Eur. Phys. J. B **14**, 439–448 (2000)

THE EUROPEAN PHYSICAL JOURNAL B

EDP Sciences

Long-range spin-pairing order and spin defects in quantum spin-$\frac{1}{2}$ ladders

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Received 19 July 1999 and Received in final form 8 October 1999

Abstract. For w-legged antiferromagnetic spin-1/2 Heisenberg ladders, a long-range spin pairing order can be identified which enables the separation of the space spanned by finite-range (covalent) valence-bond configurations into $w+1$ subspaces. Since every subspace has an equivalent counter subspace connected by translational symmetry, twofold degeneracy, breaking translational symmetry is found except for the subspace where the ground state of w = even belongs to. In terms of energy ordering, (non)degeneracy and the discontinuities introduced in the long-range spin pairing order by topological spin defects, the differences between even and odd ladders are explained in a general and systematic way.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 75.10.Jm Quantized spin models

1 Introduction

The discovery, about a decade ago, of high-Tc superconductivity [1] in lightly doped "two dimensional" antiferromagnets and materials (initially) supposed to contain coupled spin chains [2–4], have generated a renewed interest on low dimensional quantum spin-$\frac{1}{2}$ systems. One of the concerns is the non-smooth crossover from one-dimensional to two-dimensional systems (see, for instance, Ref. [5] and references therein). This fact has also been pointed out earlier in references [6–9] for different sets of long polymeric strips with graphite as the final member of these series, paralleling that of the square-lattice family. Both theoretical and experimental studies [5,10–12] suggest that the nature of antiferromagnetic spin-$\frac{1}{2}$ ladders with w = even legs differs from that of w = odd ladders. For instance, w = even ladders are gapped systems, the gap vanishing exponentially with w, while w = odd ladders display characteristics similar to one-dimensional spin-$\frac{1}{2}$ systems, namely they are gapless, with a doubly degenerate ground state, breaking translational symmetry [10,13,14]. Furthermore, spin defects are confined in ladders with w = even but they are not if w = odd. Numerical results [15] indicate that, in the infinite limit, the ground state of the two dimensional system, towards w = even and w = odd series must converge to, has long-range antiferromagnetic order and gapless excitations.

In this paper we will consider antiferromagnetic quantum spin-$\frac{1}{2}$ ladders with w legs, (even) $L \to \infty$ rungs, free boundary conditions in the inter-chain direction, and translational symmetry in the chain direction. It is assumed that the Hamiltonian appropriate to describe these systems contains only short-range interactions preserving the total spin of the system. At half filling, we assume that the Hamiltonian which governs the lowest-lying region of the spectrum is the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg Hamiltonian,

$$H = \sum_{ni,mj} J_{ni,mj} \mathbf{S}_{ni} \cdot \mathbf{S}_{mj}, \tag{1}$$

where $\mathbf{S}_{ni}$ is the spin operator for spin on site ni, n indicating the rung and i the leg, and the $J_{ni,mj}$ are the exchange-coupling parameters. The $J_{ni,mj}$ are assumed to decrease very rapidly with distance, the nearest-neighbour Heisenberg Hamiltonian with isotropic J being the dominant part of H.

Since the ground state of such a Hamiltonian for a bipartite system with equal number of sites in the two parts is known to be a singlet [16], resonating-valence-bond-type wave functions are defined in the space spanned by M-range (covalent) valence-bond (VB) configurations, with arbitrarily large but finite M. We refer to this space as *model space*, $\mathcal{H}^w$. The reasonableness of $\mathcal{H}^w$ is based on the fact that the dimer-covering configurations (or Kekulé structures [17], as have always been termed in Resonance Theory) are the lowest-lying monoconfigurational singlets. Thus, they provide a good zero-order picture. Then, on applying the Hamiltonian H, it can be noticed that the nearness of spin pairing tends to be preserved. When H is restricted to the isotropic nearest-neighbour spin-$\frac{1}{2}$ Heisenberg Hamiltonian the shorter-range RVB picture should apply best for small even w, while w = odd or

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wide even w ladders are expected to require long-range RVB pictures [18,19]. For instance, M-range RVB pictures neglect corrections lying higher than the M order in Perturbation Theory and have to be considered with caution. Nevertheless, additional terms in the Hamiltonian, as frustration, are expected to stabilise the finite-range RVB wave functions with respect to other Néel-based *ansätze* (see [20] and references therein). In addition, there exist finite-range Heisenberg models for which short-range Kekulé structures are exact ground states and also short-range RVB *ansätze* certainly apply for so-called "bond-dimer" models (see, for instance, [21–25]).

In order to separate the model space $\mathcal{H}^w$ into non-mixing different subspaces, several attempts have been made to find associated topological quantum numbers. For instance, the occurrence of a topological long-range order (LRO) was first discussed [26] to rationalise the ground-state instability to bond alternation in spin-1/2 linear Heisenberg chains. Simultaneously, this LRO has also been discussed in the context of applications to conjugated hydrocarbons [6–8,27]. Latter, Klein *et al.* [28] and independently Thouless [29] introduced the *gap* or *resonance parity*, and Kivelson *et al.* [30] and Sutherland [31], defined the *winding number*. These numbers allow the separation of the short-range VB states for odd-width strips in two subsets leading to degeneracy [32,33]. The relation between topological LRO and winding numbers is given in reference [33]. Also, in reference [33], a *resonance quantum number*, D_n, which specifies the local (at boundary n) array of singlets, has been defined for VB systems with bipartitioning conditions. Still, arguments based on a topological LRO have been applied to the qualitative analysis of distortions, excitations and their coupling for square-lattice strips [18] and, more quantitatively, to different polymers [34,35]. More recently, simple topological effects in short-range RVB were also predicated in references [19,36] for coupled Heisenberg Chains, based on numerical results from density matrix renormalization group (DMRG) techniques on clusters.

Our purpose in this paper is to show that for antiferromagnetic quantum spin-$\frac{1}{2}$ ladders a long-range spin-pairing order (LR-SPO) associated with the resonance quantum number D_n can be defined. This LR-SPO allows to separate the model space $\mathcal{H}^w$ into $w+1$ subspaces. Configurations belonging to mutually different subspaces should differ repeatedly on each of the L rungs of the ladder. Then, they are asymptotically orthogonal, and never mix by applying a few-particle operator.

The energy ordering among the lowest-lying state in every subspace is estimate by the dimer-covering-*counting* approximation [6,37,38]. Counting the dimer-covering configurations has been achieved by a transfer-matrix technique (see, *i.e.*, Refs. [34,35] and references therein). Also, since every subspace has an equivalent counter subspace connected by translational symmetry, twofold degeneracy is naturally obtained except for the subspace including the ground state of $w =$ even ladders, irrespective of the details of any Hamiltonian preserving translational symmetry. Furthermore, in the present paper it is shown that a topological spin defect introduces a discontinuity in the LR-SPO, except for the ground state of $w =$ even ladders. Then, understanding energy ordering, degeneracy, and the discontinuities introduced in the LR-SPO by topological spin defects, allow a general and systematic explanation of the differences between even and odd ladders.

This paper is organised as follows: In Section 2 we show that the (covalent) VB configurations have a LR-SPO, which allows the separation of the model space in different (asymptotically orthogonal and non-interacting) subspaces. In Section 3 the energy of the lowest lying state in every subspace is estimated within the dimer-covering-*counting* approximation. In Section 4 we obtain the discontinuity in the LR-SPO associated to the presence of a topological spin defect. In Section 5 the results are presented and discussed. Finally, the conclusions are collected in Section 6.

2 Singlets and long-range spin-pairing order

Quantum spin-$\frac{1}{2}$ ladders with $N = w \times L$ sites, with (even) $L \to \infty$ and free boundary conditions along the interchain direction, are bipartite system with a singlet ground state. Therefore, the ground state can be written as a weighted superposition of a non-orthogonal complete basis set of singlets, $|s_i\rangle$, $i = 1$ to d_N,

$$d_N = \frac{N!}{(N/2+1)!(N/2)!}\,. \tag{2}$$

In a bipartite system, sublattices A and B (starred) can be identified and a set of d_N independent singlets can be constructed by pairing to a singlet each of the $N/2$ spins in A to a spin in B. We represent one of these spin-pairings (SP) by an arrow from the site in the sublattice A to its partner in B (see, for instance, Fig. 1, where a complete set of linearly-independent singlets for six-site systems are represented). Overlap, $\langle s_i|s_j\rangle$, and matrix elements, $\langle s_i|H|s_j\rangle$ can be evaluated using the Pauling's [17,39] superposition rules.

For the sake of simplicity, we first introduce the LR-SPO of VB configurations defining the (local, at boundary n) resonance quantum numbers, D_n, when boundaries are chosen to run parallel to rungs, and the model space is restricted to the dimer-covering approximation. Later we show that the inclusion of longer pairings and/or using more general boundaries does not spoil this LR-SPO. The only effect of selecting boundaries of a different shape is changing the origin of the LR-SPO parameter. Finally, in this section, we discuss the consequences of the LR-SPO on the eigenstates of H and their degeneracy.

2.1 Dimer-covering model-space approximation

For any Kekulé structure, let us define P_n^+ (P_n^-) as the number of arrows pointing to the right (left) across a boundary, f_n, lying midway between rungs n and $n+1$

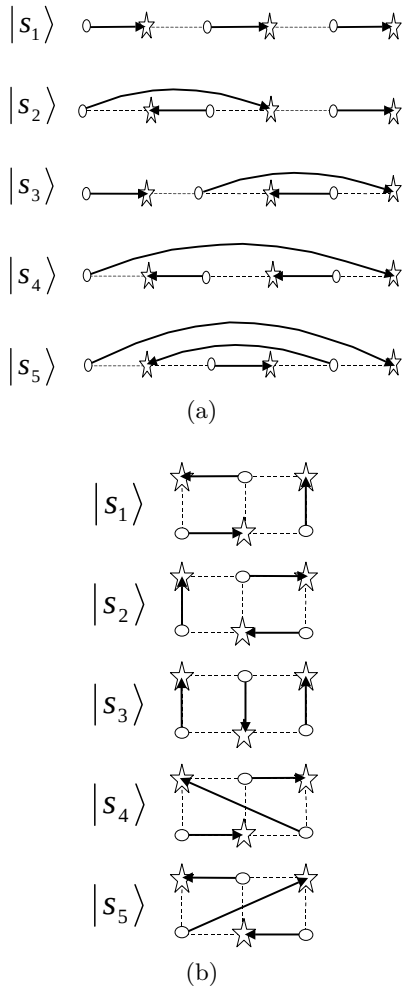

Fig. 1. A complete set of linearly independent (covalent) singlets for a six-sites system: a) 1×6; b) 2×3.

(see Fig. 2), and I_n as the number of SP with both sites in the rung n,

$$I_n = 0, 1, \ldots \frac{w-b}{2}, \tag{3}$$

where

$$b \equiv \begin{cases} 0, \, w = \text{even}, \\ 1, \, w = \text{odd}. \end{cases} \tag{4}$$

If w_n^A (w_n^B) is the number of sites belonging to the intersection of rung n and sublattice A (B), it can be easily seen that

$$\begin{aligned} w_n^A &= P_{n-1}^- + P_n^+ + I_n, \\ w_n^B &= P_{n-1}^+ + P_n^- + I_n. \end{aligned} \tag{5}$$

Choosing A and B sublattices according to

$$w_0^A - w_0^B = b, \tag{6}$$

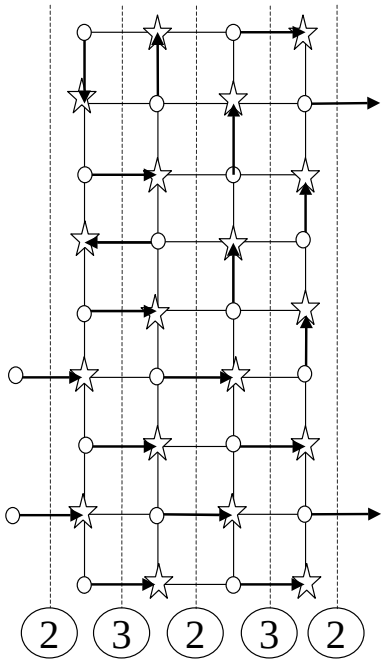

Fig. 2. A fragment of a $w = 9$ ladder, showing (inside a circle) the value of D_n at each boundary f_n. Note that $D_n = D_{n-1} + (-1)^n b$ (sublattices A and B are selected as $w_n^A - w_n^B = (-1)^n b$).

it can be written

$$\begin{aligned} w_n^A &= \frac{1}{2}\left[w + (-1)^n b\right], \\ w_n^B &= \frac{1}{2}\left[w - (-1)^n b\right]. \end{aligned} \tag{7}$$

Substracting equations (5) and using equations (7)

$$P_{n-1}^- - P_{n-1}^+ + P_n^+ - P_n^- = w_n^A - w_n^B = (-1)^n b. \tag{8}$$

Defining the resonance quantum number D_n at boundary f_n as

$$D_n \equiv P_n^+ - P_n^-, \tag{9}$$

we obtain

$$D_n = D_{n-1} + (-1)^n b. \tag{10}$$

Then a SPO parameter $D \equiv D_0$ can be associated to any dimer-covering configuration, so that

$$D_n = D - \frac{1}{2}\left[1 - (-1)^n\right] b. \tag{11}$$

Since

$$\begin{aligned} P_n^+ &= 0, 1, \ldots w_n^A, \\ P_n^- &= 0, 1, \ldots w_n^B, \end{aligned} \tag{12}$$

D can take $w+1$ different values,

$$D = \frac{w+b}{2}, \frac{w+b-2}{2}, \ldots, \frac{b-w}{2}, \tag{13}$$

and the (dimer-covering) model space can be partitioned in $w+1$ subspaces, $\mathcal{H}_D^w$, according to the value of D.

2.2 General formulation of the LR-SPO

The LR-SPO and D introduced above have been related, for the sake of simplicity, exclusively to dimer-covering configurations and to boundaries running parallel to rungs. Now we remove these restrictions. We will see that the shape of the boundaries limiting fragments of the ladder or the inclusion of long-range spin-pairings is irrelevant and that the LR-SPO can still be defined.

The dimer-covering model space is not invariant under the Hamiltonian operator. For instance, the XY terms, $S^{\pm}_{ni}S^{\mp}_{mj}$, of the nearest-neighbour Heisenberg Hamiltonian acting on a Kekulé structure yield singlets with SP between sites up to 3 bonds apart (see Fig. 3). Then, as a first step, linearly independent singlets with 3-bond-range (3BR) SP should be incorporated into $\mathcal{H}^w$ to go beyond the dimer-covering approximation. These 3BR-SP states allow sites in A-sublattice to be SP to sites in B-sublattice no more than 3 bonds apart. These states can be directly generated by the "re-coupling" [34,35] of two simply neighbouring dimers, *i.e.* unlinked bond-pairs with one and only one site in a pair being a nearest neighbour to a site in the other pair. It is worth noting that these re-couplings satisfy the non-crossing rules. Then, the 3BR-SP model subspace incorporates any singlet obtained from a dimer-covering singlet allowing an arbitrary number of unlinked re-couplings of two simply neighbouring bond-pairs. Still longer-range model spaces can be obtained allowing 5BR-SP, 7BR-SP, ..., to be included in $\mathcal{H}^w$. See, for instance, Figure 4 where a fragment of a ladder showing longer range SP is represented. Nevertheless, singlets with very long bond-range SP should contribute less, so a reasonable model space will be that including singlets with SP up to M bonds apart, M not necessarily small.

Let us now also allow the boundary f^g_n to be a line running from one side of the ladder to the other side, with $n1$ being the first site to the left of f^g_n in leg 1. We assume that f^g_n can go up and down, but it is self-avoiding and is not hitting any site. Thus, f^g_n must unambiguously break up the ladder in two regions: left region, L_n, and right region, R_n (see Fig. 5). Therefore, two non-intersecting boundaries, f^g_n and f^g_m, $n < m$, define a fragment, $F^g_{n,m}$, as the intersection of R_n and L_m.

We define P^{g+}_n (P^{g-}_n) as the number of arrows penetrating the boundary f^g_n with the arrowhead in the R_n (L_n) region. $I^g_{n,m}$ is the number of arrows with both ends in $F^g_{n,m}$. $l^g_{n,m}$ ($r^g_{n,m}$) is the number of arrows starting in R_m (L_n) and with the arrowhead in L_n (R_m), *i.e.* with no partner belonging to $F^g_{n,m}$. Finally, $F^{gA}_{n,m}$ ($F^{gB}_{n,m}$) is the number of sites belonging to the intersection of $F^g_{n,m}$ and sublattice A (B). Then

$$P^{g-}_n - l^g_{n,n+p} + P^{g+}_{n+p} - r^g_{n,n+p} + I^g_{n,n+p} = F^{gA}_{n,n+p},$$
$$P^{g+}_n - r^g_{n,n+p} + P^{g-}_{n+p} - l^g_{n,n+p} + I^g_{n,n+p} = F^{gB}_{n,n+p}. \quad (14)$$

Subtracting these two equations we obtain

$$D^g_{n+p} - D^g_n = F^{gA}_{n,n+p} - F^{gB}_{n,n+p}, \quad (15)$$

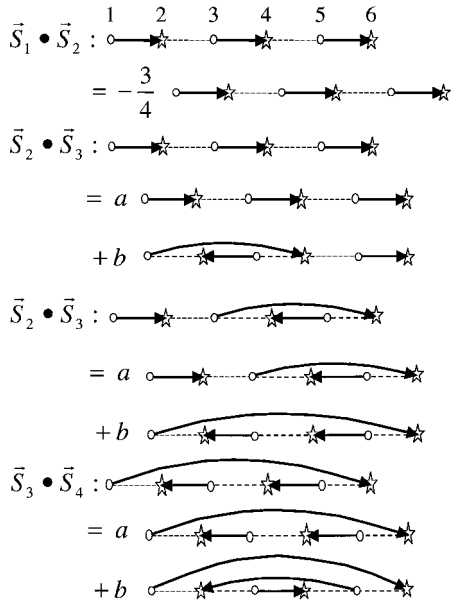

Fig. 3. A dimer-covering configuration is an eigenstate of $\mathbf{S}_j \cdot \mathbf{S}_k$ when sites j and k are spin-paired. The "off-diagonal" singlet with (i, l^*) and (k, j^*) pairings is also obtained when $\mathbf{S}_j \cdot \mathbf{S}_k$ acts on a VB configuration with spin-pairings (i, j^*) and (k, l^*).

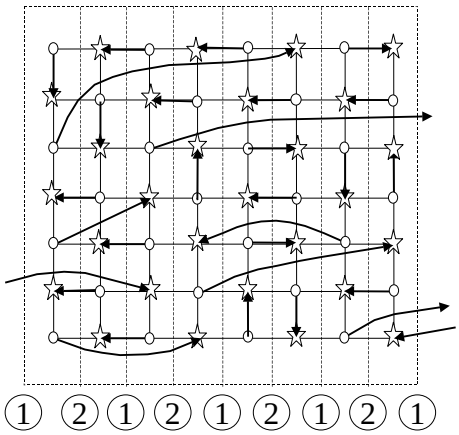

Fig. 4. A fragment of a $w = 7$ ladder, showing (inside a circle) the value of D_n at each boundary f_n. Note that still $D_n = D_{n-1} + (-1)^n b$ (sublattices A and B are selected as $w^A_n - w^B_n = (-1)^n b$), although here there are longer-range spin-pairings.

with

$$D^g_n \equiv P^{g+}_n - P^{g-}_n, \quad (16)$$

Let us analyze $F^g_{n,n+p}$ leg by leg. From Figure 5, it is readily seen that

$$F^{gA}_{n,n+2j} - F^{gB}_{n,n+2j} = 0,$$
$$F^{gA}_{n,n+2j+1} - F^{gB}_{n,n+2j+1} \equiv -b^g_n, \quad (17)$$

where j is a positive integer with the restriction f^g_n and f^g_{n+2j} do not intersect, and $b^g_n = b^g_{n+2}$ for any n. Then,

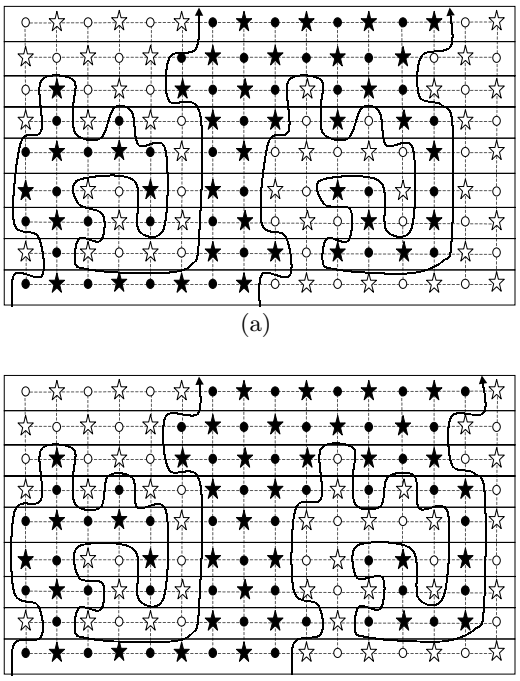

Fig. 5. Portion of a ladder showing boundaries f_n^g and f_m^g which go up and down: a) $m-n=$ even; b) $m-n=$ odd. These non-intersecting boundaries define a fragment of the ladder (the set of sites with a full dot or star), $F_{n,m}^g$, as the intersection of R_n and L_m. Analysing the fragment a leg at time, it is worth noting a series of facts: First, there are $m-n$ sites in each leg. Also, whenever a site qi belongs to $F_{n,m}^g$, neither the site $T^{m-n}qi$ nor the site $T^{-m+n}qi$ (qi translated $m-n$ steps to the right or to the left) are included in the fragment. Furthermore, in (a), $T^{m-n}qi$ remains in the same sublattice than qi while, on the contrary, in (b), $T^{m-n}qi$ belongs to a different sublattice than qi. Finally and more important, in (a) half of the $m-n$ sites belong to the sublattice A and the other belong to the B sublattice, while in (b) the fragment has different number of sites in the sublattice A than in the sublattice B.

choosing $n=0$,

$$\begin{aligned} D_{2j}^g - D_0^g &= 0, \\ D_{2j+1}^g - D_0^g &= -b_0^g. \end{aligned} \tag{18}$$

Again it follows that a SPO parameter $D^g \equiv D_0^g$ can be associated to any VB configuration, so

$$D_n^g = D^g - \frac{1}{2}\left[1-(-1)^n\right] b^g, \tag{19}$$

with $b^g \equiv b_0^g$.

The general order parameter D^g can be related to the previous one, D, in a simple way. For simplicity, without loss of generality, let us consider the fragment $F_{0,2j}$ limited by f_0^g and f_{2j}, $j>0$. We select j in such a way that as f_0^g and f_{2j} do not intersect. I_F is the number of SP with both sites in $F_{0,2j}$; l_F (r_F) is the number of arrows connecting an A site in R_{2j} (L_0) to a B site in L_0 (R_{2j}), and $F_{0,2j}^A$ ($F_{0,2j}^B$) is the number of sites belonging to the intersection of $F_{0,2j}$ and sublattice A (B). Then

$$\begin{aligned} P_0^{g-} - l_F + P_{2j}^{+} - r_F + I_F &= F_{0,2j}^A, \\ P_0^{g+} - r_F + P_{2j}^{-} - l_F + I_F &= F_{0,2j}^B. \end{aligned} \tag{20}$$

Subtracting these two equations

$$-D^g + D_{2j} = F_{0,2j}^A - F_{0,2j}^B. \tag{21}$$

Using equation (19) we obtain

$$D^g = D - \left(F_{0,2j}^A - F_{0,2j}^B\right), \tag{22}$$

which is independent of j, provided it is not too small to prevent f_0^g and f_{2j} are intersecting. Thence, there is a one to one correspondence between allowed values of D^g and D.

2.3 LR-SPO of eigenstates and degeneracy

So far, we have separated the model space in $w+1$ subspaces. At this point we note that two singlets from different subspaces must be different repeatedly at every position along the ladder. Therefore, according to Pauling's island-counting technique [17,39], they are asymptotically orthogonal and non interacting *via* any interaction mediated by a few-particle operator. Then the matrix of the Hamiltonian asymptotically block-diagonalises, so configurations belonging to different subspaces do not mix in the configuration-interaction sense. Thus D may be taken as a long-range order parameter labelling the eigenstates Ψ_D of the D block.

Furthermore, $\mathcal{H}_D^w$ and $\mathcal{H}_{b-D}^w$ subspaces are equivalent by a translation T of one rung along the legs. Then,

$$T\Psi_D = \Psi_{b-D}. \tag{23}$$

Consequently, degeneracy is always expected to occur, except for $D=0$ and $w=$ even, *i.e.* $b=0$.

3 Energy ordering

Within the dimer-covering approximation the *resonance energy* in units of J, $N\varepsilon_r(w,D)$, *i.e.* the ground-state energy correction below the energy of a single Kekulé structure ($-0.375N$), depends on the configuration interaction amongst the different Kekulé structures. It has been argued [6,38] that one might consider this energy lowering to depend solely on the dimension of the space spanned by the appropriate Kekulé structures. Let $n(w,D)$ be the dimension of the D block for a w-legged ladder. Since $n(w,D)$ is multiplicative in terms of a break up into subsystems while the energy is additive, such a functional dependence should be of the form

$$\varepsilon_r(w,D) \approx -\frac{CJ}{wL}\ln n(w,D), \tag{24}$$

where C is a fitting parameter independent of the structure to some degree, and in particular presumed to be (at least asymptotically for large w) the same for all w-legged ladders. For energy-ordering purposes the value of C is irrelevant. Nevertheless, for the nearest-neighbour isotropic Heisenberg model the value of C have been determined for a class of benzenoid hydrocarbons [6] (with $C = 0.5667$) and for finite square-lattice fragments [38] (with $C = 0.75$), by fitting the logarithm of the Kekulé-structure count to the resonance energy calculated from an equally-weighted Kekulé-structure wave function.

Arguments supporting equation (24) relay on the fact that the energy is an extensive magnitude, *i.e.* scales as the system size, while the number of Kekulé structures needs to scale exponentially with the system size. Then, C may be determined by fitting the logarithm of the Kekulé-structure count to better estimates to the energy than those used in references [6,38]. As a first attempt to do so, we obtain $C_w = 0.84$, 1.0 and 0.93 appropriate for square-lattice strips with $L \to \infty$ and $w = 2$, 3 and 4, respectively, when the "exact" energy values of Table 2 in reference [38] have been used. The weighted average of them could be used as a rough estimate of C appropriate for the two-dimensional square lattice. Assuming that the error of C_w typically behaves as $1/w$, we obtain $C = 0.94 \pm 0.19$, although a more reliable value would be desirable.

The values of $n(w, D)$ can be easily obtained (see the Appendix) as the $L/2$ power of the highest eigenvalue, Λ^2_{wD}, of the D block of the square of a dimer-covering-*counting* transfer matrix $\mathcal{T}^2_D$. Then, the resonance energy of the lowest lying state in the subspace D can be written as

$$\varepsilon_{\rm r}(w, D) \approx -\frac{CJ}{w} \ln \Lambda_{wD}. \tag{25}$$

4 Topological spin defects and LR-SPO

Let us now suppose that there is a topological spin defect on site i of rung n, *i.e.* for any reason the site ni remains not spin-paired,

$$ni \in \begin{cases} A, & n+i = \text{odd}, \\ B, & n+i = \text{even}. \end{cases} \tag{26}$$

Then, choosing boundaries parallel to rungs, equations (14) become

$$\begin{aligned} w^A_n &= P^-_{n-1} - l + P^+_n - r + I_n + \frac{1}{2}\left[1 - (-1)^{n+i}\right] \\ w^B_n &= P^+_{n-1} - r + P^-_n - l + I_n + \frac{1}{2}\left[1 + (-1)^{n+i}\right] \end{aligned} \tag{27}$$

and the recurrence relation across the rung n with a topological spin defect on site ni is

$$D_n = D_{n-1} + (-1)^n \left[b + (-1)^i\right]. \tag{28}$$

If the order parameter to the left of the spin defect is D_l, according to equation (11), the order parameter to the right of site ni, D_r, will be

$$D_r = D_l + (-1)^{n+i}. \tag{29}$$

Then, a topological spin defect can be seen as a domain wall separating sectors with order parameters D_l and D_r.

Furthermore, since the subspaces D and $b - D$ are degenerate, the energy per site associated to the sectors to the right and to the left of a spin defect located at the ni site will be degenerate if

$$D_l = \frac{1}{2}\left[b - (-1)^{n+i}\right]. \tag{30}$$

This equation has a solution only when $b = 1$, *i.e.* w is odd, and $D_l = 0$ (with $D_r = 1$) or $D_l = 1$ (with $D_r = 0$).

Furthermore, it is possible to form a local region between rungs n and m of LR-SPO $D \pm 1$ placing two spin defects in a wave function of LR-SPO D, one in a site ni and the other in a site mj, with $n + i + m + j =$ odd.

5 Results and discussion

Considering that w-legged (even) $L \to \infty$ antiferromagnetic spin-$\frac{1}{2}$ Heisenberg ladders are bipartite systems with singlet ground state, we have assumed that their ground state is described by an RVB many-body wave-function *ansätze* within the space spanned by the M-range (covalent) valence-bond configurations, $\mathcal{H}^w$, with arbitrarily large $M \ll L$.

We have shown that any (covalent) VB configuration exhibits a LR-SPO. This LR-SPO is characterised by a parameter D, which can take $w + 1$ different values, and allows to specify the local (at boundary) array of spin-pairings penetrating the boundary n, for any n. The shape of the boundary selected to define D is quite arbitrary: it can go up and down, but it is self-avoiding and is not hitting any site, so it is able to break up the ladder in two (non-longitudinal) parts. When the boundary is chosen to be parallel to the rungs, the allowed values of D are:

$$D = \frac{w+b}{2}, \frac{w+b-2}{2}, \ldots, \frac{b-w}{2}, \tag{31}$$

where b is zero (one) for $w =$ even (odd). Choosing another boundary, the values of D simply change by a boundary-dependent integer.

This long-range spin-pairing-order allows to separate $\mathcal{H}^w$ in $w+1$ subspaces, $\mathcal{H}^w_D$. Two configurations in different $\mathcal{H}^w_D$ differ repeatedly on each of the L rungs of the ladder. Consequently, they are asymptotically orthogonal and non interacting via any interaction mediated by a few-particle operator. Thence, the matrix of the Hamiltonian asymptotically block-diagonalises. Thus, the eigenstates of H do not mix configurations with different value of D. Therefore, D may be taken to be a long-range order parameter labelling the eigenstates of the D block. This gives rise to $w + 1$ RVB *Anzätze* exhibiting different LR-SPO, Ψ_D. It is also worth noting that asymptotic strong orthogonality and LR-SPO in RVB wave functions persist with a long finite cut-off.

Furthermore, subspaces $\mathcal{H}^w_D$ and $\mathcal{H}^w_{b-D}$ are equivalent by a translation of one rung along the legs, T. Then

$$T\Psi_D = \Psi_{b-D}, \tag{32}$$

Table 1. The absolute value of the resonance energy in units of C, $(\ln \Lambda_D)/w$, for the lowest lying state of subspaces with order parameters from $D = 0$ to $(w + b)/2$, and the extrapolations to $w \to \infty$ for the lowest lying subspace of both, the w = even and w = odd, series.

w \ D	0	1	2	3	4	5	6
1	0.	0.					
3	0.2195	0.2195	0.				
5	0.2529	0.2529	0.1567	0.			
7	0.2656	0.2656	0.2121	0.1181	0.		
9	0.2721	0.2721	0.2383	0.1762	0.0940	0.	
11	0.2760	0.2760	0.2527	0.2090	0.1491	0.0799	0.
∞	0.2920						
2	0.2426	0.					
4	0.2610	0.1849	0.				
6	0.2699	0.2331	0.1349	0.			
8	0.2748	0.2532	0.1930	0.1048	0.		
10	0.2778	0.2637	0.2332	0.1617	0.0852	0.	
12	0.2800	0.2700	0.2410	0.1959	0.1382	0.0717	0.
∞	0.2913						

and the energy of the corresponding wave functions must be

$$E_D = E_{b-D}. \tag{33}$$

Thus degeneracy is always predicted to occur, except for w = even and $D = 0$, irrespective of the details of any Hamiltonian preserving translational symmetry.

We have obtained the values of Λ_{wD} of Section 3 for w ranging from one to twelve and D from b to $(w + b)/2$. Table 1 summarises the zero order resonance energies $\varepsilon_r(w, D)$, in units of C, calculated by using equation (25). Since it is unlikely that the zero-order energies are drastically modified by the small corrections to the isotropic nearest-neighbour Heisenberg Hamiltonian, we expect an energy ordering

$$E_b < E_{b+1} < \cdots < E_{\frac{1}{2}(w+b)}. \tag{34}$$

Therefore, for w = even, the ground state belongs to the non-degenerate $D = 0$ subspace, with

$$T\Psi_0 = \Psi_0, \tag{35}$$

while, for w = odd, the ground-state manifold is spanned by Ψ_0 and Ψ_1, which are eigenstates of H, but not of T. The eigenstates $\Phi_\pm$ of the translation operator, are defined in the ground-state manifold,

$$\Phi_\pm \equiv \frac{1}{\sqrt{2}} \left(\Psi_0 \pm \Psi_1\right), \tag{36}$$

so

$$T\Phi_\pm = \pm\Phi_\pm. \tag{37}$$

with $k = 0$ and $k = \pi$. This RVB asymptotic degeneracy for w = odd is consistent with a very wide body of evidence.

It could be argued that the true ground state of the spin-$\frac{1}{2}$ nearest-neighbour Heisenberg Hamiltonian for $w = 1$ and $L \to \infty$ should be described in terms of two degenerate subspaces, in order to regain the non-degenerate and gapless Bethe *Ansatz* state. For finite (even) L with cyclic boundary conditions the two degenerate RVB wave functions do interact, in the configuration interaction sense, giving a splitting of the translationally-adapted states $\Phi_\pm$ (with $k = 0$ and $k = \pi$), which leads to a non-degenerate ground state. Thus, for finite L, restriction to just one subspace does not yield a true ground state. Nevertheless, when the splitting is examined as a function of L, it is seen that the gap closes at least as fast as $1/L$ and the states $\Phi_\pm$ approach to an accidental degeneracy. This feature is basically related with the dimerizing instability of the Bethe *ansatz* state. For instance, if a small dimerizing interaction occurs, then the accidental degeneracy of equation (33) no longer holds. Therefore, either Ψ_0 or Ψ_1 will be lower in energy and completely dominate the wave function, leading to a spin-Peierls broken-symmetry ground state [26].

Table 2. Parameters of the equation (38), which fits the ground-state ($D = 0$) resonance energy, in units of C, for the w = even and w = odd series and their weighted average.

	w=even	*w*=odd	weighted average
$\varepsilon_r(\infty,0)/C$	−0.29133 ± 0.00026	−0.29203 ± 0.00031	−0.2916 ± 0.0002
a_1	0.14326	0.16059	–
a_2	−0.08378	0.17130	–

The $w \to \infty$ limit is obtained by fitting $\varepsilon_r(w, 0)/C$ by a power series in $1/w$,

$$\frac{\varepsilon_r(w,0)}{C} \approx \frac{\varepsilon_r(\infty,0)}{C} + \frac{a_1}{w} + \frac{a_2}{w^2}\,. \tag{38}$$

In Table 2 the values of $\varepsilon_r(\infty, 0)/C$, a_1 and a_2 are collected for both w = even and w = odd, along with their weighted average for $\varepsilon_r(\infty, 0)/C$. For the purpose of seeing how reasonable this simple model is, a value of C is needed. When C is fitted to dimer-covering estimates of the energy for square-lattice fragments, the value 0.75 is obtained [38]. Using this value of C, the present simple model predicts an energy per site of ≈ -0.594 (in unit of J), in good agreement with the value -0.604 calculated at the same level by Liang, Doucot and Anderson [40]. When C is evaluated as the weighted average of the C_w, $w = 2$, 3 and 4, derived from the "exact" estimates of the energy of Zivkovic *et al.* [38] (see Sect. 3) we obtain $C = 0.94 \pm 0.19$. Obviously, a more reliable C value would be desirable. Using this value of C, an energy per site of $\approx -0.65 \pm 0.10$ (in unit of J) is obtained, which also compares fairly well with the best estimate (-0.668) of Liang, Doucot and Anderson [40].

We have shown that a topological spin defect, *i.e.* a non-paired site, can be seen as a domain wall separating two sectors of the ladder with order parameters D_l and D_r

$$D_r = D_l + (-1)^{n+i}. \tag{39}$$

Furthermore, the energy per site associated to the right and to the left sectors of the spin defect will be degenerate only when $b = 1$, *i.e.* w is odd, and $D_l = 0$ (with $D_r = 1$) or $D_l = 1$ (with $D_r = 0$). Also, it is possible to form a local region between rungs n and m of LR-SPO $D \pm 1$ placing two spin defects in a wave function of LR-SPO D, one in a site ni and the other in a site mj, with $n + i + m + j =$ odd.

Now, half-filled excited states (other than the $d_n - 1$ singlets orthogonal to the ground state) or even slightly doped states are analysed *via* topological spin defects. There are different types of excitations conceivable from a *Maximally-spin-paired* ground state. For instance, preserving half filling (one electron per site), there are primarily spin excitations. In this case, two topological spin defects, one in an A site and the other in a B site, are obtained by breaking one SP to form a triplet state. Away from half filling, removing (adding) one electron produces a vacant (doubly-occupied) site and the ladder becomes a doublet, with two sites, again one in an A site and the other in a B site, that cannot be SP. In this case hopping terms must be retained in the Hamiltonian and the so-called t-J *model* applies. Thence, the doublet is a weighted superposition of configurations with a single spin not SP and a vacant (doubly-occupied) site. Either a vacancy or a doubly-occupied site may also be assimilated to a topological spin defect, although there is no spin associated with them. Then, away from half filling, it may be conceivable a local region limited by two vacant (doubly-occupied) sites, or even a vacant (doubly-occupied) site and a single non-SP spin (provided that the doping is not so strong as to preclude a maximally-spin-paired ground state). Therefore, there are low-energy spin and charge excitations. Still, going up in the hierarchy of Hamiltonians, the Hubbard or even a more general Hamiltonian has to be considered. In this case, still another type of excitations (though presumably of higher energy if a Heisenberg-like Hamiltonian is assumed to govern the lowest-lying region of the spectrum) can be produced relaxing the single-occupancy constrain. This leads to the *ionic* states, *i.e.* states with at least a couple of sites, one doubly occupied and the other empty. Therefore, the couple of spin defects, associated to an excitation above a *Maximally spin-paired* state Ψ_D, are limiting a local region of LR-SPO $D \pm 1$.

When $w =$ odd and $D = 0$ ($D = 1$), there can be local regions with $D = \pm 1$ ($D = 0, 2$). Then, since subspaces $D = 0$ and $D = 1$ are degenerate, it is possible to have a local region with identical per site energy inside and outside the local region. In this case the topological spin defects limiting the local region are not confined, though it may happen that they attract one another (with an ordinary short-range potential). Two conclusions can be drawn from this result. First, for the half filling case, triplets with the two spin defects very far apart from one another are possible. Although breaking a singlet does cost some energy (due to contribution of the diagonal terms), there is a gain in kinetic energy (off-diagonal terms contributions), since (for $w =$ odd) the two spins are not confined and can move independently. Consequently, a gapless triplet spectrum is not inconsistent with the results of this work. This feature can be understood as a generalisation to any odd-legged spin-$\frac{1}{2}$ antiferromagnetic ladders of Lieb, Shultz, and Mattis theorem [13,14] holding for one-dimensional systems. Second, away from half filling, removing (adding) an electron to the system yields a *non-confined* pair of sites, one being a vacant (doubly-occupied) site and the other a non-SP site. It is worth noting that the vacant (doubly-occupied) site holds the charge, while the non-SP site holds the up or down spin, leading to charge-spin separation.

In clear contrast, when $w =$ even, the order parameter of the local region limited by the couple of spin defects is always associated to higher energy per site. This indicates that the couple of spin defects should remain as close as possible so confinement is predicted to occur. Hence, at half filling, the energy difference between the triplet and the ground state will be finite, and the $w =$ even ladders are expected to be gapped. Nevertheless, we observe that the energy difference per site between the lowest lying subspaces, $\Delta\varepsilon$, behaves as $\sim w^{-\alpha}$, with $\alpha \approx 1.8$, *i.e.* $\Delta\varepsilon$ decreases faster than $1/w$. Therefore, a lowering of confinement and the closing of the gap is predicted for increasing values of w. At this point, it could be argued that an excitation energy lowering can be achieved by allowing a Bloch superposition of analogous couples of topological spin defects. However this lowering is not expected to be as important as to close the gap, at least for $w = 2$ [38]. Nevertheles, within the scope of the present work it is not able to predict the energy ordering of the lowest singlet and triplet excited states. Now, away from half filling, when removing (adding) one electron the vacant (doubly-occupied) site will be bound to the non-SP spin, forming a "quasi-particle" with charge and spin. Again we expect the lowering of the confinement and the charge-spin separation with increasing values of w. This quasi-particle is far from being a static vacant (doubly-occupied) site bound to a static non-SP site. The hopping term of the t-J Hamiltonian allows the vacant (doubly-occupied) site to move while the exchange part mixes up all the doublet VB configurations with the constrain of keeping the vacant (doubly-occupied) site and the non-SP spin close to one another. Therefore, the appropriate wave function must be a weighted superposition of all possible static configurations in order to benefit from the hopping contribution to the energy, while lowering the exchange energy by keeping both the spin and the vacant (doubly-occupied) site bound. When removing (adding) two electrons, arguments based on the LR-SPO alone are not able to decide if the two-holes (two-electrons) state is described as two quasi-particles or two bound vacant (doubly-occupied) sites. Nevertheless, we expect the two vacant (doubly-occupied) sites to be confined to benefit from the energy lowering due to the hoping term of the Hamiltonian, as has been pointed out in reference [36], using numerical results from DMRG techniques on clusters. Another argument to take into account is the range of the RVB. Since the two quasi-particles are expected to couple to a singlet, non-bound quasi-particle would imply a long

bond, while a short-range RVB is expected for w = even ladders [18,19].

The above results also apply to open boundary conditions along the L direction. In this case, no pairing is expected to the left of rung $n = 1$, and to the right of rung $n = L$. Then, open boundary conditions determine the long-range order parameter to be $D = 0$, with a pair of spin defects still delimiting a $D = 1$ fragment, which is degenerate with that of $D = 0$ solely for w = odd, so results above still apply. Furthermore, if the boundary conditions are so that would force an order parameter of energy $\varepsilon_r(w, D)$ ($\varepsilon_r(w, b - D)$), $D \neq b$, we expect that a state with $D - b + 1$ spin defects located close to each end of the ladder, these defects limiting an extended area of resonance energy per site $\varepsilon_r(w, b)$, would be favoured.

The results of the present work relay on two conditions. First, the bipartitioning condition, which allows to establish the LR-SPO. Second, the energy ordering given by equation (34). This energy ordering is valid when the dominant part of the Hamiltonian is the isotropic sin-1/2 Heisenberg Hamiltonian. It might happen that the bipartitioning condition is not fulfilled and/or the corrections away from the isotropic spin-1/2 Heisenberg Hamiltonian are as important as the energy ordering is not that of equation (34), then the above discussion will not apply.

6 Conclusions

Identifying a LR-SPO and understanding energy ordering and degeneracy among RVB wave functions, as well as the discontinuities in the LR-SPO introduced by topological spin defects, allow a general and systematic explanation of the differences between even and odd ladders. It provides an intuitive understanding of the physics of spin ladders in general. In particular, for odd leg ladders

1) a doubly degenerate ground state, breaking translational symmetry, is obtained;
2) a gapless triplet spectrum is consistent with the results of the present work;
3) a simple understanding of the deconfinement of spin excitations as well as charge-spin separation is provided.

On the contrary, for small w = even ladders

1) a non degenerate ground state is obtained;
2) triplet spin excitations are found to be gaped;
3) a simple understanding of the confinement of spin excitations is provided;
4) a lowering of the confinement and the closing of the gap is predicted for increasing values of w.

The author acknowledges valuable discussions with D.J. Klein. This research was supported by the DGICYT (project PB95-0884).

Appendix: Dimer covering counting

Let us analyse from a local point of view the dimer-covering singlets. We can identify a dimer-covering local state, $|e_{nI})$, I ranging, according to which legs have an arrow across the f_n boundary. The direction of any arrow is fixed by n and the leg number. Then, it can be seen that there are 2^w different local states for each boundary, which can be classified according to the value of D_n, $|e^D_{nI})$. The local states of position $n + 1$ are mirror images of those of position n.

A dimer-covering-*counting* matrix, $\mathcal{T}_n$, is defined as

$$(e_{n-1I}|\mathcal{T}_n|e_{nJ}) = \begin{cases} 1, \, |e_{nJ}) \text{ can succeed } |e_{n-1I}) \\ 0, \text{ otherwise.} \end{cases} \quad \text{(A.1)}$$

Then, the number of dimer-covering states in a $\mathcal{H}^w_D$ subspace is

$$n(w, D) = \sum_{e^D_{0I}} (e^D_{0I}|\mathcal{T}_1\mathcal{T}_2 \ldots \mathcal{T}_L|e^D_{0I}). \quad \text{(A.2)}$$

Since for any dimer-covering singlet $D_{n-1} = D_{n+1}$, $\mathcal{T}_n\mathcal{T}_{n+1}$ is a block-diagonal symmetric matrix that does not depend on n (apart from the direction of the arrows in the local states that it relates) we can omit the subindex. For $L \to \infty$, the highest eigenvalue Λ^2_{wD} of the D block $\mathcal{T}^2_D$ dominates, and

$$n(w, D) \approx \Lambda^L_{wD}. \quad \text{(A.3)}$$

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