Grassmann tensor-network method for strong-coupling QCD

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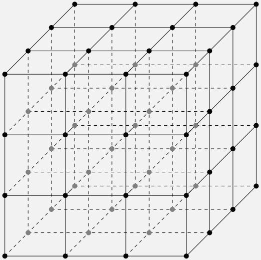
Monte Carlo versus Tensor Networks

Consider classical or quantum system in thermal equilibrium on a d-dimensional lattice described by partition function Z

- Standard method: stochastic sampling using Monte Carlo methods
- New alternative: reformulate Z as a fully contracted tensor network and use higher order tensor renormalization group (HOTRG) method to compute observables



- Tensor method can be applied when action is complex and MC simulations fail
- Cost scales logarithmically with volume
- Method based on singular value decomposition (SVD)

Strong-coupling QCD – action and partition function

Partition function for $\beta = 0$

$$Z = \int \left[\prod_x d\psi_x d\bar{\psi}_x \prod_\nu dU_{x,\nu} \right] e^{-S_F}$$

Fermion action

d-dimensional action for staggered quarks with mass m and chemical potential μ

$$S_F = \sum_x \left\{ \sum_{\nu=1}^{d} \eta_{x,\nu} \gamma^{\delta_{\nu,1}} \bar{\psi}_x \left[e^{\mu\delta_{\nu,1}} U_{x,\nu} \psi_{x+\hat{\nu}} - e^{-\mu\delta_{\nu,1}} U^{\dagger}_{x-\hat{\nu},\nu} \psi_{x-\hat{\nu}} \right] + 2m\bar{\psi}_x \psi_x \right\}$$

Change to dual variables (Rossi & Wolff (1984), Karsch & Mütter (1989))

- Infinite coupling limit → integrate out SU(3) gauge fields
- Grassmann variables contribute through mesonic combinations $(\bar{\psi}_x \psi_x)$ and baryonic/antibaryonic combinations $B_x / \bar{B}_x$ of 3 quarks/antiquarks

Tensor formulation of Z

Tensor network formulation: integrate out mesons but not baryons, as latter would introduce non-local sign factors

$$Z = \sum_{j} \int \prod_{x} S^{(x)}_{[j_x]} G^{(x)}_{[l_x]}$$

with local numeric and Grassmann tensors:

$$S^{(x)}_{[j_x]} = \delta_{x\in\mathscr{B}} w_{\mathscr{B}}([l_x]) + \delta_{x\in\mathscr{M}}\, w_{\mathscr{M}}([j_x])$$

$$G^{(x)}_{[l_x]} = (dB_x)^{\sum_\nu (l^-_{x,\nu}+l^+_{x,-\nu})}(d\bar{B}_x)^{\sum_\nu (l^+_{x,\nu}+l^-_{x,-\nu})}\prod_{\nu=1}^{d}(B_x\bar{B}_{x+\hat{\nu}})^{l^-_{x,\nu}}(\bar{B}_x B_{x+\hat{\nu}})^{l^+_{x,\nu}}$$

- Each term in sum is characterized by its indices $\boldsymbol{j} = (j_{1,1},\dots,j_{V,d})$
- Notation: indices: $[j_x] \equiv j_{x,-1}j_{x,1}\dots j_{x,-d}j_{x,d}$, etc.
- $0 \le j \le 5$
- $l \equiv l(j) \in \{-1,0,1\}$ and $l^{\pm} = \delta_{l,\pm 1}$

Grassmann HOTRG

Extend HOTRG method to handle the baryonic Grassmann variables
(using ideas introduced by Shimizu and Y. Kuramashi (2014); Sakai et al. (2017))

Decouple B and $\bar{B}$ in the Grassmann interactions by introducing one auxiliary Grassmann variable $c_{x,\nu}$ on *each link*: (recall $l^{\pm}_{x,\nu} \in \{0,1\}$)

$$(\bar{B}_x B_{x+\hat{\nu}})^{l^+_{x,\nu}} = \left(\bar{B}_x B_{x+\hat{\nu}} \int dc_{x,\nu} c_{x,\nu}\right)^{l^+_{x,\nu}} = \int (\bar{B}_x c_{x,\nu})^{l^+_{x,\nu}} (B_{x+\hat{\nu}} dc_{x,\nu})^{l^+_{x,\nu}}$$

$$(B_x \bar{B}_{x+\hat{\nu}})^{l^-_{x,\nu}} = \left(B_x \bar{B}_{x+\hat{\nu}} \int dc_{x,\nu} c_{x,\nu}\right)^{l^-_{x,\nu}} = \int (B_x c_{x,\nu})^{l^-_{x,\nu}} (\bar{B}_{x+\hat{\nu}} dc_{x,\nu})^{l^-_{x,\nu}}$$

Note: backward/forward baryon interactions are mutually exclusive on every link
→ one auxiliary Grassmann variable per link is sufficient

The factors in brackets are commuting and can be moved around freely in Z to integrate out the (anti)baryons, without generating non-local sign factors.

Partition function with auxiliary Grassmanns

After integrating out all B_x and $\bar{B}_x$

$$Z = \sum_{j} \int \prod_{x} T^{(x)}_{[j_x]} K^{(x)}_{[f_x]}$$

- Grassmann tensor:

$$K^{(x)}_{[f_x]} = \prod_{\nu} (c_{x,\nu})^{f_{x,\nu}} \coprod_{\nu} (dc_{x,-\nu})^{f_{x,-\nu}}$$
$$= (c_{x,1})^{f_{x,1}} \dots (c_{x,d})^{f_{x,d}} (dc_{x,-d})^{f_{x,-d}} \dots (dc_{x,-1})^{f_{x,-1}}$$

  with reverse ordered product $\coprod_{\nu}$ and $c_{x,-\nu} \equiv c_{x-\hat{\nu},\nu}$
  $f_{x,\nu} \equiv f_{x,\nu}(j_{x,\nu}) \in \{0,1\}$ is Grassmann parity of corresponding index $j_{x,\nu}$

- Numeric tensor:

$$T^{(x)}_{[j_x]} = \omega_{[l_x]} S^{(x)}_{[j_x]}$$

  with a local sign factor $\omega_{[l_x]}$ coming from rearrangement of auxiliaries in $K^{(x)}$.

- Components of T are nonzero only when K is Grassmann even

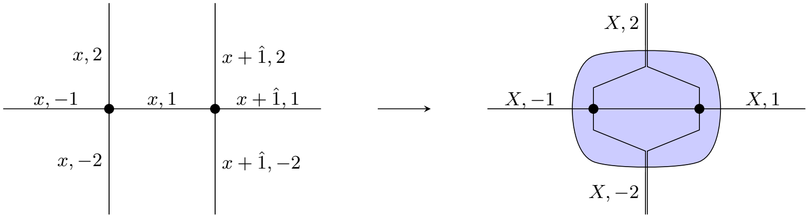
Blocking

Evaluate the partition function with iterative blocking procedure:

- the number of Grassmann variables is halved at each step
- a new local sign factor is absorbed in the coarse grid numeric tensor
- the coarse grid numeric tensor is truncated using HOSVD

Consider contraction in 1-direction: $(x, x+\hat{1}) \rightarrow X$

$$\sum_{j_{x,1}} \int_{c_{x,1}} T^{(x)}_{[j_x]} T^{(x+\hat{1})}_{[j_{x+\hat{1}}]} K^{(x)}_{[j_x]} K^{(x+\hat{1})}_{[j_{x+\hat{1}}]} \quad \rightarrow \quad \mathscr{T}^{(x,x+\hat{1})} \mathscr{K}^{(x,x+\hat{1})}$$



Grassmann blocking

Grassmann blocking

$$\mathscr{K}^{(x,x+\hat{1})} \equiv \int_{c_{x,1}} K^{(x+\hat{1})}_{[f_{x+\hat{1}}]} K^{(x)}_{[f_x]}$$

Integrate out $c_{x,1}$:

$$\mathscr{K}^{(x,x+\hat{1})}$$

$$= \int_{c_{x,1}} \prod_{\nu} (c_{x+\hat{1},\nu})^{f_{x+\hat{1},\nu}} \coprod_{\nu=2}^{d} (dc_{x+\hat{1},-\nu})^{f_{x+\hat{1},-\nu}} \underline{(dc_{x,1})^{f_{x,1}} (c_{x,1})^{f_{x,1}}} \prod_{\nu=2}^{d} (c_{x,\nu})^{f_{x,\nu}} \coprod_{\nu} (dc_{x,-\nu})^{f_{x,-\nu}}$$

$$= \sigma_{[f_x f_{x+\hat{1}}]} (c_{x+\hat{1},1})^{f_{x+\hat{1},1}} \left[\prod_{\nu=2}^{d} (c_{x,\nu})^{f_{x,\nu}} (c_{x+\hat{1},\nu})^{f_{x+\hat{1},\nu}} \right] \left[\coprod_{\nu=2}^{d} (dc_{x+\hat{1},-\nu})^{f_{x+\hat{1},-\nu}} (dc_{x,-\nu})^{f_{x,-\nu}} \right] (dc_{x,-1})^{f_{x,-1}}$$

For ⊥ directions ($\nu \geq 2$): $c_{x,\nu}$ and $dc_{x,\nu}$ are not in same $\mathscr{K}^{(x,x+\hat{1})}$
→ integration would generate non-local sign factors

Introduce coarse grid Grassmann variables

Reducing the coarse local Grassmann tensor

Integrate out all Grassmanns $c_{x,\nu} \perp$ to the contraction direction ($\nu \geq 2$), and replace these by new auxiliaries $\tilde{c}_{X,\nu}$ on the coarse lattice.

Before: Vd Grassmanns, After: $\frac{1}{2}Vd$ Grassmanns

How? In every $\mathscr{K}^{(X)}$ introduce:

$$\prod_{\nu=2}^{d}\left(\int d\tilde{c}_{X,-\nu}\tilde{c}_{X,-\nu}\right)^{\tilde{f}_{X,-\nu}} = 1$$

with

$$\tilde{f}_{X,-\nu} \equiv (f_{x,-\nu} + f_{x+\hat{1},-\nu}) \bmod 2$$

and shift the commuting combinations

$$(\tilde{c}_{X,-\nu})^{\tilde{f}_{X,-\nu}}(dc_{x+\hat{1},-\nu})^{f_{x+\hat{1},-\nu}}(dc_{x,-\nu})^{f_{x,-\nu}}$$

from coarse site X to $X - \hat{\nu}$ on the entire coarse lattice.

Reduce the perpendicular Grassmanns

Now all pairs $(c_{x,\nu}, c_{x+\hat{1},\nu})$ can be integrated out and are replaced by $\tilde{c}_{X,\nu}$.

The coarse grid partition function is now

$$Z = \sum_{\boldsymbol{j}} \int \prod_{X} \widetilde{\mathscr{T}}^{(X)} \overline{K}^{(X)}$$

with Grassmann tensor

$$\overline{K}^{(X)} = (c_{x+\hat{1},1})^{f_{x+\hat{1},1}} \left[\prod_{\nu=2}^{d} (\tilde{c}_{X,\nu})^{\tilde{f}_{X,\nu}} \right] \left[\coprod_{\nu=2}^{d} \left(d\tilde{c}_{X,-\nu} \right)^{\tilde{f}_{X,-\nu}} \right] (dc_{x,-1})^{f_{x,-1}}$$

and numeric tensor

$$\widetilde{\mathscr{T}}^{(X)}_{j_{x,-1} j_{x+\hat{1},1} (j_{x,-\nu}, j_{x+\hat{1},-\nu})(j_{x,\nu}, j_{x+\hat{1},\nu})|_{\nu\neq 1}} = \sigma_{[f_x f_{x+\hat{1}}]} \sum_{j_{x,1}} T^{(x)}_{[j_x]} T^{(x+\hat{1})}_{[j_{x+\hat{1}}]}$$

where a local sign factor $\sigma_{[f_x f_{x+\hat{1}}]}$ was generated by reordering the Grassmann variables in $\mathscr{K}^{(x,x+\hat{1})}$ to perform these integrations

Truncate numeric tensor

- Perform HOSVD of $\widetilde{\mathscr{T}}^{(X)}_{j_{x,-1} j_{x+\hat{1},1} (j_{x,-\nu}, j_{x+\hat{1},-\nu})(j_{x,\nu}, j_{x+\hat{1},\nu})|_{\nu\neq 1}}$ to reduce the dimension of perpendicular directions from $D^2 \to D$
  $\to$ truncated coarse grid numeric tensor $\overline{T}^{(X)}_{j_{x,-1} j_{x+\hat{1},1} \tilde{j}_{X,-\nu} \tilde{j}_{X,\nu}|_{\nu\neq 1}}$
- Grassmann-parity structure: after HOSVD the nonzero components of truncated coarse lattice numeric tensor still have definite Grassmann parities
- After one blocking step → shape of the (approximate) coarse-lattice partition function is identical to fine-lattice partition function, but now written as a function of the coarse lattice indices and Grassmann variables.

Blocking the complete lattice

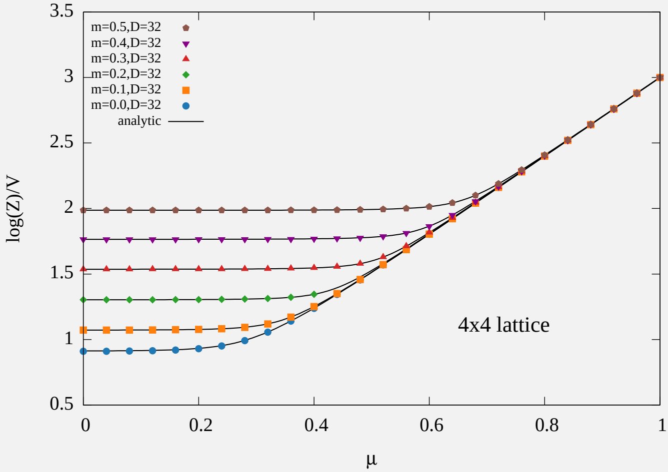
- Same procedure can be repeated to contract any other direction
- Iterate until lattice is reduced to a single point → integrate out the remaining Grassmann variables after applying the boundary conditions, then trace out the numeric tensor → Z
- Compute observables using (stabilized) finite differences or impurity method

Remark on implementation

- Grassmann-parity structure → cost of GHOTRG for sQCD similar to that of HOTRG for purely numeric tensor networks.
- Without this property: cost of algorithm would increase with factor 2^{4d-1} (2^7, 2^{11}, 2^{15} in 2,3,4 dimensions)
- Implementation more complex because local sign factors have to be built-in during the contraction and truncation of the numeric tensors

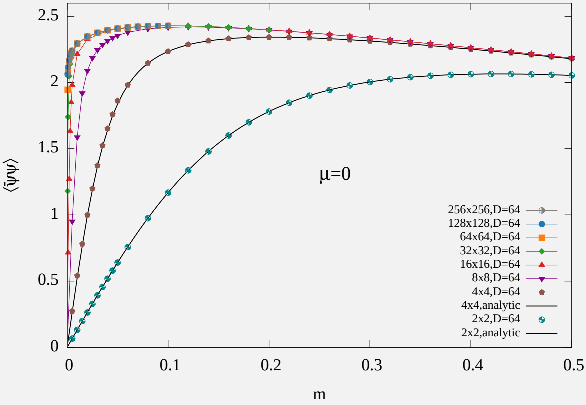
Results: sQCD GHOTRG in two dimensions

$\log Z/V$ versus μ and m – GHOTRG versus exact result

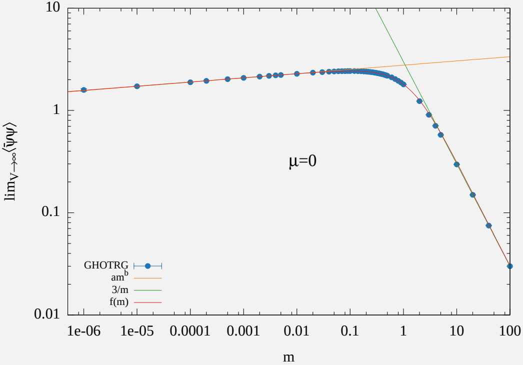


Chiral condensate versus m and V for $\mu = 0$

$$\boxed{\langle\bar{\psi}\psi\rangle = \frac{1}{V}\,\frac{\partial \ln Z}{\partial m}}$$



Study of dynamical chiral symmetry breaking for $D, V \to \infty$



Empirical fit:

$$f(m) = \frac{am^b + cm}{1 + dm + (c/3)m^2}$$

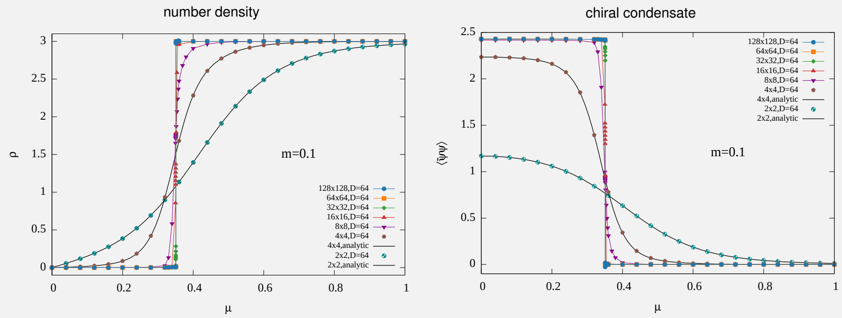
Asymptotic:

$$f(m) \sim \begin{cases} 3/m & \text{for large masses} \\ am^b & \text{for } m < 0.005 \end{cases}$$

Fitted parameter values:
$a = 2.77$, $b = 0.0409$
$c = 1.05$, $d = 0.770$

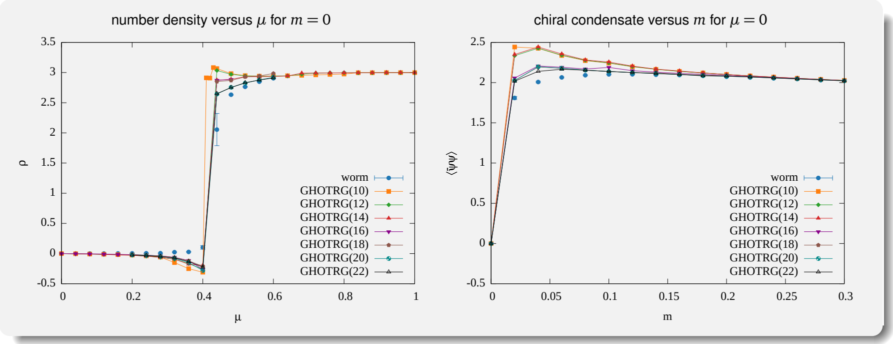
Chiral symmetry not dynamically broken in two-dimensional strong-coupling QCD with (two tastes of) staggered quarks

Number density and chiral condensate versus μ and V



Hint of first order phase transition

Preliminary results in three dimensions on 4^3 lattice


number density versus μ for $m = 0$

chiral condensate versus m for $\mu = 0$

Outlook

Hierarchical tensor (HT) factorization for HOTRG

- Clear need to increase the bond dimension D for $d = 3$
- For $d = 3$: HOTRG and GHOTRG scale as D^{11}
  → extend our existing HT-HOTRG, which scales like D^{6}, to HT-GHOTRG.

More work in progress

- Apply HT-GHOTRG to sQCD in three and four dimensions
- Develop tensor network and GHOTRG for QCD in next-to-leading order in β-expansion

Supplemental material

Change to dual variables

Integrate out the SU(3) matrices:

$$Z = \int \left[\prod_x d\psi_x d\bar{\psi}_x\right] \prod_x e^{2mM_x} \prod_{\nu=1}^{d} z_{x,\nu}$$

where

$$z_{x,\nu} = \eta_{x,\nu}\zeta_{\nu}\bar{B}_x B_{x+\hat{\nu}} - \eta_{x,\nu}\zeta_{-\nu}\bar{B}_{x+\hat{\nu}}B_x + \sum_{k_{x,\nu}=0}^{3} \frac{(3-k_{x,\nu})!}{3!k_{x,\nu}!}\left(\gamma^{2\delta_{\nu,1}}M_x M_{x+\hat{\nu}}\right)^{k_{x,\nu}}$$

with mesons $M_x = \bar{\psi}_x\psi_x$, baryons $B_x = \frac{1}{3!}\epsilon_{i_1i_2i_3}\psi_{x,i_1}\psi_{x,i_2}\psi_{x,i_3}$, antibaryons $\bar{B}_x = \frac{1}{3!}\epsilon_{i_1i_2i_3}\bar{\psi}_{x,i_3}\bar{\psi}_{x,i_2}\bar{\psi}_{x,i_1}$ and

$$\zeta_{\nu} = \begin{cases} \gamma^3 \exp(\pm 3\mu) & \text{for } \nu = \pm 1\,, \\ 1 & \text{else} \end{cases}$$

Tensor formulation of Z

Tensor network formulation: integrate out mesons but not baryons, as latter would introduce non-local sign factors

$$Z = \sum_{j} \int \prod_{x} S^{(x)}_{[j_x]} G^{(x)}_{[l_x]}$$

with local numeric and Grassmann tensors:

$$S^{(x)}_{[j_x]} = \delta_{x\in\mathscr{B}} \prod_{\nu=1}^{d} \eta_{x,\nu}^{|l_{x,\nu}|} \sqrt{\xi_\nu(l_{x,\nu})\xi_\nu(l_{x,-\nu})} + \delta_{x\in\mathscr{M}}\, h(n_x) \prod_{\nu=1}^{d} \sqrt{\alpha_\nu(k_{x,\nu})\alpha_\nu(k_{x,-\nu})}$$

$$G^{(x)}_{[l_x]} = (dB_x)^{\sum_\nu (l^-_{x,\nu}+l^+_{x,-\nu})} (d\bar{B}_x)^{\sum_\nu (l^+_{x,\nu}+l^-_{x,-\nu})} \prod_{\nu=1}^{d} (B_x \bar{B}_{x+\hat{\nu}})^{l^-_{x,\nu}} (\bar{B}_x B_{x+\hat{\nu}})^{l^+_{x,\nu}}$$

- Each term in sum is characterized by its indices $\boldsymbol{j} = (j_{1,1}, \ldots, j_{V,d})$
- Notation: indices: $[j_x] \equiv j_{x,-1} j_{x,1} \ldots j_{x,-d} j_{x,d}$ and $[l_x] \equiv l_{x,-1} l_{x,1} \ldots l_{x,-d} l_{x,d}$
- $j \in \{0,1,2,3,4,5\} \to (k,l) \in \{(0,0),(1,0),(2,0),(3,0),(0,-1),(0,+1)\}$, $l^{\pm} = \delta_{l,\pm 1}$

Tensor weigths

- Baryonic sites in $\boldsymbol{j}$:
$$k_{x,-\nu} = k_{x,\nu} = 0, \forall\, \nu$$
$$\sum_\nu (l^-_{x,\nu} + l^+_{x,-\nu}) = 1 \wedge \sum_\nu (l^+_{x,\nu} + l^-_{x,-\nu}) = 1$$
- Mesonic sites in $\boldsymbol{j}$:
$$l_{x,-\nu} = l_{x,\nu} = 0, \forall\, \nu$$
$$n_x = 3 - \sum_\nu (k_{x,-\nu} + k_{x,\nu}) \geq 0$$

Weights

baryonic:
$$\xi_\nu(l_{x,\nu}) = \begin{cases} \gamma^{3|l_{x,\nu}|} \exp(l_{x,\nu} 3\mu) & \text{if } \nu = 1 \\ 1 & \text{if } \nu \neq 1 \end{cases}$$

k-mesonic:
$$\alpha_\nu(k_{x,\nu}) = \frac{(3 - k_{x,\nu})!}{3! k_{x,\nu}!} \gamma^{2k_{x,\nu}\delta_{\nu,1}}$$

mass:
$$h(n_x) = \frac{3!}{n_x!}(2m)^{n_x}, \qquad n_x = 3 - \sum_\nu (k_{x,-\nu} + k_{x,\nu})$$

Conserved Grassmann parity

Ready to perform HOSVD of $\widetilde{\mathscr{T}}^{(X)}_{j_{x,-1} j_{x+\hat{1},1} (j_{x,-\nu}, j_{x+\hat{1},-\nu})(j_{x,\nu}, j_{x+\hat{1},\nu})|_{\nu \neq 1}}$ to reduce the dimension of perpendicular directions from $D^2 \to D$

Matrization $M^{\nu_\pm}$ of coarse grid tensor is block diagonal in Grassmann parity of the fat index → singular vectors have definite parity → nonzero components of truncated coarse lattice numeric tensor have definite Grassmann parities.

$$M^- = \left(\begin{array}{cc} \overbrace{M^-_{00}}^{(\tilde{f}_{X,2} + f_{x,-1} + f_{x+\hat{1},-1}) \bmod 2 = 0} & 0 \\ 0 & \underbrace{M^-_{11}}_{(\tilde{f}_{X,2} + f_{x,-1} + f_{x+\hat{1},-1}) \bmod 2 = 1} \end{array}\right) \begin{array}{l} \left.\vphantom{M}\right\} \tilde{f}_{X,-2} = 0 \\ \left.\vphantom{M}\right\} \tilde{f}_{X,-2} = 1 \end{array}$$

$$U = \left(\begin{array}{cc} \underbrace{U_{00}}_{\tilde{g}_{X,-2} = 0} & 0 \\ 0 & \underbrace{U_{11}}_{\tilde{g}_{X,-2} = 1} \end{array}\right) \begin{array}{l} \left.\vphantom{U}\right\} \tilde{f}_{X,-2} = 0 \\ \left.\vphantom{U}\right\} \tilde{f}_{X,-2} = 1 \end{array}$$

Applying the truncation matrices

- Due to the block-diagonal nature of U:

$$\sum_{j_{x,-2},j_{x+\hat{\imath},-2}} U_{(j_{x,-2},j_{x+\hat{\imath},-2})\tilde{j}_{X,-2}} \tilde{\mathscr{T}}^{(X)}_{j_{x,-1}j_{x+\hat{\imath},1}(j_{x,-2},j_{x+\hat{\imath},-2})(j_{x,2},j_{x+\hat{\imath},2})} \overline{K}^{(X)}_{f_{x,-1}f_{x+\hat{\imath},1}\tilde{f}_{X,-2}\tilde{f}_{X,2}}$$

$$= \overline{K}^{(X)}_{f_{x,-1}f_{x+\hat{\imath},1}\tilde{g}_{X,-2}\tilde{f}_{X,2}} \sum_{j_{x,-2},j_{x+\hat{\imath},-2}} U_{(j_{x,-2},j_{x+\hat{\imath},-2})\tilde{j}_{X,-2}} \tilde{\mathscr{T}}^{(X)}_{j_{x,-1}j_{x+\hat{\imath},1}(j_{x,-2},j_{x+\hat{\imath},-2})(j_{x,2},j_{x+\hat{\imath},2})}$$

  where $\tilde{g}_{X,-2} \equiv \tilde{g}_{X,-2}(\tilde{j}_{X,-2})$ is the Grassmann parity of the new index $\tilde{j}_{X,-2}$.

- This leads to the truncated coarse grid numeric tensor $\overline{T}^{(X)}_{j_{x,-1}j_{x+\hat{\imath},1}\tilde{j}_{X,-2}\tilde{j}_{X,2}}$

After one blocking step → shape of the (approximate) coarse-lattice partition function is identical to fine-lattice partition function, but now written as a function of the coarse lattice indices and Grassmann variables.

Convergence as a function of the bond dimension D