Renormalization group method for weakly coupled quantum chains: comparison with exact diagonalization

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We show that numerical quasi-one-dimensional renormalization group allows accurate study of weakly coupled chains with modest computational effort. We perform a systematic comparison with exact diagonalization results in two and three-leg spin ladders with a transverse Hamiltonian that can involve frustration. Due to the variational nature of the algorithm, the accuracy can be arbitrarily improved enlarging the basis of eigenstates of the density matrix defined in the transverse direction. We observe that the precision of the algorithm is directly correlated to the binding of the chains. We also show that the method performs especially well in frustrated systems.

I. INTRODUCTION

It was recently shown\textsuperscript{1} that a general Kato-Bloch matrix expansion can be applied to weakly-coupled quantum chains. This algorithm was used to study weakly-coupled Heisenberg chains\textsuperscript{2,3}. The DMRG was used as the method of solution for an isolated chain and then again for the solution of an effective 1D model which is obtained by projecting the problem to the basis of the tensor product of independent chain states. A good agreement with the stochastic series expansion (SSE) quantum Monte Carlo (QMC) was found for transverse couplings $J_{d}$ not too large. Then interchain diagonal exchange $J_{d}$ which frustrates the system was introduced. It is found, by analyzing ground state energies and spin-spin correlation functions, that there is a transition between two ordered magnetic states. When $J_{d}/J_{\perp} \lesssim 0.5$, the ground state displays a Néel order. When $J_{d}/J_{\perp} \gtrsim 0.5$, a collinear magnetic ground state in which interchain spin correlations are ferromagnetic becomes stable. In the vicinity of the transition point, $J_{d}/J_{\perp} \approx 0.5$, the ground state is disordered. The prediction of a disordered ground state is of central importance for two reasons. First, because a recent neutron scattering experiment\textsuperscript{4} on the frustrated AFM Cs\textsubscript{2}CuCl\textsubscript{4} has predicted a spin liquid ground state in this material. Second, a disordered doped spin liquid has been conjectured to be relevant for the physics of high temperature cuprate superconductors. The search of this disordered two-dimensional state by numerical methods has been challenging. Cluster QMC methods\textsuperscript{5,6}, that have been extremely useful in nonfrustrated spin systems, are hampered by sign problems for Hamiltonians with finite $J_{d}$, making very difficult their study by this technique. New algorithms have been specifically designed to deal with frustration and intense numerical research has been devoted to these systems\textsuperscript{7,8,9}. It is thus of central importance to show that the DMRG prediction is correct.

We address in this paper several questions that increase the understanding and show new potential of the method, giving additional support for the physical findings of Ref. \textsuperscript{3}. Some of these questions are technical in nature and they demand exhaustive comparison with exact results.

The class of models that we study here have transverse terms involving competing interactions. These transverse terms are projected in a optimal reduced basis of eigenstates of the independent chain. If, for instance, the chains are coupled with perpendicular and diagonal exchange constants (see the left ladder in Fig. \textbf{1}), the projection of the perpendicular ($J_{\perp}$) and the diagonal ($J_{d}$) parts of the interchain coupling is qualitatively different one to the other. More precisely, to represent coupling terms along the diagonal requires matrix elements of operators defined in different sites (those usually associated with the computation of short range correlation functions in 1D DMRG calculations). It is this competing behavior that generates negative local Boltzmann weights (sign problems) that can not be eliminated by canonical transformations when QMC is used. Therefore, it is important to check if all competing terms are represented and treated with similar accuracy by studying models that mix these terms in different ways.

We will also show that the accuracy is directly correlated to the binding energy of the chains and not to the nominal values of the transverse couplings, concluding that the method is specially good for the study of frustrated systems. In addition, based on the results of this study we have designed internal tests that signal good performance of the method when dealing with larger lattices where comparison with exact data is not possible.

Finally, we are also interested in showing the controllability of the approximation involved in the method, specifically for frustrated systems. We emphasize that its variational nature implies that the accuracy can be systematically improved by enlarging the number of states kept in the density matrix defined perpendicular to the chains($m_{s2}$). This point is not a trivial one: it demands an accurate projection of the transverse Hamiltonian in an accurate representation of the Hilbert space of the chains. The systematic comparison with exact diagonalization (ED) results in two- and three-legged ladders presented here shows that in Q1D systems excellent results can be obtained with modest values for $m_{s2}$. 



The rest of the paper is organized as follows. The different models studied in this paper are presented in 

section [II]. Then we summarize the main steps of the 

algorithm implementation in section [III]. In section [IV] we 

show how to improve systematically the numerical results 

for several magnitudes exploiting the variational property 

of the method. In section [V] we study the accuracy as we 

increase different exchange couplings in the transverse 

Hamiltonians. In section [VI] we present our conclusions.

II. MODELS

To discuss the issues that we presented in the intro- 
ductory section we need to compare the results obtained 

with two-step DMRG with exact data, that can be achieved 

by ED in small lattices [12]. In addition, we want to 

evaluate the performance of the method for a very general 

class of transverse Hamiltonians including those that 

involve frustrating couplings between the chains ( i.e. , an 

exchange constant $J_d$ along the diagonal of the square 

lattice). It is also important to study systems with different 

numbers of legs because they behave in a very different 

way as they approach the thermodynamic limit.

The natural choice as test models are then the Heisen- 
berg two- or three-legged ladders in the strong coupling 

limit:

$$H = H_{\parallel} + H_{\perp} + H_d$$

$$H_{\parallel} = J_{\parallel} \sum_{j,l} S_{j,l} S_{j+1,l}$$

$$H_{\perp} = J_{\perp} \sum_{j,l} S_{j,l} S_{j,l+1}$$

$$H_d = J_d \sum_{j,l} (S_{j,l} S_{j+1,l+1} + S_{j+1,l} S_{j,l+1})$$

where $J_{\parallel} > J_{\perp}, J_d$. $S_{j,l}$ represents the spin operator in 

the site $j$ of chain $l$ with the indices running $i = j \ldots L_x$ 

and $l = 2, 3$. We impose open boundary conditions in 

the two directions. The coupling $J_d$ connects spin operators 

along the diagonal and introduces frustration in the model.

Another frustrated model of great interest is the sys- 
	
tem of weakly coupled chains arranged in an anisotropic 

triangular lattice which can be written in the form

$$H = H_{\parallel} + H_{\perp} + H_d'$$

where the new term $H_d'$ is:

$$H_d' = J_d \sum_{j,l} S_{j,l} S_{j+1,l+1}$$

Note that the model in the square lattice with diagonal 

couplings [1] reduces to the model defined in the trian- 
gular lattice [1] when one of the two diagonal couplings is 

set to zero.

III. METHOD AND DATA ANALYSIS

A detailed description of the two-step DMRG method, 

which we will refer for short 2S-DMRG, has been given in 

Refs. 2 and 3.

The exact spectrum of a single AF chain is known 

from the Bethe ansatz, but eigenfunctions are not eas- 

illy accessible. Thus, the density-matrix renormalization 

group (DMRG) method [10,11] will be used to compute an 

approximate spectrum $\epsilon_n, |\phi_n\rangle$ of a single chain. A 

preliminary account of this approach as well as an extensive 

comparison with the Quantum Monte Carlo method was 

presented elsewhere [2]. By expressing the Hamiltonian on 

the basis generated by the tensor product of the states of 

different chains one obtains, up to the second order, the 

effective one-dimensional Hamiltonian,

$$\hat{H} \approx \sum_{[n]} E_{[[n]]} |\Phi_{[[n]]}\rangle \langle \Phi_{[[n]]}| + J_{\perp} \sum_{l} \hat{S}_l \hat{S}_{l+1} +$$

$$J_d \sum_{l} \hat{S}_l \hat{S}_{l+1} + \ldots$$

where the composite chain-spin operators on the chain 

$l$ are $\hat{S}_l = (\hat{S}_{1l}, \hat{S}_{2l}, \ldots \hat{S}_{ll})$, $L_x$ is the chain length. The 

matrix elements of the first order local spin operators are 

respectively

$$\hat{S}^{n_i, m_i}_{l,t} = \langle \phi_{n_i} | S_{l,t} | \phi_{m_i} \rangle$$

We will study the following magnitudes. The ground 

state energy per site $E_G = E_0 / L_x$, where $L_x = L_y L_z$, 

the gap to the first excited state in the sector of spin 

$S_z = 0$, $\Delta_0$ and $S_z = 1$, $\Delta_1$. To monitor both gaps, 

that have to be equal in a spin rotational invariant 

Hamiltonian, is a very stringent probe of the reliability 

of the method. The interchain spin flip coupling

FIG. 1: The two lattice geometries studied in the text. On the 

left, chains coupled with perpendicular $J_{\perp}$ and diagonal 

coupling $J_d$. On the left the chains are arranged on a triangular 

lattice.
TABLE I: Ground state energy per site ($E_G$), gaps to the $S_z = 0$ ($\Delta_0$) and $S_z = 1$ ($\Delta_1$) excitations and binding energy for a 2x10 leg-ladder with $J_{\parallel} = 0.1$, $\rho = 0.0$ as a function of the number of states kept in the parallel and perpendicular direction.

| 2x10 | $E_G$ | $\Delta_0$ | $\Delta_1$ | $E_B$ |
|------|------|-----------|-----------|-------|
| ED   | -0.4273296 | 0.283182 | 0.283182 | -0.001526 |
| $m_{s1}$ $m_{s2}$ | $E_0$ | $\Delta_0$ | $\Delta_1$ | $E_B$ |
| 8 8 | -0.42433209 | 0.4880304 | 0.28121407 | -0.0006399 |
| 8 16 | -0.42443195 | 0.47999406 | 0.27884533 | -0.0009685 |
| 8 32 | -0.42446616 | 0.47825339 | 0.27731861 | -0.0009715 |
| 16 8 | -0.42676461 | 0.29092770 | 0.2842390 | -0.0009189 |
| 16 16 | -0.42698277 | 0.2935105 | 0.28683188 | -0.0012005 |
| 16 32 | -0.42707158 | 0.28790788 | 0.28491220 | -0.0012885 |
| 16 48 | -0.42712096 | 0.28737740 | 0.28416304 | -0.0013382 |
| 16 64 | -0.42712439 | 0.28674689 | 0.28360519 | -0.0013417 |
| 32 8 | -0.42679647 | 0.2886051 | 0.28619524 | -0.0009295 |
| 32 16 | -0.42703063 | 0.29022064 | 0.29021987 | -0.0012710 |
| 32 32 | -0.42716088 | 0.28579872 | 0.28610427 | -0.0013576 |
| 32 48 | -0.42724324 | 0.28531525 | 0.28552398 | -0.0014397 |
| 32 64 | -0.42725807 | 0.28391776 | 0.28397001 | -0.0014545 |
| 32 96 | -0.42792144 | 0.28342612 | 0.28342613 | -0.0015066 |

terms (e.g. $J_{\parallel} S_{i,t}^{+} S_{i+1,t}^{-} \ldots + h.c.$) connects different sectors with different total chain magnetization $S_{T}^z = \sum_i S_i^z$ that have to be accurately and consistently described by the $m_{s1}$ states outgoing from the block renormalization step that culminates the one-dimensional part of the algorithm. This is achieved by a careful targeting of states in sectors with increasing chain magnetization $S_{T}^z$. We also computed the binding energy of the chains $E_B = (E_0(J_{\parallel}, J_{\perp}) - E_0(J_{\parallel} = 0, J_{\perp} = 0))/L$ which is primarily a 'transverse' magnitude. The ED data have been obtained using the Davidson algorithm and imposing open boundary conditions.

IV. 2S-DMRG: A CONTROLLED APPROXIMATION

The main purpose of this section is to compare the efficiency of the algorithm in frustrated and unfrustrated systems. Here we keep all the exchange couplings in the model constant and we show how the precision of the method improves systematically as we increase the number of states of the density matrix in the direction parallel ($m_{s1}$) and perpendicular to the chains ($m_{s2}$). The parallel coupling $J_{\parallel} = 1.0$ as the reference scale and we will keep it fixed as the reference energy scale in the problem. We present an exhaustive comparison of the 2x10 and the 3x6 ladders taking a common value of the perpendicular exchange coupling $J_{\perp} = 0.1$. To study the role of frustration we take two values of $J_{\perp} = \rho J_{\perp}$ corresponding with $\rho = 0$, tables II (2x10) and III (3x6) and $\rho = 0.5$, tables IV (2x10) and V (3x6), for different number of states kept in both directions. Since the Hamiltonians are anisotropic most of the energy is stored along the chains in the $J_{\parallel}$ bonds and therefore we observe larger increments in accuracy when we increase $m_{s1}$ at fixed $m_{s2}$ than when we increase $m_{s2}$ at fixed $m_{s1}$. It is also clear from this study that in all cases the singlet-triplet gap $\Delta_1$ is closer to the exact value obtained with ED than the gap in the $S_{T}^z = 0$ sector $\Delta_0$. This is a consequence of the variational nature of the method and it is also observed in the conventional 1D DMRG: $\Delta_1 = E_0(S = 1) - E_0(S = 0)$ involves two minimal energies in different sectors and it is computed with more precision than $\Delta_0 = E_1(S = 0) - E_0(S = 0)$. However, the difference between the two gaps vanishes as $m_{s1}$ and $m_{s2}$ increase. Similar dependence in $m_{s1}$ and $m_{s2}$ is found in the anisotropic triangular lattice.

We also observe that, both in the two- and the three-leg ladder, the accuracy is always higher in the frustrated case. Actually, the improvement is one order of magnitude in all the quantities computed, irrespective of the values of $m_{s1}$ and $m_{s2}$.

V. PERFORMANCE IN FRUSTRATED LATTICES.

A. Chains coupled with perpendicular and diagonal couplings

To study this point in more detail we have computed all the magnitudes listed above as a function of $\rho = J_{\perp}/J_{\parallel}$. The results are presented in table V for the 2x10 system...
TABLE III: Energies and gap dependence on the number of states kept in the 3x6 ladder with $J_x = 0.1$, $\rho = 0.0$.

| 3x6 | $E_G$  | $\Delta_0$ | $\Delta_1$ | $E_B$  |
|-----|--------|------------|------------|-------|
| ED  | -0.41733967 | 0.423312   | 0.423312   | -0.001743481 |
| $m_{x1}$ | $E_G$  | $\Delta_0$ | $\Delta_1$ | $E_B$  |
| 4 4 | -36497451 | 0.32915698 | 0.16977127 | -0.00256288 |
| 4 8 | -36518753 | 0.32932855 | 0.17029788 | -0.00277591 |
| 4 16 | -36521796 | 0.32976460 | 0.16657322 | -0.00280634 |
| 8 4 | -41690780 | 0.44817021 | 0.48170190 | -0.00111016 |
| 8 8 | -41692515 | 0.42847414 | 0.42847414 | -0.00132896 |
| 8 16 | -41720572 | 0.42941491 | 0.42941491 | -0.00163453 |
| 8 32 | -41733685 | 0.42386885 | 0.42386885 | -0.00174066 |

TABLE IV: Energies and gaps as a function of the number of states kept in the 3x6 ladder with $J_x = 0.1$ and frustration $\rho = 0.5$.

| 3x6 | $E_G$  | $\Delta_0$ | $\Delta_1$ | $E_B$  |
|-----|--------|------------|------------|-------|
| ED  | -0.41580272 | 0.47413    | 0.47413    | -0.00020653 |
| $m_{x1}$ | $E_G$  | $\Delta_0$ | $\Delta_1$ | $E_B$  |
| 4 4 | -36273211 | 0.31690894 | 0.21046881 | -0.00032049 |
| 4 8 | -36274150 | 0.31664021 | 0.21023338 | -0.00032987 |
| 4 16 | -36272196 | 0.32976460 | 0.16657322 | -0.00280634 |
| 8 4 | -41565327 | 0.47410007 | 0.47410008 | -0.00005708 |
| 8 8 | -41572257 | 0.47473022 | 0.47473022 | -0.0012638 |
| 8 16 | -41579631 | 0.47495257 | 0.47495259 | -0.00020012 |
| 8 32 | -41580249 | 0.47415896 | 0.47415897 | -0.00020630 |

and in table VII for the 3x6 system. Both $E_G$ and $E_B$ are non-monotonic functions of $\rho$ with extrema in the vicinity of $\rho = 0.6$. Actually, $E_G(\rho)$ is a function concave up and $E_B(\rho)$ is concave down. The maximum in $E_B$ is the remnant of the decoupling between staggered parts of the coarse-grained spin operator predicted by field theory at $\rho = 0.5$. In finite open-boundary systems the ‘decoupling point’ takes place at higher values of $\rho$ but still can be observed through the decrease of the binding energy of the chain. The error in the ground state energy is reduced when $\rho$ increases, making clear that 2S-DMRG can deal with coupling Hamiltonians running along the diagonal and even more, it can be performed with more frustrated than with nonfrustrated systems. A crucial observation here is that the ground state error $\delta E_0 = (E_0 - E_{0\text{ED}})/L$ does not increase with $J_d$ but exhibits nearly linear correlation with the value of $E_{B}$, i.e. it also has a minimum at $\rho \sim 0.6$. As we are going to see, this widens remarkably the range of applicability of the method.

The error in the gap $\Delta_1 - \Delta_0 < \delta \Delta_1$ follows a similar trend. However, the value of $\delta \Delta_1(\rho)$ has a minimum at a value of $\rho$ slightly higher than the error in the ground state $\delta E_0$. The consistency of the two gaps $\Delta_1, \Delta_0$ is very high and goes beyond that the error in the gap itself $\Delta_1 - \Delta_0 < \delta \Delta_1$ warranting that the spin rotational invariance of the system is preserved by the algorithm. The difference $\Delta_1 - \Delta_0 = 5.3 \times 10^{-6}$ at $\rho = 0.0$ reduces to $1 \times 10^{-6}$ at $\rho = 0.6$ in the 2x10 ladder and from $1.2 \times 10^{-7}$ at $\rho = 0.0$ to $1 \times 10^{-8}$ at $\rho = 0.6$ in the 3x6 ladder.

The method, being a perturbative renormalization approach, loses some precision as we increase the perturbation. In the square lattice, the strength of the perturbation can be encoded in a single parameter of the Hamiltonian $J_{\perp}$. To illustrate this point further, results in tables V and VI suggest that it is not the nominal value of the Hamiltonian $J_{\perp}$ that the precision reduces as $J_{\perp}$ increases. However, when we switch on the diagonal interaction $J_d$ for a fixed value of $J_{\perp}$ the precision increases. Furthermore, results in tables V and VI suggest that it is not the nominal value of the transverse couplings what limits the precision of this algorithm but the value of the binding energy, which is more directly related to the expectation value of the interchain coupling Hamiltonian. To illustrate this point we have compared values of $\delta E_0$ at $\rho = 0$ and $\rho = 0.6$ (which is nearly the value of $\rho$ with minimal binding energy). The results are presented in table VII for the 2x10 system and in table VIII for the 3x6. The precision is at least one order of magnitude higher in the $\rho = 0.6$ for both systems.
TABLE VI: Energy and gap $\Delta_1$ as a function of the ratio $\rho = J_1/J$ for the $3 \times 6$ ladder with $J_1 = 0.1$.

| $3 \times 6$ | $\rho$ | $\delta E_0$ | $\Delta_1$ | $E_B$ |
|-------------|-------|--------------|-------------|------|
| 2S-DMRG     | 0.1   | -0.41688122  | 0.432623    | -0.0128503 |
| 2S-DMRG     | 0.2   | -0.41649678  | 0.442359    | -0.0090650 |
| 2S-DMRG     | 0.3   | -0.4161880   | 0.43300687  | -0.0059181 |
| 2S-DMRG     | 0.4   | -0.41595588  | 0.463113    | -0.0035998 |
| 2S-DMRG     | 0.5   | -0.41580272  | 0.474130    | -0.0026955 |
| 2S-DMRG     | 0.6   | -0.41572872  | 0.485568    | -0.0013253 |
| 2S-DMRG     | 0.7   | -0.41573590  | 0.484843    | -0.0013920 |
| 2S-DMRG     | 0.8   | -0.4158235   | 0.471902    | -0.0022731 |
| 2S-DMRG     | 0.9   | -0.4159940   | 0.459162    | -0.0022731 |
| 2S-DMRG     | 1.0   | -0.41624674  | 0.44704680  | -0.0065028 |

TABLE VII: Error in the ground state energy and exact binding energy for the 2x10 ladder at $\rho = 0.0$ and $\rho = 0.6$.

| $2 \times 10$ | $\delta E_0$ | $E_B^{\rho=0.0}$ | $\delta E_0$ | $E_B^{\rho=0.6}$ |
|---------------|--------------|-------------------|--------------|-------------------|
| $J_1$         | 0.05         | -0.000173         | -0.001815    | -0.000093         |
|               | 0.10         | -0.000715         | -0.007880    | -0.0009639        |
|               | 0.15         | -0.001695         | -0.0019401   | -0.00022034       |
|               | 0.20         | -0.003229         | -0.0037922   | -0.00039864       |
|               | 0.25         | -0.005477         | -0.0065235   | -0.0002530        |
|               | 0.30         | -0.008634         | -0.0103230   | -0.0003881        |

TABLE VIII: Error in the ground state energy and exact binding energy for the $3 \times 6$ ladder at $\rho = 0.0$ and $\rho = 0.6$.

| $3 \times 6$ | $\delta E_0$ | $E_B^{\rho=0.0}$ | $\delta E_0$ | $E_B^{\rho=0.6}$ |
|--------------|--------------|-------------------|--------------|-------------------|
| $J_1$        | 0.05         | -0.0000023        | -0.0042351   | -0.0000003        |
|               | 0.10         | -0.0000282        | -0.00174351  | -0.000016         |
|               | 0.15         | -0.0001358        | -0.00402195  | -0.0000522        |
|               | 0.20         | -0.0004299        | -0.00729456  | -0.000127         |
|               | 0.25         | -0.0010536        | -0.01156190  | -0.000275         |
|               | 0.30         | -0.0021701        | -0.01678901  | -0.000554         |

TABLE IX: Ground state energy $E_G$, gap $\Delta_1$ and binding energy of the chains $E_B$ at different values of $J_1$ and $J_1 = 0.3$.

| $3 \times 6$ | $J_1$ | $E_G$ | $\Delta_1$ | $E_B$ |
|--------------|------|------|------------|------|
| 2S-DMRG      | 0.0  | -0.4323851 | 0.354879   | -0.0167898 |
| 2S-DMRG      | 0.1  | -0.42595045 | 0.376078  | -0.0035425 |
| 2S-DMRG      | 0.2  | -0.42604272 | 0.37907273 | -0.01048022 |
| 2S-DMRG      | 0.3  | -0.42136694 | 0.404534  | -0.00577075 |
| 2S-DMRG      | 0.4  | -0.42123679 | 0.40566085 | -0.00573060 |
| 2S-DMRG      | 0.5  | -0.41878783 | 0.441008  | -0.0031642 |
| 2S-DMRG      | 0.6  | -0.41875861 | 0.44085533 | -0.0031642 |
| 2S-DMRG      | 0.7  | -0.41871273 | 0.42255551 | -0.0031204 |
| 2S-DMRG      | 0.8  | -0.412158277 | 0.32995853 | -0.00598658 |
| 2S-DMRG      | 0.9  | -0.42805333 | 0.235580  | -0.01245714 |
| 2S-DMRG      | 1.0  | -0.42751008 | 0.25335794 | -0.01191389 |

VI. CONCLUSIONS

We have studied frustrated spin ladders using a recently proposed numerical renormalization group method for quasi-one-dimensional systems. We have presented exhaustive comparison with exact diagonalization data, a test that any other numerical method in strongly correlated systems have had to pass. The two-step DMRG method has shown good performance in a large class of frustrated systems reaching in some cases a precision comparable with the 1D case. We find a close correlation between the binding energy of the chains and the accu-
racy in the computation of ground state energy and the gap. We have also shown that a model of weakly coupled chains in a triangular geometry for $\text{Cs}_2\text{CuCl}_4$ is within the range of applicability of the method.

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