Finite-temperature lattice methods
Lecture 2.

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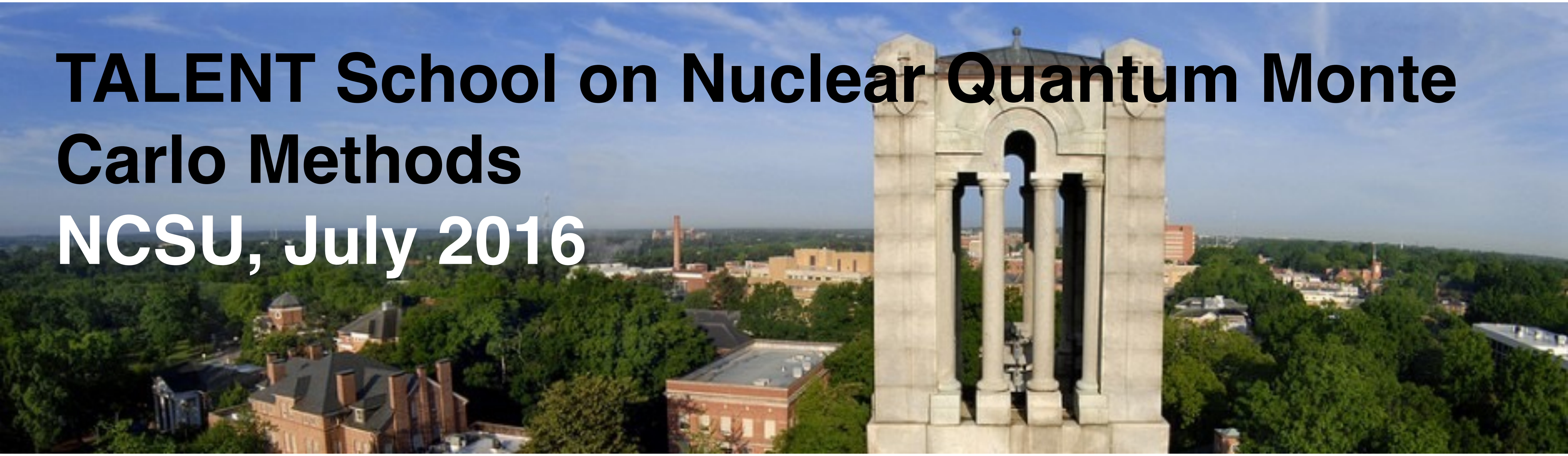

TALENT School on Nuclear Quantum Monte Carlo Methods

NCSU, July 2016

Goals

- **Lecture 1**:
  General motivation. Review of thermodynamics and statistical mechanics. Non-interacting quantum gases at finite temperature.

- **Lecture 2**:
  QRL1. Formalism at finite temperature: Trotter-Suzuki decompositions; Hubbard-Stratonovich transformations. From traces to determinants. Bosons and fermions. The sign problem.

- **Lecture 3**:
  QRL2. Computing expectation values (finally!). Particle number. Energy. Correlation functions: static and dynamic. Sampling techniques. Signal-to-noise issues and how to overcome them.

Goals

- **Lecture 4**:
  Quantum phase transitions and quantum information. Entanglement entropy. Reduced density matrix. Replica trick. Signal-to-noise issues.

- **Lecture 5**:
  QRL3. Finite systems. Particle-number projection. The virial expansion. Signal-to-noise issues. Trapped systems.

- **Lecture 6**:
  QRL5. Spacetime formulation. Finite-temperature perturbation theory on the lattice.

- **Lecture 7**:
  Applications to ultracold atoms in a variety of situations. Beyond equilibrium thermodynamics.

Finite-temperature calculations

“The underlying physical laws [...] are thus completely known, and the difficulty is only that the application of these laws leads to equations much too complicated to be soluble.”

P. A. M. Dirac, 1929

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How do we treat a strongly coupled problem?

- First we identify the degrees of freedom

  (bosons, fermions? atoms, nucleons, pions, quarks, gluons?)

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- Make sure we understand the symmetries as much as possible (sometimes there are “accidental”, also called “dynamical”, symmetries!)
  (U(N)?, SU(N)?, Galilean, Poincare, Lorentz?)

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- Then we look for the scales and dimensionless parameters that characterize the problem.

    (masses, coupling constants, etc. forming dimensionless combinations)

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- Make sure we understand the symmetries as much as possible (sometimes there are “accidental”, also called “dynamical”, symmetries!)

- Then we look for the scales and dimensionless parameters that characterize the problem.

- Sometimes one can study the limits in which those parameters are very large or very small.

  One can think of using mean-field plus fluctuations.

How do we treat a strongly coupled problem?

Example

- Hubbard Model in 1D

$$H = -\frac{t}{2}\sum_{j,\alpha}\left(\psi^\dagger_{j,\alpha}\psi_{j+1,\alpha} + h.c.\right) + U\sum_j n_{j,\uparrow}n_{j,\downarrow} + \mu\sum_{j,\alpha} n_{j,\alpha}$$

  - Exactly solvable via Bethe ansatz
  - We may consider the limits

$\frac{t}{U} \gg 1$ weak coupling

$\frac{t}{U} \ll 1$ strong coupling

How do we treat a strongly coupled problem?

- But sometimes there are no small dimensionless parameters, or at least none that are useful.

  For example: QCD
  Nuclear structure
  QED (at high energies)
  Graphene
  Ultracold atoms
  Multiple problems in condensed matter

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  Multiple problems in condensed matter

- In those cases one of the most helpful strategies is to switch to numerical methods

Problems don’t have to be too complicated for us to have to use computers!

There are many numerical methods...

- Green's function Monte Carlo
- No-core shell-model
- Coupled-cluster

.

.

.

Density Functional Theory

Not all of them are equally efficient!

...but I will focus on one kind: Lattice methods!

Main idea

- We don’t care (in principle) if the couplings are large or not (computers will solve the problem for us).

But we need to put the problem on a computer first!

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- We don't care (in principle) if the couplings are large or not (computers will solve the problem for us).

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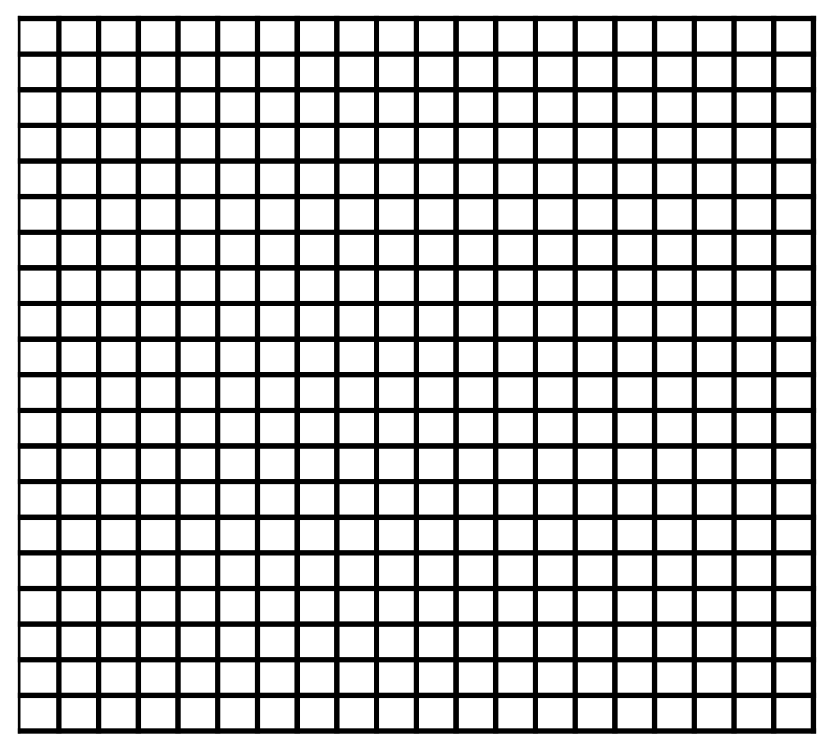
- So we need to **discretize space-time** to have a **finite** number of degrees of freedom.



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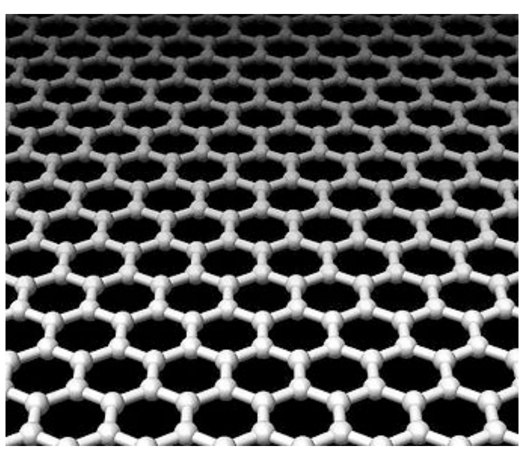

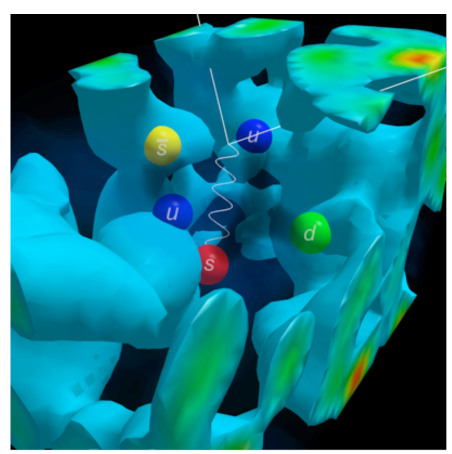

Many problems are treated this way, from graphene to QCD!

Disclaimer:
I will focus on strongly coupled non-relativistic systems.

Quick review of Lecture 1

Statistical mechanics: connection to thermodynamics

Canonical ensemble
partition function

$$\mathcal{Q}_N = \mathrm{tr}_N \left[e^{-\beta \hat{H}} \right] = \sum_j e^{-\beta E_j(N)}$$

"inverse temperature"

$$\beta = \frac{1}{k_B T}$$

Grand-canonical ensemble
partition function

$$\mathcal{Z} = \mathrm{tr} \left[e^{-\beta(\hat{H} - \mu \hat{N})} \right] = \sum_N \sum_j e^{-\beta(E_j(N) - \mu N)} = \sum_N z^N \mathcal{Q}_N$$

"fugacity"

$$z = e^{\beta \mu}$$

Connection to thermodynamics

$$-\beta F(T, V, N) = \ln \mathcal{Q}_N \qquad -\beta \Omega(T, V, \mu) = \ln \mathcal{Z}$$

Statistical mechanics: expectation values

Two equivalent ways to think about this:

1.- Define the *statistical operator*

$$\hat{\rho} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathcal{Z}}$$

Then the ensemble average of a given operator is

$$\langle\hat{O}\rangle = \mathrm{tr}\left[\hat{\rho}\;\hat{O}\right] = \frac{\mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\hat{O}\right]}{\mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]}$$

Statistical mechanics: expectation values

Two equivalent ways to think about this:

2.- Insert a *source* in the partition function

$$\mathcal{Z} \to \mathcal{Z}[j(x)] = \mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N}-X[j(x)])}\right]$$

$$X[j(x)] = \int d^d x \; j(x)\hat{O}(x)$$

Then the ensemble average we want is

$$\langle \hat{O} \rangle = \frac{1}{\beta}\frac{\delta \ln \mathcal{Z}[j(x)]}{\delta j(x)}\bigg|_{j\to 0}$$

Try it!

Simplest examples:

$$\langle \hat{N} \rangle = ? \qquad \langle \hat{H} \rangle = ?$$

Formalism on the lattice

The problem: interacting vs. non-interacting

$$\hat{H} = \hat{T} + \hat{V} \qquad\qquad [\hat{H}, \hat{N}] = 0$$

$$[\hat{T}, \hat{V}] \neq 0$$

In the non-interacting case, the Hamiltonian is trivially diagonal in all N-particle subspaces.

In the interacting case, each N needs to be diagonalized independently, and the dimension grows exponentially.

so… we need to do something different…

Towards thermodynamics on the lattice

Objective

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left[\hat{\mathcal{O}} e^{-\beta(\hat{H} - \mu \hat{N})} \right] \qquad \mathcal{Z} \equiv \mathrm{Tr}\left[e^{-\beta(\hat{H} - \mu \hat{N})} \right]$$

Towards thermodynamics on the lattice

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We can, at least formally, always write a generating functional:

$$\mathcal{Z}[j] = \mathrm{Tr} \left[e^{-\beta(\hat{H} - \mu \hat{N}) + j \hat{\mathcal{O}}} \right]$$

such that

$$\langle \mathcal{O} \rangle = \left. \frac{\delta \log \mathcal{Z}[j]}{\delta j} \right|_{j=0}$$

→ It is useful to focus on the **partition function** $\mathcal{Z}$

The transfer matrix

- Another way of saying this is that our focus should really be on the **transfer matrix**

$$\mathcal{T}_t = e^{-t\hat{H}}$$

because all our problems are in this operator.

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- **Side comment:**

Notice that most of the ground-state (i.e. T=0) methods are based on taking powers of the transfer matrix to filter out the excited states

$$\mathcal{T}_\tau^{N_\tau} |\Phi\rangle \to |GS\rangle$$

For $N_\tau \gg 1$, up to an overall constant.

The transfer matrix

The transfer matrix itself (i.e. even before we even think about taking the trace) poses a bit of a challenge

$$\hat{H} = \hat{T} + \hat{V}$$

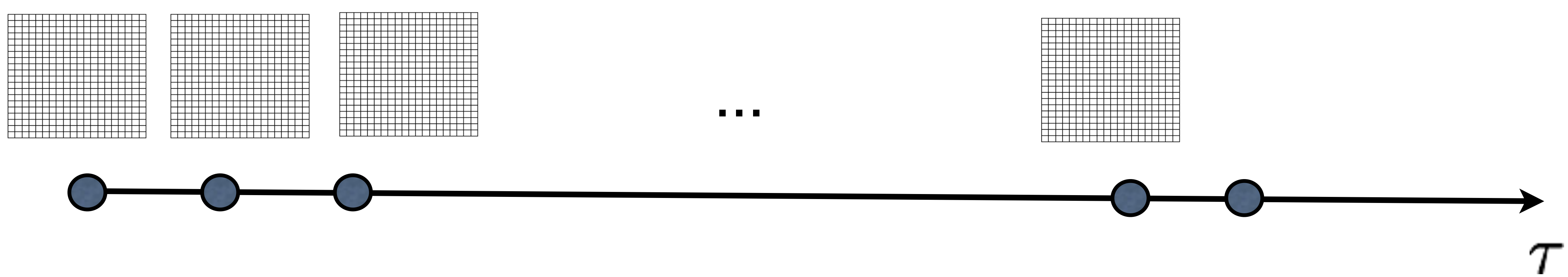
$$[\hat{T}, \hat{V}] \neq 0$$

$$\exp(-\beta \hat{H}) = \quad ???$$

Imaginary time and Trotter-Suzuki factorization

Discretize time

$$\exp(-\beta \hat{H}) = \left[\exp(-\tau \hat{H})\right]^{N_\tau}$$



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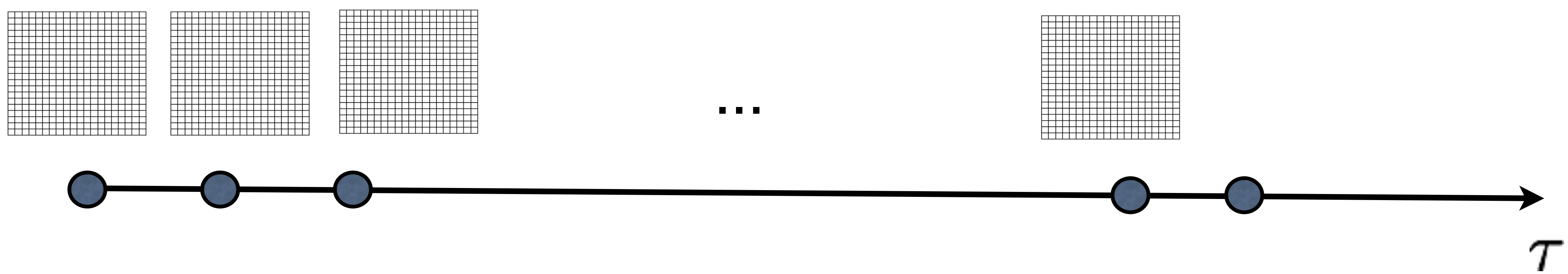

Trotter-Suzuki factorization

$$\exp(-\tau\hat{H}) = \exp(-\tau\hat{T}/2)\exp(-\tau\hat{V})\exp(-\tau\hat{T}/2)$$

The potential energy factor is of course where all our problems are.

How Trotter-Suzuki factorizations work

Simplest approximation

$$e^{-\tau \hat{H}} \simeq e^{-\tau \hat{T}} e^{-\tau \hat{V}}$$

Exercise 1:
How good are these?
How can you find out?

Next best thing you can do

$$e^{-\tau \hat{H}} \simeq e^{-\tau \hat{T}/2} e^{-\tau \hat{V}} e^{-\tau \hat{T}/2}$$

Beyond

M. Suzuki, Phys. Lett. A **146**, 319(1990).

FRACTAL DECOMPOSITION OF EXPONENTIAL OPERATORS WITH APPLICATIONS TO MANY-BODY THEORIES AND MONTE CARLO SIMULATIONS

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A new systematic scheme of decomposition of exponential operators is presented, namely $\exp[x(A+B)] = S_m(x) + O(x^{m+1})$ for any positive integer m, where $S_m(x) = e^{t_1 A} e^{t_2 B} e^{t_3 A} e^{t_4 B} \dots e^{t_M A}$. A general scheme of construction of $\{t_j\}$ is given explicitly. The decomposition $\exp[x(A+B)] = [S_m(x/n)]^n + O(x^{m+1}/n^m)$ yields a new efficient approach to quantum Monte Carlo simulations.

The Hubbard-Stratonovich transformation

This is how we can deal with this problem. Take a specific case, for example a zero-range interaction

$$\hat{V} = -g \sum_j \hat{n}_{\uparrow,j} n_{\downarrow,j} \qquad \text{where} \qquad \hat{n}_{s,j} = \psi^\dagger_{s,j} \psi_{s,j}$$

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Then, at each point in spacetime,

$$\exp\left(\tau g \hat{n}_{\uparrow,j} n_{\downarrow,j}\right) = 1 + C \hat{n}_{\uparrow,j} \hat{n}_{\downarrow,j}$$

$$= \frac{1}{2} \sum_{\sigma=\pm 1} (1 + \sqrt{C} \hat{n}_{\uparrow,j} \sigma)(1 + \sqrt{C} \hat{n}_{\downarrow,j} \sigma)$$

We have replaced a difficult problem with a tractable one.

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We have replaced a difficult problem with a tractable one.

Exercise 2: **a.** Check this!

b. Find the value of C!

c. What happens if the interaction is repulsive?

The Hubbard-Stratonovich transformation

And there are other ways to play this game

A) $$\exp(\tau g \hat{n}_{\uparrow,j}\hat{n}_{\downarrow,j}) = \frac{1}{2}\sum_{\sigma=\pm 1}(1+\sqrt{C}\hat{n}_{\uparrow,j}\sigma)(1+\sqrt{C}\hat{n}_{\downarrow,j}\sigma)$$

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B) $$\exp(\tau g \hat{n}_{\uparrow,j}\hat{n}_{\downarrow,j}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\sigma (1+\sqrt{C}\hat{n}_{\uparrow,j}\sin\sigma)(1+\sqrt{C}\hat{n}_{\downarrow,j}\sin\sigma)$$

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C) $$\exp(\tau g \hat{n}_{\uparrow,j}n_{\downarrow,j}) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\sigma e^{-\sigma^2/2} e^{-\sigma\sqrt{C}(\hat{n}_{\uparrow,j}+\hat{n}_{\downarrow,j})}$$

Exercise 3: Check all these, especially the last one!

Going back to the transfer matrix...

... putting everything back together, we obtain

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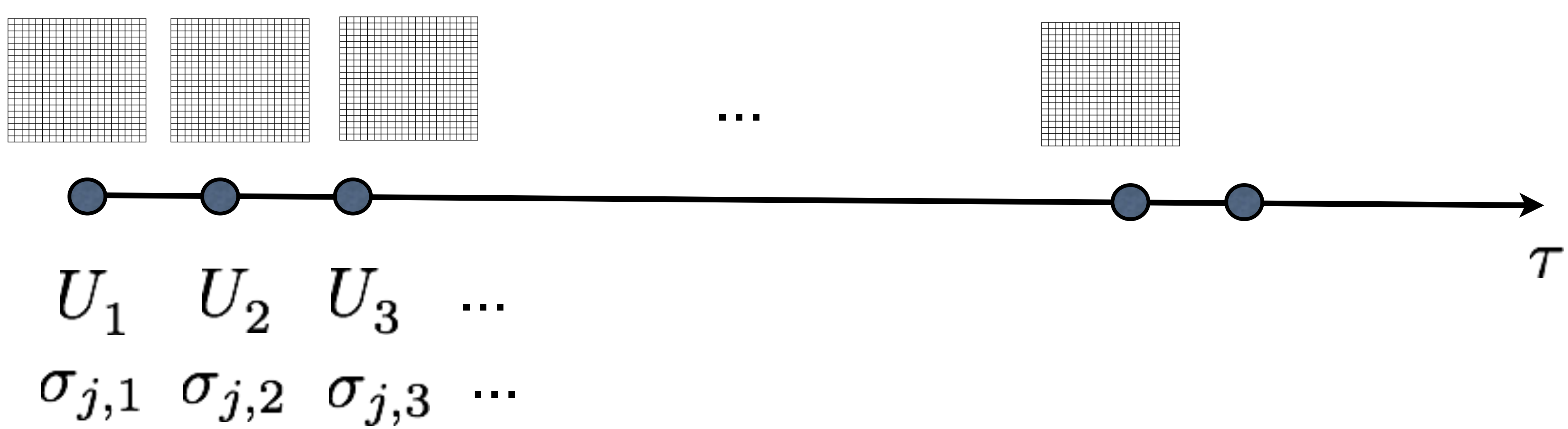

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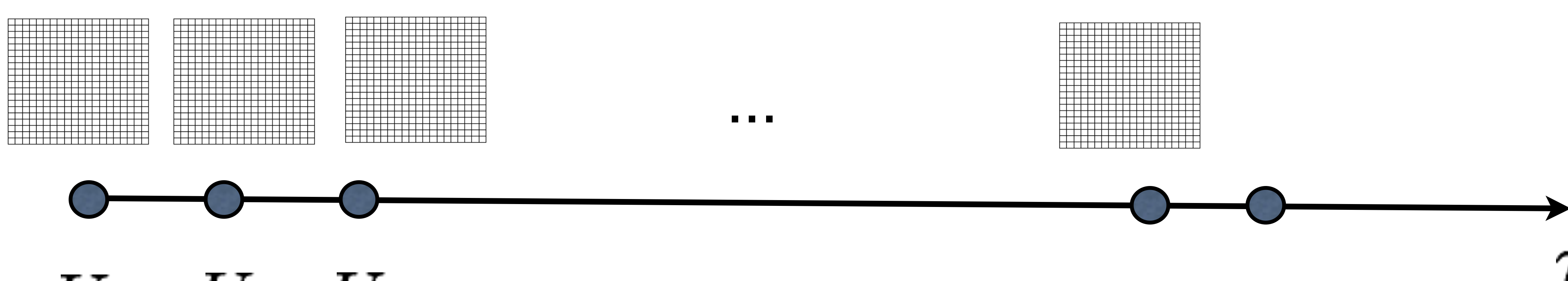

U_1 U_2 U_3 ...

$\sigma_{j,1}$ $\sigma_{j,2}$ $\sigma_{j,3}$ ...

The auxiliary field lives in all of spacetime!

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Now the auxiliary field in $\mathcal{T}[\sigma]$ is arbitrary, but…
we only have to deal with one-body operators,
so we can take that trace!

$$\mathrm{Tr}\;\mathcal{T}[\sigma] = \det M_{\uparrow} M_{\downarrow}$$

for a certain matrix M…
?!?!?!?!?!

How to take the trace over Fock space

Exercise 4

Show that, for fermions,

$$\mathrm{tr}\left[e^{A_{ij}\hat{a}_i^\dagger \hat{a}_j}\right] = \det(1 + e^A)$$

while for bosons,

$$\mathrm{tr}\left[e^{A_{ij}\hat{a}_i^\dagger \hat{a}_j}\right] = \big(\det(1 - e^A)\big)^{-1}$$

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Hint: Use a diagonal representation of the matrix A.

How to take the trace over Fock space

Exercise 5

Show that, for fermions,

$$\mathrm{tr}\left[e^{A_{ij}\hat{a}_i^\dagger \hat{a}_j} e^{B_{ij}\hat{a}_i^\dagger \hat{a}_j}\right] = \det(1 + e^A e^B)$$

where $[A, B] \neq 0$

Hint: Diagonalization won't help you.
If you already know the answer, please don't share it. Let people think.

Derive the corresponding result for bosons.

Path integrals and the reason for Monte Carlo

- So far we have managed to write

$$\mathcal{Z} = \int \mathcal{D}\sigma \; \mathcal{P}[\sigma] \qquad \text{where} \qquad \mathcal{P}[\sigma] = \det \mathcal{M}[\sigma]$$

If we put a source, take a derivative of the log, and set the source to zero, we will always end up with something of the form

$$\langle O \rangle = \left. \frac{\delta \log \mathcal{Z}[j]}{\delta j} \right|_{j=0} = \frac{1}{\mathcal{Z}} \left. \frac{\delta \mathcal{Z}[j]}{\delta j} \right|_{j=0} = \frac{1}{\mathcal{Z}} \int \mathcal{D}\sigma \; \mathcal{P}[\sigma] O[\sigma]$$

OK, but what do we do with this now?

Path integrals and the reason for Monte Carlo

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Clearly, $\mathcal{P}[\sigma]$ is a good candidate for a probability measure...

... but, is it well-defined as such?

Is it normalizable and positive semi-definite?

Probability measures and sign problems

- This is one of the most serious roadblocks to progress in lattice calculations.

  Most interesting problems, and certainly most real problems, suffer from this issue.

  This is a question of signal-to-noise ratio.

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$$\mathcal{P}[\sigma]\mathcal{O}[\sigma] = |\mathcal{P}[\sigma]| \left[\mathrm{sgn}\left(P[\sigma]\right)\mathcal{O}[\sigma]\right]$$

  Thus, we use the sign with the observable and use a positive probability (in general it will be normalizable).

  The fluctuations in the original probability will appear in the observables.

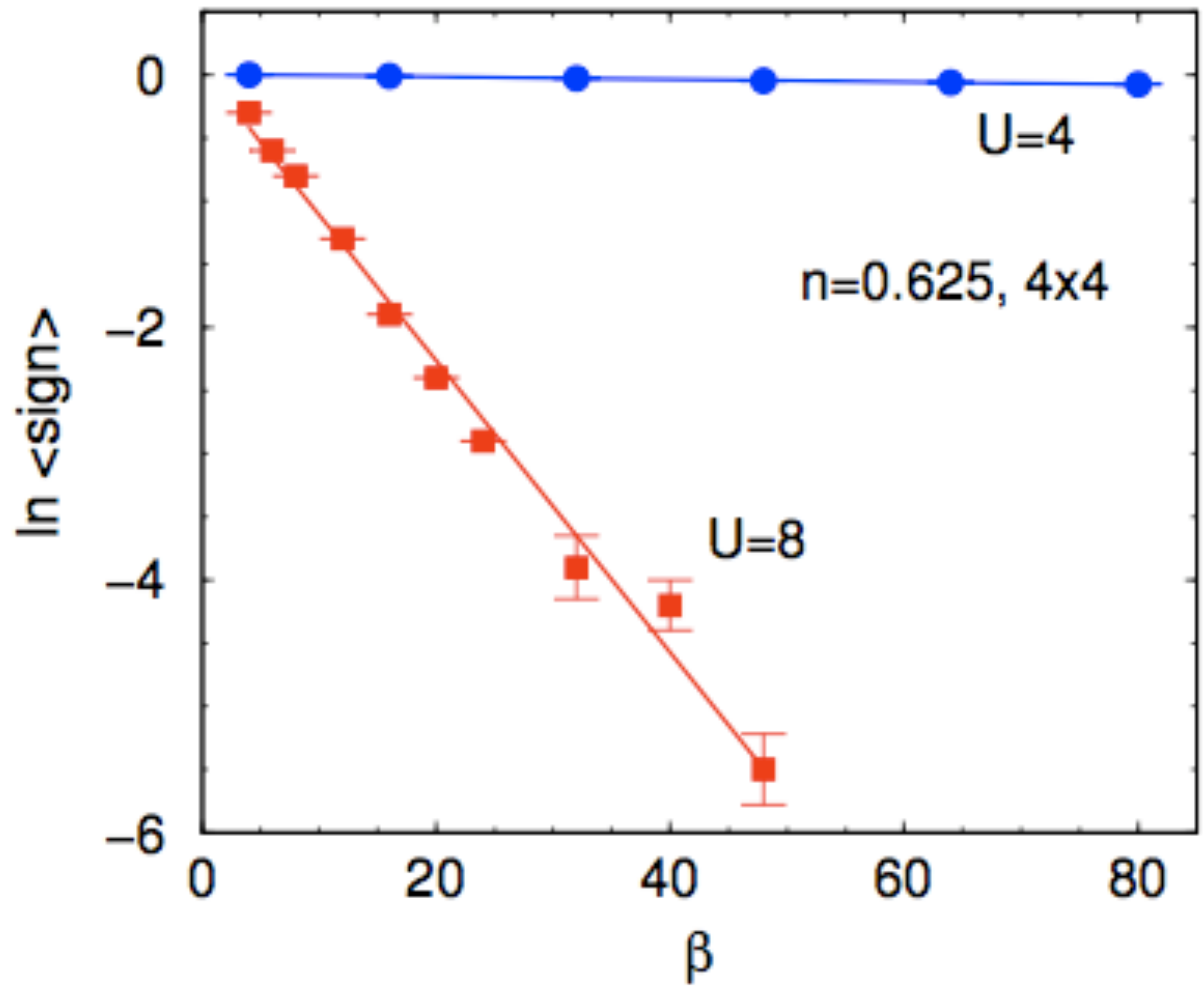
Probability measures and sign problems

- Then we can see the signal-to-noise problem explicitly by "measuring" the sign:

Example:

Repulsive Hubbard model

(There are many more examples in the LQCD literature)



R. R. dos Santos
Braz. J. Phys. **33, 36 (2003)**

Summary

- Most interesting problems are either complicated or strongly coupled, enough so that numerical methods are necessary.
- There are many methods (GFMC, CC, NCSM, Lattice, etc.). Not all of them are equally effective nor are they equally efficient.
- Lattice methods provide a route based on defining fields on a spacetime grid and decoupling the interaction via the Hubbard-Stratonovich transformation.
- This allows us to rewrite the quantum many-body problem as a multidimensional integral that can, in principle, be computed using stochastic methods (i.e. random numbers).