

## Real-space renormalization-group studies of low-dimensional quantum antiferromagnets

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We study the ground state of one- and two-dimensional (square-lattice) spin- $\frac{1}{2}$  quantum antiferromagnets using a numerical real-space renormalization-group (RG) approach. In our RG approach we consider blocks of various sizes but with an odd number of sites; we retain only the doublet ground state and we integrate out the higher-energy states by means of second-order quasidegenerate perturbation theory. That is, we assume that the role of the excited states of a block, in the RG iteration process, is to renormalize the effective coupling parameters between blocks. We compute the ground-state energy of a spin- $\frac{1}{2}$  linear chain for various block sizes and find close agreement with the Bethe-ansatz exact solution. In the case of the spin- $\frac{1}{2}$  square-lattice quantum antiferromagnet, the obtained ground-state energy is in reasonable agreement with the available numerical estimates.

### I. INTRODUCTION

In order to understand a wide variety of cooperative physical phenomena, one needs to resort to various classical or quantum lattice models that capture certain important features of the materials where such phenomena occur. Even though these models describe only certain aspects of the materials and even though most of the complexity of the various components of the physical system is neglected, one still needs to invent methods to find exact or approximate, but reliable solutions to them.

Quantum spin models, such as the Heisenberg antiferromagnet on regular lattices or lattices with frustration and the Hubbard or the  $t$ - $J$  models (which have been at the center of the theoretical studies during the last five years), present particular difficulties especially when they involve lattice fermions. Exact solutions for these models are only available in some one-dimensional (1D) or limiting cases. In two or higher dimensions, one has been, so far, limited to either approximate analytical and semianalytical treatments (which in most cases involve uncontrollable approximations) or to numerical techniques. The main numerical techniques used are Monte Carlo simulations and exact diagonalizations on finite lattices. The latter procedures are limited by computer memory and CPU time constraints, and since the number of states of the Hilbert space increases faster than exponentially with the lattice size, only calculations on very-small-size lattices are available. Monte Carlo methods, on the other hand, have been very useful in cases of quantum antiferromagnets on nonfrustrated lattices. However, when one has to take into account fermions, such as in the case of the  $t$ - $J$  or the Hubbard models,

quantum Monte Carlo procedures are seriously hindered by the well-known “minus”-sign problem and their applicability is also limited to very-small-size lattices. The technique is hindered even on pure spin systems if one cannot change the basis of the Hilbert space in order to make all the off-diagonal matrix elements of the Hamiltonian negative (such as on a triangular lattice).

The renormalization-group (RG) approach has been successfully applied to the case of classical spin systems and in field theory.<sup>1,2</sup> There have been both analytical formulations where the  $\beta$  function is calculated in perturbation theory and numerical implementations (with schemes such as real-space block-spin transformation or Monte Carlo RG transformations). The idea behind this approach—namely, that, if one is interested in phenomena of a definite energy scale, the higher, nonrelevant energy degrees of freedom can be integrated out in small steps (so that the approximations introduce very small errors)—is very attractive. In the above-mentioned quantum spin and fermion models, one is interested in extracting information at energy scales significantly smaller than the original energy scales entering in the model. For example, one may be interested in low-energy excitations or in pairing in models such as the  $t$ - $J$  or the Hubbard model. This may occur at an energy scale of a fraction of the antiferromagnetic coupling and of the hopping energy scale, and it is much smaller than the Coulomb repulsion energy scale entering in the Hubbard model. Thus, an appropriate RG method may be a promising method to study such low-energy phenomena.

There are previous attempts using real-space (RS) first-order renormalization-group transformations to study quantum spin systems. In its simplest level of

approximation, where only the lowest-energy state is retained in each iteration while the effect of the higher-energy degrees of freedom are neglected, the approach does not provide good ground-state energy estimates.<sup>3</sup> There is a more sophisticated attempt where these high-energy degrees of freedom are integrated out by a diagonalization procedure,<sup>4</sup> and as can be expected this procedure gives much better results.

In the present paper we investigate two directions of improving the RSRG calculations: First, we study the convergence of the RSRG approach by increasing the size of the block in the block-spin transformation; second, we take into account the excited states within a block by integrating them out through a second-order quasidgenerate perturbation theory<sup>5</sup> (QDPT). We shall apply the procedure to the cases of one- and two-dimensional (2D) spin- $\frac{1}{2}$  quantum antiferromagnets. The solutions obtained are in good agreement with the exact Bethe-Hulthen ansatz<sup>6</sup> for the 1D system and with reliable numerical estimates for the 2D square-lattice case.<sup>7</sup> The next section details the renormalization procedure used in this paper; the results for the ground-state energy are discussed in Sec. III. In Sec. IV we calculate the spin-spin correlation function, while conclusions are given in the last section.

## II. METHOD

Let us first start from the Hamiltonian for a Heisenberg antiferromagnet,

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

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$$H^{(n)} = E^{(n)} \sum_i \sum_{s=\pm 1/2} c_{i,s}^{(n)\dagger} c_{i,s}^{(n)} + \sum_{\langle ij \rangle} \left\{ \langle \uparrow\uparrow | H_e^{(n)} | \uparrow\uparrow \rangle (c_{i\uparrow}^{(n)\dagger} c_{i\uparrow}^{(n)} c_{j\uparrow}^{(n)\dagger} c_{j\uparrow}^{(n)} + c_{i\downarrow}^{(n)\dagger} c_{i\downarrow}^{(n)} c_{j\downarrow}^{(n)\dagger} c_{j\downarrow}^{(n)}) \right. \\ \left. + \langle \uparrow\downarrow | H_e^{(n)} | \uparrow\downarrow \rangle (c_{i\uparrow}^{(n)\dagger} c_{i\uparrow}^{(n)} c_{j\downarrow}^{(n)\dagger} c_{j\downarrow}^{(n)} + c_{i\downarrow}^{(n)\dagger} c_{i\downarrow}^{(n)} c_{j\uparrow}^{(n)\dagger} c_{j\uparrow}^{(n)}) \right. \\ \left. + \langle \uparrow\downarrow | H_e^{(n)} | \downarrow\uparrow \rangle (c_{i\uparrow}^{(n)\dagger} c_{i\downarrow}^{(n)} c_{j\downarrow}^{(n)\dagger} c_{j\uparrow}^{(n)} + c_{i\downarrow}^{(n)\dagger} c_{i\uparrow}^{(n)} c_{j\uparrow}^{(n)\dagger} c_{j\downarrow}^{(n)}) \right\}. \quad (3)$$

In the first iteration  $H^{(0)} = H$ ,  $E^{(0)} = 0$ , and  $\langle \uparrow\uparrow | H_e^{(0)} | \uparrow\uparrow \rangle = J/4$ ,  $\langle \uparrow\downarrow | H_e^{(0)} | \uparrow\downarrow \rangle = -J/4$ ,  $\langle \uparrow\downarrow | H_e^{(0)} | \downarrow\uparrow \rangle = J/2$  in the formulation of the Heisenberg Hamiltonian given by Eq. (1), while if we use the equivalent Hamiltonian given by Eq. (2) these matrix elements are, respectively, 0,  $-J/2$ , and  $J/2$ . Let us now divide the infinite lattice into nonoverlapping equivalent blocks of  $N_s$  sites (the criteria for the choice of the blocks will be detailed later).  $H^{(n)}$  can be rewritten as

$$H^{(n)} = \sum_k \bar{H}_k^{(n)} + \sum_{\langle kl \rangle} \bar{H}_{kl}^{(n)}, \quad (4)$$

where  $\mathbf{S}_i$  is the spin operator for the site  $i$  and the sum is over all nearest-neighbor pairs  $i, j$ . An equivalent representation for the case of spin- $\frac{1}{2}$  operators can be built from local singlets:

$$H = -\frac{J}{2} \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger) (c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow}), \quad (2)$$

where  $c_{i\uparrow}^\dagger$  and  $c_{i\uparrow}$  are the usual fermion creation and annihilation operators of an up spin on site  $i$ . This expression differs from the former one by a shift of the zero energy by the energy of the ferromagnetic state.

### A. Description of the RG method

The RG method is an iterative procedure where, at each iteration  $n$ , the infinite lattice is divided in equivalent nonoverlapping blocks of sites and these blocks are associated with the “supersites” constituting the lattice of the next iteration. An effective Hamiltonian  $H^{(n+1)}$ , computed from the knowledge of the Hamiltonian of the  $n$ th iteration  $H^{(n)}$ , describes the interactions between these “supersites.”

Assuming that we are at the iteration  $n+1$ , the renormalization procedure consists of constructing the effective Hamiltonian  $H^{(n+1)}$  from  $H^{(n)}$ . This is done in the following steps.

#### 1. First step

The Hamiltonian  $H^{(n)}$  has the following form:

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where the indices  $k$  and  $l$  now stand for blocks (defined as previously explained), the first sum being over all blocks and the second sum being over adjacent blocks,

$$\bar{H}_k^{(n)} = E^{(n)} \sum_{i \in k} \sum_{s=\pm 1/2} c_{i,s}^{(n)\dagger} c_{i,s}^{(n)} + \sum_{\langle ij \rangle, i, j \in k} H_{ij}^{(n)}, \quad (5)$$

$$\bar{H}_{kl}^{(n)} = \sum_{\langle i, j \rangle, i \in k, j \in l} H_{ij}^{(n)}, \quad (6)$$

and

$$H_{ij}^{(n)} = \langle \uparrow\uparrow | H_e^{(n)} | \uparrow\uparrow \rangle (c_{i\uparrow}^{(n)\dagger} c_{i\uparrow}^{(n)} c_{j\uparrow}^{(n)\dagger} c_{j\uparrow}^{(n)} + c_{i\downarrow}^{(n)\dagger} c_{i\downarrow}^{(n)} c_{j\downarrow}^{(n)\dagger} c_{j\downarrow}^{(n)}) + \langle \uparrow\downarrow | H_e^{(n)} | \uparrow\downarrow \rangle (c_{i\uparrow}^{(n)\dagger} c_{i\uparrow}^{(n)} c_{j\downarrow}^{(n)\dagger} c_{j\downarrow}^{(n)} + c_{i\downarrow}^{(n)\dagger} c_{i\downarrow}^{(n)} c_{j\uparrow}^{(n)\dagger} c_{j\uparrow}^{(n)}) \\ + \langle \uparrow\downarrow | H_e^{(n)} | \downarrow\uparrow \rangle (c_{i\uparrow}^{(n)\dagger} c_{i\downarrow}^{(n)} c_{j\downarrow}^{(n)\dagger} c_{j\uparrow}^{(n)} + c_{i\downarrow}^{(n)\dagger} c_{i\uparrow}^{(n)} c_{j\uparrow}^{(n)\dagger} c_{j\downarrow}^{(n)}). \quad (7)$$

## 2. Second Step

Next we diagonalize  $\bar{H}_k^{(n)}$  inside the Hilbert subspace of a block. Let the  $2^{N_s}$  eigenvalues and eigenstates of the block be denoted by  $\epsilon_\nu^{(n)}$  and  $|v_\nu^{(n)}\rangle$ . The blocks should be chosen in such a way that the form of the  $H^{(n)}$  Hamiltonian is conserved. Therefore, for lattices such as the 1D chain and the square lattice, we shall consider blocks with an odd number of sites so that the ground state is a doublet. Thus, we can assign a ‘‘superspin’’ on each block which takes the values  $\pm\frac{1}{2}$  in order to represent the two degenerate components of the ground state of the block. Namely, we can associate its  $S_z = 1/2$  component with an up ‘‘superspin’’ and its  $S_z = -1/2$  component with a down ‘‘superspin,’’ denoted by  $|\uparrow\rangle$  and  $|\downarrow\rangle$ . We define the associated ‘‘superparticle’’ creation and annihilation operators  $c_{i,s}^{(n+1)\dagger}$  and  $c_{i,s}^{(n+1)}$ , which by acting on the vacuum create or destroy a ‘‘superparticle’’ composed of one of the  $1/2$  or  $-1/2$  ground-state components, for instance,  $|\uparrow\rangle_i = c_{i\uparrow}^{(n+1)\dagger}|0\rangle$ .

## 3. Third Step

We now need to define the new Hamiltonian  $H^{(n+1)}$ . This Hamiltonian operates in the subspace spanned by the states which are direct products of the above-defined  $|\uparrow\rangle$  and  $|\downarrow\rangle$  states for each block. The reduced Hilbert subspace is spanned by the direct products

$$|\{S_k^z\}\rangle = \bigotimes_k |S_k^z\rangle, \quad (8)$$

where  $k$  is the block index and  $S_k^z = \pm 1/2$  is the total  $z$  component of the spin of the ground state of that block. The remaining part of the Hilbert space, which involves the excited states of the blocks, will be taken into account by QDPT. Namely, we integrate out all the excited states and their role is to renormalize the coupling between the previously defined ‘‘supersites.’’ The Hamiltonian  $H^{(n+1)}$  is of the same form as  $H^{(n)}$ ; namely, the operators  $c_{i,s}^{(n)\dagger}$  and  $c_{i,s}^{(n)}$  should be replaced by  $c_{i,s}^{(n+1)\dagger}$  and  $c_{i,s}^{(n+1)}$  defined in the previous step; in addition,  $E^{(n+1)}$  is the ground-state energy of  $\bar{H}_k^{(n)}$ , while  $H_e^{(n+1)}$  acts on a two-‘‘supersites’’ space only and will be defined below. Let us call  $\bar{H}_e^{(n)}$  the reduction of  $H^{(n)}$  into the space of two adjacent blocks, say,  $k$  and  $l$ ,

$$\bar{H}_e^{(n)} = \bar{H}_k^{(n)} + \bar{H}_l^{(n)} + \bar{H}_{kl}^{(n)}. \quad (9)$$

Let us call  $\mathcal{E}$  the space spanned by the direct products of any pair of states of the blocks  $k$  and  $l$ ;  $\mathcal{S}$  is its subspace composed of direct products of the ground-state components of  $\bar{H}_k^{(n)}$  and  $\bar{H}_l^{(n)}$ , namely, the previously defined ‘‘superspin’’ states. Let us call  $\hat{P}$  the projection operator on  $\mathcal{S}$ , i.e.,

$$\hat{P} = |\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow| + |\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|,$$

and  $\hat{Q}$  the projection operator on  $\mathcal{Q}$ , the complementary space of  $\mathcal{S}$ , i.e.,  $\hat{P} + \hat{Q} = \hat{1}$ .  $H_e^{(n+1)}$  is formed from  $\bar{H}_e^{(n)}$

by means of second-order QDPT, within the model space  $\mathcal{S}$ ,  $\bar{H}_k^{(n)} + \bar{H}_l^{(n)}$  being the zeroth-order Hamiltonian  $H_0^{(n)}$  and  $\bar{H}_{kl}^{(n)}$  the perturbation operator  $V^{(n)}$ . Therefore one has

$$H_e^{(n+1)} = \hat{P}V^{(n)}\hat{P} + \hat{P}V^{(n)}\hat{G}^{(n)}V^{(n)}\hat{P}, \quad (10)$$

where  $\hat{G}^{(n)} = \hat{Q}(E^{(n+1)} - H_0^{(n)})^{-1}\hat{Q}$ .

## 4. Fourth Step

$H_e^{(n+1)}$ ,  $E^{(n+1)}$ ,  $c_{i,s}^{(n+1)\dagger}$ , and  $c_{i,s}^{(n+1)}$  are now known; therefore, by renaming  $\uparrow$  to  $\uparrow$  and  $\downarrow$  to  $\downarrow$ ,  $H^{(n+1)}$  will be defined and has the same form as Eq. (3). One can now go back to step one and iterate the procedure until convergence of the ground-state energy per degree of freedom of the original lattice, i.e.,  $E^{(n)}/(N_s)^n$ .

## B. Application of the method

We are now going to show that the iterations of the RG method can be done formally, i.e., that the diagonalization of  $\bar{H}^{(n)}$  and the computation of the QDPT second-order corrections need to be done only once, for the first iteration. From these results, one can get the results of any other iteration  $n \geq 2$  by a simple equation and therefore the energy at convergence of the RG procedure.

*Lemma.* Because of the invariance of the original Hamiltonian under rotations in the spin space, there are constraints among the matrix elements of  $H_e^{(n+1)}$ . The following property is valid at any iteration  $n$ :

$$\langle\uparrow\uparrow|H_e^{(n)}|\uparrow\uparrow\rangle - \langle\downarrow\downarrow|H_e^{(n)}|\downarrow\downarrow\rangle = \langle\uparrow\downarrow|H_e^{(n)}|\uparrow\downarrow\rangle. \quad (11)$$

This identity is shown in the Appendix. Let us define

$$g^{(n)} = \langle\uparrow\downarrow|H_e^{(n)}|\uparrow\downarrow\rangle \quad \text{and} \quad \alpha^{(n)} = \langle\uparrow\uparrow|H_e^{(n)}|\uparrow\uparrow\rangle. \quad (12)$$

We have

$$\begin{aligned} H^{(n)} &= E^{(n)} \sum_i \sum_{s=\pm 1/2} c_{i,s}^{(n)\dagger} c_{i,s}^{(n)} \\ &+ \alpha^{(n)} \sum_{\langle ij \rangle} \sum_{s=\pm 1/2} c_{i,s}^{(n)\dagger} c_{i,s}^{(n)} c_{j,s}^{(n)\dagger} c_{j,s}^{(n)} \\ &- g^{(n)} \sum_{\langle ij \rangle} (c_{i\uparrow}^{(n)\dagger} c_{j\downarrow}^{(n)\dagger} - c_{i\downarrow}^{(n)\dagger} c_{j\uparrow}^{(n)\dagger}) \\ &\quad \times (c_{i\uparrow}^{(n)} c_{j\downarrow}^{(n)} - c_{i\downarrow}^{(n)} c_{j\uparrow}^{(n)}) \end{aligned} \quad (13)$$

and

$$\bar{H}_k^{(n)} = A^{(n)}\hat{1} + \bar{H}_k^{(n)}, \quad (14)$$

where the constant  $A^{(n)} = E^{(n)}N_s + \alpha^{(n)}N_b$  (where  $N_b$  is the number of bonds in a block) and

$$\begin{aligned} \bar{H}_k^{(n)} &= -g^{(n)} \sum_{\langle ij \rangle} (c_{i\uparrow}^{(n)\dagger} c_{j\downarrow}^{(n)\dagger} - c_{i\downarrow}^{(n)\dagger} c_{j\uparrow}^{(n)\dagger}) \\ &\quad \times (c_{i\uparrow}^{(n)} c_{j\downarrow}^{(n)} - c_{i\downarrow}^{(n)} c_{j\uparrow}^{(n)}). \end{aligned} \quad (15)$$

The eigenvectors of  $\tilde{H}_k^{(n)}$  have the form

$$|v_\nu^{(n)}\rangle_k = \sum_{\{S_i^z\}} C_\nu(\{S_i^z\}) |\{S_i^z\}\rangle_k, \quad (16)$$

where  $|\{S_i^z\}\rangle_k = |S_1^z\rangle_{1,k} |S_2^z\rangle_{2,k} \cdots |S_{N_s}^z\rangle_{N_s,k}$  and  $|S_i^z\rangle_{i,k}$  denotes the two possible ground states  $|\uparrow\rangle_{i,k}$  and  $|\downarrow\rangle_{i,k}$  of the  $i$ th sub-block constituent of the  $k$ th block at the  $n$ th iteration. Note that the coefficients  $C_\nu(\{S_i^z\})$  are independent of iteration  $n$  and the block index  $k$ . This is so because the eigenstates of the Hamiltonians  $H_k^{(n)}$  are independent of the overall scale  $g^{(n)}$ , and thus for all  $n$  and  $k$  the Hamiltonian has the same form. In addition, if  $\epsilon_\nu^{(n)}$  denotes the eigenvalues of  $\tilde{H}_k^{(n)}$  and  $e_\nu$  the eigenvalues of  $\tilde{H}_k^{(n)}$  (in units of  $g^{(n)}$ ), we have

$$\epsilon_\nu^{(n)} = E^{(n)} N_s + \alpha^{(n)} N_b + g^{(n)} e_\nu. \quad (17)$$

Let us denote by  $e_1$  the ground-state energy of  $\tilde{H}^{(0)}$ , and following our earlier introduced notation the ground-state energy  $E^{(n+1)}$  of each block at the  $n+1$  iteration is

$$E^{(n+1)} = E^{(n)} N_s + \alpha^{(n)} N_b + g^{(n)} e_1. \quad (18)$$

Let us recall that

$$\begin{aligned} \alpha^{(n+1)} &= \langle \uparrow\uparrow | \hat{P} V^{(n)} \hat{P} | \uparrow\uparrow \rangle \\ &\quad + \langle \uparrow\uparrow | \hat{P} V^{(n)} \hat{G}^{(n)} V^{(n)} \hat{P} | \uparrow\uparrow \rangle, \\ g^{(n+1)} &= \langle \uparrow\downarrow | \hat{P} V^{(n)} \hat{P} | \downarrow\uparrow \rangle \\ &\quad + \langle \uparrow\downarrow | \hat{P} V^{(n)} \hat{G}^{(n)} V^{(n)} \hat{P} | \downarrow\uparrow \rangle, \end{aligned}$$

where  $|\uparrow\rangle$  and  $|\downarrow\rangle$  are the degenerate ground states of  $\tilde{H}_k^{(n)}$ , and

$$\begin{aligned} V^{(n)} &= \sum_{(i,j) \in \text{block1}, j \in \text{block2}} \left\{ \alpha^{(n)} \sum_{s=\pm 1/2} c_{i,s}^{(n)\dagger} c_{i,s}^{(n)} c_{j,s}^{(n)\dagger} c_{j,s}^{(n)} - g^{(n)} (c_{i\uparrow}^{(n)\dagger} c_{j\downarrow}^{(n)\dagger} - c_{i\downarrow}^{(n)\dagger} c_{j\uparrow}^{(n)\dagger}) (c_{i\uparrow}^{(n)} c_{j\downarrow}^{(n)} - c_{i\downarrow}^{(n)} c_{j\uparrow}^{(n)}) \right\} \\ &= N_l \alpha^{(n)} \hat{1} + g^{(n)} V_0^{(n)}, \end{aligned}$$

where  $N_l$  is the number of bonds between the two blocks  $i$  and  $j$ . We find that

$$\langle \uparrow\uparrow | \hat{P} V^{(n)} \hat{P} | \uparrow\uparrow \rangle = N_l \alpha^{(n)} + g^{(n)} \langle \uparrow\uparrow | V_0^{(n)} | \uparrow\uparrow \rangle,$$

$$\langle \uparrow\downarrow | \hat{P} V^{(n)} \hat{P} | \downarrow\uparrow \rangle = g^{(n)} \langle \uparrow\downarrow | V_0^{(n)} | \downarrow\uparrow \rangle,$$

$$\langle \uparrow\uparrow | \hat{P} V^{(n)} \hat{P} | \mu\nu \rangle = g^{(n)} \langle \uparrow\uparrow | V_0^{(n)} | \mu\nu \rangle,$$

and

$$\langle \uparrow\downarrow | \hat{P} V^{(n)} \hat{P} | \mu\nu \rangle = g^{(n)} \langle \uparrow\downarrow | V_0^{(n)} | \mu\nu \rangle,$$

where at least one out of  $|\mu\rangle \equiv |v_\mu^{(n)}\rangle$  and  $|\nu\rangle \equiv |v_\nu^{(n)}\rangle$  is an excited state of  $\tilde{H}^{(n)}$ . Note that because of the form of  $V_0^{(n)}$  and  $|v_\nu^{(n)}\rangle$  these matrix elements are independent of the iteration and thus we can suppress the index  $n$  from them. On the other hand, from Eq. (18) we obtain

$$\begin{aligned} E^{(n)} - \langle v_\nu^{(n)} | H_0^{(n)} | v_\nu^{(n)} \rangle &= \epsilon_1^{(n)} - \epsilon_\nu^{(n)} = g^{(n)} (e_1 - e_\nu) \\ &= g^{(n)} (\epsilon_1^{(0)} - \epsilon_\nu^{(0)}). \end{aligned}$$

From the last three equations we obtain

$$\hat{P} V^{(n)} \hat{G}^{(n)} V^{(n)} \hat{P} = g^{(n)} \hat{P} \hat{V}_0 \hat{G}^{(0)} V_0 \hat{P}$$

and therefore

$$\alpha^{(n+1)} = N_l \alpha^{(n)} + g^{(n)} \beta^{(1)} \quad (19)$$

and

$$g^{(n+1)} = g^{(n)} g^{(1)}, \quad (20)$$

where

$$\beta^{(1)} = \langle \uparrow\uparrow | \hat{P} V_0 \hat{P} | \uparrow\uparrow \rangle + \langle \uparrow\uparrow | \hat{P} V_0 \hat{G}^{(0)} V_0 \hat{P} | \uparrow\uparrow \rangle.$$

Equation (19) can be transformed as follows to a more convenient form

$$\begin{aligned} \alpha^{(n+1)} &= N_l \alpha^{(n)} + \alpha^{(1)} \frac{g^{(n)}}{g^{(0)}} \\ &= \alpha^{(1)} (N_l)^n \frac{(g^{(1)}/g^{(0)})^{n+1} - 1}{g^{(1)}/g^{(0)} - 1}, \end{aligned} \quad (21)$$

while Eq. (20) is transformed as

$$g^{(n+1)} = g^{(1)} \frac{g^{(n)}}{g^{(0)}} = g^{(0)} \left( \frac{g^{(1)}}{g^{(0)}} \right)^n. \quad (22)$$

From Eqs. (17), (18), (21), and (22) one can derive the renormalized ground-state energy per site:

$$\begin{aligned} E^{(\infty)} &= \alpha^{(0)} \frac{N_b}{N_s} + \sum_{n=0}^{\infty} \frac{e_0}{N_s} g^{(0)} \left( \frac{g^{(1)}}{g^{(0)}} \right)^n + \sum_{n=1}^{\infty} \frac{\alpha^{(n)} N_b}{(N_s)^{n+1}} \\ &= \alpha^{(0)} \frac{N_b}{N_s} + \frac{e_0}{N_s} g^{(0)} \frac{1}{1 - g^{(1)}/g^{(0)} N_s} \\ &\quad + \alpha^{(1)} \frac{N_b}{N_l N_s} \frac{1}{g^{(1)}/g^{(0)} N_l - 1} \\ &\quad \times \left[ \frac{g^{(1)}}{g^{(0)} N_s - g^{(1)}} - \frac{N_l}{N_s - N_l} \right]. \end{aligned} \quad (23)$$

Thus, with our approach, we only have to carry out the diagonalization of one block and the second-order QDPT only for the first iteration. After  $g^{(1)}$  and  $\alpha^{(1)}$  are determined, the ground-state energy can be calculated from Eq. (23).

The main difficulty of the RSRG approach is associated with the calculation of the series of the effective Hamil-

tonian. Mattis and Pan have used first-order QDPT,<sup>3,8</sup> i.e., they took into account only the direct coupling between blocks, but all processes in which a block can be in an excited state are ignored. Zivković *et al.*<sup>4</sup> exactly diagonalize  $H_e^{(n)}$  and extract the effective Hamiltonian from the singlet ground state and the lowest triplet excited state. This method takes into account the processes where two blocks can excite one another by interacting with each other. As could be expected, it gives much better results than the preceding one. However, the size of the matrix to diagonalize is growing as  $\binom{2N_s}{N_s}$ . The diagonalization is therefore a procedure which requires a CPU time which scales with the block's size  $N_s$  as  $\binom{2N_s}{N_s}^2$  and thus suffers from computer time and memory constraints. Our method, however, takes into account the role of the excited states by quasidegenerate perturbation theory up to second order as outlined above. The CPU time, in our method, scales only as the square of the number of excited states in a box, i.e.,  $\binom{N_s}{N_s/2}^2$ .

### III. RESULTS

In this section we present results for the 1D chain and the 2D square lattice for several values of  $N_s$  within first- and second-order RSRG theory. The spin- $\frac{1}{2}$  antiferromagnetic Heisenberg Hamiltonian has been used in the formulation given in Eq. (2).

#### A. 1D chain

Calculations on the 1D chain have been made with different block sizes:  $N_s = 3, 5, 7$ , and 9 sites. In our units the exact Bethe-Hulthen value for the ground-state energy per site is  $-\ln 2$ .

Figure 1 gives the energy obtained at convergence of the renormalization procedure as a function of the num-

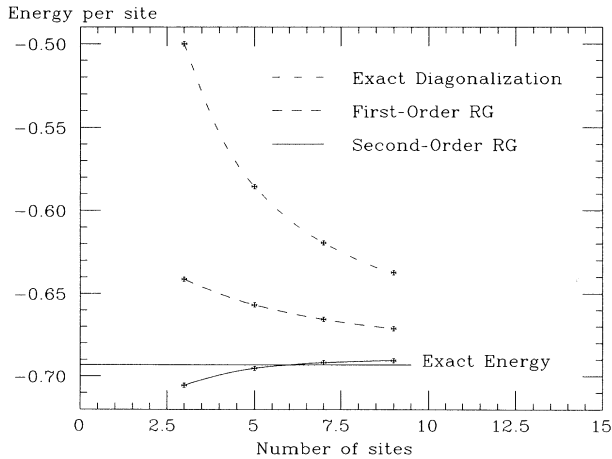


FIG. 1. Renormalized energy per site of a linear chain as a function of the number of sites ( $N_s$ ) in a unit block. The energy is given in units of J. The exact Bethe-Hulthen value is  $-\ln 2$ . Zeroth-order RG energy (exact diagonalization of the unit block) (dotted curve), first-order RG energy (dashed curve), and second-order RG energy (solid curve).

ber of sites,  $N_s$ , in the unit block. Note that the inclusion of the second-order corrections significantly improves the results; namely, going from the first order to the second the error on the estimate of the ground-state energy improves from 7.48% to  $-1.79\%$  on the three-site block. On the nine-site block, the improvement is even better since the relative error improves from 3.17% to 0.38% by including the second-order corrections. While the first-order energy decreases slowly towards the exact value, the second-order energy approaches the exact solution in an oscillating way, reaching an error of less than 0.4% by including five sites only in each block. However, the convergence as a function of  $N_s$  is very slow and calculations on boxes of seven or nine sites do not provide significant improvements.

The following extrapolation of the computed values improves the results significantly and gives a relative error of 0.052%. The extrapolation is done using a  $\chi^2$  procedure. The minimized  $\chi^2$  function is

$$\chi^2 = \sum_{N_s=3,5,7,9} \{ N_s^6 [f_1(N_s) - E_1(N_s)]^2 + N_s^8 [f_2(N_s) - E_2(N_s)]^2 \}, \quad (24)$$

where  $E_1(N_s)$  is the first-order and  $E_2(N_s)$  is the second-order renormalized energy and

$$f_1(N_s) = E_\infty + \alpha_1/N_s + \beta_1/N_s^2, \quad (25)$$

$$f_2(N_s) = E_\infty + \alpha_2/N_s + \beta_2/N_s^2 + \gamma_2/N_s^3.$$

Namely, we have assumed that the corrections to the ground-state energy estimates obtained by a first- or second-order RG for finite block size  $N_s$  is a polynomial in  $1/N_s$ . The coefficients are different for a first- or second-order RSRG, while the constant which corresponds to  $N_s = \infty$  is the same for both methods: If the block size is infinite, there should be no perturbative corrections.

The remaining error made on  $E_1(N_s)$  is then of order  $1/N_s^3$ , while the error on  $E_2(N_s)$  is of order  $1/N_s^4$ . The weighting factors  $N_s^6$  and  $N_s^8$  in  $\chi^2$  are there to ensure that the errors on  $E_1$  and  $E_2$  as a function of  $N_s$  are independent. The minimization of  $\chi^2$  gives  $E_\infty = -0.692785$ ,  $\alpha_1 = -0.1067375$ ,  $\beta_1 = 0.084772$ ,  $\alpha_2 = -0.039098$ ,  $\beta_2 = 0.304412$ , and  $\gamma_2 = -0.3909315$  (all these quantities are expressed in units of J).

#### B. 2D square lattice

We have applied both first-order and second-order renormalization procedures for the square infinite lattice using a nine-site ( $3 \times 3$ ) unit block. Figure 2 shows the convergence of the ground-state energy as a function of the number of RG iterations. One can see that the convergence is fairly fast, the limit being reached in four or five iterations. The first-order renormalization energy is  $E_1 = -1.0592$  J (see also Refs. 9 and 8), while the second-order renormalization energy is  $E_2 = -1.15465$  J. The extrapolated estimate obtained from a number of reliable calculations reviewed in Ref. 7 is  $-1.1692$  J. Note that while the first-order energy is underestimated, the

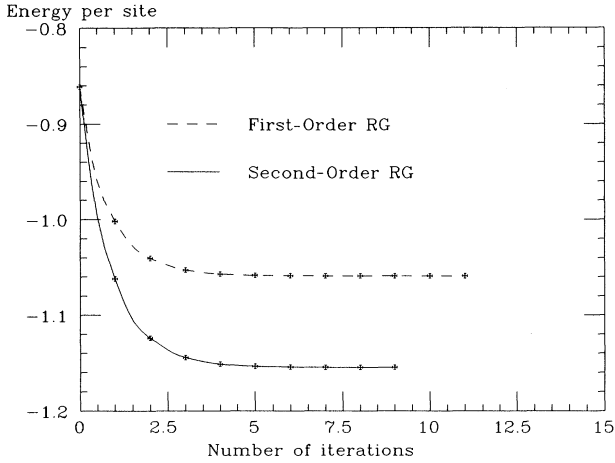


FIG. 2. Energy per site of a square lattice as a function of the RG iterations. The energy is given in units of  $J$ . First-order RG energy (dashed curve) and second-order RG energy (solid curve).

second-order energy is within the range of other estimations.

#### IV. SPIN-SPIN CORRELATIONS

The existence of long-range order in spin systems can be established by calculating the spin-spin correlation

function in the limit of infinite distance. In this section we shall evaluate the correlation function  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  using the RG procedure. The most natural way to do so is to compute at each iteration  $\langle v_1^{(n)} | \mathbf{S}_i \cdot \mathbf{S}_j | v_1^{(n)} \rangle$ . Let us first note that this expression corresponds to the correlation function of the first-order RSRG procedure. The second-order RSRG method would give the following expression for the spin-spin correlation function:  $\langle v_1^{(n)} | \mathbf{S}_i \cdot \mathbf{S}_j \Omega | v_1^{(n)} \rangle$ , where  $\Omega$  is the second-order QDPT wave operator.

As we have shown both the first- and second-order RSRG approaches preserve the form of the Hamiltonian and the coefficients  $C_\nu(\{S_i^z\})$  of the wave function are the same as long as the configuration  $\{S_i^z, i = 1, N_s\}$  of a set of  $N_s$  blocks of the  $n$ th iteration and of a set of  $N_s$  “superblocks” of the next iteration are the same.

We wish to calculate the correlation function between the sites  $i$  and  $j$ . Let  $\mathcal{N}_{ij}$  be the number of the iterations needed such that the sites  $i$  and  $j$  of the original lattice are included in the same block, for the first time. Depending on the relative values of  $\mathcal{N}_{ij}$  and  $n$ , three cases appear.

(1)  $n < \mathcal{N}_{ij}$ . The sites  $i$  and  $j$  belong to different blocks  $k$  and  $l$ . Therefore, they are not yet correlated.

(2)  $n = \mathcal{N}_{ij}$ . Let us suppose that  $k$  and  $l$  are the blocks to which sites  $i$  and  $j$  belong at the  $n-1$  iteration. Let the two ground-state components be denoted by  $|v_1^{(n)}\rangle$  and  $|\bar{v}_1^{(n)}\rangle$ , which are, respectively, characterized by values  $1/2$  and  $-1/2$  of the total  $z$  component of the spin. We find that

$$\begin{aligned} \langle v_1^{(n)} | \mathbf{S}_i \cdot \mathbf{S}_j | v_1^{(n)} \rangle &= 4 \langle v_1^{(n)} | S_k^z S_l^z | v_1^{(n)} \rangle \langle v_1^{(n-1)} | S_i^z | v_1^{(n-1)} \rangle \langle v_1^{(n-1)} | S_j^z | v_1^{(n-1)} \rangle \\ &\quad + \frac{1}{2} \langle v_1^{(n)} | S_k^+ S_l^- | v_1^{(n)} \rangle \langle v_1^{(n-1)} | S_i^+ | \bar{v}_1^{(n-1)} \rangle \langle \bar{v}_1^{(n-1)} | S_j^- | v_1^{(n-1)} \rangle \\ &\quad + \frac{1}{2} \langle v_1^{(n)} | S_k^- S_l^+ | v_1^{(n)} \rangle \langle \bar{v}_1^{(n-1)} | S_i^- | v_1^{(n-1)} \rangle \langle v_1^{(n-1)} | S_j^+ | \bar{v}_1^{(n-1)} \rangle, \end{aligned} \quad (26)$$

where  $S_k^z$  is the  $z$  component of the spin operator acting on the supersite  $k$  at the  $n-1$  iteration, i.e.,  $2S_k^z \equiv c_{k\uparrow}^{(n-1)\dagger} c_{k\uparrow}^{(n-1)} - c_{k\downarrow}^{(n-1)\dagger} c_{k\downarrow}^{(n-1)}$ . Similarly,  $S_k^+$  is the spin raising operator of the supersite  $k$ , i.e.,  $S_k^+ \equiv c_{k\uparrow}^{(n-1)\dagger} c_{k\downarrow}^{(n-1)}$  and  $S_k^- \equiv c_{k\downarrow}^{(n-1)\dagger} c_{k\uparrow}^{(n-1)}$ .

(3)  $n > \mathcal{N}_{ij}$ . Now both sites  $i$  and  $j$  belong to the same block  $k$  of the preceding iteration; therefore  $\mathbf{S}_i \cdot \mathbf{S}_j$  is an operator acting only on a “supersite” of iteration  $n$ . We obtain

$$\begin{aligned} \langle v_1^{(n)} | \mathbf{S}_i \cdot \mathbf{S}_j | v_1^{(n)} \rangle &= \langle v_1^{(n)} | c_{k\uparrow}^{(n-1)\dagger} c_{k\uparrow}^{(n-1)} + c_{k\downarrow}^{(n-1)\dagger} c_{k\downarrow}^{(n-1)} | v_1^{(n)} \rangle \langle v_1^{(n-1)} | \mathbf{S}_i \cdot \mathbf{S}_j | v_1^{(n-1)} \rangle \\ &= \langle v_1^{(n-1)} | \mathbf{S}_i \cdot \mathbf{S}_j | v_1^{(n-1)} \rangle. \end{aligned} \quad (27)$$

Thus, the correlation function at any  $n > \mathcal{N}_{ij}$  remains the same with the one at the iteration  $n = \mathcal{N}_{ij}$ .

In addition, if  $k$  is the block to which the site  $i$  belongs at the  $n-1$  iteration, we note that

$$\begin{aligned} \langle v_1^{(n)} | S_i^z | v_1^{(n)} \rangle &= \langle v_1^{(n)} | c_{k\uparrow}^{n-1\dagger} c_{k\uparrow}^{n-1} - c_{k\downarrow}^{n-1\dagger} c_{k\downarrow}^{n-1} | v_1^{(n)} \rangle \langle v_1^{(n-1)} | S_i^z | v_1^{(n-1)} \rangle \\ &= \lambda_z \langle v_1^{(n-1)} | S_i^z | v_1^{(n-1)} \rangle, \end{aligned} \quad (28)$$

$$\begin{aligned} \langle v_1^{(n)} | S_i^+ | \bar{v}_1^{(n)} \rangle &= \langle v_1^{(n)} | c_{k\uparrow}^{n-1\dagger} c_{k\downarrow}^{n-1} | v_1^{(n)} \rangle \langle v_1^{(n-1)} | S_i^+ | \bar{v}_1^{(n-1)} \rangle \\ &= \lambda_+ \langle v_1^{(n-1)} | S_i^+ | \bar{v}_1^{(n-1)} \rangle, \end{aligned} \quad (29)$$

and

$$\begin{aligned} \langle \bar{v}_1^{(n)} | S_i^- | v_1^{(n)} \rangle &= \langle \bar{v}_1^{(n)} | c_{k\downarrow}^{n-1 \dagger} c_{k\uparrow}^{n-1} | v_1^{(n)} \rangle \langle \bar{v}_1^{(n-1)} | S_i^- | v_1^{(n-1)} \rangle \\ &= \lambda_+ \langle \bar{v}_1^{(n-1)} | S_i^- | v_1^{(n-1)} \rangle, \end{aligned} \quad (30)$$

where  $\lambda_z$  and  $\lambda_+$  are independent of  $n$  and of absolute value smaller than 1. Therefore

$$\langle v_1^{(n)} | S_i^z | v_1^{(n)} \rangle = (1/2) (\lambda_0)^n, \quad (31)$$

$$\langle v_1^{(n)} | S_i^+ | \bar{v}_1^{(n)} \rangle = \langle \bar{v}_1^{(n)} | S_i^- | v_1^{(n)} \rangle = (\lambda_+)^n, \quad (32)$$

and  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  tends to zero when  $\mathcal{N}_{ij}$  tends to infinity.

## V. DISCUSSION

The results of the previous section regarding the long-range order are intrinsic to this RG method and independent of the lattice dimension or the specific shape of the lattice under consideration; since the 2D square lattice as well as other lattices allow for antiferromagnetic long-range order within the nearest-neighbor spin-1/2 Heisenberg model, this is an important drawback of the method; namely, it does not reproduce the correct long-range behavior of the spin-spin correlation function. One could ask if using a more sophisticated wave function, such as taking into account the first-order corrections to the wave function at each iteration, would change the evaluation of spin-spin correlations qualitatively.

Nevertheless, the second-order RG procedure predicts ground-state energies in good agreement with other calculations at the price of a simple diagonalization and a second-order perturbation theory calculation on a small-size finite lattice. Another advantage of the method is that its generalization to more sophisticated Hamiltonians, such as the  $t$ - $J$  model, is easy and not much more computationally costly. Simple quantum Monte Carlo (QMC) techniques when applied to the Hubbard or  $t$ - $J$  model are seriously hindered by the well-known “minus”-sign problem. Improved QMC techniques to deal with this problem, such as the Green’s function Monte Carlo (GFMC) method, are very promising and have provided useful results for the  $t$ - $J$  model.<sup>10</sup> The GFMC method, however, is a much more sophisticated stochastic technique, and it requires significantly larger computational time scales. Thus, it will be interesting to apply the present RSRG technique to the  $t$ - $J$  model with holes and such work is in progress. In addition, it is desirable to obtain results with more than one method, for the infinite-size limit regarding questions such as pairing and phase separation in the  $t$ - $J$  model.

When our work on the 1D antiferromagnetic Heisenberg model was completed and we started applying this method to the 2D case we became aware of the work of Ref. 11 where a new RSRG approach was proposed and applied to the 1D tight-binding model, an extremely simple and solvable model. In the above paper the authors suggest that the failure of the zeroth-order RSRG approach is due to the boundary conditions (BC’s) applied. Thus, in zeroth-order RSRG, the ground-state wave function is constructed out of two pieces in which each is

forced to obey the fixed BC’s in the sub-block, and thus going to the next-size block the wave function has almost a node in the middle of the larger block (in the 1D example). They allow for mixed BC’s and they have obtained very accurate results. In the approach proposed in our work, the ground state of the new “superblock” is corrected by the inclusion of the other states via perturbation theory. We have checked that after the inclusion of first-order perturbative corrections in the wave function of the larger block, the corrected wave function is close to the exact one for the tight-binding model considered in Ref. 11. Thus, with our approach one can systematically improve the estimates for the energy of a model by including higher-order corrections.

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## APPENDIX

Let us first consider a two-spin operator  $\hat{O}$  having the following symmetry properties (which are satisfied by  $H_e^n$ ):

$$\begin{aligned} \hat{O} | \uparrow \uparrow \rangle &= \alpha | \uparrow \uparrow \rangle, \\ \hat{O} | \downarrow \downarrow \rangle &= \alpha | \downarrow \downarrow \rangle, \\ \hat{O} | \uparrow \downarrow \rangle &= \beta | \uparrow \downarrow \rangle + \gamma | \downarrow \uparrow \rangle, \\ \hat{O} | \downarrow \uparrow \rangle &= \gamma | \uparrow \downarrow \rangle + \beta | \downarrow \uparrow \rangle. \end{aligned}$$

We shall show that the invariance under spin rotations is equivalent to the property

$$\langle \uparrow \uparrow | \hat{O} | \uparrow \uparrow \rangle - \langle \downarrow \downarrow | \hat{O} | \downarrow \downarrow \rangle = \langle \uparrow \downarrow | \hat{O} | \downarrow \uparrow \rangle. \quad (A1)$$

Let us call  $\hat{\omega}$  the single-spin rotation operator by an angle  $\theta$  around the  $\hat{x}$  axis. Then

$$\hat{\omega} | \uparrow \rangle = \cos \theta | \uparrow \rangle + \sin \theta | \downarrow \rangle$$

and

$$\hat{\omega} | \downarrow \rangle = -\sin \theta | \uparrow \rangle + \cos \theta | \downarrow \rangle$$

and  $\hat{\Omega} = \hat{\omega} \otimes \hat{\omega}$  is the pair-spin rotation operator by the same angle. If the property (A1) is true, we obtain

$$\begin{aligned} \hat{O} \hat{\Omega} | \uparrow \uparrow \rangle &= \alpha [\cos^2 \theta | \uparrow \uparrow \rangle + \sin^2 \theta | \downarrow \downarrow \rangle \\ &\quad + \cos \theta \sin \theta (| \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle)] \\ &= \Omega(\alpha | \uparrow \uparrow \rangle) \end{aligned} \quad (A2)$$

and

$$\begin{aligned}\hat{O}\Omega|\uparrow\downarrow\rangle &= \beta \left[ \cos\theta \sin\theta (|\downarrow\downarrow\rangle - |\uparrow\uparrow\rangle) + \cos^2\theta |\uparrow\downarrow\rangle - \sin^2\theta |\downarrow\uparrow\rangle \right] \\ &+ \gamma \left[ \cos\theta \sin\theta (|\downarrow\downarrow\rangle - |\uparrow\uparrow\rangle) - \sin^2\theta |\uparrow\downarrow\rangle + \cos^2\theta |\downarrow\uparrow\rangle \right] \\ &= \Omega(\beta|\uparrow\downarrow\rangle + \gamma|\downarrow\uparrow\rangle),\end{aligned}$$

which is equivalent to

$$\Omega\hat{O} = \hat{O}\Omega.$$

The reverse proposition is also true, since if  $\omega$  is such that it transforms the  $z$  axis into the  $x$  one, we obtain

$$\Omega|\uparrow\uparrow\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$$

and so

$$\langle\uparrow\uparrow|\Omega^\dagger\hat{O}\Omega|\uparrow\uparrow\rangle = (\alpha + \beta + \gamma)/2 = \alpha,$$

from which it follows that  $\alpha = \beta + \gamma$ , which is the identity (A1).

Note that  $H^{(0)}$  and  $H_e^0$  are both invariant under spin

rotations. Let us suppose that this is also true for  $H^{(n)}$  and  $H_e^n$ . Therefore  $\bar{H}_k^{(n)}$  and  $\bar{H}_{kl}^{(n)}$  are also invariant under spin rotations. We have then

$$\begin{aligned}H_e^{n+1}\Omega &= \hat{P}V^n\hat{P}\Omega + \hat{P}V^n\hat{G}^nV^n\hat{P}\Omega \\ &= \Omega\hat{P}V^n\hat{P} + \Omega\hat{P}V^n\hat{G}^nV^n\hat{P} \\ &= \Omega H_e^{n+1}.\end{aligned}$$

Inserting this in Eq. (3) we obtain

$$H^{(n+1)}\Omega = \Omega H^{(n+1)}.$$

Thus, we conclude that for all  $n$

$$\langle\uparrow\uparrow|H_e^n|\uparrow\uparrow\rangle - \langle\downarrow\downarrow|H_e^n|\downarrow\downarrow\rangle = \langle\uparrow\downarrow|H_e^n|\downarrow\uparrow\rangle.$$

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