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# Real-space renormalization group with effective interactions

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The real-space renormalization group for the study of periodic systems goes through the reduction of the Hilbert space to products of lowest eigenstates of identical blocks. Instead of working with the Hamiltonian, it is possible to estimate effective interactions between blocks from the spectrum of dimers or trimers of blocks, according to the effective Hamiltonian theory of Bloch. Tests on a series of spin problems [cohesive energy of the one-dimensional (1D) chain and of the 2D square lattice, excitation energies of the dimerized 1D spin chain, and behavior of the frustrated chain in the low frustration regime] show the potentiality of the method.

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## I. INTRODUCTION

To study the low-energy properties of strongly interacting quantum lattice models, several numerical methods are available. Actually, only a few cases can be solved analytically via the Bethe ansatz as the one-dimensional (1D) Hubbard and Heisenberg models[1] and none of the proposed methods may be applied universally. Among the most important ones, one may cite the density-matrix renormalization-group (DMRG) method,[2,3] for which a remarkable accuracy can be achieved for 1D systems. The generalization of its applicability to more than 1D systems remains, however, a subject of active development. The quantum Monte Carlo (QMC) method[4,5] has been successfully applied to the study of 2D systems, but this method is hindered by the minus sign problem when fermions are concerned. One may also cite the coupled-cluster (CC) method,[6–9] which has given accurate descriptions of the ground states of several models when an adapted reference function can be defined, and the exact diagonalization of finite-size systems,[10–12] which is powerful for calculating dynamical correlations. Of course, the exponential growth of the number of states for interacting quantum lattice systems that limits the latter justifies the general attempt to develop procedures in which the Hilbert space is truncated.

The real-space renormalization-group (RSRG) method, which was first proposed by Wilson,[13] is a variational scheme that truncates the Hilbert space. The basic idea is to integrate out unimportant degrees of freedom progressively using a succession of renormalization-group transformations. The method works well in the single-impurity Kondo problem but fails for most quantum lattice models.[14,15] The reason[16] for the breakdown is attributed to the use of fixed boundary conditions of the blocks, i.e., if one keeps only the ground state of the block in a 1D system, for example, the wave function of the next-iteration larger block has almost a node at the connection between the blocks. When the lattice does not present an intrinsic separation in energy scales, it is necessary to keep a large number of block states to describe accurately the low-lying states of the next-size block. Several attemps to solve that problem have been proposed. White and Noak formulated two types of RG procedures[16] that work quite well for the single-particle problem, namely the *combination of boundary conditions* (CBC) and the *superblock* methods. In the latter, the general behavior at the boundaries is provided by embedding the block of interest in a larger block (the superblock). While the projection of the wave function of the superblock onto the system block is a single-valued coordinate projection in the noninteracting system, it becomes more complicated for the interacting system. The DMRG is based on the choice of an optimal way to do this projection.

Several other investigations to improve the RSRG calculations have been formulated. Quite accurate results are obtained in Ref. 17, where the authors take into account the excited states within a block through a second-order quasidegenerate perturbation theory. In the same kind of philosophy, another method[18] integrates the effect of excited states by defining a new transformed Hamiltonian from calculations on dimers of blocks. The interaction of the transformations yields a sequence of renormalized Hamiltonians. This proposition, which gives reliable results, has been presented as a renormalization-group estimate in the particular case of a 2D square spin lattice. From our point of view, it is possible to formalize this idea in a more general way that extends widely its domain of applications. This is in fact the purpose of the present paper. We formulate a renormalization-group procedure in which the renormalized Hamiltonian is defined as a Bloch effective Hamiltonian.[19] Using effective Hamiltonian theory, one may truncate the Hilbert space in a controlled way, and take into account the effect of the omitted part of the space through accurate extractions of effective interactions.

A detailed presentation of the method is given in the next section while applications on several spin problems are presented in Sec. III. In order to show the efficiency of this procedure, we have first applied it to the 1D spin chain for which exact results are available from the Bethe ansatz. The cohesive energy of the 2D square spin lattice obtained with the method is compared with the best available results. We then study the spin gap of the dimerized 1D chain and calculate the first excitation energies of the polyacetylene chain for several values of the dimerization parameter. Finally, the behavior of the frustrated spin chain is studied and conclusions are given in the final section.

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## II. PRESENTATION OF THE METHOD

The renormalization-group procedure that is used in this work is an iterative procedure that starts with the exact treatment of a finite-size system (called the superblock) made up of a few identical blocks of sites. At the next iteration, these blocks are considered as ‘‘supersites’’ of the lattice for which the allowed states are the lowest eigenstates of the blocks; this represents a drastic truncation of the space. The main difference between this method and the previous proposals consists in the evaluation of the interactions between these supersites. Instead of using the real Hamiltonian, we propose to extract renormalized interactions from the spectrum of the superblock (SB). Such a procedure should enable us to take into account the effect of the neglected excited states of the blocks. The basic idea is to pass from the exact Hamiltonian $H_{\mathrm{SB}}$ of the superblock expressed in its complete Hilbert space to an effective Hamiltonian describing the interactions between the lowest states of the blocks (i.e., operating on the truncated basis). The extracted effective Hamiltonian is then used to describe the superblock, now built in terms of blocks, at the next iteration and the procedure is iterated until the convergence of the property is achieved.

The formalism of effective Hamiltonian used in this work has been proposed by Bloch.[19] Let us now explain step by step how the Bloch effective Hamiltonian is built up and integrated to the renormalization procedure.

### A. The choice of a target space

One first isolates a portion of an infinite system of $N_T$ sites that can be divided in a few ($N_B$) identical blocks. The size of this system that constitutes the superblock must be such that the calculation of a set of exact eigenvectors of the Hamiltonian matrix is possible. Using the efficient Lanczos[20] or Davidson[21] diagonalization technique for sparse matrices, one calculates $N_m$ eigenstates $\Psi_m^{(0)}$ among which are those that are relevant to describe the physical phenomenon of interest (for instance, for the calculation of the gap),

$$H_{\mathrm{SB}}^{(0)}|\Psi_m^{(0)}\rangle = E_m^{(0)}|\Psi_m^{(0)}\rangle, \tag{1}$$

where ‘‘(0)’’ indicates the iteration.

The choice is crucial since, in the effective Hamiltonian construction, all the information concerning the other states will be forgotten. The space $S$ spanned by these $N_m$ vectors is called the target space,

$$S = \{\Psi_m^{(0)}\}, \quad \dim(S) = N_m .$$

Let us call $P_S$ the projector associated with $S$,

$$P_S = \sum_{m=1}^{N_m} |\Psi_m^{(0)}\rangle\langle\Psi_m^{(0)}|. \tag{2}$$

### B. The choice of a model space

The superblock is divided into a few ($N_B$) identical blocks that are treated exactly. Let us call $H_{\mathrm{block}}^{(0)}$ the Hamiltonian of the isolated block,

$$H_{\mathrm{block}}^{(0)}|\phi_i^{(0)}\rangle = e_i^{(0)}|\phi_i^{(0)}\rangle. \tag{3}$$

The $N_i$ lowest eigenstates $\phi_i^{(0)}$ of each block are used to build a restricted Hilbert space for the superblock, called the model space $S_0$. $S_0$ is spanned by the direct products of the $N_i$ functions $\phi_i^{(0)}$ of each block and $N_i$ and $N_m$ must be such that $S$ and $S_0$ are isodimensional (this assertion will be justified later on),

$$S_0 = \{\Phi_m^{(0)}\} = \{\bigotimes_i \phi_i^{(0)}\}, \quad \dim(S_0) = N_i^{N_B} = N_m .$$

Let $P_0$ be the projector on the model space $S_0$,

$$P_0 = \sum_{m=1}^{N_m} |\Phi_m^{(0)}\rangle\langle\Phi_m^{(0)}|. \tag{4}$$

At this step, it is possible to revise the choice of both the target and the model space. Actually the definition of an accurate effective Hamiltonian is not always possible. The target space $S$ must have $N_m$ nonzero and linearly independent projections on the model space, i.e., a one-to-one correspondence between $S$ and $S_0$ must exist.

If one calls $\tilde{\Psi}_m^{(0)}$ the projection of the eigenvector $\Psi_m^{(0)}$ of the superblock onto the model space $S_0$,

$$|\tilde{\Psi}_m^{(0)}\rangle = P_0|\Psi_m^{(0)}\rangle, \tag{5}$$

an alternative way to write $P_0$ is

$$P_0 = \sum_{m=1}^{N_m} |\tilde{\Psi}_m^{(0)}\rangle\langle(\tilde{\Psi}_m^{(0)})^{\perp}|, \tag{6}$$

where $(\tilde{\Psi}_m^{(0)})^{\perp}$ is the biorthogonal state of $\tilde{\Psi}_m^{(0)}$. Actually the projections $\tilde{\Psi}_m^{(0)}$ of the (orthogonal) states $\Psi_m^{(0)}$ have no reason (except for symmetry reasons) to be orthogonal; they define an overlap matrix $s$,

$$s_{mn} = \langle\tilde{\Psi}_m^{(0)}|\tilde{\Psi}_n^{(0)}\rangle, \tag{7}$$

and the biorthogonal vectors are defined by

$$|(\tilde{\Psi}_m^{(0)})^{\perp}\rangle = s^{-1}|\tilde{\Psi}_m^{(0)}\rangle. \tag{8}$$

The values of the norms of the projections, i.e., the diagonal elements of the $s$ matrix, give an indication of the quality of the description of these states by the truncated space $S_0$. The model space and the target space must be in strong correspondence, i.e., one must choose both spaces so that the vectors $\Psi_m^{(0)}$ have the largest projections on $S_0$.

### C. Extraction of an effective Hamiltonian for the next iteration

Let us recall that our purpose is to obtain effective interactions between the blocks (i.e., the supersites of the next iteration) so that the Hamiltonian of the iteration 1 $(H_{\mathrm{SB}})^{(1)}$ will have the same expression as the effective Hamiltonian. It seems then natural to decompose $(H^{\mathrm{eff}})^{(1)}$ as follows:

$$(H^{\text{eff}})^{(1)} = \sum_{i=1}^{N_B} (H_i^{\text{eff}})^{(1)} + \sum_{\langle ij\rangle} (H_{ij}^{\text{eff}})^{(1)}, \tag{9}$$

where $i$ and $j$ stand for the blocks and $N_B$ is their total number. Since this Hamiltonian operates on the direct products of the wave functions of the blocks, the first term is only a diagonal matrix, its elements being a sum over the eigenenergies of the blocks. In the second term, the sum runs over all the couples of interacting blocks. Of course, this expression could be generalized to describe more complicated Hamiltonians involving $N$-site interactions by extending this sum to groups of three $\langle ijk\rangle$ or more blocks. In this paper, the Hamiltonian used will only involve two-site interactions even when trimers of blocks are considered.

In the formalism proposed by Bloch,[19] an effective Hamiltonian defined on a model space $S_0$ of dimension $N_m$ is entirely determined by the $N_m$ eigenenergies and eigenvectors of the exact Hamiltonian that span the isodimensional target space $S$ having $P_S$ as associated projector.

The two spaces (model and target) are in a one-to-one correspondence, the wave operator $\Omega$ transforming $S_0$ into $S$, according to the equation

$$P_S = \Omega P_0 . \tag{10}$$

The effective Hamiltonian, defined on the model space, is such that its $N_m$ eigenvalues are the $N_m$ exact eigenvalues of the exact Hamiltonian $H_{\text{SB}}^{(0)}$, and its eigenvectors are the projections of the exact eigenvectors $\Psi_m^{(0)}$ on the model space,

$$(H^{\text{eff}})^{(1)} |\tilde{\Psi}_m^{(0)}\rangle = E_m^{(0)} |\tilde{\Psi}_m^{(0)}\rangle . \tag{11}$$

Note that the spectral decomposition of $(H^{\text{eff}})^{(1)}$ is

$$(H^{\text{eff}})^{(1)} = \sum_{m=1}^{N_m} E_m^{(0)} |\tilde{\Psi}_m^{(0)}\rangle\langle(\tilde{\Psi}_m^{(0)})^{\perp}| . \tag{12}$$

Thus, if the projections are not orthogonal, this Hamiltonian is not Hermitian. However, its hermitization[22] can easily be obtained by imposing the solutions of the new effective Hamiltonian to be the symmetrically orthogonalized solutions of the Bloch Hamiltonian.

The effective interactions between blocks belong to the second term of Eq. (9) and are calculated by expressing the effective Hamiltonian matrix in the basis of the vectors $\Phi_m^0$,

$$\langle \Phi_k^{(0)} | (H^{\text{eff}})^{(1)} | \Phi_l^{(0)} \rangle = \sum_m \langle \Phi_k^0 | \tilde{\Psi}_m^{(0)} \rangle E_m^{(0)} \langle (\tilde{\Psi}_m^{(0)})^{\perp} | \Phi_l^0 \rangle . \tag{13}$$

Let us consider the case in which the superblock is composed of two blocks only, $A$ and $B$. The vectors $\Phi_m^{(0)}$ are products of eigenstates of each block, for instance

$$|\Phi_k^{(0)}\rangle = |\phi_{t_A}^{(0)} \otimes \phi_{s_B}^{(0)}\rangle , \tag{14}$$

$$|\Phi_l^{(0)}\rangle = |\phi_{t_A}^{(0)} \otimes \phi_{u_B}^{(0)}\rangle , \tag{15}$$

and the effective Hamiltonian will be written as a matrix, the elements of which are

$$\langle \Phi_k | (H^{\text{eff}})^{(1)} | \Phi_k \rangle$$
$$= \langle \phi_{r_A}^{(0)} \phi_{s_B}^{(0)} | (H_A^{\text{eff}})^{(1)} + (H_B^{\text{eff}})^{(1)} + (H_{AB}^{\text{eff}})^{(1)} | \phi_{r_A}^{(0)} \phi_{s_B}^{(0)} \rangle \tag{16}$$

$$= E_{r_A} + E_{s_B} + \langle \phi_{r_A}^{(0)} \phi_{s_B}^{(0)} | (H_{AB}^{\text{eff}})^{(1)} | \phi_{r_A}^{(0)} \phi_{s_B}^{(0)} \rangle , \tag{17}$$

$$\langle \Phi_k | (H^{\text{eff}})^{(1)} | \Phi_l \rangle$$
$$= \langle \phi_{r_A}^{(0)} \phi_{s_B}^{(0)} (H_{AB}^{\text{eff}})^{(1)} | \phi_{t_A}^{(0)} \phi_{u_B}^{(0)} , \tag{18}$$

where $E_{r_A}$ and $E_{s_B}$ are the energies of the block eigenstates $\phi_{r_A}$ and $\phi_{s_B}$, respectively. Another way to calculate these interactions is to solve Eq. (11) for the $N_m$ vectors $\Psi_m$, i.e., to solve the system of $N_m^2$ equations since the effective Hamiltonian matrix is of dimension $N_m$. Note that to get the right number of equations, the sizes of the model and the target spaces must be equal, and the number of interactions requested to describe the lattice should be lower than or equal to $(N_m)^2$. As we will see in the applications, this number is in practice much smaller than $(N_m)^2$ due to space and spin symmetry properties, and very simple solutions can be found.

### D. Renormalization procedure and iteration

The lattice is now made up of $N_T$ supersites that are the blocks of the iteration 0. The Hamiltonian is a renormalized effective Hamiltonian involving the extracted effective interactions. It has the general expression of Eq. (9), where the sums over $i$ and $j$ now run over the $N_T$ supersites of the superblock,

$$(H_{\text{SB}})^{(1)} = \sum_{i=1}^{N_T} (H_i^{\text{eff}})^{(1)} + \sum_{\langle ij\rangle} (H_{ij}^{\text{eff}})^{(1)} . \tag{19}$$

We can then go back to the first step and iterate the procedure.

Let us notice that the Hamiltonians $(H_{\text{SB}})^{(1)}$ and $(H_{\text{SB}})^{(0)}$ have no reason to be of the same nature. For instance, the division of the lattice into blocks may induce a different topology, leading to interactions that could differ in nature and number from the original ones; the shape of the blocks will also determine the new spin nature of the states. This degree of freedom should enable us to modify the model, i.e., to go from a Hubbard to a Heisenberg model, for example, or to study lattices through a different arrangement of their sites. Nevertheless, as will be shown in the applications, it is sometimes possible to define the blocks and the model space in such a way that the new Hamiltonian is isomorphic to the initial one.

## III. APPLICATIONS OF THE METHOD

The method has been applied to various spin problems. In all the presented cases, the division of the lattice into blocks has been realized in such a way that the nature of the Hamiltonian is conserved throughout the iterative procedure.

### A. Cohesive energy of the 1D spin chain

The considered Heisenberg Hamiltonian has the following expression:

$$(H)^{(0)}=\sum_{\langle ij\rangle}\ (2J^{(0)}\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}) \tag{20}$$

$$\begin{aligned}=\sum_{\langle ij\rangle}\ J^{(0)}[a_i^+a_{\bar j}^+a_ja_{\bar i}+a_j^+a_{\bar i}^+a_ia_{\bar j}\\ -a_i^+a_{\bar j}^+a_{\bar j}a_i-a_{\bar i}^+a_j^+a_ja_{\bar i}],\end{aligned} \tag{21}$$

where $\langle ij\rangle$ stands for the couple of nearest-neighbor sites $i$ and $j$. The interaction parameter $J^{(0)}$ is the positive exchange and $a_i^+$ and $a_i$ ($a_{\bar i}^+$ and $a_{\bar i}$) are the usual creation and annihilation operators of a spin up (spin down) on site $i$. Let us note that this Hamiltonian differs from the usual one, $H=\Sigma_{\langle ij\rangle}J\mathbf{S}_i\cdot\mathbf{S}_j$, by both the interaction parameter, which here is one-half, and a shift of the zero energy to the energy of the ferromagnetic state.

Let us consider a portion of a chain of $N_T$ sites as the superblock, made up of two identical blocks $A$ and $B$ of $N_S$ (odd) sites. In the $S_z=0$ block Hamiltonian matrix, the ground state of the superblock is a singlet and the first excited state is a triplet. These two states, denoted $\Psi_S^{AB}$ and $\Psi_T^{AB}$, respectively, constitute our target space. Let us call $E_S^{AB}$ and $E_T^{AB}$ the corresponding eigenvalues.

One needs now to define the model space. After an exact treatment of one of the identical blocks, for example $A$, we have kept the doublet ground state denoted $a$ associated to the $S_z=\frac{1}{2}$ component. Let us call $b$ the $S_z=\frac{1}{2}$ component of the doublet ground state of the block $B$, $\bar a$ and $\bar b$ the corresponding $S_z=-\frac{1}{2}$ components, and $E_D^A$ and $E_D^B$ the energies of these two blocks in their ground state. From the four previous states, one may build four direct products, namely $a\bar b$, $\bar a b$, $ab$, and $\overline{ab}$. The projections of the two exact lowest states $\Psi_S^{AB}$ and $\Psi_T^{AB}$ of the superblock on the last two direct products are of course zero because of spin. Thus, to build a model space $S_0$, one may keep only $a\bar b$ and $\bar a b$, which generate the following projector:

$$P_0=|a\bar b\rangle\langle a\bar b|+|\bar a b\rangle\langle\bar a b|. \tag{22}$$

One should notice that keeping the two doublet components for each block corresponds to assigning effective spins up and down to the supersites at the next iteration, thus insuring the isomorphism between the iterations.

The effective Hamiltonian is therefore a Heisenberg Hamiltonian of the same nature. It may be written as a function of only two effective interactions,

$$\begin{aligned}(H^{\rm eff})^{(1)}=\sum_{i=1}^{N_B}\ (H_i^{\rm eff})^{(1)}+\sum_{\langle ij\rangle}\ (B^{(1)}+J^{(1)}[a_i^+a_{\bar j}^+a_ja_{\bar i}\\ +a_j^+a_{\bar i}^+a_ia_{\bar j}-a_i^+a_{\bar j}^+a_{\bar j}a_i-a_i^+a_j^+a_ja_{\bar i}]),\end{aligned} \tag{23}$$

where $a_i^+(a_i)$ now creates (annihilates) a doublet $S_z=\frac{1}{2}$ on the block $i$, $J^{(1)}$ is the effective exchange parameter $J^{(1)}=\langle\bar a b|(H_{ij}^{\rm eff})^{(1)}|a\bar b\rangle=-\langle\bar a b|(H_{ij}^{\rm eff})^{(1)}|\bar a b\rangle$ in our convention, and the energy of the ferromagnetic solution [the triplet of $(H_{ij}^{\rm eff})^{(1)}$] is $B^{(1)}=\langle ab|(H_{ij}^{\rm eff})^{(1)}|ab\rangle=\frac{1}{2}\langle\bar a b+a\bar b|(H_{ij}^{\rm eff})^{(1)}|\bar a b+a\bar b\rangle$.

The matrix representation of this Hamiltonian is

$$(H^{\rm eff})^{(1)}=\begin{pmatrix}2E_D^A+B^{(1)}-J^{(1)} & J^{(1)}\\ J^{(1)} & 2E_D^A+B^{(1)}-J^{(1)}\end{pmatrix}. \tag{24}$$

The effective interactions $B^{(1)}$ and $J^{(1)}$ are obtained by replacing by $E_S^{AB}$ and $E_T^{AB}$ the solutions $E$ of

$$\det(\mathbf{H}^{\rm eff}-E\mathbf{I})=\mathbf{0}, \tag{25}$$

$\mathbf{I}$ being the representative matrix of the identity operator. One obtains

$$E_S^{AB}=2E_D^A+B^{(1)}-2J^{(1)}, \tag{26}$$

$$E_T^{AB}=2E_D^A+B^{(1)}. \tag{27}$$

The isomorphism from one iteration to another implies the generation of a sequence of identical effective Hamiltonians. The eigenvalues $\alpha$ of $(H_{ij}^{\rm eff})^{(n)}$ for a single block being equal in units of $J^{(n)}$ at any iteration $n$, one may therefore calculate the energy $A^{(n)}$ of a block as follows:

$$A^{(n)}=N_sA^{(n-1)}+n_BB^{(n-1)}+\alpha J^{(n-1)}, \tag{28}$$

$$B^{(n)}=n_cB^{(n-1)}+\beta J^{(n-1)}, \tag{29}$$

$$J^{(n)}=\gamma J^{(n-1)}, \tag{30}$$

where $n_B$ is the number of first-neighbor pairs (or bonds) $\langle ij\rangle$ inside the blocks and $n_c$ is the number of bonds connecting two blocks. Note that $\alpha$, $\beta$, and $\gamma$ are iteration-independent parameters. Notice that this procedure is applicable to any dimensional lattice in which only one type of interaction connects the blocks.

Expressions (30)–(32) are also true at the first iteration,

$$A^{(1)}=N_sA^{(0)}+n_BB^{(0)}+\alpha J^{(0)}, \tag{31}$$

$$B^{(1)}=n_cB^{(0)}+\beta J^{(0)}, \tag{32}$$

$$J^{(1)}=\gamma J^{(0)}, \tag{33}$$

with $A^{(0)}=0$ and $B^{(0)}=0$ to get $H^{(0)}$.

Expressing $A^{(n)}$, $B^{(n)}$, and $J^{(n)}$ as functions of the initial parameters, one obtains

$$\begin{aligned}A^{(n)}\rightarrow N_S^n\Bigg(A^{(0)}+\frac{n_B}{N_S-n_c}B^{(0)}+\frac{\alpha}{N_S-\gamma}J^{(0)}\\ +\frac{\beta n_B}{(N_S-n_c)(N_S-\gamma)}J^{(0)}\Bigg),\end{aligned} \tag{34}$$

$$B^{(n)}\rightarrow n_c^n\bigg(B^{(0)}+\frac{\beta}{n_c-\gamma}J^{(0)}\bigg), \tag{35}$$

TABLE I. Asymptotic energy per site of the 1D spin chain for several block sizes and the infinite estimate.

| Block size | 5 | 7 | 9 | 11 | ∞ estimate |
|---|---|---|---|---|---|
| Block energy per site | −1.171 154 4 | −1.238 925 6 | −1.274 738 1 | −1.296 744 2 | |
| Superblock energy per site | −1.301 607 0 | −1.325 246 3 | −1.338 556 8 | −1.347 097 8 | |
| Renormalized energy per site | −1.392 270 2 | −1.390 113 8 | −1.388 950 9 | −1.388 253 1 | −1.386 205 |

$$J^{(n)}=\gamma^{n}J^{(0)}. \tag{36}$$

In the case of a 1D chain, the number of connecting bonds between two consecutive blocks is $n_c=1$ and the number of bonds per blocks is $n_B=N_S-1$, so the large-limit ground-state energy per site in units of $J^{(0)}$ is

$$\epsilon_{1\mathrm{D}}=\lim_{n\to\infty}N_S^{-n}A^{(n)}=\frac{\alpha+\beta}{N_S-\gamma}=\frac{2[E_T^{AB}-E_D^{A}]}{2N_S-E_T^{AB}+E_S^{AB}}. \tag{37}$$

We have performed calculations on superblocks of $N_T=10$, 14, 18, and 22 sites, so the number of sites per block is $N_S=5$, 7, 9, and 11, respectively. The obtained values of the large-limit energies per site are reported in Table I. The exact value of the ground-state energy per site given by the Bethe ansatz[1] is $-2\ln 2$ in our Hamiltonian. The error as a function of the number of sites is going from $6\times10^{-3}$ for $N_S=5$ to $2\times10^{-3}$ for $N_S=11$. It is always 20 times smaller than the energy error obtained from the starting dimer. We have estimated the infinite-size energy per site using the standard BST extrapolation method.[23] This method evaluates the limit of a function $T(h)=T+a_1h^{\omega}+a_2h^{2\omega}+\dots$, where $h=1/N_s$ and $\omega$ is a free parameter, by approximating the function $T(h)$ by a sequence of rational functions.

A minimal error of $8\times10^{-8}$ is obtained for $\omega=1.606$; the corresponding estimated value of the energy is $-1.386\,205$. This result compares very well with the exact one ($-1.386\,294$). One should recall that it has been obtained for a very low computational cost, with only one diagonalization of the block and the superblock systems for each size.

### B. Cohesive energy of the 2D square lattice

A similar development has been performed to calculate the large-limit energy per site of the 2D square spin lattice. The superblock has $N_T=18$ sites and is divided in two identical blocks of $N_S=9$ sites arranged in a $(3\times3)$ sublattice. The effective Hamiltonian has been extracted from the two lowest eigenstates $\Psi_S^{AB}$ and $\Psi_T^{AB}$ of the superblock. It has the expression of Eq. (23) and the two associated eigenvalues are given by Eqs. (26) and (27).

Since in that case also one gets an isomorphism from one iteration to another, it is possible to calculate the energy of a block at any iteration *n* using the expressions (34)–(36), as did the authors of Ref. 18. Now the characteristic numbers of the lattice are as follows:

$$N_S=9,\quad n_B=12,\quad n_C=3, \tag{38}$$

which leads to an expression of the large-limit energy per site in units of $J^{(0)}$ of the form

$$\epsilon_{2\mathrm{D}}=\lim_{n\to\infty}N_S^{-n}A^{(n)}=\frac{\alpha+2\beta}{9-\gamma}=\frac{4E_T^{AB}-6E_D^{A}}{18-E_T^{AB}+E_S^{AB}}. \tag{39}$$

The obtained value for $N_s=9$ is $-2.332\,31$ while the energy per site for an 18-site cluster is $-1.8926$. The best available QMC method[24] and dressed cluster (DCM) method[25] results are, respectively, $-2.338\,68$ and $-2.338\,56$. For comparison, the CC method gives $-2.334\,00$ in the LSUB6 approximation and $-2.33634$ in the LSUB8 approximation.[26] Notice that we did not perform any extrapolation as a function of the block size, which would have probably improved the estimated value. Actually, the next-size block would be $N_S=25$ sites, i.e., $N_T=50$ for an identical treatment, which is not possible to compute exactly at the moment. It would, however, be possible to treat the $N_S=11$- and 13-site systems by changing the model of the lattice, and this will be the subject of a future work.

### C. Spin gap of the dimerized 1D chain: Application to the polyacetylene

As we have seen in the presentation of the method, the excited states should be accurately described by this method since the effective Hamiltonian theory is designed to reproduce several states simultaneously. The simplest verification may concern the dimerized 1D spin chain, i.e., an infinite system with alternating spin couplings $J_1^{(0)}=\overline{J^{(0)}}(1+\delta^{(0)})$ and $J_2^{(0)}=\overline{J^{(0)}}(1-\delta^{(0)})$, where $\overline{J^{(0)}}$ is a mean coupling (which here is fixed to 1) and $\delta^{(0)}$ is a dimerization parameter varying from 0 to 1. There is no spin gap for the nondimerized chain ($\delta^{(0)}=0$). Actually the lowest singlet-triplet transition energy calculated from Eqs. (26) and (27) is $2J^{(n)}=2\gamma^{n}\overline{J^{(0)}}$ at iteration *n* with $\gamma<1$, i.e., zero for an infinite number of iterations. As soon as $\delta^{(0)}$ is different from zero, a gap appears. For the fully dimerized chain ($\delta^{(0)}=1$), the strong bonds with $J_1^{(0)}=2\overline{J^{(0)}}$ become independent ($J_2^{(0)}=0$) and the excitation energy is $\Delta E_{ST}^{(0)}(\delta^{(0)}=1)=4\overline{J^{(0)}}$. The power law $\Delta E_{ST}=\alpha\delta^{2/3}$ (Ref. 27) has been established in the case of the dimerized and frustrated 1D chain at the critical ratio $J=J_2/J1\simeq0.2411$ ($J_2$ and $J_1$ being, respectively, the second- and first-nearest-neighbor couplings). When the ratio $J$ is lower than that critical value, logarithmic corrections appear. In order to study that problem within our RSRG approach, we have to consider a block with an odd number of sites $N_S$, presenting a strong interaction $J_1^{(0)}$ on one border and a weak interaction $J_2^{(0)}$ on the other border. Actually when the $J_2^{(0)}/J_1^{(0)}$ ratio increases, the unpaired electron (effective spin) tends to localize on the

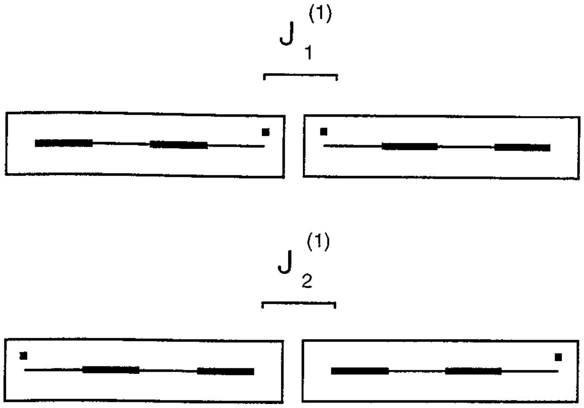

FIG. 1. Two types of 10-site dimeric superblocks for the study of the dimerized spin chain.

external site connected to the system by a weak bond. There are, therefore, two possible types of dimers (see Fig. 1). The first one concerns those terminating with strong interactions for which the splitting into two blocks goes through a strong interaction. The singlet-triplet splitting of such a skeleton obtained at the first iteration is actually finite and

$$2J_1^{(1)} = \Delta E_{ST}^{(0)}(2N_S). \tag{40}$$

On the contrary, in the other type of dimers, terminating with two weak interactions, the two blocks are connected by a weak interaction and the interaction between the two remote effective spins will be weak; and actually,

$$2J_2^{(1)} = \Delta E_{ST}'^{(0)}(2N_S) \tag{41}$$

is much weaker and will tend to zero when $N_S$ tends to infinity. From $J_2^{(1)}$ and $J_1^{(1)}$, one redefines new values of $\delta^{(1)}$ and $\overline{J^{(1)}}$ and iterates the process. $J_2^{(n)}$ decreases rapidly to zero, i.e., one obtains a finite gap $\Delta E_{ST}^{(n)}$.

The logical structure of the problem can be pictured as a single figure (Fig. 2) in which $\overline{J^{(1)}}$, $\delta^{(1)}$, and $\Delta E_{ST}^{(n_a)}/4$ (where $n_a$ is the iteration where the procedure is converged) are represented as functions of $\delta^{(0)}$ for $N_s=7$ and 9. One sees that both $\overline{J^{(1)}}$ and $\delta^{(1)}$ increase toward 1 when $\delta^{(0)}$ increases. The iteration procedure can be visualized as a stair growth toward the $\delta^{(0)}=1$, $\delta^{(1)}=1$, and $\overline{J^{(1)}}=1$ accumulation point. At each step, $\delta^{(n)}$ is changed into a new value $\delta^{(n+1)}$ rapidly equal to 1 and one may calculate the corresponding value of $\overline{J^{(n+1)}}$ from the newly read value $\overline{J^{(1)}}$ for this $\delta^{(n)}$,

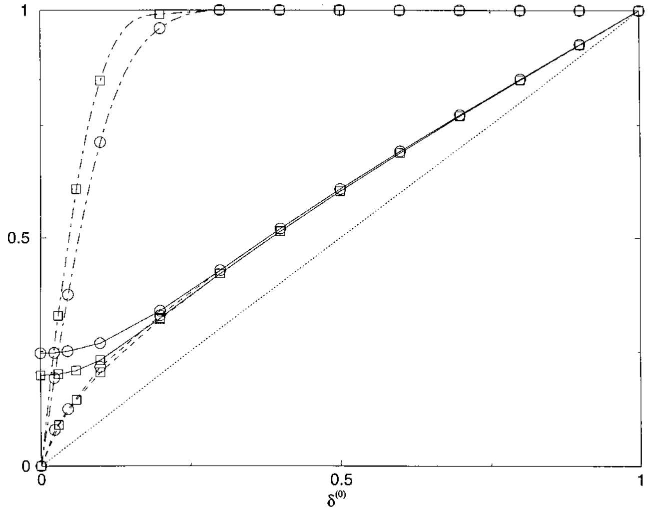

FIG. 2. Dimerization parameter $\delta^{(1)}$ (dot-dashed line) and mean coupling $\overline{J^{(1)}}$ (plain line), both obtained at the first iteration, and converged values $\Delta E_{ST}^{n_a}/4$ (dashed line) as functions of the coupling dimerization parameter $\delta^{(0)}$ for the dimerized 1D chain. Circles and squares correspond, respectively, to seven- and nine-site blocks.

$$\overline{J^{(n+1)}} = \overline{J_{\delta^{(n)}}^{(1)}} \times \overline{J^{(n)}}. \tag{42}$$

Since the procedure converges in three or four iterations to the accumulation point, the asymptotic value of $\overline{J^{(n_a)}}$ and the gap are finite. While the values of $\overline{J^{(1)}}$ and $\delta^{(1)}$ are quite different for $N_S=7$ and 9, the values of the converged gaps are very close. Figure 3 presents, for $N_S=7$, a very simple interpolation of the gaps $\Delta E_{ST}^{(n_c)} = 4\overline{J} * \delta^{\alpha}$, where the $\alpha = 0.71$ optimized value is close to the canonical value $\frac{2}{3}$.

As a more realistic illustration of this study, we will calculate the first excitation energy of the polyacetylene chain $(\mathrm{CH})_n$ in the Heisenberg regime. The low-lying states of that polymer may be studied by considering only a half-filled band involving the $2p_z$ atomic orbitals of the carbon atoms, which are orthogonal to the polymer chain. The other electrons (of the carbon and the hydrogen atoms) belong to the $\sigma$ system. The Heisenberg Hamiltonian[28] that we use in this study treats the electronic delocalization of the $\pi$ electrons through the exchange parameter $2J_{ij}$. A scalar term $R_{ij}$ describes the $\sigma$ system energy,

$$(H)^{(0)} = \sum_{ij} J_{(ij)}(r_{ij})[a_i^+ a_{\bar{j}}^+ a_j a_{\bar{i}} + a_j^+ a_{\bar{i}}^+ a_i a_{\bar{j}} - a_i^+ a_{\bar{j}}^+ a_{\bar{j}} a_i - a_{\bar{i}}^+ a_j^+ a_j a_{\bar{i}}] + R_{ij}(r_{ij}). \tag{43}$$

TABLE II. First excitation energies (in a.u.) of the polyacetylene chain calculated for several black sizes and the infinite-size estimate for different values of the bond alternation $d$ (in Å).

| Block size | 3 | 5 | 7 | 9 | 11 | ∞ estimate |
|---|---|---|---|---|---|---|
| $d=0.01$ | $2.649\,834E-2$ | $2.306\,438E-2$ | $2.157\,016E-2$ | 2.055 638E−2 | $2.009\,299E-2$ | $1.971\,703E-2$ |
| $d=0.02$ | $4.053\,322E-2$ | $3.612\,172E-2$ | $3.397\,360E-2$ | $3.312\,325E-2$ | $3.273\,165E-2$ | $3.215\,941E-2$ |
| $d=0.032$ | $5.407\,111E-2$ | $4.880\,9E-2$ | $4.676\,770E-2$ | $4.581\,6E-002$ | $4.451\,167E-2$ | $4.295\,732E-2$ |

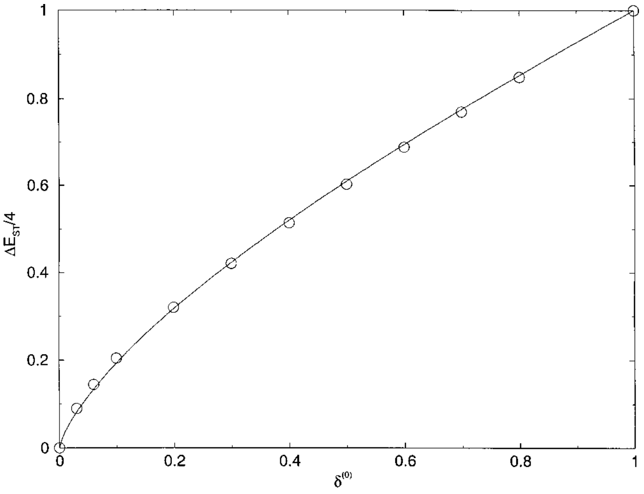

FIG. 3. Converged gaps (divided by 4) obtained from nine-site blocks. The circles correspond to calculated values while the plain line is a power-law interpolation $\Delta E_{ST}^{n_a}=4\overline{J}*\delta^{0.71}$.

The parameters $R_{ij}(r_{ij})$ and $J_{(ij)}(r_{ij})$ are functions of the interatomic distances $r_{ij}$; they have been extracted from accurate *ab initio* calculations on the lowest singlet and triplet states of the ethylene molecule. The scalar term $R_{ij}(r_{ij})$ plays a role in the determination of the optimal bond-length alternations but not in the calculation of transition energies at a fixed geometry.

Previous calculations[29] (exact diagonalizations and extrapolations) have predicted an optimized geometry of the chain. Let us define $r_{i,i\pm 1}=\overline{r}\pm d$. The optimized average interatomic distance and bond-length alternation parameter $d$ (half difference between the long and short bond lengths) are, respectively, $\overline{r}=1.4$ Å and $d=0.032$ Å. We have concentrated our study on the $d$ parameter keeping $\overline{r}=1.4$ Å constant. Since the bond-length alternation increases the antiferromagnetic coupling in every other bond, one gets two alternating $J_1^{(0)}$ and $J_2^{(0)}$ couplings so that $J_1^{(0)}=J_{ij}(\overline{r}-d)$ and $J_2^{(0)}=J_{ij}(\overline{r}+d)$, respectively, for short and long bonds.

Our calculations have been performed for superblocks of $N_T=10$, 14, 18, and 22 sites, so that $N_S=5$, 7, 9, and 11 sites, respectively. The values of the calculated gaps for several values of the dimerization and for the different block sizes are reported in Table II. The values of these energies when $N_T$ tends to infinity, estimated by the BST extrapolation algorithm, as a function of the dimerization parameter $d$ are plotted in Fig. 4. For $d=0.01$, 0.02, and 0.032, the minimal errors are $\epsilon=2\times 10^{-8}$, $9\times 10^{-9}$, and $1\times 10^{-7}$, respectively, for the corresponding values of $\omega=4.695$, 2.642, and 1.375. Previous estimates of the excitation energies may be found in Ref. 30, where a dressed cluster method was used. The calculated $\Delta E_{ST}$ were somewhat smaller than the present values, but they did not behave as $\delta^{2/3}$, as they should, while the results of the present work nicely follow this power law.

### D. The 1D spin-$\frac{1}{2}$ Heisenberg chain with nearest-neighbor (NN) and next-nearest-neighbor (NNN) couplings

Let us start with the Hamiltonian of this model,

$$(H)^{(0)}=\sum_{ij,\mathrm{NN}} J_1[a_i^+ a_{\bar{j}}^+ a_j a_{\bar{i}}+a_j^+ a_{\bar{i}}^+ a_i a_{\bar{j}}-a_i^+ a_{\bar{j}}^+ a_{\bar{j}} a_i - a_{\bar{i}}^+ a_j^+ a_j a_{\bar{i}}]+\sum_{ij,\mathrm{NNN}} J_2[a_i^+ a_{\bar{j}}^+ a_j a_{\bar{i}}+a_j^+ a_{\bar{i}}^+ a_i a_{\bar{j}} - a_i^+ a_{\bar{j}}^+ a_{\bar{j}} a_i - a_{\bar{i}}^+ a_j^+ a_j a_{\bar{i}}]. \tag{44}$$

To get an isomorphic Hamiltonian since the first iteration, one should have both NN and NNN block couplings. We have so considered superblocks made up of three identical blocks of an odd number of sites, namely *A*, *B*, and *C*, where the NN blocks *A* and *B*, as well as *B* and *C*, interact through the effective exchange $J_1^{(1)}$, and the NNN blocks *A* and *C* interact through the effective exchange $J_2^{(1)}$ (see Fig. 5).

Here also, only the doublet ground state of each block has been kept. The model space of the $S_z=\frac{1}{2}$ component states is made up of the three direct products $\overline{a}bc$, $a\overline{b}c$, and $ab\overline{c}$.

We now need to identify the three states of the superblock having the right projections on this model space. The position of these states in the spectrum of the superblock is not as trivial as in the previously considered cases. Actually, it changes as a function of the ratio $J^{(1)}=J_2^{(1)}/J_1^{(1)}$, and is different for different-sized systems, so systematic projections of the low-lying states of the superblock matrix were performed to control the method.

The expression of the effective Hamiltonian matrix is

$$(H^{\mathrm{eff}})^{(1)}=\begin{pmatrix} 3E_D^A+2B^{(1)}-J_1^{(1)}-J_2^{(1)} & J_1^{(1)} & J_2^{(1)} \\ J_1^{(1)} & 3E_D^A+2B^{(1)}-2J_1^{(1)} & J_1^{(1)} \\ J_2^{(1)} & J_1^{(1)} & 3E_D^A+2B^{(1)}-J_1^{(1)}-J_2^{(1)} \end{pmatrix}, \tag{45}$$

where $E_D^A$ is the ground-state energy of a block, $J_1^{(1)}$ and $J_2^{(1)}$ are the NN and NNN exchange couplings to extract, and $2B^{(1)}$ is the energy of the ferromagnetic solution $\langle abc|(H_{ij}^{\mathrm{eff}})^{(1)}|abc\rangle$. The diagonalization of this matrix gives three eigenstates of different symmetries: an antisymmetric doublet ground state $\widetilde{\Psi}_{DA}^{ABC}$, a symmetric doublet $\widetilde{\Psi}_{DS}^{ABC}$, and an antisymmetric quartet $\widetilde{\Psi}_{QA}^{ABC}$. These states are the projections of the three states of the superblock to be identified,

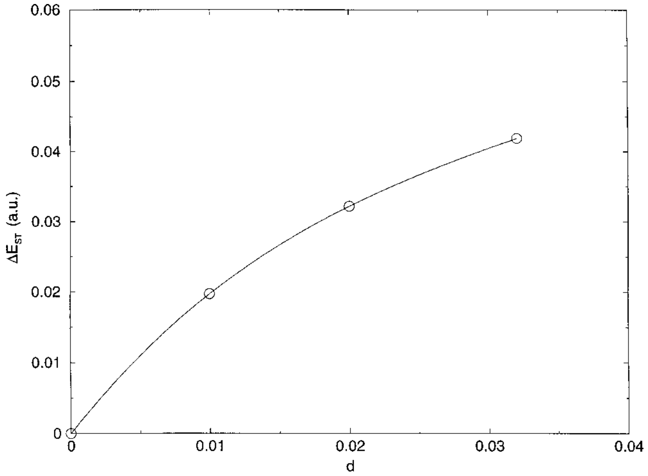

FIG. 4. Extrapolated values of the first excitation energies (in a.u.) of the polyacetylene chain when $N_T$ tends to infinity, as a function of the bond-length alternation parameter $d$ (in Å).

$$|\tilde{\Psi}^{ABC}_{DA}\rangle = \sqrt{\tfrac{2}{3}}|a\overline{b}c\rangle - \frac{1}{\sqrt{6}}(|\overline{a}bc\rangle + |ab\overline{c}\rangle), \tag{46}$$

$$|\tilde{\Psi}^{ABC}_{DS}\rangle = \frac{1}{\sqrt{2}}(|\overline{a}bc\rangle - |ab\overline{c}\rangle), \tag{47}$$

$$|\tilde{\Psi}^{ABC}_{QA}\rangle = \frac{1}{\sqrt{3}}(|\overline{a}bc\rangle + |a\overline{b}c\rangle + |ab\overline{c}\rangle). \tag{48}$$

Once the corresponding states are identified, one can extract the three effective interactions by replacing the solutions $E$ of

$$\det(\mathbf{H}^{\mathrm{eff}} - E\mathbf{I}) = \mathbf{0}$$

by the three corresponding eigenvalues $E^{ABC}_{DA}$, $E^{ABC}_{DS}$, and $E^{ABC}_{QA}$. One finally gets

$$J_1^{(1)} = \frac{E^{ABC}_{QA} - E^{ABC}_{DA}}{3}, \quad J_2^{(1)} = \frac{2E^{ABC}_{QA} - 3E^{ABC}_{DS} + E^{ABC}_{DA}}{6}.$$

We have performed calculations on superblocks made up of $N_T = 9$, 15, and 21 sites. Let us consider what happens at the first iteration when $J^{(0)} = J_2^{(0)}/J_1^{(0)}$ increases from 0 to 0.5. We have concentrated on that domain because the nature of the ground state changes after 0.5 and the definition of a new model space would be necessary beyond that value. For a given value of $N_S, J_1^{(1)}$ depends weakly on $J^{(0)}$ while $J_2^{(1)}$ increases. When the number of sites per block increases, they both tend to zero for small values of the initial ratio $J^{(0)}$, while they seem to converge to a finite value for larger values of this ratio. Unfortunately, we did not manage to get any infinite-size estimates for both couplings from the BST extrapolation algorithm. The ratio $J^{(1)} = J_2^{(1)}/J_1^{(1)}$ as a function of $J^{(0)}$ presents an interesting behavior, as may be seen in Fig. 6. For each value of $N_S$, the distance of the corresponding curve to the straight line of slope 1 goes through a minimum around $J^{(0)} \simeq 0.24$ and this distance decreases when $N_S$ increases. The three values of $J^{(0)}$ giving the minimal distance are reported in Table III. An extrapolation of the position of the closest contact $J_c^{(0)}$ when $N_S$ increases has been performed using the BST algorithm. The estimated asymptote $J_c^{(0)} = 0.241\,915$ (with a minimal error $\epsilon = 5 \times 10^{-7}$ and a value $\omega = 2.362$) compares quite well with the accurate value $J_c = 0.241\,167$.[31] The minimal difference $J^{(1)} - J^{(0)}$ decreases slowly (as $N_S^{-0.25}$) when $N_S$ increases. One may therefore expect that the extrapolated $J^{(1)} = F(J^{(0)})$ curve will present an accumulation point at $J_c^{(0)}$. This point will be attractive when one comes from a lower value of the ratio and repulsive when starting from a larger value. Starting the iteration procedure from a value $J^{(0)} < J_c^{(0)}$, an infinite number of iterations is required to reach the accumulation point.

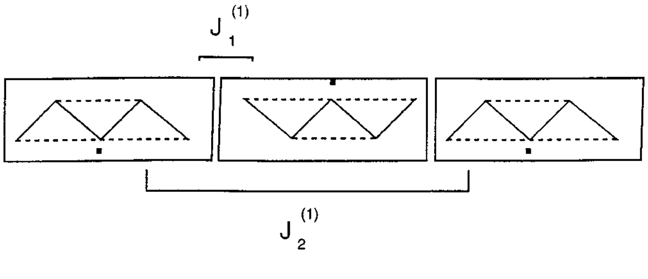

FIG. 5. Example of a trimer (15-sites) superblock for the study of a frustrated spin chain.

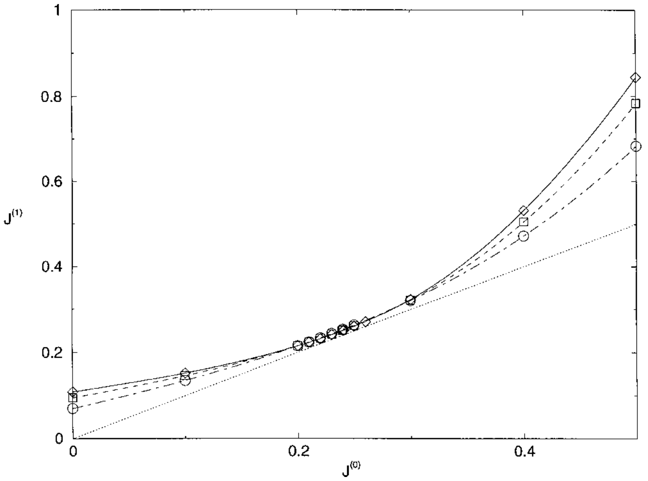

FIG. 6. 1D spin frustrated chain: effective couplings $J^{(1)} = J_2^{(1)}/J_1^{(1)}$ obtained at the first iteration as a function of the initial ratios $J^{(0)} = J_2^{(0)}/J_1^{(0)}$ for different sizes of the blocks. The circles are used for $N_S = 3$, the squares for $N_S = 5$, and the diamonds for $N_S = 7$. The dotted line is a straight line of slope 1.

TABLE III. Critical ratios of the NNN and NN couplings obtained at the first iteration of the RG transformation for several block sizes and their infinite-size estimate, for the frustrated 1D chain.

| Block size | 3 | 5 | 7 | ∞ estimate |
|---|---|---|---|---|
| $J_c^{(0)}$ | 0.233 55 | 0.239 35 | 0.240 75 | 0.241 91 |

At each step the new value of $J_1^{(n+1)}$ is obtained by multiplying $J_1^{(n)}$ by the value of $J_1^{(1)}$ (which is always smaller than 1) corresponding to a value of $J^{(0)}$ equal to $J^{(n)}$,

$$J_1^{(n+1)} = J^{(1)}_{1_{J^{(n)}}} \times J_1^{(n)}.$$

The effective interactions decrease at each iteration leading to a zero value of $J_1^{\infty}$. Consequently the gap defined as the energy difference between the quartet and the lowest doublet $\Delta E_{DQ} = 3J_1^{\infty}$ is zero.

Starting from a $J^{(0)}$ value greater than the critical one, a few iterations lead outside of the studied domain. The converged value of $J_1^{\infty}$ would be obtained from the next accumulation point. Unfortunately, to get the new accumulation point, it would be necessary to define a different model space (this one being irrelevant beyond $J^{(0)} = 0.5$). Nevertheless, since the effective couplings $J_1^{(1)}$ seem to converge to a finite value when $N_s$ increases, a finite gap is expected.

## IV. CONCLUSION

This work proposes an improvement of the numerical real-space renormalization-group method. It first proceeds through the exact treatment of a finite-size system, which may be divided into a few blocks. Then one restricts the Hilbert space to products of the lowest eigenstates of these blocks. At the next iteration, these blocks are considered as the new sites of the system and the procedure is repeated. The main difference with the traditional RSRG method consists in the determination of an effective interaction between the selected eigenstates of the blocks. Treating exactly a dimer or a trimer of blocks, it becomes possible, according to Bloch's formalism, to define an effective Hamiltonian, having one-body and two-body (and eventually *n*-body) interactions where the bodies are the blocks in their selected eigenstates. At this stage, it is possible to check the relevance of the chosen model space by calculating the projections on it of the interesting eigenstates of the superblock. The numerical advantage of this procedure (i.e., of the substitution of the Hamiltonian interactions by renormalized interactions) is that it takes into account the energetic effect of the neglected eigenstates of the blocks. It is possible to show in the model problem of the lowest energy of the monoelectronic Hamiltonian for a 1D chain that this procedure circumvents quite efficiently the fixed boundary condition problem since the effective interaction between the two lowest states of the blocks no longer behaves as $N_S^{-2}$ (where $N_S$ is the dimension of the block) but as $N_S^{-1}$.

Computationally, the bottleneck is the exact treatment of the superblock that attempts to consider blocks of smaller size than the traditional RSRG method. Larger systems could, however, be treated if the space of the Hamiltonian of the superblock were truncated, the neglected terms being, for instance, included by an appropriate dressing of the matrix.[32] It may be worth noting the flexibility of the method, since it presents several degrees of freedom—the topology of the blocks, the number of the selected eigenstates, and the division of the superblock in a variable number of blocks—which govern the nature and complexity of the effective Hamiltonian. Playing with these different factors should also give the opportunity to check the stability of the results.

The method has been tested on several spin problems. We have seen that in the case of the 1D and 2D spin lattices, infinite summations were possible, due to the isomorphism of the Hamiltonian from one iteration to another. In such cases, only one iteration of the procedure was necessary to calculate the converged results.

The formalism of the effective Hamiltonian has been designed to study several states at a time, so that the calculation of gaps is possible, as illustrated in the study of the excitation energies of the 1D dimerized spin chain. Finally, the example of the 1D frustrated spin chain has shown the possible use of the method for the study of phase transition. The domain of application of this method is wide; it can be applied to 2D and 3D systems and its extension to more sophisticated models such as the Hubbard or the $t$-$J$ model would be easy and not computationally more demanding. It would be worthwhile to use the eigenstates of the blocks' reduced density matrix to define the model space $S$ instead of the eigenstates of the blocks, as done in the DMRG method.

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