↳ With $U = (|\phi_1\rangle, \dots, |\phi_\chi\rangle)$ $(d\chi \times \chi)$-matrix,

project operators such as $\underset{d\chi \times d\chi \text{ matrix}}{H_{A\bullet}} \to \tilde{H}_{A\bullet} = \underbrace{U^\dagger H_{A\bullet} U}_{\chi \times \chi \text{ matrix}}$

(and possible other operators to be "measured") down to the truncated space.

↳ Proceed likewise for $\rho_{\bullet B}$ (or use reflection symmetry)

↳ Identify $\tilde{H}_{\bullet A} \to H_A$, $\tilde{H}_{\bullet B} \to H_B$ and restart by adding two new sites.

↳ Iterate until $\frac{E}{N}$ becomes stationary and thus represents the ground state energy per site of an infinite system.

⇝ For other operators (such as correlation functions), keep a large distance from the boundaries to avoid finite size effects.

- Computational cost of "infinite" DMRG:

$\mathcal{O}(N(d\cdot\chi)^3)$, memory $\mathcal{O}((d\chi)^2)$.

$\uparrow$
\# sites

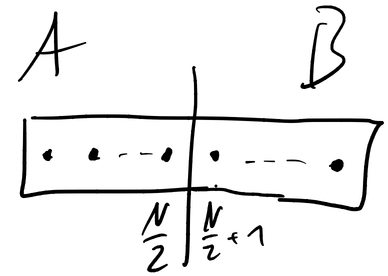
Concrete example: $H = \sum_{j=1} \sum_{\alpha = x,y,z} J_\alpha S_\alpha^{(j)} S_\alpha^{(j+1)}$ (xyz-model) (in 1D)

spin-$\frac{1}{2}$

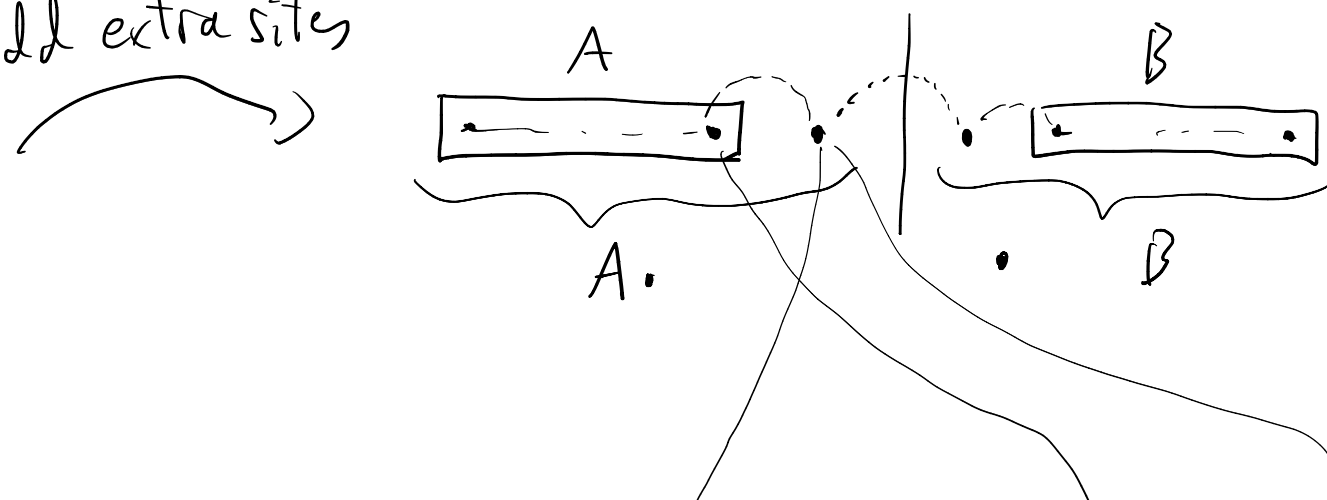
- We exemplify the block growth procedure from length $\frac{N}{2}$ to $\frac{N}{2}+1$.

↳ H_A, H_B, $S_\alpha^{(\frac{N}{2})}$, $S_\alpha^{(\frac{N}{2}+1)}$ retrieved from memory

[in Block A] [in Block B]



add extra sites



↳ Build $H_{A\bullet} = H_A \otimes \mathbb{1}_2 + \sum_\alpha J_\alpha S_\alpha^{(\frac{N}{2})} \otimes S_\alpha$,

$H_{\bullet B} = \mathbb{1}_2 \otimes H_B + \sum_\alpha J_\alpha S_\alpha \otimes S_\alpha^{(\frac{N}{2}+1)}$

and with that $H_{A\bullet\bullet B} = H_{A\bullet} \otimes \underbrace{\mathbb{1}_2}_{\text{extra B}} \otimes \mathbb{1}_B + \mathbb{1}_A \otimes \underbrace{\mathbb{1}_2}_{\text{extra A}} \otimes H_{\bullet B} + \sum_\alpha J_\alpha \mathbb{1}_A \otimes \underbrace{S_\alpha}_{\text{extra A}} \otimes \underbrace{S_\alpha}_{\text{extra B}} \otimes \mathbb{1}_B$

↳ Find ground state of $H_{A\bullet\bullet B}$ by Lanczos

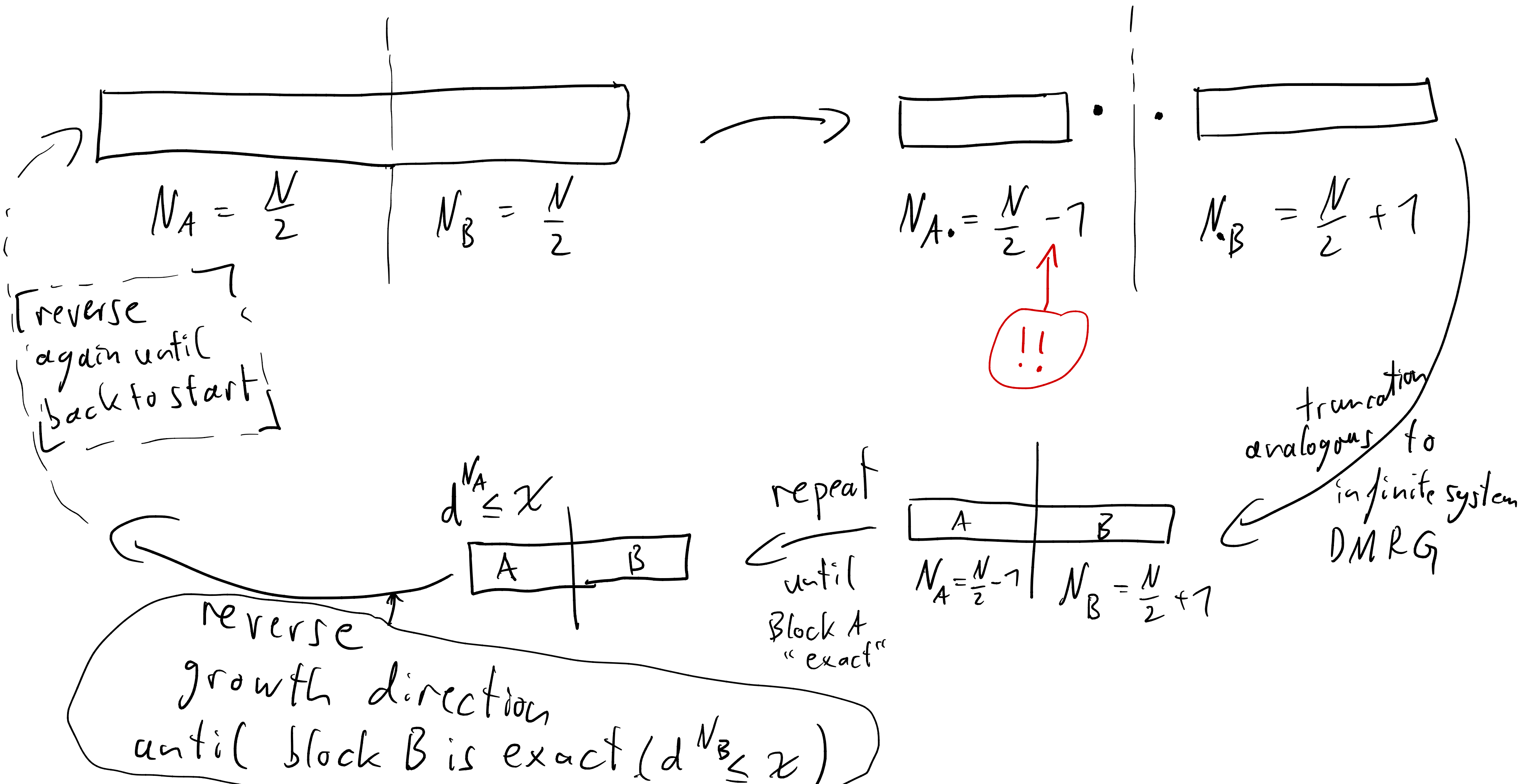
Compute $H_{A\bullet\bullet B} |\Psi\rangle$ using the matrix representation Ψ_{ij} (in $A\bullet$, in $\bullet B$), i.e. no need to store explicitly $H_{A\bullet\bullet B}$ as a $(d\chi)^2 \times (d\chi)^2$ matrix.

↳ Compute $\rho_{A\bullet} = \Psi\Psi^\dagger$ and $\rho_{\bullet B} = \Psi^\dagger\Psi$ ..... (truncate)

↳ Eventually project $\mathbb{1}_A \otimes S_\alpha \to U^\dagger \mathbb{1}_A \otimes S_\alpha U$, and $H_{A\bullet} \to U^\dagger H_{A\bullet} U$ into truncated basis and store in memory (similar for B).

- Problems with infinite system DMRG
  - System to described by state $|\psi\rangle$ changes (grows) during iteration ⇝ This can lead to severe artefacts and in som cases qualitatively wrong results.
  - Even if $\frac{E}{N}$ is correct for $N \to \infty$, stopping at finite N we cannot expect to have a good approximation of finite system with size N.
- Solution: Stop infinite system DMRG at desired finite N and follow up with <u>finite-system DMRG</u> (see next page)

- Finite system DMRG algorithm:
  - Proceed analogous to infinite system DMRG until size N is reached.
  - Follow up with cyclic sweeps:



- Additional book-keeping: Representations of operators for all block sizes N_A, $N_B = N - N_A$ need to be stored in order to reconstruct $H_{A \bullet \bullet B}$ during the sweeps.
- Overall computational cost per sweep $\mathcal{O}(N \cdot (\chi \cdot d)^3)$, typically 10 to 100 sweeps typically needed to achieve satisfactory convergence.

C.3: General Matrix Product State Methods

- Relation between DMRG truncation and MPS (Östlund and Rommer, PRL 1995)

extra site

Block of $n-1$ sites $\bullet$ ← [basis states $|\sigma\rangle$, $\sigma = 1, \dots, d$]

[basis states $|\alpha\rangle^{(n-1)}$, $\alpha = 1, \dots, \chi$, $\in \mathbb{C}^{\chi}$] ⟶ extended block states

$$\underbrace{|\alpha\rangle^{(n-1)} \otimes |\sigma\rangle}_{\mathbb{C}^{\chi \cdot d}}$$

– DMRG truncation can be seen as a mapping from $\mathbb{C}^{\chi \cdot d} \to \mathbb{C}^{\chi}$ written as

$$|\alpha\rangle^{(n)} = \sum_{\beta, \sigma} A^{(n), \sigma}_{\alpha, \beta} |\beta\rangle^{(n-1)} \otimes |\sigma\rangle$$

$1, \dots, \chi$

- If $A^{(n)}$ becomes stationary at some $n_0 \gg 1$, we may express the basis states in the "bulk region" $n_0+1, \dots, n$ (with $A^{\sigma} := \left(A^{(j),\sigma}_{\alpha,\beta}\right)_{\alpha,\beta}$, $j > n_0$) as

$$|\alpha\rangle^{(n)} = \sum_{\sigma_{n_0+1}, \dots, \sigma_n} \left(A^{\sigma_n} A^{\sigma_{n-1}} \cdots A^{\sigma_{n_0+1}}\right)_{\alpha,\beta} |\beta\rangle^{(n_0)} \otimes |\sigma_n, \dots, \sigma_{n_0+1}\rangle$$

- A generic state for the bulk region may then be written as (shifting $n_0 \to 0$)

$$|\Psi_Q\rangle = \sum_{\{\sigma_j\}} \mathrm{Tr}\left(Q A^{\sigma_n} \cdots A^{\sigma_1}\right) |\sigma_n, \dots, \sigma_1\rangle .$$