Universality Classes of Diagonal Quantum Spin Ladders

M.A. Martín-Delgado*, J. Rodríguez-Laguna* and G. Sierra*
*Departamento de Física Teórica I, Universidad Complutense. 28040 Madrid, Spain.
*Instituto de Física Teórica, C.S.I.C.- U.A.M., Madrid, Spain.

We find the classification of diagonal spin ladders depending on a characteristic integer \( N_p \) in terms of ferrimagnetic, gapped and critical phases. We use the finite algorithm DMRG, non-linear sigma model and bosonization techniques to prove our results. We find stoichiometric contents in cuprate \( \text{CuO}_2 \) planes that allow for the existence of weakly interacting diagonal ladders.

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The determination of the ground state and low lying excited states properties in strongly correlated systems is known to be a central problem in condensed matter since they are responsible for their thermodynamical properties at low temperature, their interaction with weak external fields and generically, for the presence or not of long-range correlations in the system. Thus, any time a new quantum system is brought about, their low energy properties are one of the first issues at stake. In this work we adress this problem for the case of diagonal quantum spin ladders with antiferromagnetic Heisenberg interactions:

\[
H = J \sum_{(i,j) \in \text{diagonal ladder}} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}
\]

![Diagram of diagonal quantum spin ladders](image)

**FIG. 1:** a) Diagonal ladder with \( N_p = 4 \) plaquettes. b) The \( N_p = 2 \) diagonal ladder as a decorated zig-zag ladder. c) Rectangular ladder with \( n_1 = 2 \) legs.

an array of sites hosting quantum spins \( S = \frac{1}{2} \) and links, characterized by their number of plaquettes \( N_p \) as depicted in Fig. 1. On the contrary, standard square ladders are characterized by the number of legs \( n_1 \). The interest in this type of spin systems is manifold: i/ They represent an alternative route to reaching 2D quantum physics from 1D systems [2]. ii/ They appear related to the physics of stripes in cuprate materials (e.g. \( \text{La}_{1.6-x} \text{Nd}_{0.4} \text{Sr}_x \text{CuO}_4 \) [3]. iii/ They also show up in numerical simulations of the \( t - J \) model in planes [4]. iv/ The necklace diagonal ladder is the simplest member of the class having \( N_p = 1 \) plaquettes. It is realized in both organic and inorganic compounds (e.g.: metal-free poly(\( m \)-aniline) or poly[1,4-bis-(2,2,6,6-tetramethyl-1-4-oxo-4-piperidyl-1-oxyl)-butadiyne]) [5]. v/ Standard square ladders have been synthesized in cuprate superconductors like \( \text{Sr}_{n-1} \text{Cu}_n \text{O}_{2n}, n \in \{3, 5, 7, \cdots \} \) [6]. Here we shall provide an explicit experimental proposal to study the whole class of diagonal ladders in cuprates.

In this paper we cast the main results of our investigations in a diagram of universality classes for AF diagonal ladders depending on their number of plaquettes \( N_p \):

\[
\begin{array}{|c|c|c|}
\hline
\text{Diag. Ladders} & \text{Odd} N_p & \text{Even} N_p \\
\hline
\text{Ferrimag., Gapless (F), Gapped (AF)} & \begin{cases} N_p = 2 \ (\text{mod 4}) & \text{AF, Haldane phase} \\ N_p = 0 \ (\text{mod 4}) & \text{AF, Gapless} \end{cases} & \end{array}
\tag{2}
\]

The first classification of diagonal ladders occurs depending on whether they show ferrimagnetism or not: for \( N_p \) odd they show ferrimagnetic order while for \( N_p \) even, they do not. The reason is as follows: although all diagonal ladders are bipartite systems, the number of sites in each sublattice is different. This imbalance between the number of sites in each sublattice is responsible for the \( N_p \) odd ladders exhibiting ferrimagnetism. Moreover, these \( N_p \) odd ladders present two types of excitations: a/ ferromagnetic gapless excitations which are the Goldstone bosons associated to the ferromagnetic order of the ground state; b/ antiferromagnetic gapped excitations.

The second classification corresponds to \( N_p \) even ladders, which are not ferrimagnetic. Their classification is not as simple as the \( N_p \) odd case since the gapless and gapped excitations do not coexists. In fact, for \( N_p = 0 \ (\text{mod 4}) \) the diagonal ladders are gapless systems with long-range interactions and critical, while for \( N_p = 2 \ (\text{mod 4}) \) they are gapped, with finite correlation length and we can describe them as a Haldane phase. Both types of excitations are antiferromagnetic.

Therefore, it is apparent that the classification of diagonal ladders is richer than that of standard square lad-
ders, which show gapless behaviour for \( n_1 \) odd legs and gapped for \( n_2 \) even \( \ell \). In fact, we want to stress that the study of diagonal ladders is much more difficult than for square ladders. To see this, we introduce a topological deformation of the diagonal ladders as shown in Fig. 1(b) for \( N_p = 2 \). This is achieved by flattening the outer links. The net result is a new sort of zigzag ladder that we call decorated zigzag ladder due to the extra sites. In the horizontal legs we put coupling constants \( J \) while in the zigzag inter-leg links they are \( J' \). This distribution must be compared with the corresponding distribution for the square ladder in Fig. 1(c) where \( J' \) stands for the rung coupling constants. The difficulties in studying diagonal ladders can now be attributed to the absence of a simple strong coupling limit \( J'/J \gg 1 \): when \( J \gg J' \) the ladder is equivalent to 2 weakly coupled chains (gapless point) similar to what happens with the square ladder; when \( J' \gg J \) it is again equivalent to one weakly coupled chain (gapless point) unlike the square ladder which has a well-defined strong coupling limit around singlet states on the vertical rungs producing a gapped phase. The absence of a strong coupling limit for diagonal ladders have important consequences for their study: neither it is possible to perform a perturbation theory as in \( \ell \) nor a mean-field calculation based on the condensation of spin singlets on the rungs as in \( \ell \). All this makes diagonal ladders a hard problem compared to square ladders. One of the fundamental open questions we address is: are there gapless phases around the limits \( J \gg J' \) and \( J' \gg J \)? We need hereby to resort to a series of numerical an analytical nonperturbative methods.

DMRG: We focus on \( N_p \) even diagonal ladders and start the DMRG calculations for \( N_p = 2 \) case which is equivalent to a decorated zigzag ladder Fig. 1(b). We use the finite algorithm version of the DMRG method which is more accurate than the infinite version. We have devised a sweeping process through the lattice adapted to the topology of the diagonal ladders for arbitrary \( N_p \) which improves the accuracy of the algorithm: (a) all sites should be included just once (i.e., a Hamiltonian graph); (b) ideally, all links should be included also (i.e., an Eulerian graph), but since this latter is impossible, we reduce our pretensions to (c) most of the links should be included in the path, favouring the ones in the “short direction”, (d) path links which are not graph links are allowed, but not favoured. The maximum number of sites is \( N = 122 \) (which corresponds to a horizontal length of \( L = 30 \) unit cells), the number of states kept is \( m = 200 \), discarded weights of the density matrix are always below \( 10^{-8} \) and we achieve a convergence of 6 digits in the energies of the eigenstates. Moreover, we have used an independent Lanczos method to check our DMRG results for small number of sites up to \( N = 28 \). In Fig. 2 we present our DMRG results for the gap \( \Delta = E(L, S = 1) - E(L, S = 0) \) between the first excited state (spin triplet) and the ground state (spin singlet) as a function of the coupling constant ratio \( J'/J \). Each point in the plot is the result of a extrapolated fit of the gap as a function of 1/\( L \) given by \( \Delta(L) = a_0 + a_1 L^{-1} + a_2 L^{-2} \). With these results we can answer now the above open question: we clearly see that the gap vanishes only at the extreme cases of \( J' \rightarrow 0 \) and \( J \rightarrow 0 \). Thus, we have a dense gapped phase \( \forall J'/J \), except at two limiting points.

The next interesting fact we find is the existence of a maximum corresponding to the isotropic point \( J = J' \). This must be compared with the results for the standard zigzag ladder in \( \ell \) where the physics of the gapped phase is dominated by the Majumdar-Gosh point (fully dimerized state) and in additional, there is a gapless phase separated by a critical point \( (J/J')_c \approx 0.24 \). The reason for the standard zigzag ladder having two phases is because it is a frustrated lattice, unlike our decorated zigzag ladder which is bipartite and thus nonfrustrated. This makes a big difference and is responsible for the
presence of an single gapped phase in our ladder. Likewise, we may wonder whether our gapped phase in Fig. 3 is a real Haldane phase or dimerized. To clarify this issue we have computed with DMRG the dimerized order parameter $D^\alpha(L)$ for a given length as the difference between two consecutive spin-spin correlators in the measured in the middle of the ladder as

$$D^\alpha(L) := \langle S_{i-1}^\alpha \cdot S_i^\alpha \rangle_{\frac{L}{2}} - \langle S_i^\alpha \cdot S_{i+1}^\alpha \rangle_{\frac{L}{2}}$$

where $\alpha = u, d, z$ stands for up, down or zigzag directions in the ladder. For the Majumdar-Gosh state this parameter takes a maximum value and detects its dimerization. In our $N_p = 2$ ladder we find values $D^u,d(L = 25) = 4 \cdot 10^{-6}$, $D^z(L = 25) \approx 2 \cdot 10^{-5}$. Thus, our ladders are not dimerized, a result compatible with a Haldane phase. Moreover, we have also computed with DMRG the string order parameter (SOP) defined as

$$S(L) := \langle (S_1^u + S_1^d) e^{i \sum_{j=2}^{L-1} (S_j^u + S_j^d)} (S_L^u + S_L^d) \rangle$$

Non-vanishing values of SOP detect the hidden order characteristic of the Haldane phase. In Fig. 2 (inset) we plot the extrapolated values $S(\infty)$ and find finite values in whole range corresponding to the gapped phase. It is remarkable that our values of the SOP are bigger than for the square ladder, while the gap in the diagonal ladder is more than ten times smaller than in the square ladder.

For $N_p = 4$ diagonal ladder, we have performed similar DMRG calculations up to $N = 184$ sites with $m = 400$ states. Our results are shown in Fig. 3 where we present the corresponding gap vs. $1/L$, and also the same for $N_p = 2$ for comparison. We find that the extrapolated value points to a negligible gap for the $N_p = 4$ ladder. This is a crucial difference w.r.t. the previous case and it means that there is a sharp difference between the whole class of $N_p$ even diagonal ladders. Is it possible to give an explanation for this difference?

**Non-Linear Sigma Model:** We turn to the sigma model (NLSM) to answer this question. The low energy properties of a Heisenberg lattice can be mapped onto the effective Hamiltonian of a non-linear sigma model given by

$$H = \frac{v}{2} \int dx \left[ g \left( \ell - \frac{\theta}{4\pi} \phi' \right)^2 + \frac{1}{2} \phi'^2 \right],$$

where $\phi$ is an $O(3)$ sigma field with the constraint $||\phi||^2 = 1$, $\ell$ is the angular momentum, $v$ the spin wave velocity, $g$ the coupling constant and $\theta$ is the topological term which is defined only mod $2\pi$. These $(v, g, \theta)$ are phenomenological parameters that will depend on the microscopic parameters like $(J, J', S)$ via the sigma model mapping. The behaviour of the system depends on whether the topological constant $\theta = 0$ (mod $2\pi$) for gapped or $\theta = \pi$ (mod $2\pi$) for gapless. This mapping can be done with a real-space blocking procedure. For the diagonal ladders we need to use the topological deformation introduced earlier in Fig. 1b) in order to bring them to the form of generalized decorated ladders with $n_l = \frac{N_p}{2} + 1$ legs as shown also in Fig. 1 where we also show the splitting of the original Hamiltonian into a block $H_B$ and interblock $H_{BB}$ parts. In order to make an appropriate ansatz we need to take into account several subtleties occurring in diagonal ladders: a/ the Neel state has AF character in the horizontal direction but Ferromagnetic in the vertical direction despite being the same for $N_p = 2$ ladder we find values $p = 4$ diagonal ladder, we have performed similar calculations for $L = 25$; b/ the even-site spin operators are inequivalent to the odd-site spins due to the peculiar zigzag interleg couplings (Fig. 4). With these provisos in mind, we find the correct ansatz to be:

$$\left\{ \begin{array}{l}
S_a(2n) = A_a^u \ell(x) + \ell_a(x) + S(\phi(x) + \phi_a(x)) \\
S_a(2n + 1) = A_a^d \ell(x) + \ell_a(x) - S(\phi(x) + \phi_a(x))
\end{array} \right.$$
TABLE I: NLSM data \((v_g, g, \theta)\) in \(N_p\)-even diagonal ladders.

\[
\begin{array}{|c|c|c|}
\hline
 & N_p = 2 \text{ Diagonal Ladder} & N_p = 4 \text{ Diagonal Ladder} \\
\hline
\theta & 4\pi S & 6\pi S \\
\hline
g & \frac{1}{3} \left(1 + \frac{J'}{J}\right)^{-1/2} & \frac{1}{3} \left(1 + \frac{4J'}{3J}\right)^{-1/2} \\
\hline
v_p & 2SJ \left(1 + \frac{J'}{3J}\right)^{1/2} & 2JS \left(1 + \frac{4J'}{3J}\right)^{1/2} \\
\hline
\end{array}
\]

Thus, it vanishes in the strong coupling limit \(J' \gg J\) meaning that the system becomes less disordered. This is in sharp contrast with the behaviour of square ladders. With this NLSM calculations we see that \(N_p\) even ladders can have a very different behaviour as shown in Fig. 4 and the DMRG calculations in Fig. 8.

\(\text{Bosonization:}\) We can obtain additional information about the gap formation in the \(N_p = 2\) diagonal ladder (decorated zigzag) using abelian bosonization techniques. Each leg of the decorated zigzag ladder (Fig. 1b)) can be described in the continuum limit in terms of massless Bosonic fields \(\varphi_a(x), a = 1, 2\) with a non-interacting Hamiltonian \(H_0 = \frac{\pi}{2} \sum_{a=1,2} \int dx \left[\Pi_{\varphi}^2(x) + (\partial_x \varphi_a(x))^2\right]\).

The corresponding SU(2) currents \(J_{\varphi}^{(L,R)}(x)\) and staggered field \(n_{\varphi}(x)\) satisfy \(S_{\varphi}(x) = J_{\varphi}^{(L,R)}(x) + J_{\varphi}^{(R,L)}(x) + (-1)^n n_{\varphi}(x)\). For weak coupling regime \(J'/J \ll 1\), we may switch on the interchain coupling

\[
H_{\text{int}} = J' \sum_n \left[ S_1(2n+1) + S_1(2n+3) \right] \cdot S_2(2n+2),
\]

and bosonize it with the result \(H_{\text{int}} \approx -4J'a_0 \int dx \ n_1(x) \cdot \ n_2(x)\), where we have kept only the strongly relevant staggered parts and the marginal current-current terms are discarded. The nice feature of this result is that when we compare it with the bosonization of the standard square 2-leg ladder \(H_{\text{int}} \approx J'a_0 \int dx \ n_1(x) \cdot \ n_2(x)\) and the standard zig-zag ladder \(H_{\text{int}} \approx J'a_0 \int dx \left[ -\partial_1 n_2(x) \right] \cdot \ n_2(x) + (-1)^n n_1(x)\) we find that our decorated zigzag ladder \((N_p = 2)\) produce a gap of the same type as the square ladder (both unfrustrated) and not related to the standard zigzag ladder which is dimerized. Therefore, this supports the existence of a Haldane phase in our \(N_p = 2\) diagonal ladder.

\(\text{Experimental Proposal:}\) Let us now turn to the experimental realization of diagonal ladders mentioned at the beginning based on cuprate materials. We find that it is possible to modify the basic \(CuO_2\)-stoichiometry of the cuprate planes in order to arrange the \(Cu\) sites and the \(O\) sites in links of 180 degrees with the precise shape of a diagonal ladder, while each diagonal ladder are weakly interacting among each other because they share links of \(Cu - O - Cu\) making 90 degrees that are much weaker. This construction for the Heisenberg interaction \(H\), is based on the superexchange mechanism among \(Cu\) sites mediated by interstitial \(O\) sites which is stronger when the sites \(Cu-O\) are aligned in 180 degrees. An example of our construction for the first \(N_p = 1, 2\) diagonal ladders \(2\) is shown in Fig. 5 corresponding to a stoichiometry of \(Cu_3O_4\) and \(Cu_2O_3\), respectively.

FIG. 5: \(N_p = 1\) (left) and \(N_p = 2\) (right) weakly interacting diagonal ladders in cuprate planes. Solid circles are \(Cu\) sites and the lattice sites are the \(O\) interstitial sites.

The outcome of our general construction is summarized in the following series of cuprate materials based on Stroncium:

\[
\begin{align*}
S_{r_{n-1}Cu_{n+1}O_{2n}}: n = 2, 4, \ldots & \rightarrow N_p = 1, 3, \ldots \\
S_{r_{n-1}Cu_{n+1}O_{2n}}: n = 3, 5, \ldots & \rightarrow N_p = 2, 4, \ldots
\end{align*}
\]

Interestingly enough, the series of cuprates with \(n\) odd has been studied experimentally as a set of square ladders with variable number of legs \(n_1\), both even and odd. What we have found is that our diagonal ladders with \(N_p\) even are allomorphic with all the square ladders. This makes sense since we have found both gapped and gapless behaviour in \(N_p\) even diagonal ladders \(2\). It is remarkable that each of the series in our classification \(2\) of universality classes corresponds to a different series in the same family of cuprate materials and it may allow for an experimental test of those complex behaviours found in diagonal quantum spin ladders.

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[1] E. Dagotto and T.M. Rice, Science 271, 618 (1996).
[2] G. Sierra, M. A. Martin-Delgado, S. R. White, D. J. Scalapino, J. Dukelsky, Phys. Rev. B 59, 7973 1999.
[3] J.M. Tranquada et al., Nature 375, 561 (1995).
[4] S.R. White and D.J. Scalapino, Phys. Rev. Lett. 80, 1272(1998).
[5] E.P. Raposo and M.D. Coutinho-Filho, Phys. Rev. B 59, 14384 (1999).
[6] M. Azuma et al. Phys. Rev. Lett. 73, 3463 (1994).
[7] T.M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. 23, 445 (1993).
[8] S. Gopalan, T.M. Rice and M. Sigrist, Phys. Rev. B 49, 8901 (1994).
[9] S.R. White, R.M. Noack, D. J. Scalapino; Phys. Rev. Lett. 73, 886 (1994).
[10] S.R. White, Phys. Rev. Lett. 69, 2863 (1992).
[11] S.R. White, Phys. Rev. B 48, 10345 (1993).
[12] S. R. White and I. Affleck Phys. Rev. B 54, 9862 (1996).
[13] F.D.M. Haldane, Phys. Lett. 93A, 464 (1983); Phys. Rev. Lett. 50, 1153 (1983).
[14] I. Affleck, T. Kennedy, E.H. Lieb and H. Tasaki, Commun. Math. Phys. 115, 477 (1988).
[15] M. den Nijs, K. Rommelse, Phys. Rev. B 40, 4709 (1989); T. Kennedy, H. Tasaki, Phys. Rev. B 45, 304 (1992).
[16] G. Sierra, J. Math. Phys. A 29, 3299 (1996).