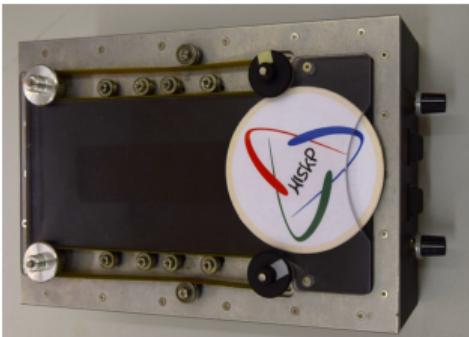


Simulating both parity sectors of the Hubbard Model with Tensor Networks

arXiv:2106.13583 [physics.comp-ph]

Manuel Schneider, Johann Ostmeyer, Karl Jansen, Thomas Luu, and Carsten Urbach

Helmholtz-Institut für Strahlen- und Kernphysik
Bonn University



July 7, 2021

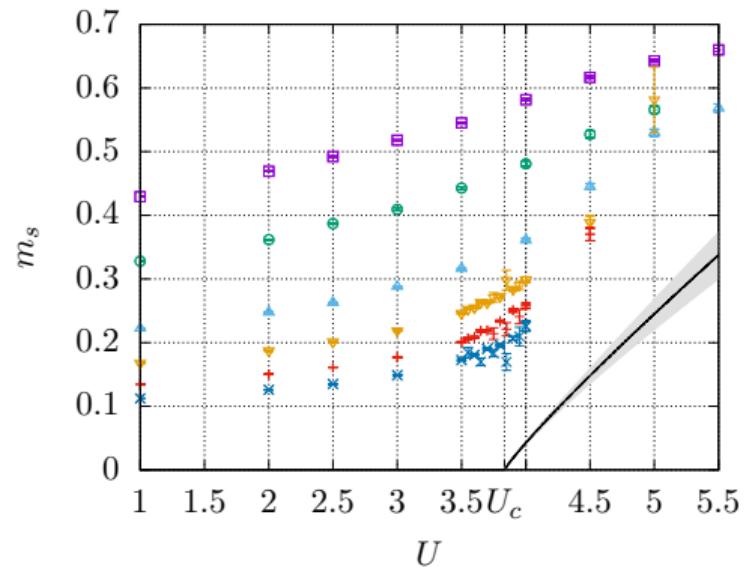
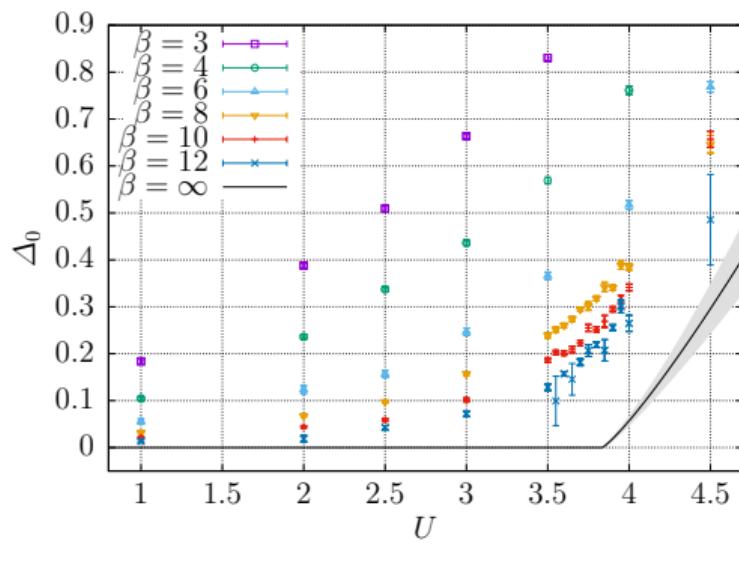


Hybrid Monte Carlo simulations of the Hubbard model [Ostmeyer et al. 2020, 2021]

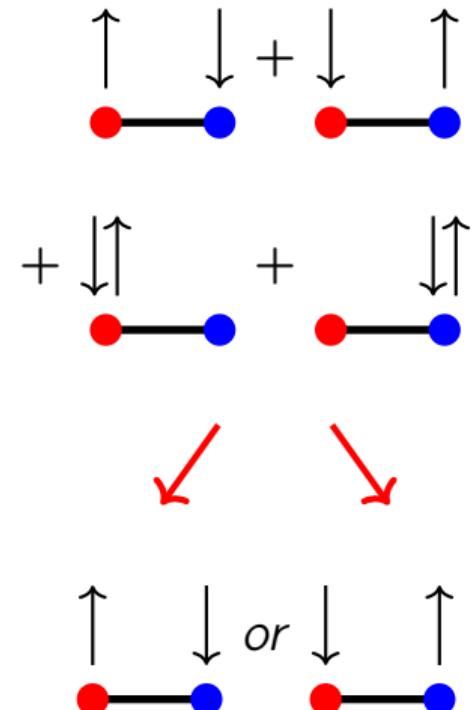
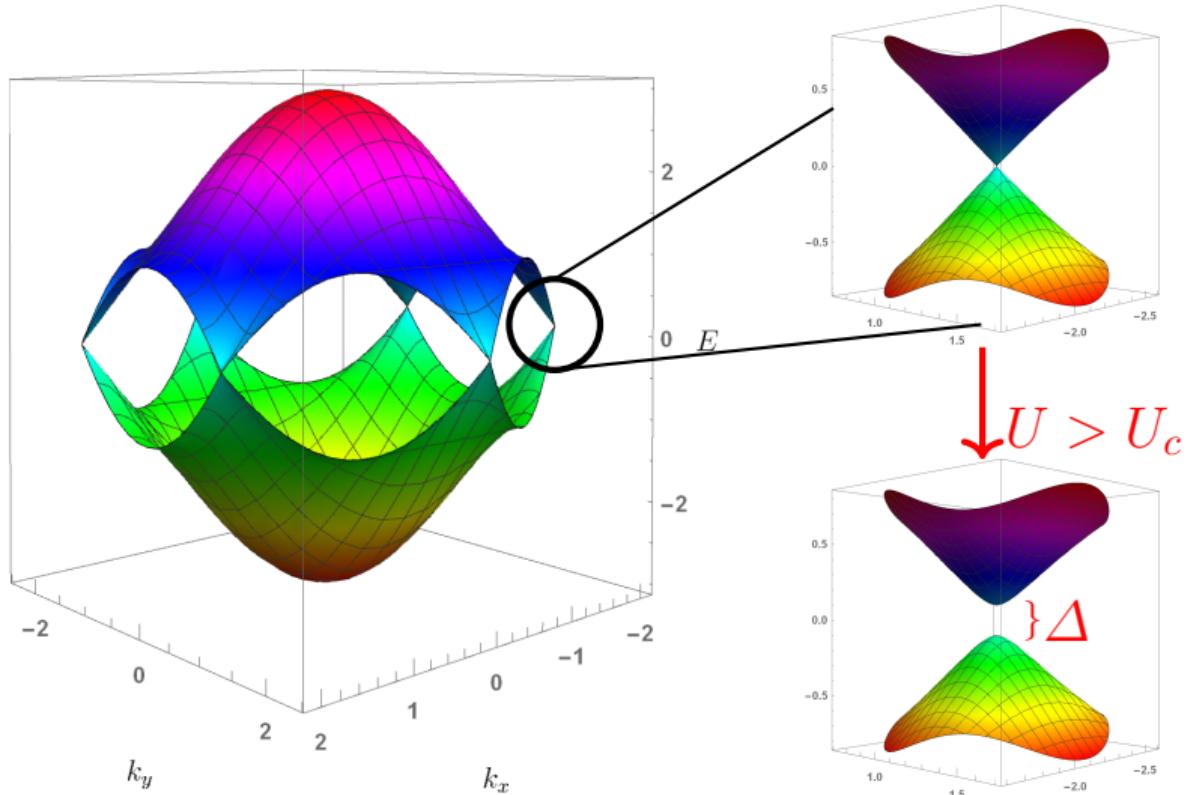
$$H = - \sum_{\langle x,y \rangle, s} c_{x,s}^\dagger c_{y,s} + \frac{1}{2} U \sum_x q_x^2$$

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[Alexandru *et al.* 2016; Cristoforetti *et al.* 2013; Ulybyshev *et al.* 2020; Wijnen *et al.* 2021]

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[Alexandru *et al.* 2016; Cristoforetti *et al.* 2013; Ulybyshev *et al.* 2020; Wijnen *et al.* 2021]
- ▶ Tensor Networks
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Projected Entangled Pair States (PEPS) [Orús 2014; Verstraete & Cirac 2004]

$$|\psi\rangle = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} A_{s_1, s_2, \dots, s_N} |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle$$

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

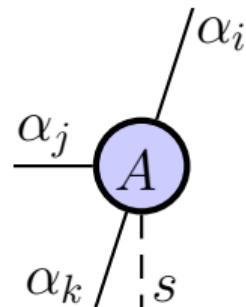
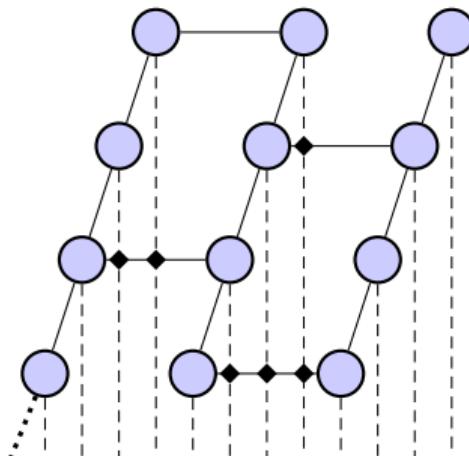
$$\begin{aligned} |\psi\rangle &= \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} A_{s_1, s_2, \dots, s_N} |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle \\ &\approx \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} A_{s_1; \alpha_1}^1 A_{s_2; \alpha_1, \alpha_2}^2 \cdots A_{s_N; \alpha_{N-1}}^N |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle \end{aligned}$$

Truncate $\alpha_i \leq D \forall i$

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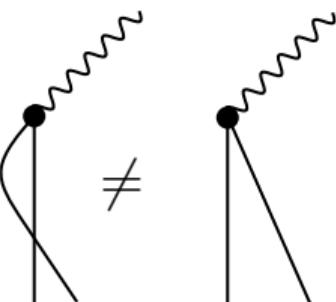
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Truncate $\alpha_i \leq D \forall i$

Fermionic PEPS [Corboz *et al.* 2010]

$$c_i c_k = -c_k c_i$$


A diagram illustrating the fermionic commutation relation $c_i c_k = -c_k c_i$. It consists of two parts separated by a large inequality sign (\neq). The left part shows a black dot at the top connected by a vertical line to a horizontal line that curves downwards and then turns right. The right part shows a black dot at the top connected by a vertical line to a horizontal line that goes straight down and then turns right. Both diagrams have a wavy line above them, representing a fermion exchange between the two sites.

Fermionic PEPS [Corboz *et al.* 2010]

$$c_i c_k = -c_k c_i$$
$$(c_i c_j) c_k = c_k (c_i c_j)$$

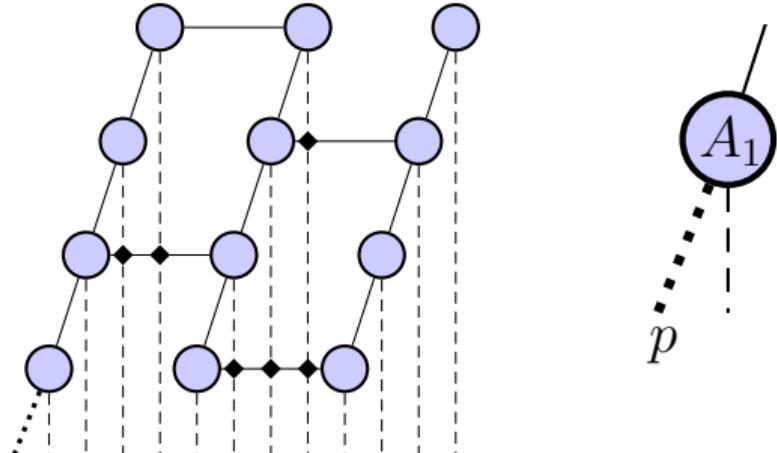
Fermionic PEPS [Corboz *et al.* 2010]

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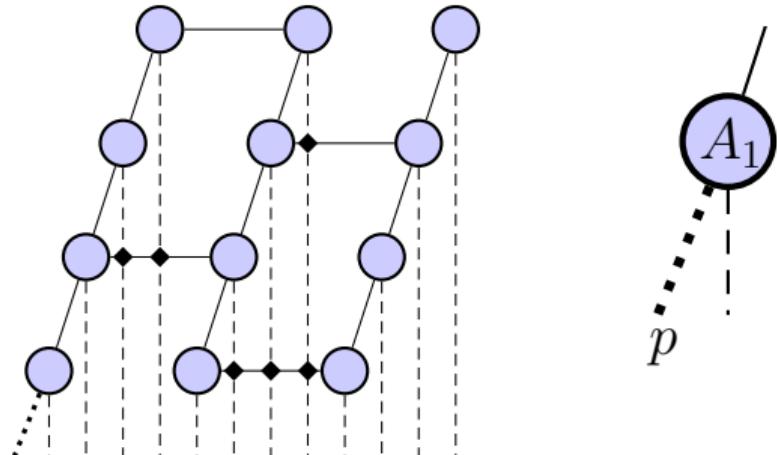
$$(c_i c_j) c_k = c_k (c_i c_j)$$

$$S = \begin{pmatrix} & \overbrace{\hspace{1cm}}^{\text{even}} & & \overbrace{\hspace{1cm}}^{\text{odd}} & \\ 1 & \dots & 1 & 1 & \dots & 1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 1 & \dots & 1 \\ 1 & \dots & 1 & -1 & \dots & -1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & -1 & \dots & -1 \end{pmatrix}$$

Parity link



Parity link



$p = \pm 1$
⇒ even- and odd-parity
subspaces without
communication

Ground state search

- ▶ Fix bond dimension D

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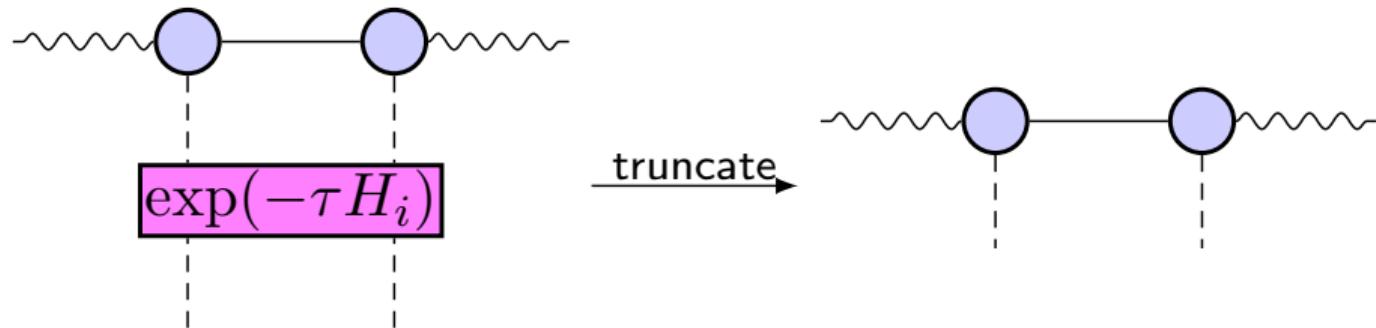
Ground state search

- ▶ Fix bond dimension D
- ▶ Initialise PEPS randomly
- ▶ Trotter-decomposed imaginary time evolution
- ▶ Local updates

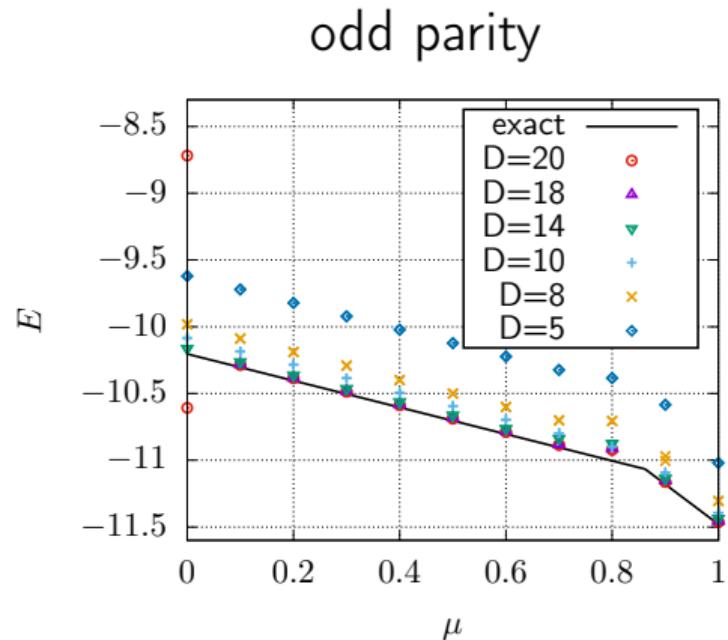
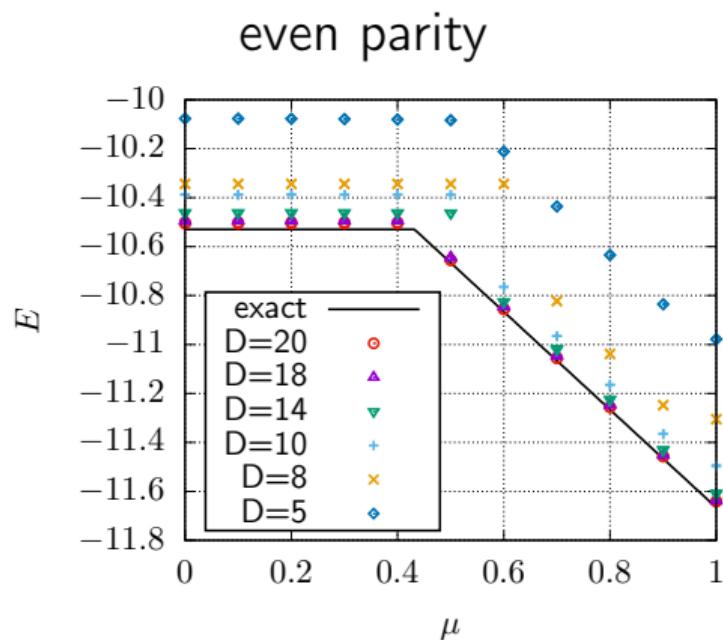
Ground state search

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

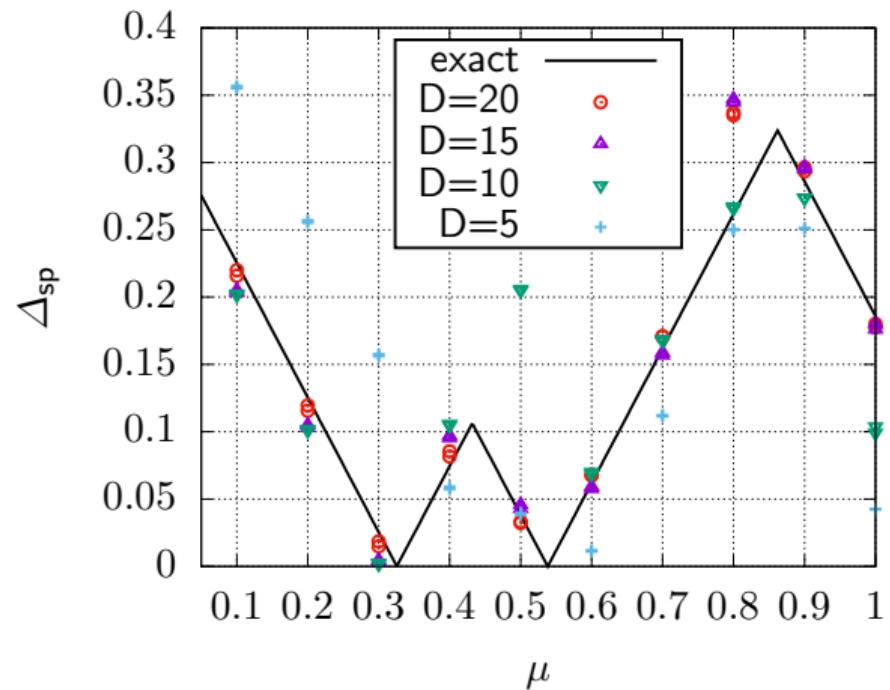
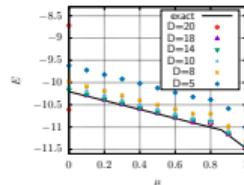
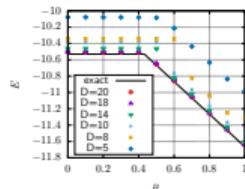
Simple Update



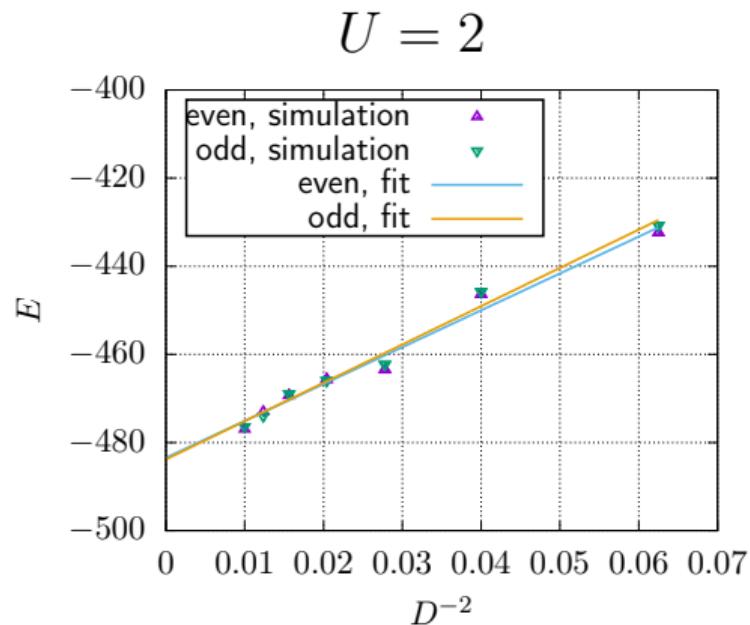
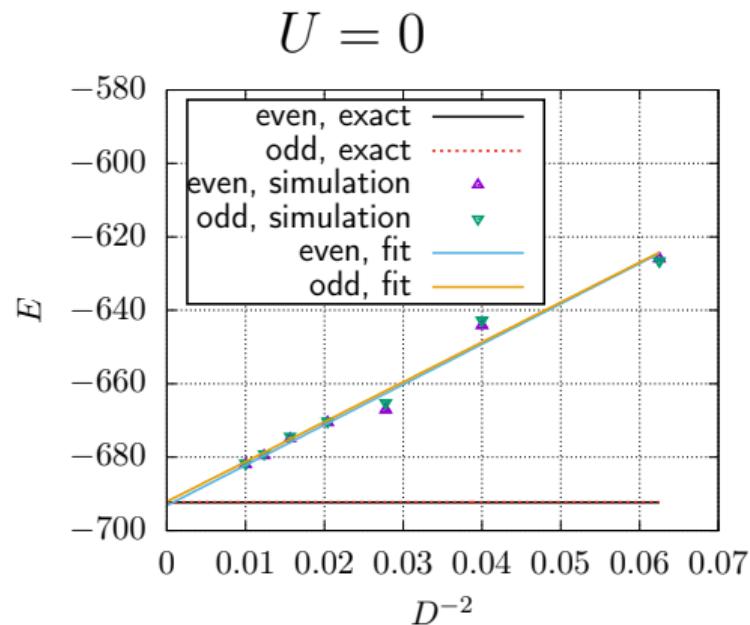
Simulations with chemical potential (3×4 hex. lattice, $U = 2$)



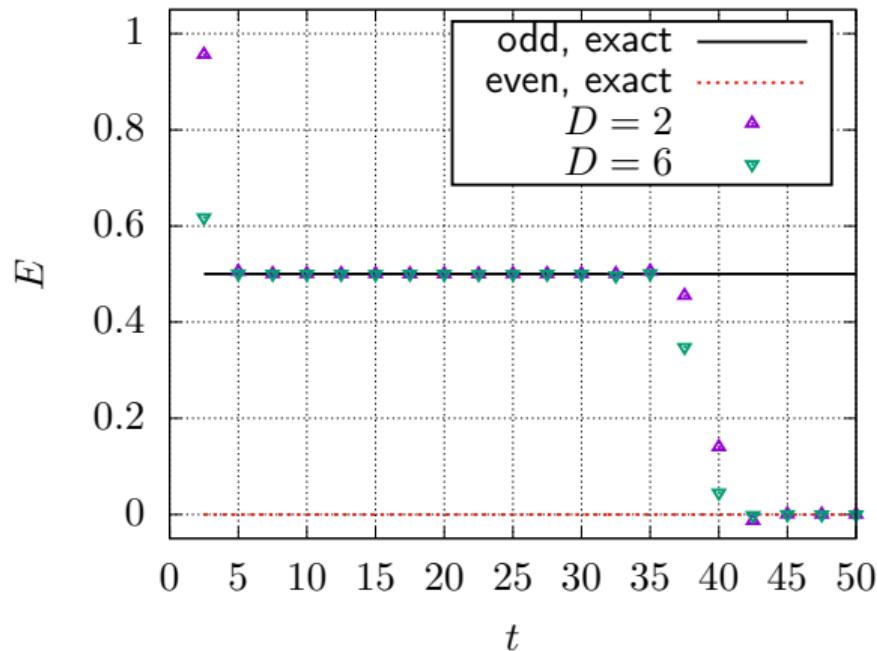
Simulations with chemical potential (3×4 hex. lattice, $U = 2$)



Simulations with chemical potential (30×15 hex. lattice, $\mu = 0.5$)

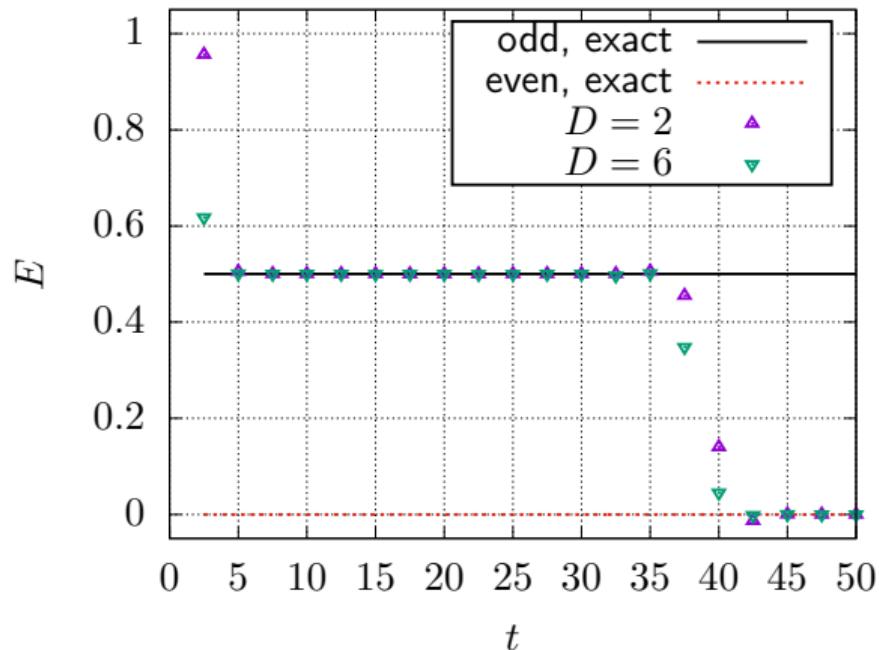


Stability issues with odd parity



3×4 hex. lattice, $U = 1$, no hopping

Stability issues with odd parity



3×4 hex. lattice, $U = 1$, no hopping

Large gap (strong coupling)
⇒ jump to even parity
ground state

Possible solutions

- ▶ Non-local Full Update

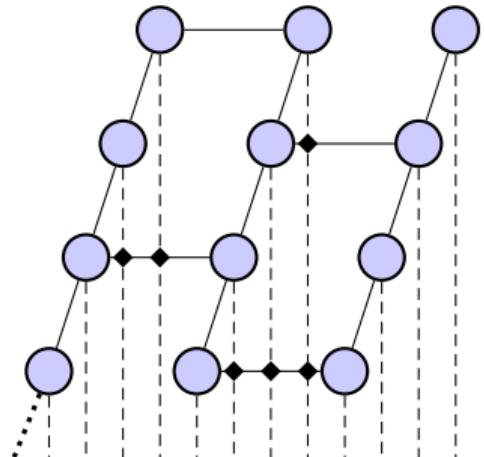
Possible solutions

- ▶ Non-local Full Update
- ▶ Use only even parity ground state
→ alternative observables required

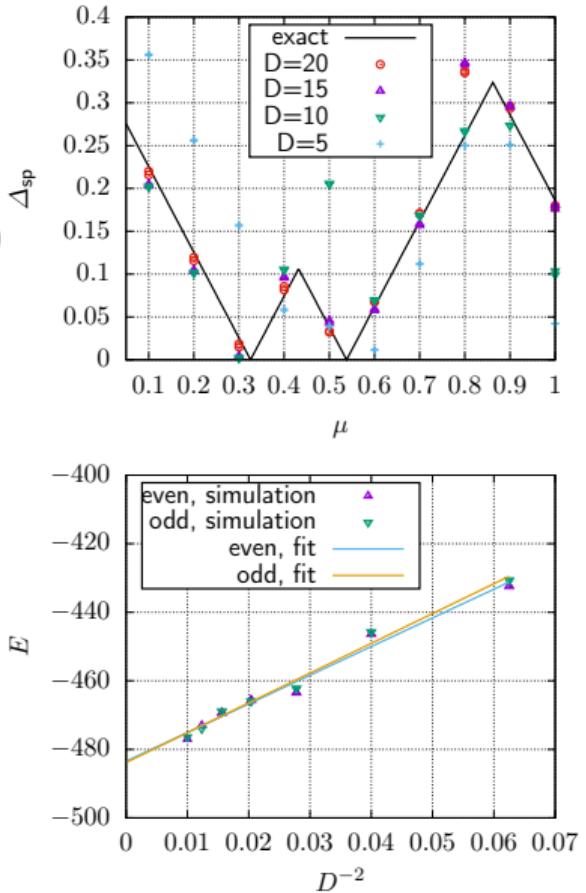
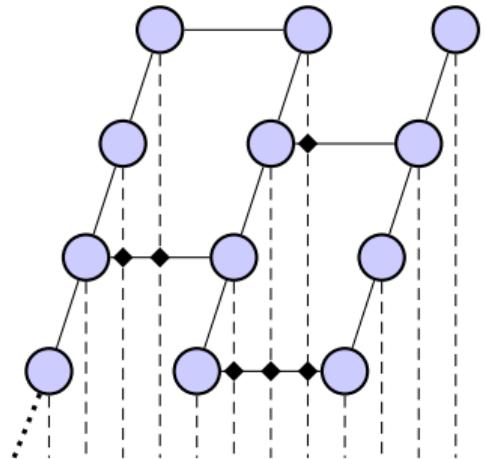
Possible solutions

- ▶ Non-local Full Update
- ▶ Use only even parity ground state
→ alternative observables required
- ▶ Open for suggestions!

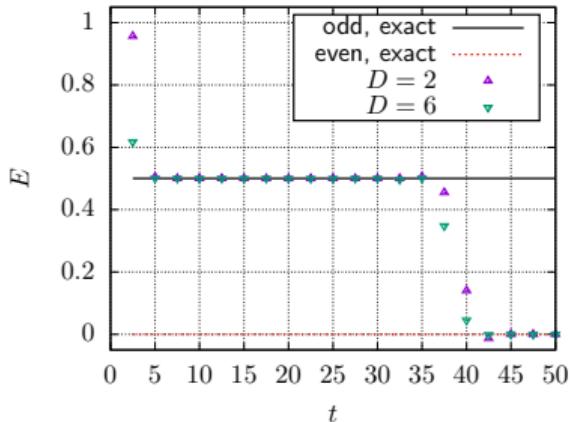
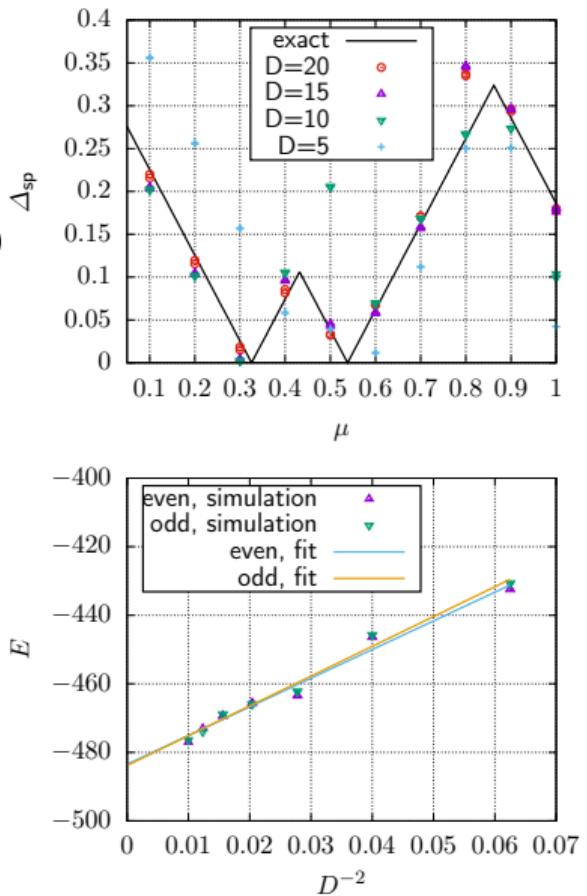
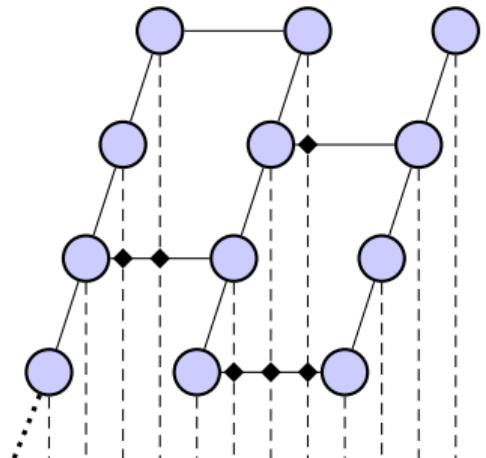
Summary



Summary



Summary



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