Determining entanglement measures in SU(N) lattice gauge theory for N>4: *difficulties and solutions*

Swiss National Science Foundation
Grant No. 210064

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UNIVERSITÄT BERN
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LATTICE 2024, July 28 - August 3, 2024

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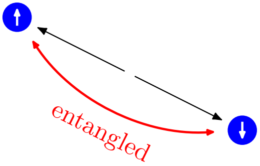
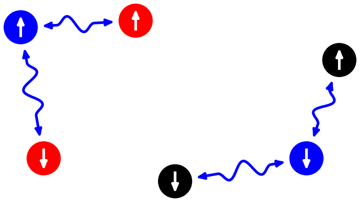
What is entanglement?

➔ Quantum physical implementation of conservation laws

- Decay of spin-0 particle: $s = 0 \longrightarrow s_1 + s_2 = 0$
- Pair creation from vacuum: $s = 0 \longrightarrow s_1 + s_2 = 0$



- In a quantum field theory ➔ correlations



Introduction

How to quantify entanglement?

- Bipartite quantum system: $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$

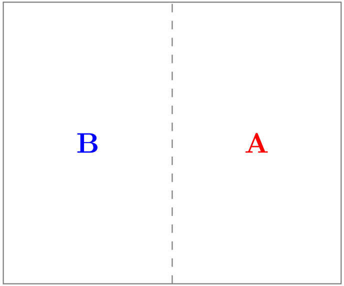
  pure state: $|\psi\rangle_{AB} \in \mathcal{H}_{AB}$, $\rho_{AB} = |\psi\rangle_{AB}\langle\psi|$ $\rightarrow$ $\mathrm{tr}(\rho_{AB}^2) = 1$

  orthonormal bases: $|n\rangle_A \in \mathcal{H}_A, |m\rangle_B \in \mathcal{H}_B$

  ➔ $|\psi\rangle_{AB} = \sum_{mn} c_{mn} |m\rangle_A \otimes |n\rangle_B$, $\sum_{mn} |c_{mn}|^2 = 1$

  ➔ $\rho_{AB} = |\psi\rangle_{AB}\langle\psi| = \sum_{mnkl} c_{mn} c_{kl}^* |m\rangle_A\langle k| \otimes |n\rangle_B\langle l|$

  (notation: $|\psi\rangle_C\langle\psi| = |\psi\rangle_C \otimes {}_C\langle\psi|$)



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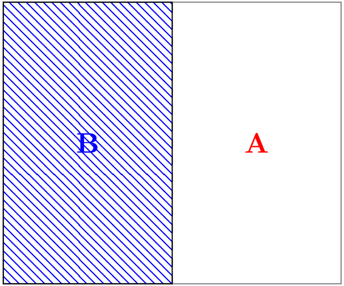
- Reduced density matrix: $\rho_A = \mathrm{tr}_B(\rho_{AB}) = \sum_{mkl} c_{ml} c_{kl}^* |m\rangle_A\langle k|$



$\mathrm{tr}\left(\rho_A^2\right) = 1 \quad \Rightarrow \quad$ no entanglement ($c_{mn} = a_m\, b_n$) $\quad \Longleftrightarrow \quad \mathrm{tr}\left(\rho_A^2\right) < 1 \quad \Rightarrow \quad$ entanglement

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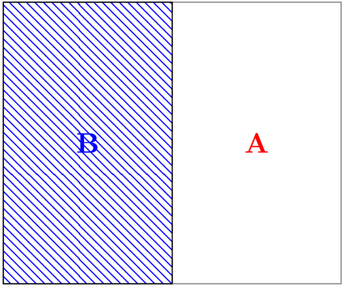

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- Entanglement measures:

  ➔ Purity: $\mathrm{tr}\left(\rho_A^2\right)$

  ➔ Rényi entropies: $H_s(A) = -\frac{1}{s-1} \log \mathrm{tr}\left(\rho_A^s\right)$, $s = 2, 3, \ldots$

  ➔ Entanglement entropy: $S_{EE}(A) = -\lim_{s\to1} \frac{\partial \log \mathrm{tr}(\rho_A^s)}{\partial s} = \lim_{s\to1} \frac{\partial((s-1)H_s(A))}{\partial s} = \lim_{s\to1} H_s(A)$

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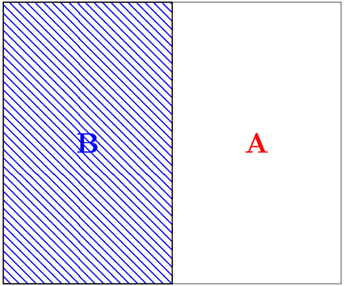

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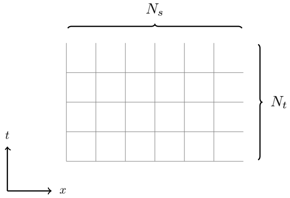
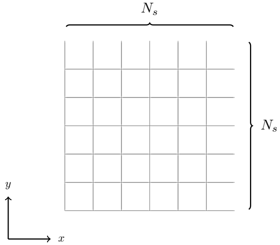
Entanglement entropy on the lattice **[P. Calabrese, J. Cardy (2004)]**

- SU(N) gauge theory on $N_s^{d-1} \times N_t$ lattice

  Partition function: $Z(N_t, N_s) = \int \mathcal{D}[U]\ \mathrm{e}^{-S_G[U]}$





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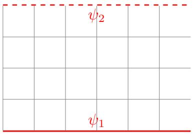
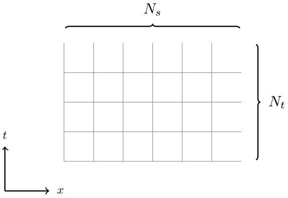
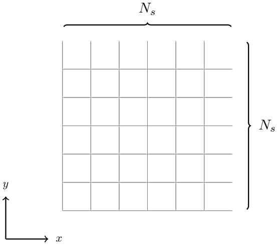
➔ Density matrix element:

$$\langle \psi_1 | \rho | \psi_2 \rangle = \int_{\substack{U(\bar{x}, N_t) = \psi_2(\bar{x}) \\ U(\bar{x},\ 0\ ) = \psi_1(\bar{x})}} \mathcal{D}[U]\ \mathrm{e}^{-S_G[U]} =$$







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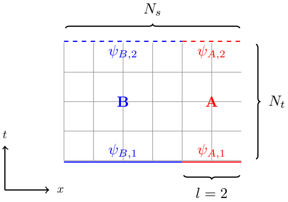

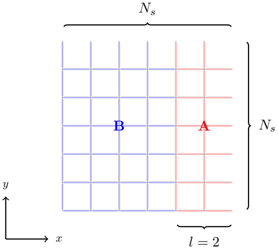

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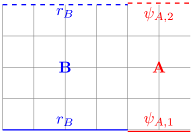
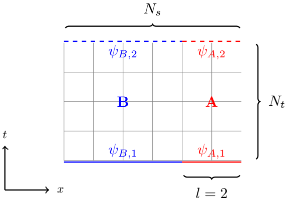
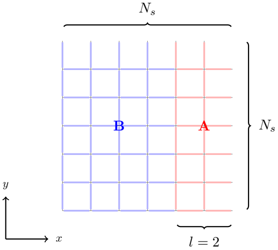
$$\langle \psi_{A,1} | \rho_A | \psi_{A,2} \rangle =$$







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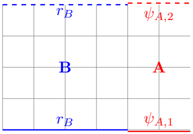
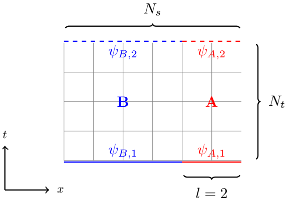
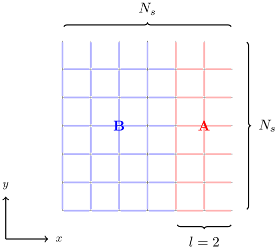


  ➔ Entanglement entropy:

$$S_{EE} = -\,\mathrm{tr}_A(\rho_A \log \rho_A) \quad \text{(how ?)}$$





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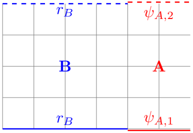

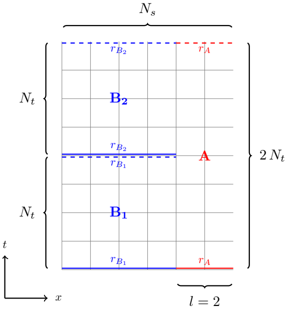

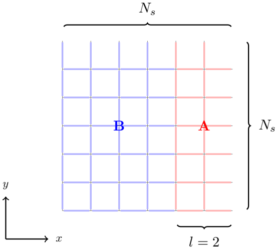

  ➔ Replica method for s-th Rényi entropy:

$$H_s(l, N_t, N_s) = \frac{1}{1-s} \log \mathrm{tr}(\rho_A^s) = \frac{1}{1-s} \log \frac{Z_c(l, s, N_t, N_s)}{Z^s(N_t, N_s)}$$

with "cut partition function" $Z_c(l, s, N_t, N_s)$

$\rightarrow \quad Z_c(l = 0, s, N_t, N_s) = Z^s(N_t, N_s) \quad \forall s \in \mathbb{N}$

$\rightarrow \quad Z_c(l = N_s, s, N_t, N_s) = Z(s\, N_t, N_s) \quad \forall s \in \mathbb{N}$

Entanglement entropy on the lattice **[P. Calabrese, J. Cardy (2004)]**

➔ Entanglement entropy (EE):

$$
\begin{aligned}
S_{EE}(l, N_t, N_s) &= -\lim_{s\to 1} \frac{\partial \log \mathrm{tr}\left(\rho_A^s\right)}{\partial s} \\
&= -\left(\lim_{s\to 1} \frac{\partial \log Z_c(l, s, N_t, N_s)}{\partial s} - \log Z(N_t, N_s)\right) \\
&\approx \; -\log Z_c(l, 2, N_t, N_s) \; - \; (-2 \, \log Z(N_t, N_s)) \\
&= -\log \mathrm{tr}\left(\rho_A^2\right) = H_2(l, N_t, N_s)
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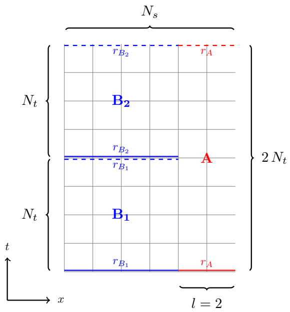
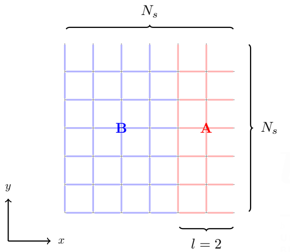
$$\approx \boxed{-\log Z_c(l, 2, N_t, N_s)} - \left(-2 \log Z(N_t, N_s)\right)$$

$$= -\log \mathrm{tr}\left(\rho_A^2\right) = H_2(l, N_t, N_s)$$

➔ free energy difference





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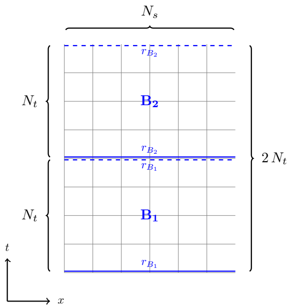

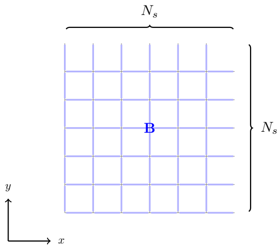

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➔ Instead of EE, measure discrete derivative w.r.t. $l > 0$:

$$\left.\frac{\partial S_{EE}(l', N_t, N_s)}{\partial l'}\right|_{l'=l+1/2} \approx$$

$$-\log Z_c(l+1, 2, N_t, N_s) \; - \; (-\log Z_c(l, 2, N_t, N_s))$$

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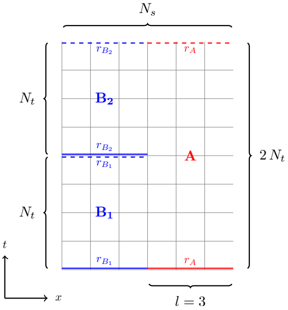

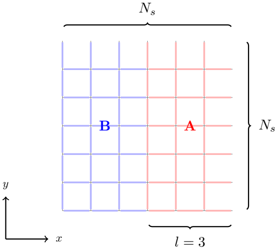

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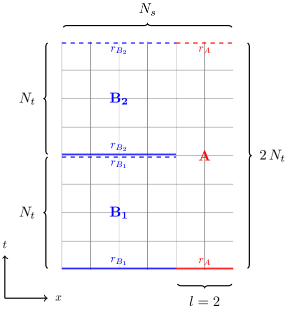

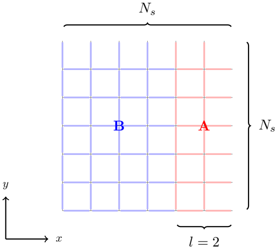

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$$= -\log \operatorname{tr}\left(\rho_A^2\right) = H_2(l, N_t, N_s)$$

➔ free energy difference

➔ Instead of EE, measure discrete derivative w.r.t. $l > 0$:

$$\left.\frac{\partial S_{EE}(l', N_t, N_s)}{\partial l'}\right|_{l'=l+1/2} \approx$$

$$-\log Z_c(l+1, 2, N_t, N_s) \; - \; (-\log Z_c(l, 2, N_t, N_s))$$

➔ $l \to l+1$ is non-local change $\Longrightarrow$ overlap problem

Overcoming the overlap problem

- Original approach

  [P. V. Buividovich, M. I. Polikarpov (2008)],[Y. Nakagawa et al. (2009)],[E. Itou et al. (2015)],[A. Rabenstein et al. (2018)]

  ➔ interpolating partition function:

$$Z_l^*(\alpha) = \int \mathcal{D}[U] \, \exp\Big(-(1-\alpha)\ S_l[\,U\,]\ - \alpha\ S_{l+1}[\,U\,]\ \Big) \quad \text{with} \quad \alpha \in [\,0, 1\,]$$

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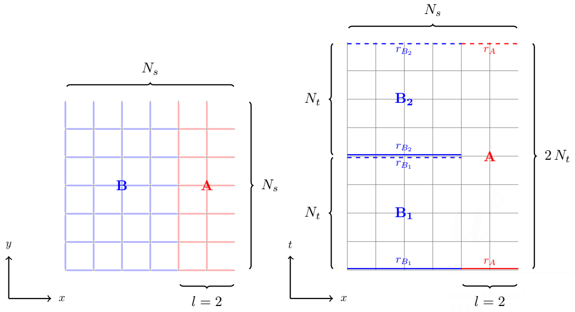

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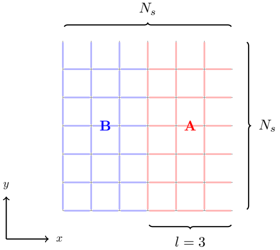

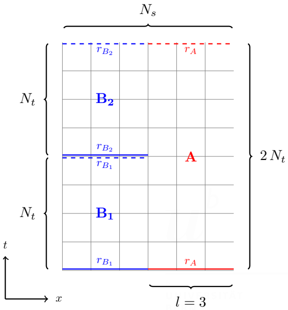

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  ➔ interpolate and integrate:

$$\left.\frac{\partial S_{EE}(l', N_t, N_s)}{\partial l'}\right|_{l'=l+1/2} \approx -\int_0^1 \mathrm{d}\alpha \frac{\partial \log Z_l^*(\alpha)}{\partial \alpha} = \int_0^1 \mathrm{d}\alpha \langle S_{l+1} - S_l \rangle_\alpha$$

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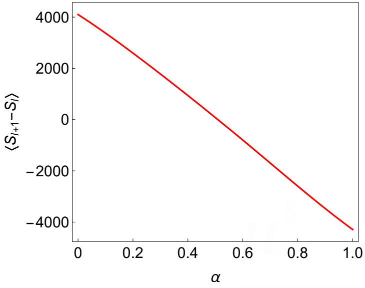
Issue: huge free energy barrier $\rightarrow$ bad signal to noise ratio

➔ Gets worse with increasing volume and increasing N (number of colors)



data from [Y. Nakagawa et al. (2009)]

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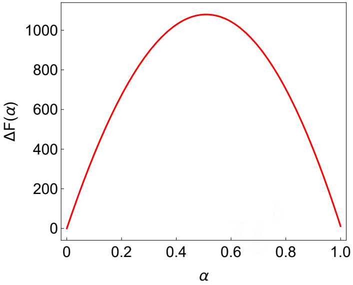

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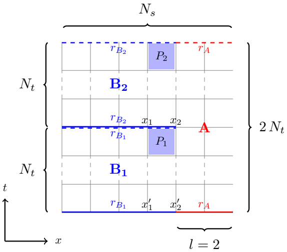
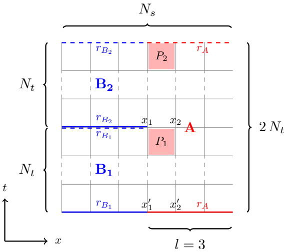
Overcoming the overlap problem

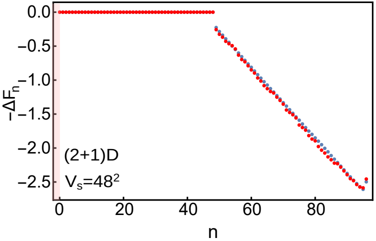


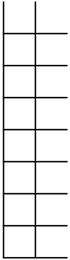
- Entanglement surface deformation method

➔ interpolate by deforming entangling surface

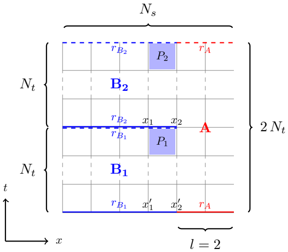


Example in (2+1) dimensions



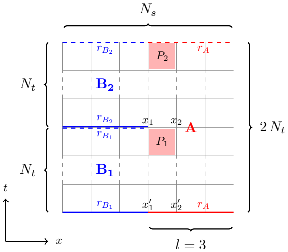


Overcoming the overlap problem



- Entanglement surface deformation method

➔ interpolate by deforming entangling surface



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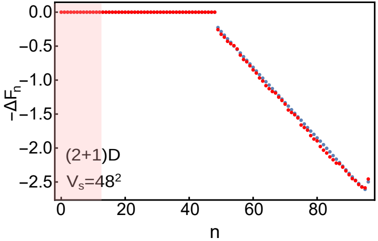
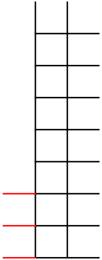
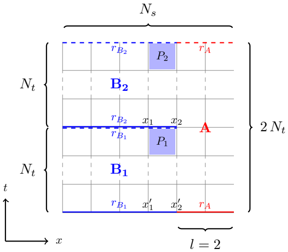


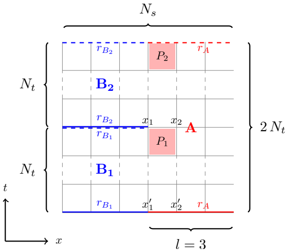


Overcoming the overlap problem

- Entanglement surface deformation method

➔ interpolate by deforming entangling surface





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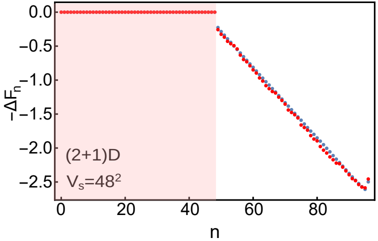
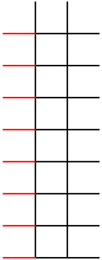
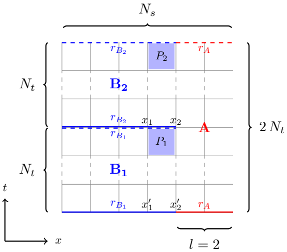




Overcoming the overlap problem



- Entanglement surface deformation method

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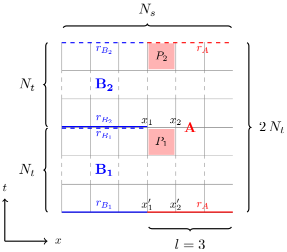

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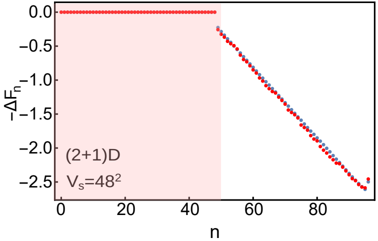
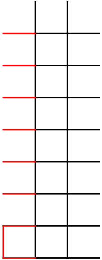
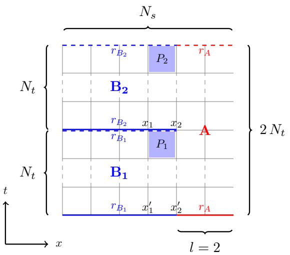




Overcoming the overlap problem



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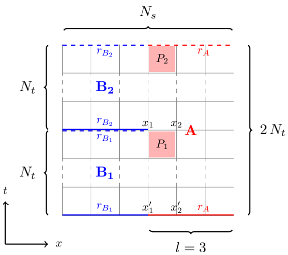
➔ interpolate by deforming entangling surface



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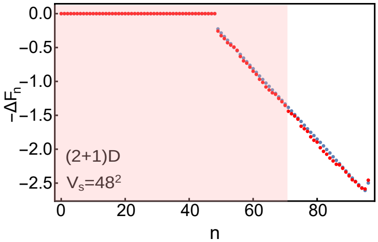

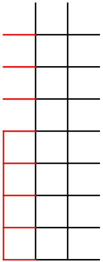

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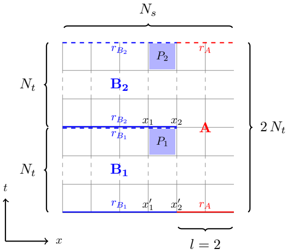

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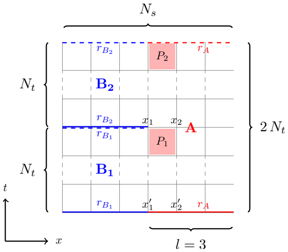

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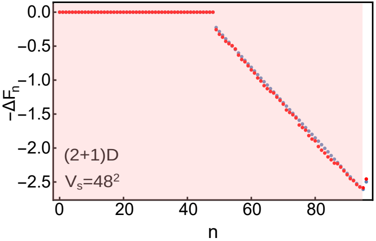
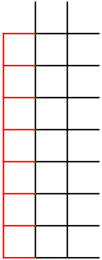
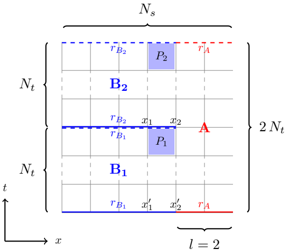




Entanglement entropy on the lattice

Overcoming the overlap problem



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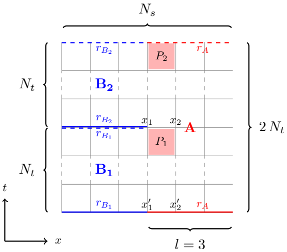

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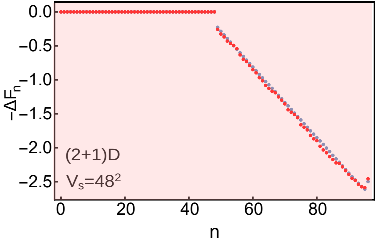

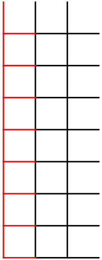

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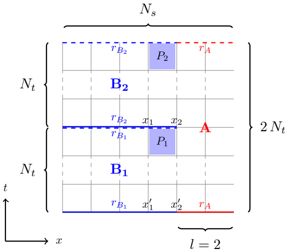
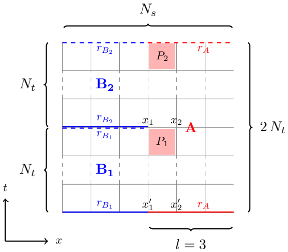
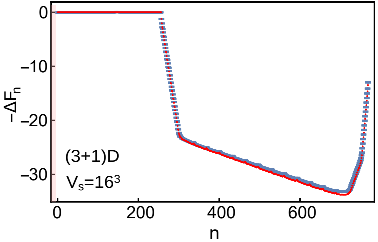


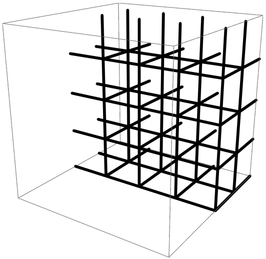
- Entanglement surface deformation method

➔ interpolate by deforming entangling surface



Example in (3+1) dimensions





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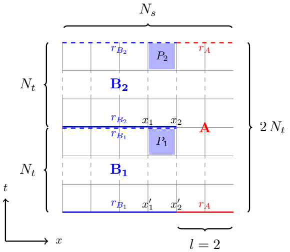

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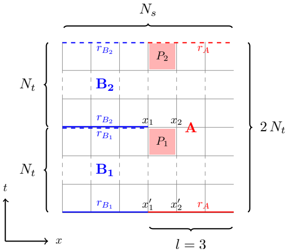
→ interpolate by deforming entangling surface



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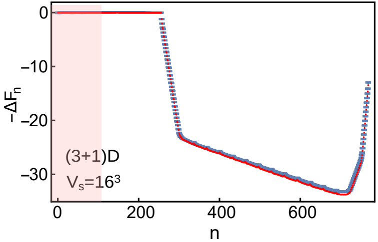

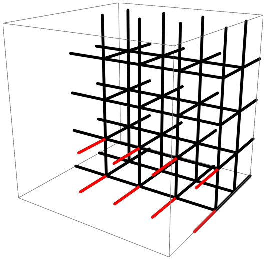

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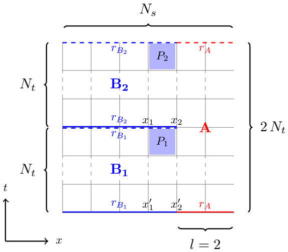

- Entanglement surface deformation method

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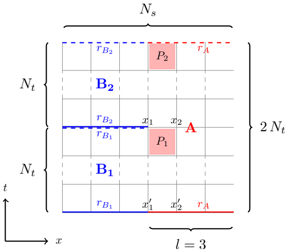

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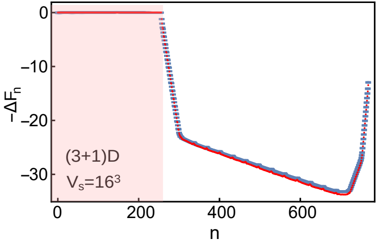

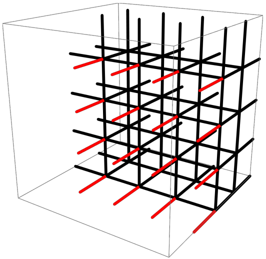

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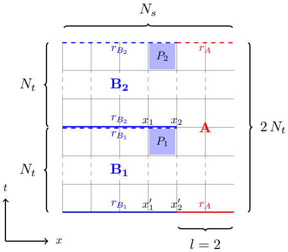

- Entanglement surface deformation method

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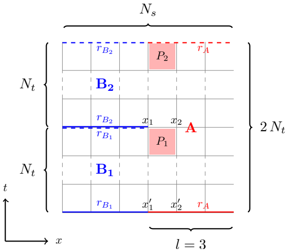

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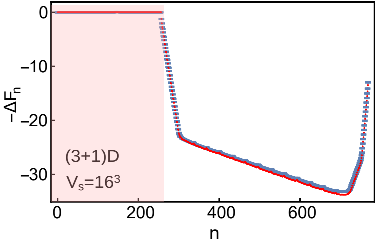

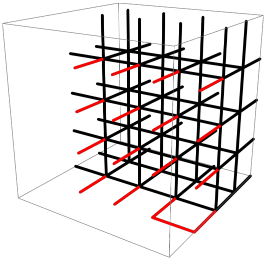

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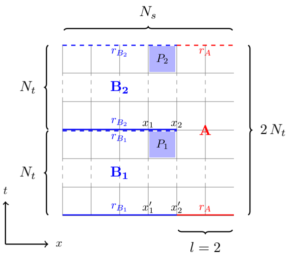
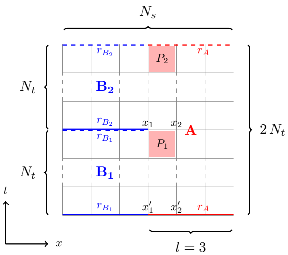


- Entanglement surface deformation method

  ➔ interpolate by deforming entangling surface



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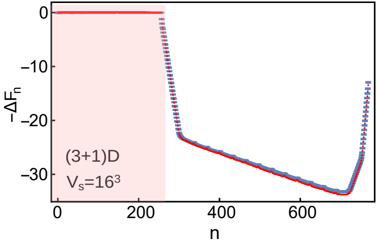
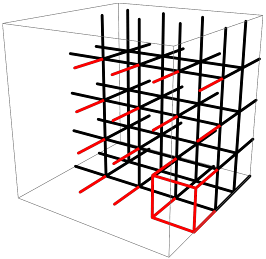
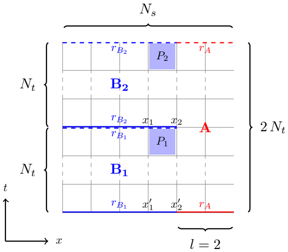




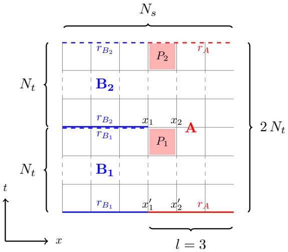
Entanglement entropy on the lattice

Overcoming the overlap problem

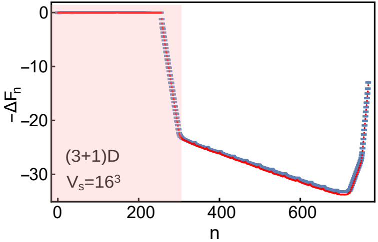


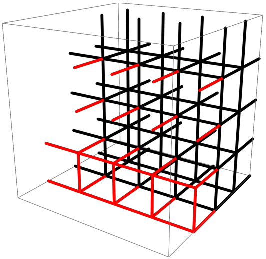
- Entanglement surface deformation method

  ➔ interpolate by deforming entangling surface

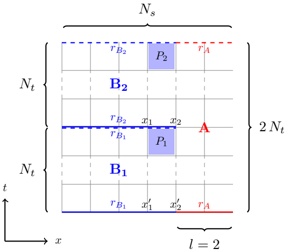


Example in (3+1) dimensions





Overcoming the overlap problem



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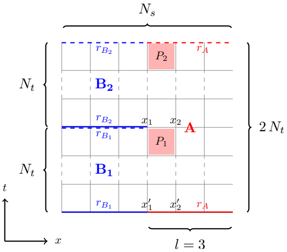

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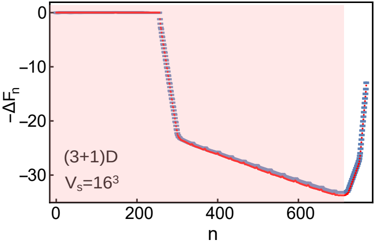

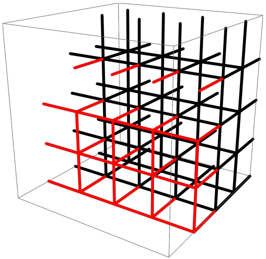

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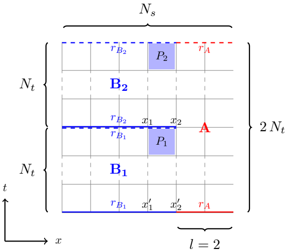

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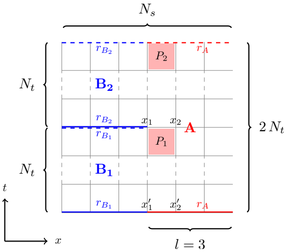

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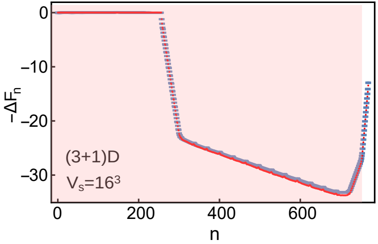

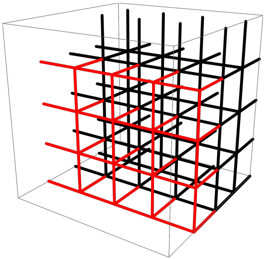

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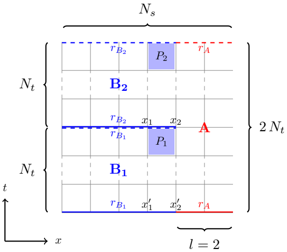

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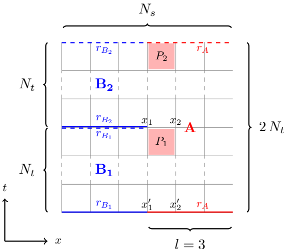

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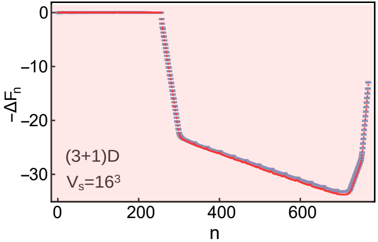
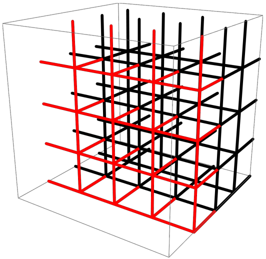
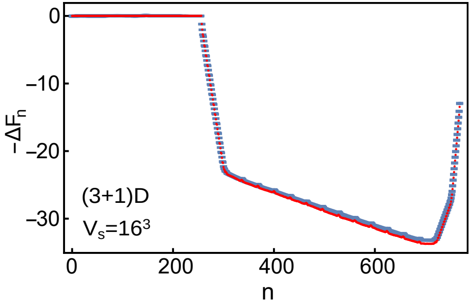




Avoiding remnant free energy barriers

- Remnant free energy barriers due to changing numbers of corners and edges in entangling surface



Entangling surface deformation

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- Remnant free energy barriers due to changing numbers of corners and edges in entangling surface
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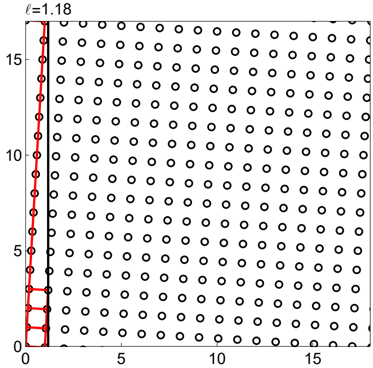

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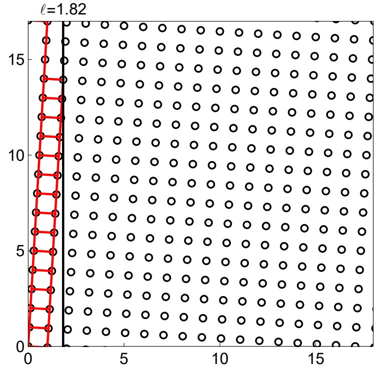

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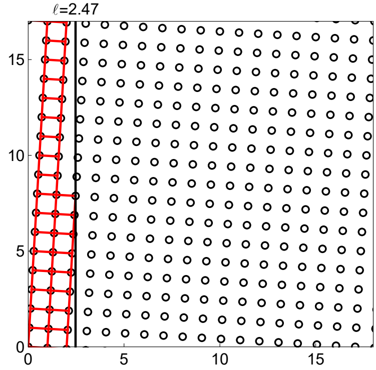

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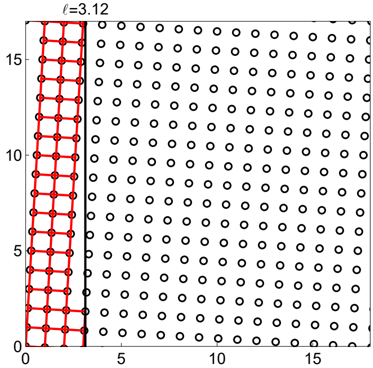

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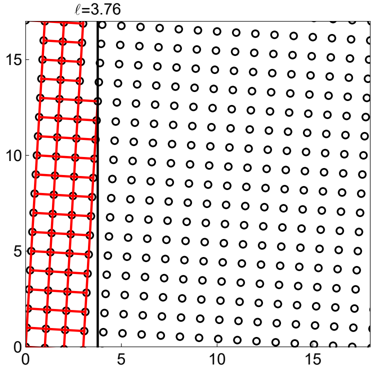

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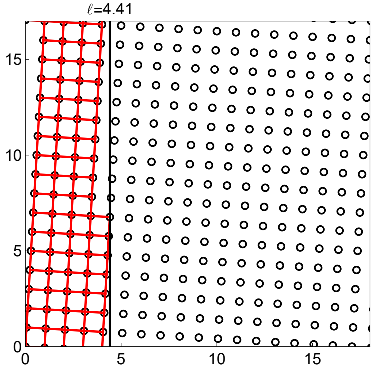

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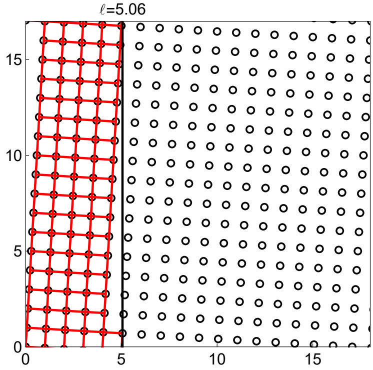

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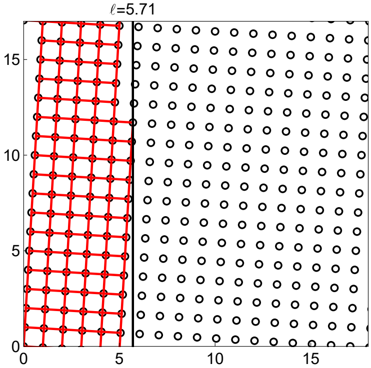

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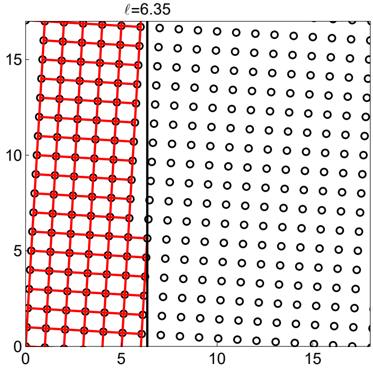

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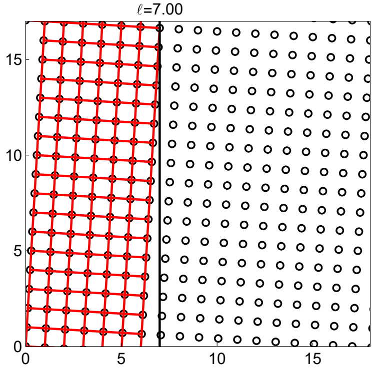

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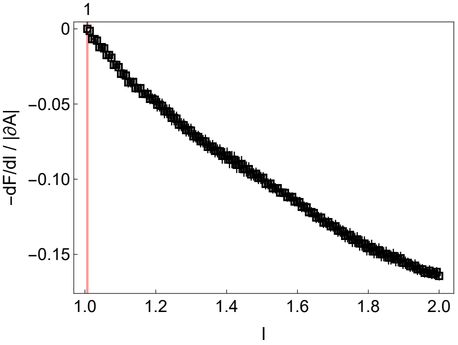

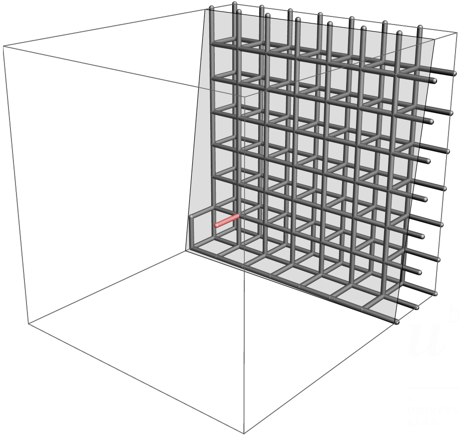

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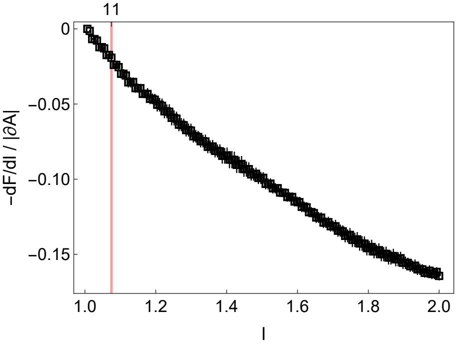

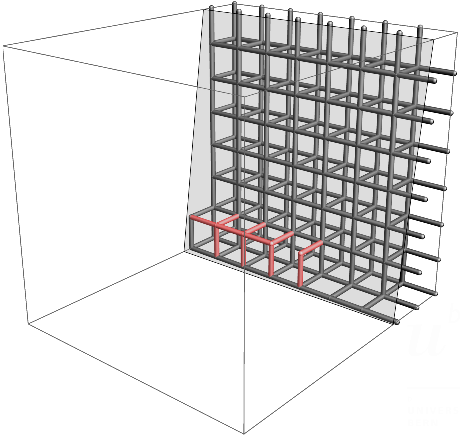

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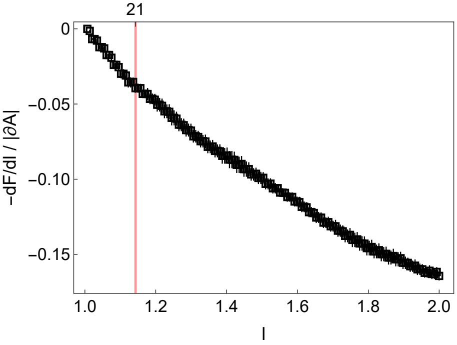

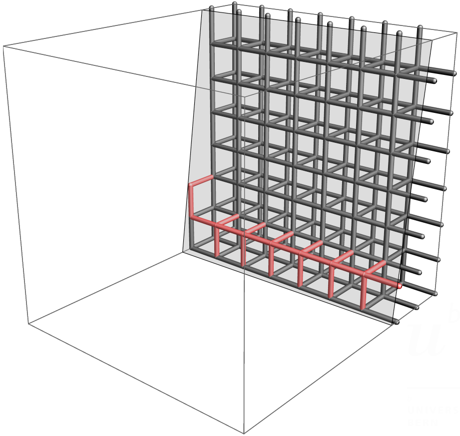

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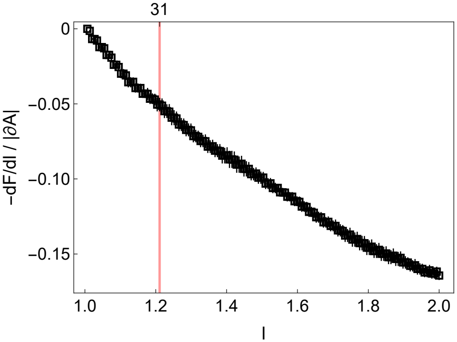

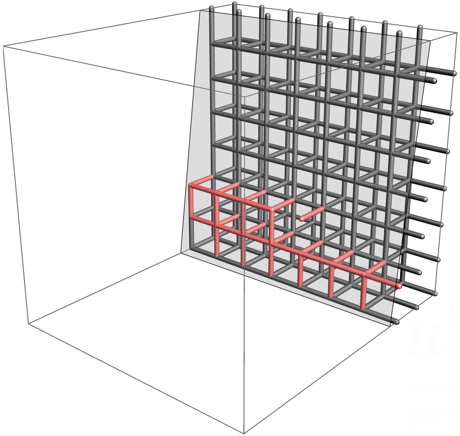

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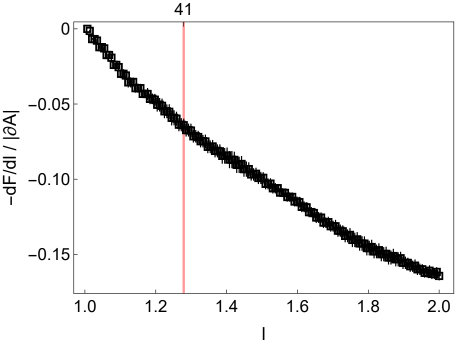

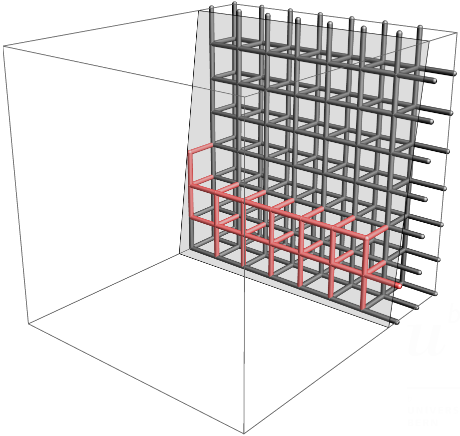

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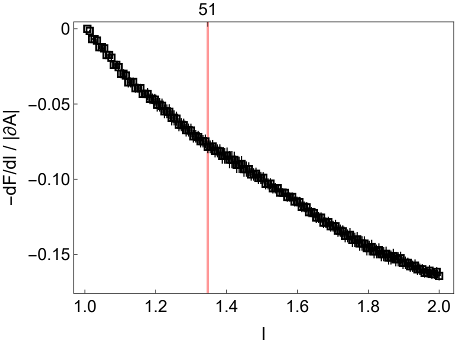

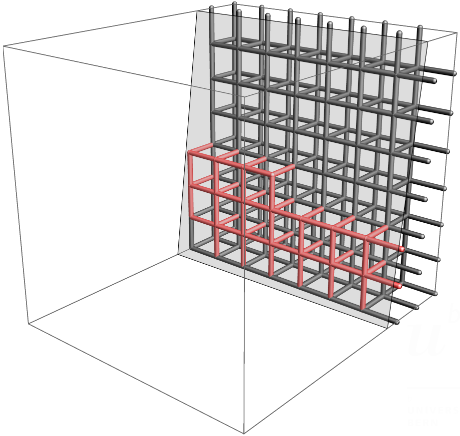

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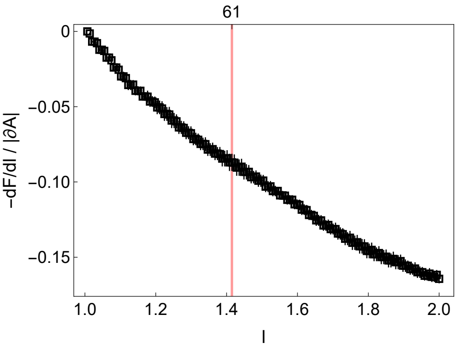

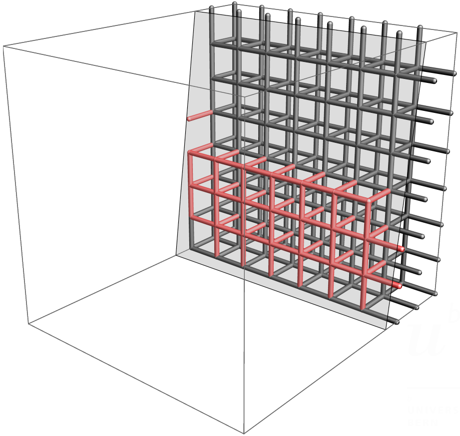

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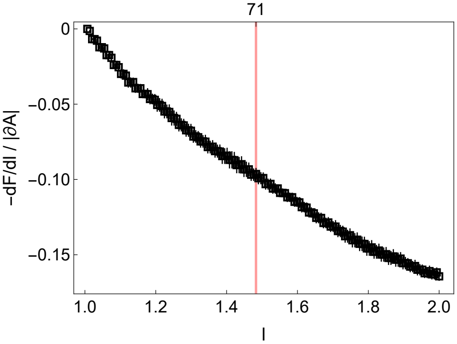

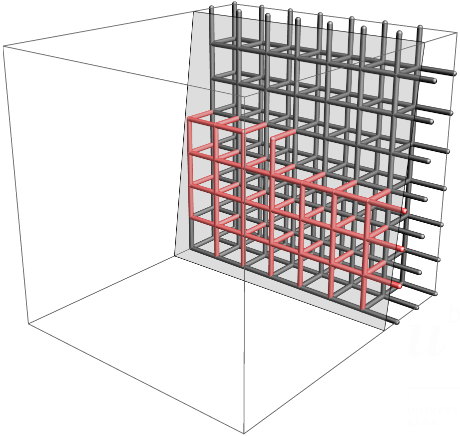

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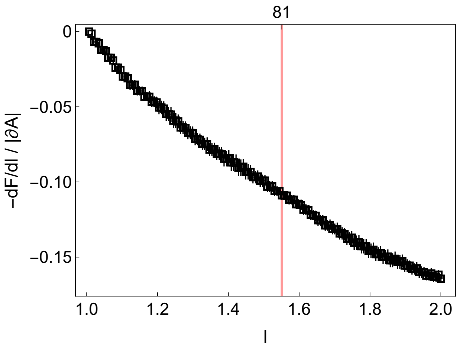

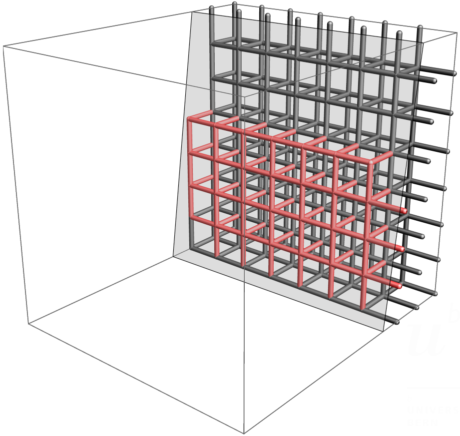

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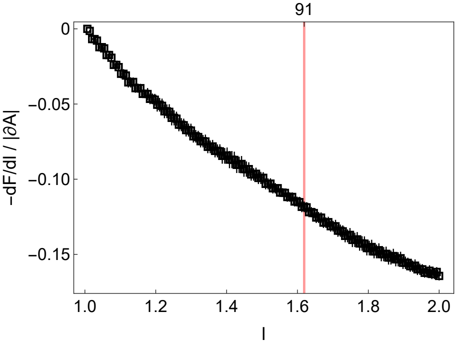

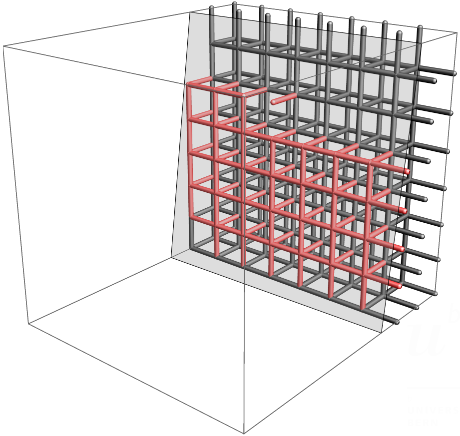

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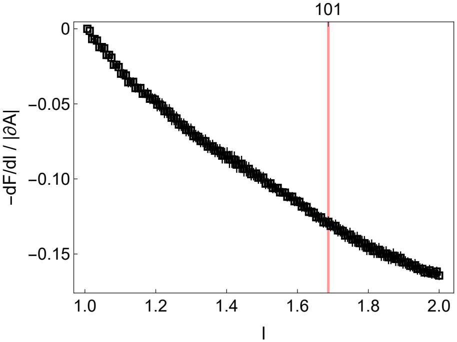

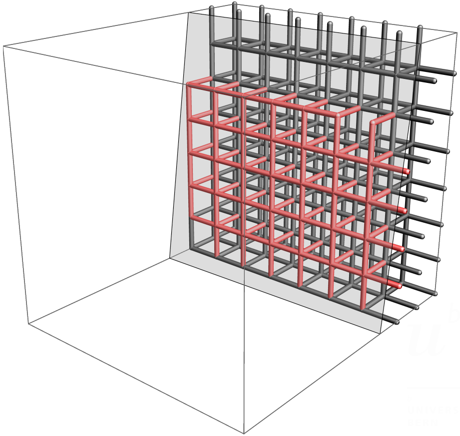

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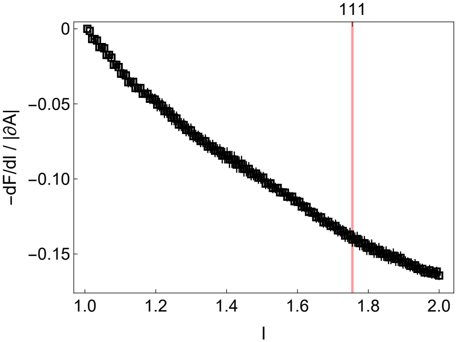

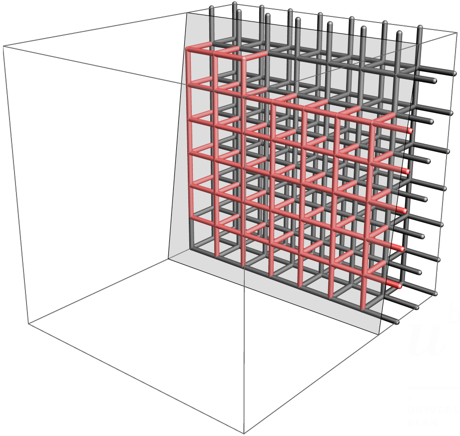

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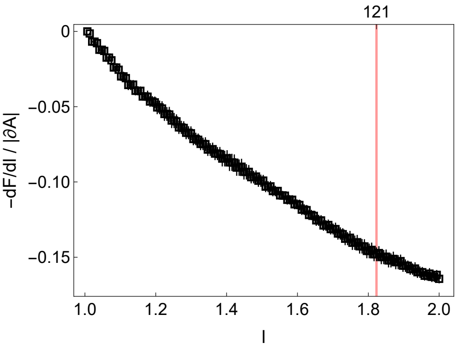

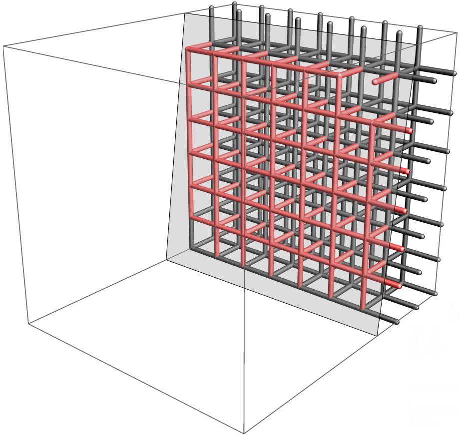

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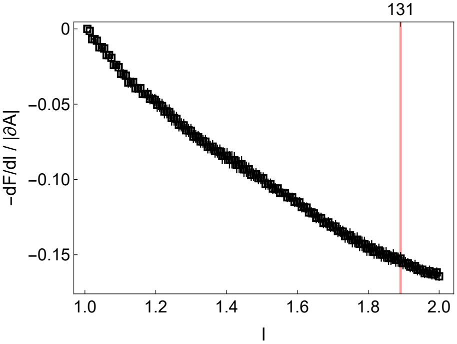

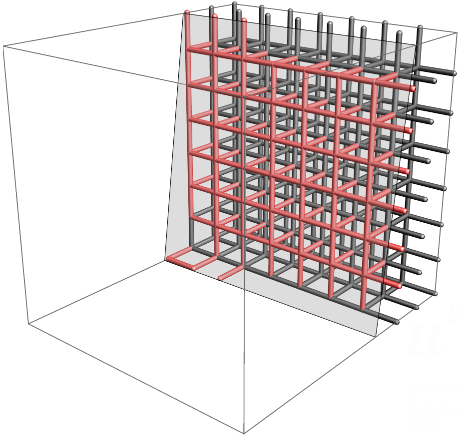

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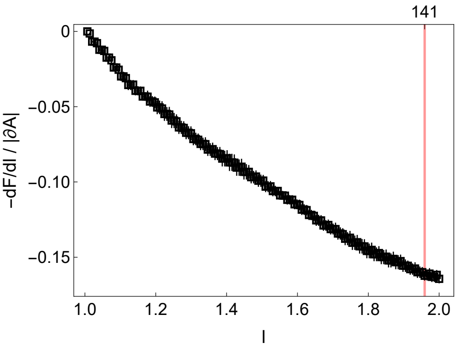

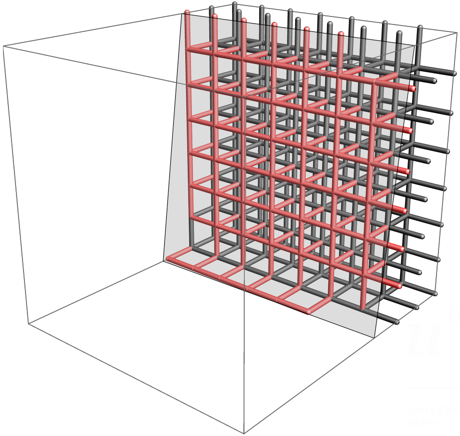

Entangling surface deformation

Avoiding remnant free energy barriers

- Remnant free energy barriers due to changing numbers of corners and edges in entangling surface
- Can be avoided by appropriate tilting of lattice with respect to principal directions of "torus"

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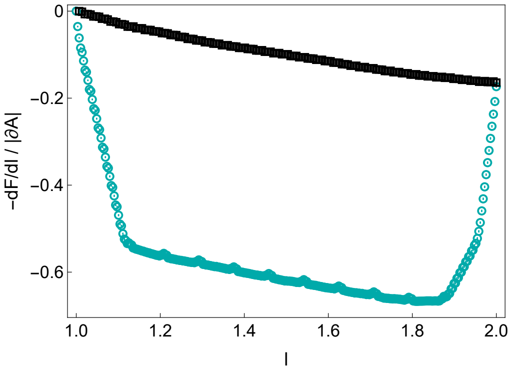
comparison of boundary update methods: non-tilted lattice ⟷ tilted lattice



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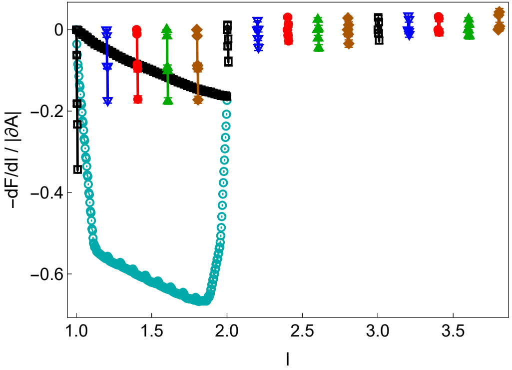
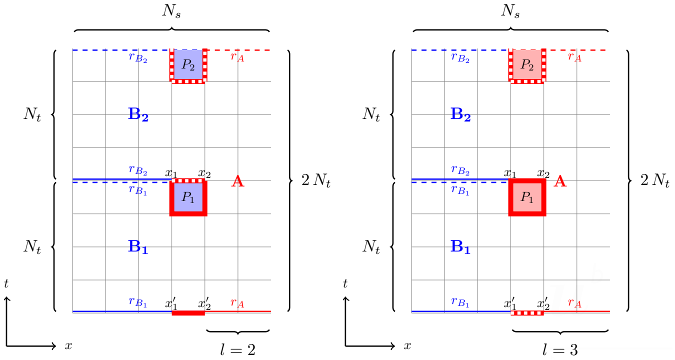


Remaining problems

Single link overlap problem

- BC swap over single non-perpendicular spatial link becomes difficult for $N > 3$

$$p(B \to A) \sim \mathrm{e}^{\frac{\beta}{N}\,\mathrm{Re\,tr}\left(P_{1,A}+P_{2,A}\right) - \frac{\beta}{N}\,\mathrm{Re\,tr}\left(P_{1,B}+P_{2,B}\right)} \quad \text{(naive Metropolis)}$$



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- modified SU(2) sub-group heat-bath update incl. BC swap:

(only slightly better than simple Metropolis)

$SU(2) \to p_{acc} \sim 0.3$

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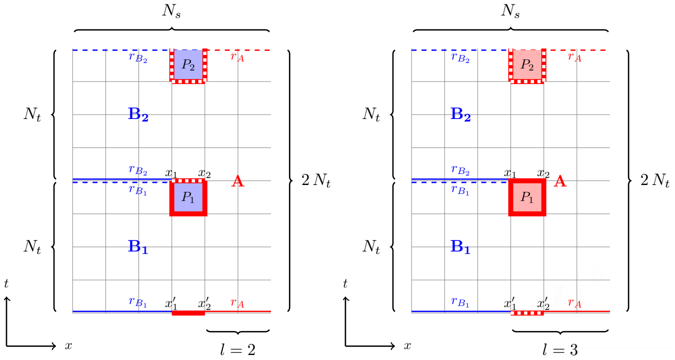

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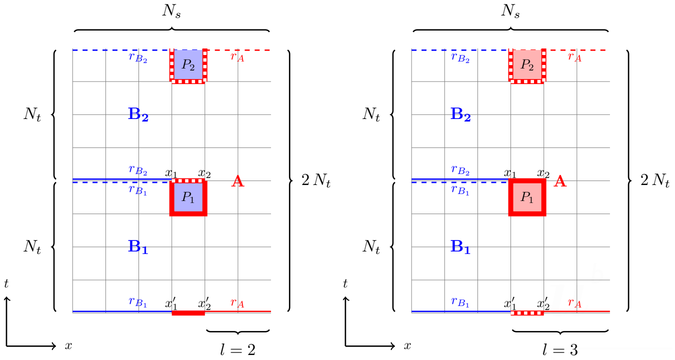
➔ Worm-like update:

$SU(2) \to p_{\text{acc}} \sim 0.45$

$SU(3) \to p_{\text{acc}} \sim 0.35$

$SU(5) \to p_{\text{acc}} \sim 0.1$



Worm-like BC update (simplified: move choice probab. factors not shown)

- pick permutation $\sigma \in \Pi(1, \ldots, s)$, set $i = 1$
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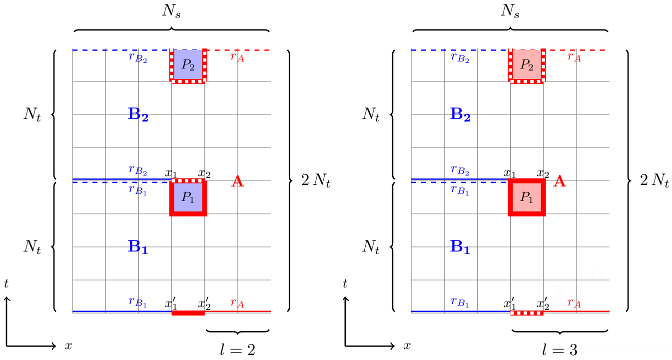

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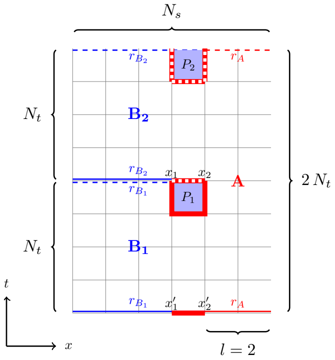
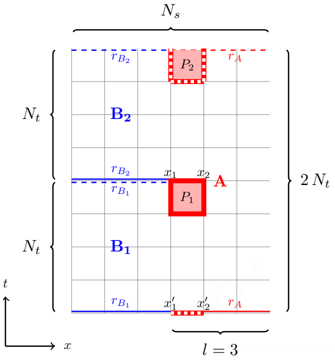
    end worm
  - set $i' = i + (\delta i - 1)/2$





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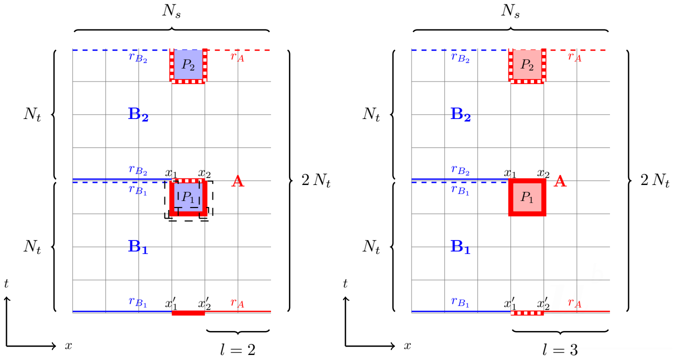

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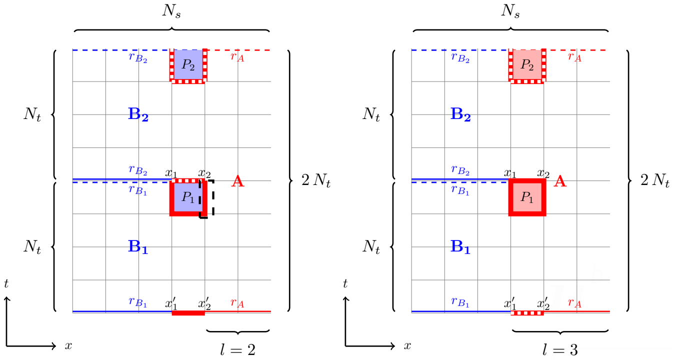

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  - compute one-link integrals

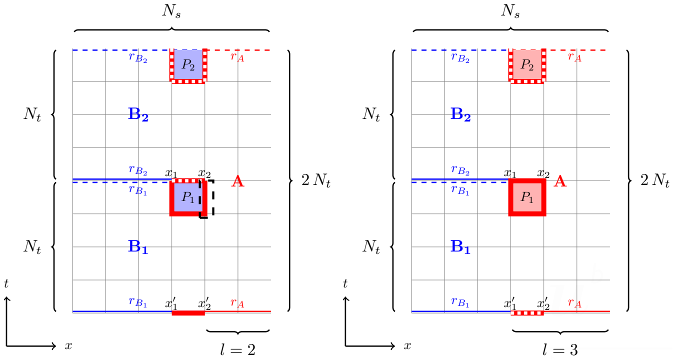
    $Z_{A,B} = \int \mathcal{D}[U]\, \mathrm{e}^{\frac{\beta}{N}\,\mathrm{Re}\,\mathrm{tr}(U\,S_{A,B})}$

    $S_{A,B}$ is staple sum around U w.r.t. $\mathrm{BC_A}$, $\mathrm{BC_B}$

    (one-link int. with Cayley-Hamilton: [TR (2024)])
  - with probab. $p(\delta i) = \min(1,(Z_A/Z_B)^{\delta i})$:

    change BC for $P_{\sigma(i')}$

    set $i = i + \delta i$



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  - with probab. $p(\delta i) = \min(1, (Z_A/Z_B)^{\delta i})$:

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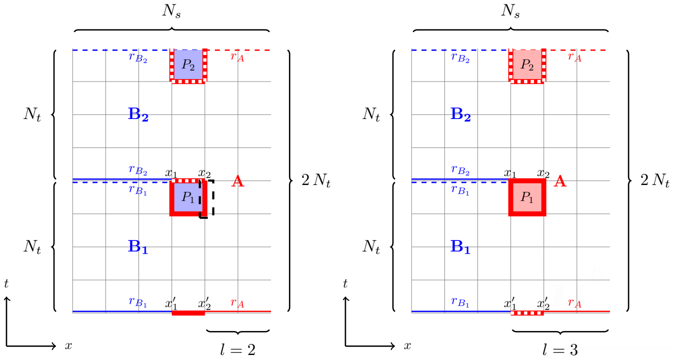
  - generate new value for U

    (using heat-bath dist. w.r.t. current BC)

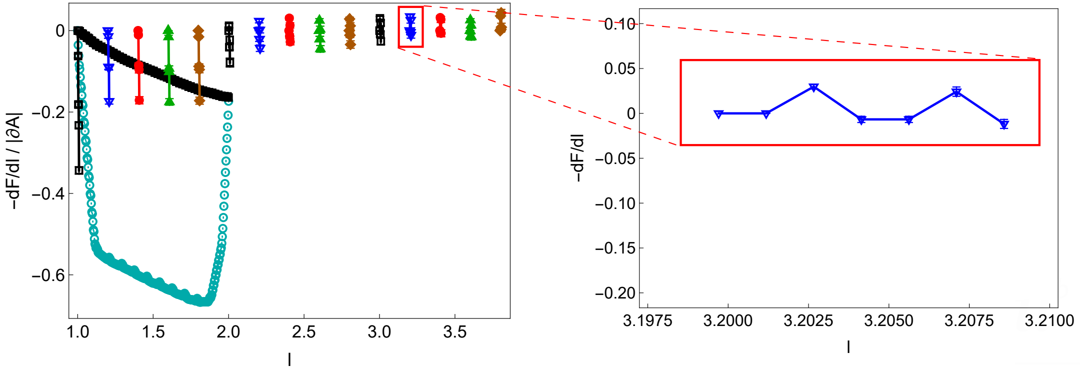


Remnant "single cube" free energy barrier?

- For $\ell > 2$ non-monotonic change in free energy during BC change for single spatial cube

  ➔ auto-correlation issue?

  ➔ can it be avoided?



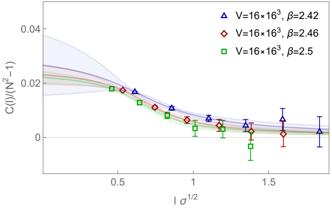
Conclusions & outlook

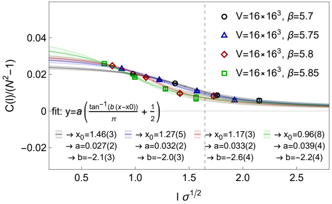
Conclusions

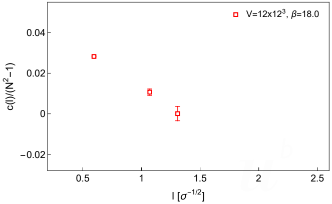
- Entangling surface deformation method with tilted lattice and/or local derivative essentially avoids free energy barriers in determination of entanglement measures (Rényi entropies) in SU(N) lattice gauge theories.
- Worm-like update for temporal BC flip over spatial link results in significantly higher acceptance rates. (but still small as N increases)
- Remnant "single cube" free energy barrier can show up for $\ell > 2$.

Outlook

- Some ideas to overcome the "single cube" free energy barriers and improve acceptance rates for BC updates further.
- Aplications: entropic c-function for SU(2) , SU(3) , SU(5) , mutual information, ...







Thank you!