The Hubbard Model in Low Dimensions

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Theoretical background
Hubbard model
Correlation functions

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Motivation

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Results

- Simplified model still exhibits interesting physics
- Examples: metal-insulator transition, antiferromagnetism and superconductivity
- \bullet Exact diagonalization is too time-/storage expensive \to Monte Carlo Integration

Hubbard model - A simplified model

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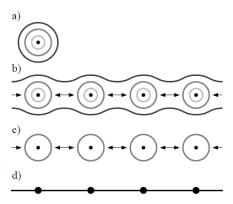


Figure: From valence electrons and bound electrons to the Hubbard simplification

Hubbard model - 2

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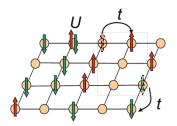


Figure: Illustration of the model on a 2D lattice

$$H = -t \sum_{\langle ij\rangle,\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Hubbard model - Fock space

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 Fock space containing all many body states of the Hamiltonian

• Example 1 site lattice:

$$|0\rangle$$
, $|\uparrow\rangle$, $|\downarrow\rangle$ oder $|\uparrow\downarrow\rangle$

ullet For L lattice sites 4^L possible states, but

$$H = \begin{pmatrix} H_{N=0} & 0 & 0\\ 0 & H_{N=1} & 0\\ 0 & 0 & H_{N=2} \end{pmatrix}$$

 \Rightarrow Basis splits up

Correlation functions

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Partition function

$$Z := \mathsf{Tr}(\mathsf{e}^{-\beta H}) = \sum_n \mathsf{e}^{-\beta E_n}$$

Energy expectation value

$$\langle E \rangle = \frac{1}{Z} \text{Tr}(He^{-\beta H}) = \frac{1}{Z} \sum_{n} E_n e^{-\beta E_n}$$
 (1)

Correlator

$$\left\langle C_{\alpha\beta}(\tau) \middle| C_{\alpha\beta}(\tau) \right\rangle = \frac{1}{Z} \sum_{i} \left\langle i | a_{\alpha}(\tau) a_{\beta}^{\dagger}(0) | i \middle| i | a_{\alpha}(\tau) a_{\beta}^{\dagger}(0) | i \right\rangle \tag{2}$$

Analytic solution of the model for small lattices

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Analytic solutions

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Hubbard-Stratonovich transformation

Importance

Results

- For 1 (2) lattice sites only 4(16) states in Fock space
- can find expressions for correlaors analytically

Solving the 1 site model

Analytic solutions

Enumeration
 State
 Number of eletrons

$$|1\rangle$$
 $|0\rangle$
 0

 $|2\rangle$
 $|\uparrow\rangle$
 1

 $|3\rangle$
 $|\downarrow\rangle$
 1

 $|4\rangle$
 $|\uparrow\downarrow\rangle$
 2

Table 1: Enumeration of Fock states in the onesited model

$$\langle i|H|j\rangle = \begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & -\frac{U}{2} & 0 & 0\\ 0 & 0 & -\frac{U}{2} & 0\\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$Z_1 = 2(1 + e^{\beta U/2}) \tag{3}$$

Methods

Methods

- Hubbard-Stratonovich transformation
- Importance sampling

Hubbard-Stratonovich transformation

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Calculating expectation values

$$\begin{split} \langle O(t) \rangle &= \frac{1}{Z} \operatorname{Tr} \left[O(t) e^{-\beta H} \right] \\ &= \frac{1}{Z} \int \left[\prod_i d\psi_i^\dagger d\psi_i \right] e^{-\Sigma_j \left(\psi_j^\dagger \psi_j \right)} \left\langle -\psi \right| O(t) e^{-\beta H} \left| \psi \right\rangle \end{split}$$

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Trick to reduce the number of fermion fields

$$e^{\frac{1}{2}Un^2} = \frac{1}{\sqrt{2\pi U}} \int_{-\infty}^{\infty} d\phi \, e^{-\frac{1}{2U}\phi^2 \pm \phi n}$$

Correlator:

$$C_{\alpha\beta}(\tau) = \lim_{N_t \to \infty} \int_{-\infty}^{\infty} \mathcal{D}[\phi] e^{-\frac{1}{2\bar{U}}\phi^2} M_{\alpha\tau,\beta_0}^{-1}[\phi] \det(M[\phi]M[-\phi])$$

Importance sampling

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$$\bullet \ \sqrt{2\pi \tilde{U}}^{-1}$$
 included in $\mathcal{D}[\phi] \Rightarrow$ sample from $\mathcal{N}_{0,\sqrt{\tilde{U}}}$

• Then calculate matrix part and average

Importance sampling - 2

Motivation

Theoretical

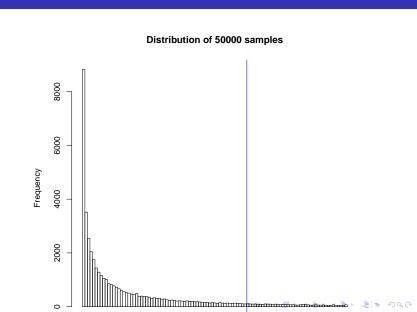
Hubbard model Correlation function

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Importance sampling

2 2 2 3 4 4 5



Results - Partition function

8

17

9

15

10 20 30

Results

1-Site U=2 beta=2 N=50000

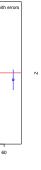
N_t

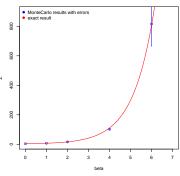
MonteCarlo results with errors exact result

50



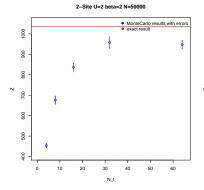
1-Site N=50000 U=2 Nt=32

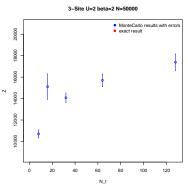




Results - Partition function - 2

Results





Results - Correlator

Motivation

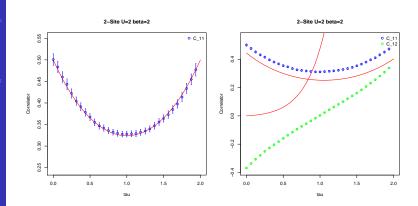
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Conclusion and Outlook

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Successes

- 1- and 2-site partition function matching
- 1- site correlators matching
- Extension to larger 1D lattices possible

Outlook

- Optimize in precision
- Optimize in computing time
- Higher dimensional model
- Grand-canonical ensemble

References



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