Fermionic Tensor Networks and optimized discrete Time Evolution

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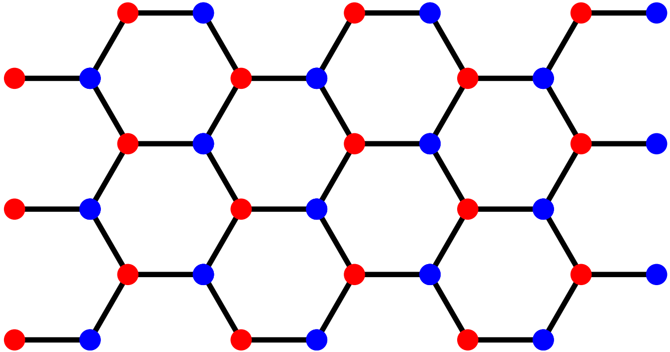
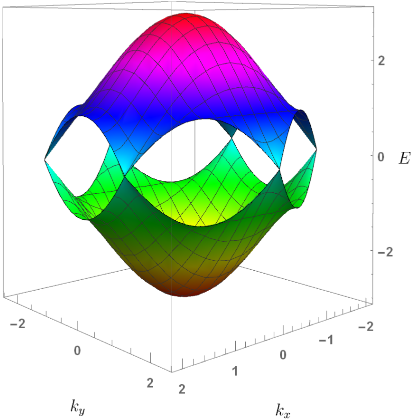
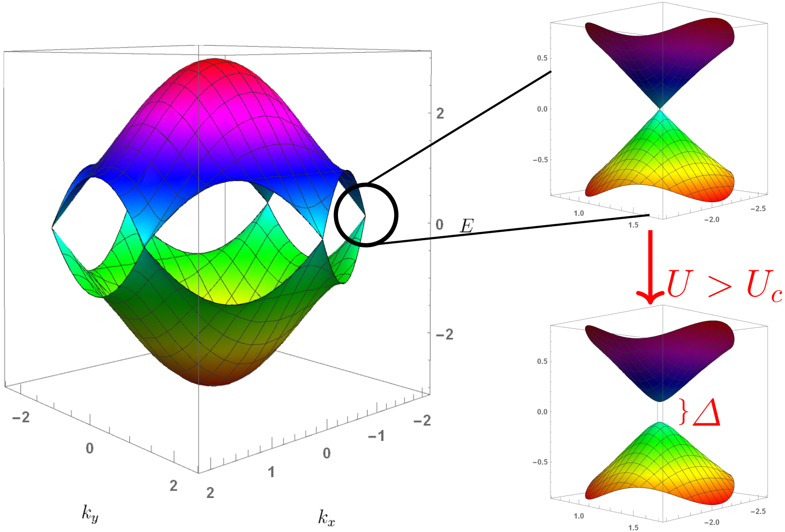
Hubbard model [Hubbard *ProcRSoc* **276** (1963); Wallace *PhysRev* **71** (1947)]

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

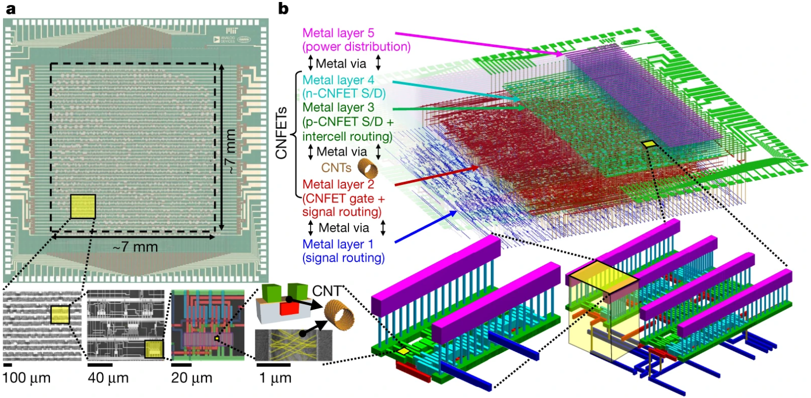




Metal-insulator phase transition



Carbon Nanotube Computer



"Hello, world!
I am RV16XNano."

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

Path integral formalism

[Brower et al. *PoS* **LATTICE2011** (2011); Buividovich et al. *PRB* **86** (2012); Krieg, JO et al. *CPC* **236** (2019); Luu et al. *PRB* **93** (2016); Smith et al. *PhysRev* **B89** (2014)]

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

$$\mathrm{e}^{-\frac{1}{2}\sum_{x,y} V_{x,y} q_x q_y} \propto \int \mathcal{D}\phi_t \, \mathrm{e}^{-\frac{1}{2}\sum_{x,y} V^{-1}_{x,y} \phi_{x,t}\phi_{y,t} + \mathrm{i}\sum_x \phi_{x,t} q_x}$$

- Fermion matrix

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

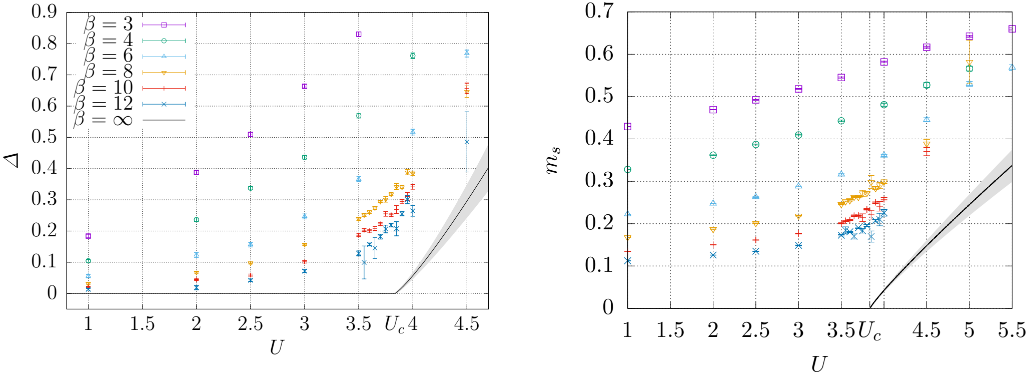
- **Hybrid Monte Carlo** simulation according to probability density

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

Quantum phase transition at half filling

[JO, Berkowitz et al. *PRB* **102** (2020), *PRB* **104** (2021)]

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



Beyond half filling?

Sign problem!

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

$$p[\phi] \propto \det\left(M[\phi,\mu]\, M[\phi,-\mu]^\dagger\right) \not\geq 0$$

- Reweighting: $\langle\mathcal{O}\rangle = \frac{\langle \mathcal{O} e^{i\theta}\rangle}{\langle e^{i\theta}\rangle}$
- Density of States, Complex Langevin, Line integrals,...
- Tensor Networks

  [Akiyama et al. *JHEP* **10** (2021); Butt et al. *PRD* **101** (2020); Dai et al. *cond-mat*/**2211**.00043; Emonts et al. *PRD* **107** (2023); Magnifico et al. *NatCom* **12** (2021); Meurice et al. *RevModPhys* **94** (2022)]
- Lefschetz Thimbles & Holomorphic Flow

  [Alexandru et al. *PRD* **93** (2016); Cristoforetti et al. *PRD* **88** (2013); Ulybyshev et al. *PRD* **101** (2020)]

  [Rodekamp, JO et al. *PRB* **106** (2022); Wynen, JO et al. *PRB* **103** (2021)]

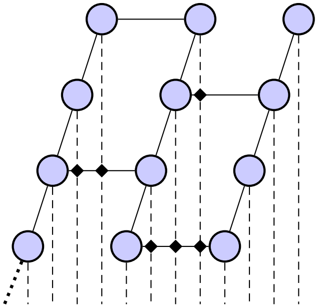
No sign problem

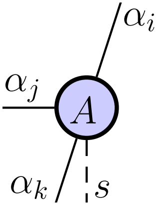
"Simulating both parity sectors of the Hubbard Model with Tensor Networks"
Manuel Schneider, JO, Karl Jansen, Thomas Luu, Carsten Urbach
[*PRB* **104** (2021)]

Projected Entangled Pair States (PEPS)

[Corboz *PRB* **93** (2016); Orús *AnnPhys* **349** (2014)]

$$|\psi\rangle = \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} A_{s_1,s_2,\ldots,s_N} |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle$$
$$\approx \sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} A^1_{s_1;\alpha_1} A^2_{s_2;\alpha_1,\alpha_2} \cdots A^N_{s_N;\alpha_{N-1}} |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_N\rangle$$

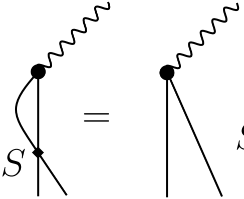




Truncate $\alpha_i \leq D \; \forall i$

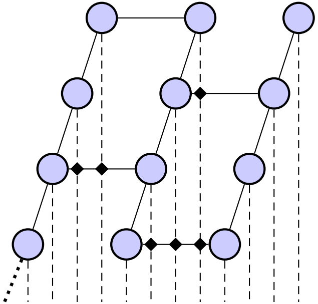
Fermionic PEPS [Corboz et al. *PRB* **81** (2010)]

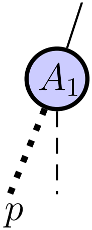
$$c_i c_k = -c_k c_i$$
$$(c_i c_j) c_k = c_k (c_i c_j)$$



$$S = \begin{array}{c} \begin{array}{cc} \overbrace{\hphantom{1 \;\; \dots \;\; 1}}^{\text{even}} & \overbrace{\hphantom{-1 \;\; \dots \;\; -1}}^{\text{odd}} \end{array} \\ \begin{pmatrix} 1 & \dots & 1 & 1 & \dots & 1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 1 & \dots & 1 \\ 1 & \dots & 1 & -1 & \dots & -1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & -1 & \dots & -1 \end{pmatrix} \end{array} \begin{array}{l} \\ \left.\begin{array}{c} \\ \\ \\ \end{array}\right\} \text{even} \\ \left.\begin{array}{c} \\ \\ \\ \end{array}\right\} \text{odd} \end{array}$$

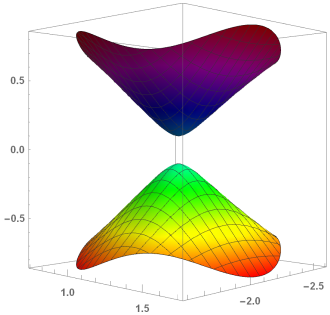
Parity link





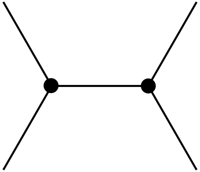
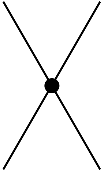
$p = \pm 1$

$\Rightarrow$ even- and odd-parity subspaces are disjoint



Contractions

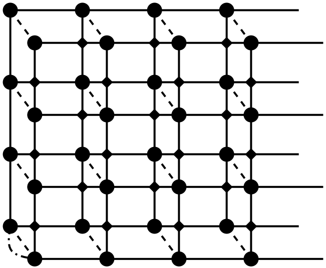
$d = 1$  $=$ 

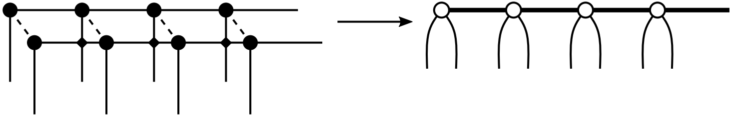
$d > 1$  $=$ 

Contractions using boundary Matrix Product States

[Verstraete et al. *cond-mat*/**0407066**]

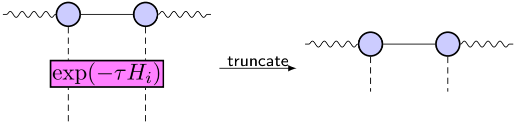
$$\langle \psi \mid \psi \rangle =$$

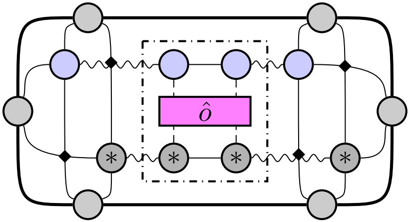




Ground state search

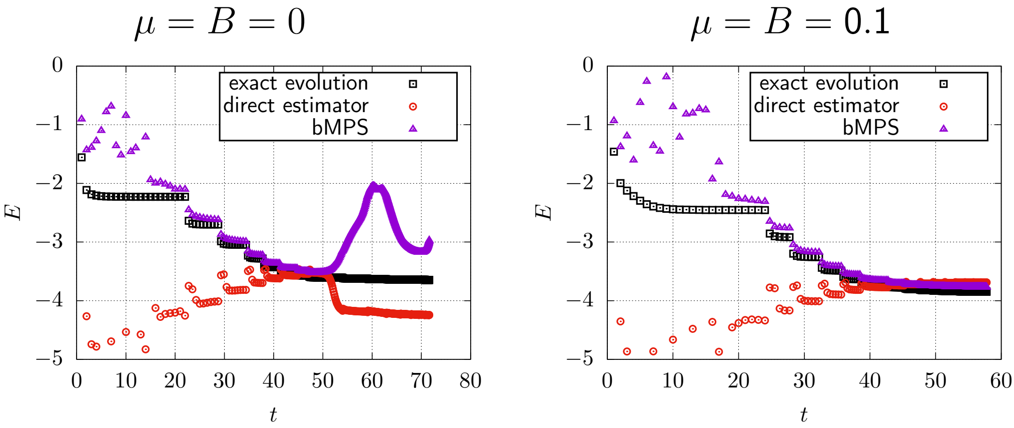
- Fix bond dimension D
- Initialise PEPS randomly
- Trotter-decomposed imaginary time evolution
- Local (simple) updates
- Contract network to calculate expectation values





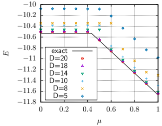
Degenerate ground state

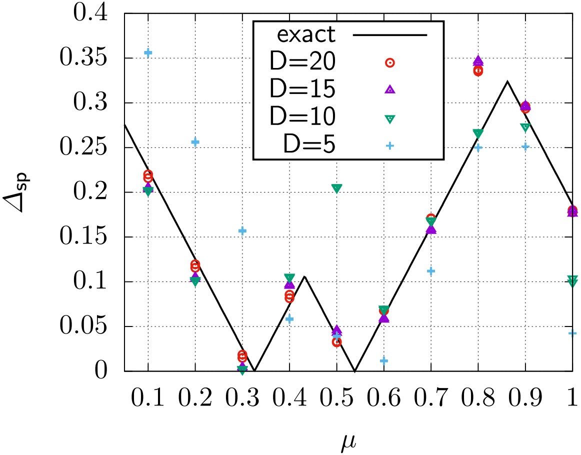
[Schneider, JO et al. *PRB* **104** (2021)]

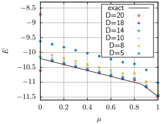


Simulations with chemical potential (3×4, $U = 2$)

[Schneider, JO et al. *PRB* **104** (2021)]

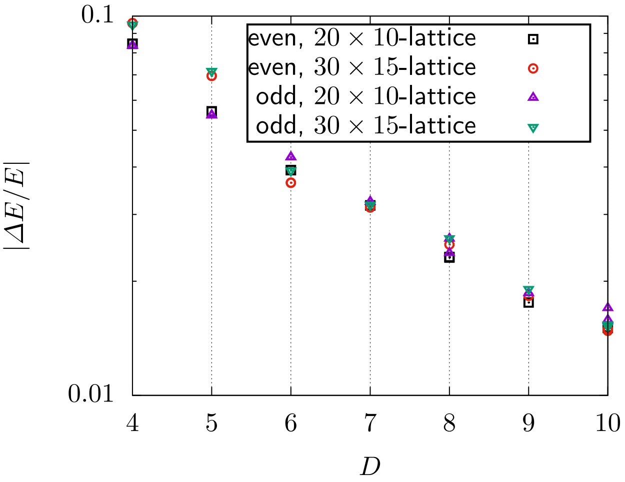






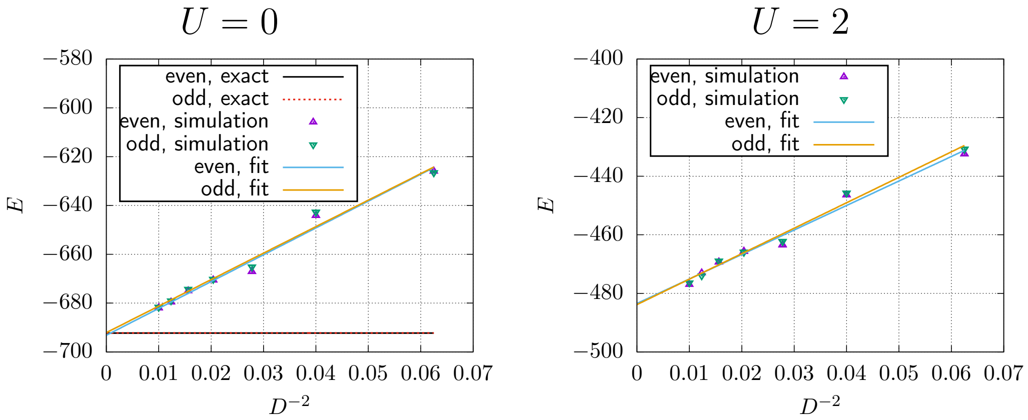
Convergence (non-interacting $U = 0$, $\mu = 0.5$)

[Schneider, JO et al. *PRB* **104** (2021)]



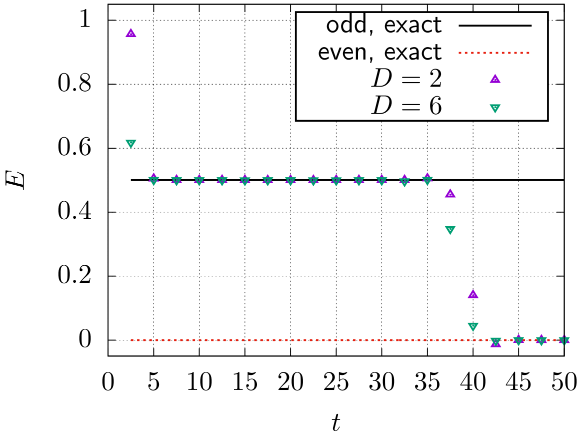
Simulations with chemical potential (30×15, $\mu = 0.5$)

[Schneider, JO et al. *PRB* **104** (2021)]



Stability issues with odd parity

[Schneider, JO et al. *PRB* **104** (2021)]



Large gap (strong coupling) $\Rightarrow$ jump to even parity ground state

3×4 hex. lattice, $U = 1$, no hopping

Discrete time evolution

[Suzuki *CommunMathPhys* **51** (1976); Trotter *ProcAMS* **4** (1959)]

$$H = \sum_{i}^{\Lambda} A_i \,, \quad [A_i, A_j] \neq 0$$

$$U(h) \equiv \mathrm{e}^{\mathrm{i}\,Hh}$$

$$U(h) = \mathrm{e}^{\mathrm{i}\,A_1 h}\,\mathrm{e}^{\mathrm{i}\,A_2 h} \cdots \mathrm{e}^{\mathrm{i}\,A_\Lambda h} + \mathcal{O}\left(h^2\right)$$

$$U(h) = \mathrm{e}^{\mathrm{i}\,A_1 h/2}\,\mathrm{e}^{\mathrm{i}\,A_2 h/2} \cdots \mathrm{e}^{\mathrm{i}\,A_\Lambda h/2}\,\mathrm{e}^{\mathrm{i}\,A_\Lambda h/2} \cdots \mathrm{e}^{\mathrm{i}\,A_2 h/2}\,\mathrm{e}^{\mathrm{i}\,A_1 h/2} + \mathcal{O}\left(h^3\right)$$

$$\vdots$$

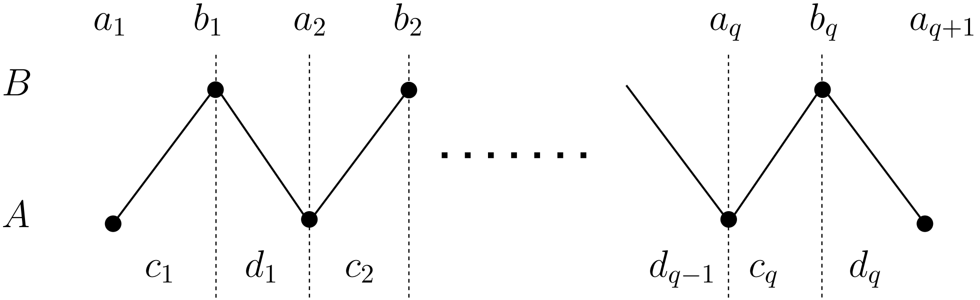
Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

$$\begin{aligned}
\mathcal{O}_1 &= (\nu-1)A + (\sigma-1)B \\
\mathcal{O}_3 &= \alpha[A,[A,B]] + \beta[B,[A,B]] \\
\mathcal{O}_5 &= \gamma_1[A,[A,[A,[A,B]]]] + \gamma_2[A,[A,[B,[A,B]]]] \\
&\quad + \gamma_3[B,[A,[A,[A,B]]]] + \gamma_4[B,[B,[B,[A,B]]]] \\
&\quad + \gamma_5[B,[B,[A,[A,B]]]] + \gamma_6[A,[B,[B,[A,B]]]] \\
\mathrm{Eff}_2 &= \frac{1}{q^2\sqrt{|\alpha|^2+|\beta|^2}} \\
\mathrm{Eff}_4 &= \frac{1}{q^4\sqrt{\sum_{j=1}^{6}|\gamma_j|^2}}
\end{aligned}$$

Decompositions into 2 stages

$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\,\mathrm{e}^{Aa_2h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$
$$= \mathrm{e}^{Ac_1h}\,\mathrm{e}^{Bc_1h}\,\mathrm{e}^{Bd_1h}\,\mathrm{e}^{Ad_1h}\cdots\mathrm{e}^{Bd_qh}\,\mathrm{e}^{Ad_qh}$$

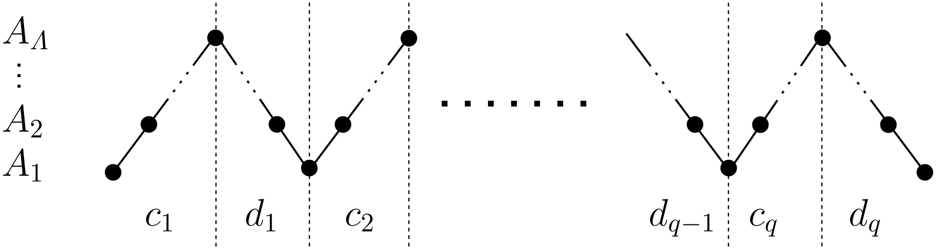


$$c_1 = a_1\,,\qquad d_1 = b_1 - c_1\,,$$
$$c_2 = a_2 - d_1\,,\qquad d_2 = b_2 - c_2\,,$$
$$\vdots\qquad\qquad\vdots$$

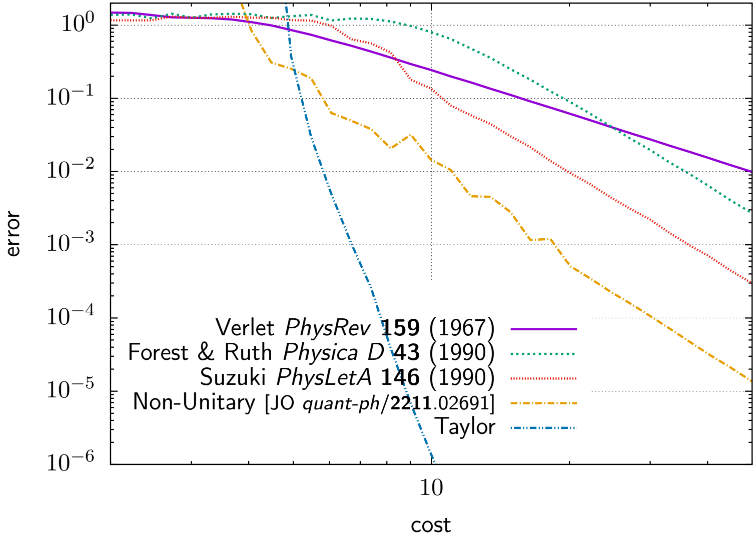
Decompositions into Λ stages [JO *quant-ph*/**2211**.02691]

$$\mathrm{e}^{h\sum\limits_{k=1}^{\Lambda} A_k + \mathcal{O}\left(h^{n+1}\right)}$$

$$= \left(\prod_{k=1}^{\Lambda} \mathrm{e}^{A_k c_1 h}\right)\left(\prod_{k=\Lambda}^{1} \mathrm{e}^{A_k d_1 h}\right)\cdots\left(\prod_{k=1}^{\Lambda} \mathrm{e}^{A_k c_q h}\right)\left(\prod_{k=\Lambda}^{1} \mathrm{e}^{A_k d_q h}\right)$$



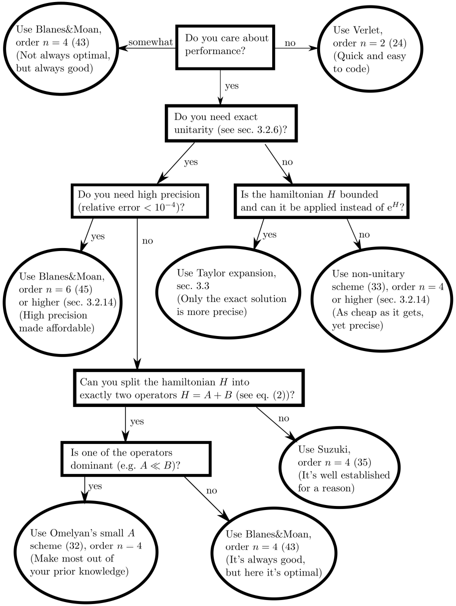
Benchmarking the Heisenberg model



$$\mathrm{e}^{Hh} = \lim_{k\to\infty} \sum_{i=0}^{k} \frac{(Hh)^i}{i!}$$

$$\left| \frac{(\lambda_{\mathsf{max}}(H)h)^k}{(k+1)!} \right| < \varepsilon$$

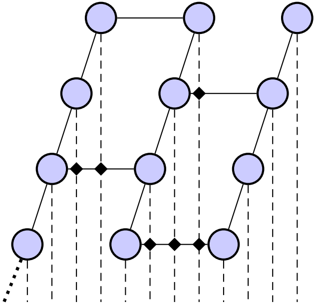
How to choose... [JO *quant-ph*/**2211**.02691]



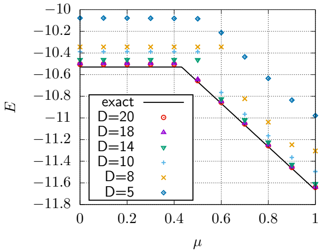
“Fermionic Tensor Networks and optimized discrete Time Evolution”

[JO *quant-ph*/**2211**.02691; Schneider, JO et al. *PRB* **104** (2021)]

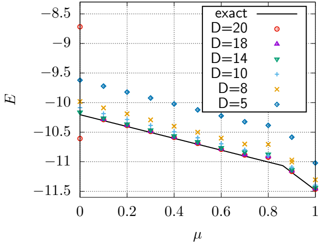
Projected Entangled Pair States (PEPS)

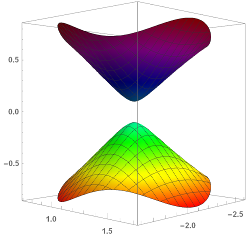


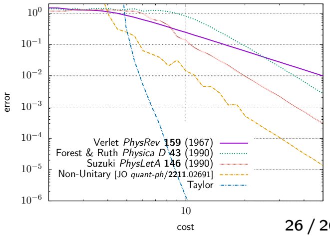
even parity



odd parity







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