Finite size scaling

Statistical physics; temperature dependent correlation length $\Rightarrow$ energy gap as a function of a control parameter

$$\xi(T) \to \Delta(g) = 1/\xi(T)$$

for 2nd order QPT with $N \to \infty$

$$\Delta(g) \sim |g - g_c|^{\nu}$$

Kosterlitz-Thouless phase transition

$$\Delta(g) = \begin{cases} \text{const} \cdot \exp\left[-c(g-g_c)^{\sigma}\right] & \text{if } g > g_c \\ 0 & \text{if } g < g_c \end{cases}$$

- for PBC $\Delta(N) = \Delta + c\frac{1}{N^{1/2}}\exp(-N/\xi)$
- for OBC $\Delta(N) = \Delta + a/N^2 + O(N^{-4})$

where does this come from:

if $\epsilon(k) = \sqrt{\Delta^2 + v^2k^2}$ magnon's dispersion is quadratic around its minim

due to boundary node at boundary

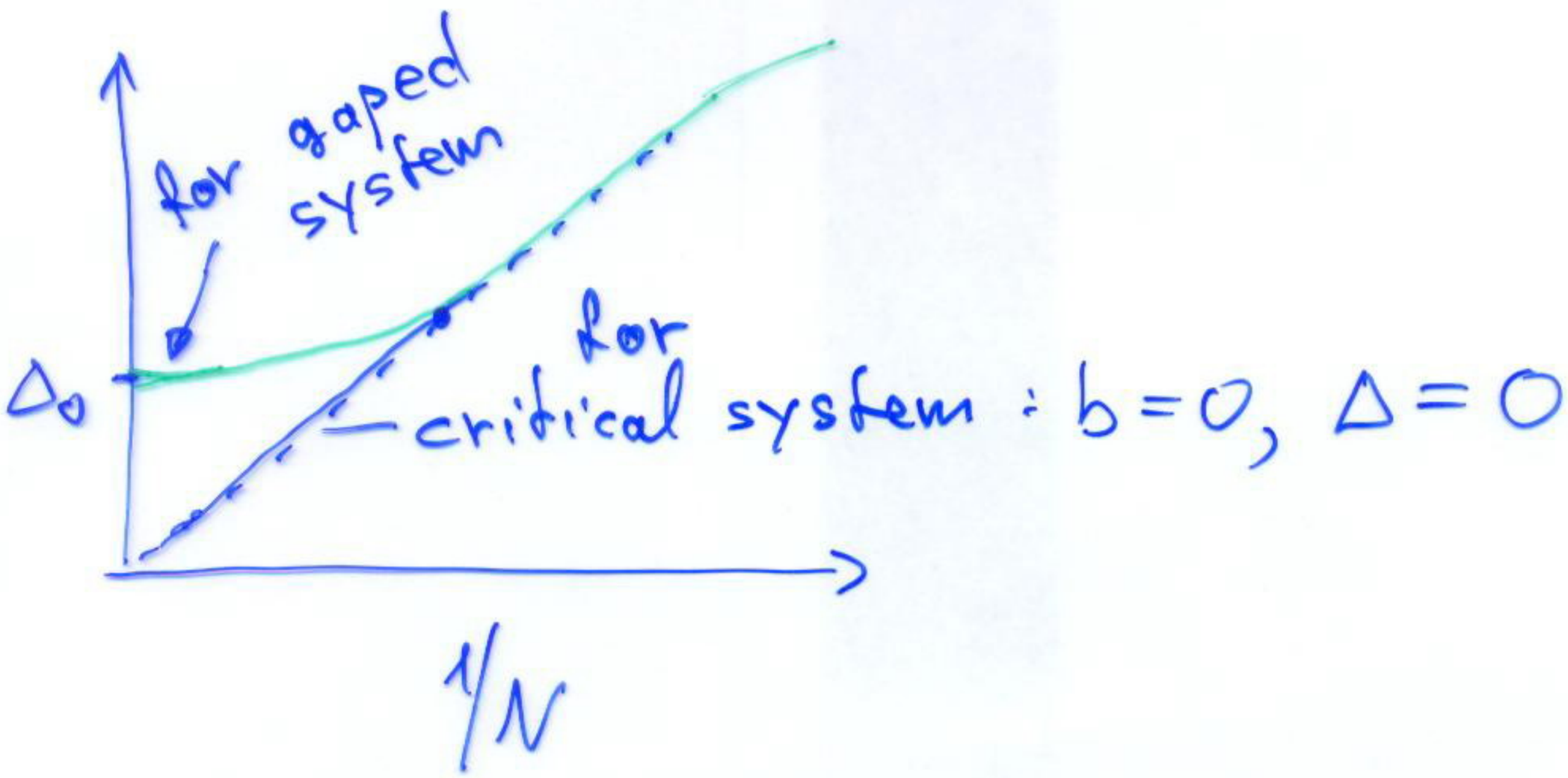
~~due~~ so lowest possible magnon momentu

⇒ lowest excitation gap:

$$\Delta(N) = \sqrt{\Delta^2 + v^2(\pi/N^2)} \approx \Delta + \pi^2 v^2 / 2\Delta N^2 + O(N^{-4})$$

general fitting form:

$$\Delta_N = \Delta + aN^{-1} + bN^{-2}$$



- What is information?
- We all carry information
- (different properties)
- Need interaction (correlation)
  to "measure" it
- Dominant and Recessive properties
- Need constraius to determine
  which are relevant and irrelevant

Examples:

properties:

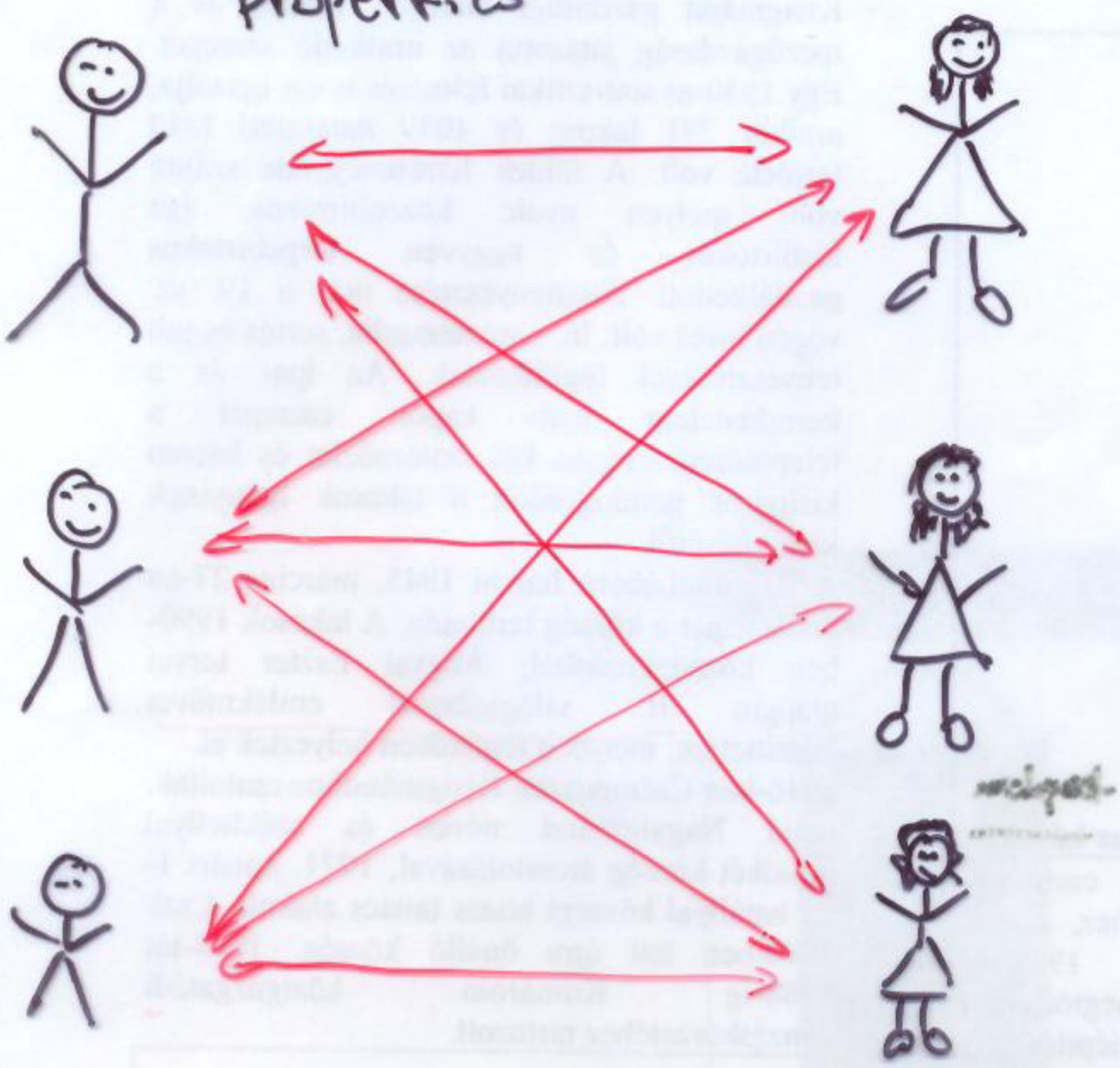
nice

smart

tall

ugly

...



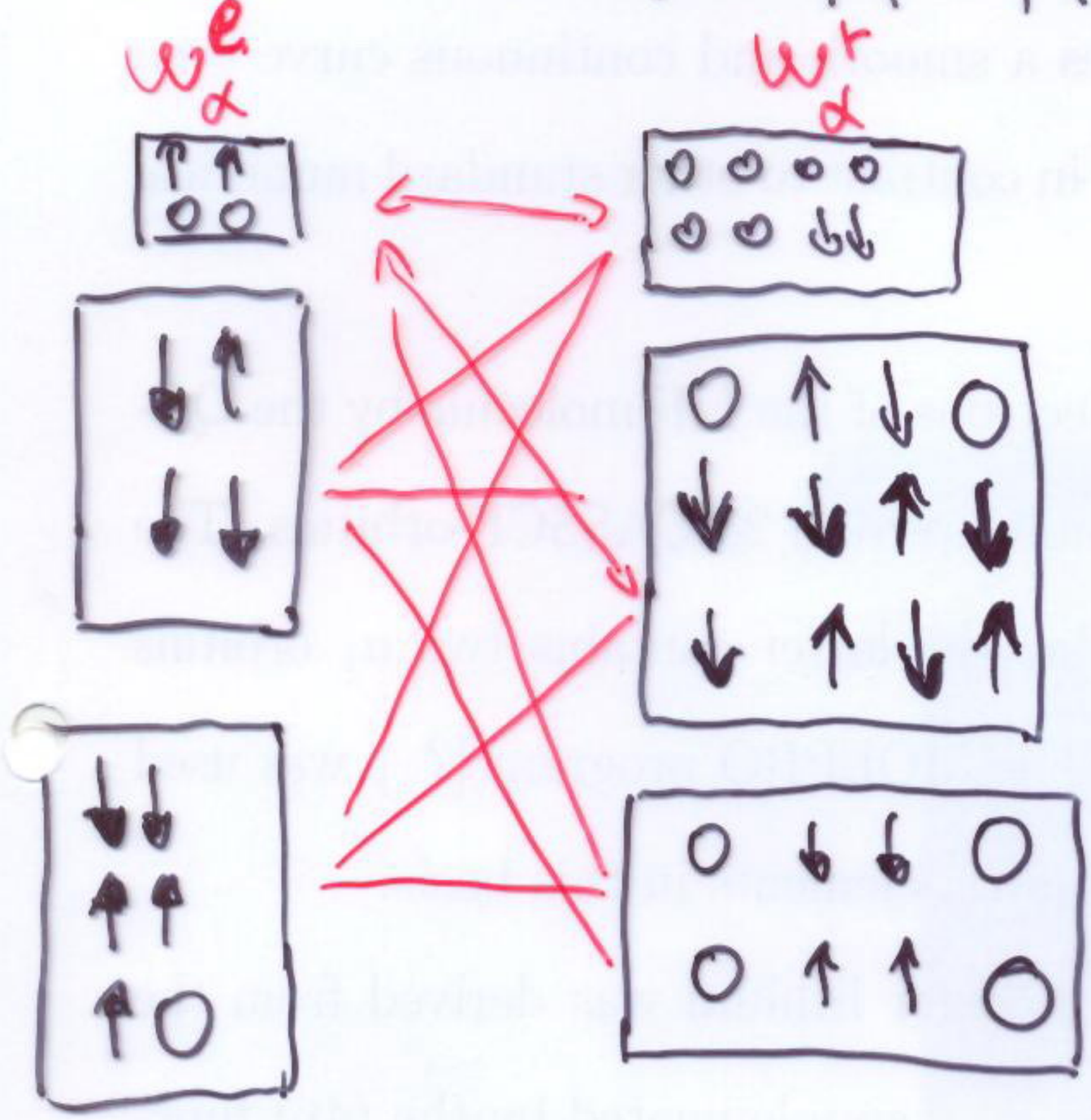
Exchanging information, interaction,

Correlation

Need selection rules to weight properties

Example 2 : Quantum chain : $L = 6$

$q = 4$ $\quad |0\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle$



- for a given partitioning

$\ell = 2$, $r = 4$

$L = \ell + r$

- individuals ≡ blocks having different subsets of the q^ℓ and q^r states
- Need selection rules to weight w_α^ℓ and w_α^r
- total quantum numbers, energy, code words, etc.

Total information of the system is shared between two ~~parts~~ blocks

- Quantum coding and decoding:
  take L letters states → q^L states
  but only a subset form codewords
  (has meaning) the rest is just junk

- In DMRG for a given target
  State only a subset is required,
  the rest have zero weight

- SENDER —message→ Receiver

- meaning to a message can be assigned iff response of receiver is taken into account

- mutual information

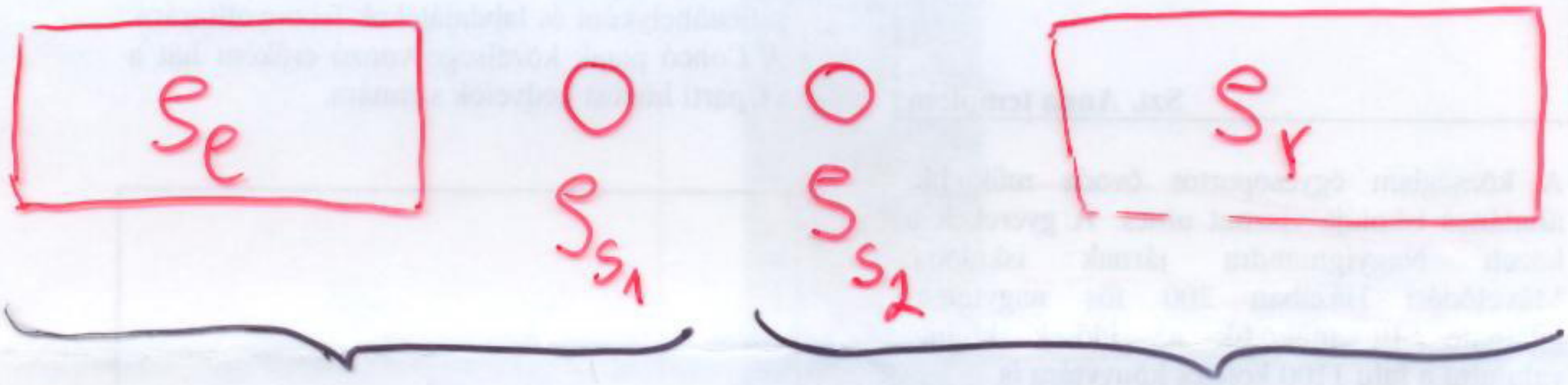
Measuring information:

- von Neumann entropy

$$S = Tr(s \ln s) \longrightarrow \sum_{\alpha} w_\alpha (\ln w_\alpha)$$

w_α are eigenvalues of s

- For DMRG



$$\mathcal{H}_* = \mathcal{H}_\ell * \mathcal{H}_R + \mathcal{H}_{LR}$$

$$G = G_\ell \otimes G_r$$

Site entropy : $S_i = Tr(s_i \ln s_i)$

for $q=4$, $S_{max} = 1.38$ $\quad S_{min} = 0$

Optimizing momentum space DMRG using quantum information entropy

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I. THEORETICAL BACKGROUND

A. Separability versus entanglement

$$\mathcal{G} = \otimes_{i=1}^{m} \mathcal{G}_i, \quad \dim \mathcal{G} = \prod_{i=1}^{m} N_i = N. \tag{1}$$

In general, states of $\mathcal{G}$ can be pure states or mixed states which are described by making use of the density matrix written as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{2}$$

$$\rho \equiv \sum_{i=1}^{N} \omega_i P_i, \quad \sum_{n=1}^{N} \omega_n = 1, \quad \omega_n \geq 0, \tag{3}$$

$$\rho = \sum_i p_i \otimes_{l=1}^{m} \rho_i^l \tag{4}$$

with $N_1 \equiv M_l$, $N_2 \equiv q_l$, $N_3 \equiv q_r$, $N_4 \equiv M_r$.

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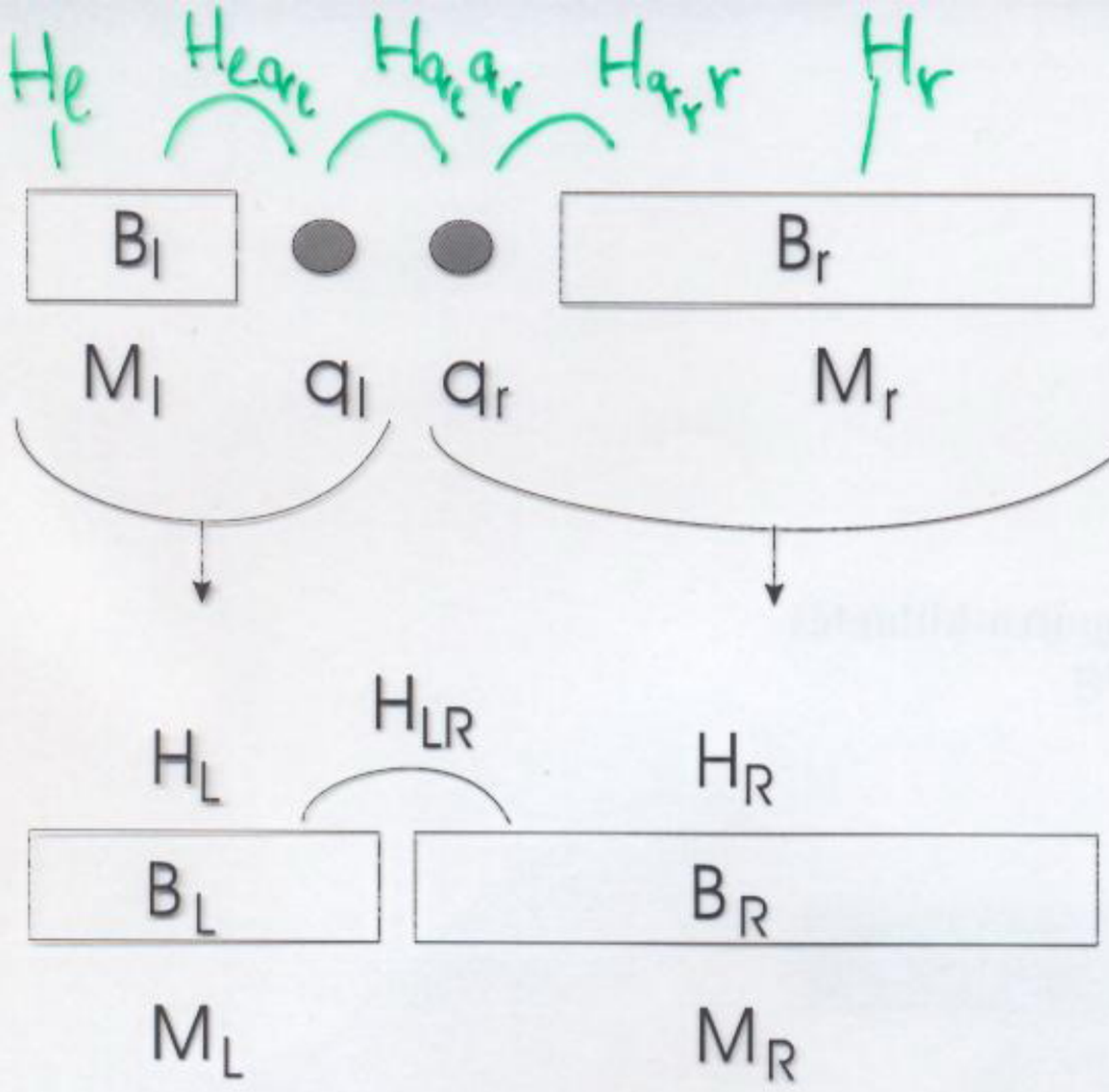


FIG. 1. Schematic plot of system and environment block of DMRG and related quantities described in the text.

- Block and interaction energies

$$\langle \mathcal{H}_i \rangle = \frac{\langle \Psi_T | \mathcal{H}_i | \Psi_T \rangle}{\langle \Psi_T | \Sigma_i \, \mathcal{H}_i | \Psi_T \rangle}, \tag{5}$$

where $i \equiv L, R, LR$ and $\Sigma_i \langle \mathcal{H}_i \rangle = \langle \Sigma_i \, \mathcal{H}_i \rangle$.

$|\Psi_T\rangle \in \mathcal{G} = \mathcal{G}_L \otimes \mathcal{G}_R$, with $\dim \mathcal{G}_L = M_L$, $\dim \mathcal{G}_R \equiv M_R$, $M_L \times M_R = N$,

$$|\Psi_T\rangle = \sum_{i=1}^{r \leq \min(M_L, M_R)} \omega_i |e_i\rangle \otimes |f_i\rangle, \tag{6}$$

where $|e_i\rangle \otimes |f_i\rangle$ form a bi-orthogonal basis $\langle e_i | e_j \rangle \equiv \langle f_i | f_j \rangle \equiv \delta_{ij}$, and $0 \leq \omega_i \leq 1$ with the condition $\Sigma_i \, \omega_i^2 = 1$.

$$\Lambda = \langle \Psi | \rho^{-1} | \Psi \rangle^{-1} > \frac{1}{1 + \max_{i \neq j}(\omega_i \omega_j)} \tag{7}$$

$$\Lambda = \quad \langle \Psi | \rho | \Psi \rangle > \max_i \omega_i^2 \tag{8}$$

- A quantitative characterization of the degree of mixtures is provided by the von Neumann entropy

$$S(\rho) = -\mathrm{Tr}(\rho \ln \rho) \tag{9}$$

and participation number

$$R(\rho) = \frac{1}{\mathrm{Tr}(\rho^2)} \tag{10}$$

- A fundamental concept related to inseparability and non-locality of quantum mechanics is the entanglement.

$$|\psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle. \tag{11}$$

$E : \rho(\mathcal{G}_L \otimes \mathcal{G}_R) \to R_+$ with
(i) $E(\rho) = 0$ if ρ is separable,
(ii) E is convex and
(iii) E is non-increasing (on average) under LOCC

$$E_F(\rho) \equiv \min \sum_i p_i S(\mathrm{Tr_L}|\psi_i\rangle\langle\psi_i|), \;\; \rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{12}$$

where the minimum is taken over all the possible realizations of the state (ρ),

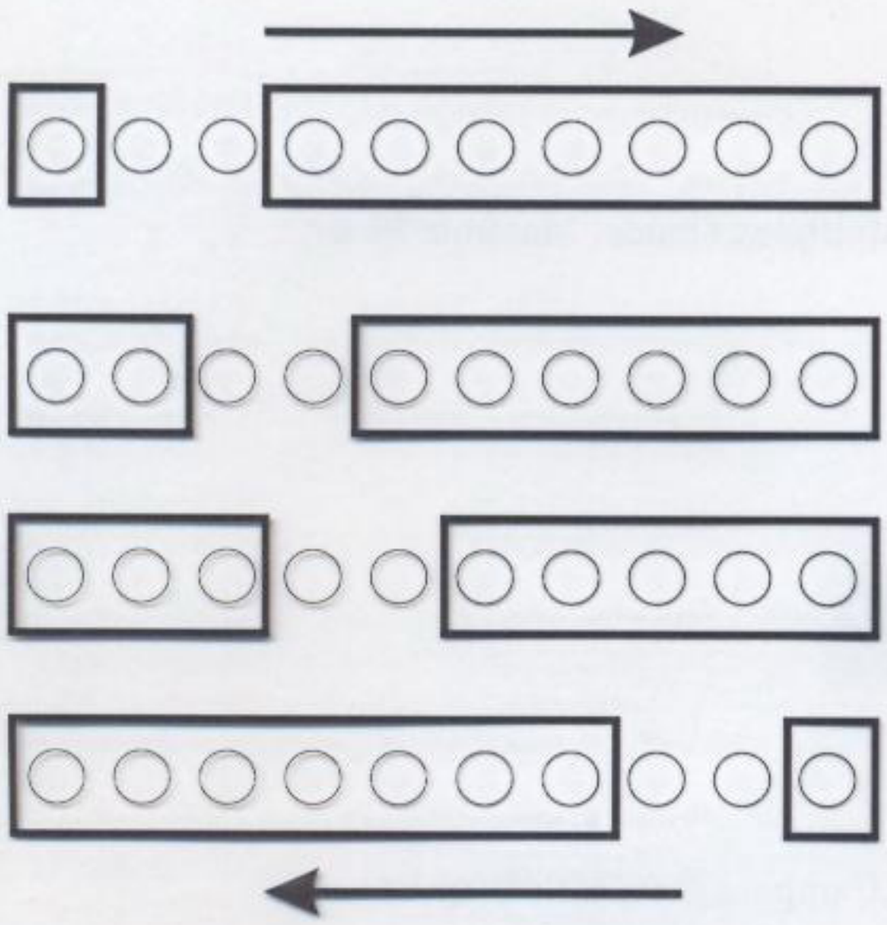


FIG. 2. The decomposition of the finite system to subsystems as a function of iteration steps corresponding to various partitioning.

- Shannon entropy[1] for the two sets is defined as

$$S_i = -\sum_{j=1}^{M_i} p(x_j^i) \ln p(x_j^i), \ \sum_j p(x_j^i) = 1 \tag{13}$$

where $i \equiv L, R$ and labels the information entropy of the left and right sets, respectively.

$$S = \sum_j p(x_j) f_j, \ \ f_j = -\ln p(x_j), \ \ p(x_j) \neq 0 \tag{14}$$

and the weight is $p(x_j)$.

$$\Delta_j = \ln p(x'_j) - \ln p(x_j). \tag{15}$$

- Mean change of information, Kullback information gain:

$$K(p(x'), p(x)) = \sum_j p(x'_j)\Delta_j = \sum_j p(x'_j) \ln \frac{p(x'_j)}{p(x_j)} \tag{16}$$

where $\Sigma_j \, p(x_j) = 1$ and $\Sigma_j \, p(x'_j) = 1$.

- If X^L and X^R are not independent:

$$\begin{aligned} I(L,R) &= S_L - S(L|R) \\ &= S_L + S_R - S_{LR} \\ &= S_L - S(L|R)\,, \end{aligned} \tag{17}$$

where $S(L|R)$ the conditional entropy is given by

$$\begin{aligned} S(L|R) &= S_{LR} - S_R \\ &= -\Sigma_{j,j'}\, p(x_j^L, x_{j'}^R) \ln p(x_j^L, x_{j'}^R) \\ &\quad -\Sigma_j\, p(x_j^R) \ln p(x_j^R) \end{aligned} \tag{18}$$

and $p(x_j^L, x_{j'}^R)$ is the joint probability distribution of the two events.

- $I(L,R)$ is symmetric under the interchange of X^L and X^R and zero if and only if $p(x^L, x^R) = p(x^L)p(x^R)$.

- Within the context of DMRG treating quantum systems:

$$K(\rho||\sigma)) \equiv \mathrm{Tr}(\rho \ln \rho - \rho \ln \sigma). \tag{19}$$

target state is a pure state it corresponds to zero Neumann entropy with $S_{LR} = 0$, thus $I(L,R) = S_L + S_R$.

$$S = \sum_j \omega_j \ln \omega_j = S_L = S_R. \tag{20}$$

as a consequence that $\omega_i = \omega_i^L = \omega_i^R$.

- Calculate also $\rho_l, \rho_{ql}, \rho_{qr}, \rho_r$

C. Information generation and annihilation

- DMRG behaves dynamically.

• Then the relative importance ω_j is defined as

$$\omega_j = \sum_k L_{jk}\omega'_k = \sum_k \frac{M_{jk}}{\Sigma_{j'} M_{j'k} + \epsilon}\omega'_k \tag{21}$$

where $\epsilon \to 0$.

• If there are several system coupled one after the other, then for instance in the two step procedure we obtain

$$\omega_j = \sum_k L^{(1)}_{jk}\omega'_k = \sum_{k,k'} L^{(1)}_{jk} L^{(2)}_{kk'}\omega''_k. \tag{22}$$

• Recursion from $\omega^{(n)}$ to ω may depend on the path, namely on the ordering of lattice sites or molecule orbitals.

$$S^{(0)} = -\sum_j \omega_j \ln \omega_j, \;\; S^{(1)} = -\sum_k \omega_k \ln \omega_k. \tag{23}$$

If $\Sigma_k \omega_k \equiv 1$ and $\Sigma_j \omega_j \equiv 1$ there is annihilation of information if $S(1) < S(0)$ or generation of information if $S^{(1)} > S^{(0)}$. Depending on features of a dynamical system it can be "sensitive" or "insensitive" for a given message.

II. NUMERICAL INVESTIGATION OF NEUMANN ENTROPY AND ENTANGLEMENT

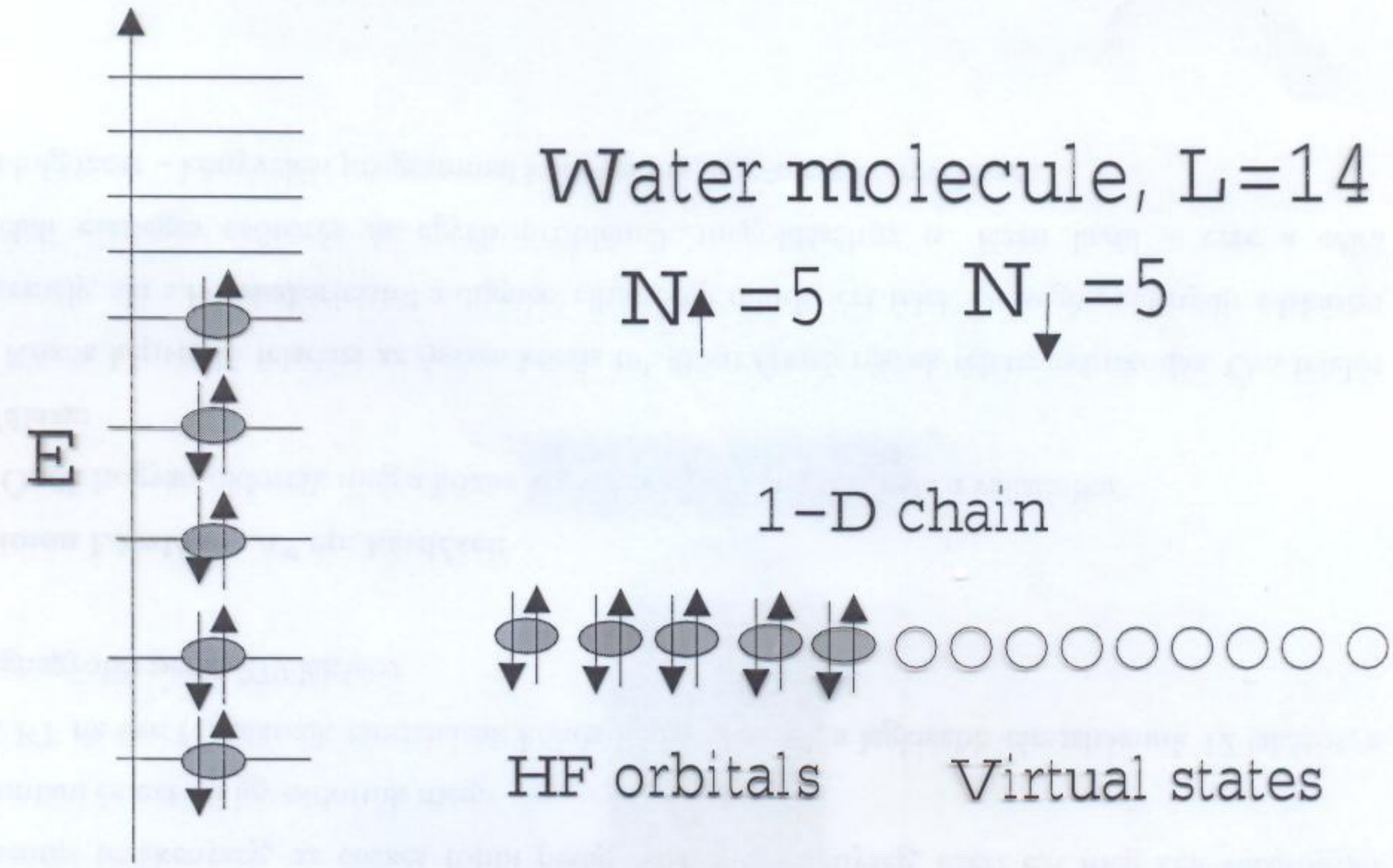
$$\mathcal{H} = \sum_{ij\sigma} T_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{ijkl\sigma\sigma'} V_{ijkl} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{k\sigma'} c_{l\sigma} \tag{24}$$

• T_{ij} denotes the matrix elements of the one-particle Hamiltonian

• V_{ijkl} stands for the matrix elements of the electron interaction operator.

• molecules within the context of quantum chemistry,

• the Hubbard and extended Hubbard models in one or higher dimensions



A. Transformation to 1D lattice

• A one dimensional chain containing L molecular orbitals is generated by ordering the orbitals employed to build up the multi-particle states with increasing energy or by other rules, analogous to k points in k-DMRG. These molecular orbitals are calculated by standard numerical methods of quantum chemistry.

• One site has 4 degrees of freedom, namely the doubly occupied, spin up, spin down and empty orbital situation.

• In the Full-CI solution the dimension of the Hilbert space would be $4^L|_{N_{up},N_{down}}$.

- coupled fermion chains.

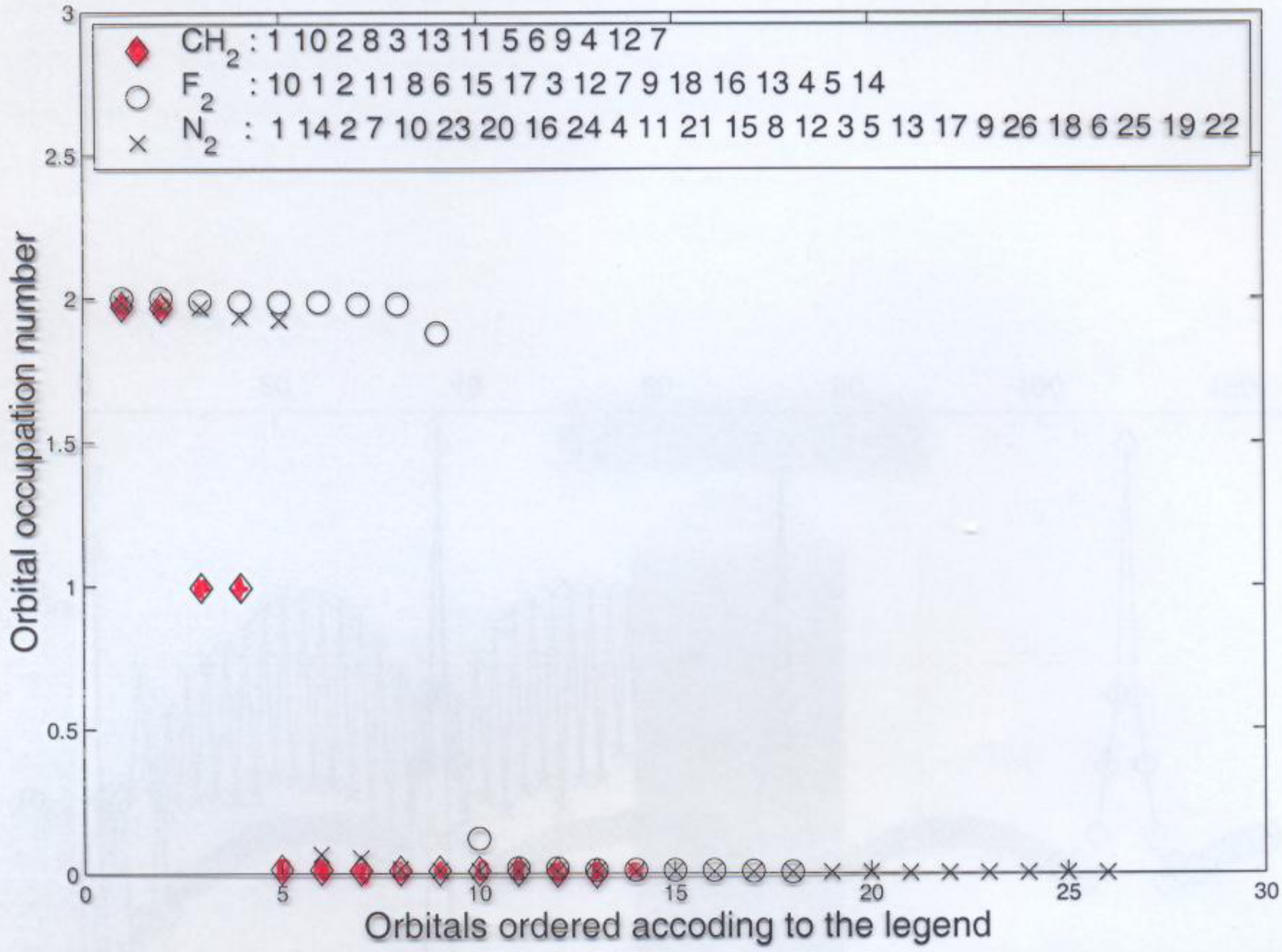
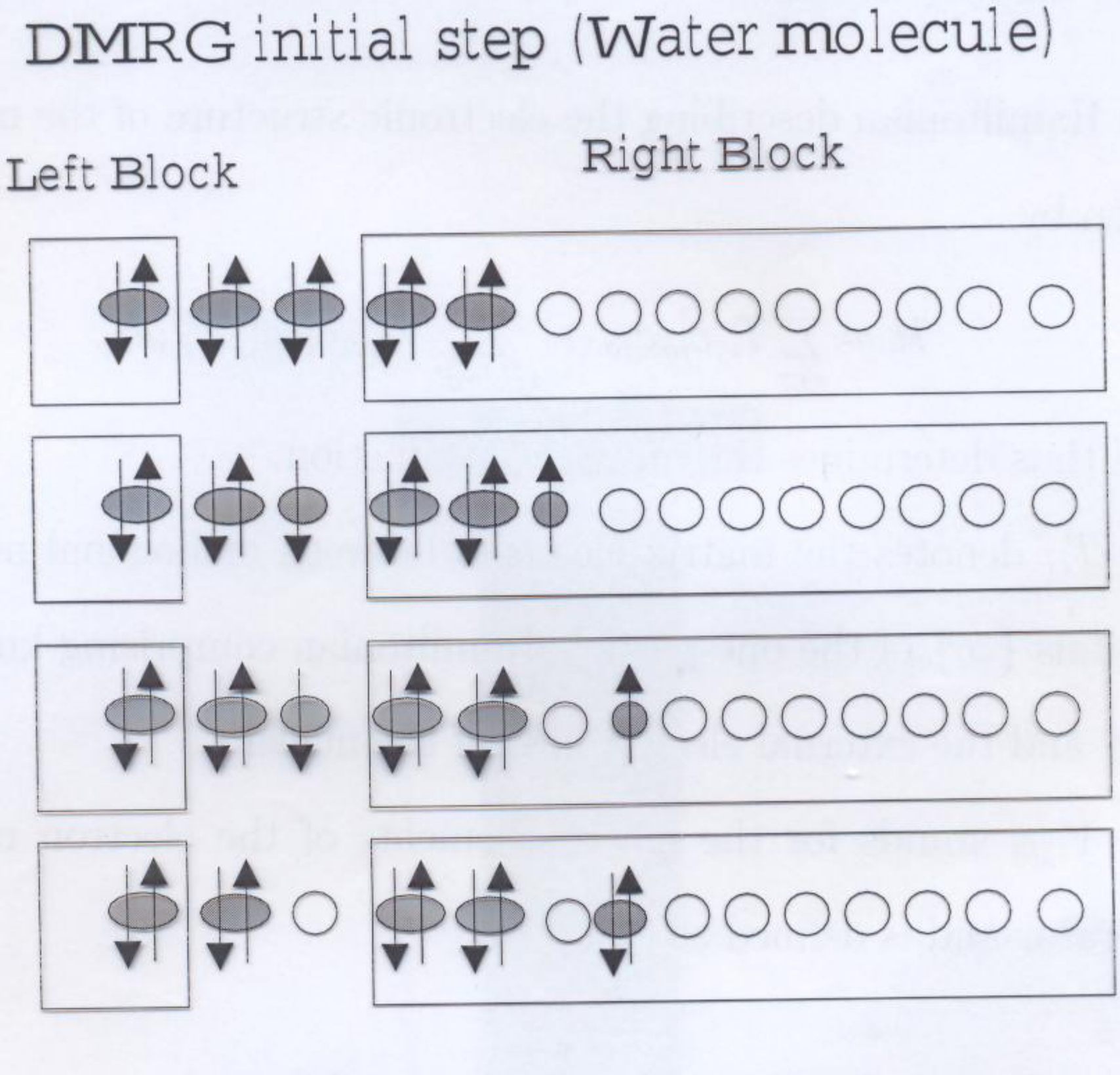


FIG. 3. Decay of orbital occupation number obtained in the full CI limit and the corresponding ordering of orbitals for molecules studied in the paper.



M_L<q^L .q .q M_R<q^R

far away from each other in the chain and include their contribution to the correlation energy, the size of the left block is increased as long as $l \leq N - 3$ and the length of the right block is decreased so that $r + l + 2 = N$ always holds.

F. Target state

• This sweeping procedure implies that in each DMRG iteration step the wave function of the molecule is built up from the linear com-

• Besides ordering, the optimal performance of DMRG is also effected to a great extent by the initial conditions or in other words by the initial block configurations.

A. The CAS-DMRG

• most probable excitations

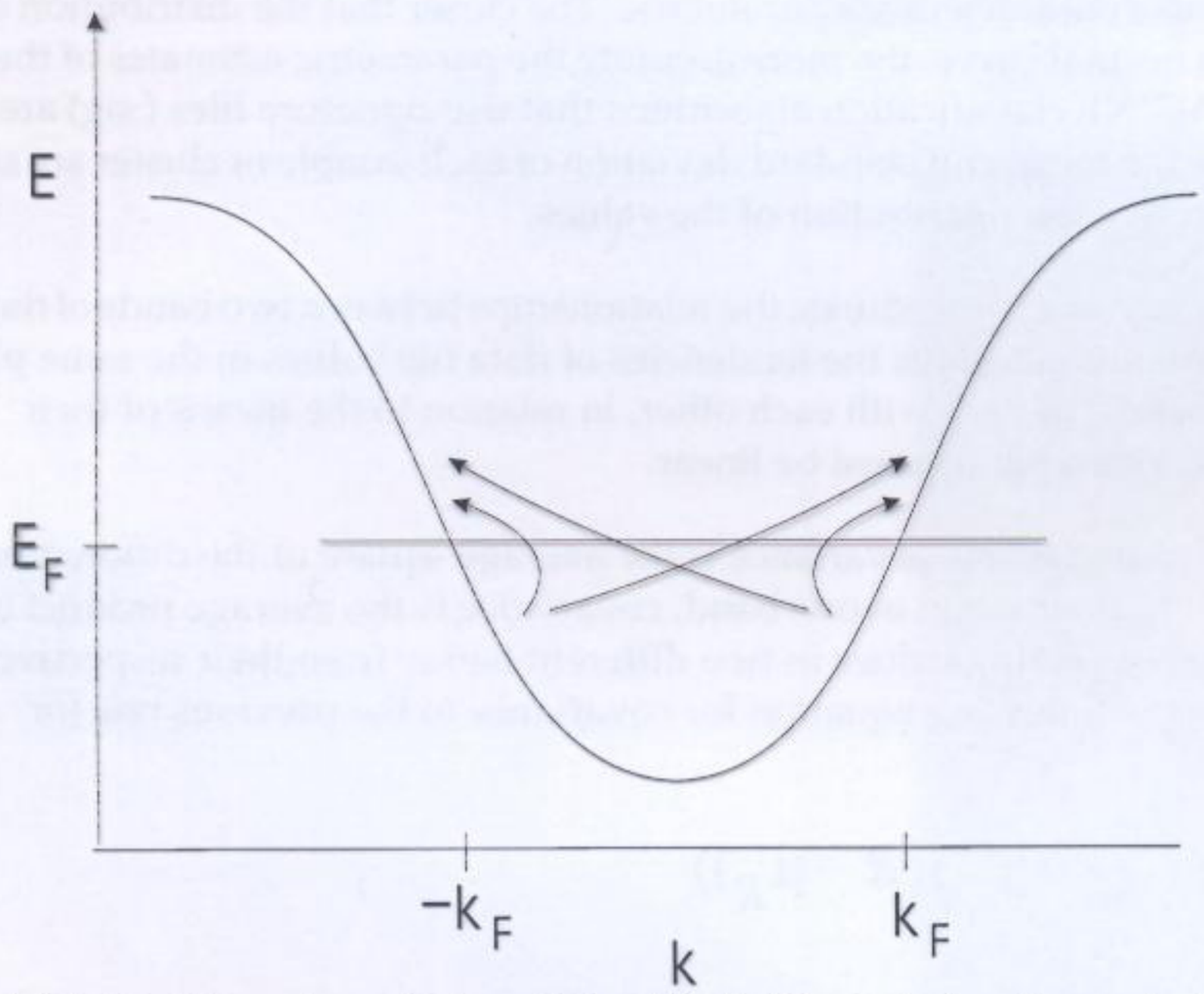


FIG. 11. Dispersion relation of the 1-D Hubbard chain. Arrows indicate the most probable electron-hole excitations with small momentum transfer in the small U limit.

• partitioning when the left block (system block) contains one lattice site and the right block (environment) $L-3$ lattice sites

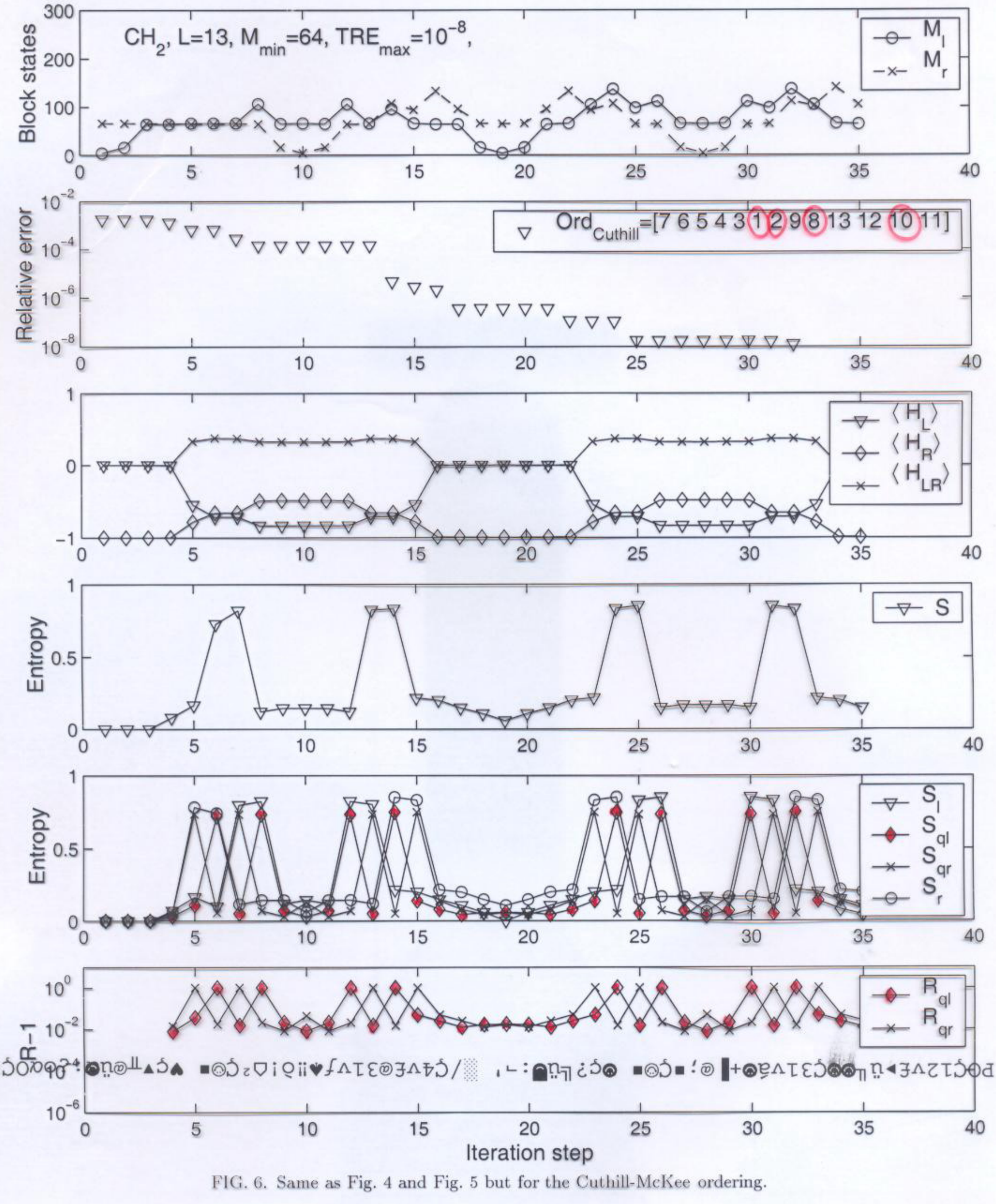


FIG. 6. Same as Fig. 4 and Fig. 5 but for the Cuthill-McKee ordering.

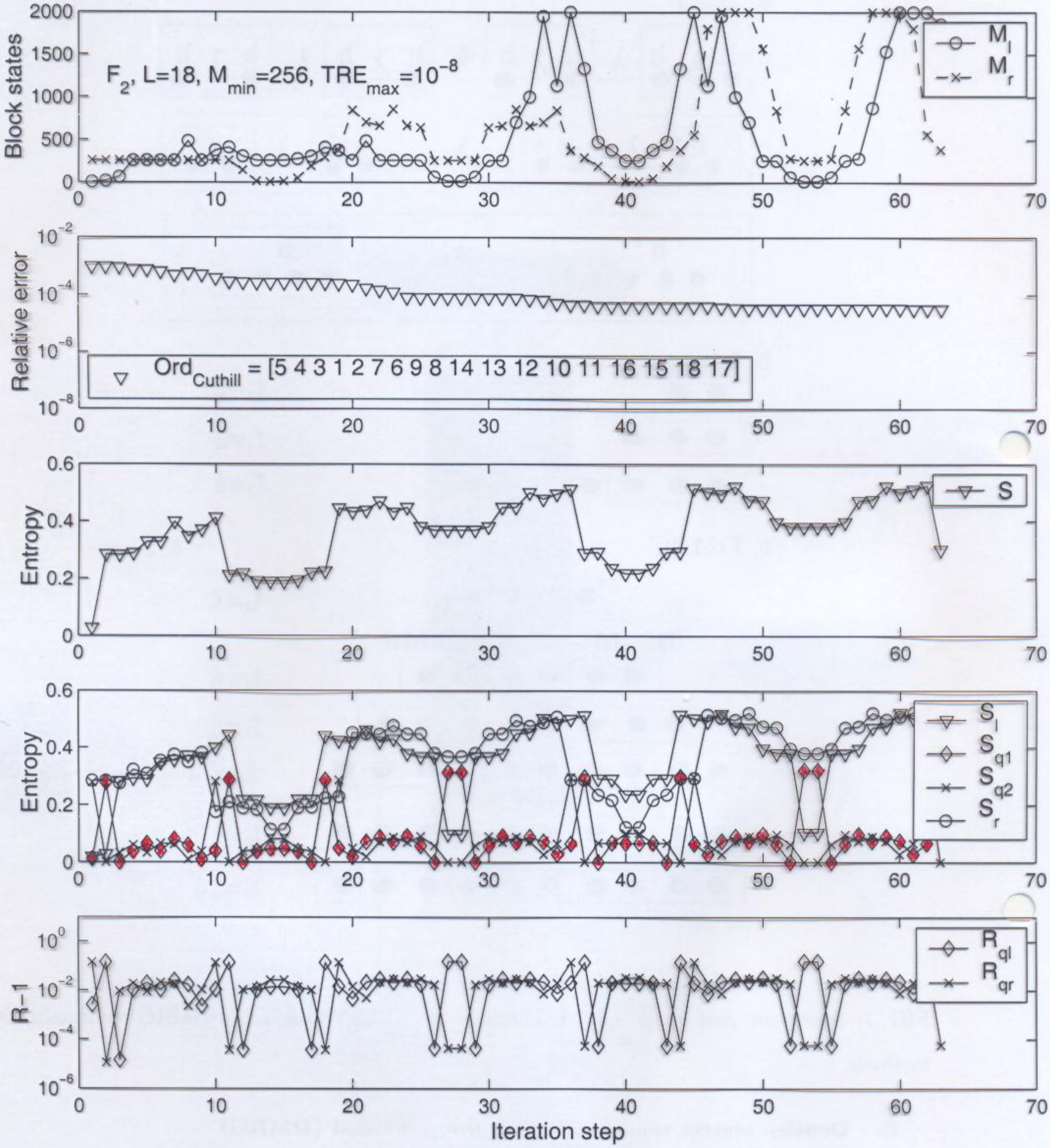


FIG. 7. Result for F_2 molecule correlating 18 electrons on 18 orbitals using Cuthill-McKee ordering.

B. Analysis on the 1-D Hubbard chain

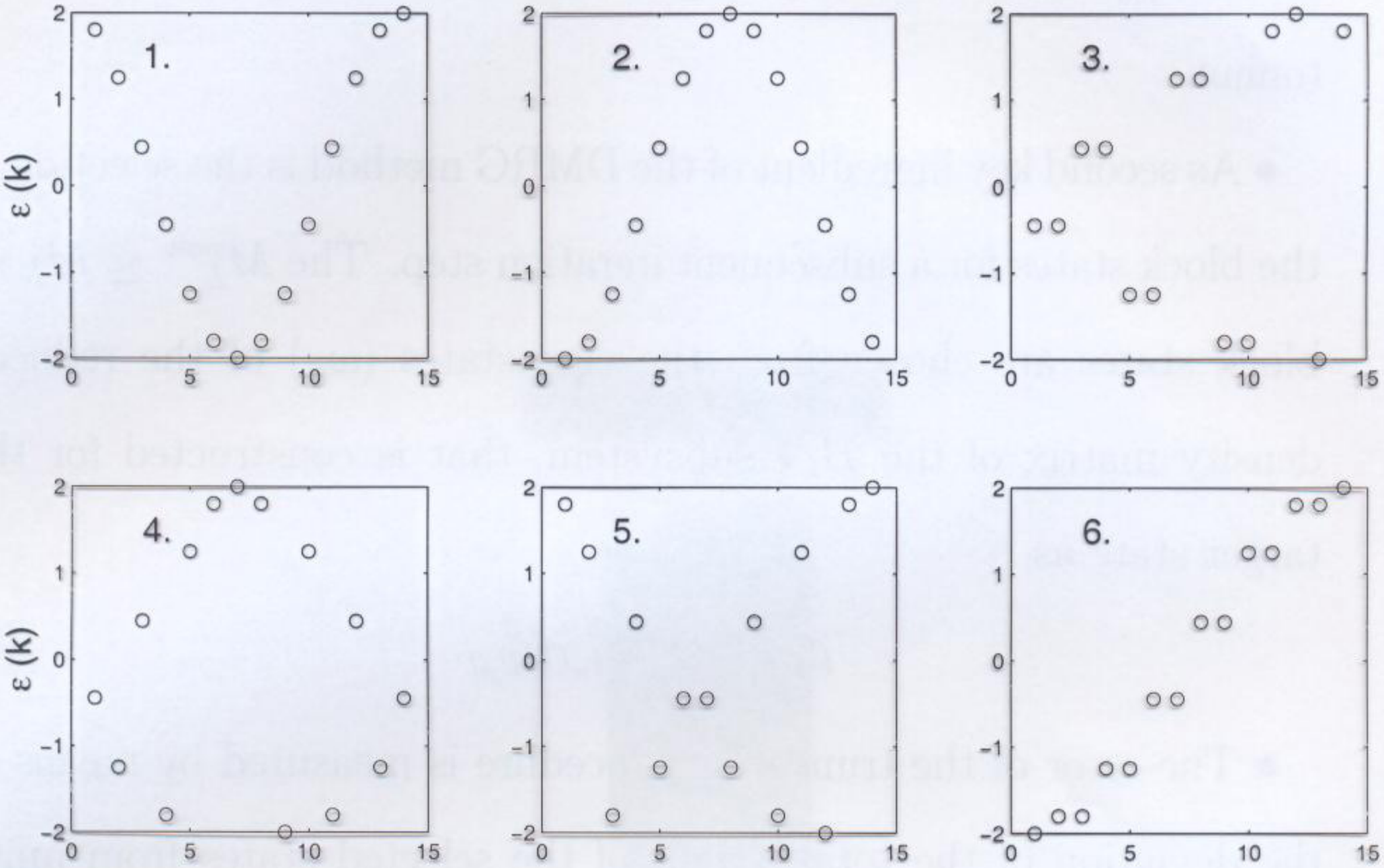


FIG. 8. Example for various orderings of k_i points for the half-filled Hubbard chain with L=14. Doubly filled sites in the HF limit in the natural ordering are 4,5,6,7,8,9,10.

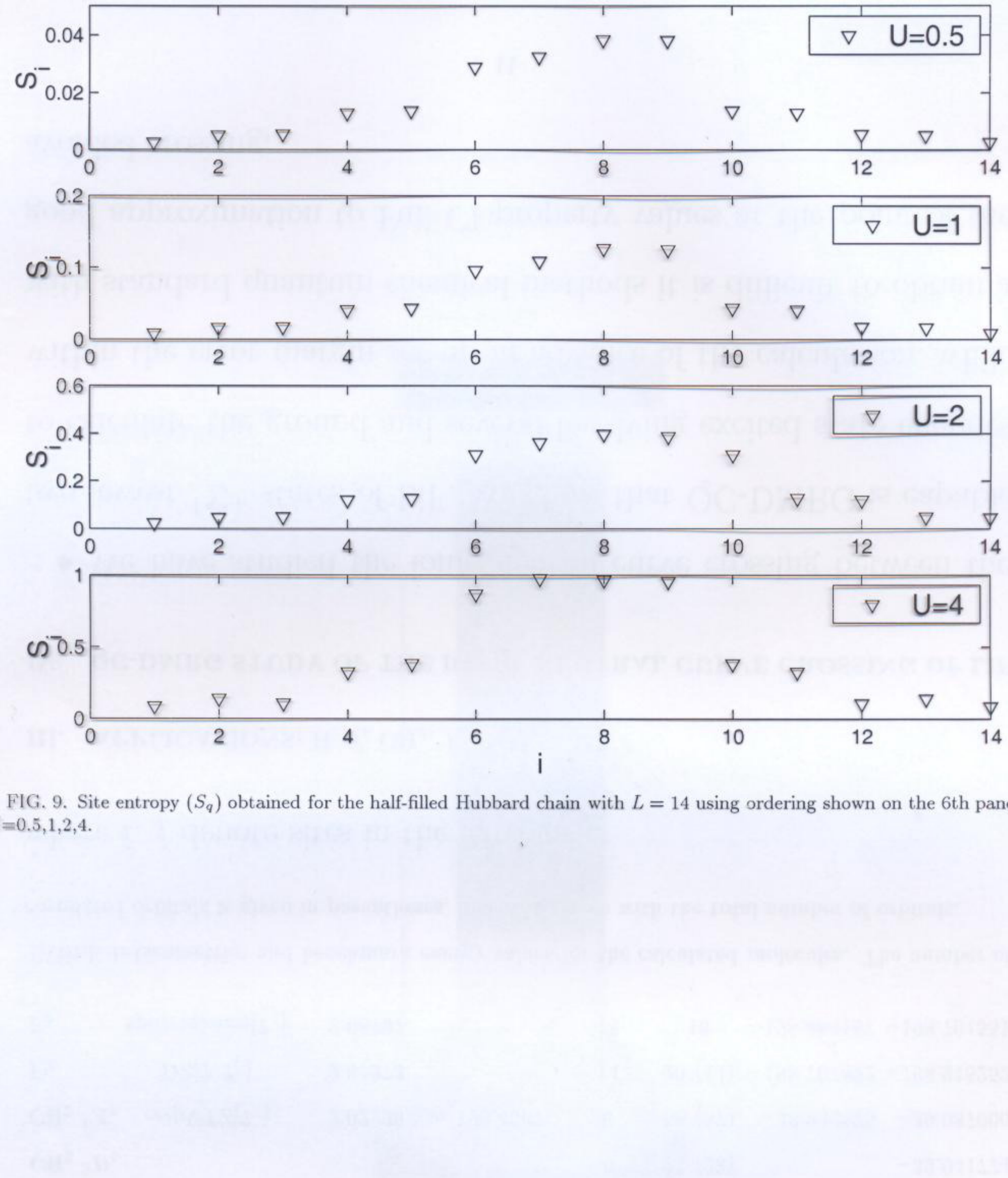


FIG. 9. Site entropy (S_q) obtained for the half-filled Hubbard chain with $L = 14$ using ordering shown on the 6th panel with U=0.5,1,2,4.

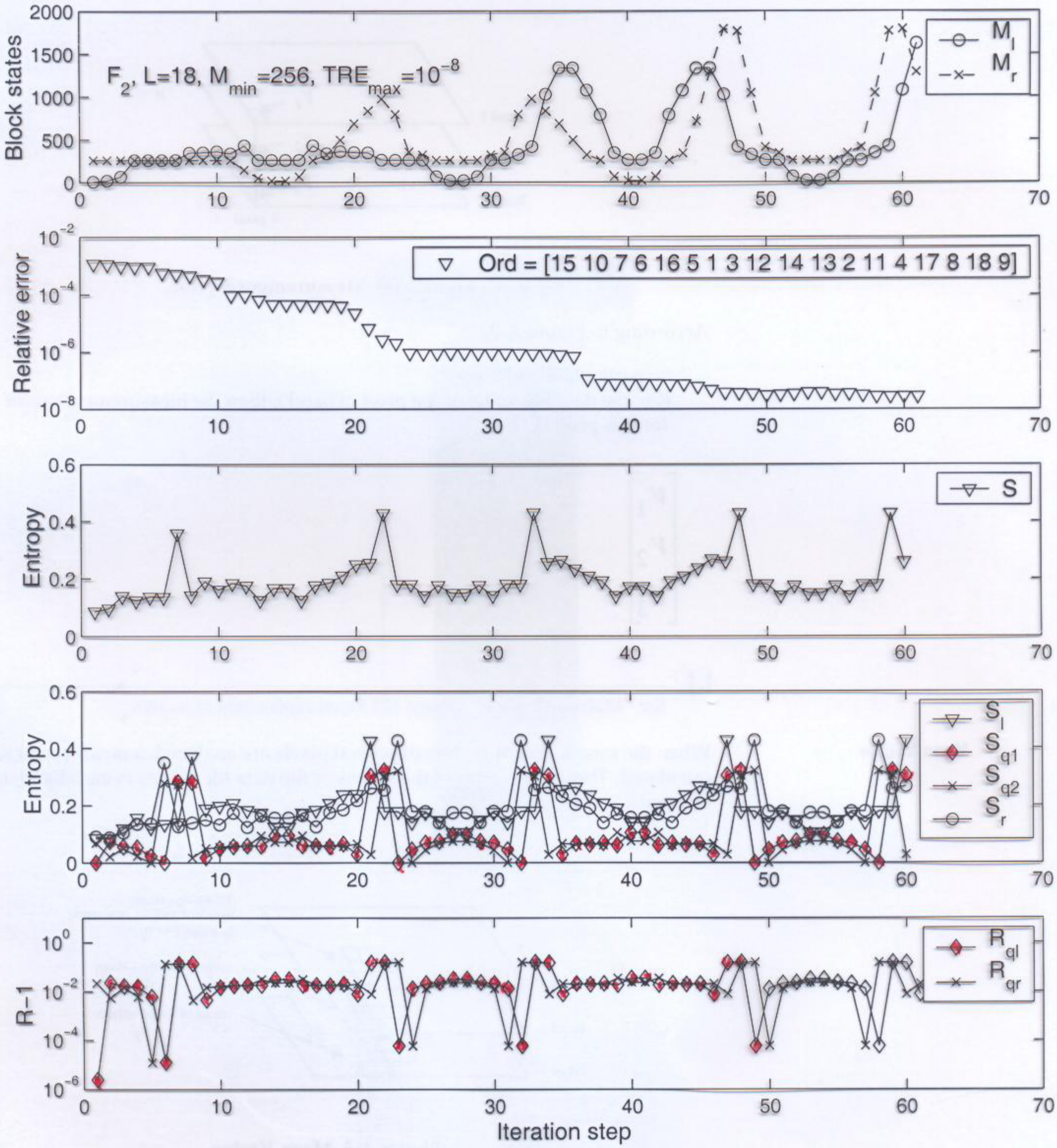


FIG. 10. Result for F_2 molecule correlating 18 electrons on 18 orbitals using our numerically optimized ordering.

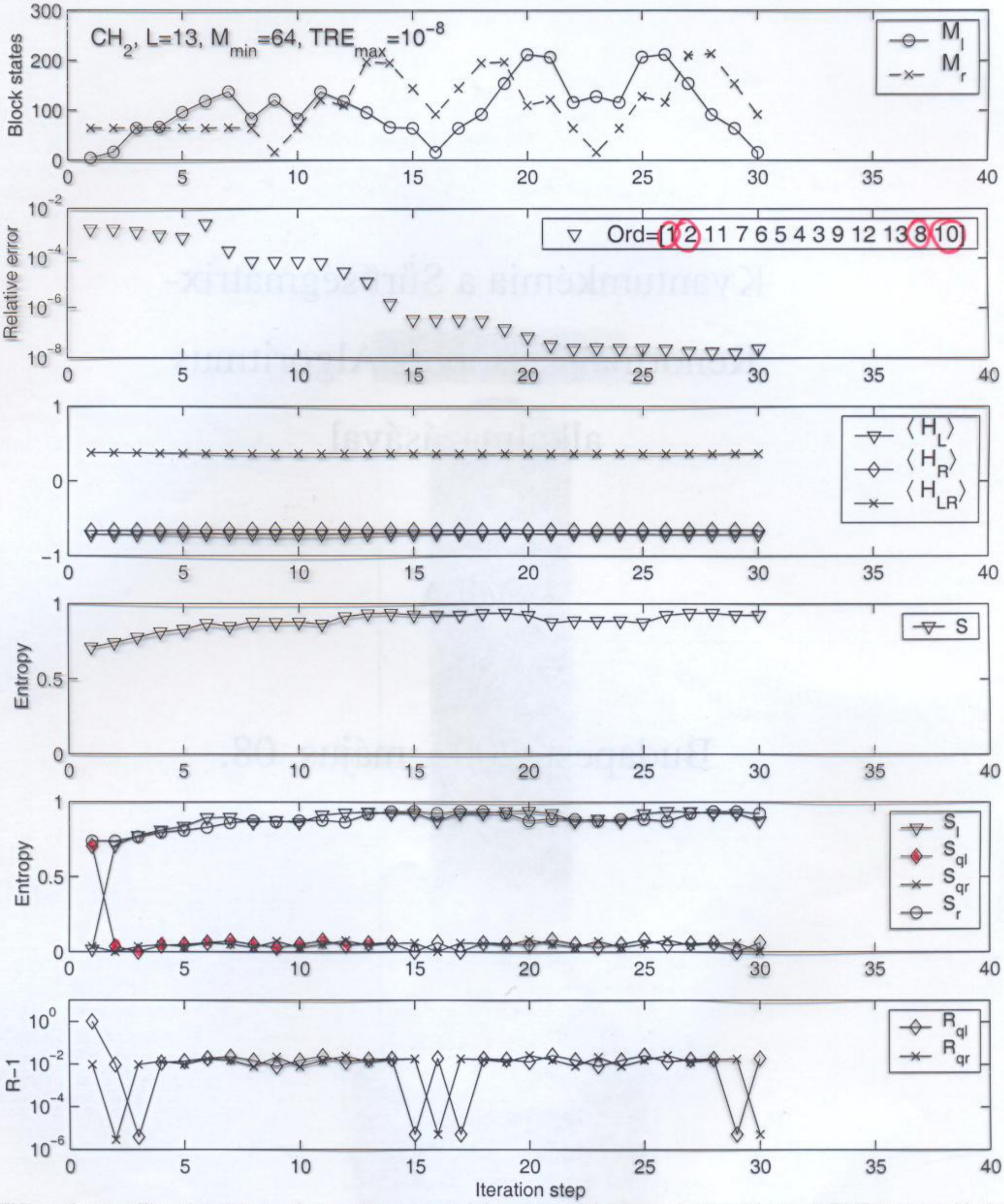


FIG. 5. Same as Fig. 4 but for an ordering when relevant information of the system is shared between DMRG system blocks giving rise to strong interblock interaction and large quantum information exchange between the blocks.

Cuthill-McKee algorithm

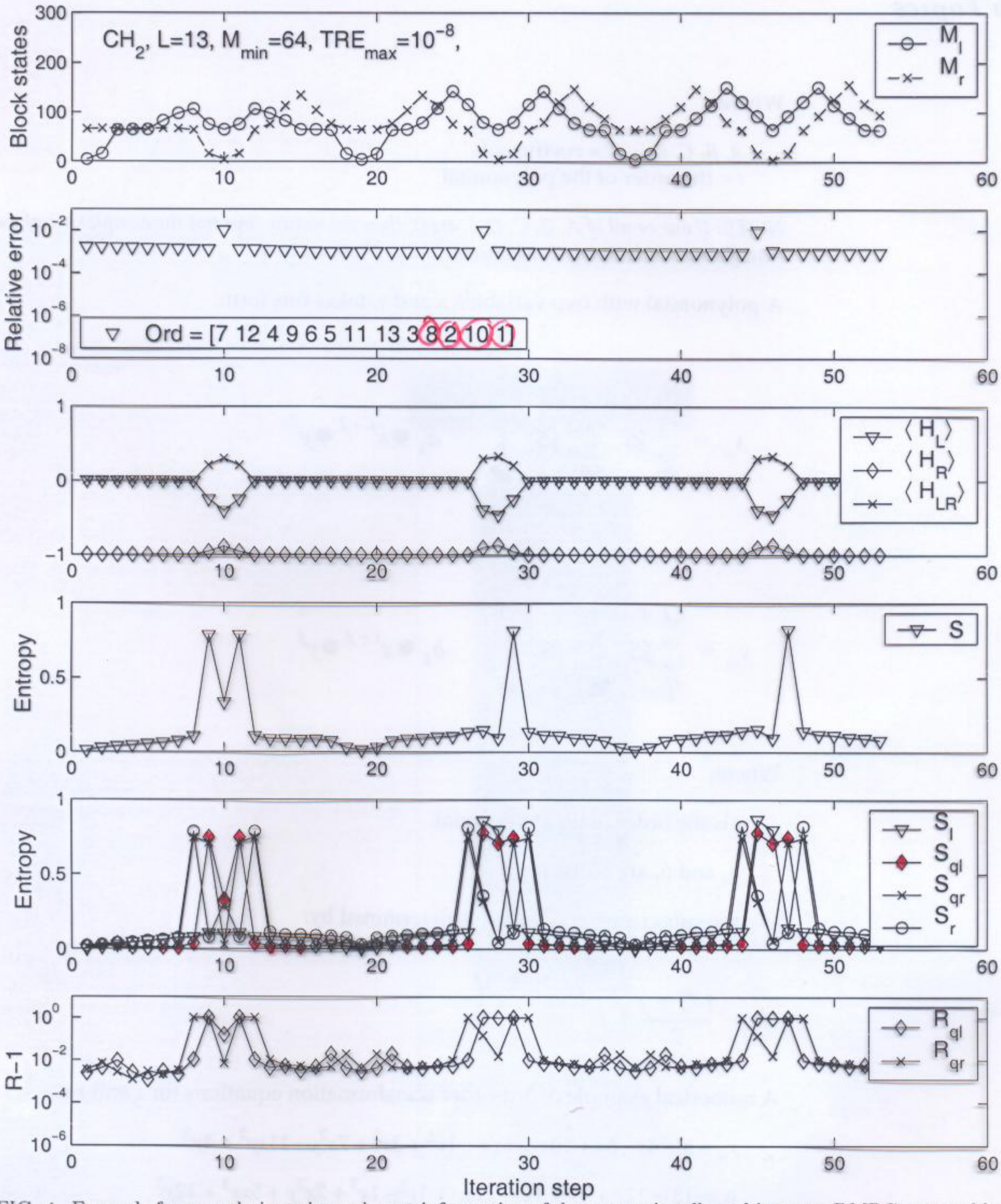


FIG. 4. Example for an ordering when relevant information of the system is collected into one DMRG system block giving rise to vanishing interblock interactions and very low entropy indicating high separability of the target state and lack of quantum information exchange between the blocks.

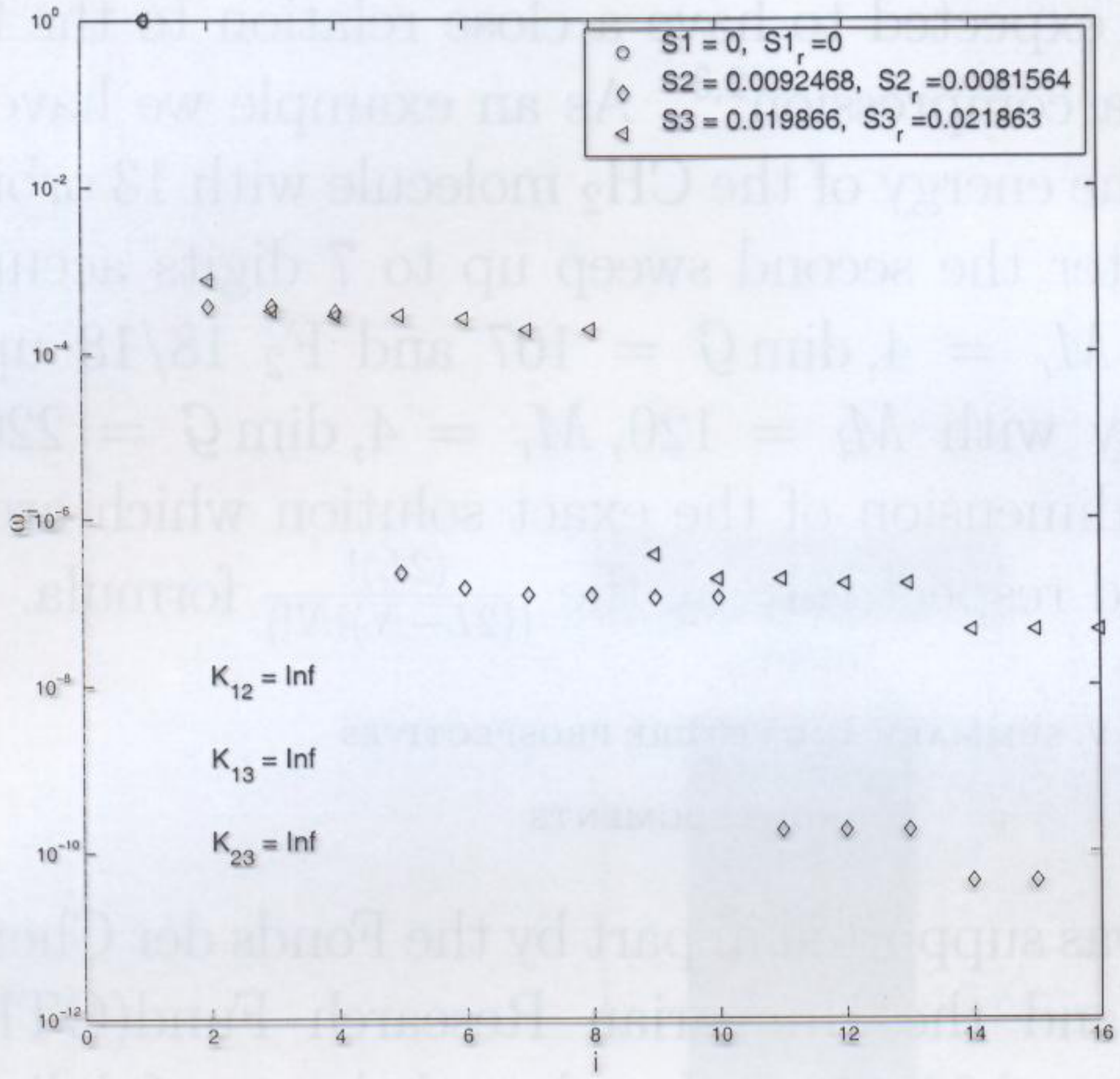


FIG. 12. The mutual Neumann entropy (S), environment block entropy (S_r) and Kullback-Leibler (K) entropy calculated for three specially constructed environment blocks for the half-filled Hubbard chain with $U = 1$ and $L = 14$ using original ordering.

- right block configuration
- In practical application of DMRG $M_r \ll q^r$, many orbitals will remain unfilled
- Vacuum sites, Doubly filled sites, Active sites $\rightarrow$ reducing effective system size

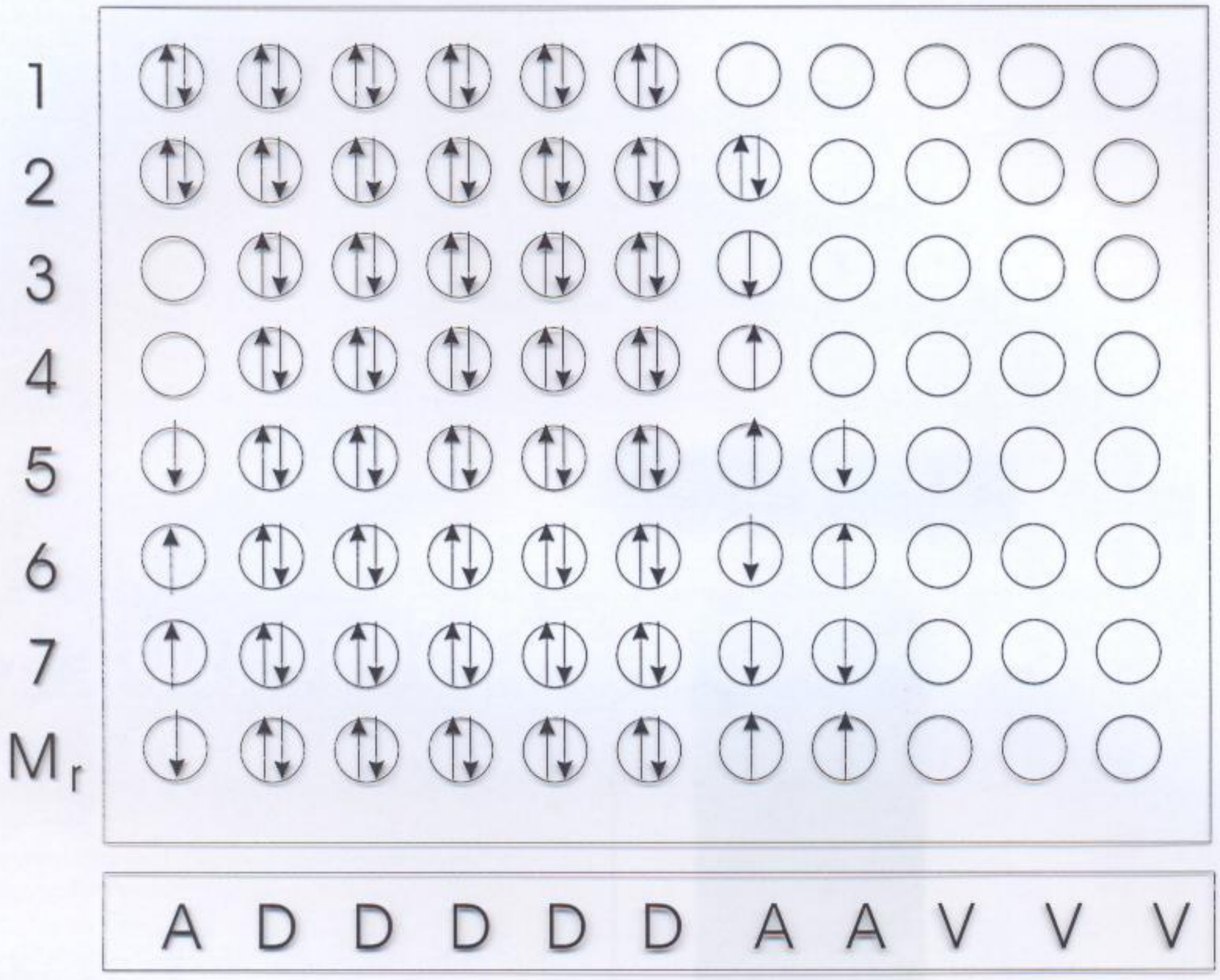


FIG. 13. Example for a right block configuration space obtained by CAS-DMRG for the half-filled Hubbard chain with $L = 14$, $N_\uparrow = N_\downarrow = 7$, $M_r^{min} = 8$, $l = 1$, $r = 11$ and HF vector $\equiv [4, 5, 6, 7, 8, 9, 10]$ and CAS vector $\equiv [4, 10, 3, 11, 5, 9]$.

B. Application of Abelian point-group symmetry within the context of QC- DMRG

The k_i quantum numbers operator for an orbital defined on the $(0, \downarrow, \uparrow, \downarrow\uparrow)$ basis states in QC-DMRG is written as

$$K_i = k_i \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \tag{25}$$

where k_i can take values from one to eight according to the symmetry of the orbital. The symmetry quantum number operator for basis states of two orbitals is determined by using the standard character table as

$$K_{ij} \equiv \mathcal{T}(K_i, K_j), \tag{26}$$

with

$$\mathcal{T} = \begin{pmatrix} 1&2&3&4&5&6&7&8 \\ 2&1&4&3&6&5&8&7 \\ 3&4&1&2&7&8&5&6 \\ 4&3&2&1&8&7&6&5 \\ 5&6&7&8&1&2&3&4 \\ 6&5&8&7&2&1&4&3 \\ 7&8&5&6&3&4&1&2 \\ 8&7&6&5&4&3&2&1. \end{pmatrix} \tag{27}$$

$$K_{TOT} = \mathcal{T}(K^L, K^R). \tag{28}$$

C. Numerical results on CAS-DMRG

As an example Fig. 14 shows result obtained for the half-filled, $L = 18$ chain with with $M_{min} = 400$ and $TRE_{max} = 10^{-5}$ in order to obtain an absolute error of 10^{-4} for various $U = 0.5, 1, 2, 4$ values using the ordering shown on the 6th panel on Fig. 8. The CAS vector was $CAS \equiv [13, 5, 14, 4, 12, 6, 15, 3, 11, 7, 16, 2, 10, 8, 17, 1]$ and the HF vector $[1, 2, 3, 4, 5, 6, 7, 8, 9]$.

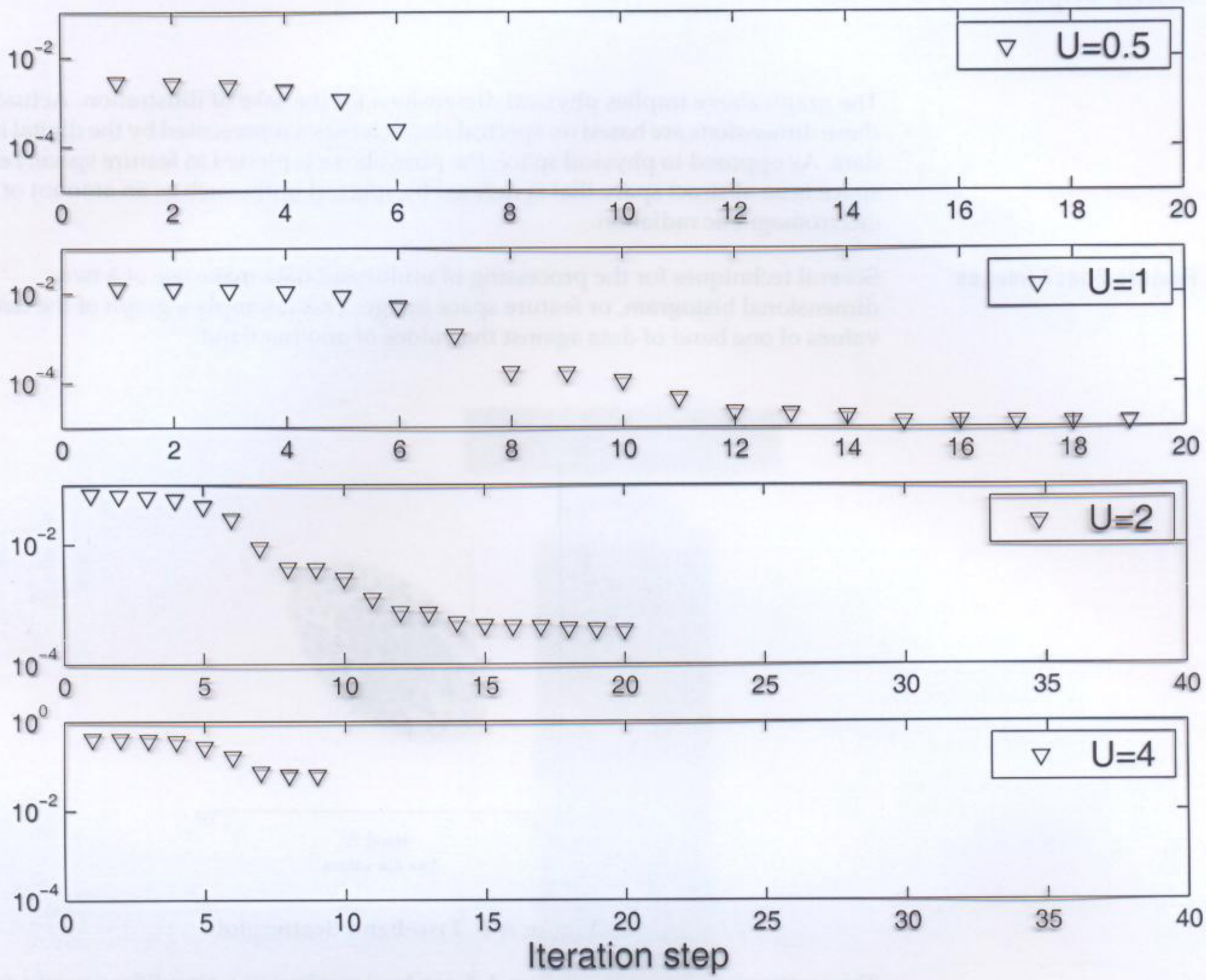


FIG. 14. L=18 Half-filled Hubbard chain for $U = 0.5, 1, 2, 4$ using CAS-DMRG.

calculated momentum distribution ($n_k = \Sigma_{i,\alpha}\, c^{\dagger}_{i\alpha} c_{i\alpha}$)
Results for CH_2 6/13 and 6/23, H_2O with 8/24, N_2 with 10/26 and F_2 with 18/18 are shown on

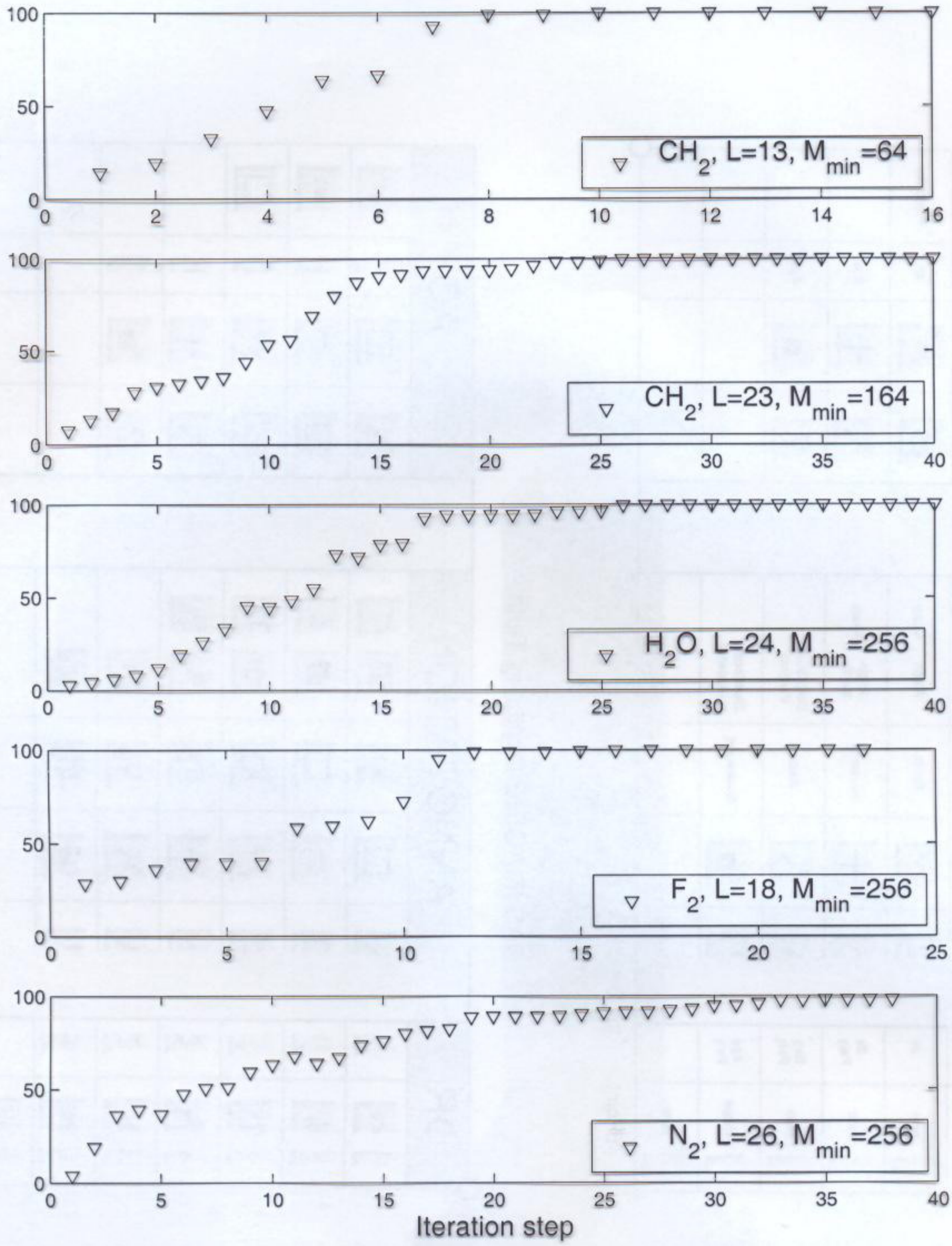


FIG. 15. Percent of correlation energy as a function of iteration step obtained by CAS-DMRG for the CH_2, H_2O, N_2, F_2 molecules.

This feature is expected to have a close relation to the field of quantum data compression[2,3]. As an example we have set $M_{min} = 4$ and the energy of the CH_2 molecule with 13 orbitals

was obtained after the second sweep up to 7 digits accuracy with $M_l = 21, M_r = 4, \dim \mathcal{G} = 107$ and F_2 18/18 up to 5 digits accuracy with $M_l = 120, M_r = 4, \dim \mathcal{G} = 220$ in contrast to the dimension of the exact solution which are ..., and ... calculated respectively by the $\frac{(2L)!}{((2L-N)!N!)}$ formula.

V. SUMMARY AND FUTURE PROSPECTIVES

ACKNOWLEDGMENTS

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[1] E. Shannon, Bell Syst. Tech. J. **27**, 379 (1948).
[2] B. Schumacher, Phys. Rev. A. **51**, 2738 (1995).
[3] R. Jozsa, J. Mod. Opt. **41**, 2315 (1994).

Optimizing momentum space DMRG using quantum information entropy
Ö. Legeza and J. Sólyom
preprint (2003).

Controlling the accuracy of the density-matrix renormalization-group method:
The dynamical block state selection approach.
Ö. Legeza, J. Röder, and B. A. Hess
Phys. Rev. B 67, 125114 (2003).

QC-DMRG study of the ionic--neutral curve crossing of LiF.
Ö. Legeza, J. Röder, and B. A. Hess
Mol. Phys. , accepted for publication (2003).

String order in spin liquid phases of spin ladders.
G. Fáth, Ö. Legeza, and J. Sólyom
Phys. Rev. B 63, 134403 (2001).

Minimal model to describe the magnetism of CuGeO3.
G. Bouzerar, Ö. Legeza, and T. Ziman
Phys. Rev. B 60, 15278-15284 (1999).

Density-Matrix spectra for integrable models.
I. Peschel, M. Kaulke. Ö. Legeza
Ann. Physik (Leipzig) 8 (1999) 153.

Response of finite spin-S Heisenberg chains to local perturbations
Ö. Legeza and J. Sólyom
Phys. Rev. B 59, 3606-3611 (1999).