Quantum Monte Carlo Simulations of the Hubbard Model

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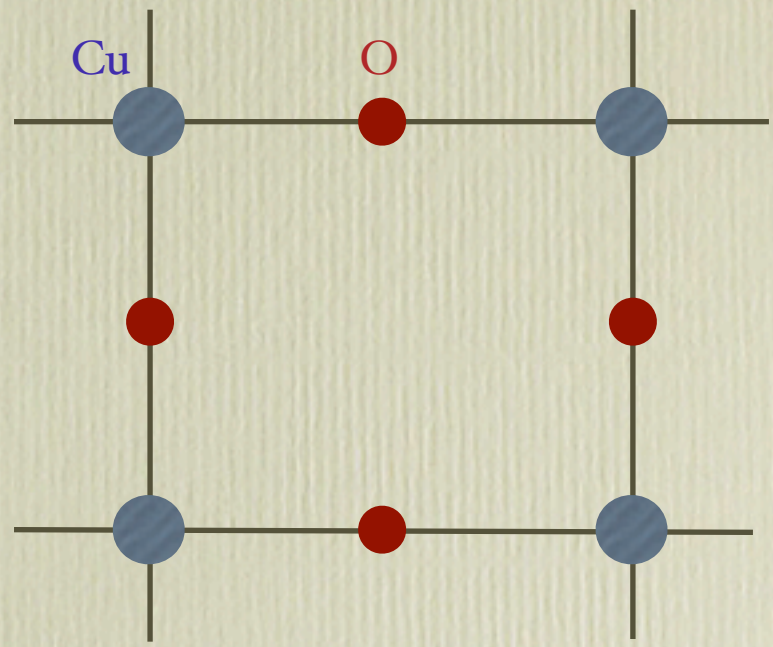
Overview

- Physical System - Cuprates
- Hubbard Model
- Questions for simulations
- Details of simulation
- Results as a function of chemical potential

Cuprates

- $YBa_2Cu_3O_7$, $Bi_2Sr_2Ca_2Cu_3O_8$
- e^- hop between Cu atoms in 2D sheets
- One partially filled band
- Can exhibit antiferromagnetism and superconductivity



Hubbard Model

$$H = -t \sum_{<ij>,\sigma} (c^{\dagger}_{i\,\sigma}\, c_{j\,\sigma} + c^{\dagger}_{j\,\sigma}\, c_{i\,\sigma}) + U \sum_{i} (n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2})$$

Kinetic

Coulomb

- <ij> denotes nearest neighbor sites, σ denotes spin up or down
- Kinetic term allows hopping between lattice sites
- Coulomb term makes two electrons on a lattice site unfavorable
- Exhibits some properties of the cuprates

Questions for Simulation

We want to be able to calculate thermodynamic averages.

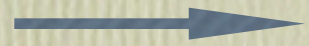
$$\langle O \rangle = \frac{\mathrm{Tr}\, O\, e^{-\beta(H-\mu n)}}{\mathrm{Tr}\, e^{-\beta(H-\mu n)}}$$

"Tr" means take the sum of the argument over all configurations of electrons and $\beta = 1/T$

O can be any observable such as density, magnetic susceptibility, or energy

Simulation Method

Electrons are quantum mechanical



Introduce auxiliary field to decouple the electrons

$$e^{-\Delta\tau\, U\,(n_{i\uparrow}-\frac{1}{2})(n_{i\downarrow}-\frac{1}{2})} \propto \sum_{x_i(\ell)=\pm 1} e^{-\Delta\tau\, x_i(\ell)\,\lambda\,(n_{i\uparrow}-n_{i\downarrow})}$$

Now electrons are non-interacting so the trace can be done exactly.

$$\mathrm{Tr}\, e^{-\beta H(x)} \Rightarrow W(x)$$

Monte Carlo

We want to do sums

$$\langle O \rangle = \frac{\sum_x O(x) W(x)}{\sum_x W(x)}$$

Sample configurations with probability distribution

$$P(x) = \frac{W(x)}{\sum_x W(x)}$$

then

$$\langle O \rangle = \frac{1}{N_{\mathrm{MC}}} \sum_x^{\mathrm{MC}} O(x)$$

Sign Problem

$W(x)$ is not always positive: it cannot be a valid probability distribution

Use absolute-value probability distribution:

$$P_{||} = \frac{|W(x)|}{\sum_x |W(x)|}$$

so

$$\langle O \rangle = \frac{\sum_x P_{||}(x)\, O(x)\, S(x)}{\sum_{x'} P_{||}(x')\, S(x')} = \frac{\langle OS \rangle_{||}}{\langle S \rangle_{||}}$$

with $S(x) = W(x)/|W(x)| = \pm 1$

Canonical Ensembles

Canonical ensembles have a fixed number of electrons

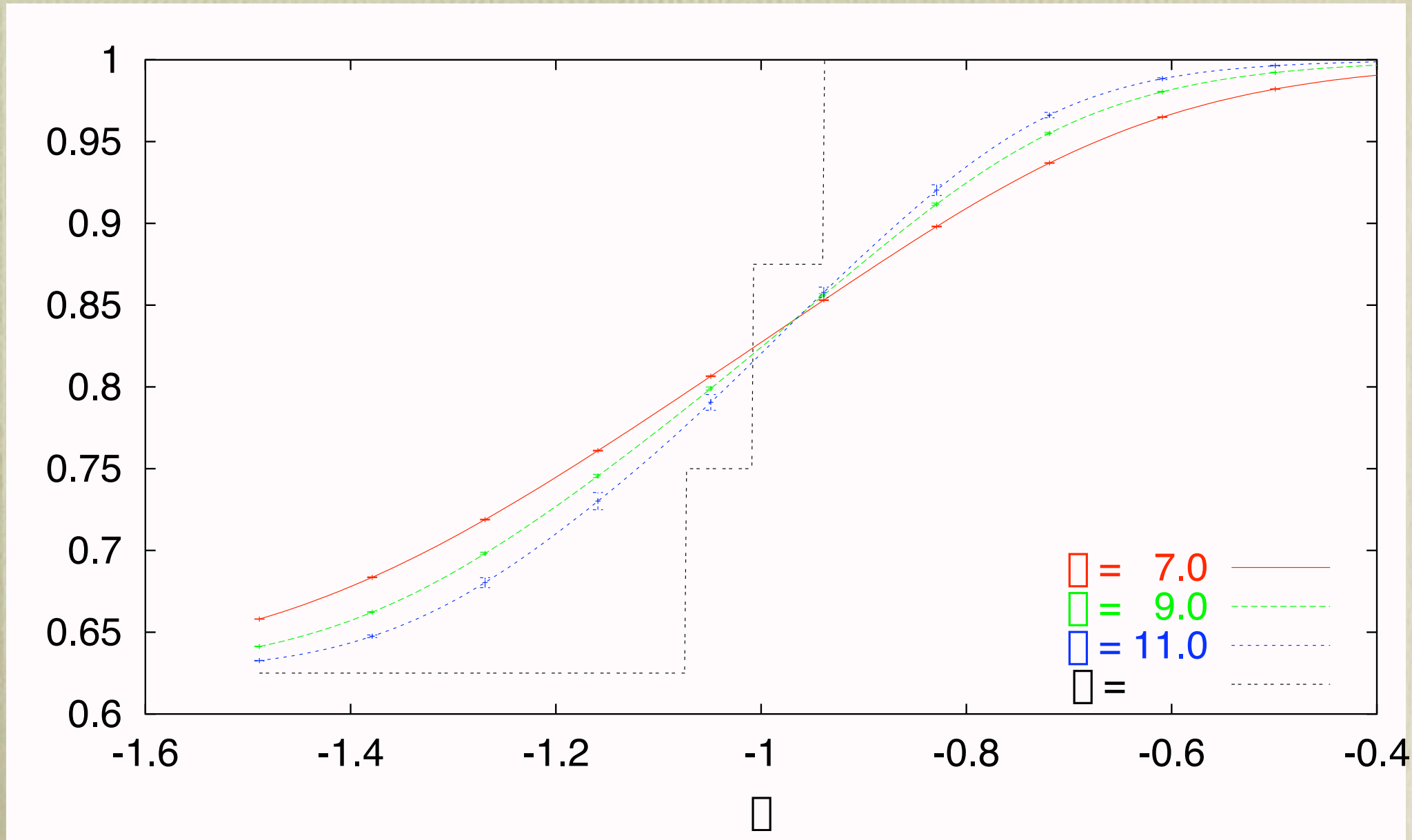
Extract canonical expectation results with expansion:

$$Z(\mu) = \sum_N Z_N \, e^{\beta N \mu} \qquad Z(\mu)\, O(\mu) = \sum_N O_N \, e^{\beta N \mu}$$

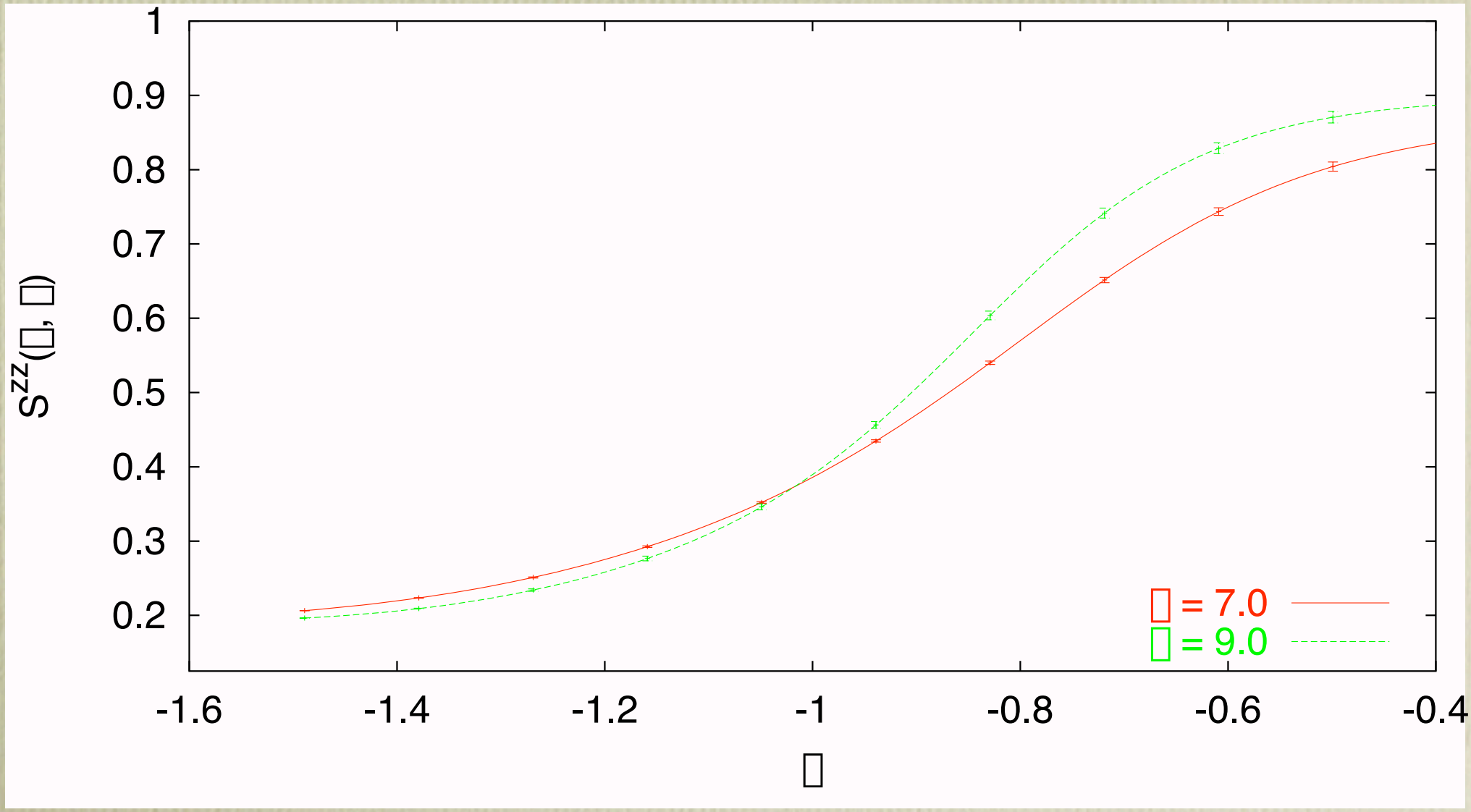
Measure Z(μ) at many values of μ and invert equation to get Z_N

Recombine Z_N to get Z(μ) at any μ

Results: density



Results: Antiferromagnetic susceptibility



Conclusions

- The Hubbard model is a model for high-temperature superconductors.
- Quantum Monte Carlo is a powerful tool to study quantum mechanical systems.
- Extracting canonical ensemble results allows for efficient generation of results as a function of the chemical potential.