Constant path integral contour shifts

Johann Ostmeyer

Helmholtz-Institut für Strahlen- und Kernphysik, University of Bonn, Germany

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SIGN25

Gefördert durch

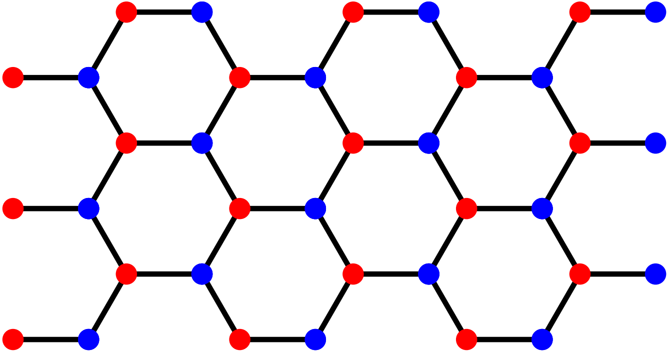
⟨NuMeriQS⟩

DFG Deutsche Forschungsgemeinschaft

Hubbard model

[Hubbard *ProcRSoc* **276** (1963); Novoselov + *Science* **306** (2004); Wallace *PhysRev* **71** (1947)]

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



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

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- Lefschetz thimbles & contour deformation

  [Alexandru + *PRD* **93** (2016); Cristoforetti + *PRD* **88** (2013); Rodekamp, JO + *PRB* **106** (2022);

  Ulybyshev + *PRD* **101** (2020); Wynen, JO + *PRB* **103** (2021)]

  [Gäntgen, JO + *PRB* 109 (2024); Rodekamp, JO + *EPJB* accepted (2024)]

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- Tensor Networks

  [Corboz *PRB* **93** (2016); Schneider, JO + *PRB* **104** (2021)]

  [Suladze, JO + (forthcoming)]

The Team

Evan Berkowitz

Stefan Krieg

Thomas Luu

Giovanni Pederiva

Manuel Schneider

Carsten Urbach

[Gäntgen, JO + *PRB* **109** (2024)]

Christoph Gäntgen

[Rodekamp, JO + *EPJB* **accepted** (2024)]

Marcel Rodekamp

[Suladze, JO + (forthcoming)]

Archil Suladze

Disclaimers

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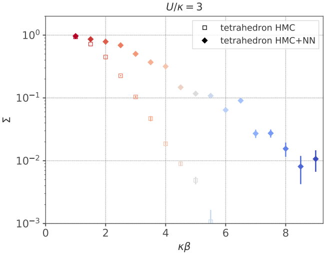
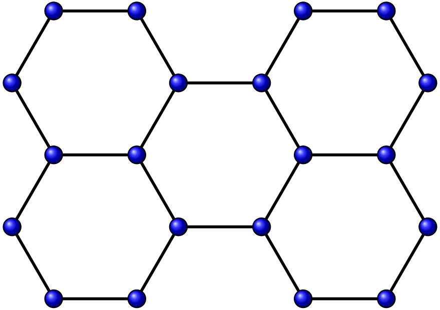
2. Sign problem still exponentially bad.



[Wynen, JO + *PRB* **103** (2021)]

Perylene

[Cao & Yang *RSC Adv* **12** (2022); Sato + *IEEE JSelTopQEl* **4** (1998); Shchuka + *ChemPhysLet* **164** (1989)]



Candidate for organic LEDs, solar cells,. . .

Lefschetz thimbles

[Alexandru + *PRD* **93** (2016); Lefschetz *AMS* **22** (1921); Tanizaki + *NewJPhys* **18** (2016); talk by M. Ulybyshev]

- Path integral formalism
  $\phi \sim \mathrm{e}^{-S[\phi]}$

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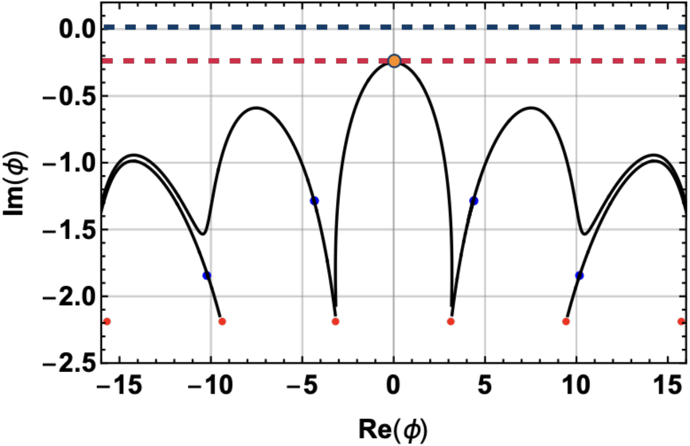

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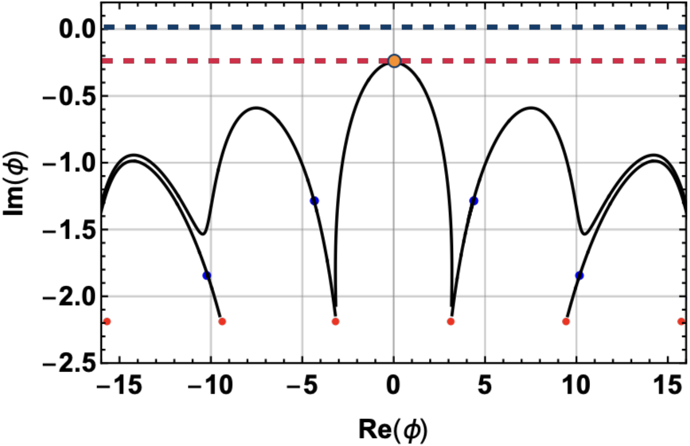
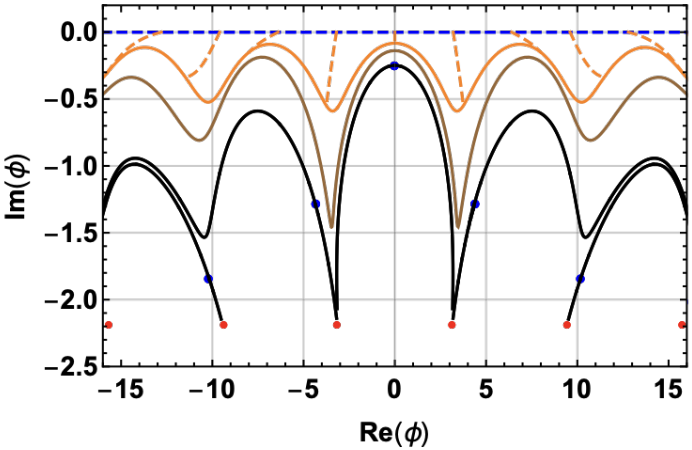
- Complex manifolds of constant $\mathrm{Im} S$
- Same path integral by Cauchy's theorem



Holomorphic flow [Cristoforetti + *PRD* **86** (2012)]



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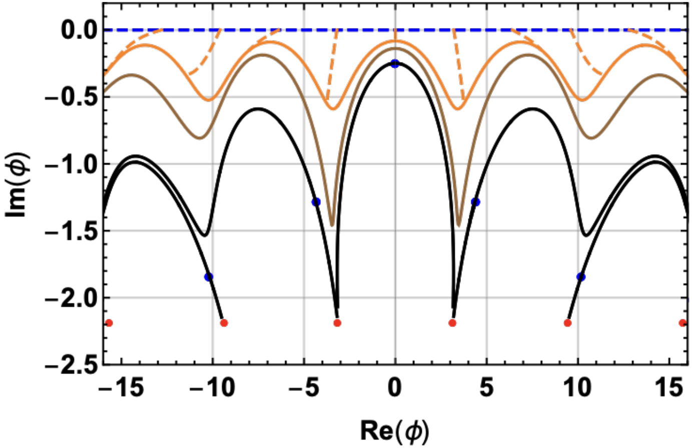

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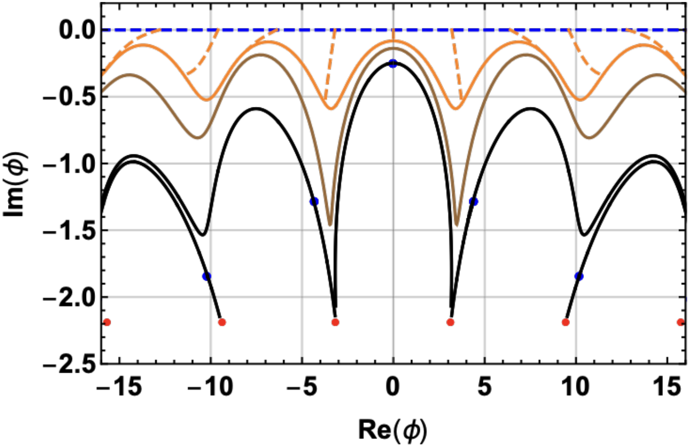

Extremely expensive!

Use Machine Learning

[Alexandru + *PRD* **96** (2017); Rodekamp, JO + *PRB* **106** (2022); Wynen, JO + *PRB* **103** (2021)]

- Flow some random field configurations

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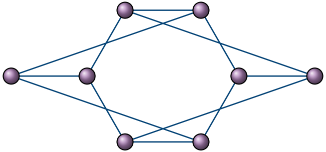
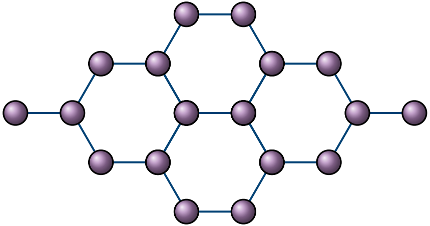
- Apply reweighting $\Rightarrow$ SHIFT doesn’t have to be perfect

Benchmark lattices [Rodekamp, JO + *PRB* **106** (2022)]

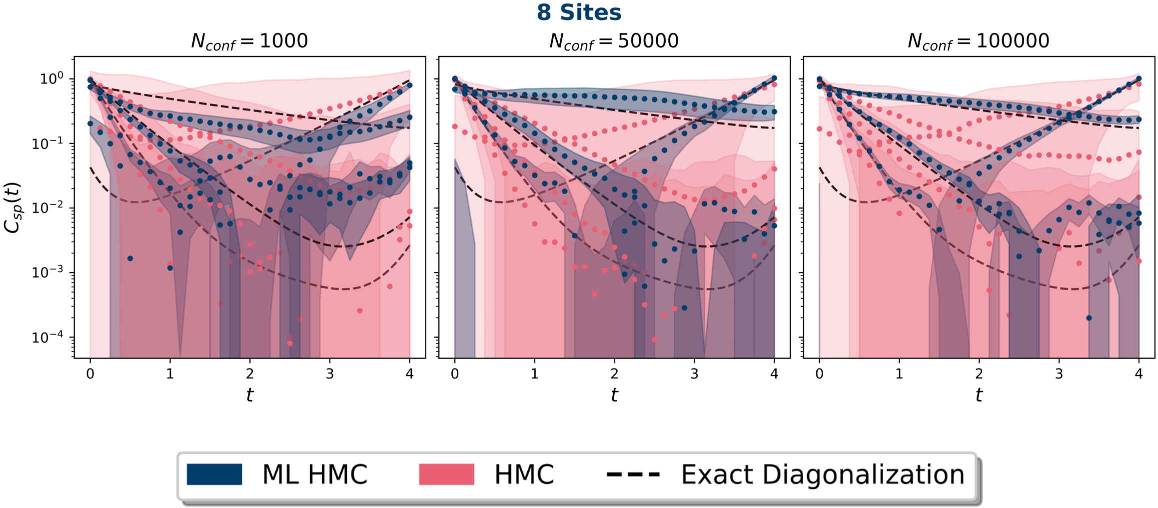


(a) 8 Sites



(b) 18 Sites (boundary suppressed)

Single Particle Correlators [Rodekamp, JO + *PRB* **106** (2022)]



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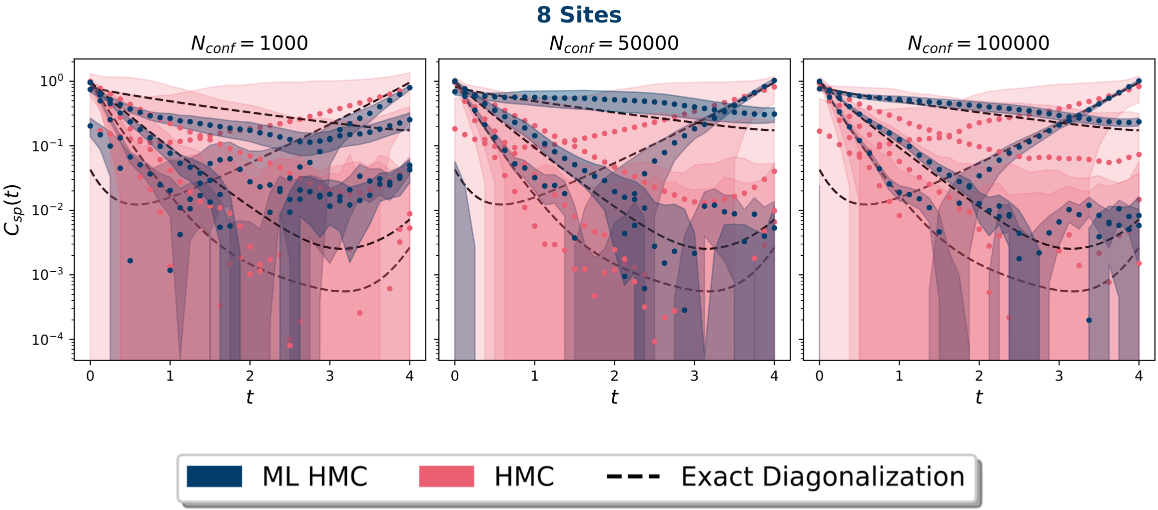

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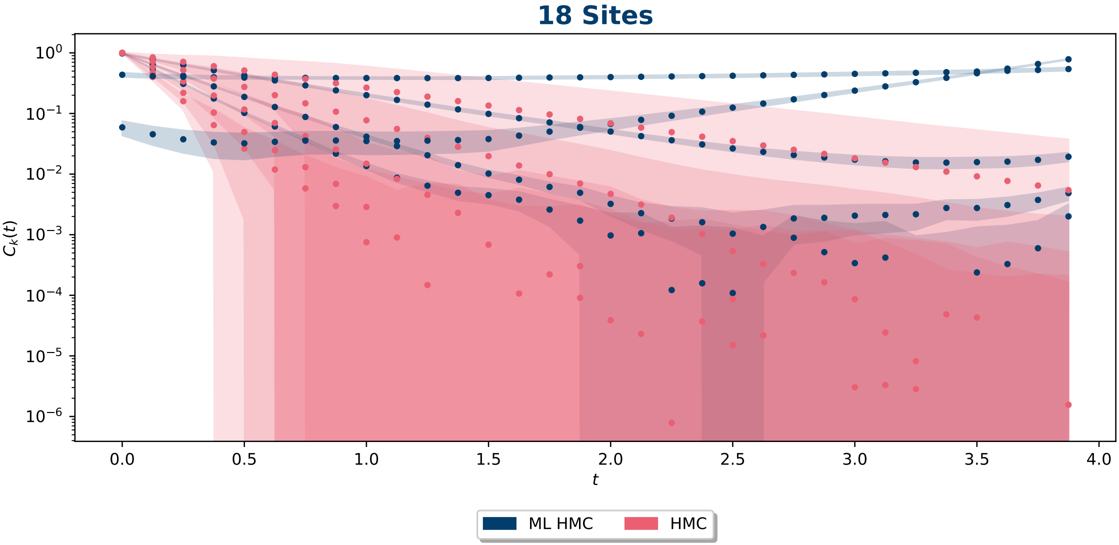
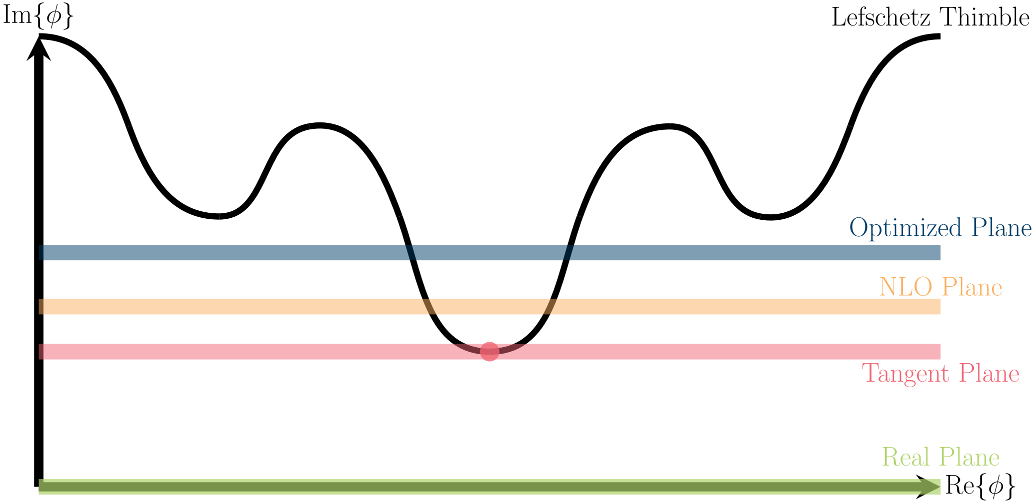
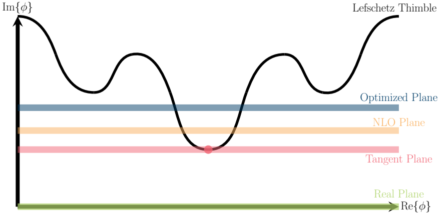


Sketch of manifolds [Gäntgen, JO + *PRB* **109** (2024)]



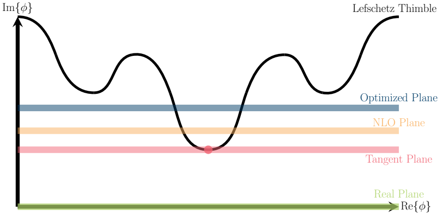
Analytic formulae [Gäntgen, JO + *PRB* **109** (2024)]



Analytic formulae [Gäntgen, JO + *PRB* **109** (2024)]

Tangent plane (saddle point of S):

$$\phi_0/\delta = -\frac{U}{N_x}\sum_k \tanh\left(\frac{\beta}{2}\left[\epsilon_k + \mu + \phi_0/\delta\right]\right)$$



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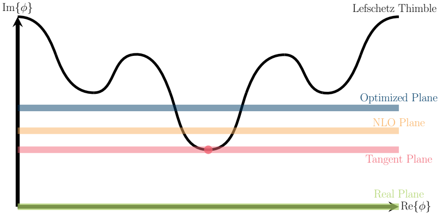

Next-to-leading order (NLO) plane
(saddle point of $S_{\text{eff}} = S + \frac{1}{2}\log\det\mathbb{H}$)

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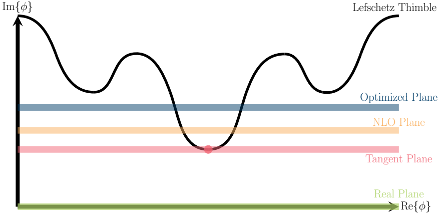

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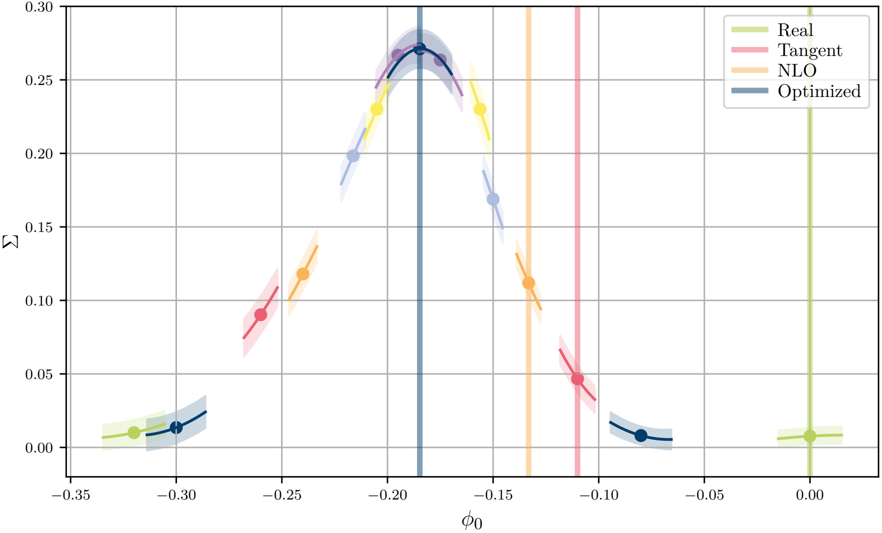
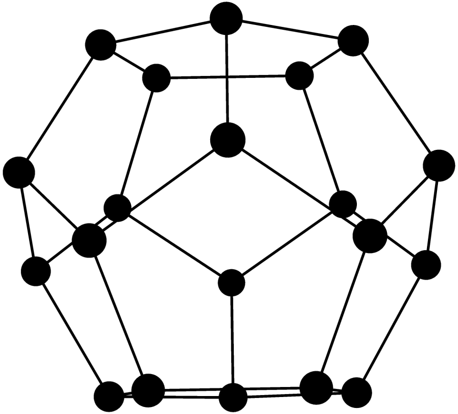
$$\mathbb{H}_{x't',xt} = \left(\frac{1}{\tilde{U}} - 1\right)\delta_{x',x}\delta_{t',t} - T_{+;xt,x't'}T_{+;x't',xt} - T_{-;xt,x't'}T_{-;x't',xt}\,,$$

$$T_{\pm;x't',xt} = \sum_{kn} \Lambda^\dagger_{x't',kn}\frac{e^{\pm(\delta\epsilon_k+\delta\mu+\phi_1+i\tilde{\omega}_n)}}{1-e^{\pm(\delta\epsilon_k+\delta\mu+\phi_1+i\tilde{\omega}_n)}}\Lambda_{kn,xt}$$

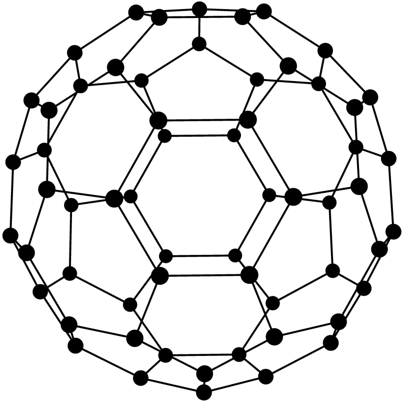
Numerical search [Gäntgen, JO + *PRB* **109** (2024)]



Bigger benchmark lattices [Gäntgen, JO + *PRB* **109** (2024)]

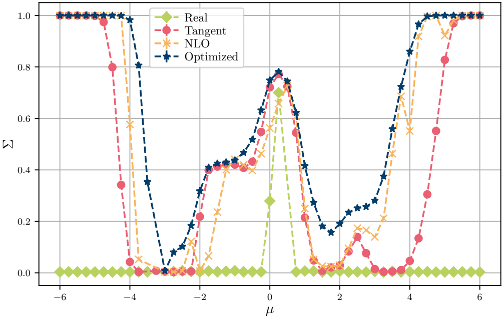


C_{20}



C_{60}

Statistical power [Gäntgen, JO + *PRB* **109** (2024)]



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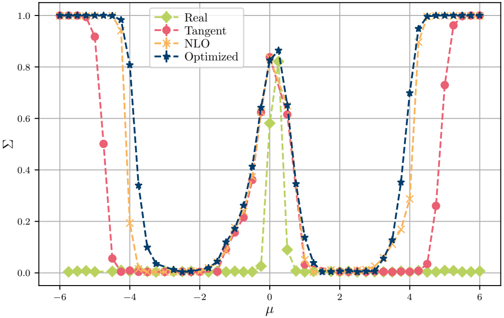

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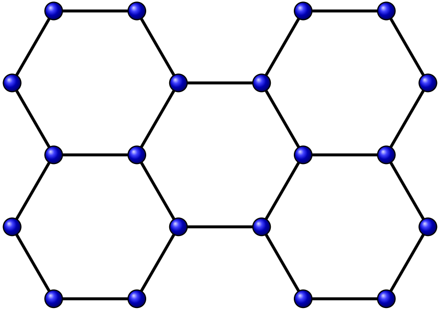
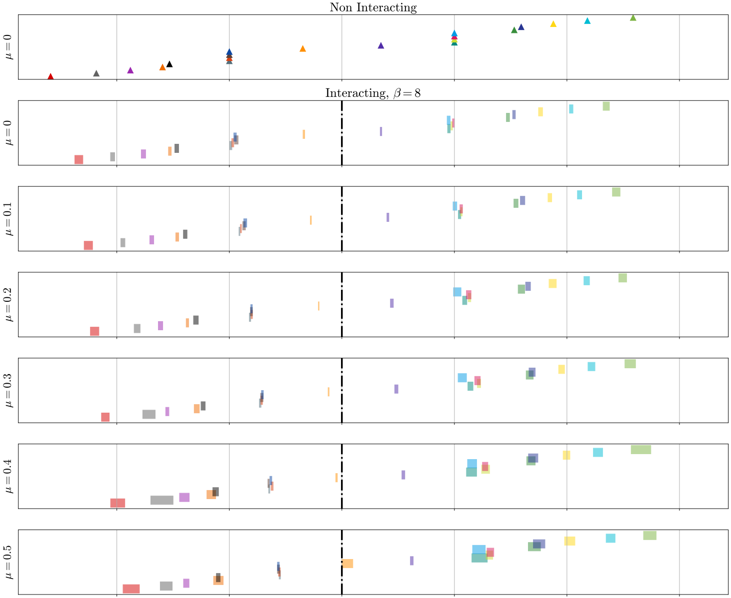
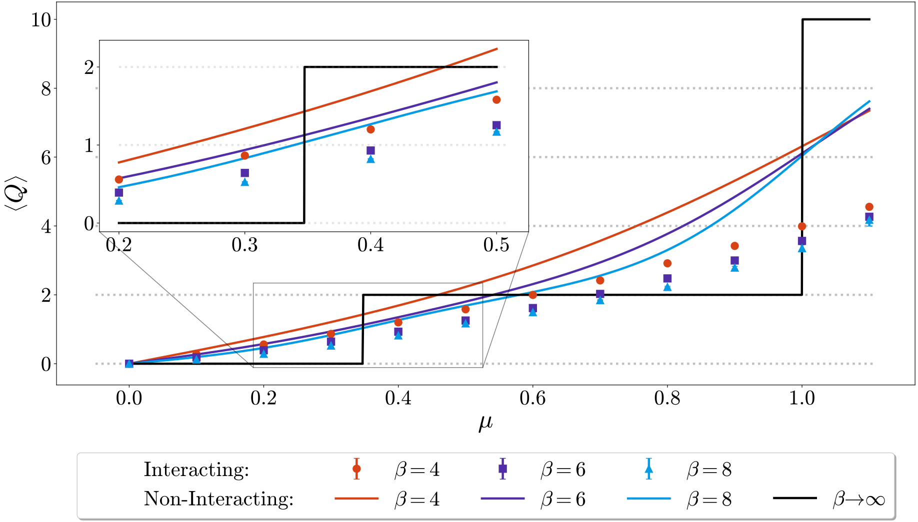


Candidate for organic LEDs, solar cells,. . .

Single particle spectrum [Rodekamp, JO + *EPJB* **accepted** (2024)]



Charge with doping [Rodekamp, JO + *EPJB* **accepted** (2024)]



SIGN25

Tensor Networks (TN) have no sign problem [Chen + *PRXQuantum* **6** (2025)]

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Contraction complexity depends on average sign.

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Projected Entangled Pair States (PEPS)

[Orús *AnnPhys* **349** (2014); Verstraete & Cirac *cond-mat*/**0407066**]

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

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

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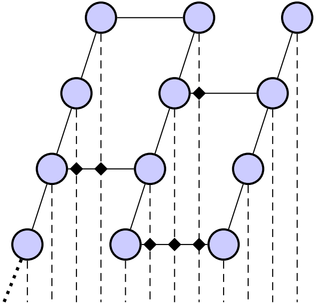
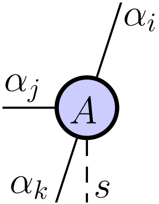


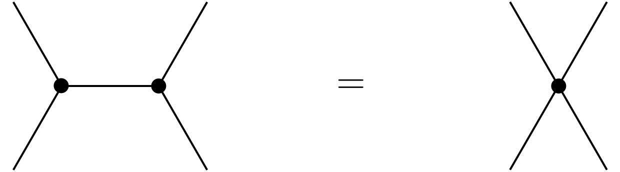


Truncate $\alpha_i \leq D\ \forall i$

Contractions [Schuch + *PRL* **98** (2007)]

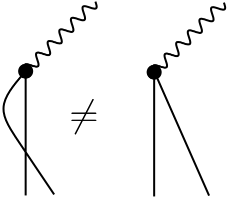
$d = 1$

$d > 1$



Fermionic PEPS [Corboz + *PRB* **81** (2010)]

$$c_i c_k = -c_k c_i$$



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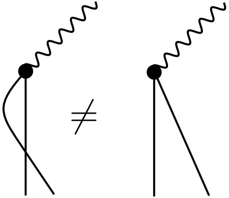

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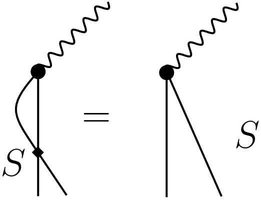
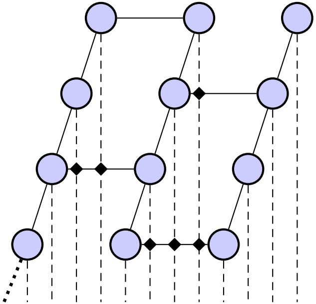
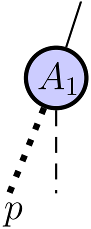


$$S = \begin{array}{cc}
\begin{array}{cc} \overbrace{\hphantom{1 \quad \dots \quad 1}}^{\text{even}} & \overbrace{\hphantom{-1 \quad \dots \quad -1}}^{\text{odd}} \end{array} & \\
\begin{pmatrix} 1 & \dots & 1 & 1 & \dots & 1 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 1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

Parity link





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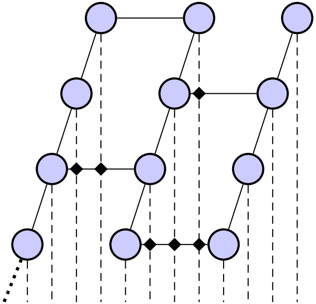
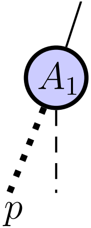
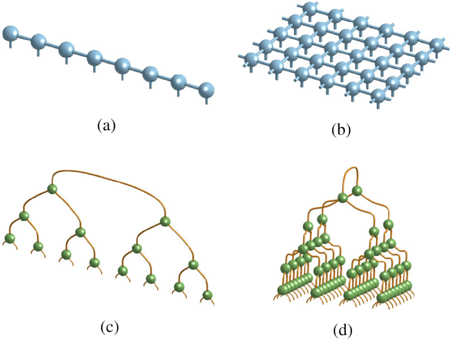




$p = \pm 1$

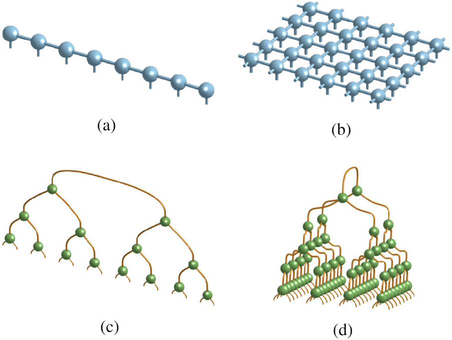
$\Rightarrow$ even- and odd-parity subspaces are disjoint

Augmented Tree Tensor Networks (aTTN) [Felser + *PRL* **126** (2021)]



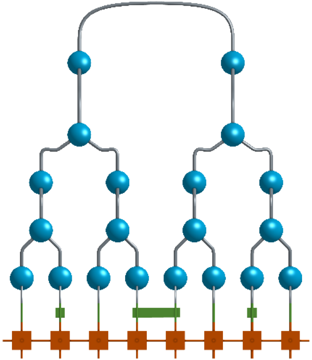
[Felser + *PRX* **10** (2020)]

Augmented Tree Tensor Networks (aTTN) [Felser + *PRL* **126** (2021)]



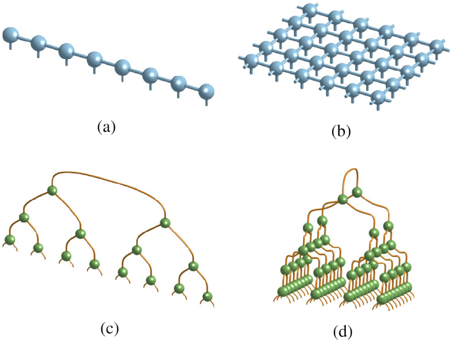
(a) (b) (c) (d)

[Felser + *PRX* **10** (2020)]



[Felser *PhD* **thesis** (2021)]

Augmented Tree Tensor Networks (aTTN) [Felser + *PRL* **126** (2021)]



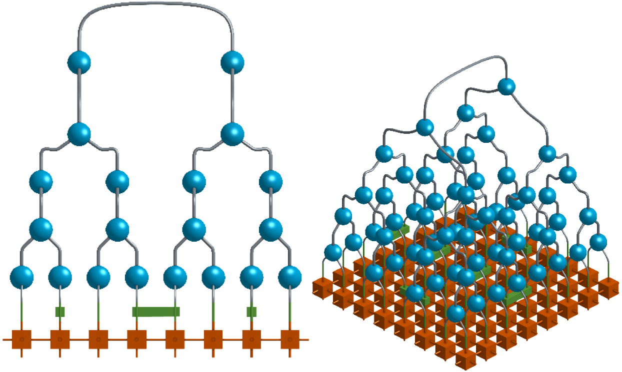
(a)

(b)

(c)

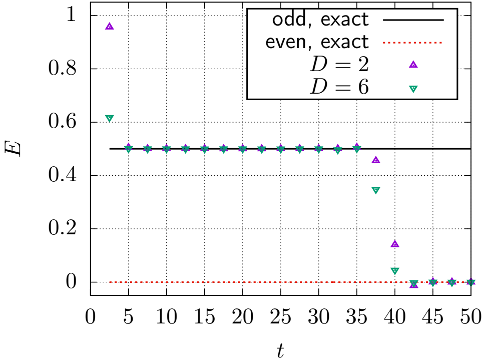
(d)

[Felser + *PRX* **10** (2020)]

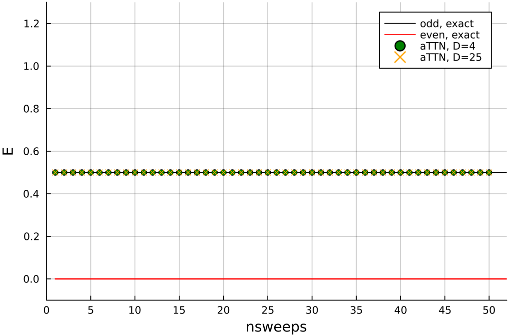


[Felser *PhD* **thesis** (2021)]

Stability in the odd parity sector

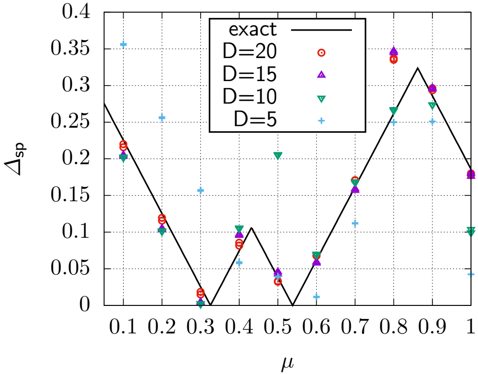


PEPS [Schneider, JO + *PRB* **104** (2021)]

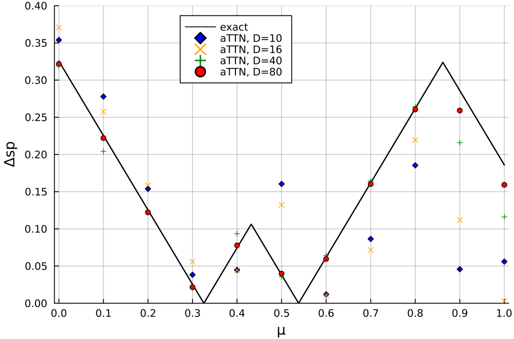


aTTN [Suladze, JO + (forthcoming)]

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

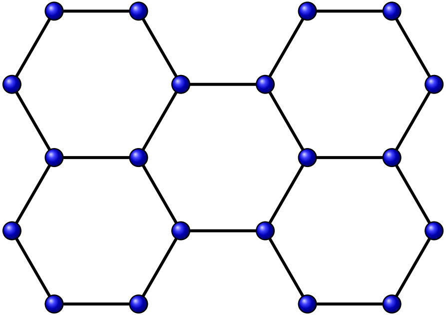


PEPS [Schneider, JO + *PRB* **104** (2021)]

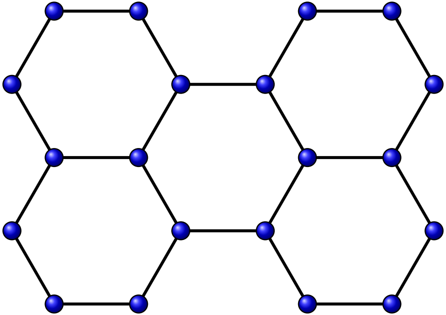


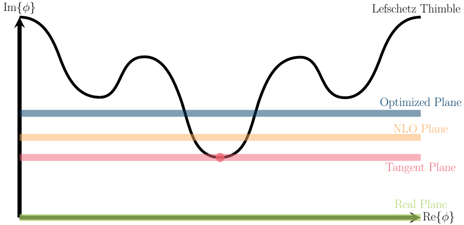
aTTN [Suladze, JO + (forthcoming)]

Constant path integral contour shifts

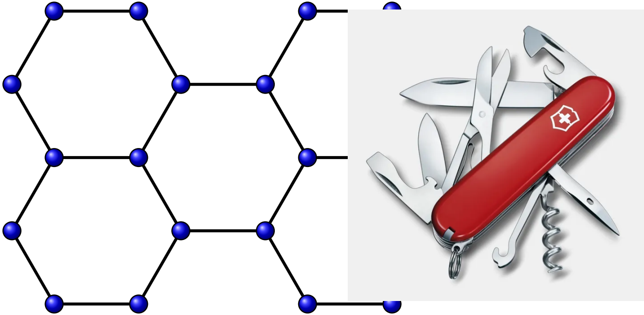


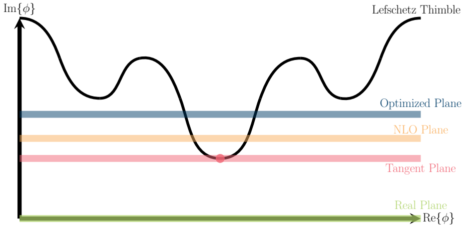
Constant path integral contour shifts



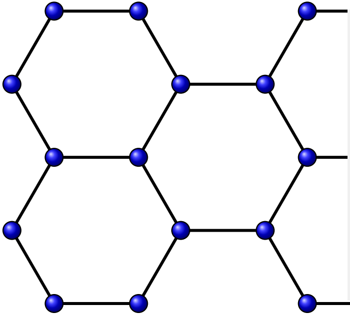


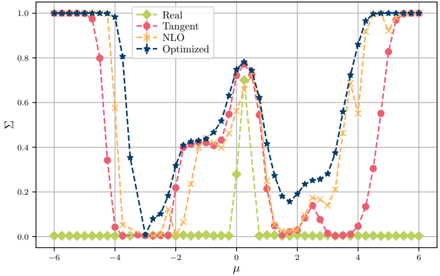
Constant path integral contour shifts

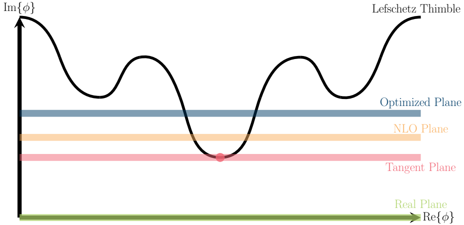




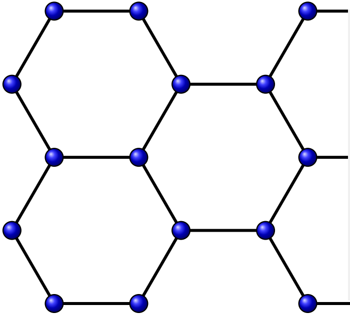
Constant path integral contour shifts

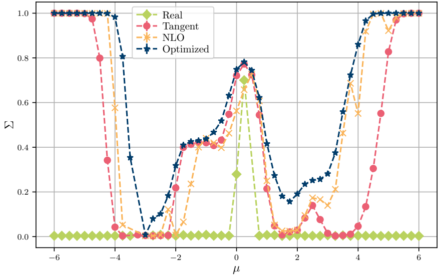


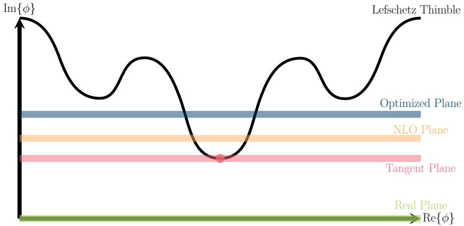


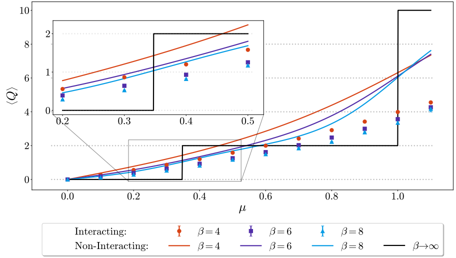


Constant path integral contour shifts

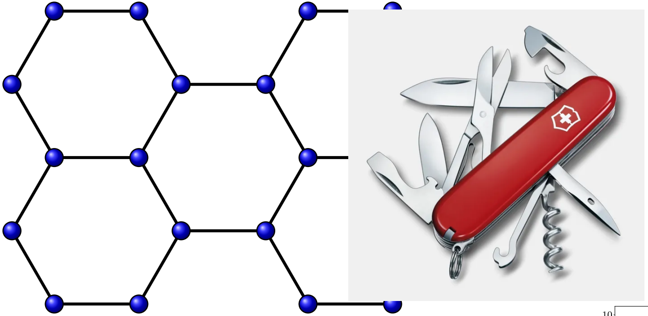


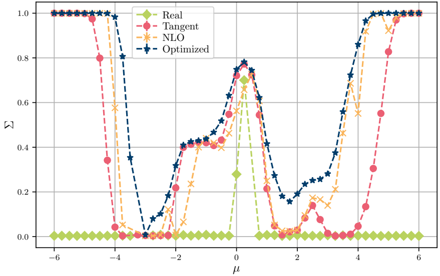


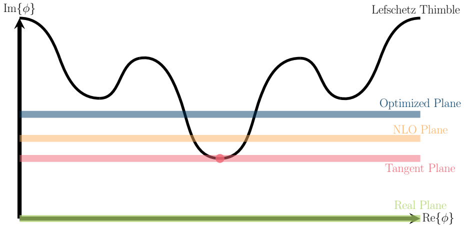


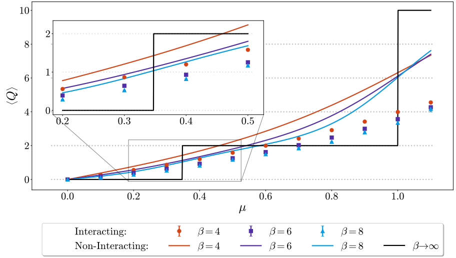


Constant path integral contour shifts









Stay tuned for updates on fermionic aTTNs!

Radial updates [JO *physics.comp-ph*/**2411**.18218]

```
parameters: dimension $d$, potential $V$ with $V(x) \approx c|x|^a$ for large $|x|$
input     : initial configuration $x^{\mathsf{i}} \in X$, standard deviation $\sigma$
            (default $\sigma = \sqrt{\frac{2}{ad}}$)
output    : final configuration $x^{\mathsf{f}} \in X$
sample $\gamma \sim \mathcal{N}(0,\sigma^2)$ ;                    // normal distribution
$x \leftarrow x^{\mathsf{i}} \cdot \mathrm{e}^{\gamma}$;
$\Delta V \leftarrow V(x) - V(x^{\mathsf{i}})$;
if $\mathrm{e}^{-\Delta V + d\gamma} \geq \mathcal{U}_{[0,1]}$ then              // uniform distribution
    $x^{\mathsf{f}} \leftarrow x$;
else
    $x^{\mathsf{f}} \leftarrow x^{\mathsf{i}}$;
end
```

Path integral formalism

[Krieg, JO + *CPC* **236** (2019); Luu & Lähde *PRB* **93** (2016); Smith & Smekal *PRB* **89** (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 of probability

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

Chemical potential

- $H_\mu = \mu \sum_x \left(c^\dagger_{x,\uparrow} c_{x,\uparrow} + c^\dagger_{x,\downarrow} c_{x,\downarrow} \right) = \mu \sum_x \left(p^\dagger_x p_x - h^\dagger_x h_x \right) + \text{const.}$
- μ introduces net charge in the ground state
- breaks particle-hole symmetry
- Probability weight

$$\det \left(M \left[\mu \right] M \left[-\mu \right]^\dagger \right) \ngeq 0$$

$\longrightarrow$ Sign Problem

Statistical Power

$$\langle \mathcal{O} \rangle = \frac{\left\langle e^{-i\mathrm{Im}S}\mathcal{O}\right\rangle_{\mathrm{Re}S}}{\left\langle e^{-i\mathrm{Im}S}\right\rangle_{\mathrm{Re}S}} = \frac{1}{\Sigma}\left\langle e^{-i\mathrm{Im}S}\mathcal{O}\right\rangle_{\mathrm{Re}S}$$

$$\Sigma := \left\langle e^{-i\mathrm{Im}S}\right\rangle_{\mathrm{Re}S} \equiv \frac{\int \mathcal{D}\Phi\ e^{-\mathrm{Re}S}e^{-i\mathrm{Im}S}}{\int \mathcal{D}\Phi\ e^{-\mathrm{Re}S}}$$

$$N^{\mathrm{eff}} = |\Sigma|^2 \cdot N$$

statistical error $\sim 1/\sqrt{N^{\mathrm{eff}}} \propto 1/|\Sigma|$

Transform path integral contour

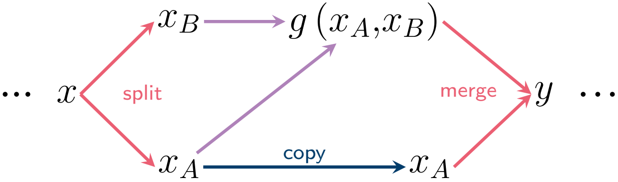
$$\begin{aligned} \mathcal{Z} &= \int_{\mathcal{M}} \mathcal{D}\Phi \; e^{-S[\Phi]} \\ &= \int_{\mathbb{R}^n} \mathcal{D}\phi \;\; \det J \left[\Phi\left(\phi\right)\right] e^{-S[\Phi(\phi)]} \;, \quad J_{ij} = \frac{\partial \Phi_i}{\partial \phi_j} \\ \Rightarrow S^{\text{eff}}\left[\phi\right] &= S\left[\Phi(\phi)\right] - \log\det J\left[\Phi(\phi)\right] \end{aligned}$$

Runtime of determinant as V^3!

Affine coupling layers [Albergo + *hep-lat*/**2101**.08176; Dinh + *cs.LG*/**1410**.8516]

$$f(x) = \begin{cases} y_A = x_A \\ y_B = g(x_A, x_B) \end{cases}$$

$$g(x_A, x_B) = x_B \odot s(x_A) + t(x_A)$$



$$\Rightarrow \det\left(\frac{\partial f}{\partial x}\right) = \det\begin{pmatrix} \mathbb{1} & 0 \\ \frac{\partial y_B}{\partial x_A} & s(x_A) \end{pmatrix} = \prod_j s(x_A)_j$$

$$\det \frac{\partial \mathcal{N}\mathcal{N}}{\partial x} = \det\left(\frac{\partial f^n(x)}{\partial x}\right) \det\left(\frac{\partial f^{n-1}(x)}{\partial x}\right) \cdots \det\left(\frac{\partial f^1(x)}{\partial x}\right)$$

$$\det J = \det\left(\mathbb{1} + i\frac{\partial \mathcal{N}\mathcal{N}}{\partial x}\right) \neq \prod_k \det\left(\mathbb{1} + i\frac{\partial f^k(x)}{\partial x}\right)$$

Complex-valued Neural Networks

[Bassey + *stat.ML*/**2101**.12249; Bouboulis *cs.LG*/**1005**.5170; Brandwood *IET* **130** (1983)]

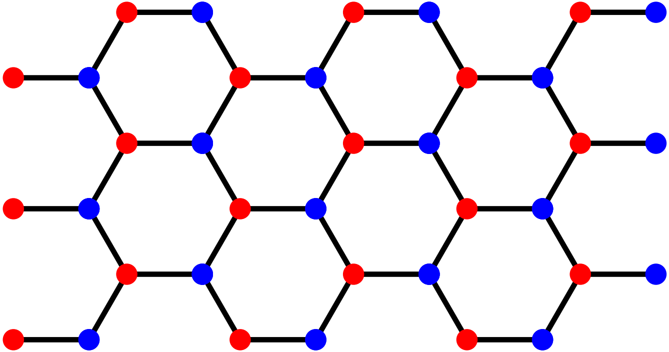
[Rodekamp, JO + *PRB* **106** (2022)]

	real	complex
Trafo	$\phi \mapsto \phi + i\mathcal{N}\mathcal{N}(\phi)$	$\phi \mapsto \mathcal{N}\mathcal{N}(\phi)$
Derivative	$\frac{\partial f(x)}{\partial x}$	$\frac{\partial f(z)}{\partial z} = \frac{1}{2}\left(\frac{\partial f(z)}{\partial \mathrm{Re} z} - i\frac{\partial f(z)}{\partial \mathrm{Im} z}\right)$ $\frac{\partial f(z)}{\partial z^*} = \frac{1}{2}\left(\frac{\partial f(z)}{\partial \mathrm{Re} z} + i\frac{\partial f(z)}{\partial \mathrm{Im} z}\right)$
Layers	dense	affine
$\det J$ runtime	$\mathcal{O}\left(V^3\right)$	$\mathcal{O}\left(V\right)$

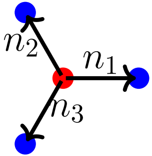
Tight binding model [Bloch 1929]

$$H^0 = -\sum_{\langle x,y \rangle} c_x^\dagger c_y$$

$\langle x,y \rangle$ denotes nearest neighbours

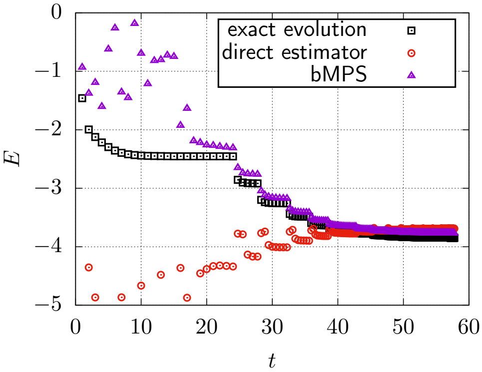


Sub-lattices **A** and **B**



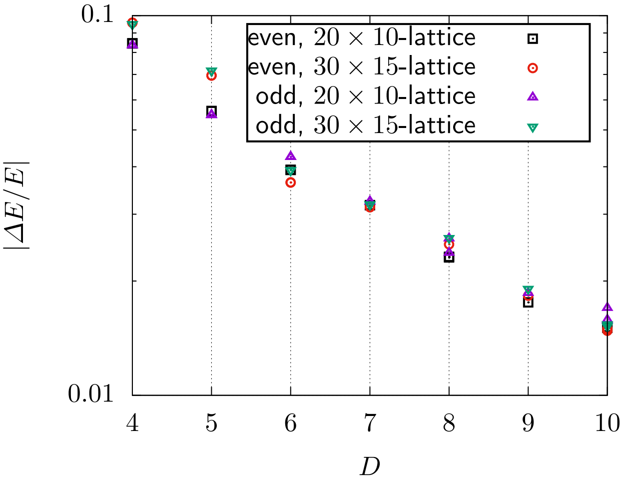
Ground state search [Schneider, JO + *PRB* **104** (2021)]

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



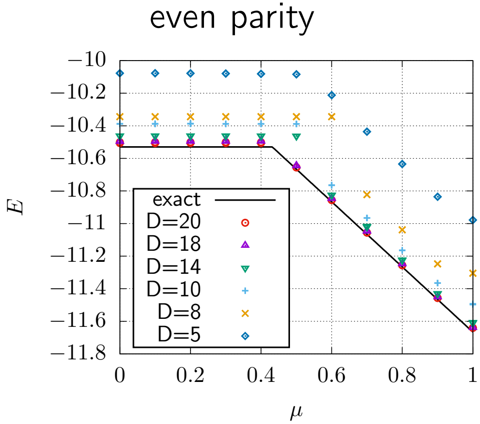
Convergence (non-interacting $U = 0$, $\mu = 0.5$)

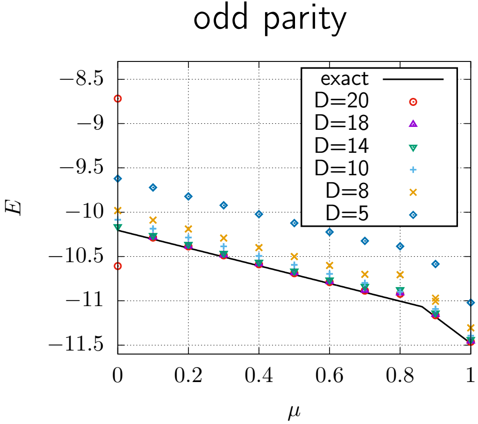
[Schneider, JO + *PRB* **104** (2021)]



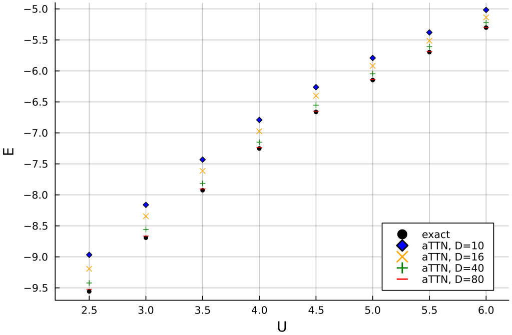
Simulations with chemical potential $(3 \times 4,\, U = 2)$

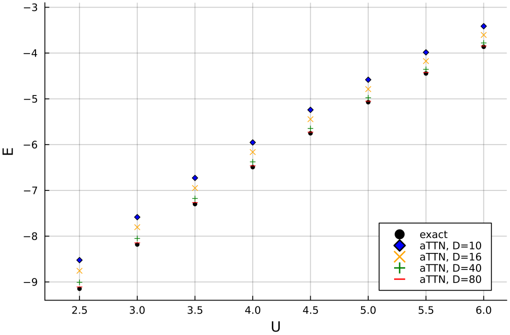
[Schneider, JO + *PRB* **104** (2021)]





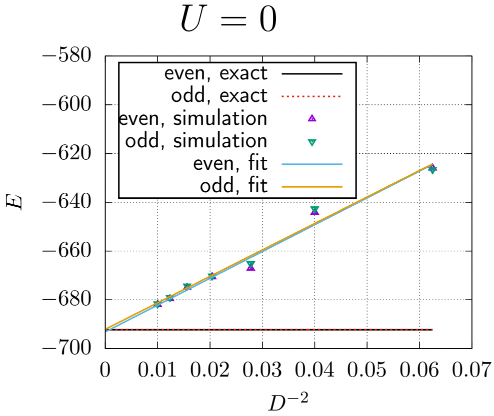
More preliminary fermionic aTTN results [Suladze, JO+ (forthcoming)]

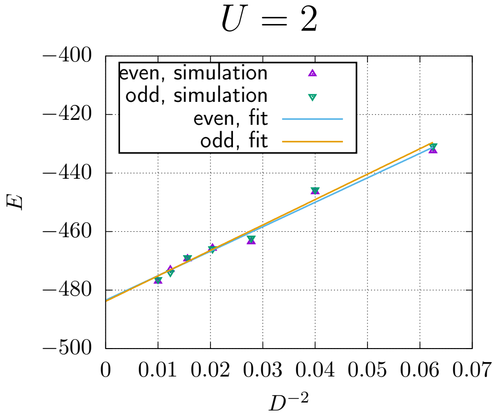




Simulations with chemical potential (30×15, $\mu = 0.5$)

[Schneider, JO + *PRB* **104** (2021)]





Overview

	Hybrid Monte Carlo	Fermionic PEPS
lattice size	$L \lesssim 100$	$L \lesssim 30$
boundary conditions	periodic	open
thermodynamic limit	easy	hard
continuum limit	controlled, expensive	easy
temperature	only finite	only zero
other extrapolations	no	uncontrolled in D
excited states	few lowest, expensive	some specific, unstable
sign problem	yes	no
performance	CPU-intensive	RAM-intensive

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