Matrix product state simulations with general non-Abelian symmetries

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[1] **MAW**, C. P. Moca, Ö. Legeza, and G. Zaránd, arXiv:2007.12418 (accepted to PRB)

bme-mta exotic quantum phases group
BME PHYSICS
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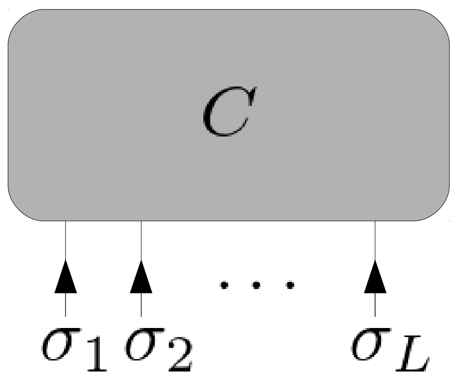
Outline

- **Short introduction to Matrix Product States**
- **MPS for general non-Abelian symmetries**
- **NA tensors and their algebraic properties**
- **Demonstration: NA-TEBD simulation of the post quench dynamics in the SU(3) Hubbard model**

Introduction to Matrix Product States

Generic pure state:

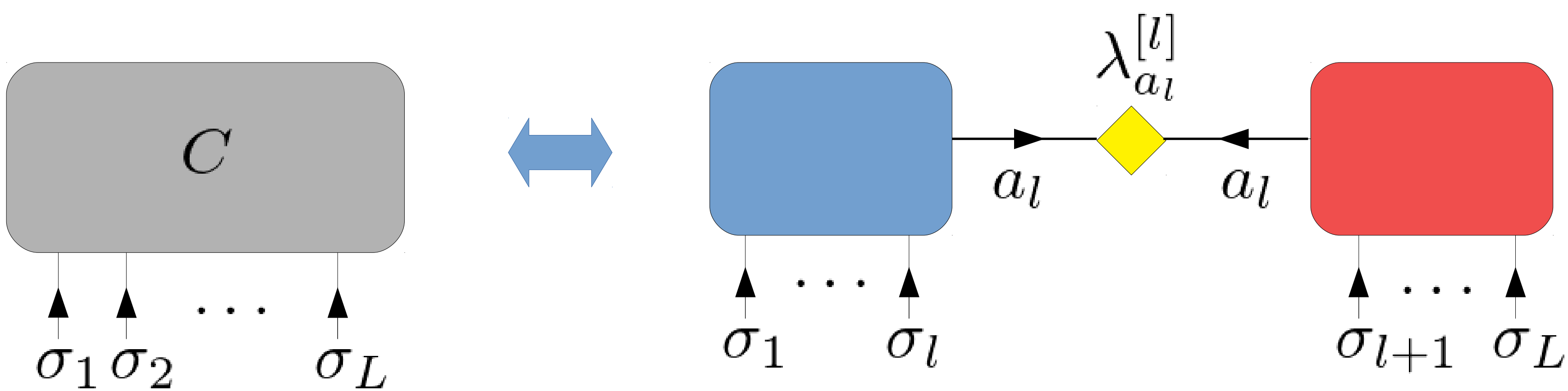
$$|\Psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} C_{\sigma_1\sigma_2\ldots\sigma_L} |\sigma_1\rangle \otimes \cdots \otimes |\sigma_L\rangle \qquad \dim = d^L$$



Cut in two parts! $\text{left} = [1, \ldots, l]$
$\text{right} = [l+1, \ldots, L]$

Schmidt decomposition

$$|\Psi\rangle = \sum_{a_l} \lambda^{[l]}_{a_l} |a_l\rangle_{\text{left}} \otimes |a_l\rangle_{\text{right}}$$



Introduction to Matrix Product States

Moving the cut:

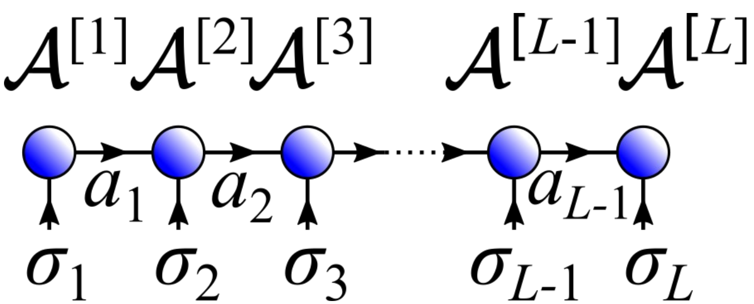
$$|a_{l+1}\rangle_{\text{left}} = \sum_{a_l,\sigma_{l+1}} \mathcal{A}^{[l]\,a_{l+1}}_{a_l\,\sigma_{l+1}} |a_l\rangle_{\text{left}} |\sigma_{l+1}\rangle$$

"Left unitarity":

$$\sum_{\sigma,a} \mathcal{A}^{[l]\,a'}_{\;a\,\sigma} \left(\mathcal{A}^{[l]\,a''}_{\;a\,\sigma}\right)^* = \delta^{a'}_{a''} \,.$$

Left canonical MPS ansatz:

$$|\Psi\rangle = \sum_{a_1,\ldots a_{L-1}} \sum_{\sigma_1,\ldots\sigma_L} \mathcal{A}^{[1]\,a_1}_{\sigma_1} \mathcal{A}^{[2]\,a_2}_{a_1\sigma_2} \ldots \mathcal{A}^{[L]}_{a_{L-1}\sigma_L} |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \cdots \otimes |\sigma_L\rangle$$



Approximation: truncation

$$|\Psi\rangle \approx \sum_{a_l=1}^{M} \lambda^{[l]}_{a_l} |a_l\rangle_{\text{left}} \otimes |a_l\rangle_{\text{right}}$$

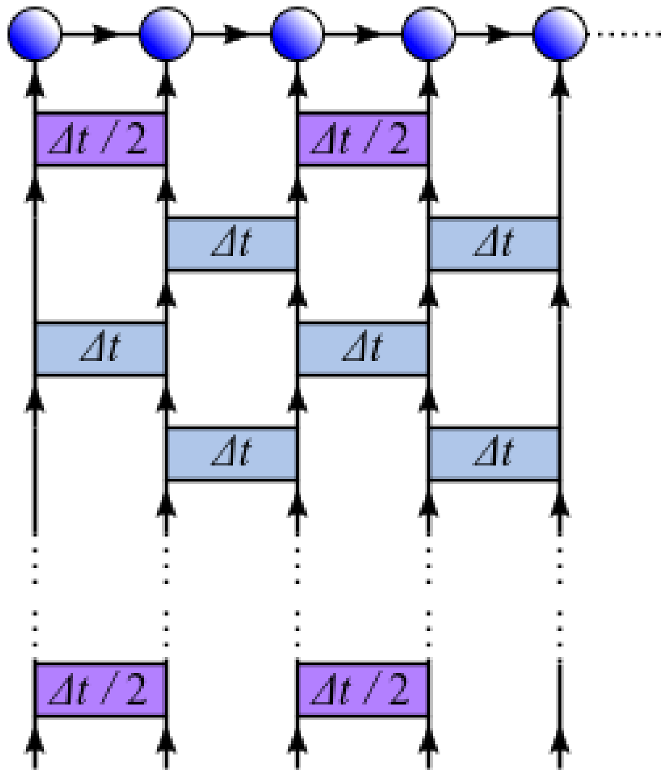
Truncation error: $\displaystyle\sum_{a_l>M} \left|\lambda^{[l]}_{a_l}\right|^2$

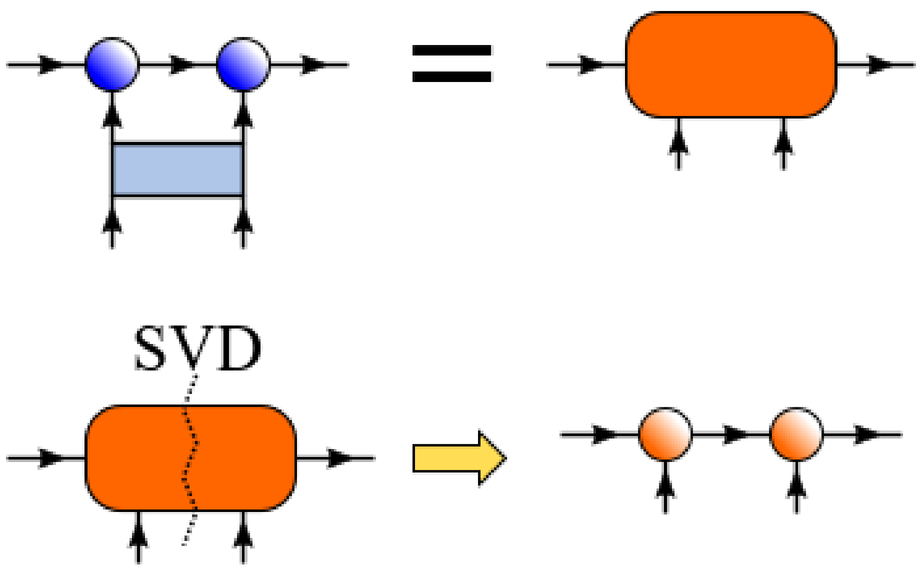
Real time dynamics: the TEBD algorithm

$$\hat{H} = \sum_i \hat{h}^{(2)}_{i,i+1} = \hat{H}_{\text{even}} + \hat{H}_{\text{odd}} = \sum_k \hat{h}^{(2)}_{2k,2k+1} + \sum_k \hat{h}^{(2)}_{2k-1,2k}$$

$$e^{-i\hat{H}\Delta t} \approx e^{-i\hat{H}_{\text{even}}\Delta t/2} e^{-i\hat{H}_{\text{odd}}\Delta t} e^{-i\hat{H}_{\text{even}}\Delta t/2}$$

The Time Evolving Block Decimation algorithm:





Symmetries

Symmetry group: $\mathcal{G}$ ⟺ **Symmetry transformations:** $\hat{U}(g) \quad g \in \mathcal{G}$

Symmetric model: ⟺ $\left[\hat{H}, \hat{\mathcal{U}}(g)\right] = 0\,, \quad \forall g \in \mathcal{G}$

Locally generated symmetries:

$$\hat{\mathcal{U}}(g) = \hat{\mathcal{U}}_1(g) \otimes \hat{\mathcal{U}}_2(g) \otimes \cdots \otimes \hat{\mathcal{U}}_L(g)$$

Single-site transformations

Examples

- U(1) charge $\quad \hat{U}_i(\varphi) = e^{i\varphi \hat{n}_i}$
- U(1) spin-z $\quad \hat{U}_i(\varphi) = e^{i\varphi \hat{S}^z_i}$
- SU(2) spin $\quad \hat{U}_i(\varphi, \vec{n}) = e^{i\varphi \vec{n}\cdot\vec{\hat{S}}_i}$
- **SU(3) x U(1)** $\quad \hat{U}_i(\varphi, \underline{\underline{\mathbf{U}}}) = e^{i\varphi \hat{n}_i} \sum_{a,b} \mathbf{U}_{ab}\, c^\dagger_a c_b$

  Color charge

Transformation in the color space

Symmetries

Structure of the Hilbert space

$$\mathcal{H} = \mathrm{span}\left\{|\Gamma; t, m\rangle\right\}$$

- Γ : Representation index
- t : Multiplet index (within sector Γ)
- m : Internal index, $m = [1 \ldots \mathrm{dim}_\Gamma]$

Hilbert space of a single site

$$\mathcal{H}_i = \mathrm{span}\left\{\left|\Gamma_i^{\mathrm{loc}}; \tau_i, \mu_i\right\rangle\right\}$$

Schmidt-decomposition of singlet (trivial) states

$$|\Psi\rangle = \sum_{\Gamma_l} \sum_{t_l} \sum_{m_l=1}^{\mathrm{dim}_{\Gamma_l}} \lambda^{[l]}(\Gamma_l)_{t_l} \, |\Gamma_l; t_l, m_l\rangle_{\mathrm{left}} \left|\overline{\Gamma}_l; t_l, \overline{m}_l\right\rangle_{\mathrm{right}}$$

States in the conjugate representation

Non singlet states? $\left|\Psi_{\Gamma,M}\right\rangle$

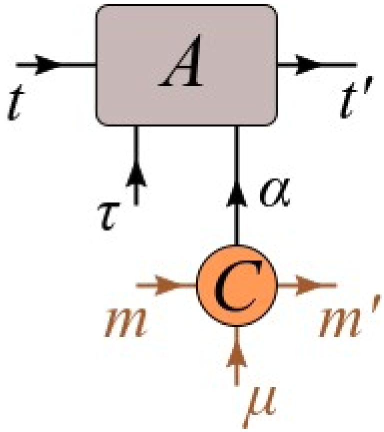
$$\left|\tilde{\Psi}\right\rangle = \sum_M \frac{1}{\sqrt{\mathrm{dim}_\Gamma}} \left|\Psi_{\Gamma,M}\right\rangle \otimes \left|\overline{\Gamma}, \overline{M}\right\rangle$$

Auxiliary site

Non-Abelian MPS states

Moving the cut

$$|\Gamma';t',m'\rangle = \sum_{\Gamma,\Gamma^{\rm loc}} \sum_{t,\tau} \sum_{\alpha} A(\Gamma,\Gamma^{\rm loc},\Gamma')^{t'}_{t\,\tau\,\alpha} \sum_{m,\mu} C(\Gamma,\Gamma^{\rm loc},\Gamma')^{m'\,\alpha}_{m\,\mu} \, |\Gamma;t,m\rangle \otimes |\Gamma^{\rm loc};\tau,\mu\rangle$$



Generalized Clebsch-Gordan coefficients

$$C(\Gamma,\Gamma^{\rm loc},\Gamma')^{m'\,\alpha}_{m\,\mu} = \left(\Gamma,m;\Gamma^{\rm loc},\mu \middle| \, \Gamma',m'\right)_{\alpha}$$

Outer multiplicity: α

- Labels the multiplets of the same Γ' in the product $\Gamma \otimes \Gamma^{\rm loc}$.
- It is always trivial for Abelian groups and also for SU(2).

U(1) charge: $|n_1\rangle \otimes |n_2\rangle = |n_1 + n_2\rangle$

SU(2) spin: $|S_1\rangle \otimes |S_2\rangle \Rightarrow |S\rangle \;, \quad |S_1 - S_2| \leq S \leq S_1 + S_2$

- **Nontrivial multiplicities for SU(3) (and also SU(n>3))**

Non-Abelian MPS states

$$|\Gamma';t',m'\rangle = \sum_{\Gamma,\Gamma^{\mathrm{loc}}} \sum_{t,\tau} \sum_{\alpha} A(\Gamma,\Gamma^{\mathrm{loc}},\Gamma')^{t'}_{t\,\tau\,\alpha} \sum_{m,\mu} C(\Gamma,\Gamma^{\mathrm{loc}},\Gamma')^{m'\,\alpha}_{m\,\mu} \, |\Gamma;t,m\rangle \otimes |\Gamma^{\mathrm{loc}};\tau,\mu\rangle$$

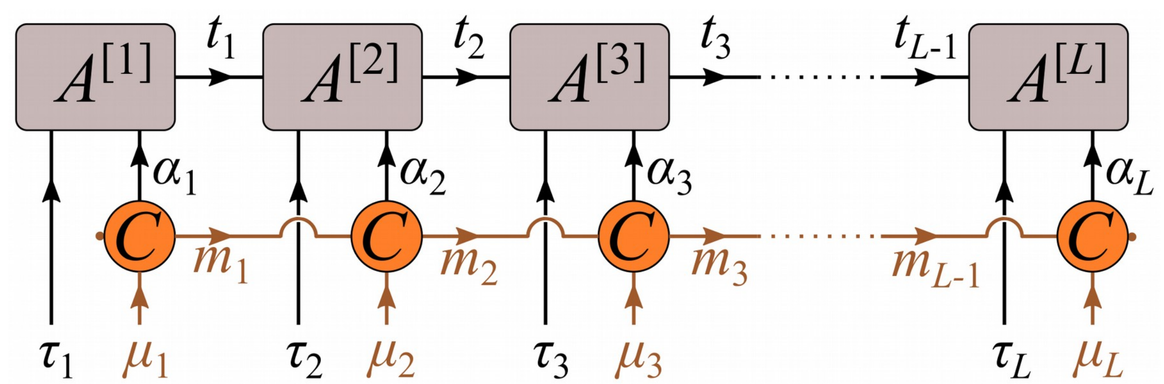
Iteration

$$|\Psi\rangle = \sum_{\{\Gamma_l^{\mathrm{loc}}\}} \sum_{\{\Gamma_l\}} \sum_{\{t_l\}} \sum_{\{\tau_l\}} \sum_{\{\alpha_l\}} A^{[1]}(\{\Gamma\}^{[1]})^{t_1}_{\tau_1\,\alpha_1}\, A^{[2]}(\{\Gamma\}^{[2]})^{t_2}_{t_1\,\tau_2\,\alpha_2} \cdots A^{[L]}(\{\Gamma\}^{[L]})_{t_{L-1}\,\tau_L\,\alpha_L}$$

$$\sum_{\{m_l\}} \sum_{\{\mu_l\}} C(\{\Gamma\}^{[1]})^{m_1\,\alpha_1}_{0\,\mu_1}\, C(\{\Gamma\}^{[2]})^{m_2\,\alpha_2}_{m_1\,\mu_2} \cdots C(\{\Gamma\}^{[L]})^{0\,\alpha_L}_{m_{L-1}\,\mu_L}$$

$$|\Gamma_1^{\mathrm{loc}};\tau_1,\mu_1\rangle \otimes |\Gamma_2^{\mathrm{loc}};\tau_2,\mu_2\rangle \otimes \cdots \otimes |\Gamma_L^{\mathrm{loc}};\tau_L,\mu_L\rangle \;,$$

$$\{\Gamma\}^{[i]} = (\Gamma_{i-1}, \Gamma_i^{\mathrm{loc}}, \Gamma_i)$$

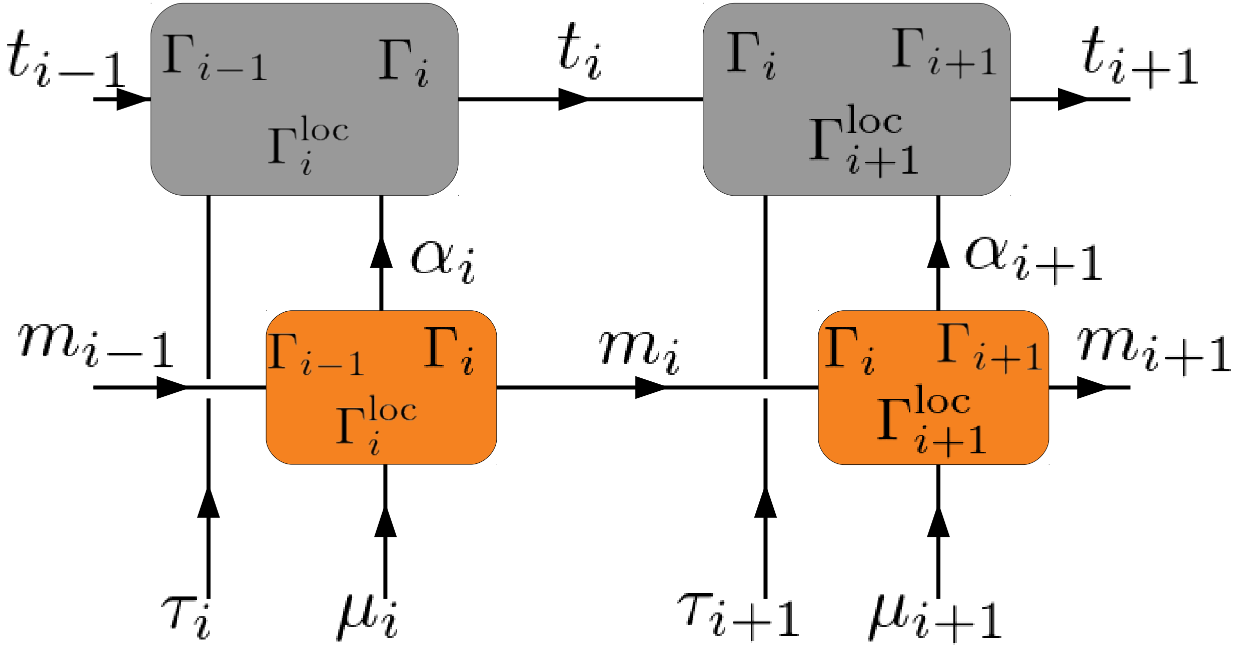


- **The upper layer contains all the relevant information**
- **Bond-dimension reduction: multiplets vs. states**
- **Block structure (NA-tensors)**

NA-tensors

$$|\Gamma';t',m'\rangle = \sum_{\Gamma,\Gamma^{\rm loc}} \sum_{t,\tau} \sum_{\alpha} A(\Gamma,\Gamma^{\rm loc},\Gamma')^{t'}_{t\,\tau\,\alpha} \sum_{m,\mu} C(\Gamma,\Gamma^{\rm loc},\Gamma')^{m'\,\alpha}_{m\,\mu} |\Gamma;t,m\rangle \otimes |\Gamma^{\rm loc};\tau,\mu\rangle$$

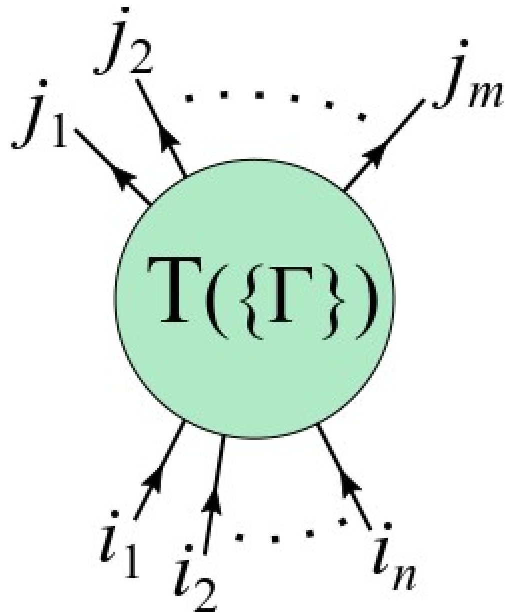
- **Block-sparse tensors, block key:** $\{\Gamma\} = (\Gamma, \Gamma^{\rm loc}, \Gamma')$
- **Matching of irrep labels**
  - The A and C tensors on the same site share all three irrep labels
  - The two A tensors on adjacent sites share the "bond" irrep label Γ_i
  - The two C tensors on adjacent sites share the "bond" irrep label Γ_i



- **Dependencies** $\mathrm{dep}(t_i) = \Gamma_i$ $\quad \mathrm{dep}(\tau_i) = \Gamma_i^{\rm loc}$

$$\mathrm{dep}(m_i) = \Gamma_i \qquad \mathrm{dep}(\mu_i) = \Gamma_i^{\rm loc}$$

$$\mathrm{dep}(\alpha_i) = (\Gamma_{i-1}, \Gamma_i^{\rm loc}, \Gamma_i)$$



$$T(\{\Gamma\})^{j_1 \dots j_m}_{i_1 \dots i_n} \qquad \{\Gamma\} = (\Gamma_1 \dots \Gamma_k)$$

1) Incoming and outgoing legs can be contracted. Their dependencies must match.

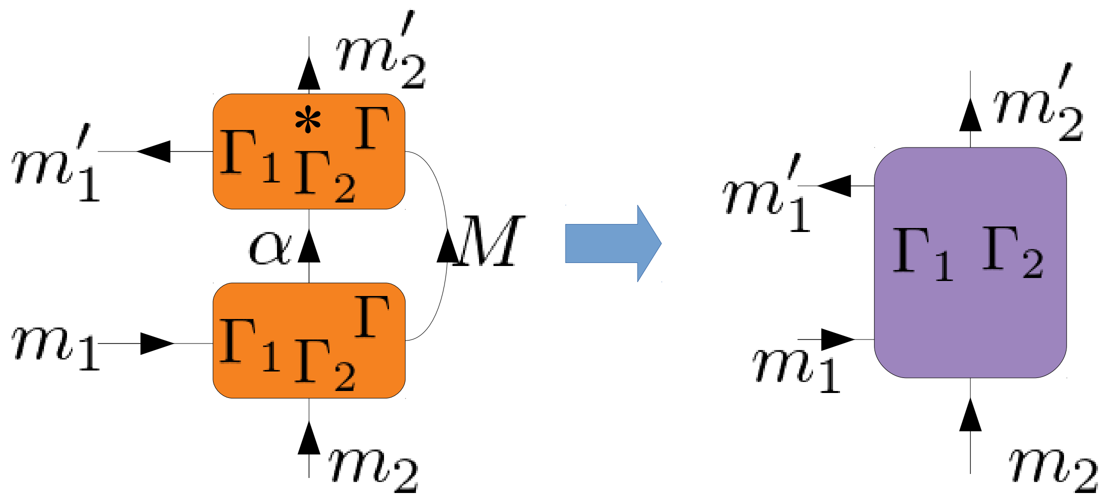
2) The result tensor's blocks are labeled by all the irreps, but the matched irrep labels appear just once.

Additional rule:

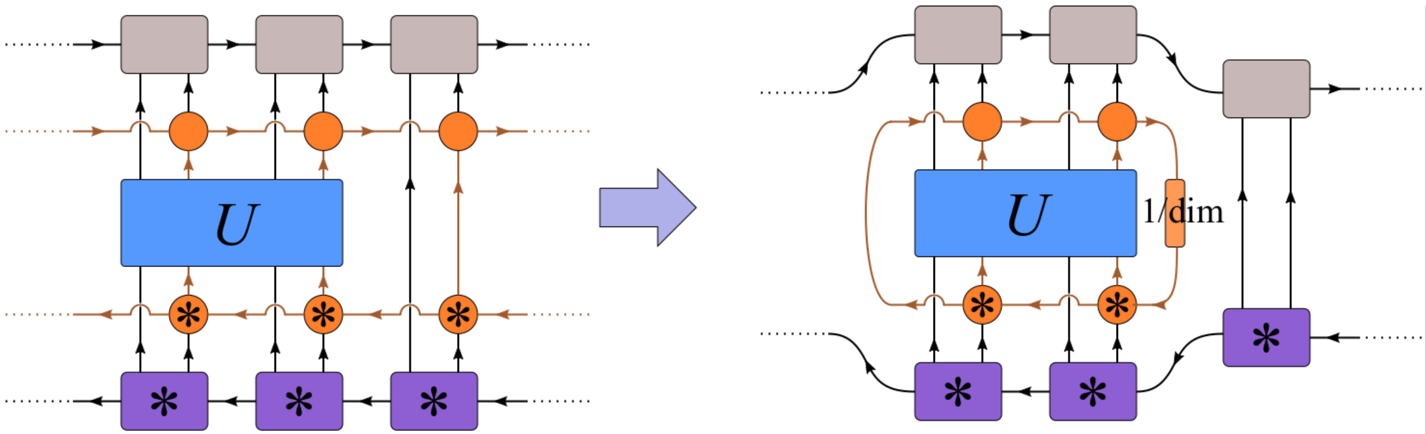
3) If there is one or more representation indices in the result tensor that no remaining (uncontracted) legs depend on, then blocks must be summed over these representation indices.

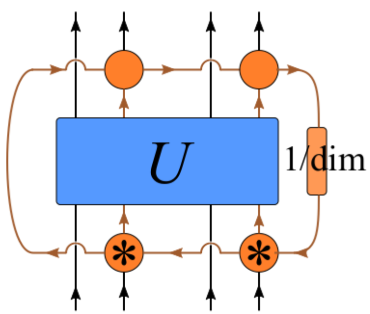
Motivation to 3)

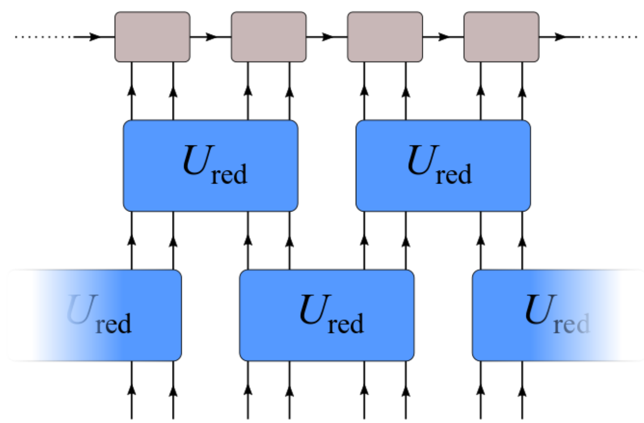
$$\sum_{M,\alpha,\Gamma} (\Gamma_1, m_1; \Gamma_2, m_2 | \, \Gamma, M)_\alpha \left[(\Gamma_1', m_1'; \Gamma_2', m_2' | \, \Gamma, M)_\alpha \right]^* = \delta^{(\Gamma_1' \, m_1' \;\; \Gamma_2' \, m_2')}_{(\Gamma_1 \, m_1 \;\; \Gamma_2 \, m_2)}$$



Non-Abelian TEBD



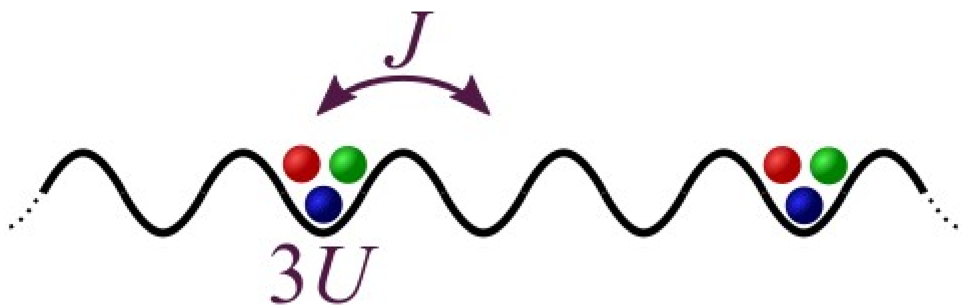
$U_{\mathrm{red}} =$ 



$$U_{\mathrm{red}}(\{\Gamma\})^{\tau_1\alpha_1\ \tau_2\alpha_2}_{\tau_1'\alpha_1'\ \tau_2'\alpha_2'}$$

$$\{\Gamma\} = (\Gamma_{\mathrm{left}}, \Gamma_1^{\mathrm{loc}}, \Gamma_1^{\mathrm{loc}\prime}, \Gamma_{\mathrm{center}}, \Gamma'_{\mathrm{center}}, \Gamma_2^{\mathrm{loc}}, \Gamma_2^{\mathrm{loc}\prime}, \Gamma_{\mathrm{right}})$$

Quantum Quench in the SU(3) Hubbard model



$$\hat{H} = -t \sum_{i,a} \left(c^\dagger_{i,a} c_{i+1,a} + c^\dagger_{i+1,a} c_{i,a} \right) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

$$|\Psi_0\rangle = \left(\prod_{i=3k} \prod_{a=1}^{3} c^\dagger_{i,a} \right) |0\rangle$$

$$n_i = \sum_{a=1}^{3} c^\dagger_{i,a} c_{i,a}$$

Measurements:

$$\langle n_i(t) \rangle = ?$$

$$\langle n_i(t) n_j(t) \rangle = ?$$

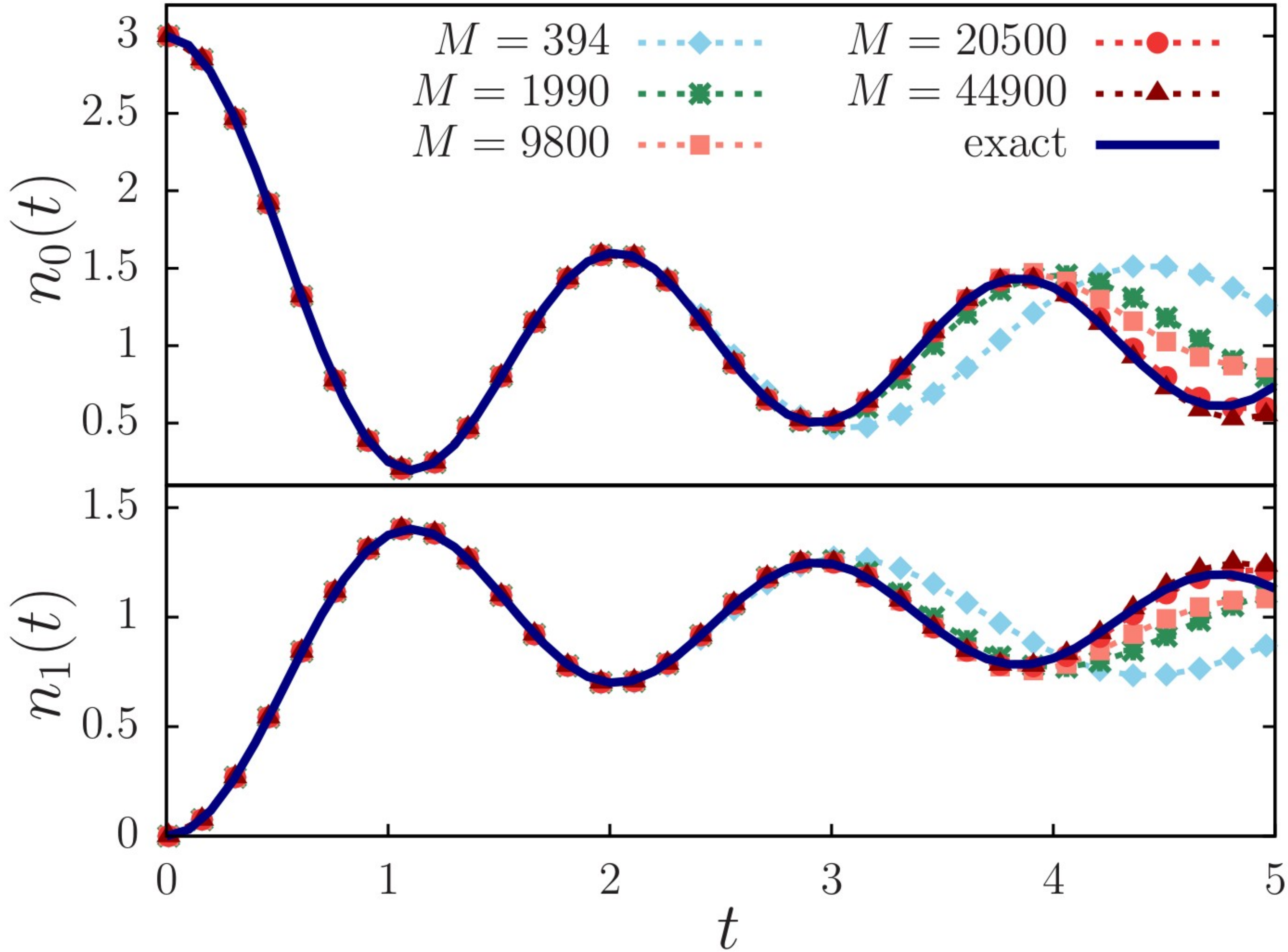
$$S_{\mathrm{vN}} = ?$$

Technical questions:

- How do these depend on the bond-dimension?
- How long can we simulate?

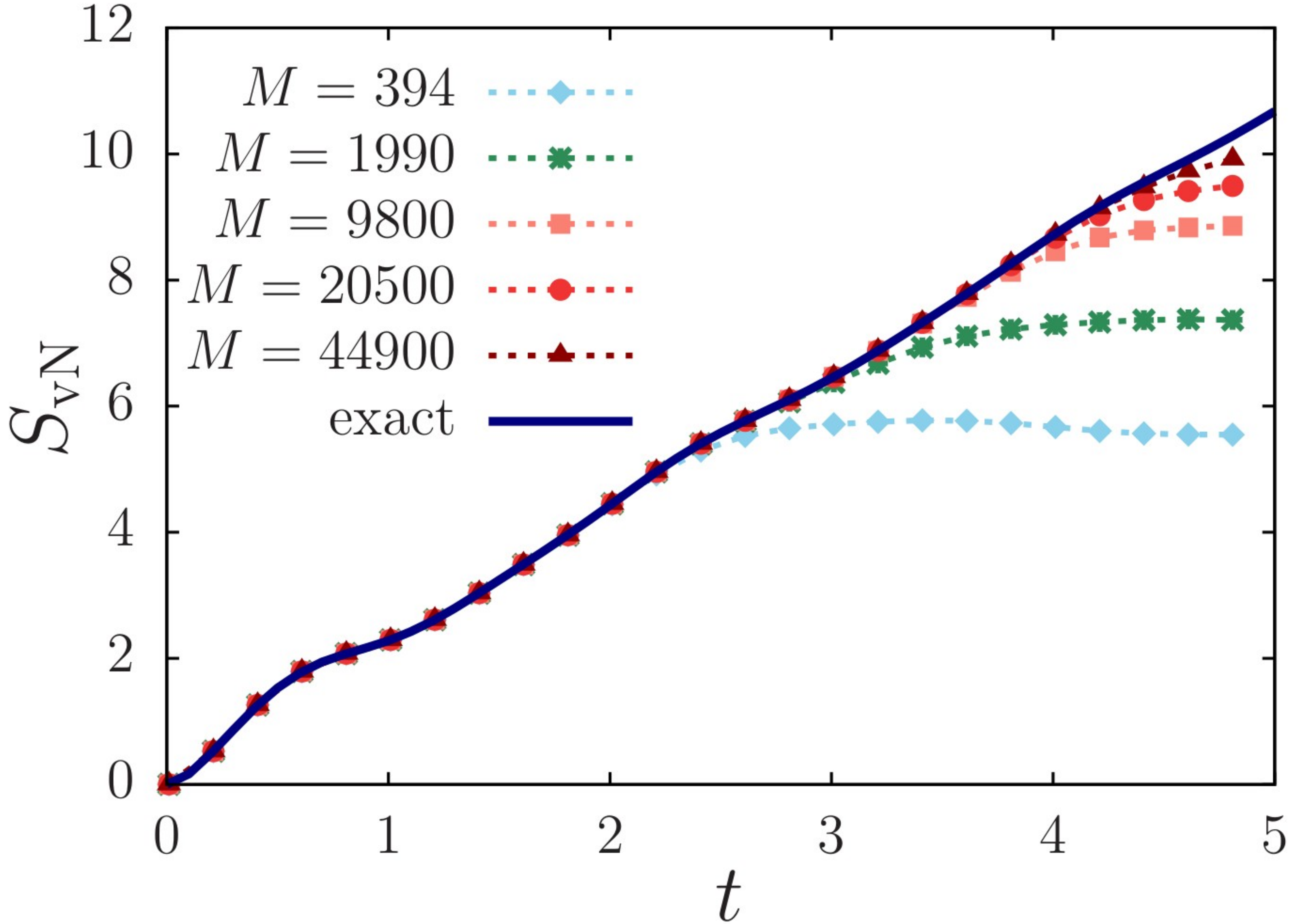
Quantum Quench in the SU(3) Hubbard model

Data for $U = 0$



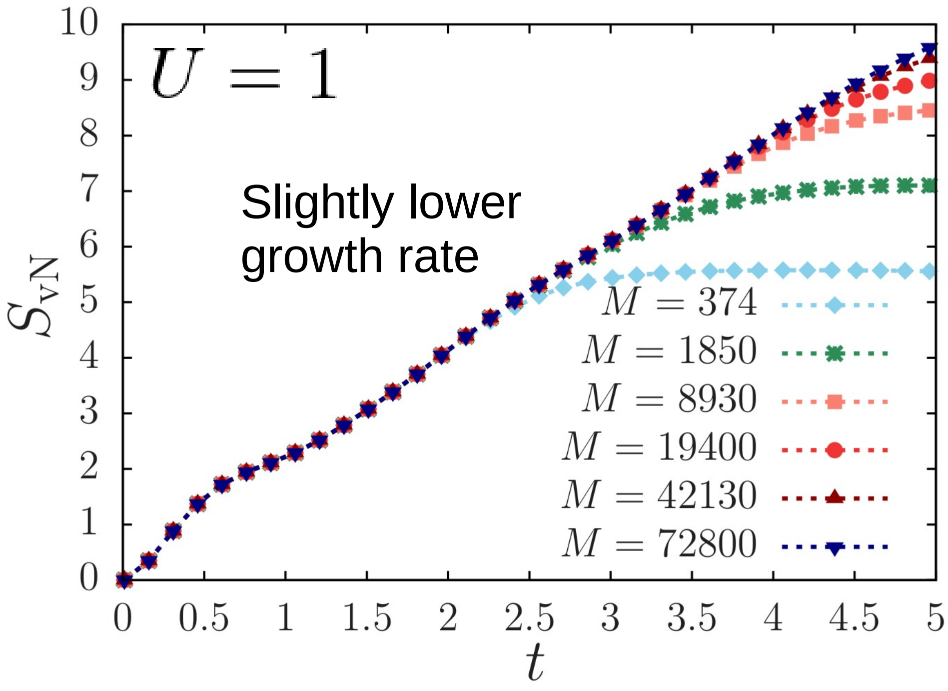
Quantum Quench in the SU(3) Hubbard model

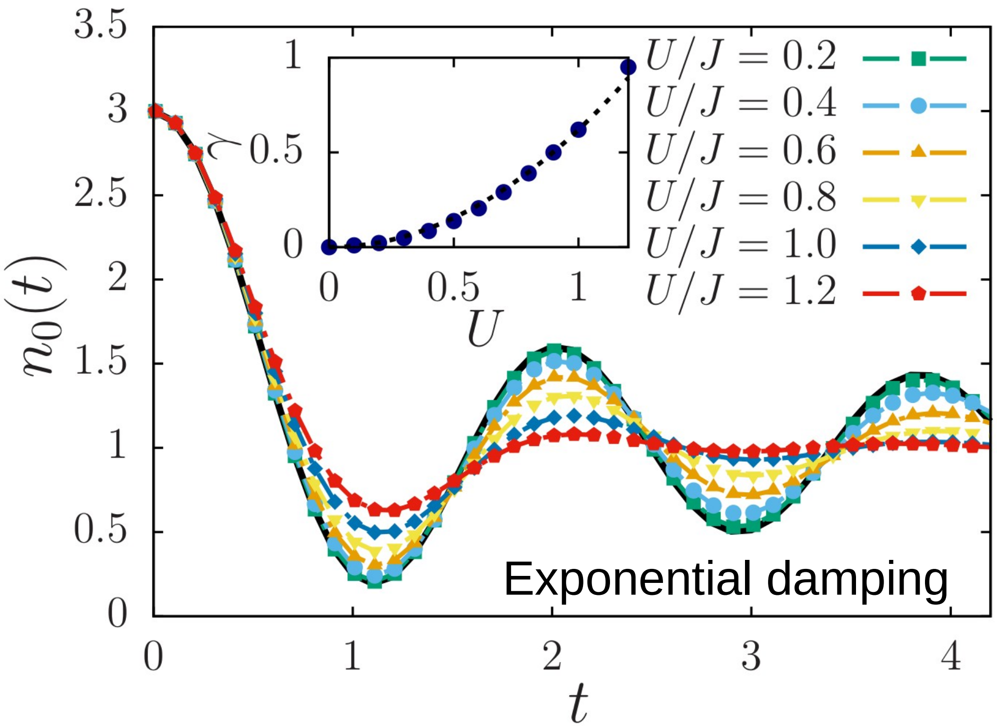
Data for $U = 0$

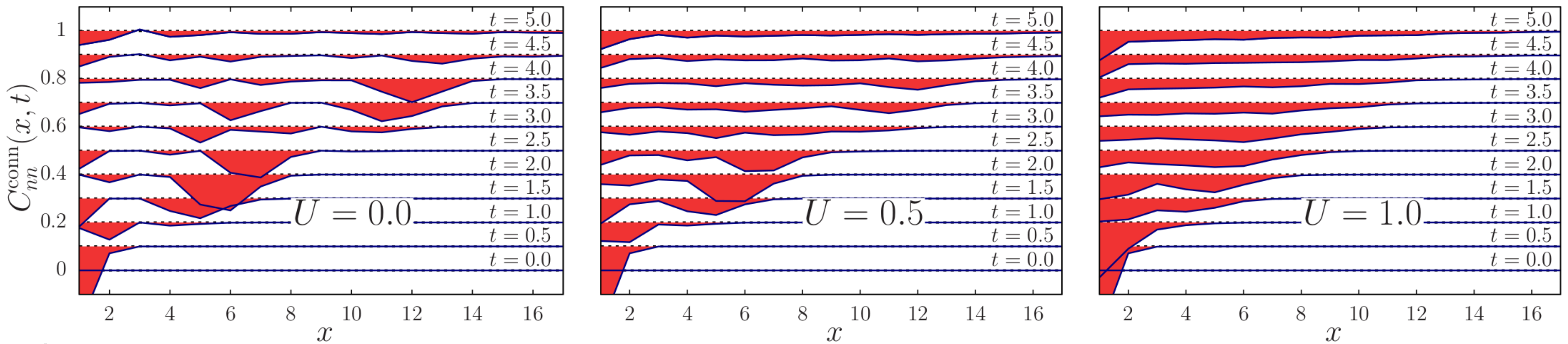


Quantum Quench in the SU(3) Hubbard model

Data for $U > 0$



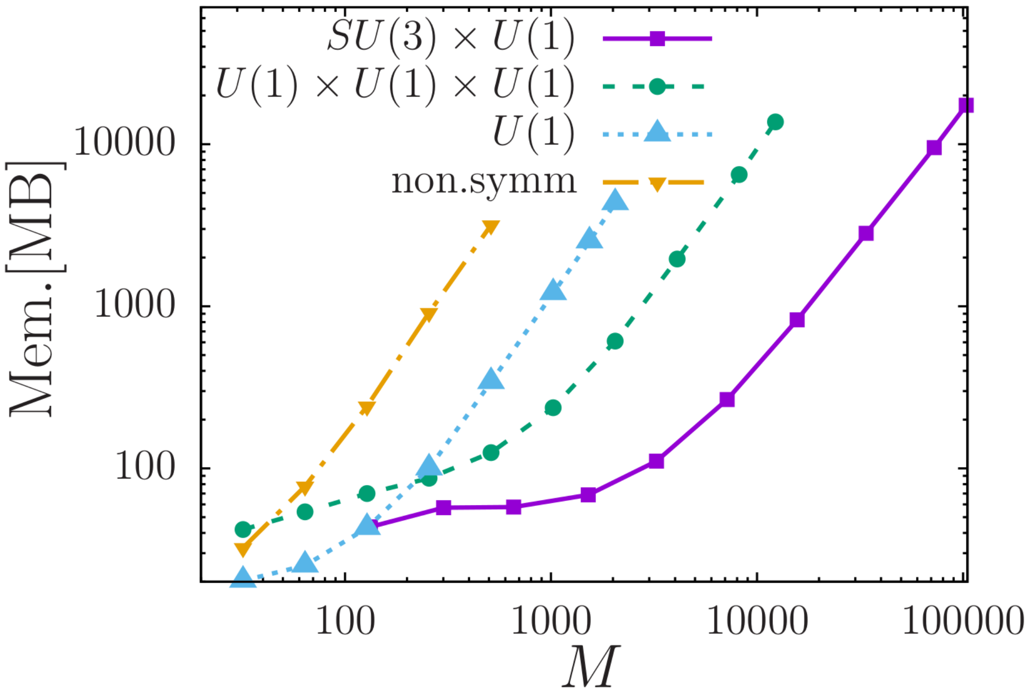


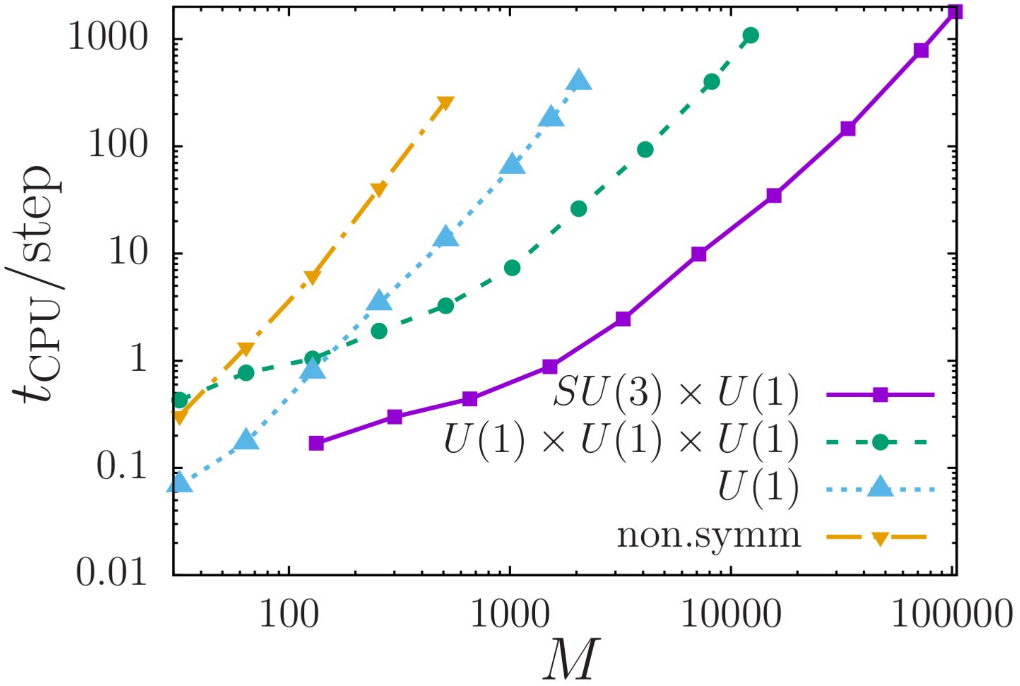


Numerical efficiency test

We can “lower” the used symmetry

$$SU(3) \times \underbrace{U(1) \times U(1) \times U(1)}_{\text{Color charges}} \Rightarrow \underbrace{U(1)}_{\text{Total charge only}} \Rightarrow \text{non.symm.}$$





Summary

- **Matrix Product States for general non-Abelian symmetries**

- **NA tensors and their algebraic properties**
    - General objects, do not dependent on a specific symmetry.
    - They have simple contraction rules.
    - Various MPS algorithms can be formulated with them.

- **Demonstration: NA-TEBD simulation of the post quench dynamics in the SU(3) Hubbard model**

- **Test of efficiency: almost two orders of magnitude speedup compared to the best Abelian case**

Acknowledgements

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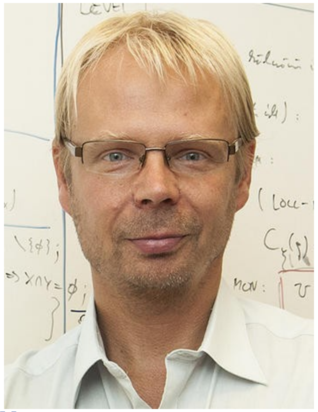

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**Thank you very much
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