Finite-temperature lattice methods
Lecture 5.

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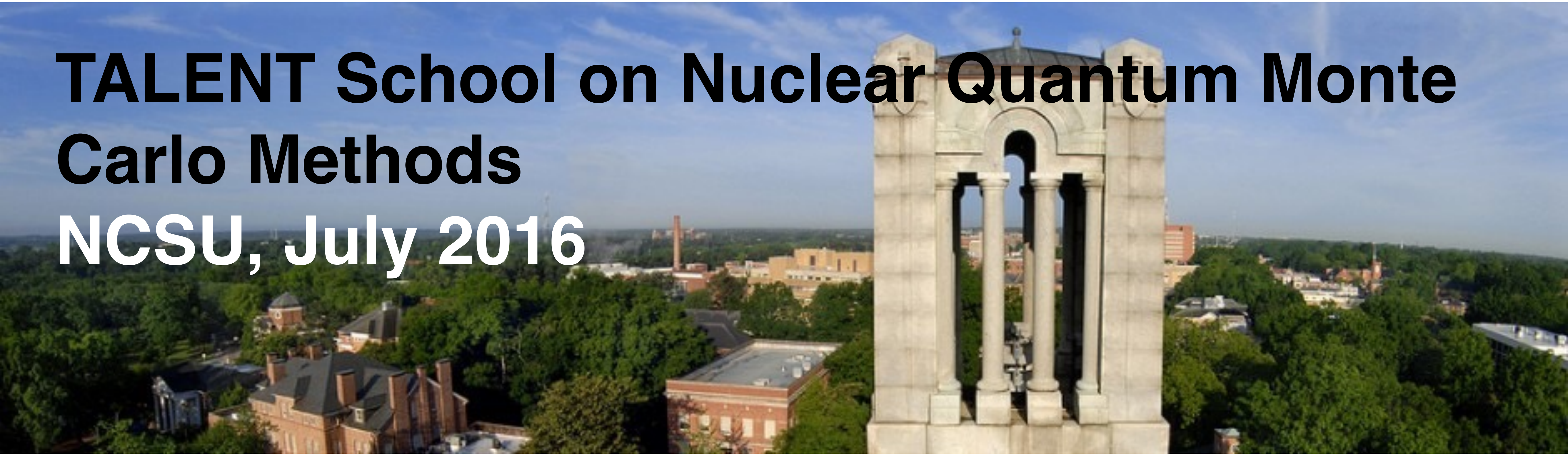

TALENT School on Nuclear Quantum Monte Carlo Methods

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-systems
&
the virial expansion

Statistical mechanics: connection to thermodynamics

Canonical ensemble
partition function

"inverse temperature"

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

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

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: the virial expansion

The virial expansion is simply an expansion in powers of the fugacity z, i.e. assume z << 1.

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

It implies a low-density approximation in which the few-particle dynamics dominates.

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What do we need in order to compute the coefficients of this expansion?

Statistical mechanics: the virial expansion

The "direct" way

N = 0 Empty system

$$\mathcal{Q}_0 = \langle 0|e^{-\beta \hat{H}}|0\rangle = 1$$

N = 1

$$\mathcal{Q}_1 = \sum_{\mathbf{p}} \langle \mathbf{p}|e^{-\beta \hat{H}}|\mathbf{p}\rangle = \sum_{\mathbf{p}} e^{-\beta \mathbf{p}^2/2m}$$

Sum over single-particle states

N = 2

Same thing: solve the 2-body problem, sum over all states. Can do.

N = 3

Well, this is where everyone stops.

Statistical mechanics: the virial expansion

The “direct” way

General N

We can separate* the center-of-mass (CM) motion:

$$\mathcal{Q}_N = \mathcal{Q}_{\mathrm{CM}} \mathcal{Q}_{\mathrm{rel}}$$

Moreover, the CM contribution is equivalent to that of 1 particle of mass M (= total mass of the system)

* When is this possible?

Statistical mechanics: the virial expansion

The "direct" way

What we really want is an expansion for the pressure…

$$-\beta\Omega = \ln \mathcal{Z} = \ln\left(1 + \sum_{N=1}^{\infty} z^N \mathcal{Q}_N\right)$$

$$\ln(1+x) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{x^k}{k}$$

$$= \mathcal{Q}_1 \sum_{n=1}^{\infty} b_n z^n$$

Virial coefficients

$$b_1 = 1$$

$$b_2 = \frac{\mathcal{Q}_2 - \mathcal{Q}_1^2/2}{\mathcal{Q}_1}$$

$$\vdots$$

Note: the virial coefficients are intensive parameters, even though the partition functions are not.

Statistical mechanics: the virial expansion

The "stochastic" way

$$\mathcal{Z} = \int \mathcal{D}\sigma \, \det{}^{N_f}(1 + zU[\sigma])$$

Once again, expand in powers of the fugacity…

$$\mathcal{Q}_1 = N_f \int \mathcal{D}\sigma \; \mathrm{tr} U[\sigma]$$

$$\mathcal{Q}_2 = \frac{1}{2} \int \mathcal{D}\sigma \; \left(N_f^2 \mathrm{tr}^2 U[\sigma] - N_f \mathrm{tr} U^2[\sigma] \right)$$

$$\vdots$$

Statistical mechanics: the virial expansion

The "stochastic" way

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$$\vdots$$

Two problems here:

1. Remember: the virial coefficients are intensive parameters, even though the partition functions are not.

2. Where did the probability go?

Back to the original problem:
How to code this thing

How to code this thing (finally!): Finite-temperature determinantal Monte Carlo

Overall code structure

- Decide what size of spacetime you need: set lattice sizes Nx and Nt
- Initialize auxiliary field σ
- Enter Metropolis loop
  - Propose auxiliary field “update”
  - **Compute Fermi matrix M = 1 + U**
  - Compute matrix determinant (e.g. using LU decomposition)
  - Accept/reject step (using matrix determinant as probability)
- End Metropolis loop

How to code this thing (finally!): Finite-temperature determinantal Monte Carlo

Computing the Fermi matrix

- Choose a single-particle (s.p.) basis:
  e.g. plane waves, or coordinate-space deltas
  (remember you are taking a trace, i.e. basis independent).

- Define an array that stores your s.p. waves:
  Size = (spatial volume) x (spatial volume)

- “**Evolve**” the s.p. waves in imaginary time, i.e.
  apply the sequence of operations:

$$\hat{U}_t = \exp(-\tau \hat{T}/2) \exp(-\tau \hat{V}_{\text{ext}}[\sigma]) \exp(-\tau \hat{T}/2)$$

  for t = 1, … , Nt, to all the waves

- The evolved waves are the Fermi matrix!

How to code this thing (finally!): Finite-temperature determinantal Monte Carlo

Imaginary-time evolution

- Loop over s.p. waves
  - Enter imaginary-time loop: t = 1 to Nt
    - Apply **kinetic energy factor**
    - Apply field-dependent **potential energy factor**
    - Apply **kinetic energy factor**
  - End imaginary-time loop
- End loop over s.p. waves.