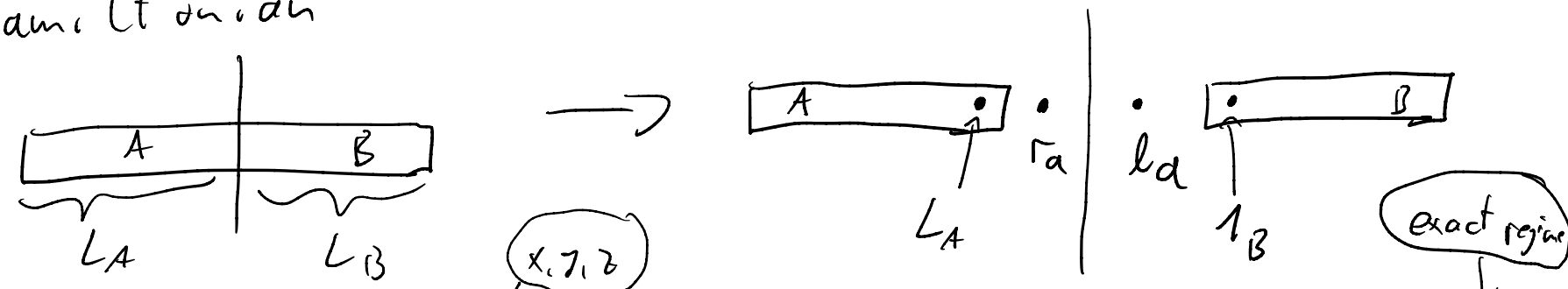
Solutions - Sheet 5

$$H = -J \sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right) + \Delta \sum_j S_j^z S_{j+1}^z =$$

$$= \sum_j H_{j,j+1}, \quad \text{with } H_{j,j+1} = -J \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right) + \Delta S_j^z S_{j+1}^z$$

1. 2-site update: Ground state of superblock Hamiltonian



- Input: H_A, $S^\mu_{L_A}$ in $|n_A\rangle$, $n = 0, \dots, \min(\chi-1, 2^{L_A}-1)$

$\mu = x, y, z$

H_B, $S^z_{r_B}$ in basis $\{|n_B\rangle\}$ " " " "

- Superblock Hilbert space: $\mathcal{H}_S = \mathcal{H}_A \otimes \mathcal{H}_{r_A} \otimes \mathcal{H}_{\ell_B} \otimes \mathcal{H}_B$

- Superblock Hamiltonian: $H_{A\bullet\bullet B} = H_{A\bullet} + H_{\bullet\bullet} + H_{\bullet B}$,

where $H_{A\bullet} = H_A \otimes \mathbb{1}_{r_A} \otimes \mathbb{1}_{\ell_B} \otimes \mathbb{1}_B + H_{\ell_A, r_A} \otimes \mathbb{1}_{\ell_B} \otimes \mathbb{1}_B$

↑ see $H_{\vec{0}\,\vec{0}+1}$ notation above

$H_{\bullet B} = \mathbb{1}_A \otimes \mathbb{1}_{r_A} \otimes \mathbb{1}_{\ell_B} \otimes H_B + \mathbb{1}_A \otimes \mathbb{1}_{r_A} \otimes H_{\ell_B, 1_B}$

$H_{\bullet\bullet} = \mathbb{1}_A \otimes H_{r_A, \ell_B} \otimes \mathbb{1}_B$

- ED to find ground state of $H_{A\bullet\bullet B}$ in $\mathcal{H}_S$.

↳ Quick and dirty: Store $H_{A\ldots B}$ explicitly as $4\chi^2 \times 4\chi^2$ (sparse) matrix and use predefined Lanczos routine to find GS $|\psi_0\rangle$

⇝ Worst case: Memory and runtime scale as $\mathcal{O}(\chi^4)$.

⇝ Reality here is $\mathcal{O}(\chi^3)$ due to $\mathbb{1}\otimes\ldots$ structure.
(Still critical since not subleading).

↳ Alternative: Use product structure of Hamiltonian in basis representation $|\psi\rangle = \sum_{a,b} \psi_{a,b} \underbrace{|a\rangle}_{\in \mathcal{H}_A \otimes \mathcal{H}_{rA}} \otimes \underbrace{|b\rangle}_{\in \mathcal{H}_{lB} \otimes \mathcal{H}_B}$ to

write $H_S|\psi\rangle = \Big\{ \big[(H_A)_{aa'} \psi_{a'b} + (H_B)_{bb'} \psi_{ab'} + \ldots$

$$\left(\epsilon\,\partial\right)\Big[\left(\mathbb{1}_A \otimes S^{x}_{r_A}\right)_{aa'}\left(S^{x}_{\ell_B}\otimes \mathbb{1}_B\right)_{bb'} + x\leftrightarrow y\Big] + \Delta\ldots\Big)\psi_{a'b'}\Big\}|a\rangle|b\rangle$$

i.e. $$\left(H_S\psi\right)_{ab} = \Big(H_A\cdot\psi + \psi H_B^{T} + \left[(-\partial)\,S^{x}_{r_A}\,\psi\,S^{xT}_{\ell_B} + x\leftrightarrow y + \Delta\ldots\right]\Big)_{ab}$$

$\rightsquigarrow$ Note that $\mathbb{1}_A \otimes S^{\mu}_{r_A}$, $S^{\nu}_{\ell_B}\otimes\mathbb{1}_B$ only have $\mathcal{O}(x)$ non-vanishing elements each. To further optimize, the product structure $|a\rangle = \underbrace{|n_A\rangle}_{\in \mathcal{H}_A} \otimes \underbrace{|G_{r_A}\rangle}_{\in \mathcal{H}_{r_A}}$,

$$|b\rangle = \underbrace{|G_{\ell_B}\rangle}_{\in \mathcal{H}_{\ell_B}} \otimes \underbrace{|n_B\rangle}_{\in \mathcal{H}_B}$$

may be used to reduce the effort of two-sided

(sparse)- operators to $\mathcal{O}(1)$.

↳ Use one of the above $H_s|\psi\rangle$ routines in a Lanczos iteration.

Output: $|\psi_0\rangle$, with $H_s|\psi_0\rangle = E_0|\psi_0\rangle$.

2. Reduced density operators:

With $|\psi_0\rangle = \sum_{a,b=0}^{2^{x-1}} \psi_{ab} |a\rangle \otimes |b\rangle$, we have

$$\rho_A = Tr_B \left(|\psi_0\rangle\langle\psi_0| \right) = Tr_B \left(\sum_{\substack{a,b \\ a',b'}} \psi_{ab} \psi^*_{a'b'} \left(|a\rangle \otimes |b\rangle \right)\left(\langle a'| \otimes \langle b'| \right) \right)$$

$$= Tr_B \left(\sum_{\substack{a,b \\ a',b'}} \psi_{ab} \psi^*_{a'b'} |a\rangle\langle a'| \otimes |b\rangle\langle b'| \right) \overset{\text{Def of } Tr_B}{=}$$

$$= \sum_{\tilde{b}} \sum_{\substack{a,b \\ a',b'}} \psi_{ab} \psi^*_{a'b'} |a\rangle\langle a'| \underbrace{\langle \tilde{b}|b\rangle}_{\delta_{\tilde{b},b}} \underbrace{\langle b'|\tilde{b}\rangle}_{\delta_{b',\tilde{b}}} = \quad \uparrow \; b=b'=\tilde{b}$$

$$= \sum_{a,a',b} \psi_{ab} \psi^*_{a'b} |a\rangle\langle a'| = \sum_{a,a'} \underbrace{\left(\sum_b \psi_{ab} \psi^\dagger_{ba'} \right)}_{(\psi\psi^\dagger)_{aa'}} |a\rangle\langle a'|$$

$$= \sum_{a,a'} (\psi\psi^\dagger)_{aa'} |a\rangle\langle a'| \,, \text{ i.e. in terms of re-}$$

presentation matrices $(\rho_{A\cdot})_{aa'} = (\psi\psi^\dagger)_{aa'}$.

Similarly: $(\rho_{\cdot B})_{bb'} = (\psi^\dagger\psi)_{bb'}$

$\rightsquigarrow$ Full diagonalization of $\rho_{\cdot A}, \rho_{B\cdot}$.

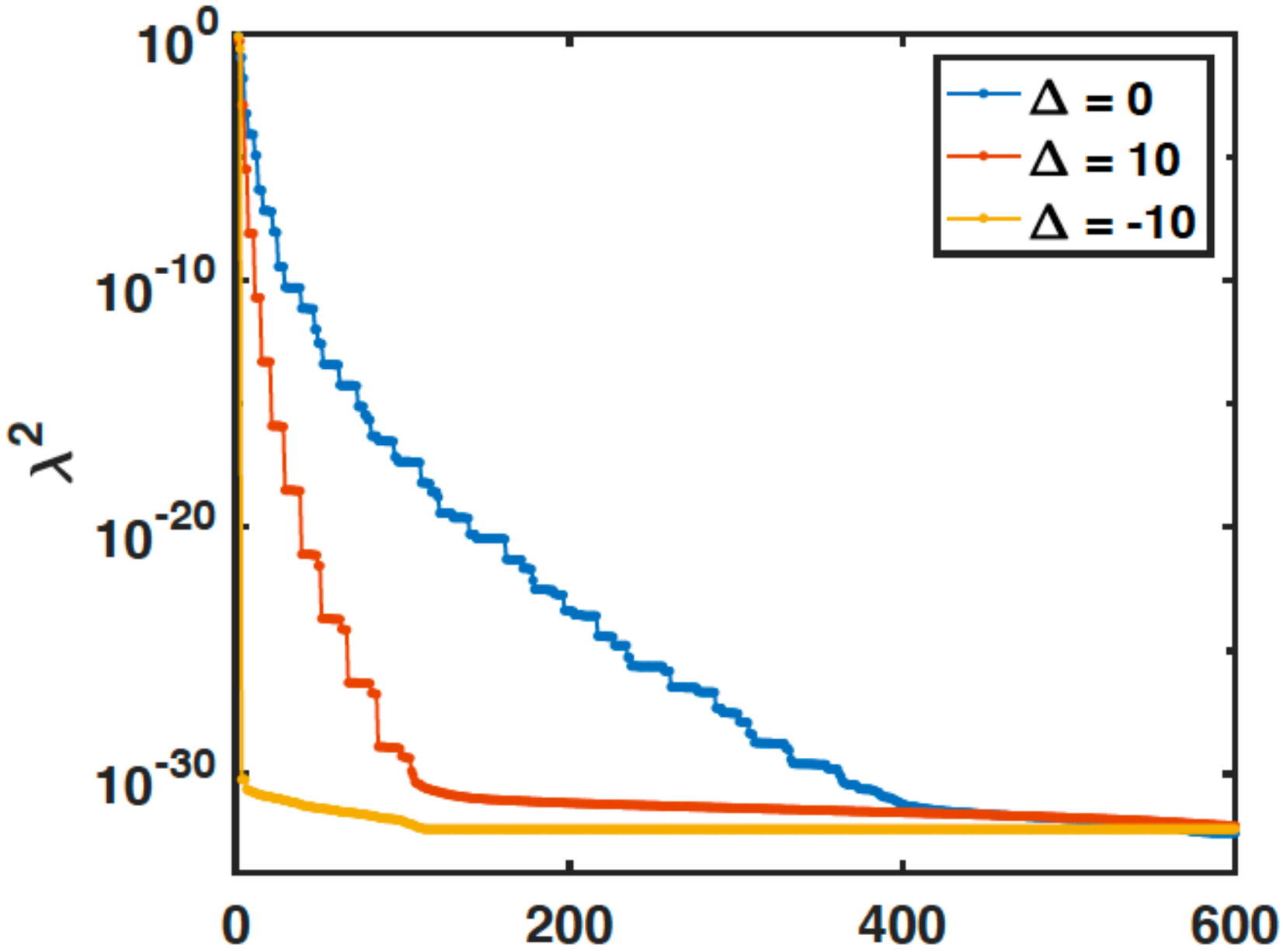


Figure 1: Spectrum of $\rho_{A\bullet}$ for $L_A = L_B = 9$ (i.e. suberblock length $L = 20$ and reduced density matrix of half of the system) in the cases $\Delta = 0$ and $\Delta = \pm 10$.

↳ Output of step 2: Spectral representations

$$\rho_{A\cdot} = \sum_{j=0}^{2\chi-1} \lambda_j^2 \, |j_A\rangle\langle j_A| \,, \quad \rho_{\cdot B} = \sum_{j=0}^{2\chi-1} \lambda_j^2 \, |j_B\rangle\langle j_B|$$

3. Hilbert space truncation

- Represent operator on $\mathcal{H}_A \otimes \mathcal{H}_{r_A}$ in $\rho_{A\cdot}$ eigenbasis,

i.e. $$O = \sum_{a,a'} O_{aa'} |a\rangle\langle a'| = \sum_{j,j'} (U^\dagger O U)_{jj'} \, |j_A\rangle\langle j_A'|$$

(Similarly $O = \sum_{b,b'} O_{bb'} |b\rangle\langle b'| = \sum_{j,j'} (V^\dagger O V^*)_{jj'} \, |j_B\rangle\langle j_B'|$ on $\mathcal{H}_{\ell_B} \otimes \mathcal{H}_B$)

- Relation to SVD: $\Psi = U S V^\dagger$, with $S = \begin{pmatrix} \lambda_0 & & \\ & \lambda_1 & \\ & & \ddots \\ & & & \lambda_{2\chi-1} \end{pmatrix}$.

- Relation to above eigen-decomposition: $\sum_a U_{aj} |a\rangle = |j_A\rangle$,

$$\sum_b V^*_{bj} |b\rangle = |j_B\rangle .$$

- Assuming $\lambda_0 \geq \lambda_1 \geq \dots \geq \lambda_{2\chi-1}$, discard all columns $j \geq \chi$ of (U_{aj}) and (V^*_{bj}), respectively

$\rightsquigarrow$ Truncated $2\chi \times \chi$ matrices $\tilde{U}$, $\tilde{V}^*$.

- Project all tracked operators (at least $S^{\mu}_{r_A}$, $S^{\nu}_{l_B}$, $H_{A\cdot}$, $H_{\cdot B}$) to the truncated basis by computing

Output: $\tilde{O} = \tilde{U}^\dagger O \tilde{U}$ (on $A\cdot \rightarrow$ new A)

and $\tilde{O} = \tilde{V}^T O \tilde{V}^*$ (on $\cdot B \rightarrow$ new B), respectively.

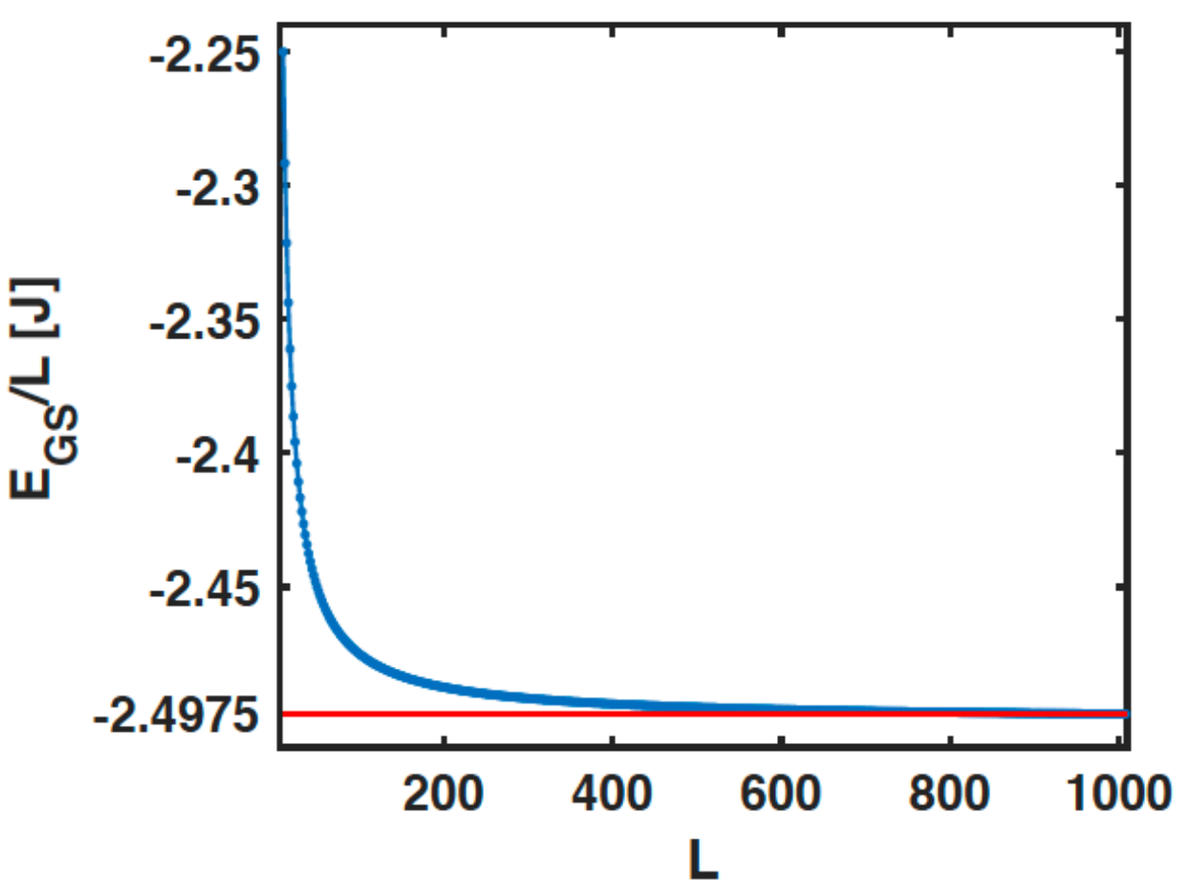
4. Putting together the infinite system DMRG algorithm.

- Structure of iteration:
  - Start with $L_A, L_B = 2$, $H_A = H_{1_A, 2_A}$, $H_B = H_{1_B, 2_B}$
  - As long as $2^{L_A} < \chi$, no truncation is necessary.
  - Iterate growth procedure from subproblems (1) - (3), where the new inputs given in (1) are the $\tilde{O}$ operators from the previous step (3), in particular $\tilde{H}_{A\bullet} \to H_A$, $\tilde{H}_{\bullet B} \to H_B$, $\tilde{S}^{\mu}_{r_A} \to S^{\mu}_{L_A}$, $\tilde{S}^{\nu}_{l_B} \to S^{\nu}_{1_B}$.
  - Iterate until observables such as $\frac{E_0}{L}$ (with $L = L_A + L_B$) are converged to satisfactory precision.

↳ Keep track of $\varepsilon_{\text{trunc}} = 1 - \sum_{j=0}^{\chi-1} \lambda_j^2$, and track how large χ needs to be to satisfy $\lambda_\chi^2 < \varepsilon_c = 10^{-13}$.

↳ Special for integrable XXZ-model: Track difference to exact $\frac{E_0}{L}$ (known from Bethe-Ansatz solution).

(see attached plots)



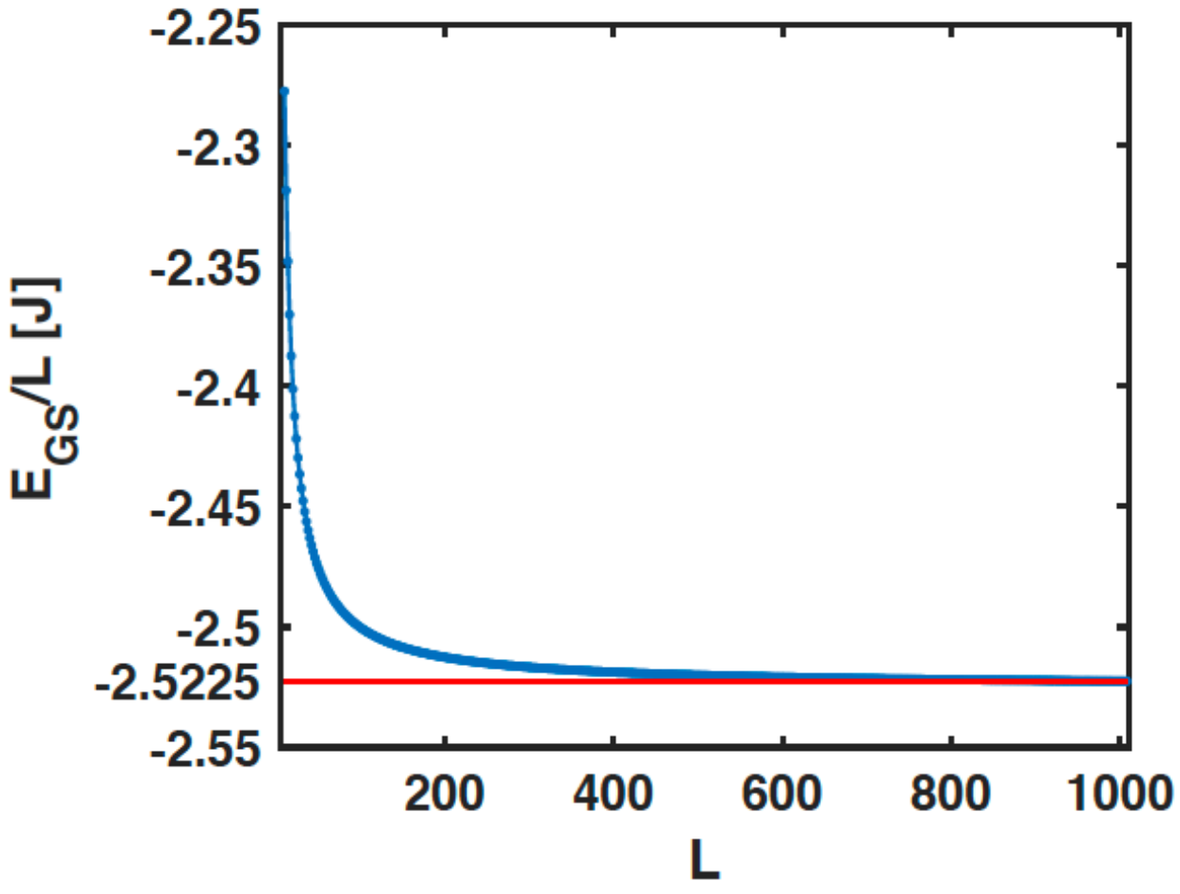
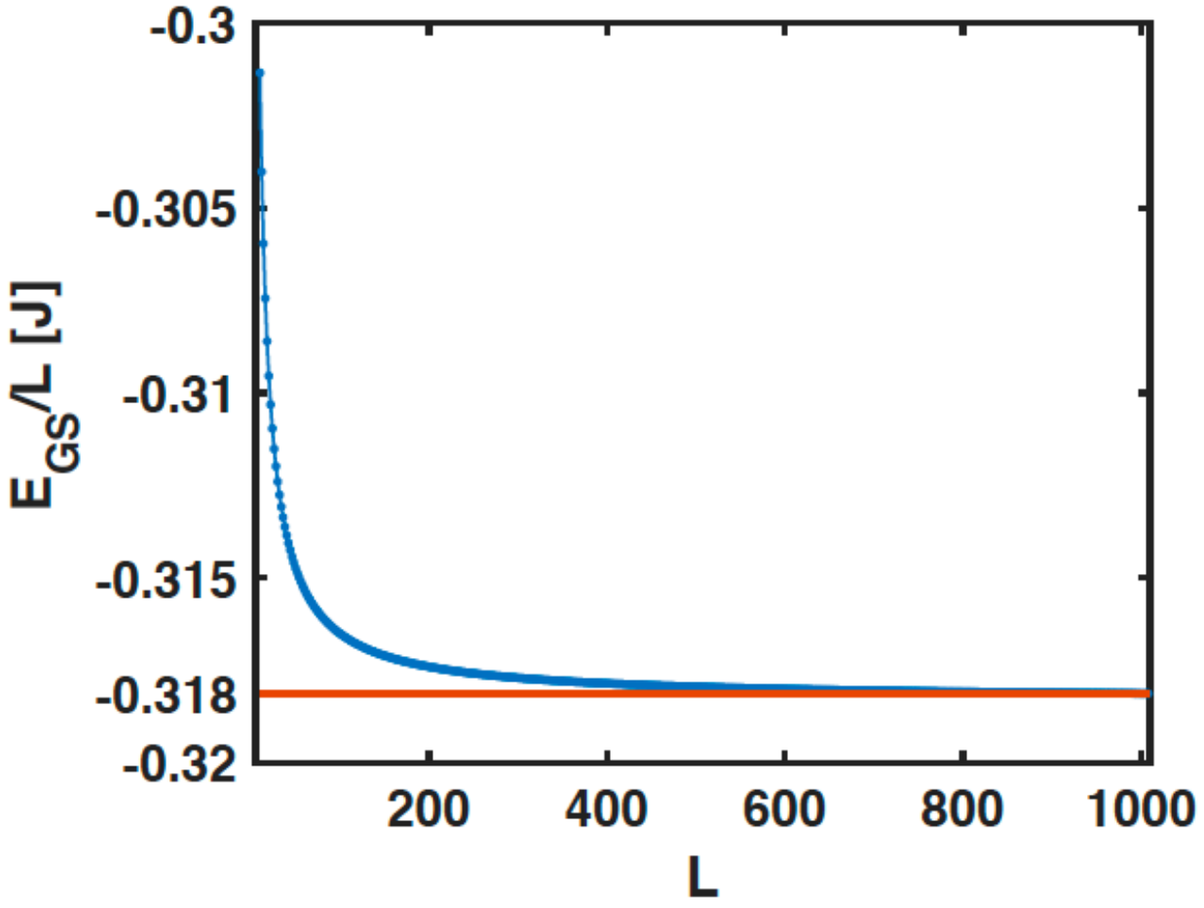


Figure 2: Ground-state energy per site $e_{GS} = E_{GS}/L$ as a function of the superblock length L during the iDMRG iterations, for $\Delta = -10$ (left panel) and $\Delta = 10$ (right



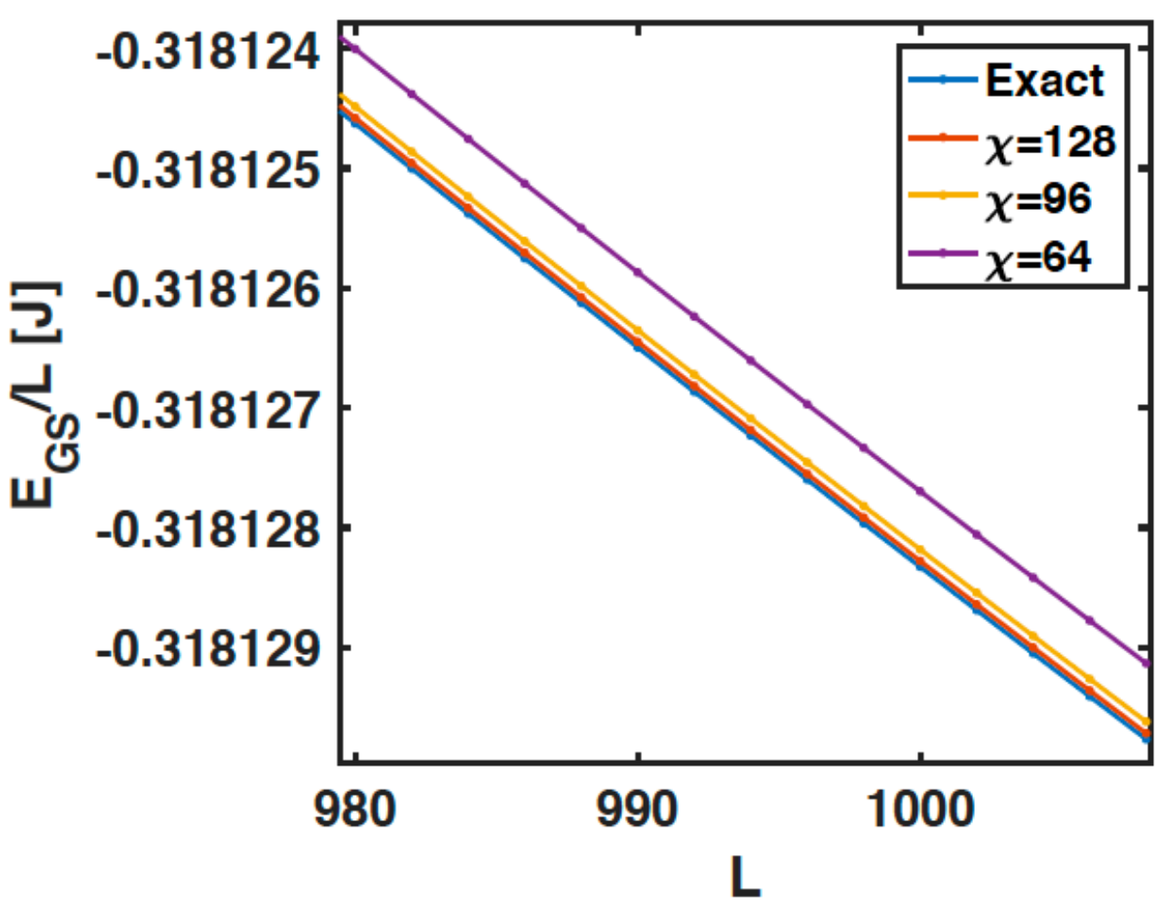


Figure 3: Ground-state energy per site $e_{GS} = E_{GS}/L$ as a function of the superblock length L during the iDMRG iterations, for $\Delta = 0$.

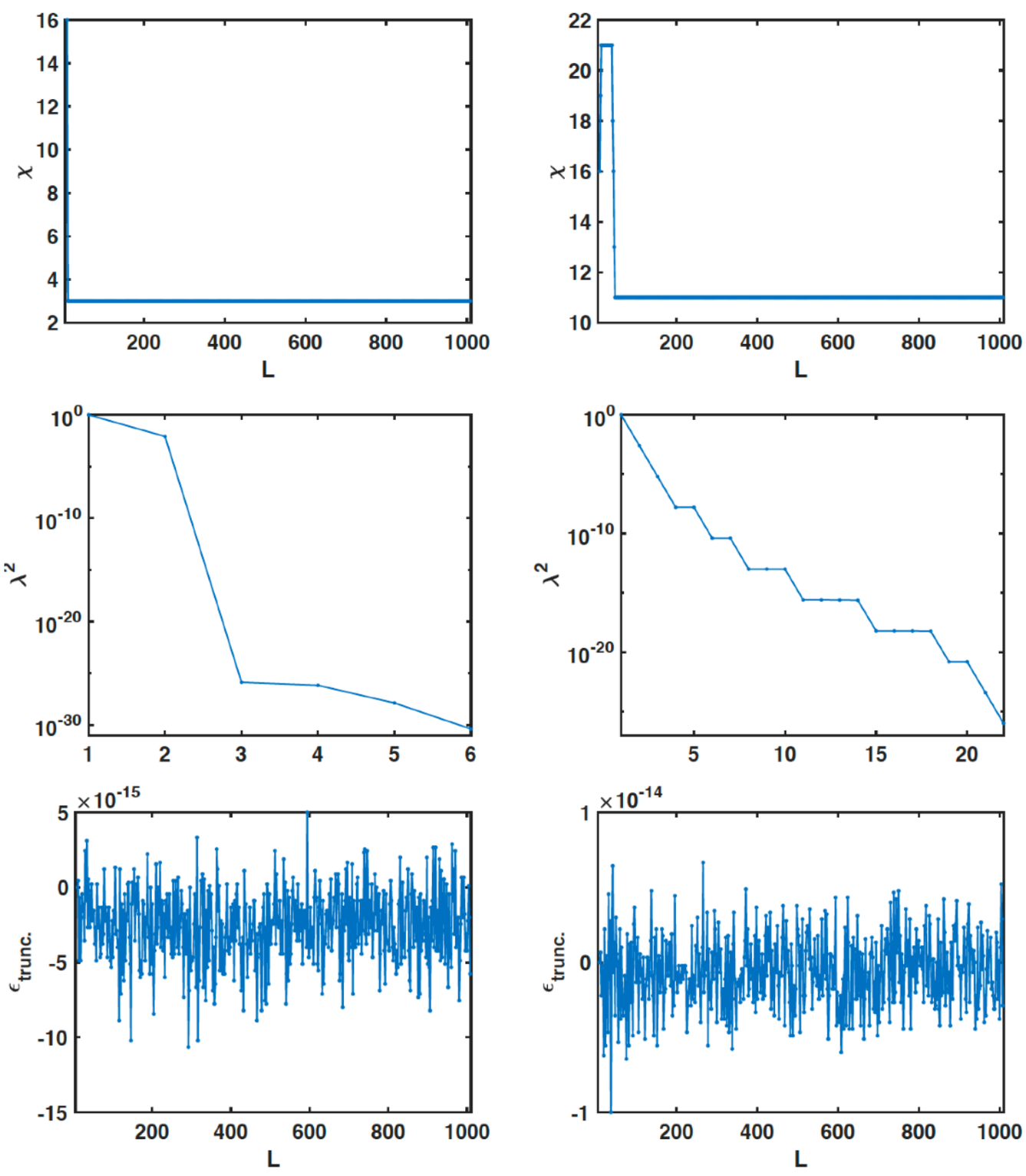


Figure 4: Upper row: Number of states kept χ as a function of the superblock length L during the iDMRG iterations, for $\Delta = -10$ (left panel) and $\Delta = 10$ (right panel), for an accuracy fixed to `acc`$= 10^{-14}$. *Here $J = 1$,* `Lin`$= 4$, `maxiter`$= 500$. *The maximum for the number of states kept* `chi`$= 64$ *is never reached.*
Middle row: Largest reduced density matrix eigenvalues at last iDMRG iteration for $\Delta = -10$ (left panel) and $\Delta = 10$ (right panel).
Last row: Truncation errors during the iDMRG iterations, for $\Delta = -10$ (left panel) and $\Delta = 10$ (right panel).

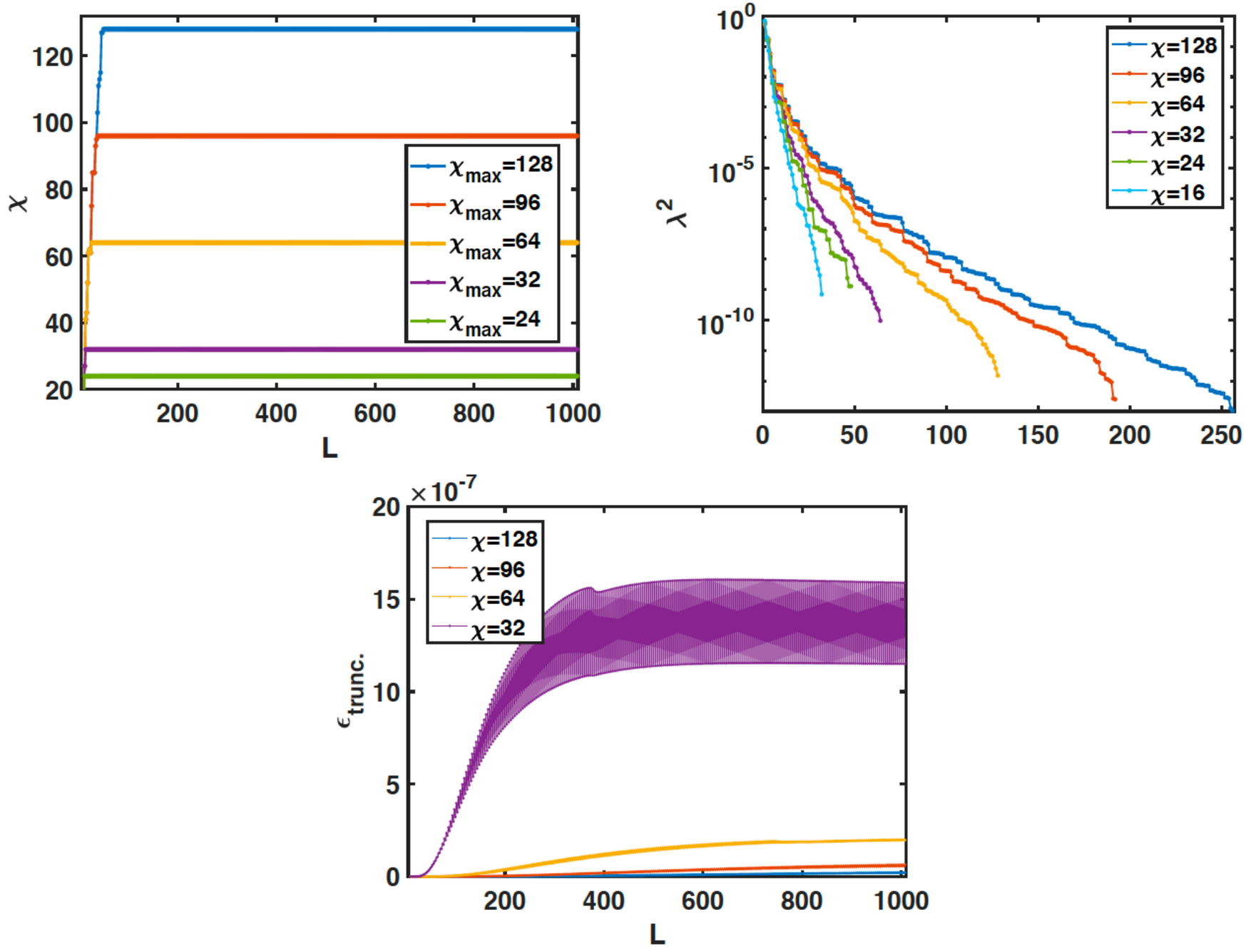


Figure 5: Upper-left panel: Number of states kept χ as a function of the superblock length L during the iDMRG iterations, for $\Delta = 0$, for an accuracy fixed to `acc`$= 10^{-14}$. *Here* $J = 1$, `Lin`$= 4$, `maxiter`$= 500$. *Upper-right: Largest reduced density matrix eigenvalues at last iDMRG iteration for* $\Delta = 0$ *for different numbers* `chi` *of states kept during the iterations. Last row: Truncation errors during the iDMRG iterations, for* $\Delta = 0$, *for different numbers* `chi` *of states kept. The truncation error obviously reduces as* `chi` *increases, but it is much bigger that the error in the cases* $\Delta = \pm 10$, *given the much slower decay of the eigenvalues of the reduced density matrices.*

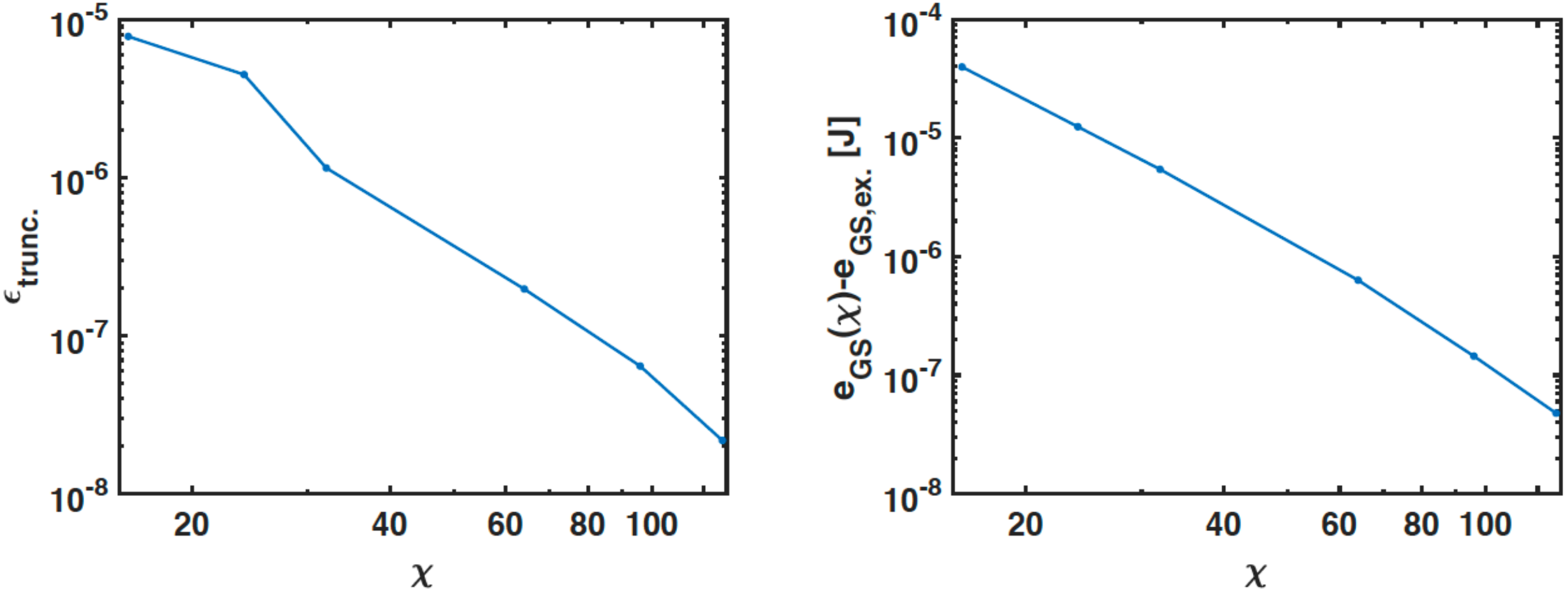


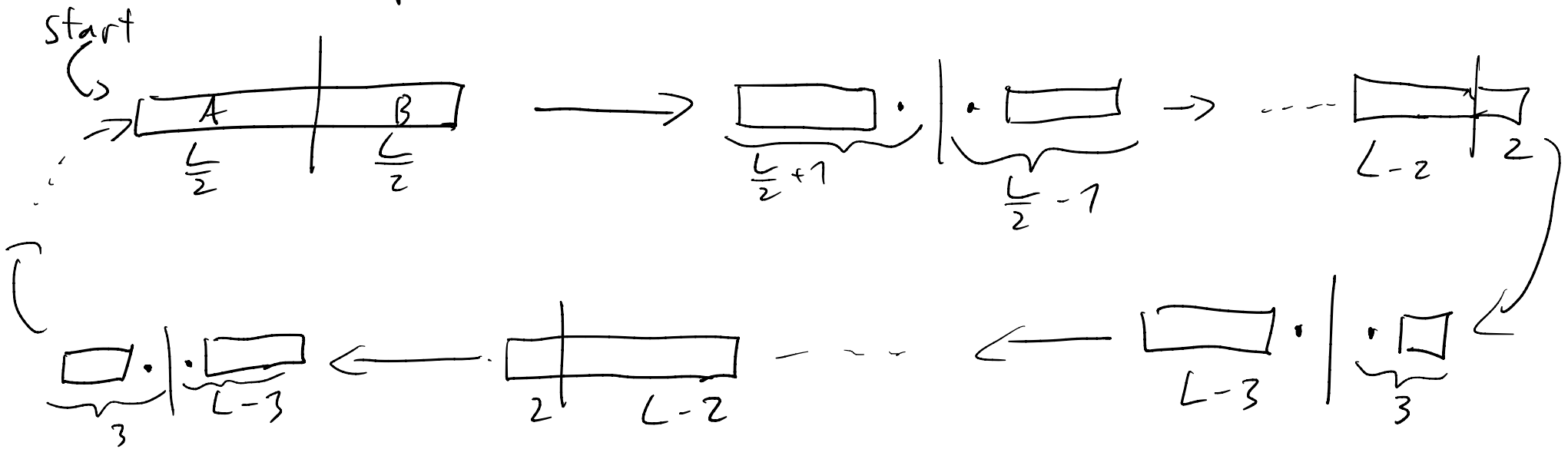
Figure 6: Left panel: Truncation error at last iDMRG iteration vs. the max. number of states kept χ, for $\Delta = 0$. Right panel: Difference between the ground-state energy per site $e_{GS}(\chi)$ for a given χ and the exact value of e_{GS} computed via Jordan-Wigner transformation, as a function of the max. number of states kept χ, for $\Delta = 0$.

5. Finite size DMRG (Bonus)

- Proceed as in (4) up to fixed L (typically $L = 100$ to 1000 and OBC).

↳ Only difference to (4): Store operators H_A, H_B, $S^\mu_{L_A}, S^\mu_{1_B}$ for all block sizes $2, \dots, \frac{L}{2}$.

- Follow up with DMRG sweeps (cycles):



↳ Store tracked operators for all occuring block sizes L_A, L_B, updating them in every sweep.

↳ Iterate until E_0 converged.

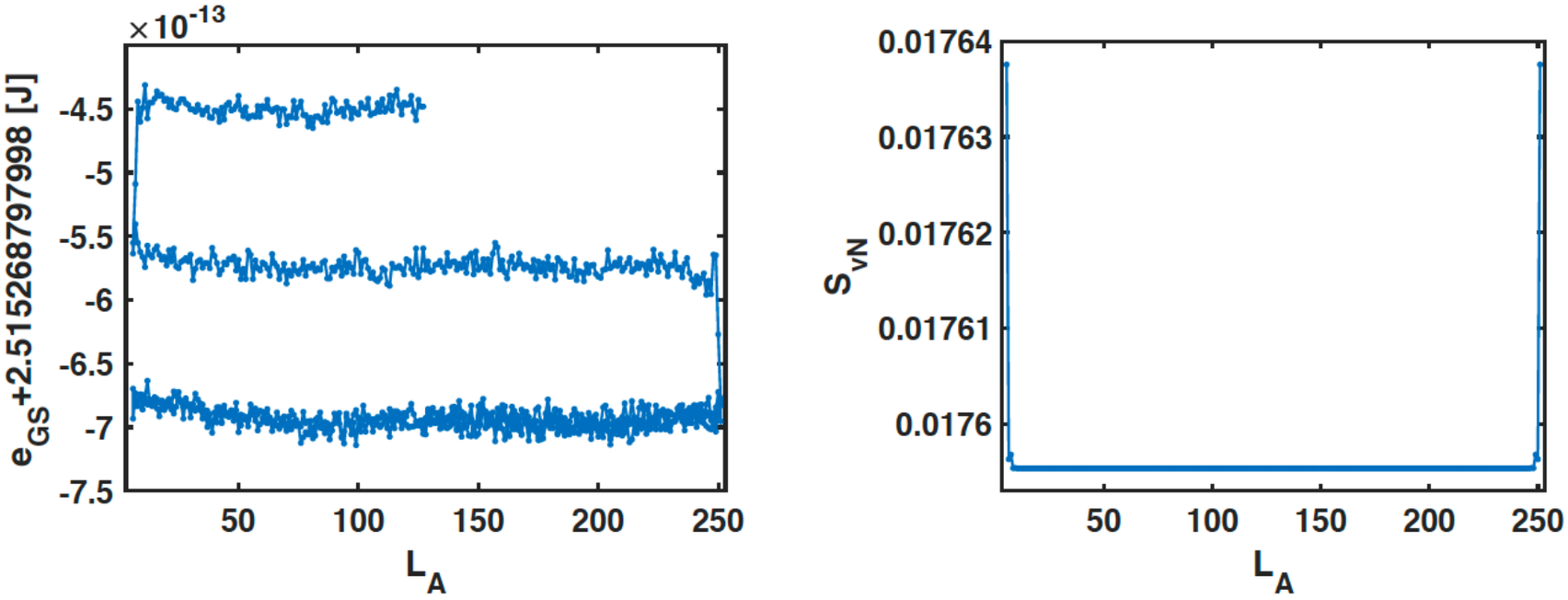


Figure 7: Finite-size DMRG for the XXZ model with $\Delta = 10$ *and* $L = 256$*. The accuracy set for the reduced density matrix eigenvalues is* `acc`$= 10^{-12}$ *and the threshold number of states kept is* `chi`$= 64$ *(never reached). The results are converged after* 2 *sweeps. Upper-left panel: Plot of* e_{GS} *during the sweeps (with an offset added for better readability). The energy reduces to its converged value during the first sweep, and stays constant in the second indicating convergence. Upper-right panel: von Neumann entropy* S_{vN} *as a function of the length* L_A *of* $A\bullet$ *during the last sweep. Apart from boundary effects, the entanglement enropy is constant with* L_A*, indicating that in this gapped phase an area law is satisfied. Lower panel: Truncation error during the last sweep. Its value gives an estimate of the error on the observables.*