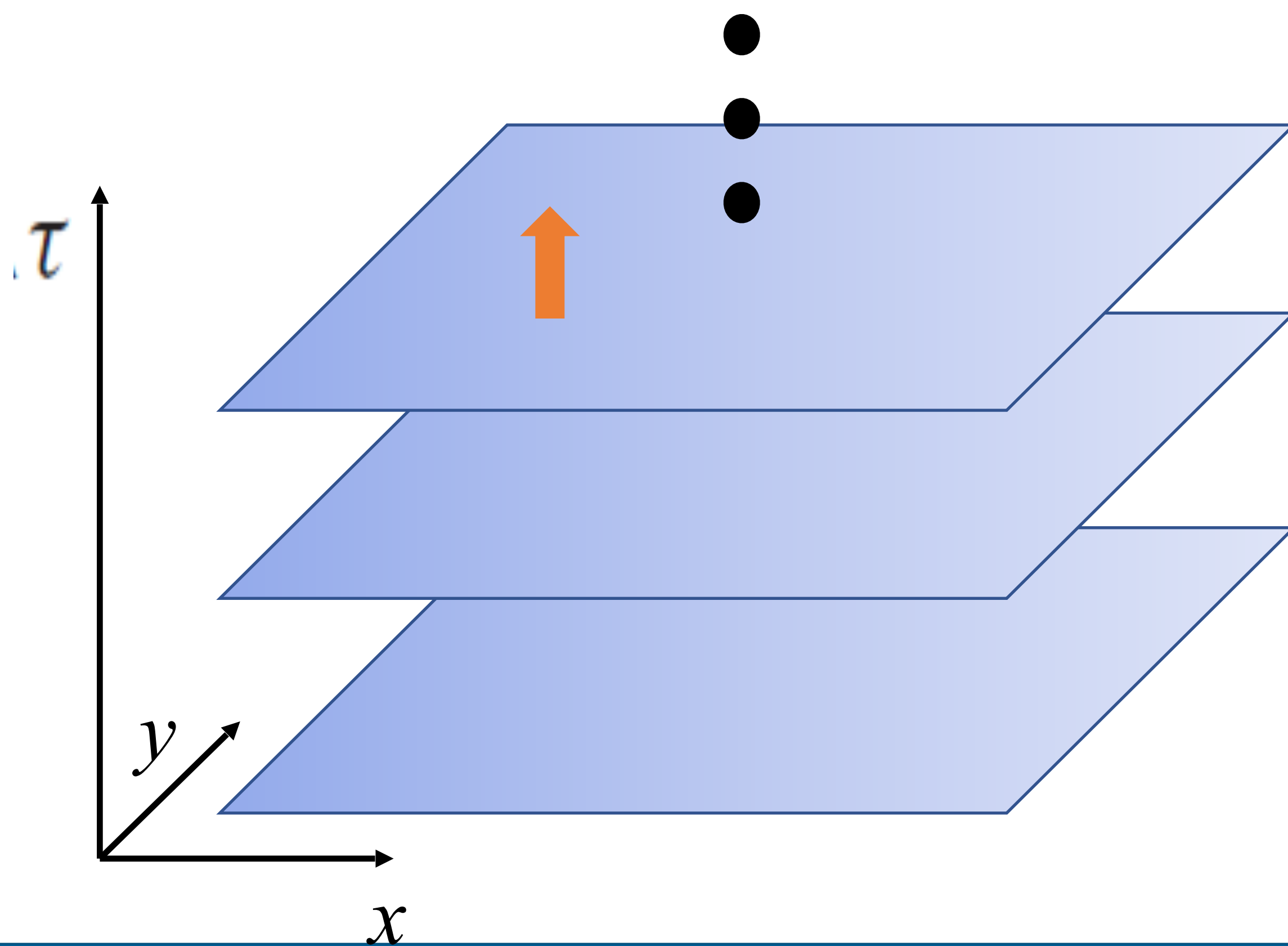
$$\left\{ \begin{array}{l} \mathbf{B}_\ell^\sigma \equiv e^{-\Delta\tau \mathbf{K}} e^{-\Delta\tau V^\sigma(\ell)} \\ \mathbf{O}^\sigma(\{s\}) \equiv 1 + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \cdots \mathbf{B}_1^\sigma \end{array} \right.$$

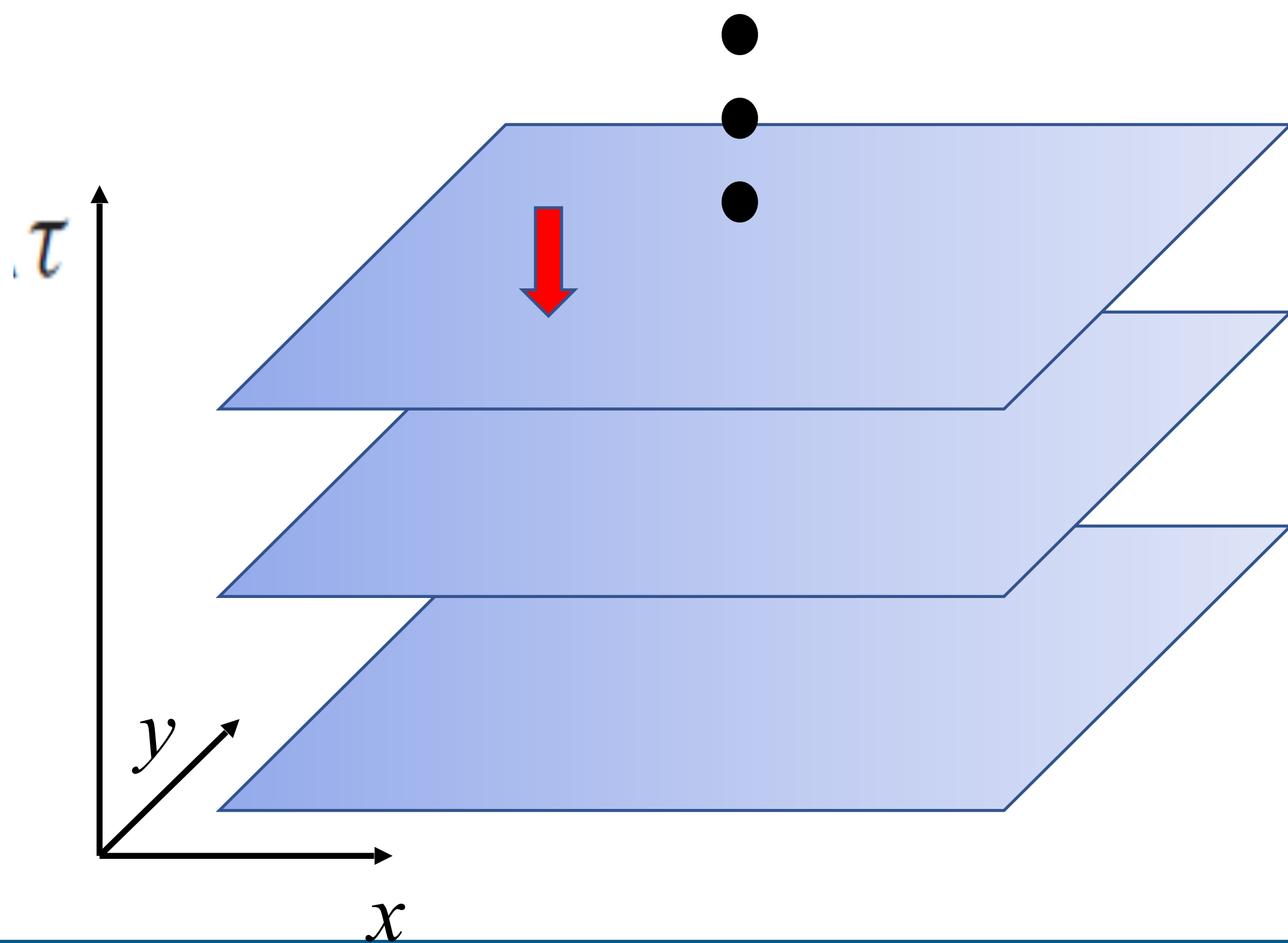
$$\begin{aligned} \mathcal{Z} &= \left(\frac{1}{2}\right)^{L^d M} \mathbf{Tr}_{\{s\}} \det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\}) = \\ &= \mathbf{Tr}_{\{s\}} \rho(\{s\}), \end{aligned}$$

$\rho \rightarrow$ Effective density matrix

Start with a distribution of the Ising variables

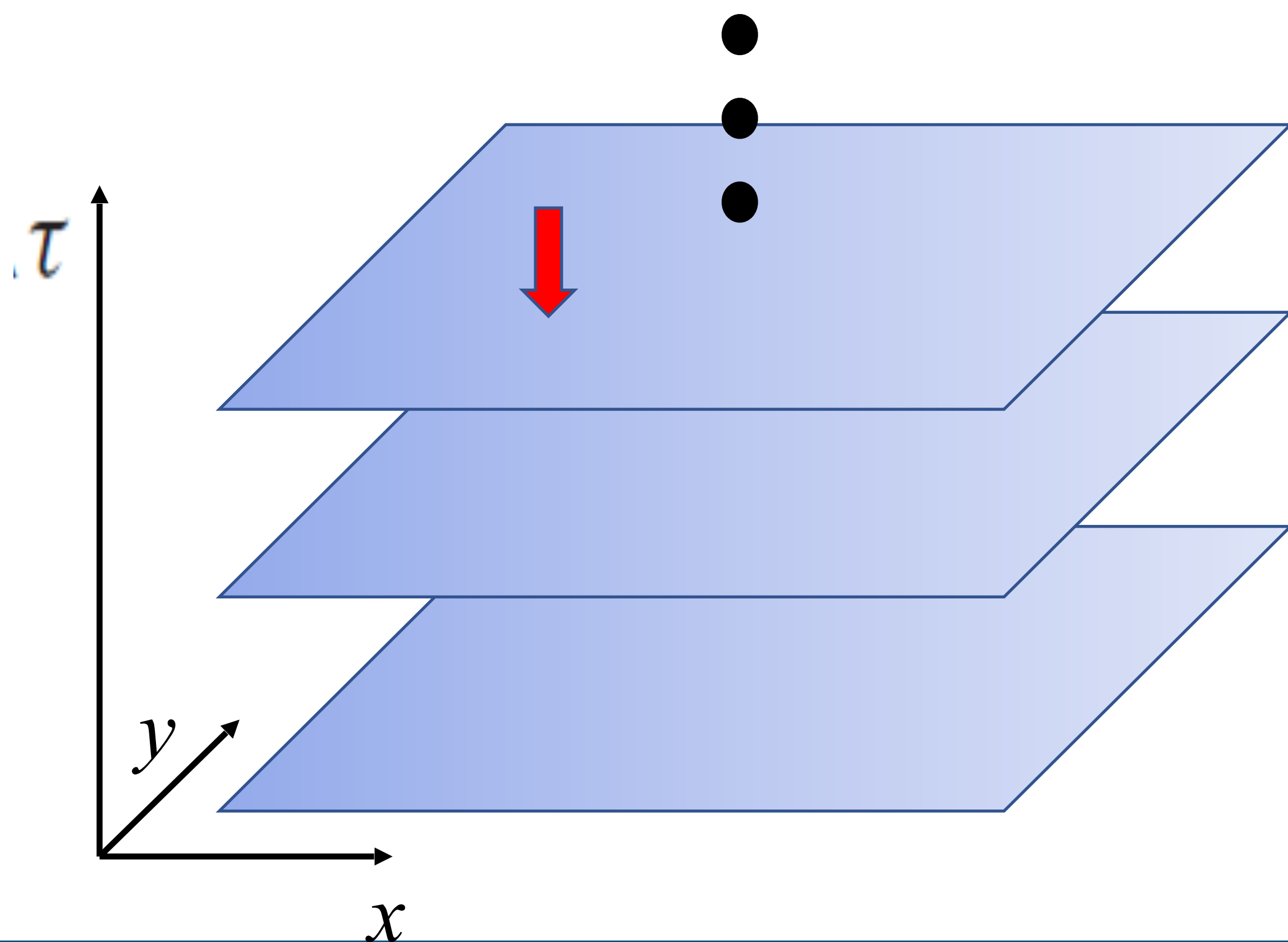
Propose flips in each site at each time-slice





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

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



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

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

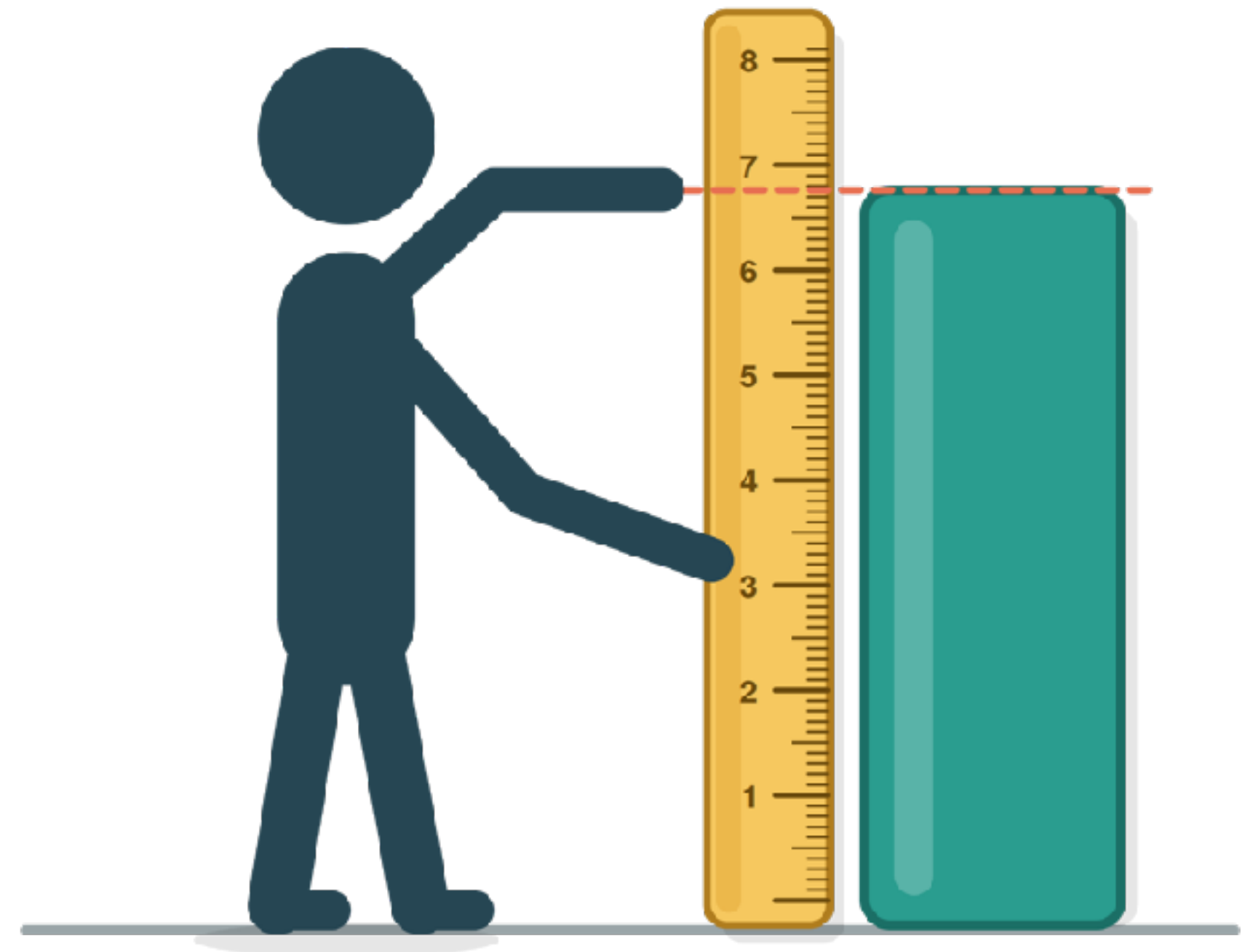
$$r = \mathcal{R}^\uparrow \mathcal{R}^\downarrow \quad \text{Metropolis}$$

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

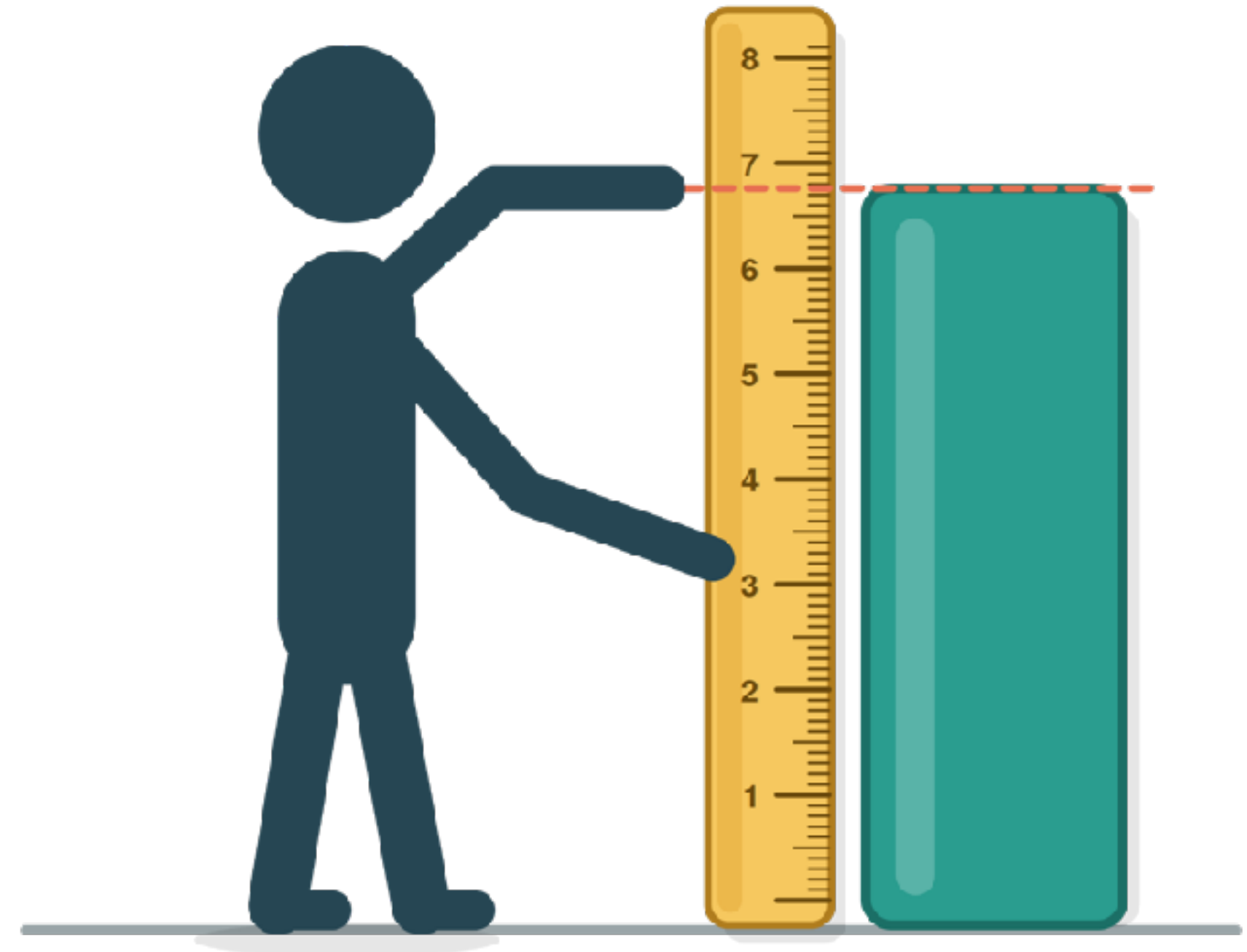
Do an initial number of thematization sweeps

Do measurement sweeps

Measuring quantities



Measuring quantities



Next classes!

End of second class