Stochastic and Tensor Network simulations of the Hubbard Model

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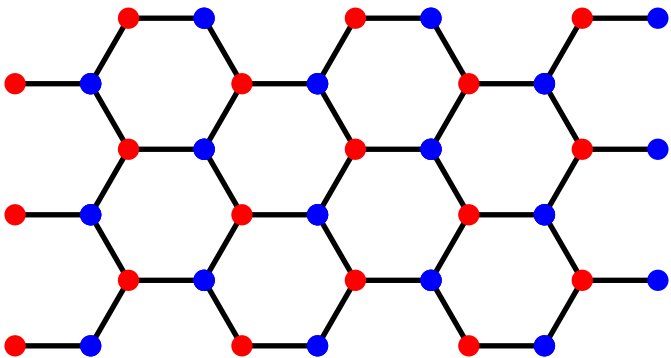
Hubbard model [Hubbard *ProcRSoc* **276** (1963); Wallace *PhysRev* **71** (1947)]

$$H = -\sum_{\langle x,y\rangle,s} c^{\dagger}_{x,s} c_{y,s}$$



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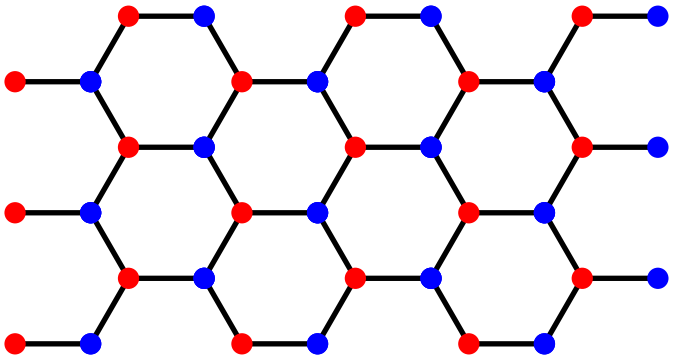

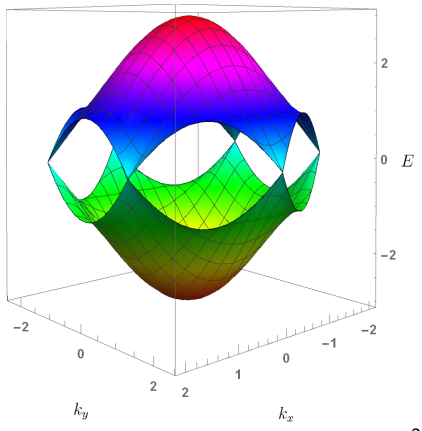

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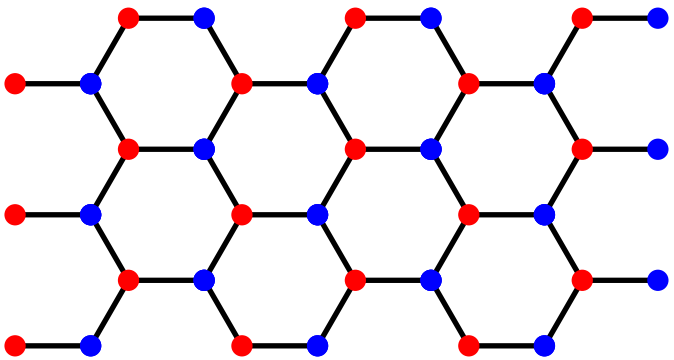
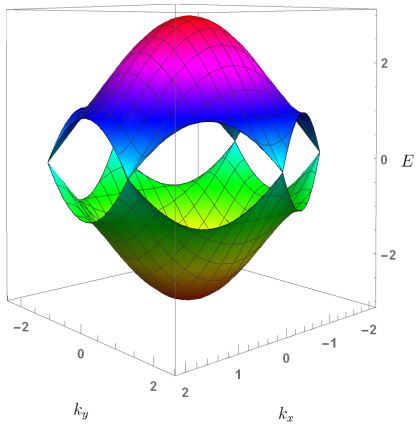
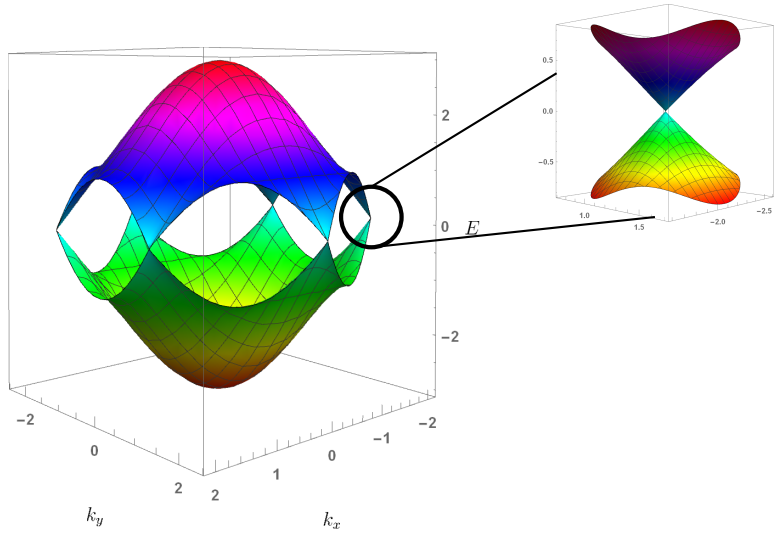




Expected phase transition



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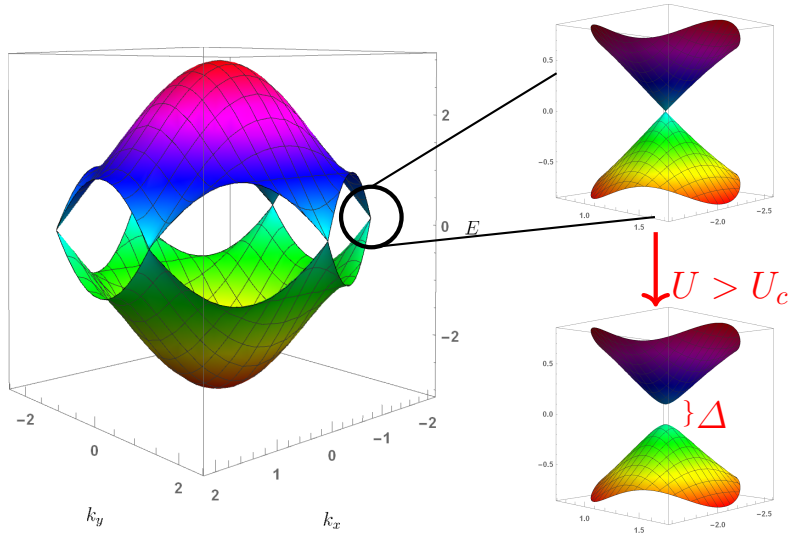

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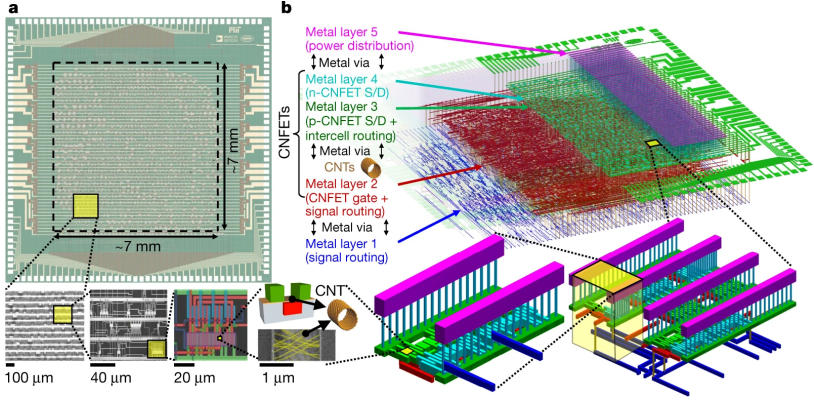

"Hello, world!
I am RV16XNano."

[Hills *et al. Nature* **572** (2019)]

Path integral formalism [Krieg, JO *et al.* *CPC* **236** (2019); Luu & Lähde *PRB* **93** (2016)]

- Discretise imaginary time into steps $\delta = \beta/N_t$, $\beta = 1/T$

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$$p_x^\dagger \equiv c_{x,\uparrow}^\dagger \, , \, p_x \equiv c_{x,\uparrow} \, , \, h_x^\dagger \equiv c_{x,\downarrow} \, , \, h_x \equiv c_{x,\downarrow}^\dagger$$

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$$M_{(x,t)(y,t')} = \delta_{xy}\delta_{tt'} - \mathrm{e}^{-\mathrm{i}\,\delta\cdot\phi_{x,t}}\delta_{xy}\delta_{t-1,t'} - \delta\cdot\delta_{\langle x,y\rangle}\delta_{t-1,t'}$$

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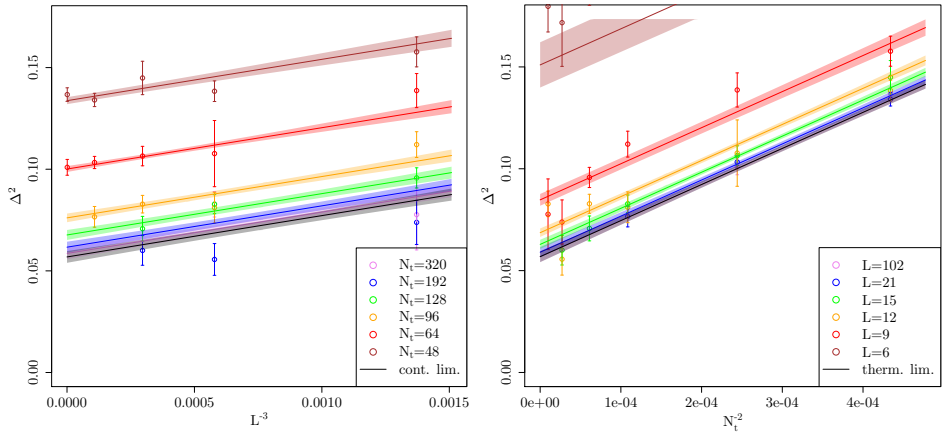
- **Hybrid Monte Carlo** simulation according to probability density

$$p[\phi] \equiv \mathrm{e}^{-S[\phi]} = \det\left(MM^\dagger\right)\mathrm{e}^{-\frac{\delta}{2U}\phi^2}$$

Extrapolation towards the physical limit [JO, Berkowitz *et al.* *PRB* **102** (2020)]

$$\Delta^2 = \Delta_0^2 + c_T\, N_t^{-2} + c_L\, L^{-3}$$



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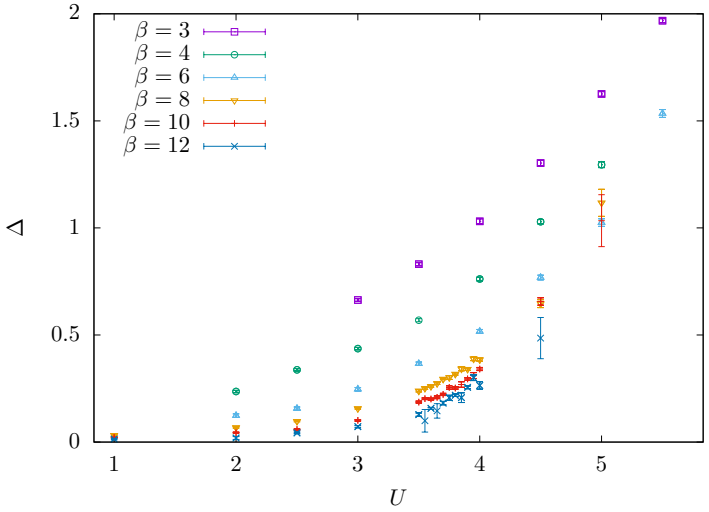
$$\Delta \sim \beta^{-1}$$



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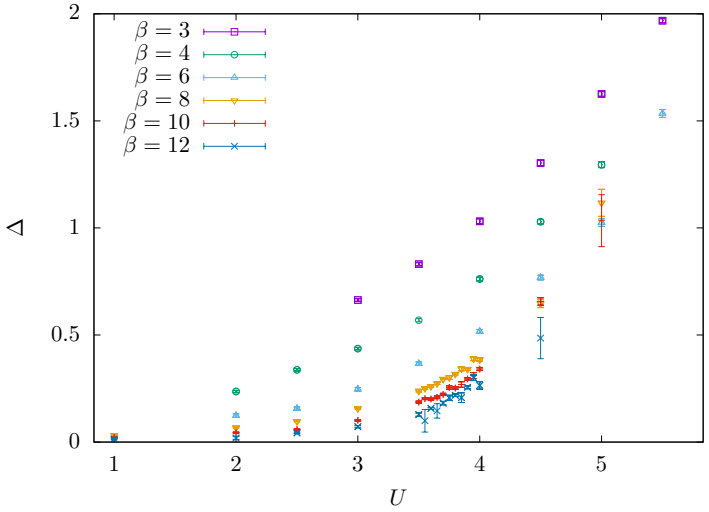

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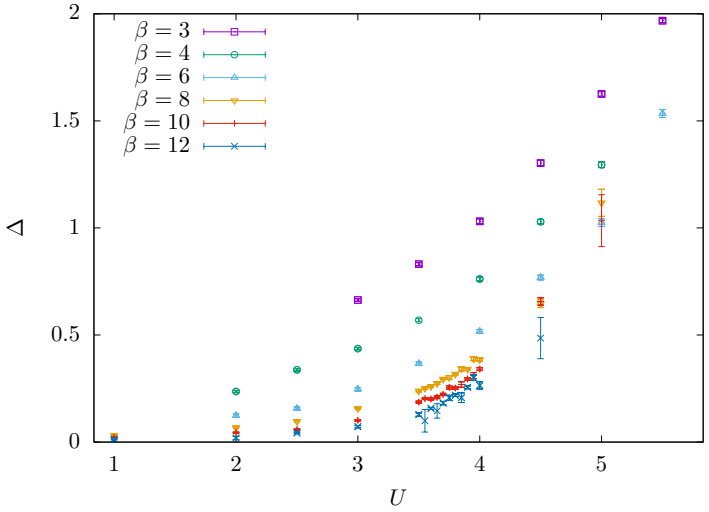

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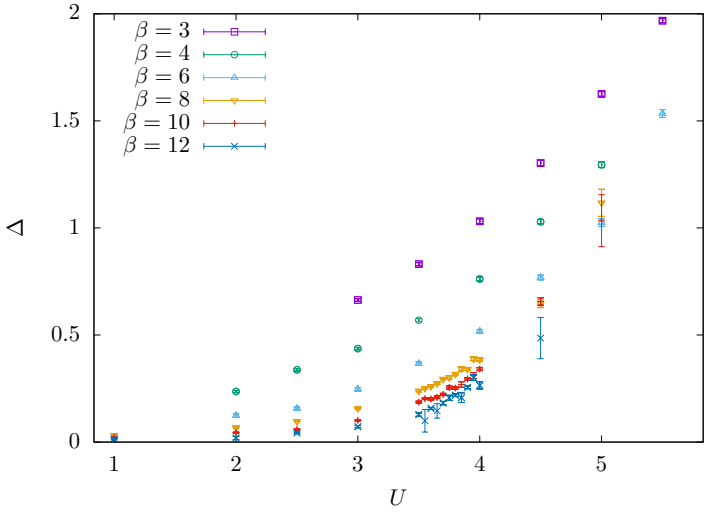

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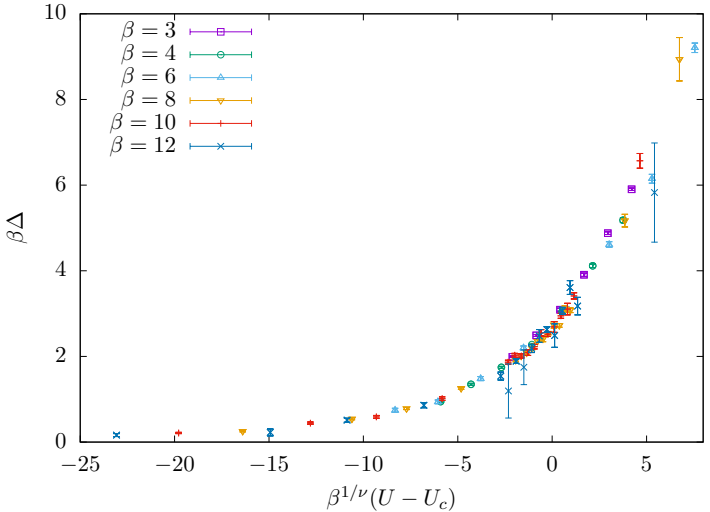

$$\Rightarrow U_c = 3.834(14)\ , \quad \nu = 1.185(43)\ , \quad \beta = 1.095(37)$$

Quantum phase transition at half filling

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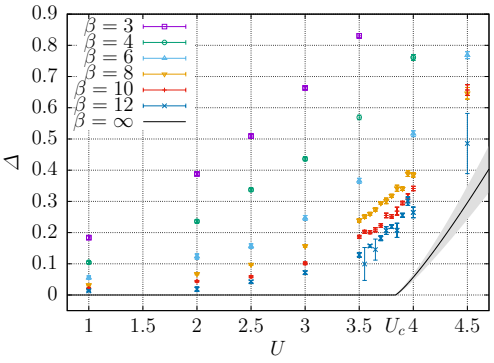

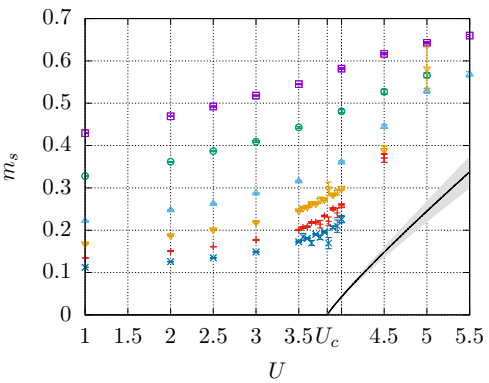

Beyond half filling?

Sign problem!

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

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- Tensor Networks
  [Corboz *PRB* **93** (2016); Schneider, JO *et al. PRB* **104** (2021); talks by T. Angelides, R. Sakai, J. Bloch, T. Kuwahara]

Projected Entangled Pair States (PEPS)

[Orús *AnnPhys* **349** (2014); Verstraete & Cirac *arXiv* **0407066** (2004); talk by L. Funcke]

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

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Truncate $\alpha_i \leq D\ \forall i$

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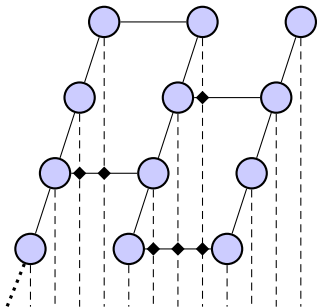

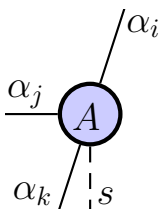

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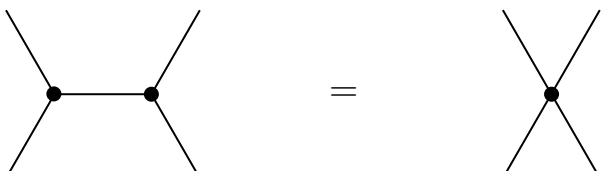
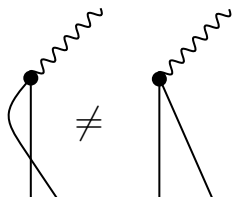
Contractions

$d = 1$ 

$d > 1$ 

Fermionic PEPS [Corboz *et al.* *PRB* **81** (2010)]

$$c_i c_k = -c_k c_i$$



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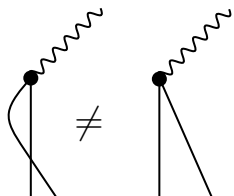

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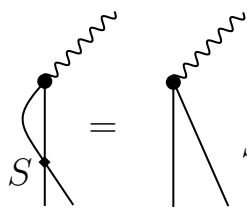
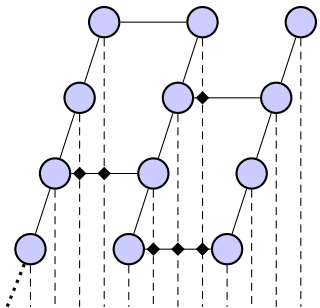


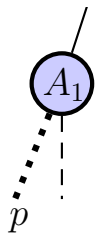
$$S = \begin{pmatrix} 1 & \dots & 1 & 1 & \dots & 1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 1 & \dots & 1 \\ 1 & \dots & 1 & -1 & \dots & -1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & -1 & \dots & -1 \end{pmatrix}$$

even (columns) odd (columns)

even (rows) odd (rows)

Parity link





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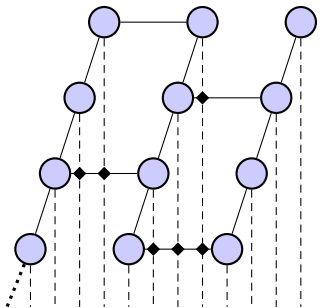

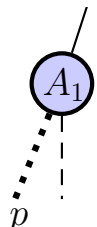

$p = \pm 1$
$\Rightarrow$ even- and odd-parity subspaces are disjoint

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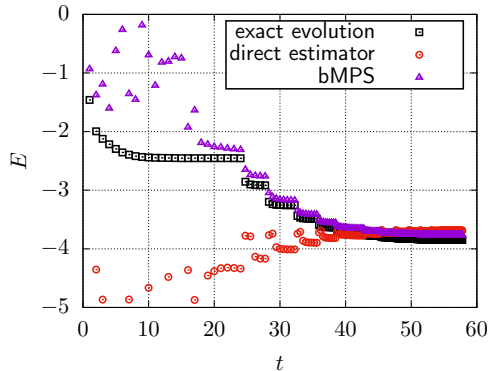
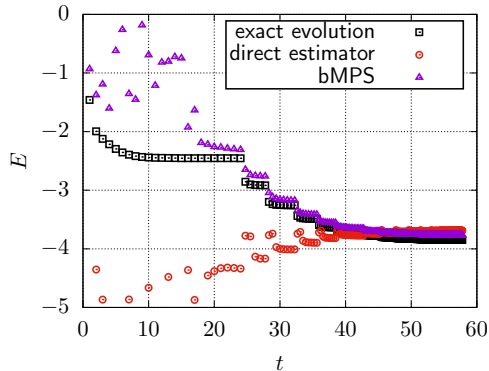


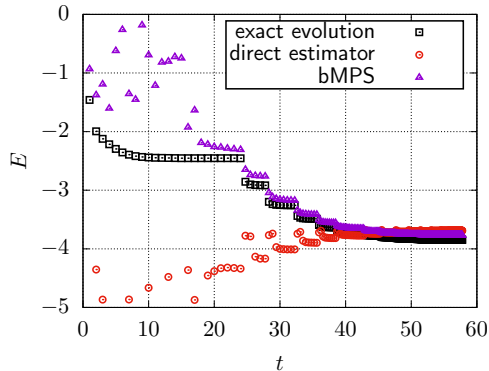
Ground state search

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

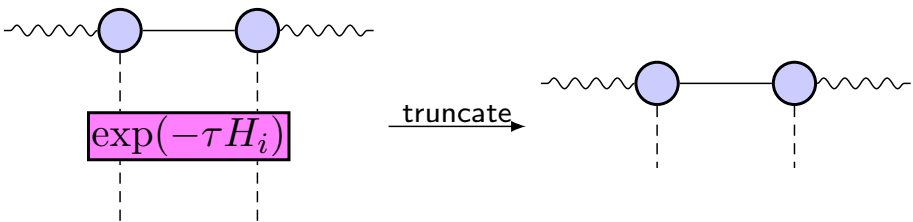


Ground state search

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

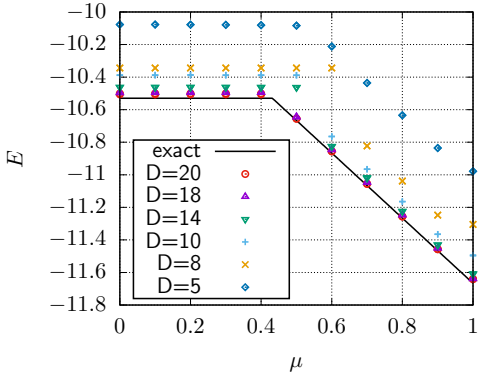


Simple Update

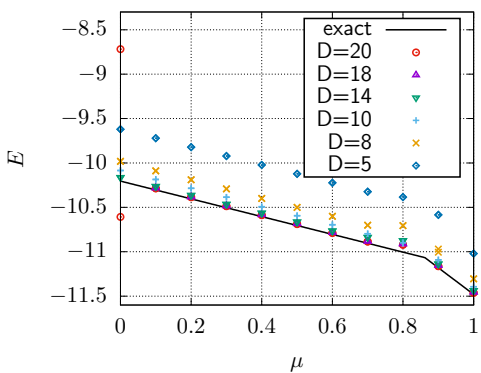


Simulations with chemical potential (3×4 hex. lattice, $U = 2$)

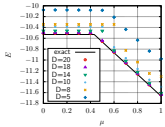
even parity

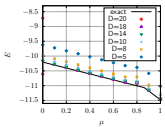


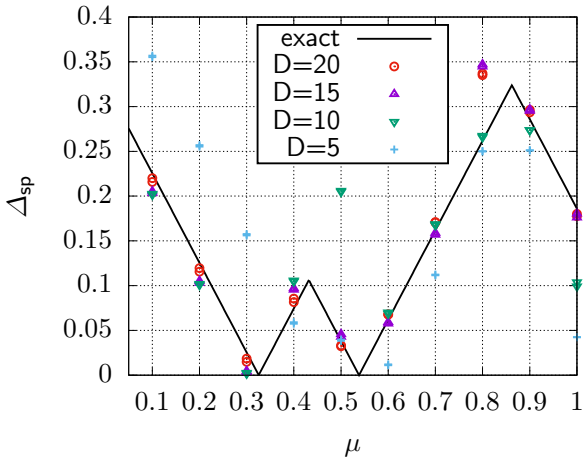
odd parity



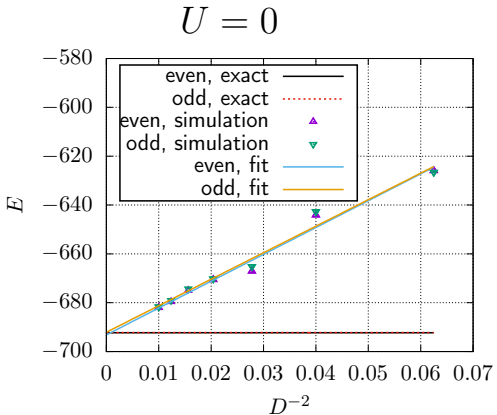
Simulations with chemical potential (3×4 hex. lattice, $U = 2$)

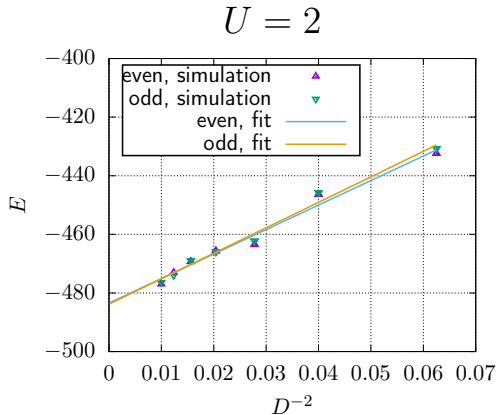




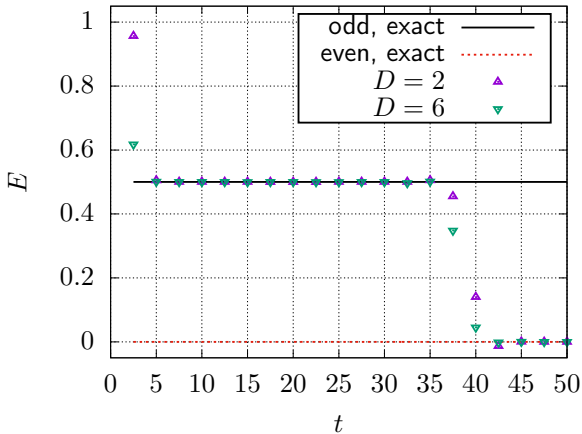


Simulations with chemical potential (30×15 hex. lattice, $\mu = 0.5$)



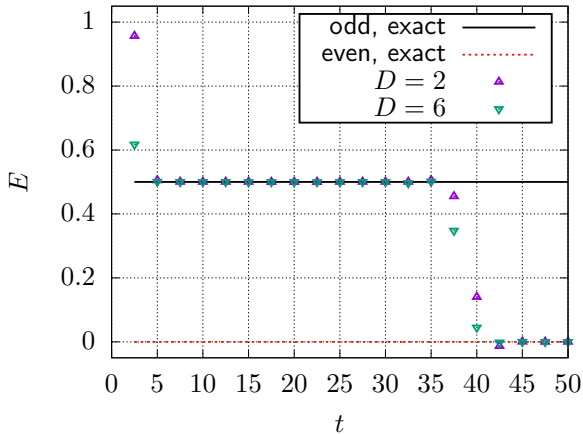


Stability issues with odd parity



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)
$\Rightarrow$ jump to even parity ground state

Overview

	Hybrid Monte Carlo	Fermionic PEPS

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lattice size	$L \lesssim 100$	$L \lesssim 30$

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sign problem	yes	no
performance	CPU-intensive	RAM-intensive

Full comparison of results

Method	U_c/κ	ν	β
Grand canonical BRS HMC [JO, Berkowitz *et al. PRB* **104** (2021)]	3.834(14)	1.185(43)	1.095(37)
Grand canonical BSS HMC [Buividovich *et al.* 2018]	3.90(5)	1.162	1.08(2)
Grand canonical BSS QMC [Buividovich *et al.* 2019]	3.94	0.93	0.75
Projection BSS QMC [Otsuka *et al.* 2016]	3.85(2)	1.02(1)	0.76(2)
Projection BSS QMC [Otsuka *et al.* 2020]		1.05(5)	
Projection BSS QMC [Parisen Toldin *et al.* 2015]	3.80(1)	0.84(4)	0.71(8)
Projection BSS QMC [Liu *et al.* 2019]		0.88(7)	
Projection BSS QMC [Assaad & Herbut 2013]	3.78	0.882	0.794
GN $4-\epsilon$, 1st order [Herbut *et al.* 2009]		0.882	0.794
GN $4-\epsilon$, 1st order [Rosenstein *et al.* 1993]		0.851	0.824
GN $4-\epsilon$, 2nd order [Rosenstein *et al.* 1993]		1.01	0.995
GN $4-\epsilon$, ν 2nd order [Rosenstein *et al.* 1993]		1.08	1.06
GN $4-\epsilon$, $1/\nu$ 2nd order [Rosenstein *et al.* 1993]		1.20	1.17
GN $4-\epsilon$, ν 4th order [Zerf *et al.* 2017]		1.2352	
GN $4-\epsilon$, $1/\nu$ 4th order [Zerf *et al.* 2017]		1.5511	
GN FRG [Janssen & Herbut 2014]		1.31	1.32
GN FRG [Knorr 2018]		1.26	
GN Large N [Gracey 2018]		1.1823	

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