The Hubbard Model with fermionic Tensor Networks

arXiv:2106.13583 [physics.comp-ph]

Manuel Schneider, Johann Ostmeyer, Karl Jansen, Thomas Luu, and Carsten Urbach
manuel.schneider@desy.de

DESY Zeuthen
NIC group

Humboldt-Universität zu Berlin
Faculty of Mathematics and Natural Sciences
Department of Physics

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Motivation

- Hubbard Model on the Honeycomb Lattice is a model for Graphene
- Phase Transition from Semi-Metallic to Mott-Insulator $\rightarrow$ fast transistors [Han *et al.* 2014]

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$$H = -\kappa \sum_{\langle x,y \rangle, s} c^\dagger_{x,s} c_{y,s} + \frac{U}{2} \sum_x q_x^2 + \mu \sum_{x,s} \left(c^\dagger_{x,s} c_{x,s} - \frac{1}{2} \right)$$

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- At $\mu = 0$: good results with HMC [Johann Ostmeyer, Tue, 6am], [Ostmeyer *et al.* 2021]
- $\mu \neq 0$: sign problem
- Tensor Network methods do not suffer from the sign problem

Projected Entangled Pair States (PEPS) [Orús 2014; Verstraete & Cirac 2004]

$$|\psi\rangle = \sum_{s_1 \dots s_N} \underbrace{A_{s_1, s_2, \dots, s_N}}_{4^N \text{coefficients}} |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle$$

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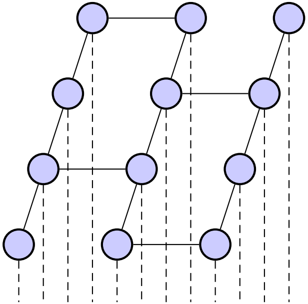
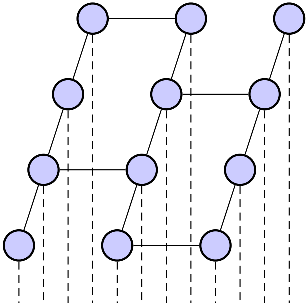


fermionic PEPS [Corboz *et al.* 2010]

$$c_i^\dagger c_k^\dagger = -c_k^\dagger c_i^\dagger$$



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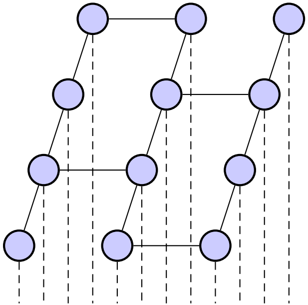
- define parity on all links



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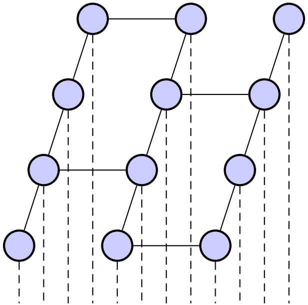

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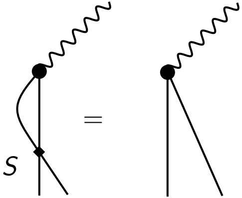
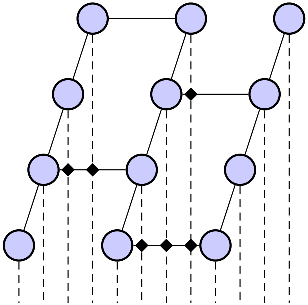
- line crossing $\rightarrow$ swap gates



$$S = \begin{pmatrix} \overbrace{1 & \dots & 1}^{\text{even}} & \overbrace{1 & \dots & 1}^{\text{odd}} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 1 & \dots & 1 \\ 1 & \dots & 1 & -1 & \dots & -1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & -1 & \dots & -1 \end{pmatrix} \begin{matrix} \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} \text{even} \\ \left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} \text{odd} \end{matrix}$$



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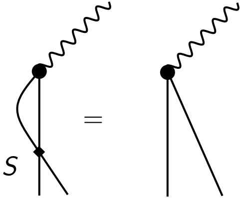
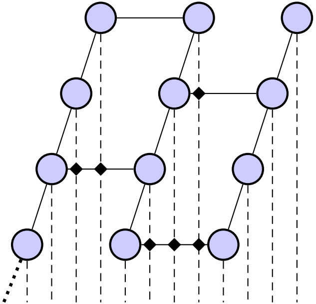


- parity link → choose overall parity

$$S = \overbrace{}^{\text{even}}\ \overbrace{}^{\text{odd}} \\ S = \begin{pmatrix} 1 & \dots & 1 & 1 & \dots & 1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 1 & \dots & 1 \\ 1 & \dots & 1 & -1 & \dots & -1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & -1 & \dots & -1 \end{pmatrix} \begin{matrix} \left.\vphantom{\begin{matrix}1\\ \vdots\\ 1\end{matrix}}\right\} \text{even} \\ \left.\vphantom{\begin{matrix}1\\ \vdots\\ 1\end{matrix}}\right\} \text{odd} \end{matrix}$$



imaginary time evolution of PEPS

- Fix bond dimension D

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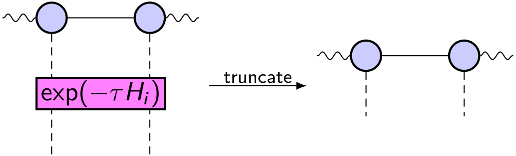
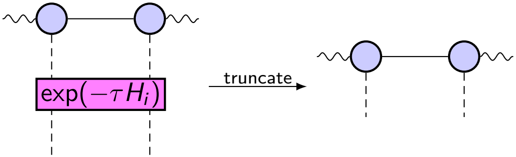
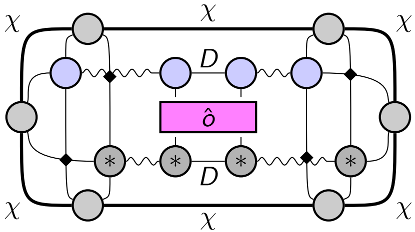


imaginary time evolution of PEPS

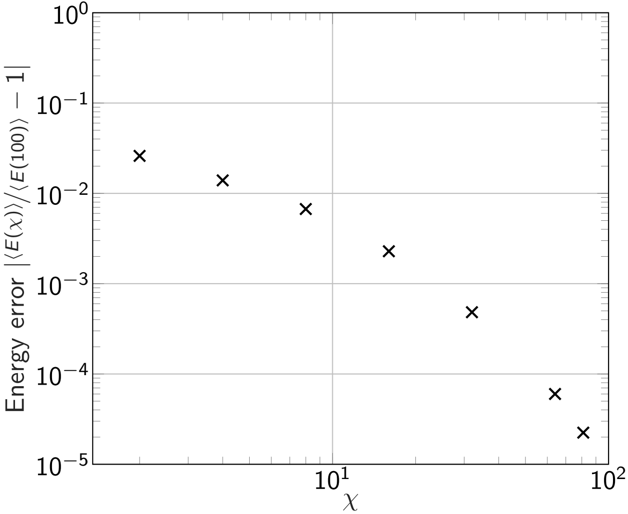
- Fix bond dimension D
- Initialize PEPS randomly
- Trotter-decomposed imaginary time evolution
- Local updates
- Contract network to calculate expectation values





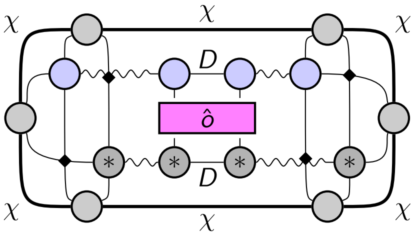
boundary MPS effect

$D = 12, L = 12 \times 6$ hexagonal,
$\kappa = 1, U = 2, \mu = 0.1, B = 0.01$

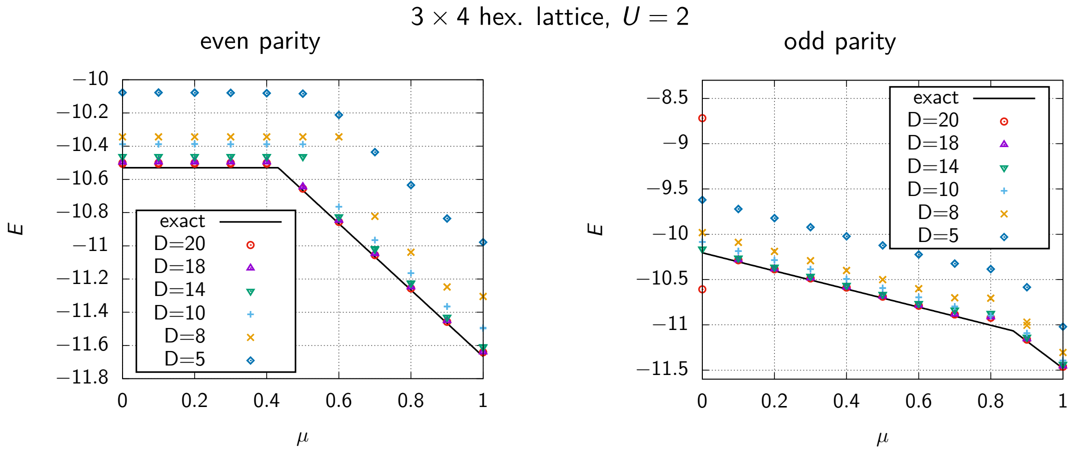


Runtime $\propto N\chi^3 D^4$

Memory $\propto \chi^2 D^4$

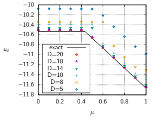


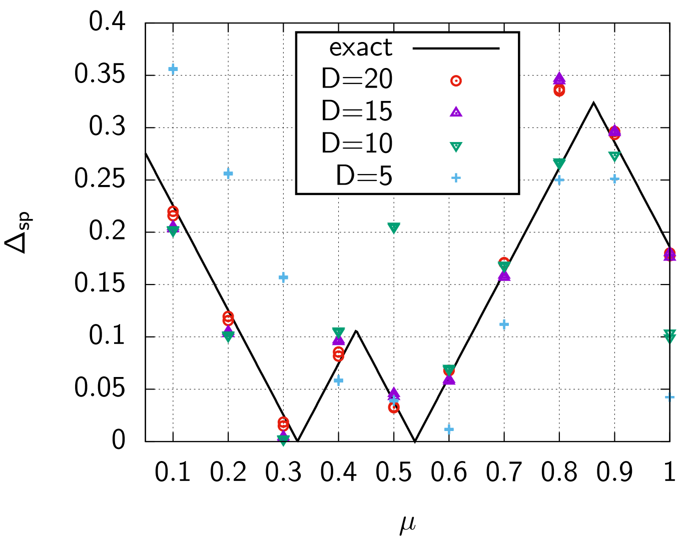
Simulations with chemical potential



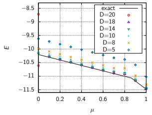
Simulations with chemical potential

even parity





odd parity



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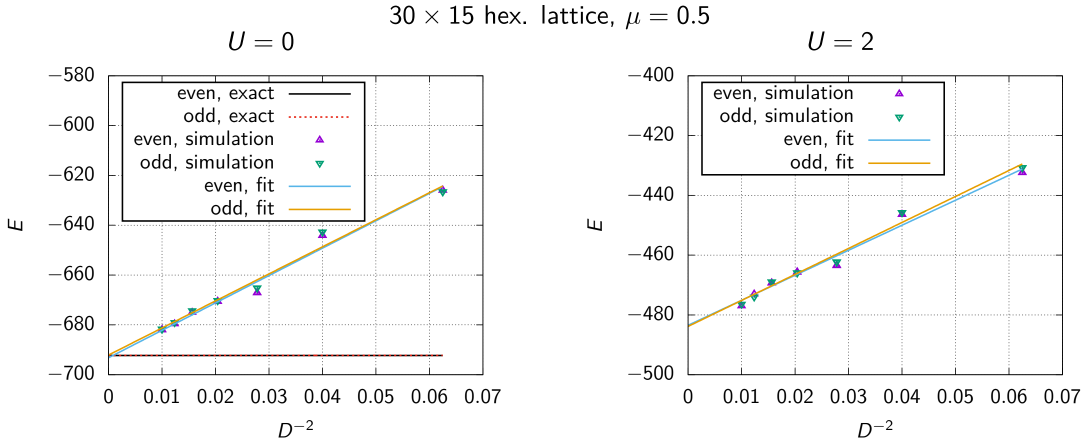

Summary

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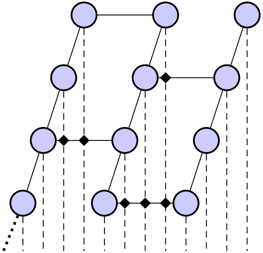

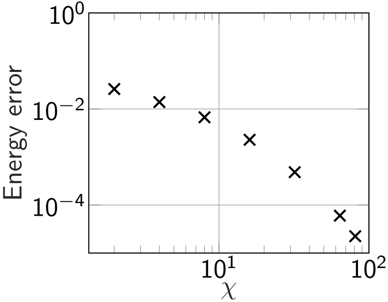

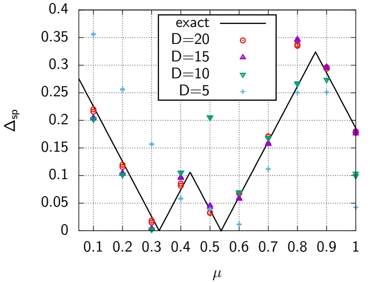

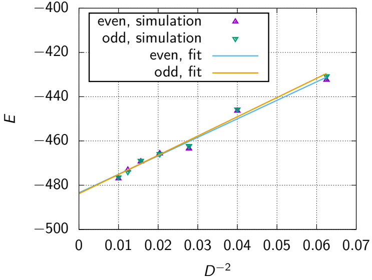

Outlook:

- explore phase diagram
- study exciting new physics at $\mu \neq 0$

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