The Hubbard Model in Low Dimensions

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Inhalt

Motivation

- Simplified model - still exhibits interesting physics
- Examples: metal-insulator transition, antiferromagnetism and superconductivity
- Exact diagonalization is too time-/storageexpensive $\rightarrow$ Monte Carlo Integration

Hubbard model - A simplified model

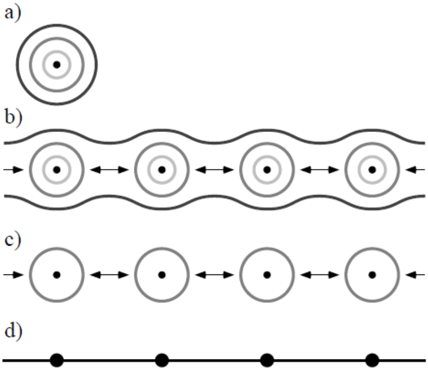


Figure: From valence electrons and bound electrons to the Hubbard simplification

Hubbard model - 2

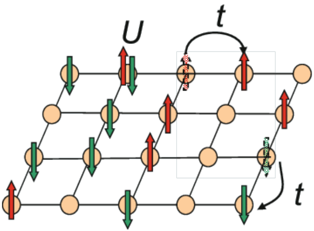


Figure: Illustration of the model on a 2D lattice

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

Hubbard model - Fock space

- Fock space containing all many body states of the Hamiltonian
- Example 1 site lattice:

$$|0\rangle\,,\ |\uparrow\rangle\,,\ |\downarrow\rangle\ \text{oder}\ |\uparrow\downarrow\rangle$$

- 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

- Partition function

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

- Energy expectation value

$$\langle E \rangle = \frac{1}{Z}\mathrm{Tr}(H\mathrm{e}^{-\beta H}) = \frac{1}{Z}\sum_n E_n \mathrm{e}^{-\beta E_n} \tag{1}$$

- 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

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

Solving the 1 site model

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

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

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

Methods

- Hubbard-Stratonovich transformation
- Importance sampling

Hubbard-Stratonovich transformation

- Calculating expectation values

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

Hubbard-Stratonovich transformation - 2

- Trick to reduce the number of fermion fields

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

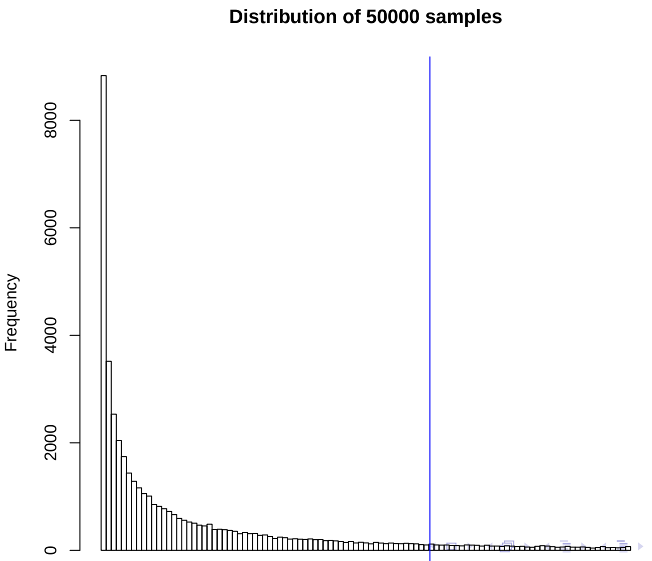
- Correlator:

$$C_{\alpha\beta}(\tau) = \lim_{N_t \to \infty} \int_{-\infty}^{\infty} \mathcal{D}[\phi] e^{-\frac{1}{2\tilde{U}}\phi^2} M^{-1}_{\alpha\tau,\beta 0}[\phi] \det\big(M[\phi]M[-\phi]\big)$$

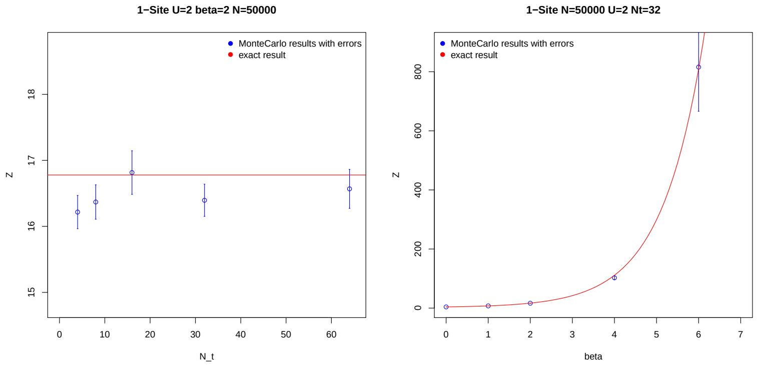
Importance sampling

- $\sqrt{2\pi\tilde{U}}^{-1}$ included in $\mathcal{D}[\phi] \Rightarrow$ sample from $\mathcal{N}_{0,\sqrt{\tilde{U}}}$
- Then calculate matrix part and average

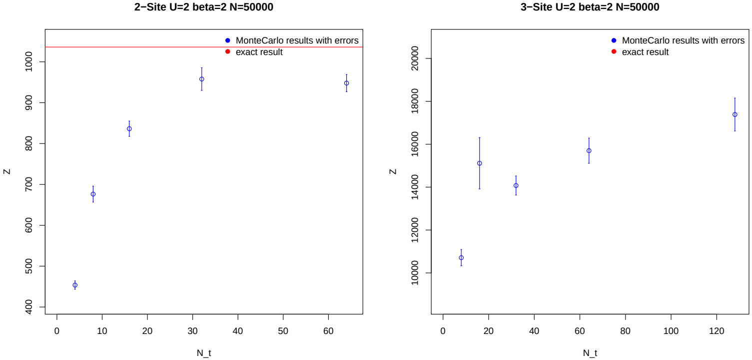
Importance sampling - 2



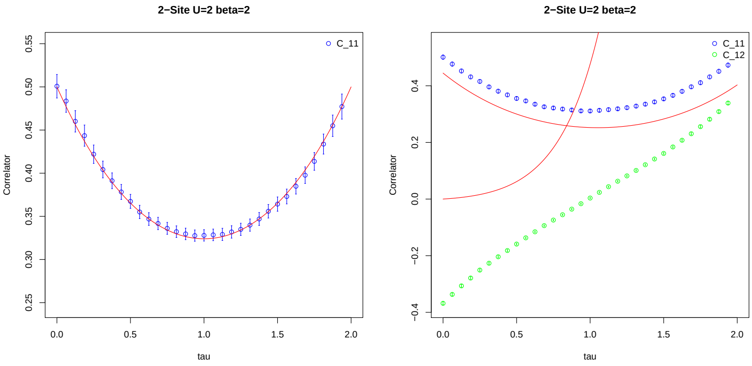
Results - Partition function



Results - Partition function - 2



Results - Correlator



Conclusion and Outlook

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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