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Quantifying and improving the accuracy of the Matrix Product Operator Renormalization Group of random spin chains

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Abstract. A relatively simple real-space renormalization procedure, due to Ma and Dasgupta and known as Strong-Disorder Renormalization Group (SDRG), provides in principle exact results on the critical properties at the infinite-randomness fixed point of random spin chains. Numerically, SDRG can be efficiently implemented as a renormalization of Matrix Product Operators (MPO-RG). By considering larger blocks than SDRG, MPO-RG was recently used to compute non-critical quantities that are inaccessible to SDRG. In this work, we study the accuracy of the approach and propose two simple and fast improvements. We observe that the accuracy on the ground state energy is improved by a factor at least equal to 4.

PACS numbers:

1. Introduction

The critical behavior of the random quantum Ising chain in a transverse field (RIMTF) is known to be governed by a very peculiar renormalization-group fixed point where randomness becomes infinitely strong [1, 2, 3]. The properties of this Infinite-Disorder quantum critical point were elucidated using a relatively simple real-space renormalization group, previously introduced by Ma and Dasgupta [4, 5], and known as Strong-Disorder Renormalization Group (SDRG) [6, 7]. The term H_0 of the Hamiltonian with the largest coupling is isolated from the rest of the chain. The full Hilbert space of the spin chain is then projected out onto the subspace spanned by the ground states of H_0 . A strong transverse field h_i leads to a freezing of the spin on which it acts while a strong exchange coupling J_i freezes the relative states of the two spins at its edges. The latter can be considered as a two-state effective macro-spin. Effective interactions with the rest of the chain are generated by second-order perturbation theory. An effective exchange coupling $J_{\text{eff}} = J_{i-1}J_i/h_i$ is induced between the two neighboring spins of a spin frozen by a strong transverse field h_i . Similarly, an effective transverse field $h_{\text{eff}} = h_i h_{i+1}/J_i$ acts on the macro-spin formed by a strong exchange coupling. As the renormalization is iterated, the probability distribution of the couplings evolves towards an infinitely broad law. As a consequence, a strong coupling is more and more likely to be surrounded by weak couplings. Therefore, the SDRG is believed to become exact, not only at the IRFP but in the whole Griffiths phase [8].

Following the general principles of renormalization group, the critical exponents are extracted from the flow equations of couplings during the renormalization process. The dynamical exponent z for instance is obtained from the scaling of the number of remaining sites while the magnetic exponent β is given by the scaling of the total magnetic moment of the chain. In the case of the random Ising chain in a transverse field, the flow equations have been solved by Fischer. For more general models, as for instance the random Ashkin-Teller model, these equations cannot be solved but SDRG rules can easily be implemented numerically [9, 10]. Even though very approximate effective interactions are generated during the first iterations of the SDRG, they are expected to become more and more accurate as the IRFP is approached. It is therefore necessary to apply the technique to very large chains, typically of the order of tens of thousands or millions of spins. The procedure is nevertheless able to give accurate estimates of critical exponents. For strong disorder, this approach is the most efficient. The Density Matrix Renormalization Group (DMRG) algorithm [13, 14, 15, 16] suffers from stringent convergence problems in presence of strong disorder. In the case of the above-mentioned random Ashkin-Teller model, only small lattices could be considered [17, 18]. Moreover, SDRG can be implemented numerically to study lattice models in higher dimensions [19].

The spirit of MPO renormalization, as introduced by [11] and then considered by [12], is different from SDRG: the goal is to construct an effective Hamiltonian acting on a small Hilbert space from which quantum averages in the ground state, rather than critical exponents, can be estimated. MPO renormalization is meant as an alternative to DMRG at strong disorder. Like the Hamiltonian, the observables should be expressed as MPO. Powers of global observables $(\sum_i O_i)^n$ can also be written as MPO. At each step of the renormalization process, the same transformation is applied to the matrix product of the Hamiltonian and of all observables. At the end of the renormalization, i.e. when only one site remains, the Hamiltonian is diagonalized and the averages of the observables are computed in the ground state. In the case of the random anti-ferromagnetic Ising chain in a transverse field, the Binder cumulant was estimated with this algorithm and the location of its crossing points were shown to be in good agreement with the exact transition point [12].

In the first section of this paper, SDRG is reviewed. The emphasis is put on the construction of effective interactions by perturbation theory. In the second section, the MPO renormalization algorithm is presented. The equivalence with SDRG in the limit of strong couplings is shown in the particular case of the Ising chain in a transverse field. In the third section, two improvements of this algorithm are presented: a new criterion is introduced to choose the blocks to be merged in the renormalization procedure and the construction of effective interactions taking into account the highest excited states to be discarded is presented. In the fourth section, the accuracy of the estimates of the average ground state energy and of the gap with the first excited state of these two algorithms is compared with the original MPO-RG. Conclusions follow.

2. Review of Strong-Disorder Renormalization rules

Consider the random Ising chain in a transverse field whose Hamiltonian reads

$$H = - \sum_{i=1}^{N-1} J_i \sigma_i^x \sigma_{i+1}^x - \sum_{i=1}^N h_i \sigma_i^z \quad (1)$$

where the couplings J_i and h_i are random variables. The SDRG algorithm is the following: find the strongest coupling $\Omega = \max_i \{J_i, h_i\}$. Isolate the term H_0 of H involving Ω . Restrict the Hilbert space to the subspace spanned by the ground states of H_0 . Generate effective interactions with the rest of the chain using second-order perturbation theory. Iterate until leaving only one site.

In the case of $\Omega = h_i$ for example, the local Hamiltonian on site i is

$$H_0 = -h_i \sigma_i^z \quad (2)$$

so the ground state is $|\uparrow\rangle_i$ (if $h_i > 0$). The Hilbert space is projected out onto the subspace spanned by $\{|\uparrow\rangle_i\}$ with the projection operator

$$P = |\uparrow\rangle_i \langle \uparrow|_i = \mathbb{I}^{\otimes i-1} \otimes |\uparrow\rangle \langle \uparrow| \otimes \mathbb{I}^{\otimes N-i}. \quad (3)$$

As a result, the spin is frozen in the state $|\uparrow\rangle_i$. An effective coupling between the spins $i-1$ and $i+1$ is computed with the perturbing Hamiltonian

$$W = -J_{i-1} \sigma_{i-1}^x \sigma_i^x - J_i \sigma_i^x \sigma_{i+1}^x. \quad (4)$$

It is convenient to consider the Dyson expansion of the perturbed Green function

$$(z - W_{\text{eff}})^{-1} = PG(z)P = \frac{1}{z - H_0} + \frac{1}{z - H_0} PWP \frac{1}{z - H_0} \\ + \frac{1}{z - H_0} PW \frac{1}{z - H_0} WP \frac{1}{z - H_0} + \dots \quad (5)$$

The first order term of the matrix element $\langle \uparrow|_i G(z) |\uparrow\rangle_i$ vanishes and, since $\sigma_i^x |\uparrow\rangle_i = |\downarrow\rangle_i$,

$$\langle \uparrow|_i G(z) |\uparrow\rangle_i = \frac{1}{z + h_i} + \frac{1}{z + h_i} [J_{i-1} \sigma_{i-1}^x + J_i \sigma_{i+1}^x] \frac{1}{z - h_i} [J_{i-1} \sigma_{i-1}^x + J_i \sigma_{i+1}^x] \frac{1}{z + h_i}. \quad (6)$$

Note that $1/(z - h_i)$ is the unperturbed Green function evaluated in the excited state. Since we are interested in an effective interaction in the ground state, the parameter z of this unperturbed Green function is set to $z = -h_i$:

$$\langle \uparrow|_i G(z) |\uparrow\rangle_i = \frac{1}{z + h_i} - \frac{1}{(z + h_i)^2} \frac{J_{i-1}^2 + J_{i+1}^2 + 2J_{i-1}J_i \sigma_{i-1}^x \sigma_{i+1}^x}{2h_i}. \quad (7)$$

The last term can be interpreted as a first-order term $G_0(z)W_{\text{eff}}G_0(z)$ for the effective Hamiltonian

$$W_{\text{eff}} = - \frac{J_{i-1}^2 + J_{i+1}^2 + 2J_{i-1}J_i \sigma_{i-1}^x \sigma_{i+1}^x}{2h_i} \\ = \text{Cste} - \frac{J_{i-1}J_i}{h_i} \sigma_{i-1}^x \sigma_{i+1}^x \quad (8)$$

i.e. an effective exchange coupling $J_{\text{eff}} = J_{i-1}J_i/h_i$.

Similarly, if the strongest coupling is J_i , the ground states of $H_0 = -J_i \sigma_i^x \sigma_{i+1}^x$ are $|\tilde{\uparrow}\rangle_{i+1} = |\uparrow_x\rangle_i \otimes |\uparrow_x\rangle_{i+1}$ and $|\tilde{\downarrow}\rangle_{i+1} = |\downarrow_x\rangle_i \otimes |\downarrow_x\rangle_{i+1}$. The Hilbert space is projected

out onto the subspace spanned by these two states. $\tilde{\sigma}_{i+1}$ behaves as a macro-spin. The excited states induce an effective interaction

$$W_{\text{eff}} = \text{Cste} - \frac{h_i h_{i+1}}{J_i} \tilde{\sigma}_i^z. \quad (9)$$

The method becomes exact as the infinite-randomness fixed point is approached because the probability distribution of the couplings is broader and broader. A strong coupling is more likely to be surrounded by weak couplings, justifying the use of perturbation theory.

3. RG algorithms for MPO

3.1. MPO formulation of renormalization

Consider an open spin chain of N spins with the Hamiltonian

$$H = \sum_{i=1}^N H_i + \sum_{i=1}^{N-1} L_i R_{i+1} \quad (10)$$

where $R_i = \mathbb{I}^{\otimes i-1} \otimes R \otimes \mathbb{I}^{\otimes N-i}$ for instance acts on the i -th spin. Using successive Singular Value Decompositions (SVD), the matrix elements of any linear operator

$$\hat{O} = \sum_{\substack{\sigma_1, \dots, \sigma_N, \\ \sigma'_1, \dots, \sigma'_N}} O_{\sigma_1, \dots, \sigma_N; \sigma'_1, \dots, \sigma'_N} |\sigma_1, \dots, \sigma_N\rangle \langle \sigma'_1, \dots, \sigma'_N| \quad (11)$$

acting on the Hilbert space $\mathcal{H}_1^{\otimes N}$ of the N spins can be cast as a product of matrices [20, 21, 22]

$$O_{\sigma_1, \dots, \sigma_N; \sigma'_1, \dots, \sigma'_N} = (A_1)_{a_1}^{\sigma_1, \sigma'_1} (A_2)_{a_1, a_2}^{\sigma_2, \sigma'_2} \dots (A_N)_{a_N}^{\sigma_N, \sigma'_N}. \quad (12)$$

The lower indices correspond to an auxiliary vector space associated to the bonds of the chain. This decomposition is referred to as Matrix Product Operator. For the Hamiltonian (10), the smallest dimension of this auxiliary vector space is $\chi = 3$ and the matrices read

$$A_i = \begin{pmatrix} \mathbb{I} & L_i & H_i \\ 0 & 0 & R_i \\ 0 & 0 & \mathbb{I} \end{pmatrix} \quad (13)$$

for $1 < i < N$ while at the two edges of the chain

$$A_1 = (\mathbb{I} \quad L_1 \quad H_1), \quad A_N = \begin{pmatrix} H_N \\ R_N \\ \mathbb{I} \end{pmatrix} \quad (14)$$

The simplest renormalization algorithm is as follows. The system is divided into blocks of two spins. The local Hamiltonian of the block spanning over the sites i and $i+1$ is given by the matrix element

$$(A_i \otimes A_{i+1})_{1, \chi} = H_i \otimes \mathbb{I} + L_i \otimes R_{i+1} + \mathbb{I} \otimes H_{i+1}. \quad (15)$$

For each block, the local Hamiltonian is diagonalized and the largest gap is found in the energy spectrum. The renormalization is performed on the block with the largest energy gap. Its Hilbert space is truncated to the subspace spanned by the eigenvectors

whose eigenvalues are below the gap. The local Hamiltonian, as well as all other non-zero matrix elements of $A_i \otimes A_{i+1}$, are projected out onto this subspace. This defines a renormalized matrix

$$A'_i = U^+(A_i \otimes A_{i+1})U \quad (16)$$

where U is a rectangular matrix whose rows are the selected eigenvectors of the local Hamiltonian. The transformation is not unitary. Note that U acts on the spin indices and not on the auxiliary vector space. The matrix A'_i has dimension $\chi \times \chi$, except at the left and right edges of the chain, and keeps the same structure as the original A_i 's. The process is iterated until the chain has a single site.

3.2. Equivalence with SDRG

Even though *a priori* simpler than SDRG, this approach is actually equivalent in the limit of strong randomness. Consider again the Ising chain in a transverse field (1). The Hamiltonian can be cast as a MPO with the matrices

$$A_i = \begin{pmatrix} \mathbb{I} & -\sqrt{J_i}\sigma^x & -h_i\sigma^z \\ 0 & 0 & \sqrt{J_{i-1}}\sigma^x \\ 0 & 0 & \mathbb{I} \end{pmatrix} \quad (17)$$

for $1 < i < N$ and

$$A_1 = (\mathbb{I} \quad -\sqrt{J_1}\sigma^x \quad -h_1\sigma^z), \quad A_N = \begin{pmatrix} -h_N\sigma^z \\ \sqrt{J_{N-1}}\sigma^x \\ \mathbb{I} \end{pmatrix}. \quad (18)$$

Suppose that the largest gap is found for the block obtained after merging sites i and $i+1$. The local Hamiltonian of this block is then

$$H_{i,i+1} = (A_i \otimes A_{i+1})_{1\chi} = -h_i\sigma^z \otimes \mathbb{I} - h_{i+1}\mathbb{I} \otimes \sigma^z - J_i\sigma^x \otimes \sigma^x \quad (19)$$

whose four eigenvalues are

$$\pm E_1 = \pm\sqrt{(h_i + h_{i+1})^2 + J_i^2}, \quad \pm E_2 = \pm\sqrt{(h_i - h_{i+1})^2 + J_i^2}. \quad (20)$$

Keeping the two states below the largest gap, i.e. with energies $-E_1$ and $-E_2$, the effective matrix is

$$A'_i = U^+ A_i A_{i+1} U = \begin{pmatrix} \mathbb{I} & -\sqrt{J_{i+1}}U^+(\mathbb{I} \otimes \sigma^x)U & \begin{pmatrix} -E_1 & 0 \\ 0 & -E_2 \end{pmatrix} \\ 0 & 0 & \sqrt{J_1}U^+(\sigma^x \otimes \mathbb{I})U \\ 0 & 0 & \mathbb{I} \end{pmatrix} \quad (21)$$

By construction, the renormalized local Hamiltonian is diagonal in this basis and can therefore be written as

$$H_{i,i+1} = -\frac{1}{2}(E_1 + E_2)\mathbb{I} - \frac{1}{2}(E_1 - E_2)\sigma^z = \text{Cst}\mathbb{I} - h_{\text{eff}}\sigma^z \quad (22)$$

with the effective transverse field

$$h_{\text{eff}} = \frac{1}{2}(E_1 - E_2) = \frac{1}{2}\sqrt{(h_i + h_{i+1})^2 + J_i^2} - \frac{1}{2}\sqrt{(h_i - h_{i+1})^2 + J_i^2} \quad (23)$$

It turns out that the renormalized operators $U^+(\sigma^x \otimes \mathbb{I})U$ and $U^+(\mathbb{I} \otimes \sigma^x)U$ are proportional to σ^x so the expression of the original Hamiltonian is preserved †.

† If the rotated Hamiltonian $H = -J\sum_i \sigma_i^z \sigma_{i+1}^z - h\sum_i \sigma_i^x$ is considered instead of (1), an additional 45° rotation is needed at each renormalization step to bring back the local Hamiltonian to its original form.

When the exchange coupling J_i is stronger than both h_i and h_{i+1} , a Taylor expansion to lowest-order in $(h_i \pm h_{i+1})/J_i$ gives the SDRG renormalized transverse field

$$h_{\text{eff}} \simeq \frac{J_i}{2} \left(1 + \frac{(h_i + h_{i+1})^2}{2J_i^2} \right) - \frac{J_i}{2} \left(1 + \frac{(h_i - h_{i+1})^2}{2J_i^2} \right) = \frac{h_i h_{i+1}}{J_i}. \quad (24)$$

When the transverse field h_i is stronger than both h_{i+1} and J_i , the gap between the two lowest eigenvalues $-E_1$ and $-E_2$ is now

$$\frac{1}{2}(E_1 - E_2) \simeq \frac{h_i}{2} \left[1 + \frac{h_{i+1}}{h_i} + \mathcal{O}\left(\frac{1}{h_i^2}\right) \right] - \frac{h_i}{2} \left[1 - \frac{h_{i+1}}{h_i} + \mathcal{O}\left(\frac{1}{h_i^2}\right) \right] = h_{i+1} \quad (25)$$

i.e. equal to the original transverse field acting on site $i + 1$. In the basis $\{|\uparrow\uparrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\downarrow\rangle\}$, the associated eigenvectors are proportional to

$$\begin{aligned} (E_1 + h_i + h_{i+1} \quad 0 \quad 0 \quad J_i) &\simeq (2(h_i + h_{i+1}) \quad 0 \quad 0 \quad J_i) \\ (0 \quad E_2 - h_i + h_{i+1} \quad J_i \quad 0) &\simeq (0 \quad \frac{J_i^2}{2h_i} \quad J_i \quad 0) \end{aligned} \quad (26)$$

to lowest-order in $1/h_i$. The 2-spin block is coupled to σ_{i-1}^x via the operator σ_i^x . After renormalization, σ_i^x is transformed into $U^+(\sigma^x \otimes \mathbb{I})U$. The latter is proportional to σ^x . The coefficient is computed as the off-diagonal matrix element between the two (normalized) eigenvectors

$$\frac{1}{2h_i} (2h_i \quad 0 \quad 0 \quad J_i) \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \frac{1}{J_i} \begin{pmatrix} 0 \\ \frac{J_i^2}{2h_i} \\ J_i \\ 0 \end{pmatrix} = \frac{J_i}{h_i} \quad (27)$$

The Hamiltonian coupling σ_{i-1} and the 2-spin block is therefore

$$-J_{i-1} \sigma_{i-1}^x U^+(\sigma^x \otimes \mathbb{I})U = -\frac{J_{i-1} J_i}{h_i} \sigma_{i-1}^x \tilde{\sigma}_{i+1}^x \quad (28)$$

as predicted par SDRG.

A comparison of the renormalized couplings given by SDRG and MPO-RG is shown on figure 1 and 2.

4. Improvements of the MPO renormalization algorithm

4.1. New criterion for selecting the block to be renormalized

In the above-described renormalization algorithm, a low-energy effective Hamiltonian is constructed by successive projections onto the lowest eigenstates of local Hamiltonians. At each iteration, the two-spin block to be renormalized is therefore treated as completely decoupled from the rest of the chain. Close to the IRFP, randomness becomes very large so, if one of the inter-block couplings is strong, one can safely assume that the couplings with the rest of the chain are much smaller. Away from the IRFP, this is no more the case and the interaction with the rest of the chain cannot be neglected. The renormalization procedure is then expected to introduce systematic deviations on the ground state of the whole chain.

To partially circumvent the problem, a simple approach consists in renormalizing in priority the block with, not only the largest gap in the spectrum of its local Hamiltonian, but also with the smallest couplings with the rest of the chain. We suggest the following modification to the algorithm: the ground state energy $\varepsilon_0^{(i,i+1)}$

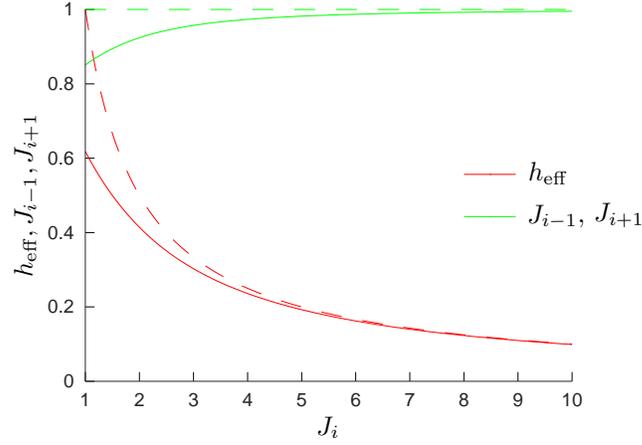


Figure 1. Effective couplings of a 2-spin block after renormalization versus the exchange coupling J_i binding the two spins. All other couplings (transverse fields and couplings with the spins at the left and the right of the block) are taken equal to one. The dashed lines are the predictions of SDRG. Note that the latter predicts an absence of renormalization of the left and right couplings (J_{i-1} and J_{i+1} if the block spans over the sites i and $i + 1$).

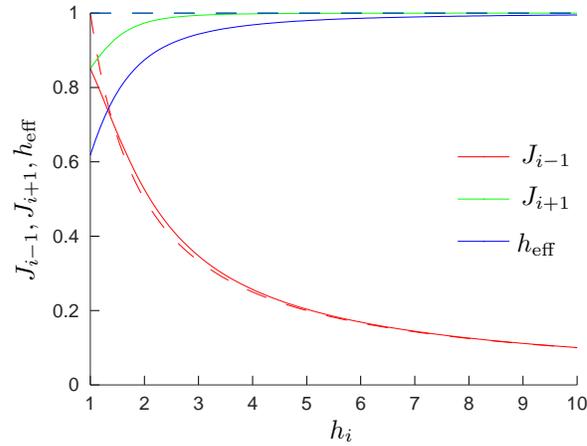


Figure 2. Effective couplings of a 2-spin block after renormalization versus the transverse field h_i originally coupled to the left spin of the block. All other couplings (transverse field and couplings inside and outside the block) are taken equal to one. The dashed lines are the predictions of SDRG.

is first computed for each block of two sites $(i, i + 1)$. The strength of the coupling between the two spins is estimated as the difference

$$\Delta\varepsilon_0^{(i,i+1)} = \varepsilon_0^{(i)} + \varepsilon_0^{(i+1)} - \varepsilon_0^{(i,i+1)} \quad (29)$$

where $\varepsilon_0^{(i)}$ is the energy of the single spin at site i . Then, to compare the inter-block coupling with the couplings of the two neighboring blocks, the ratio

$$\rho^{(i,i+1)} = \frac{\Delta\varepsilon_0^{(i,i+1)}}{\max(\Delta\varepsilon_0^{(i-1,i)}, \Delta\varepsilon_0^{(i+1,i+2)})} \quad (30)$$

is computed for each block. Last, the renormalization is performed on the block with the largest ratio $\rho^{(i,i+1)}$. This simple modification is observed to give lower ground state energies, closer to the estimate of DMRG. Note that the energies $\varepsilon_0^{(i,i+1)}$ and the ratios $\rho^{(i,i+1)}$ do not need to be computed at each renormalization step. Only the two of them that are affected by the renormalization of a block needs to be recomputed. Moreover, the ratio $\rho^{(i,i+1)}$ can be stored in a binary tree in order to speed up the search for the largest one.

4.2. Effective interactions between effective spins

A second improvement consists in generating the effective interactions mediated by the highest eigenstates between a block and its neighboring spins. The algorithm is as follows. A two-spin block, say $(i, i + 1)$ is chosen according to the above-described criterion. A new macro-spin is defined by merging the two spins i and $i + 1$. Its local Hamiltonian $H_{i,i+1} = (A_i \otimes A_{i+1})_{1,\chi}$ is diagonalized:

$$H_{i,i+1} = \sum_{j=0}^{d_i d_{i+1} - 1} \varepsilon_j^{(i,i+1)} |\phi_j\rangle\langle\phi_j|. \quad (31)$$

The Hamiltonian of the macro-spin, including the interaction with its two neighbors, is

$$H = L_{i-1}R_i + H_{i,i+1} + L_{i+1}R_{i+2} \quad (32)$$

Define the projectors

$$\begin{aligned} P &= \sum_{j \leq \Lambda} \mathbb{I}^{\otimes i-1} \otimes |\phi_j\rangle\langle\phi_j| \otimes \mathbb{I}^{\otimes N-i-1}, \\ Q &= \sum_{j > \Lambda} \mathbb{I}^{\otimes i-1} \otimes |\phi_j\rangle\langle\phi_j| \otimes \mathbb{I}^{\otimes N-i-1} = \mathbb{I}^{\otimes N} - P \end{aligned} \quad (33)$$

where the cut-off Λ separates the eigenstates to be kept from those to be discarded. In the original MPO renormalization-group algorithm, the Hamiltonian is projected out onto the subspace spanned by the lowest eigenstates, i.e. H is replaced by

$$PHP = L_{i-1}PR_iP + PH_{i,i+1}P + PL_{i+1}PR_{i+2}. \quad (34)$$

To take into account perturbatively the highest eigenstates, one can decompose the Hamiltonian as $H = H_0 + W$ where the unperturbed Hamiltonian

$$H_0 = L_{i-1}PR_iP + H_{i,i+1} + PL_{i+1}PR_{i+2} \quad (35)$$

does not couple the lowest and highest eigenstates and the perturbation reads

$$W = L_{i-1}(PR_iQ + QR_iP + QR_iQ) + (PL_{i+1}Q + QL_{i+1}P + QL_{i+1}Q)R_{i+2}. \quad (36)$$

The Dyson expansion of the perturbed Green function is

$$\begin{aligned}
 PG(z)P &= P(z - H_0 - W)^{-1}P \\
 &= P[\mathbb{I} - (z - H_0)^{-1}W]^{-1}(z - H_0)^{-1}P \\
 &= \sum_{n=0}^{+\infty} P[G_0(z)W]^n G_0(z)P
 \end{aligned} \tag{37}$$

where $G_0(z) = (z - H_0)^{-1}$ is the unperturbed Green function. The first-order term vanishes because $[P, G_0] = 0$ and $PWP = 0$. At second order, the Dyson expansion is

$$\begin{aligned}
 PG(z)P &= G_0(z) + G_0(z)PWG_0(z)WPG_0(z) \\
 &= G_0(z) + G_0(z)\Sigma_{\text{eff}}G_0(z)
 \end{aligned} \tag{38}$$

with the self-energy

$$\Sigma_{\text{eff}}(z) = PWG_0(z)WP. \tag{39}$$

Note that $PWP = 0$ so the latter can be written

$$\Sigma_{\text{eff}}(z) = PWQG_0(z)QWP. \tag{40}$$

Since we are interested in the ground state of the chain, a low-energy effective Hamiltonian is $W_{\text{eff}} = \Sigma_{\text{eff}}(z)$ where z should be chosen equal to the ground state energy of the chain. Different interactions are generated:

$$L_{i-1}^2 PR_i QG_0(z) QR_i P + R_{i+2}^2 PL_i QG_0(z) QL_{i+1} P = L_{i-1}^2 X_i + Y_i R_{i+2}^2 \tag{41}$$

that couple the macro-spin with the spins on sites $i - 1$ and $i + 1$. A three-spin interaction

$$L_{i-1} [PR_i QG_0(z) QL_i P + PL_i QG_0(z) QR_i P] R_{i+2} = L_{i-1} Z_i R_{i+2} \tag{42}$$

is also generated. Taking into account these terms requires to increase the dimension χ of the auxiliary vector space of the matrices A_{i-1} , A_i , A_{i+1} . The matrices A_{i-1} , A_i , and A_{i+2} become, after renormalization,

$$A_{i-1} = \begin{pmatrix} \mathbb{I} & L_{i-1} & L_{i-1}^2 & H_{i-1} \\ 0 & 0 & 0 & R_{i-1} \\ 0 & 0 & 0 & \mathbb{I} \end{pmatrix}, \tag{43}$$

$$A_i = \begin{pmatrix} \mathbb{I} & PL_i P & Y_i & 0 & PH_{i,i+1} P \\ 0 & 0 & 0 & Z_i & PR_i P \\ 0 & 0 & 0 & 0 & X_i \\ 0 & 0 & 0 & 0 & \mathbb{I} \end{pmatrix}, \tag{44}$$

$$A_{i+2} = \begin{pmatrix} \mathbb{I} & L_{i+2} & H_{i+2} \\ 0 & 0 & R_{i+2} \\ 0 & 0 & R_{i+2}^2 \\ 0 & 0 & R_{i+2} \\ 0 & 0 & \mathbb{I} \end{pmatrix} \tag{45}$$

where

$$\begin{aligned}
 X_i(z) &= PR_i QG_0(z) QR_i P, \\
 Y_i(z) &= PL_i QG_0(z) QL_i P, \\
 Z_i(z) &= PR_i QG_0(z) QL_i P + PL_i QG_0(z) QR_i P.
 \end{aligned} \tag{46}$$

The procedure is iterated. If the sites i and $i + 2$ are later merged for example, A_{i-1} will be replaced by a 6×4 matrix.

The numerical calculation of the matrix element $\langle \phi_k | X_i | \phi_j \rangle$ ($k, j \leq \Lambda$) has been performed in the following way: first, R_i is applied onto the eigenvector $|\phi_j\rangle$ of the local Hamiltonian. The resulting vector is then projected out onto the levels to be discarded:

$$|\varphi\rangle = QR_i|\phi_j\rangle = \left[\mathbb{I} - \sum_{k \leq \Lambda} |\phi_k\rangle\langle\phi_k| \right] R_i|\phi_j\rangle. \quad (47)$$

The unperturbed Green function $G_0(z)$ is estimated by first finding the eigenvectors $|\psi_i\rangle$ associated to the eigenvalues e_i of smallest algebraic magnitude of the operator $z - H_0$. The numerical calculation was performed using the implicit restarted Arnoldi algorithm as implemented in the `arpack` library. $G_0(z)QR_i|\phi_j\rangle$ is estimated as

$$|\varphi'\rangle = \sum_j e_j^{-1} |\psi_j\rangle\langle\psi_j|\varphi\rangle \quad (48)$$

The estimation is refined using a conjugate gradient algorithm. Finally, since $G_0(z)$ is diagonal in the unperturbed basis, we do need to apply the projector Q again. The matrix element $\langle \phi_k | X_i | \phi_j \rangle$ is finally given by $\langle \phi_k | \varphi' \rangle$.

5. Accuracy of the approach

In the following, the accuracy of the different approaches discussed above is studied. Three versions of the MPO-RG algorithm are compared: the first is the original one introduced in section 3.1, the second implements the improved choice of the block to be renormalized of section 4.1 and the third takes into account effective interactions as discussed in section 4.2. In the following, these three variants of the MPO-RG algorithm will be referred to as Algo 1, 2, and 3. The parameter z of Algo 3 is set to the estimate of the ground state energy given by Algo 2. For simplicity, the three-site effective interaction (operator Z in (46)) was neglected. The latter indeed introduces 4-site, 5-site, ... effective interactions as the renormalization procedure is iterated. In contrast, the two-site effective interactions (operators X and Y) keep the same form during the renormalization. We allowed for a maximum of 8 different interactions between neighboring blocks and neglected any further interaction that would be generated by the renormalization process. The accuracy of the different MPO-RG algorithms is tested by comparing the estimated ground state energies. The latter is easily computed at the end of the renormalization when only one site is left.

5.1. Shift of the ground state energy during the renormalization

To monitor the shift of the ground state energy induced by the renormalization, the different MPO-RG algorithms were coupled to a DMRG algorithm. After each renormalization step, a full DMRG calculation is performed on the renormalized MPO to estimate the ground state energy. The code is drastically slowed down by the DMRG calculations so the lattice was limited to 32 sites. The random Ising chain in a transverse field is considered:

$$H = - \sum_{i=1}^{L-1} J_i \sigma_i^z \sigma_{i+1}^z - \sum_{i=1}^L h_i \sigma_i^x - B \sum_{i=1}^L \sigma_i^z \quad (49)$$

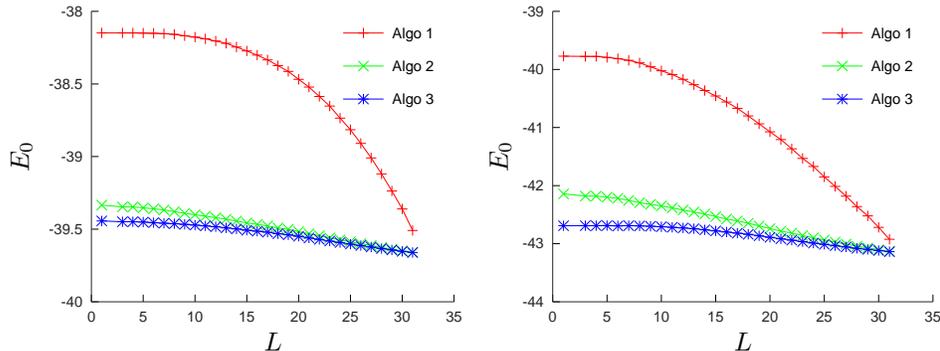


Figure 3. Average ground state energy of a random Ising chain of 32 spins as estimated by the three variants of the MPO-RG algorithm versus the number of remaining sites L during the RG process. The system is in the ferromagnetic phase ($h_i \in [0.3; 0.4]$) on the left figure and in the ordered Griffiths phase ($h_i \in [0.5; 1]$) on the right.

with a uniform probability distribution of exchange couplings ($J_i \in [0.5; 2]$). The transverse fields were also uniformly distributed but in different intervals corresponding to different regions of the phase diagram: ferromagnetic phase ($h_i \in [0.3; 0.4]$), ordered Griffiths phase ($h_i \in [0.5; 1]$), critical point ($h_i \in [0.5; 2]$), disordered Griffiths phase ($h_i \in [1; 2]$), and paramagnetic phase ($h_i \in [2.5; 3]$). This disorder is relatively weak so we expect the original SDRG algorithm to lead to important deviations for small chains. On the other hand, the DMRG algorithm, used to probe these deviations, is more efficient at weak disorder. A small longitudinal field $B = 10^{-4}$ is added to further improve the convergence of the DMRG algorithm. 128 states were kept in the left and right blocks (64 for the environment and 2 for the central spin) in the DMRG algorithm and 16 sweeps were performed. For the three algorithms, the renormalization consisted in merging two neighboring 2-state blocks and truncating the Hilbert state to the subspace spanned by the two eigenstates with lower energies. Results with more states per block will be considered in the next section. Finally, the ground state energy is averaged over 32 disorder realizations in order to show that the results are typical and not due to a particular disorder configuration.

The results are presented on figures 3 to 5. The average ground state energy is plotted versus the number of remaining sites L during the RG process for the three MPO-RG algorithms. All points from $L = 31$ (after the first renormalization step) to $L = 4$ were computed by applying the DMRG algorithm to the renormalized MPO. The last point $L = 1$ corresponds to the average ground state energy given by the MPO-RG algorithm at the end of the renormalization, i.e. when there is only one site left. Since the first point on the right corresponds to the energy after only one renormalization step, its value is therefore close to the exact value. The figures show a monotonous evolution with L of the estimates of the ground state energy. However, a jump is sometimes observed for Algo 1 and 3 at the end of the calculation, i.e. L small. It seems therefore safer to stop the calculation at $L \geq 5$ and compute exactly the quantum averages rather than pursuing the renormalization up to $L = 1$.

As can be seen on the figures, the original MPO algorithm (Algo 1) induces much larger systematic deviations of the ground state energy than the two other algorithms.

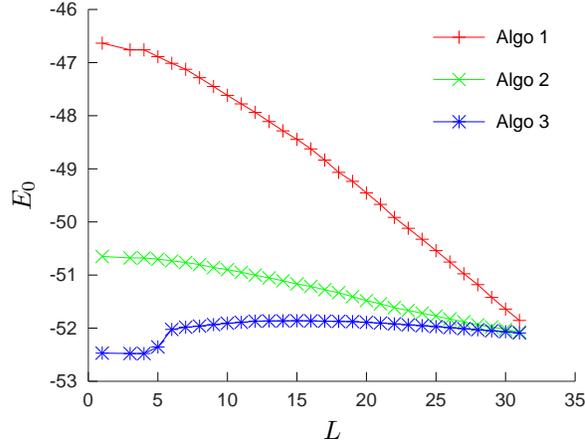


Figure 4. Average ground state energy of a random Ising chain of 32 spins as estimated by the three variants of the MPO-RG algorithm versus the number of remaining sites L during the RG process. The system is at the critical point ($h_i \in [0.5; 2]$).

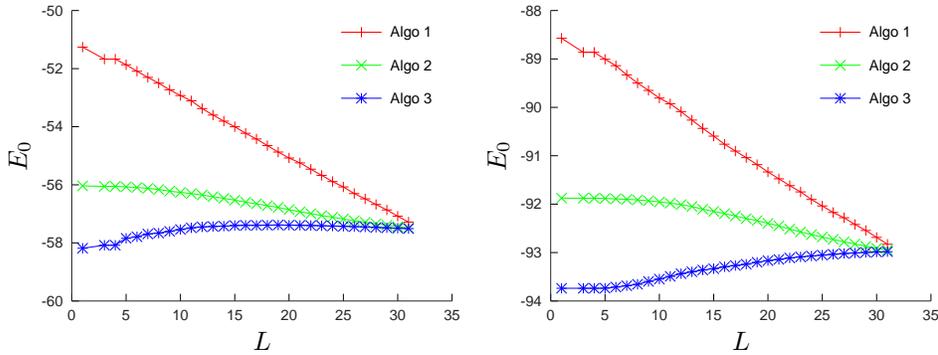


Figure 5. Average ground state energy of a random Ising chain of 32 spins as estimated by the three variants of the MPO-RG algorithm versus the number of remaining sites L during the RG process. The system is in the disordered Griffiths phase ($h_i \in [1; 2]$) on the left and in the paramagnetic phase ($h_i \in [2.5; 3]$) in the right.

In the paramagnetic phase, the systematic deviation grows approximately linearly with the number of RG steps, i.e. each iteration is followed by the same shift of the ground state energy. The relative deviation at the end of the calculation is about 4.7%. In the ferromagnetic phase, the deviation tends to be larger at the beginning of the renormalization process. Almost no shift is observed in the last iterations. Nevertheless, the relative deviation of the ground state energy at the end of the calculation is about 3.8%.

Despite a small modification with respect to Algo. 1, the algorithm with an improved choice of the block to be renormalized (Algo. 2) turns out to be surprisingly much more efficient. As can be seen on figures 3 to 5, the average ground state

Table 1. Average ground state energies of a random Ising chain of 240 spins as estimated by the three variants of the MPO-RG algorithm for different numbers of states kept during the truncation of the Hilbert space.

	$h \in [0.3; 0.4]$	$h \in [0.5; 1]$	$h \in [0.5; 2]$	$h \in [1; 2]$	$h \in [2.5; 3]$
Algo 1					
4 states	$-3.00643.10^2$	$-3.12685.10^2$	$-3.60362.10^2$	$-4.04007.10^2$	$-6.80757.10^2$
8 states	$-3.02988.10^2$	$-3.21175.10^2$	$-3.75499.10^2$	$-4.18228.10^2$	$-6.88960.10^2$
16 states	$-3.04019.10^2$	$-3.24527.10^2$	$-3.82430.10^2$	$-4.23943.10^2$	$-6.93308.10^2$
32 states	$-3.04537.10^2$	$-3.26313.10^2$	$-3.85995.10^2$	$-4.26790.10^2$	$-6.95864.10^2$
Algo 2					
4 states	$-3.03551.10^2$	$-3.23612.10^2$	$-3.85713.10^2$	$-4.27185.10^2$	$-6.95643.10^2$
8 states	$-3.04476.10^2$	$-3.26770.10^2$	$-3.89493.10^2$	$-4.30330.10^2$	$-6.97327.10^2$
16 states	$-3.04827.10^2$	$-3.28022.10^2$	$-3.91017.10^2$	$-4.31602.10^2$	$-6.97933.10^2$
32 states	$-3.04980.10^2$	$-3.28684.10^2$	$-3.91891.10^2$	$-4.32286.10^2$	$-6.98192.10^2$
Algo 3					
4 states	$-3.03697.10^2$	$-3.24632.10^2$	$-4.01471.10^2$	$-4.40873.10^2$	$-6.99829.10^2$
8 states	$-3.04560.10^2$	$-3.27368.10^2$	$-3.98940.10^2$	$-4.35034.10^2$	$-6.98487.10^2$
16 states	$-3.04877.10^2$	$-3.28406.10^2$	$-3.96255.10^2$	$-4.34810.10^2$	$-6.98376.10^2$
32 states	$-3.05011.10^2$	$-3.28941.10^2$	$-3.94581.10^2$	$-4.34575.10^2$	$-6.98377.10^2$

energy displays a much smaller shift as the renormalization is performed. The total deviation of the ground state energy at the end of the calculation is about 1.2% in the paramagnetic phase and 0.8% in the ferromagnetic phase.

The MPO-RG algorithm with effective interactions (Algo. 3) brings some improvements with respect to the two other algorithms. In the ferromagnetic phase, the average ground state energy is systematically lower during the renormalization process and the relative deviation at the end of the calculation is about 0.5%. However, in the paramagnetic phase, the average ground state energy goes below the exact one and the relative deviation is about -0.8% , i.e. the same deviation as Algo. 2 but with a different sign.

5.2. Stability of the algorithms with more states per block

In this section, the three variants of the MPO-RG algorithm are compared for a larger lattice of 240 sites and with 4,8,16 or 32 states per block during renormalization. The ground state energy is averaged over 1000 disorder configurations.

On table 1, the average ground state energies are presented at the same points of the phase diagram as in the previous section. For the three algorithms, all estimates evolve monotonously as the number of states per block is increased. The energies only decrease for Algo 1 and 2 while they increase for Algo 3 at the critical point, in the disordered Griffiths phase and in the paramagnetic phase. Nevertheless, the estimates of the three algorithms seem to converge towards the same value with a convergence which is faster for Algo 3.

On table 2, the average gaps between the first excited state and the ground state energies are presented. Note that in the ferromagnetic and ordered Griffiths phases,

Table 2. Average energy gap between the first excited state and the ground state of a random Ising chain of 240 spins as estimated by the three variants of the MPO-RG algorithm for different numbers of states kept during the truncation of the Hilbert space.

	$h \in [0.3; 0.4]$	$h \in [0.5; 1]$	$h \in [0.5; 2]$	$h \in [1; 2]$	$h \in [2.5; 3]$
Algo 1					
4 states	0.058270	0.10491	0.10131	0.46837	2.9748
8 states	0.058662	0.079809	0.038335	0.39790	2.7150
16 states	0.057870	0.081128	0.029123	0.33381	2.6969
32 states	0.059596	0.076776	0.022698	0.29653	2.7078
Algo 2					
4 states	0.051948	0.058287	0.011563	0.18225	2.5420
8 states	0.051221	0.052873	0.012093	0.18069	2.5071
16 states	0.050813	0.052706	0.012025	0.18297	2.4829
32 states	0.050232	0.052737	0.012001	0.17774	2.4633
Algo 3					
4 states	0.051741	0.066224	0.012145	0.18851	2.4050
8 states	0.050549	0.053929	0.013135	0.17546	2.3987
16 states	0.050494	0.051849	0.012938	0.17560	2.3797
32 states	0.050058	0.051016	0.013564	0.16924	2.3828

the gap is due to the energy splitting induced by the small magnetic field B . In contrast to the average ground state energies, the estimates of the three algorithms do not display any monotonous evolution with the number of states per block. However, we note that the average gap is about 6000 times smaller than the ground state energy. The ground state and the first excited state show the same monotonous evolution with the number of states and their difference, i.e. the gap, evolves only according to their statistical fluctuations. In this case, increasing the number of states does not lead to a significant improvement of the gap.

Conclusions

We have presented two variants of the MPO renormalization algorithm. In the first one (Algo 2), the choice of the blocks to be merged and renormalized takes into account the couplings with the neighboring blocks of the chain. The renormalization differs therefore only by the order in which the blocks are grouped together. Nevertheless, it is observed that this simple modification improves the accuracy of the ground state energy by a factor at least 4 in all regions of the phase diagram of the random Ising chain in a transverse field. In the second algorithm (Algo 3), effective interactions are generated to take into account the highest eigenstates to be discarded during the renormalization. We observe a small improvement of the accuracy of the ground state energy. However, in contrast to Algo 1 and 2, this algorithm gives smaller estimates of the ground state energy than the exact one in the paramagnetic and disordered Griffiths phases. The smallest energy is therefore not the necessarily the best one in this case. We note that the algorithm may be improved by taking into account the

three-site interaction, as well as higher orders in the Dyson expansion. Finally, it was shown that the two algorithms are stable as the number of states kept during the renormalization is increased.

Recently, a different route, based on entanglement renormalization [23], has been investigated to improve the accuracy of MPO-RG [24]. The ground-state is constructed as a tensor network involving not only unitaries but also disentanglers. The computational effort is increased with the number of variational parameters. We note that the structure of the tensor network is determined by first applying SDRG to the random chain. The results of the present paper shows that the accuracy can be improved in a simple way by replacing SDRG by Algo 2. It would be therefore very interesting to test the use of Algo 2 to construct the tensor network for entanglement renormalization.

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