Reducing the Sign Problem of the Hubbard Model

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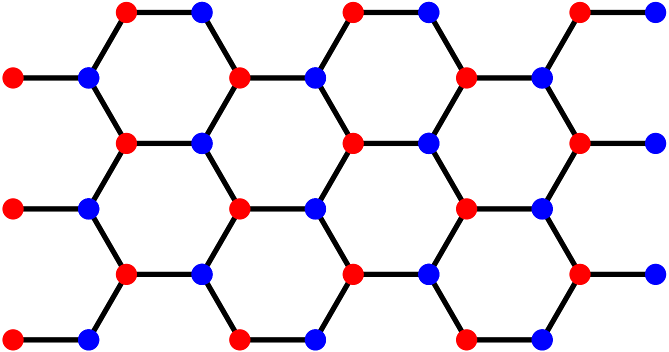
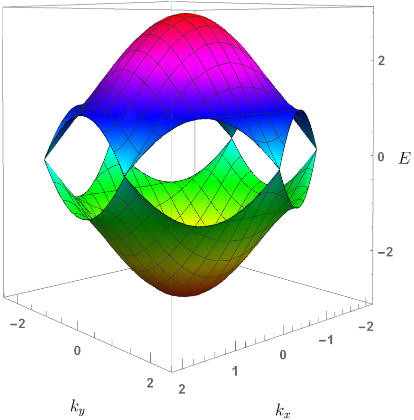
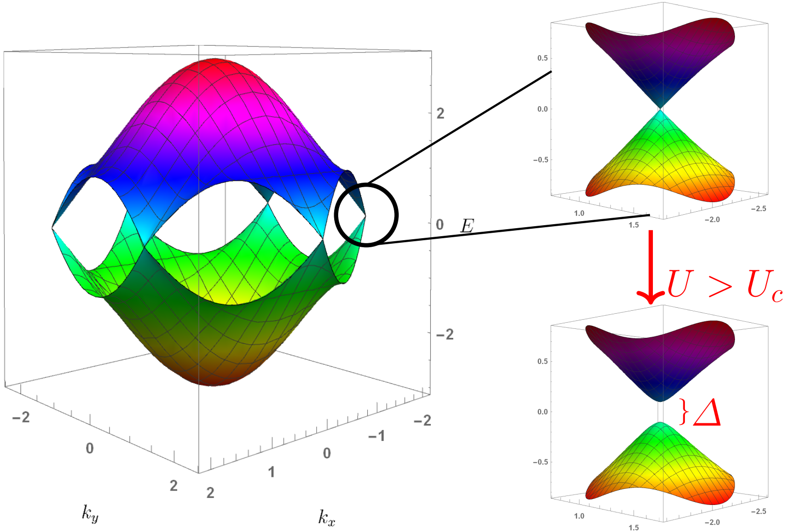
Hubbard model [Hubbard *ProcRSoc* **276** (1963); Wallace *PhysRev* **71** (1947)]

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





Expected phase transition



Path integral formalism

[Brower *et al.* *PoS* **LATTICE2011** (2011); Buividovich & Polikarpov *PRB* **86** (2012); Krieg, JO *et al.* *CPC* **236** (2019); Luu & Lähde *PRB* **93** (2016); Smith & von Smekal *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

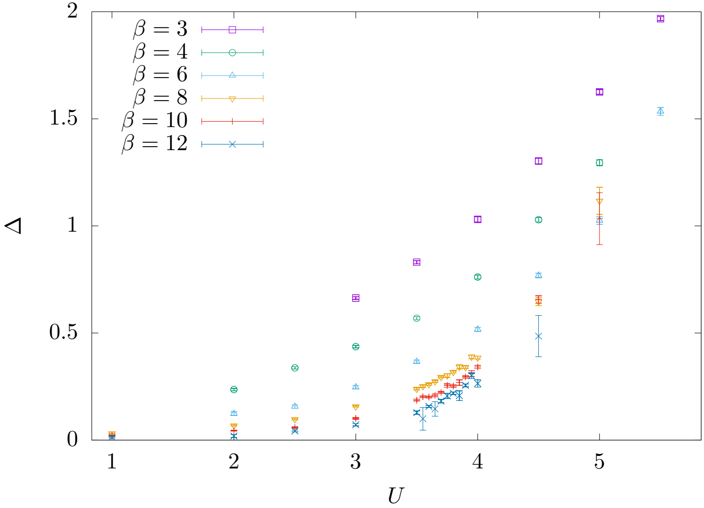
$$p[\phi] \equiv \mathrm{e}^{-S[\phi]} = \det\left(MM^\dagger\right)\mathrm{e}^{-\frac{\delta}{2U}\phi^2}$$

Data collapse [Herbut *et al.* *PRB* **79** (2009); JO, Berkowitz *et al.* *PRB* **102** (2020), *PRB* **104** (2021)]

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

$$\Delta \sim (U - U_c)^{\nu}$$

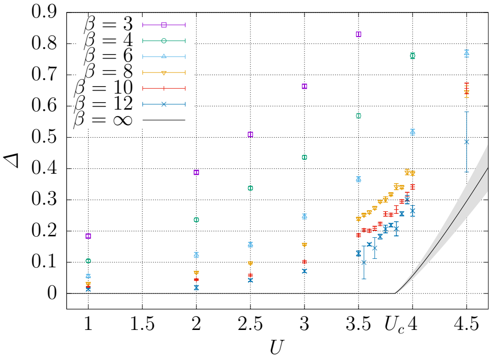
$$\Delta = \beta^{-1} F(\beta^{1/\nu}(U - U_c))$$

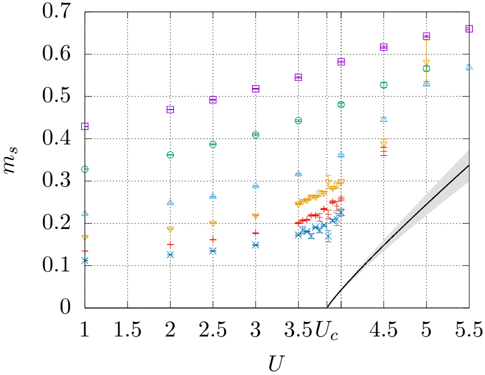


$$\Rightarrow U_c = 3.834(14)\ , \quad \nu = 1.185(43)\ , \quad \beta = 1.095(37)$$

Quantum phase transition at half filling

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





Beyond half filling?
Sign problem!

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

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

- Reweighting: $\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} e^{i\theta} \rangle}{\langle e^{i\theta} \rangle}$
- Machine Learning, Density of States, Complex Langevin, Line integrals,...
- Lefschetz Thimbles & Holomorphic Flow

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

  [Corboz *PRB* **93** (2016); Verstraete & Cirac *cond-mat*/**0407066**]

Milder sign problem

"Mitigating the Hubbard Sign Problem with Complex-Valued Neural Networks"

Marcel Rodekamp, Evan Berkowitz, Christoph Gäntgen, Stefan Krieg, Thomas Luu, JO

[*PRB* **106** (2022)]

"Minimizing the Sign Problem with a Shift of the Integration Contour"

Christoph Gängten, Evan Berkowitz, Thomas Luu, JO, Marcel Rodekamp, Neill Warrington

[forthcoming]

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)]

Statistical power

$$S_{\mathbb{C}} = S - i\theta$$

$$\langle \mathcal{O} \rangle_{\mathbb{C}} = \frac{\left\langle \mathcal{O} e^{i\theta} \right\rangle}{\left\langle e^{i\theta} \right\rangle} = \frac{1}{\Sigma} \left\langle e^{i\theta} \mathcal{O} \right\rangle$$

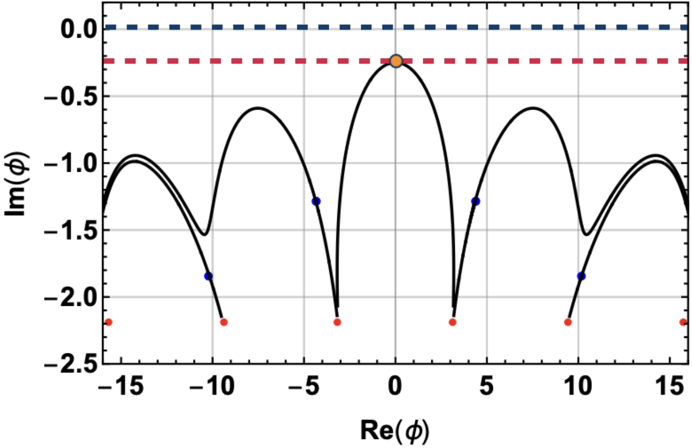
$$\Sigma := \left\langle e^{i\theta} \right\rangle \equiv \frac{\int \mathcal{D}\Phi \; e^{-S} e^{i\theta}}{\int \mathcal{D}\Phi \; e^{-S}}$$

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

$$\text{statistical error} \sim 1/\sqrt{N^{\text{eff}}}$$

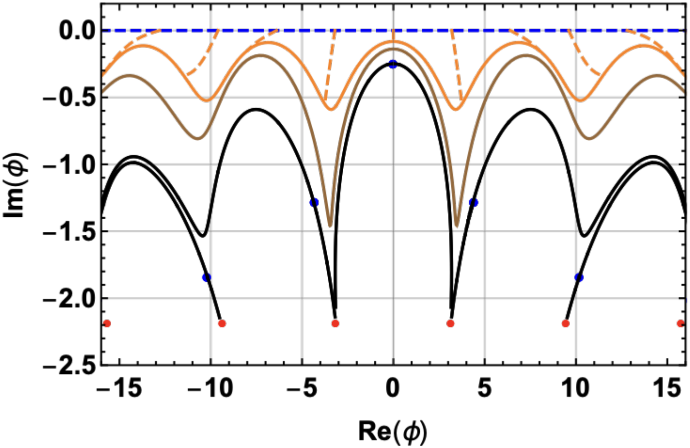
Lefschetz thimbles [Alexandru *et al.* *PRD* **93** (2016); Lefschetz *AMS* **22** (1921); Tanizaki *et al.* *NewJPhys* **18** (2016)]

- Manifolds of constant θ
- In the complex hyper-plane
- Same path integral by Cauchy's theorem



Holomorphic flow [Cristoforetti *et al.* *PRD* **86** (2012)]

$$\frac{d\Phi(\tau)}{d\tau} = \left(\frac{\partial S\left[\Phi(\tau)\right]}{\partial \Phi(\tau)}\right)^{*}$$



Extremely expensive!

Use machine learning [Alexandru *et al.* *PRD* **96** (2017); Wynen, JO *et al.* *PRB* **103** (2021)]

- Flow some random field configurations
- ‘Learn’ structure of Lefschetz Thimbles from flowed data
- neural network: $\phi \mapsto \mathcal{N}\mathcal{N}(\phi)$
- Apply reweighting $\Rightarrow \mathcal{N}\mathcal{N}$ doesn't have to be perfect

Affine neural network [Albergo *et al.* *hep-lat*/**2101**.08176; Dinh *et al.* *cs.LG*/**1410**.8516]

$$f(\phi) = \begin{cases} \phi'_A = \phi_A \\ \phi'_B = g(\phi_A, \phi_B) \end{cases}$$

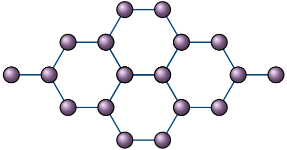
$$g(\phi_A, \phi_B) = \phi_B \odot s(\phi_A) + t(\phi_A)$$

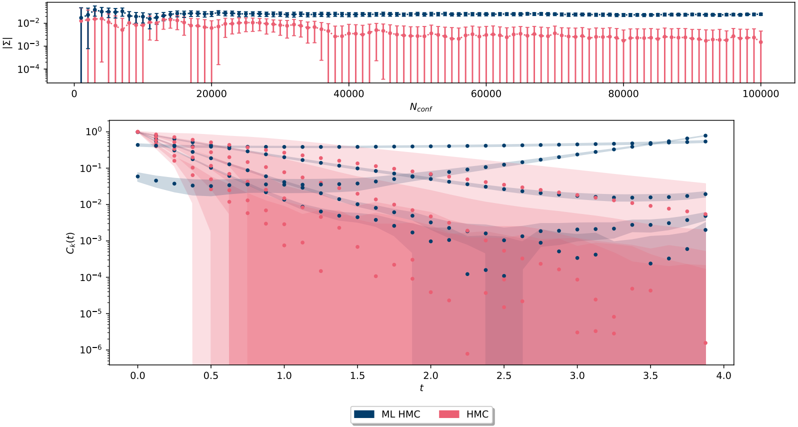
$$\begin{tikzcd}
 & & \phi_B \arrow[r] & g\left(\phi_A,\phi_B\right) \arrow[dr] & & \\
\cdots & \phi \arrow[ur] \arrow[dr] \arrow[r, phantom, "\text{split}"] & & \arrow[r, phantom, "\text{merge}"] & \phi' & \cdots \\
 & & \phi_A \arrow[r, "\text{copy}"] \arrow[uur] & \phi_A \arrow[ur] & &
\end{tikzcd}$$

$$\Rightarrow \det\left(\frac{\partial f}{\partial \phi}\right) = \det\begin{pmatrix} \mathbb{1} & 0 \\ \frac{\partial \phi'_B}{\partial \phi_A} & s(\phi_A) \end{pmatrix} = \prod_j s(\phi_A)_j$$

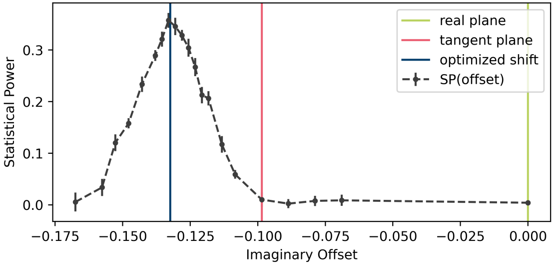
$$\det \frac{\partial \mathcal{N}\mathcal{N}}{\partial \phi} = \det\left(\frac{\partial f^n(\phi)}{\partial \phi}\right) \det\left(\frac{\partial f^{n-1}(\phi)}{\partial \phi}\right) \cdots \det\left(\frac{\partial f^1(\phi)}{\partial \phi}\right)$$

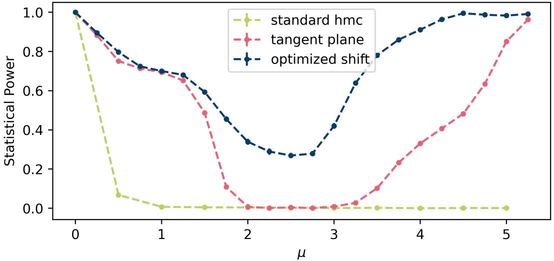
Benchmarking 18 sites, $U = \mu = 3$ [Rodekamp, JO *et al. PRB* **106** (2022)]

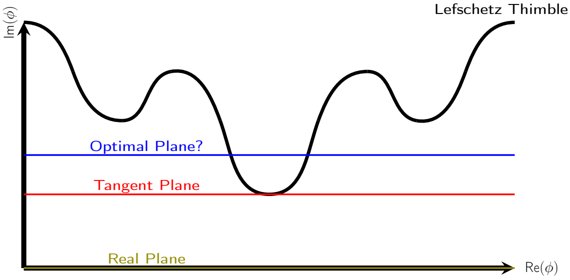




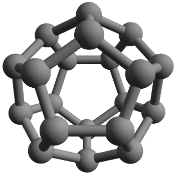
Optimal plane [Gängten, JO *et al.* (forthcoming)]

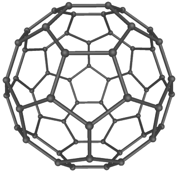


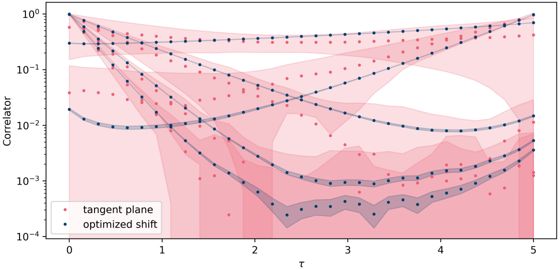


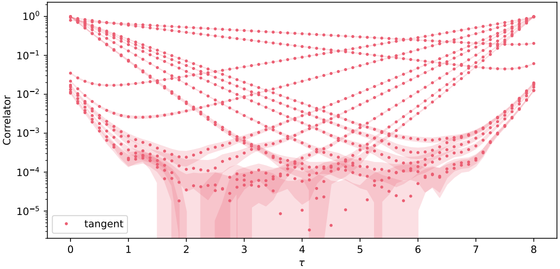


First Fullerene calculations: C_{20} and C_{60} [Gängten, JO *et al.* (forthcoming)]







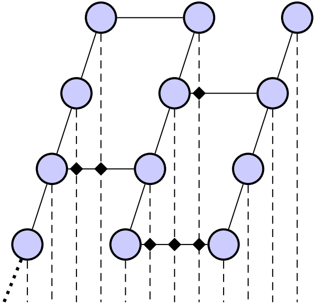


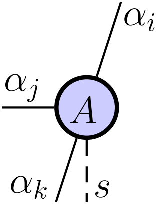
Projected Entangled Pair States (PEPS)

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

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

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



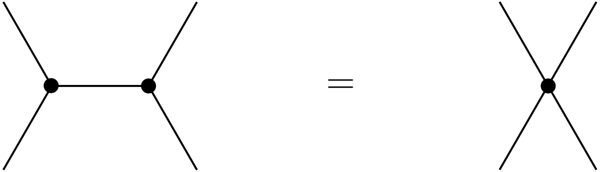


Truncate $\alpha_i \leq D\ \forall i$

Contractions

$d = 1$

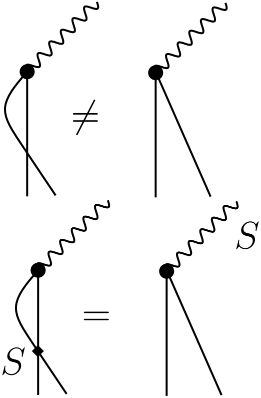
$d > 1$



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

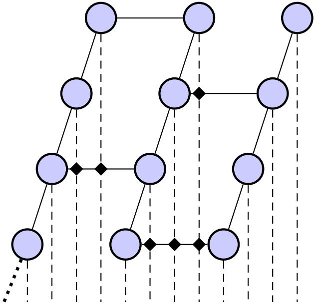
$$c_i c_k = -c_k c_i$$

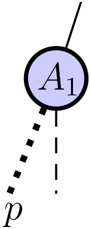
$$(c_i c_j) c_k = c_k (c_i c_j)$$



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

Parity link



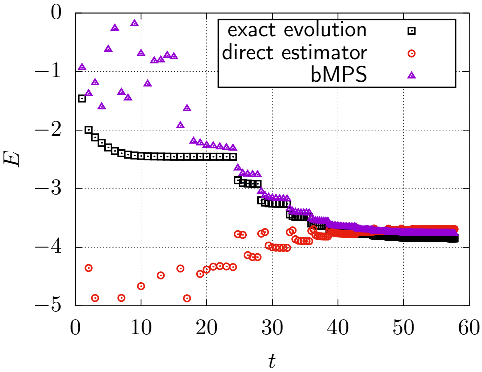


$p = \pm 1$

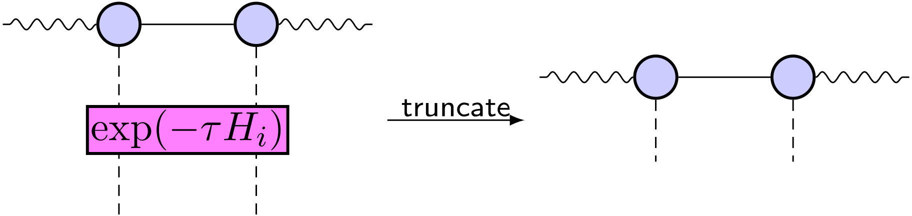
$\Rightarrow$ even- and odd-parity subspaces are disjoint

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

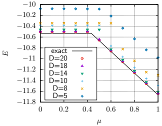


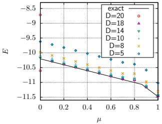
$\exp(-\tau H_i)$

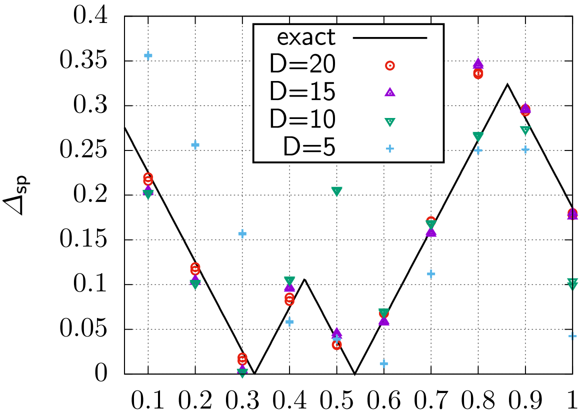
truncate

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

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

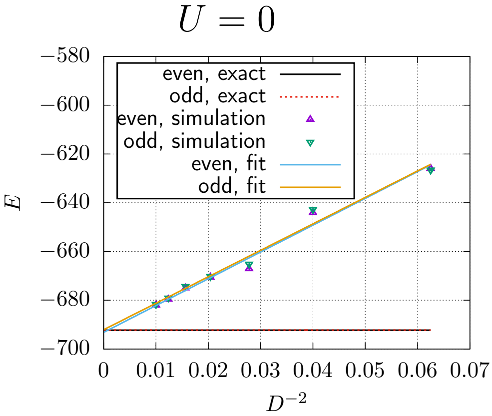


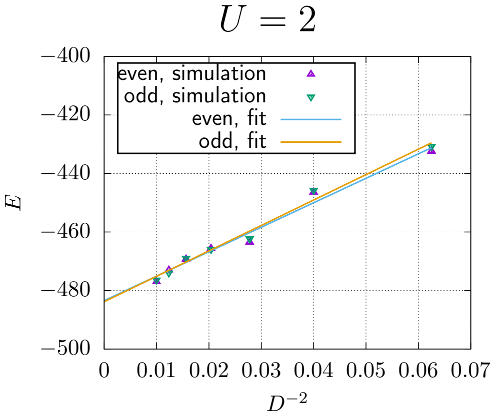




Simulations with chemical potential (30×15, $\mu = 0.5$)

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





“Reducing the Sign Problem of the Hubbard Model”

[Gängten, JO *et al.* (forthcoming); Rodekamp, JO *et al.* *PRB* **106** (2022); Schneider, JO *et al.* *PRB* **104** (2021)]

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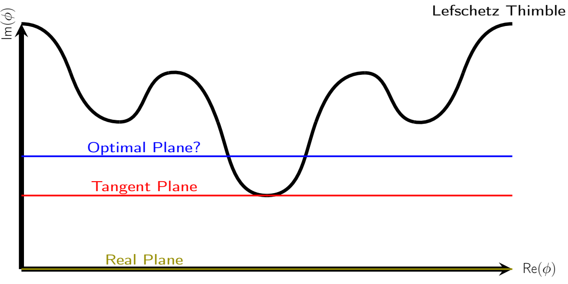

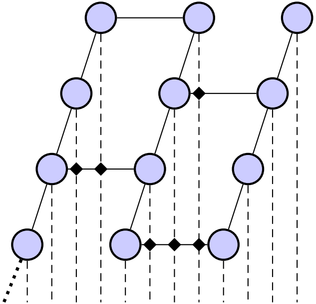

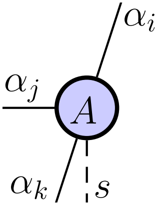

U	**K**	
$\bar{\psi}$	U_μ	ψ
L	**F**	**T**

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