Finite-temperature lattice methods
Lecture 6.

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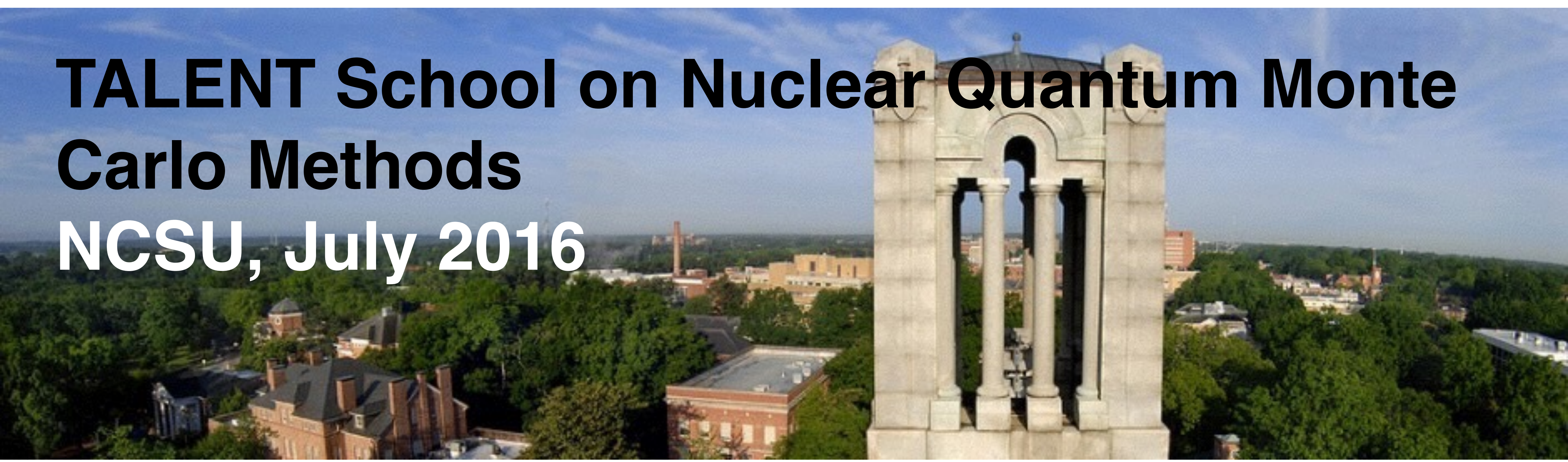

TALENT School on Nuclear Quantum Monte Carlo Methods
NCSU, July 2016

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.

Observables

Computing expectation values

- Simplest observables we discussed:

$$\langle \hat{N} \rangle = \frac{\partial(-\beta\Omega)}{\partial(\beta\mu)} = \frac{\partial(\ln \mathcal{Z})}{\partial(\beta\mu)}$$

$$\langle \hat{H} \rangle = -\frac{\partial(\ln \mathcal{Z})}{\partial\beta}$$

but…

$$\mathcal{Z} = \int \mathcal{D}\sigma \det M_\uparrow[\sigma] M_\downarrow[\sigma]$$

How do we proceed from here towards computing observables?

Computing expectation values

- Particle number

$$\langle \hat{N} \rangle = \frac{\partial(-\beta\Omega)}{\partial(\beta\mu)} = \frac{\partial(\ln \mathcal{Z})}{\partial(\beta\mu)}$$

Exercise 1: Derive the explicit form of this observable in the auxiliary field-integral representation.

Perturbation theory on the lattice

Spacetime formulation

From a previous lecture

$$\mathcal{Z} = \int \mathcal{D}\sigma \ \mathcal{P}[\sigma]$$ where $$\mathcal{P}[\sigma] = \det(1 + W_\uparrow)\det(1 + W_\downarrow)$$

$$W_s = U_1 U_2 U_3 \ldots U_{N_\tau}$$

Quick question: What is the size of the W matrix?

Can we use this form to gain some analytic insight?

Spacetime formulation

$$M \equiv \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & U_{N_\tau} \\ -U_1 & 1 & 0 & 0 & \dots & 0 \\ 0 & -U_2 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & -U_{N_\tau-2} & 1 & 0 \\ 0 & 0 & \dots & 0 & -U_{N_\tau-1} & 1 \end{pmatrix}$$

$$\det M = \det(1 + W_s)$$

Exercise 2: Prove this identity.
What is the physical meaning of this larger matrix?

Spacetime formulation

In fact, we can show that

$$M = M_0 + \sqrt{C} M_1[\sigma]$$

where M_0 does not depend on the auxiliary field.

Exercise 3: Find M_0 and M_1 above based on the previous slide.

Spacetime formulation

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where M_0 does not depend on the auxiliary field.

Exercise 3: Find M_0 and M_1 above based on the previous slide.

Then,

$$\det M = \det(M_0 + \sqrt{C} M_1[\sigma]) = \det M_0 \det(1 + \sqrt{C} M_0^{-1} M_1[\sigma])$$

which we can expand in powers of $\sqrt{C}$

What does the expansion look like?