Renormalized excitonic method in terms of block excitations: Application to spin lattices

Mohamad Al Hajj, Jean-Paul Malrieu, and Nathalie Guihéry
Laboratoire de Physique Quantique, IRSAMC/UMR5626, Université Paul Sabatier, 118 route de Narbonne, F-31062 Toulouse Cedex 4, France

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Dividing the lattice into blocks with a singlet ground state and knowing the exact low-energy spectrum of the blocks and of dimers (or trimers) of blocks, it is possible to approach the lowest part of the lattice spectrum through an excitonic type effective model. The potentialities of the method are illustrated on the one-dimensional (1D) frustrated chain and the 1/5-depleted square and the plaquette 2D lattices. The method correctly locates the phase transitions between gapped and nongapped phases.

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I. INTRODUCTION

The idea that one may see a periodic lattice as built from interacting blocks of sites, rather than as interacting sites, is computationally and intellectually attractive. Various methods take advantage of this idea in order to perform a scale change. Among them, Wilson's bright proposal of real space renormalization group[1] (RSRG) is certainly the most elegant one, since it can be infinitely iterated and converges asymptotically on meaningful fixed points. In its original version, the RSRG theory consists in a severe truncation of the Hilbert space since only the lowest states of each block are selected at each iteration. The resulting eigenfunction is therefore expanded on the products of the selected block eigenfunctions. While the method works well in the single impurity Kondo problem, it fails for most quantum systems defined on lattices. Recent works have shown that its efficiency can be dramatically improved when one introduces effective interactions between the blocks. The so-called contractor renormalization (CORE) method[2–5] also starts by the exact treatment of blocks of sites, selects a few eigenstates $|I_A\rangle$ in each block A and then defines interblock effective interactions $\langle I_A J_B|H^{\text{eff}}|K_A L_B\rangle$. The calculation of these effective interactions requires the determination of the spectrum of the AB system and the use of the Bloch's theory[6] of effective Hamiltonians. In most applications the size of the blocks remains small, several states per blocks are kept, and three and/or four blocks effective interactions are extracted from the lowest states of the trimers and/or tetramers of blocks spectrum. A specific variant of the method has been proposed by two of the authors under the name of RSRG-EI (Refs. 7–9) (RSRG with effective interactions). This method treats spin lattices by considering blocks with an odd number of sites and a doublet ground state which is the only one to be explicitly selected. The blocks are then considered as quasispins. From the spectrum of dimers or trimers of blocks one may define an interblock Heisenberg Hamiltonian. A proper design of the blocks frequently results in an isomorphism between the original lattice and the lattice of blocks. Hence the process may be iterated, exhibiting critical ratios of the elementary interactions and fixed points. The methodological studies have examined the following dilemma in the search for accuracy. (i) Consider larger blocks and only dimers of blocks (i.e., two-body effective interactions only) or (ii) consider smaller blocks and trimers or tetramers (i.e., three and four blocks interactions). In most cases the former solution is more efficient. Among the methods that are based on a similar philosophy, one may mention the block correlated coupled cluster method[10] which also starts from the product of the ground state in each block and uses the coupled cluster formalism,[11–13] as well as the self-consistent perturbation method.[14] These last two methods do not provide any information on the gaps, while CORE and RSRG-EI give good estimates of them.

The present work presents a method that is also inspired by the scale change concept. The renormalized excitonic method (REM) is focused on a determination of the gap. It starts from the definition of blocks constituted of an even number of sites and presenting a nondegenerate singlet ground state. The blocks may be identical or not, but they must lead to a periodic picture of the lattice in terms of blocks (hence with larger unit cells). The ground state is still built from products of block ground states and the interblock effective interactions are extracted from exact energies of dimers or trimers of blocks, the energy appearing as the sum of block energies plus interaction energies between blocks. The main difference between REM and previous methods concerns the treatment of excited states. The model space involves the states which are obtained by low-energy excitation on a *single* block, the other blocks remaining in their ground state. The excitation may, of course, concern any block. The effective interactions now describe the interaction between an excited state of a specific block and the neighbor blocks ground states and the possible jump of an excitation from one block to an other one. These interactions are still determined through the use of Bloch's theory of effective Hamiltonians. Then, the lattice lowest excitations are treated through an excitonic model that makes use of these effective quantities.

The theory is developed in Sec. II. In Sec. III the efficiency of the method is then illustrated on three spin lattices, namely, the 1D frustrated chain, the 1/5-depleted 2D square lattice, and the 2D plaquette lattice. The three problems exhibit phase transitions (of second and first order) which are satisfactorily treated with the renormalized excitonic method proposed here.

II. METHOD

A. Principle

Let us consider a lattice constituted of blocks $A,B,\ldots$, having a nondegenerate singlet ground state. ψ_A^0 is the ground state for the block A, of Hamiltonian H_A,

$$H_A\psi_A^0 = E_A^0\psi_A^0. \tag{1}$$

The zero-order description of the lattice *ground state* is the product of all blocks ground states

$$\Psi^0 = \prod_A \psi_A^0. \tag{2}$$

The corresponding zero-order energy is additive

$$E^0 = \sum_A E_A^0 \tag{3}$$

but, since the Hamiltonian involves interaction operators between blocks

$$H = \sum_A H_A + \sum_A \sum_{<B} V_{AB}, \tag{4}$$

the mean energy implies interblock interactions

$$\langle\Psi^0|H|\Psi^0\rangle = \sum_A E_A^0 + \sum_A \sum_{<B} \langle\psi_A^0\psi_B^0|V_{AB}|\psi_A^0\psi_B^0\rangle$$

$$= \sum_A E_A^0 + \sum_A \sum_{<B} v_{AB}^0. \tag{5}$$

Here v_{AB}^0 is a first-order interaction energy between blocks A and B.

Solving the AB problem exactly

$$H_{AB}|\Psi_{AB}^0\rangle = (H_A^0 + H_B^0 + V_{AB})|\Psi_{AB}^0\rangle = E_{AB}^0|\Psi_{AB}^0\rangle \tag{6}$$

enables one to define an improved interaction energy v_{AB}

$$v_{AB} = E_{AB}^0 - E_A^0 - E_B^0, \tag{7}$$

which takes into account at all orders the perturbative effect of excitations on A and B, i.e., of the vectors $|\psi_A^i\psi_B^j\rangle$. Then, from the exact treatment of trimers of blocks $H_{ABC}|\Psi_{ABC}^0\rangle = E_{ABC}^0|\Psi_{ABC}^0\rangle$, it becomes possible to define three-body quantities

$$v_{ABC} = E_{ABC}^0 - E_A^0 - E_B^0 - E_C^0 - v_{AB} - v_{BC} - v_{AC}. \tag{8}$$

The generalization of the procedure to many-block interactions would lead to the additive ground-state energy

$$E = \sum_A E_A^0 + \sum_A \sum_{<B} v_{AB} + \sum_A \sum_{<B} \sum_{<C} v_{ABC} + \cdots \tag{9}$$

according to the simplest version of the CORE method.[2,3] Let us notice that the ground state wave function remains the zero-order function Ψ^0 given by Eq. (2).

For the description of the *excited states* a different model space is required. The block A may be either in its ground state or in the lowest excited state (of the desired multiplicity) ψ_A^*, obtained from the eigenequation relative to H_A

$$H_A|\psi_A^*\rangle = E_A^*|\psi_A^*\rangle. \tag{10}$$

One may introduce local excitation T_A^+ and deexcitation T_A operators $|\psi_A^*\rangle = T_A^+|\psi_A^0\rangle$, $|\psi_A^0\rangle = T_A|\psi_A^*\rangle$.

Let us call Δ_A^*, the on-block excitation lowest energy $\Delta_A^* = E_A^* - E_A^0$. The model space S_0^* is constituted of products of one block excited state and ground states on all the other blocks:

$$S_0^* = \{\Psi_I^*\}, \quad \Psi_I^* = T_I^+\Psi^0 = \psi_I^* \prod_{J\neq I} \psi_J^0. \tag{11}$$

We intend to represent the lowest excitations on an ensemble of blocks from the set of locally singly excited configurations of the type Ψ_I^* where the excitation is localized on block I. This will lead to an excitonic treatment of the excitation, ruled by the effective Hamiltonian

$$H^* = \sum_I \Delta E_I^* T_I^+ T_I + \sum_{\langle IJ\rangle} h'_{IJ}(T_I^+ T_J + T_J^+ T_I), \tag{12}$$

where ΔE_I^* is a local excitation energy on block I in the presence of the other blocks in their ground state and h'_{IJ} is an excitation transfer integral between blocks I and J. The eigenvectors of the Hamiltonian will be linear combinations of local excitations

$$\Psi_{\vec{k}}^* = \sum_I \lambda_I^{\vec{k}} \Psi_I^* = \left(\sum_I \lambda_I^{\vec{k}} T_I^+\right)\Psi^0, \tag{13}$$

and the eigenvalues will be collective excitation energies.

The amplitudes of the quantities ΔE_I^* and h'_{IJ} will be obtained from the spectral properties of dimers and trimers of blocks, using the effective Hamiltonian theory. Let us consider first the extraction of information from pairs of interacting blocks.

B. Extraction of information from dimers of blocks

For a dimer AB the ground state is described as $\psi_A^0\psi_B^0$. The model space for the lowest energy excited states is spanned by the two vectors $\psi_A^*\psi_B^0$ and $\psi_A^0\psi_B^*$. The corresponding projector is

$$P_{AB}^* = |\psi_A^*\psi_B^0\rangle\langle\psi_A^*\psi_B^0| + |\psi_A^0\psi_B^*\rangle\langle\psi_A^0\psi_B^*|. \tag{14}$$

If one identifies the two eigenvectors Ψ_{AB}^* and $\Psi_{AB}^{*\prime}$ of eigenenergies E_{AB}^* and $E_{AB}^{*\prime}$

$$H_{AB}|\Psi_{AB}^*\rangle = E_{AB}^*|\Psi_{AB}^*\rangle, \tag{15}$$

$$H_{AB}|\Psi_{AB}^{*\prime}\rangle = E_{AB}^{*\prime}|\Psi_{AB}^{*\prime}\rangle, \tag{16}$$

which have the largest projections onto the model space, it is possible to define an effective Hamiltonian built on the model space and according to Bloch's definition

$$H^{\text{eff}}|P_{AB}^*\Psi_{AB}^*\rangle = E_{AB}^*|P_{AB}^*\Psi_{AB}^*\rangle, \tag{17}$$

$$H^{\text{eff}}|P_{AB}^*\Psi_{AB}^{*\prime}\rangle = E_{AB}^{*\prime}|P_{AB}^*\Psi_{AB}^{*\prime}\rangle. \tag{18}$$

In order to have an hermitian effective Hamiltonian its eigenvectors must be orthogonal. We shall assume that $P_{AB}^*|\Psi_{AB}^{*\prime}\rangle$

is orthogonal or Schmidt orthogonalized to $P^*_{AB}|\Psi^*_{AB}\rangle$. One may write, after normalization,

$$|P^*_{AB}\Psi^*_{AB}\rangle = a|\psi^*_A\psi^0_B\rangle + b|\psi^0_A\psi^*_B\rangle, \tag{19}$$

$$|P^*_{AB}\Psi^{*\prime}_{AB}\rangle = -b|\psi^*_A\psi^0_B\rangle + a|\psi^0_A\psi^*_B\rangle. \tag{20}$$

The spectral definition of H^{eff} leads to the following equations:

$$\langle\psi^*_A\psi^0_B|H^{\text{eff}}|\psi^*_A\psi^0_B\rangle = a^2E^*_{AB} + b^2E^{*\prime}_{AB} = E^*_A + E^0_B + v_{(A^*)B}, \tag{21}$$

$$\langle\psi^0_A\psi^*_B|H^{\text{eff}}|\psi^0_A\psi^*_B\rangle = b^2E^*_{AB} + a^2E^{*\prime}_{AB} = E^0_A + E^*_B + v_{A(B^*)}, \tag{22}$$

$$\langle\psi^*_A\psi^0_B|H^{\text{eff}}|\psi^0_A\psi^*_B\rangle = (E^*_{AB} - E^{*\prime}_{AB})ab = h_{AB}. \tag{23}$$

The terms $v_{(A^*)B}$ ($v_{A(B^*)}$) represent the effective interactions between A^* and B (between A and B^*) and h_{AB} is the effective interaction responsible for the transfer of excitation from A to B which may be significantly different from the direct interaction $h^0_{AB}=\langle\psi^*_A\psi^0_B|H|\psi^0_A\psi^*_B\rangle$. If A and B are identical blocks and if the AB dimer presents an element of symmetry transforming A in to B and vice versa, $|a|=|b|=1/\sqrt{2}$, one eigenvector is an in-phase combination of $\psi^*_A\psi^0_B$ and $\psi^0_A\psi^*_B$, of energy E^{*g}_{AB}, the other one being the out-of-phase combination, of energy E^{*u}_{AB}:

$$P^*_{AB}\Psi^{*g}_{AB} = \frac{1}{\sqrt{2}}(\psi^*_A\psi^0_B + \psi^0_A\psi^*_B), \tag{24}$$

$$H_{AB}|\Psi^{*g}_{AB}\rangle = E^{*g}_{AB}|\Psi^{*g}_{AB}\rangle, \tag{25}$$

$$P^*_{AB}\Psi^{*u}_{AB} = \frac{1}{\sqrt{2}}(\psi^*_A\psi^0_B - \psi^0_A\psi^*_B), \tag{26}$$

$$H_{AB}|\Psi^{*u}_{AB}\rangle = E^{*u}_{AB}|\Psi^{*u}_{AB}\rangle, \tag{27}$$

$$v_{(A^*)B} = v_{A(B^*)} = \frac{1}{2}(E^{*g}_{AB} + E^{*u}_{AB}) - E^*_A - E^0_B, \tag{28}$$

$$h_{AB} = \frac{1}{2}(E^{*g}_{AB} - E^{*u}_{AB}). \tag{29}$$

It is then possible to consider the infinite lattice in which each block is surrounded by nearest-neighbor blocks B with equal or different respective interactions. The ground-state energy is given from Eq. (9)

$$\mathcal{E}_0 = \sum_K E^0_K + \sum_K \sum_{<L} v_{KL}. \tag{30}$$

The local excitation energy appearing in the effective excitonic Hamiltonian Eq. (12) is

$$\Delta E^*_I = E^*_I - E^0_I + \sum_{K\neq I}(v_{K(I^*)} - v_{KI}). \tag{31}$$

It involves the excitation energy of the isolated block $(E^*_I - E^0_I)$ and the modification of the interaction energy between the block I and the other blocks under the excitation of the block I $[\Sigma_{K\neq I}(v_{K(I^*)} - v_{KI})]$. The amplitude of the term h'_{IJ} in Eq. (12) is taken from the two-block problem [Eq. (23)] $h'_{IJ}=h_{IJ}$. The effective Hamiltonian matrix has a near-diagonal structure, similar to that of a tight-binding monoelectronic Hamiltonian. It generates bands which only represent the states of the lattice having large projections onto the vectors Ψ^*_I, i.e., on the intrablocks lowest energy excitations. This description of the lowest-energy states of the lattice should be relevant. If the blocks are identical and engaged in the same interactions of negative sign with their first neighbors, the excitation energy to the lowest $\vec{k}=0$ state should be

$$\Delta^{*\infty}_{\vec{k}=0} = (E^*_I - E^0_I) + \sum_{K\neq I}(v_{K(I^*)} - v_{KI}) + \sum_{K\neq I} h_{IK}. \tag{32}$$

If the KI couples present an element of symmetry transforming K into I, using Eqs. (32) and (28) one obtains

$$\Delta^{*\infty}_{\vec{k}=0} = \Delta^*_I + \sum_K (\Delta^*_{KI} - \Delta^*_I), \tag{33}$$

where $\Delta^*_I = E^*_I - E^0_I$ and $\Delta^*_{KI} = E^{*g}_{KI} - E^0_{KI}$ are excitation energies on the blocks and dimers of blocks, respectively. One notices that the other root E^{*u}_{KI} of the dimer disappears in this expression.

One sees that the derivation leads to a renormalized excitonic method, where the excitation transfer integrals h'_{IJ} are renormalized. The effective interactions include to all orders some indirect processes going through higher-energy (multiple) excitations on neighbor blocks as well as inter-block excitations, as will be shown hereafter. Of course, the results are dependent on the shape and size n of the blocks.

C. Extraction of information from trimers of blocks

It is possible to use the eigenstates of trimers of blocks to extract three-blocks interactions. For a given shape of the elementary blocks one must of course consider the various types of trimers of blocks. While for the ground state the three-block correction is given by Eq. (8), for the excited states the model space involves three vectors. The projector on the model space is

$$P^*_{ABC} = |\psi^*_A\psi^0_B\psi^0_C\rangle\langle\psi^*_A\psi^0_B\psi^0_C| + |\psi^0_A\psi^*_B\psi^0_C\rangle\langle\psi^0_A\psi^*_B\psi^0_C| + |\psi^0_A\psi^0_B\psi^*_C\rangle\langle\psi^0_A\psi^0_B\psi^*_C|, \tag{34}$$

one must identify the three eigenstates of the ABC problem having the largest projections on the model space. Notice that these three states are not necessarily the three lowest ones. Let us call these three states Ψ^*_{ABC}, $\Psi^{*\prime}_{ABC}$, and $\Psi^{*\prime\prime}_{ABC}$ and the corresponding eigenenergies E^*_{ABC}, $E^{*\prime}_{ABC}$, and $E^{*\prime\prime}_{ABC}$. For hermiticity the projected eigenvectors $P^*_{ABC}\Psi^*_{ABC}$, $\Psi^{*\prime\prime}_{ABC}P^*_{ABC}$, and $P^*_{ABC}\Psi^{*\prime}_{ABC}$ are orthonormalized, leading to three vectors Φ^*_{ABC}, $\Phi^{*\prime}_{ABC}$, and $\Phi^{*\prime\prime}_{ABC}$ and from the spectral definition of H^{eff}:

$$H^{\text{eff}}_{ABC} = E^*_{ABC}|\Phi^*_{ABC}\rangle\langle\Phi^*_{ABC}| + E^{*\prime}_{ABC}|\Phi^{*\prime}_{ABC}\rangle\langle\Phi^{*\prime}_{ABC}| + E^{*\prime\prime}_{ABC}|\Phi^{*\prime\prime}_{ABC}\rangle\langle\Phi^{*\prime\prime}_{ABC}|, \quad (35)$$

one may calculate the diagonal matrix elements of H^{eff}_{ABC} and reexpress them as

$$\langle\psi^*_A\psi^0_B\psi^0_C|H^{\text{eff}}_{ABC}|\psi^*_A\psi^0_B\psi^0_C\rangle = E^*_A + E^0_B + E^0_C + v_{(A^*)B} + v_{(A^*)C} + v_{BC} + v_{(A^*)BC}, \quad (36)$$

which defines a three-body interaction $v_{(A^*)BC}$, and revised excitation hopping integrals

$$\langle\psi^*_A\psi^0_B\psi^0_C|H^{\text{eff}}_{ABC}|\psi^0_A\psi^*_B\psi^0_C\rangle = h_{AB} + h_{AB(C)}. \quad (37)$$

The last term represents the effect of C on the hopping between A and B. One also obtains effective hopping between non directly interacting blocks (for instance, A and C through B in a linear ABC configuration). This indirect propagation may proceed, for instance for triplet states, through the process $\psi^*_A\psi^0_B\psi^0_C \leftarrow\rightarrow \psi^*_A\psi^*_B\psi^*_C \leftarrow\rightarrow \psi^0_A\psi^0_B\psi^*_C$. These effective interactions are used in the excitonic treatment.

The matrix elements of the effective excitonic Hamiltonian (12) are

$$\Delta E^*_I = E^*_I - E^0_I + \sum_J (v_{(I^*)J} - v_{IJ}) + \sum_{JK} (v_{(I^*)JK} - v_{IJK}) \quad (38)$$

and

$$h'_{IJ} = h_{IJ} + \sum_K h_{IJ(K)}. \quad (39)$$

In periodic lattices when all blocks are equivalent, the excitation energy for the vector $\vec{k}=0$ (which is not necessarily the lowest one) is

$$\Delta^{*\infty}_{\vec{k}=0} = E^*_I - E^0_I + \sum_J (v_{(I^*)J} - v_{IJ}) + \sum_{JK} (v_{(I^*)JK} - v_{IJK}) + \sum_J \left(h_{IJ} + \sum_K h_{IJ(K)} \right). \quad (40)$$

The method is generalizable to four (and more) blocks. One should however remark that when one increases the number of blocks the identification of the eigenstates having the largest projections onto the model space may become ambiguous. When changing the ratio of the intersite interactions the (say) third best eigenvector may jump from the eigenvector number 3 to the eigenvector number 4, a problem which will be documented below. In such a case the effective Hamiltonian will be a discontinuous function of the intersite interactions, which is a rather unpleasant feature.

D. Comment

Of course, the method is only applicable to the study of gapped systems and to locate the phase transition between a gapped phase and a gapless phase. This limitation is due to the fact that one uses different model spaces for the ground state and for the excited states. The method cannot provide the low energy physics of gapless antiferromagnetic lattices.

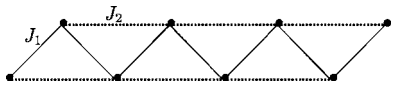

FIG. 1. The nondimerized frustrated 1D chain.

For such phases the method is unable to give a strictly zero gap nor the density of states. As will be shown in the following examples the calculated gap becomes extremely small and in some cases it may be spuriously negative. This limitation (which is not present in the CORE method) should be kept in mind.

III. TEST APPLICATIONS

A. The 1D frustrated spin chain

The 1D antiferromagnetic (AF) spin chain with J_1 spin couplings between nearest-neighbor sites and J_2 couplings (also AF) between next-nearest-neighbor sites (see Fig. 1), is ruled by the Heisenberg Hamiltonian

$$H = 2J_1 \sum_i \vec{S}_i\vec{S}_{i+1} + 2J_2 \sum_i \vec{S}_i\vec{S}_{i+2}. \quad (41)$$

It presents a second order phase transition for $(J_2/J_1)_c = j_c = 0.2411$.[15–17] There is no gap for $J_2/J_1 = j < j_c$ while a finite gap exists beyond this critical ratio. Close to the critical point the gap increases very slowly, presenting an *essential singularity* at j_c. It behaves at this origin[17] as

$$\Delta \simeq \beta \exp \frac{-\alpha}{j - j_c}. \quad (42)$$

Density matrix renormalization group (DMRG) calculations have been reported for this system,[17] as well as analytic treatments.[18] The renormalized excitonic method has been applied to ($n=4$, 6, 8, and 10 sites) blocks, and extrapolated. For a given value of n, the calculated gap $\Delta^{*\infty}(n)$ for the lattice, estimated from Eq. (33), using the $\Delta^*(n)$ and $\Delta^*(2n)$ excitation energies, is dramatically reduced with respect to $\Delta^*(2n)$, due to the cancellation of the (n^{-1}) components of the $\Delta^{*\infty}$ excitation. Actually in such a simple problem $\Delta^{*\infty}(n) = 2\Delta^*(2n) - \Delta^*(n)$. If $\Delta^*(n) = A + Bn^{-1} + Cn^{-2}$,

$$\Delta^{*\infty}(n) = A + C\left(\frac{1}{4n^2} - \frac{1}{16n^2}\right) + \cdots = A + \frac{3C}{16n^2}. \quad (43)$$

From the different calculations of $\Delta^{*\infty}(n)$ it is possible to estimate an extrapolated value of the gap. We have used a polynomial fit

$$\Delta^{*\infty}(n) = a_1 + a_2(n+1)^{-2} + a_3(n+1)^{-3} + a_4(n+1)^{-4}, \quad (44)$$

which gives the results reported in Fig. 2 (somewhat better than a fit in terms of inverse powers of n). One may notice that the extrapolated value of the gap $\Delta^{*\infty} = a_1$ for $j < j_c$ is not strictly zero. The largest error is for $j=0$ where $\Delta^{*\infty} = 0.0068J_1$. This value is within the accuracy of the extrapolation techniques of DMRG (see Fig. 3 of Ref. 17). The calculated gap goes through a minimum at $j=0.24$, close to

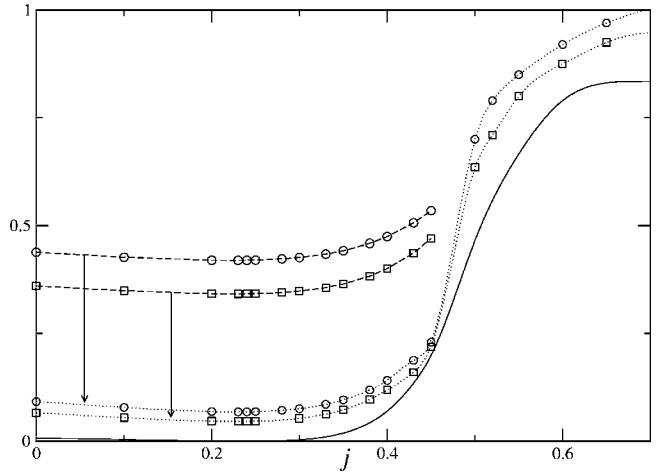

FIG. 2. Dependence of the gap of the frustrated 1D chain on the $j=J_2/J_1$ ratio. --○-- and --□-- direct gaps from 16 and 20 sites segments, ···○··· and ···□··· REM gaps from 8 and 10 sites blocks. The arrows indicate the benefit of the REM treatment. The full line gives the extrapolated gap from REM.

the critical value, where $|\Delta^{*\infty}|=3\times10^{-6}$. It increases for larger values of J_2. Immediately beyond J_{2c} the gap follows the expected law. We found $\alpha=0.21022$, $\beta=0.10253$ for the parameters of Eq. (42). The calculated gap for the Majumdar-Ghosh point ($2J_2=J_1$) is $0.465J_1$, which compares well with the DMRG (Ref. 17) estimate ($0.48J_1$) and the result of an analytic development ($\simeq 0.45J_1$).[18]

B. The 1/5-depleted square 2D lattice

The 1/5-depleted square 2D lattice, built from square plaquettes and octagons (see Fig. 3), was first considered as representing the 2D lattice of the CaV_4O_9 crystal. It appeared later on that next-nearest-neighbor spin couplings are important in this material, but the simple picture, with J_p AF couplings on plaquette bonds and J_d AF couplings between adjacent plaquettes, already presents an interesting physics with three phases. When the plaquettes are weakly coupled, i.e., $J_p/(J_p+J_d)=j>j_c$, one may speak of a plaquette phase and the system is gapped. It is also gapped when the dimers

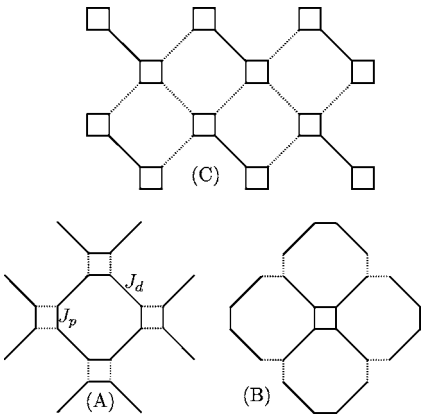

FIG. 3. 1/5-depleted 2D square lattice, various definitions of blocks.

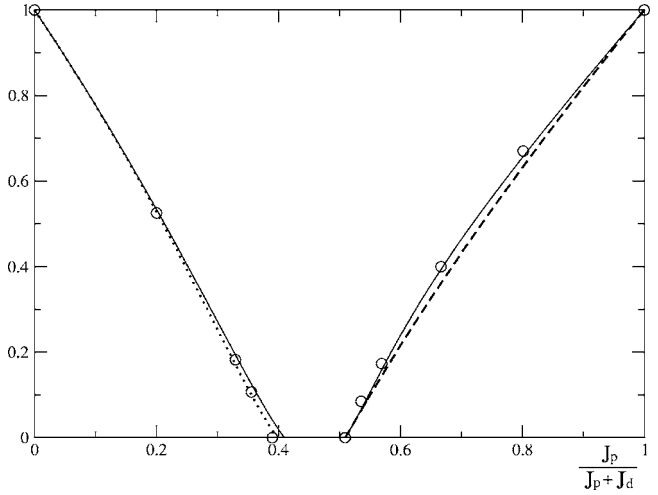

FIG. 4. Gap in the 1/5-depleted 2D square lattice. (—) from octagonal blocks (A), (…) from blocks of type (B), (--) from blocks of type (C), (○) QMC calculations from Ref. 20.

connecting the plaquettes are weakly coupled, i.e., when $j<j_c'$. This phase is called dimer-phase. In between, i.e., for $j_c<J_p/(J_p+J_d)<j_c'$, the lattice keeps a Néel order and this phase is gapless. Several studies, using perturbative expansions[19] or quantum Monte Carlo (QMC) calculations[20] agree on this picture and propose $j_c\simeq 0.4\pm0.01$ and $j_c'\simeq 0.51\pm0.01$. We have tested our method on this problem. The simplest block that one may consider is the octagon [see schema (A) of Fig. 3]. Its ground state is nondegenerate whatever the J_p/J_d ratio. Actually starting from these blocks, REM provides a correct picture of the physics, since the gap disappears between $j_c=0.40967$ and $j_c'=0.50945$ (see Fig. 4). This result is obtained from eight-site blocks.

In order to check wether this excellent agreement was not fortuitous we have introduced next-nearest-neighbor interactions between octagons, applying the formalism of Sec. II C. Two types of trimers (linear and perpendicular) have to be considered. The results appear in Table I, and they deserve the following comments.

The dependence of the gap on the j ratio is almost the same as when working with dimers only. The gapless domain in slightly reduced to the interval $0.39572<j<0.49784$.

The third target vector for the perpendicular trimer (i.e., the third vector presenting the largest projection on the model space) is the third eigenvector (Ψ_3) of the perpendicular trimer problem for $j\leqslant 0.41$ and the fourth (Ψ_4) one for $j>0.41$. This may be seen as a signature for a finite (24 sites) cluster of the vicinity of the phase transition in the periodic lattice. A similar phenomenon is observed for the linear trimer between $j=0.40$ and $j=0.41$. Regarding the Néel-plaquette phase transition, a similar change of the target vectors appears for $0.50<j<0.51$ in the perpendicular trimer superblock. This phenomenon of discontinuity of H^{eff} does not appear when working with dimers only. One might eventually circumvent this problem by taking a weighted energy for the third "root" appearing in the spectral definition of H^{eff}. If P_0 is the projector on the model space $\alpha=\|P_0\Psi_3\|=\langle P_0\Psi_3|P_0\Psi_3\rangle$, $\beta=\|P_0\Psi_4\|=\langle P_0\Psi_4|P_0\Psi_4\rangle$ and if $H_{ABC}|\Psi_3\rangle=E_3|\Psi_3\rangle$, $H_{ABC}|\Psi_4\rangle=E_4|\Psi_4\rangle$, one might define

TABLE I. Calculated spin gap for the 1/5-depleted square lattice as a function of $j=J_p/(J_p+J_d)$.

	gap		number of the third relevant eigenvector	
j	dimers	trimers	linear	perpendicular
0	1.0	1.0	3	3
0.1	0.777541	0.794138	3	3
0.2	0.533681	0.561073	3	3
0.3	0.272110	0.289024	3	3
0.39	0.041669	0.015530	3	3
0.39572	0.028882	0.0	3	3
0.4	0.019637	−0.01160	3	3
0.40967	0.0	−0.03536	4	3
0.41	−0.00068	−0.03610	4	3
0.42	−0.01882	−0.05463	4	4
0.49	−0.03646	−0.02158	4	4
0.49784	−0.02361	0.0	4	4
0.5	−0.01961	0.005945	4	4
0.50945	0.0	0.027081	4	3
0.51	0.001129	0.028707	4	3
0.52	0.024859	0.057802	4	3
0.55	0.105265	0.139275	3	3
0.7	0.463095	0.461658	3	3
0.8	0.654426	0.648198	3	3
0.9	0.831083	0.830046	3	3
1	1.0	1.0	3	3

$E''^{*}_{ABC}=\alpha E_3+\beta E_4$. One may alternatively change the shape of the blocks. A stared eight-site block with four dimer bonds around a plaquette pictured in scheme (B) of Fig. 3 is expected to be relevant for the dimer phase. The gap calculated from these blocks almost coincides with the previously calculated one, with a critical value $j_c=0.40$ (see Fig. 4).

For the plaquette phase we have considered blocks with two plaquettes, as pictured in scheme (C) of Fig. 3. The gap is slightly smaller than from the octagons, but the critical values of disappearance of the gap, $j'_c=0.508$, coincide. We have compared our calculated gaps with the ones reported (in Fig. 2 of Ref. 20) from QMC calculations, and the two methods practically coincide (within the uncertainties of reading of the abovementioned figure).

C. The plaquette lattice

The square type lattice built from interacting phaquettes is characterized by intraplaquette J and interplaquette j AF couplings (see Fig. 5). The properties depend on the $\lambda=j/J$ ratio. For $j=0$, the plaquettes are independent and the lattice is gapped. It is not gapped for the $j=J$ 2D square lattice, and phase transitions are expected to occur for $(j/J)_c=\lambda_c$ and for $(J/j)_c=1/\lambda_c$ (this last relation being due to the intrinsic symmetry between j and J). Several works have been devoted to this problem. Third-order series expansions[21] and QMC calculations[22] suggest that $\lambda_c\simeq 0.55$. Extrapolations of finite

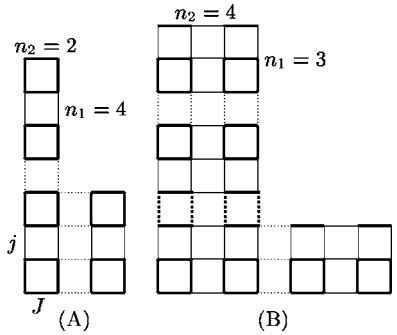

FIG. 5. Definitions of blocks for the study of the plaquette lattice.

size exact diagonalizations[23] fail to give a zero spin gap whatever the value of λ. A recent work has used the CORE method[24] together with order parameter susceptibilities, suggesting a critical behavior between $\lambda=0.5$ and $\lambda=0.6$. The problem of the gap is reexamined here using REM. Two types of blocks have been considered. The *first one* involves one, two or three plaquettes ($n=4$, 8, and 12 sites), fragments of a ladder [see schema (A) of Fig. 5]. There are two types of dimers, collinear or side by side. Let us call ΔE_A the excitation energy of the block and ΔE_{AB} and $\Delta E'_{AB}$ the excitation energies for these dimers. For a block of n_1 sites along the longitudinal direction, n_2 sites along the transverse one, our model leads to the following expression of the gap $\Delta E(n_1,n_2)$:

$$\Delta E(n_1,n_2)=2\Delta E_{AB}(2n_1,n_2)+2\Delta E_{AB}(n_1,2n_2)-3\Delta E_A(n_1,n_2). \tag{45}$$

Figure 6 reports the gap calculated for $n_1=2$, 3, 4 and $n_2=2$. One sees that the gap vanishes when λ tends to 1. An extrapolation is possible in terms of n_1^{-1} and n_1^{-2}, for $n_2=2$,

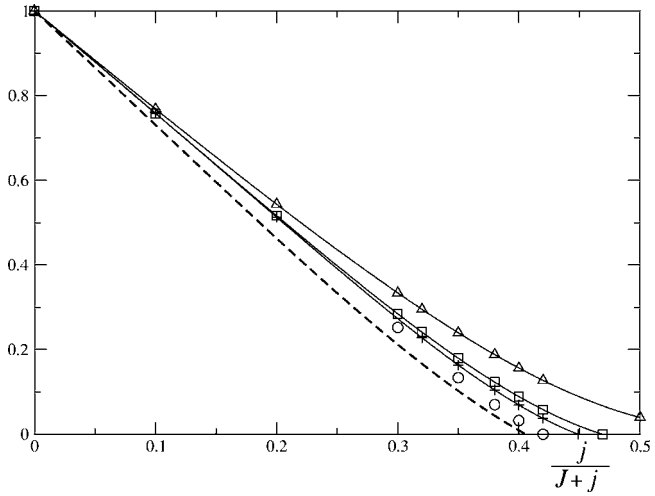

FIG. 6. Singlet-triplet spin gap in the plaquette lattice from 2×2 block (△), 4×2 block (□), 6×2 block (+), 4×3 block (○). Dashed line: extrapolation from $n\times 2$ block.

$$\Delta E(n_1,n_2=cte)=A_0+\frac{A_1}{n_1}+\frac{A_2}{n_1^2}. \tag{46}$$

$\bar{\Delta}E(n_2)=A_0$ is the n_1 extrapolated value of the gap for a fixed value of n_2. Assuming that

$$\Delta E(n_1,n_2)=\left(\alpha+\frac{\beta}{n_1}+\frac{\gamma}{n_1^2}+\cdots\right)\left(\alpha+\frac{\beta}{n_2}+\frac{\gamma}{n_2^2}\cdots\right), \tag{47}$$

$$\Delta E(n_1,n_2)=\bar{\Delta}E+\frac{a_1}{n_1}+\frac{a_1}{n_2}+\frac{a_2}{n_1^2}+\frac{a_2}{n_2^2}+\frac{b}{n_1n_2} \tag{48}$$

one obtains

$$\Delta E(n_1,n_2)=\bar{\Delta}E-\frac{a_2}{2n_1^2}-\frac{a_2}{2n_2^2}-\frac{b}{n_1n_2}. \tag{49}$$

Confronting Eqs. (46) and (49) gives $A_0=\bar{\Delta}E-a_2/2n_2^2$, $A_1=-b/n_2$, and $A_2=-a_2/2$. Hence the final value of the extrapolation gap is $\bar{\Delta}E=A_0-A_2/n_2^2$. Figure 6 reports the so-calculated gap as well as the values $\Delta E(n_1,n_2)$ for $n_2=2$ and $n_1=2,4,6$ as a function of the $j/(J+j)$ ratio. One sees that a gapless phase appears for $n_1>2$. After extrapolation the lattice is found to be gapless for $j/J>2/3=0.666$. The value of λ_c is somewhat larger than the commonly accepted value but it represents a considerable improvement over the extrapolations of finite lattices exact diagonalizations. One may mention that, as a by-product of the present calculations, one obtains, for $j=J$, a value of the gap of the two-leg ladder. The extrapolation leads to $\Delta E=0.47J$, close to the best QMC estimate $(0.50J)$.[25] A *second type* of rectangular blocks have been considered, involving odd numbers of sites in one direction and even numbers in the other one [see schema (B) of Fig. 5]. In such a case there are three types of dimers. These 12-site ($n_1=3$, $n_2=4$) blocks are more compact than the previous ($n_1=6$, $n_2=2$) ones and the calculated gap, which appears in Fig. 6, is somewhat lower. Extrapolation is difficult in this case, due to the difference in the physical nature of the dimers, but the evaluations from different blocks are quite consistent.

IV. CONCLUSION

We have presented a simple method for the study of the gap in gapped periodic lattices. The method rests on the consideration of blocks and a truncation of the Hilbert space to products of a few eigenstates of the blocks as practiced in the RSRG. In the past we have considered $(2n+1)$-site blocks, with spatially nondegenerate doublet ground states, in spin lattices. The blocks can then be seen as $S_z=\pm 1/2$ quasispins. Using the theory of effective Hamiltonians, and the exact spectrum of dimers (or trimers) of blocks, we have proposed to renormalize the interactions between blocks, and the so-obtained variant of CORE (RSRG-EI) happens to keep the conceptual elegance of Wilson's idea while gaining, at a very low cost, numerical accuracy.[7,8]

The present work is closely related but different. It considers blocks with even number of sites, presenting a nondegenerate ground state. Again the exact treatment of the block and of the dimers or trimers of blocks is employed to define block effective energies and interblock effective interactions. However different model spaces are used for the ground state and for the lowest excited states. For the ground state Ψ^0, built from the product of block ground states, the energy is a simple sum of intra and interblock energies. The excited states are linear combinations of locally singly excited functions, products of an excited state on one block by the ground states functions on the other blocks. This space is a small fraction of those handled in RSRG techniques. The knowledge of the excited states of dimers or trimers of blocks enables one to define the effective interactions between an excited block and its ground-state neighbors, as well as effective excitation hopping integrals, which delocalize the excitations. The effective interactions incorporate complex processes, including multiple excitations or/and interblock excitations. These informations are used to build an excitonic Hamiltonian for the infinite lattice, and to estimate the gap.

The method has been presented (and tested) in its simplest version on spin lattices, with identical blocks, one excited state per block, and extraction from dimers and trimers. It is possible to generalize it to blocks of different sizes or topologies, and one may keep several excited states per block. The renormalized excitonic method has been tested so far to the research of singlet-triplet gaps but it is applicable as well to singlet to singlet excitations. The bottleneck is the size of the dimers or trimers of blocks, the lowest states of which have to be calculated. In the few benchmark problems tested in the present work the results are surprisingly accurate and the method seems to be able to locate phase transitions between gapped and gapless phases in 1D and 2D lattices at a very low computational cost. Another application concerning the Shastry-Sutherland lattice,[26] shows the relevance of the here proposed method for the study of phase transition in frustrated 2D spin lattices.

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