# C.2 Density Matrix Renormalization Group (DMRG)

- Prelude: "Naive" real space RG and its failure (see U. Schollwoeck, RMP 77, 259 (2005))

  - Consider particles in a box with discrete sites and

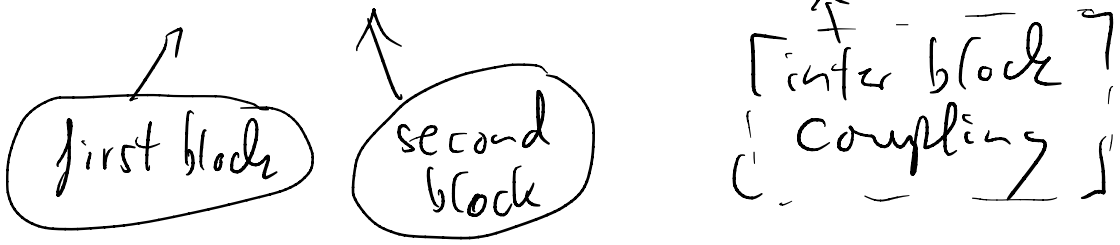
$$H = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & \ddots \\ & & & \ddots & \ddots \end{pmatrix} \sim p^2$$

  - Basic "real space RG" procedure:

    (i) Consider block A of length $\ell$ described by $M \times M$ Hamiltonian $H_A$.

(ii) Form compound block AA with length $2\ell$ and

$$H_{AA} = H_A \otimes \mathbb{1} + \mathbb{1} \otimes H_A + \tilde{H}$$




(iii) Diagonalize $H_{AA}$ to find $M$ lowest (in energy) states

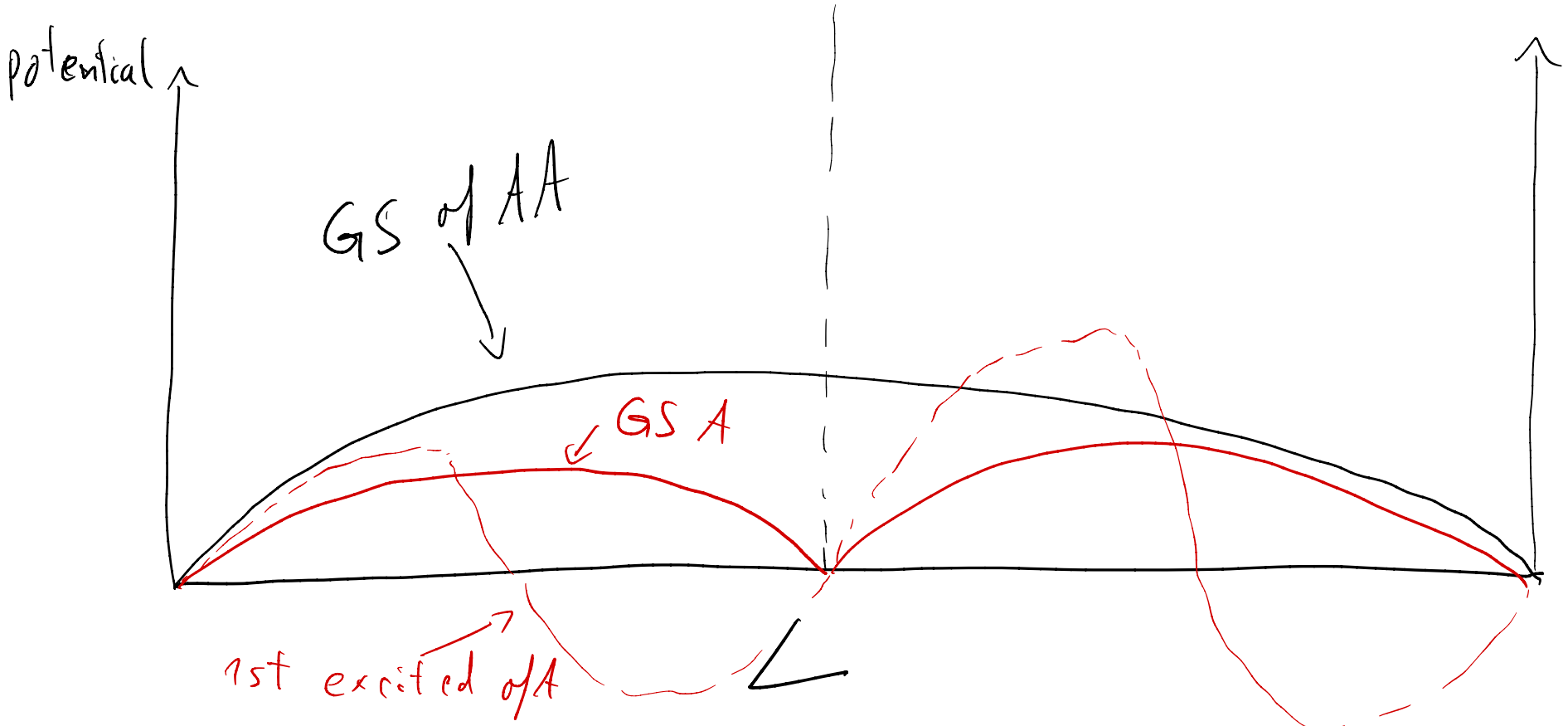
(iv) Project $H_{AA}$ onto subspace spanned $M$ lowest states: $H_{AA} \to H_{AA}^{tr}$ (truncation back to $M \times M$)

(v) Restarting from (ii) with doubled block size: $2\ell \to \ell$, $AA \to A$, $H_{AA}^{tr} \to H_A$, until full box size $L$ is reached.

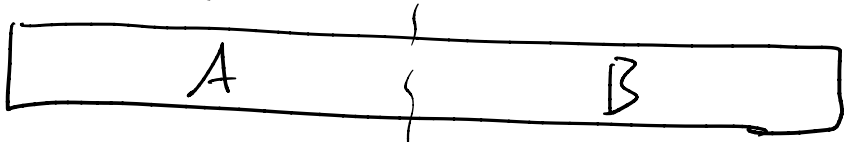
$\rightsquigarrow$ Find $H_{AA}^{tr}$ is effective $M \times M$ Hamiltonian of

the full system

↳ This gives poor results, since the ground state of the compound block is not well approximated by low-lying states of sub-blocks.



- More clever truncation procedure in DMRG: Select states by their contribution to entanglement rather than by their energy.
- Truncation procedure in DMRG:
  - Consider generic state $|\Psi\rangle = \sum_{ij} \Psi_{ij} |\phi_{iA}\rangle \otimes |\phi_{jB}\rangle$ (orthonormal basis states) of bipartite system!




$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$

$\dim \mathcal{H}_A = M_A$, $\dim \mathcal{H}_B = M_B$,

$m := \min(M_A, M_B)$

$\rightsquigarrow \Psi = (\Psi_{ij})$ is $M_A \times M_B$ matrix.

↳ Singular value decomposition (SVD) of $(\psi_{ij})$ gives

$$\psi = U \, S \, V^\dagger$$

$U$: $[M_A \times m$ with $U^\dagger U = \mathbb{1}]$

$V^\dagger$: $[m \times M_B$ with $V^\dagger V = \mathbb{1}]$

with $S$ diagonal $m \times m$ matrix with non-negative entries.

[cf. Eigendecomposition $M = U D U^\dagger$]

$$\hookrightarrow |\psi\rangle = \sum_{a=1}^{m} \underbrace{S_{aa}}_{=: s_a} \Big( \underbrace{\sum_i U_{ia} |\phi_{iA}\rangle}_{=: |a^A\rangle} \Big) \otimes \Big( \underbrace{\sum_j V^*_{ja} |\phi_{jB}\rangle}_{=: |a^B\rangle} \Big) =$$

$$= \sum_{a=1}^{m} s_a |a^A\rangle \otimes |a^B\rangle \quad \text{(Schmidt decomposition)}$$

↳ Reduced density matrix : $\rho_A = Tr_B(|\psi\rangle\langle\psi|) =$

$= \sum_{a=1}^{m} s_a^2 \, |a^A\rangle\langle a^A|$ . Similarly $\rho_B = Tr_A(|\psi\rangle\langle\psi|) = \sum_{a=1}^{m} s_a^2 \, |a^B\rangle\langle a^B|$

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$$|\psi\rangle\langle\psi| = \sum_{a,b} s_a s_b \, |a^A\rangle \otimes |a^B\rangle\langle b^A| \otimes \langle b^B|$$

$$\rightsquigarrow Tr_B(|\psi\rangle\langle\psi|) = \sum_{a,b,c} s_a s_b \, |a^A\rangle\langle b^A| \otimes \underbrace{\langle c^B|a^B\rangle}_{\delta_{c,a}} \underbrace{\langle b^B|c^B\rangle}_{\delta_{c,b}}$$

$a=b=c$

$$= \sum_{a} s_a^2 \, |a^A\rangle\langle a^A|$$

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General : $\rho_A = \psi\psi^\dagger$ .

↳ Number of non-vanishing singular values $s_a$ is called the Schmidt-rank $r$ of $|\psi\rangle$, where $1 \le r \le m$.

- Key question: What is the best approximation of a rank $r$ state $|\psi\rangle$ within the states $|\tilde{\psi}\rangle$ that have a lower Schmidt rank $\tilde{r} < r$ ?

$\rightsquigarrow$ Exact answer from SVD:

For $\psi = U \begin{pmatrix} s_1 & & \\ & \ddots & \\ & & s_r \\ 0 & \cdots & 0 \end{pmatrix} V^\dagger \xrightarrow{\text{truncation}} \tilde{\psi} = U \begin{pmatrix} s_1 & & & \\ & \ddots & & \\ & & s_{\tilde{r}} & \\ 0 & \cdots & 0 & 0 \end{pmatrix} V^\dagger$

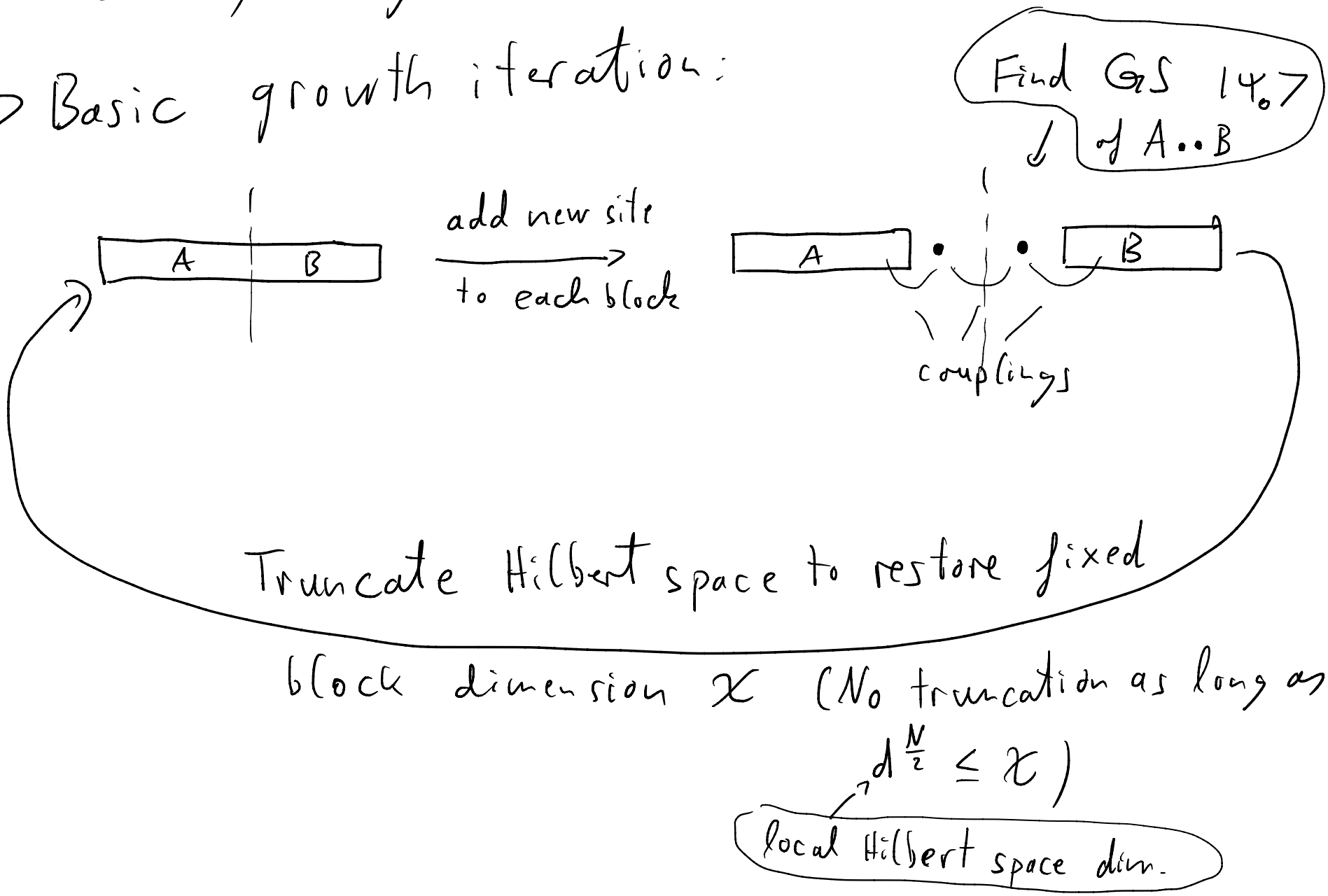
(Use same $U, V^\dagger$, but set $s_{\tilde{r}+1}, \dots, s_r$ to zero, assuming $s_1 \geq s_2 \cdots \geq s_r$)

$\rightsquigarrow$ Truncation by discarding smallest Schmidt coefficients.

- Infinite system DMRG algorithm.
  - General structure
    - Consider system of increasing length $N = 2, 4, 6, \dots$

and discard sufficiently many states in truncation procedure to keep effective Hilbert space dimension ($\sim \chi$) manageable.

↳ Basic growth iteration:



- Growth and truncation procedure in formulae:

↳ Starting point of an iteration: (Effective) Hamiltonians $H_A$, $H_B$ of blocks A, B.

↳ Add new site to each block to form superblock

Hamiltonian $H_{A\bullet\bullet B} = H_{A\bullet} \otimes \mathbb{1}_{\bullet B} + \mathbb{1}_{A\bullet} \otimes H_{\bullet B} + \mathbb{1}_A \otimes \tilde{H}_{\bullet\bullet} \otimes \mathbb{1}_B$

($\tilde{H}_{\bullet\bullet}$: coupling between new sites)

(assuming a local Hamiltonian that couples only NN sites)

↳ General ansatz for state $|\Psi\rangle = \sum \Psi_{a_A \sigma_A, \sigma'_B b_B} |a^A\rangle \otimes |\sigma^A\rangle \otimes |\sigma'^B_1\rangle \otimes |\sigma'^B_2\rangle$ (A ... B)

($a_A$: A; $\sigma_A$: ↑; $\sigma'_B$: ↑; $b_B$: B)

$a_A, b_B = 1, \dots, \chi$

$\sigma_A, \sigma'_B = 1, \dots, d$

↳ Find ground state $|\psi_0\rangle$ of $(\chi^2 \cdot d^2) \times (\chi^2 \cdot d^2)$ matrix $H_{A\cdots B}$

by Lanczos (cost $\mathcal{O}(\chi^2 \cdot d^2 \cdot \log(\chi^2 d^2))$.

↳ Compute $\rho_{A\cdots} = \mathrm{Tr}_{\cdots B}(|\psi_0\rangle\langle\psi_0|) = \Psi\Psi^\dagger$ and

fully diagonalize $(d\chi \times d\chi)$ matrix $\rho_{A\cdots}$, ordering

its non-negative eigenvalues by magnitude (cost $\mathcal{O}((\chi \cdot d)^3)$).

$d \cdot \chi$

⇝ Result: $\rho_{A\cdots} = \sum_{a=1} s_a^2 \, |\phi_a\rangle\langle\phi_a|$ with $\langle\phi_a|\phi_b\rangle = \delta_{ab}$

↳ Discard the $(d-1)\cdot\chi$ smallest eigenvalues to

obtain truncated $\tilde{\rho}_{A\cdots} = \sum_{a=1}^{\chi} s_a^2 \, |\phi_a\rangle\langle\phi_a|$.