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# **Twisted-order parameter applied to dimerized ladders**

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#### Abstract

We apply the twisted-order parameter (TOP) for dimerized quantum spin ladders to locate the critical points that separate gapped phases representing quantum spin liquids of various types. Using the density matrix renormalization group (DMRG), method, we find that the TOP is a good order parameter for these systems regardless of the number of legs. As a check, we reproduce with the DMRG and periodic boundary conditions the computations previously done with quantum Monte Carlo for one-dimensional S = 1/2, S = 1, S = 3/2 and S = 2 Heisenberg chains with alternating bonds.

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(Some figures in this article are in colour only in the electronic version)

# 1. Introduction

The physics of quantum spin ladders with dimerization [1] is an emblematic example of quantum phase transitions with a rich structure of both gapless and gapped phases [2–4, 35]. The main issue in their quantum phase diagrams is to determine the location of critical points or lines, which typically separate massive phases. These phases exhibit quite strongly correlated properties like Haldane phases [5], an example of quantum spin liquid of great interest in condensed matter systems. Analytical methods have been applied to uncover this rich phase structure, some of them non-perturbative [1, 6–9]. However, they are not sufficient to study with enough precision the whole range of coupling parameters entering in their quantum lattice Hamiltonians and, consequently, they have to be complemented with numerical studies [10–13], which sometimes modify the conclusions achieved with analytical methods, either quantitatively and/or qualitatively.

Quantum spin ladder systems are not mere theoretical constructs, but they have been experimentally synthesized in several types of materials [14–16, 18, 19], some of them as interesting as the superconducting cuprate compounds or other classes of materials which allow not only for antiferromagnetic couplings but also for ferromagnetic ones as we shall be considering in this work. Ladder systems are also valuable candidates to implement their

physics in simulable optical lattices [20, 21], where the coupling constants of the models could be externally manipulated more easily than with standard materials. Furthermore, quantum spin chains and ladders have played a central role for ground test numerical simulations when the density matrix renormalization group (DMRG) was introduced [22–26].

A diversity of variants of quantum spin liquids appear as gapped phases in these dimerized spin ladders. These types of spin orders have been initially classified resorting to the string-order parameter (SOP) [27, 28]. However, this initial SOP parameter was only valid for systems with spin magnitude S = 1. Then, a generalization valid for both integer and half-integer spin systems was introduced [29] and recently, we have been able to check their validity in a large class of dimerized spin ladders [13] and we have found that the generalized SOP serves as a good order parameter to distinguish the many quantum phases appearing in those ladders when their number of legs and spin couplings are varied.

When moving from one gapped phase to another, this process generically implies crossing a critical point or line. Although the SOP parameter can detect the change associated with this phase crossing, however it does not perform so well when trying to locate the position of those critical points. To this end, another order parameter called twisted-order parameter (TOP) has been introduced for spin chains [30] and some ladders [31, 32]. The TOP being non-local, it can be considered as a close relative of the SOP. In fact, both the SOP and the TOP are suitable to identify the valence bond solid content of a quantum phase. However their own peculiarities make each of them more suitable for certain tasks: the SOP gives more information about the valence bond solid content of a given quantum state and, moreover, allows us to unequivocally classify each particular type of valence bond solid. On the other hand, the TOP performs better than the SOP in the task of accurately locating the critical points in a quantum phase transition between valence bond solid phases. In the end, both parameters together provide a very powerful machinery to study the physics of these particular spin liquid systems.

The idea behind the TOP comes from the twist operator introduced in the proof of the Lieb–Schulz–Mattis theorem (LSM) [33, 34] in one-dimensional quantum spin systems. Under certain circumstances, namely, for half-integer *S*-spin chains, the system is proved to be gapless by creating a sort of twisted excited state along the chain, whose energy gap with respect to the ground state vanishes in the thermodynamic limit as 1/N, where *N* is the length of the chain. Although this twist operator cannot be conclusive for the case of integer *S*-spin chains, thereby opening the door for the celebrated Haldane conjecture [5], it turns out that it can be used to locate the critical points of dimerized chains of arbitrary spins, either integer or half-integer. The way to see this connection is by means of the valence bond solid (VBS) states used as trial wavefunctions to qualitatively represent those gapped quantum phases.

The existence of extensions of the LSM theorem for spin ladders [35] can also be used as a hint to trying to extend the notion of the TOP parameter to more complicated lattices beyond one-dimensional systems. For spin ladders with  $S = \frac{1}{2}$  spins, this generalized LSM theorem only works for an odd number of legs. Interestingly enough, we have found that the generalized TOP parameter works for locating the critical points, regardless of the number of legs.

This paper is organized as follows: in section 2 we introduce a set of quantum lattice Hamiltonians for spin ladders which present two different patterns of dimerization, either staggered or columnar, as well as antiferromagnetic or ferromagnetic couplings between their legs (chains); in section 3 we present our numerical results for the TOP parameter measured in those dimerized spin ladders using DMRG calculations. With this information we can plot the TOP versus the dimerization strength and detect critical points by the vanishing of the TOP parameter. Upon varying the dimerization patterns and the ferro- or antiferro-types of rung couplings, the number of zeros and shape of the TOP also changes in characteristic forms

that serve us to distinguish among the set of quantum ladder Hamiltonians introduced in the previous section. Section 4 is devoted to conclusions.

#### 2. Models of dimerized spin ladders

In this paper, we study quantum spin ladders that can be viewed as a certain number of bond-alternated Heisenberg chains stacked one on top of another and coupled between them via a coupling constant J' corresponding to a Heisenberg-like spin interaction. The bond alternation between neighbor spins on the same leg is such that every strong bond is followed by a weaker one. Every leg can then begin either with a strong or weak coupling, and that initial choice determines the dimerization pattern all the way through the ladder.

Then, to characterize completely our ladders we have to specify some parameters: the number of legs  $n_l$ , the ferromagnetic J' < 0 or antiferromagnetic J' > 0 nature of the Heisenberg coupling between legs and the dimerization pattern of every leg, given by the coupling constant  $\gamma$ .

The Hamiltonian that gives raise to this general set of families of dimerized Heisenberg ladders is

$$H^{\text{OBC}} = \sum_{\ell} \sum_{i} J_{i,\ell} \mathbf{S}_i(\ell) \cdot \mathbf{S}_{i+1}(\ell) + J' \sum_{\ell,i} \mathbf{S}_i(\ell) \cdot \mathbf{S}_i(\ell+1),$$
(1)

where  $S_i(\ell)$  denotes a S = 1/2 spin operator at the site *i* in the leg  $\ell$ , with i = 1, ..., N and  $\ell = 1, ..., n_l$ . The set of couplings denoted by  $J_{i,\ell}$  endows the ladders with certain dimerization patterns to be specified below.

We shall focus our attention on two- and three-leg ladders, in addition to spin chains. These cases will suffice to clarify the behavior of the TOP parameter under diverse dimerization patterns. Moreover, among the different possibilities of establishing a dimerization pattern on every leg, we will only be interested in two particular arrangements of bonds. We will denote the *staggering* dimerization pattern that with a  $J_{i,\ell}$  distribution of the form  $J_{i,\ell} = 1 + (-1)^{i+\ell}\gamma$  while the *columnar* pattern has a distribution  $J_{i,\ell} = 1 - (-1)^i \gamma$ , i.e., all the legs begin with a strong bond. In both cases the parameter  $\gamma$  is constrained to be within  $-1 \leq \gamma \leq 1$ .

We will also be interested in using not only open boundary conditions but also periodic ones. In this case, we have to modify the Hamiltonian (1) to take into account the interactions between both ends:

$$H^{\text{PBC}} = H^{\text{OBC}} + \sum_{\ell} J_{N,\ell} \mathbf{S}_N(\ell) \cdot \mathbf{S}_1(\ell).$$
<sup>(2)</sup>

Equation (1) is not translationally invariant. In contrast, if we consider ladders with an even number (greater than two) of sites per leg and using periodic boundary conditions, the Hamiltonian (2) is invariant under translations of the form  $S_i(\ell) \rightarrow S_{i+2}(\ell)$  and also under reversal of the dimerization strength  $\gamma \leftrightarrow -\gamma$ .

The number of possible combinations of those ingredients described above is still high, and not all of them may have critical properties. This fact will depend essentially on the staggering pattern and coupling constant J'. In particular, for ladders with two and three legs, the models that may have critical phases for certain configurations of the microscopic parameters are the following ones: (i) the staggered antiferromagnetic two-leg ladder, (ii) the columnar ferromagnetic two-leg ladder, (iii) the staggered antiferromagnetic three-leg ladder and (iv) the columnar ferromagnetic three-leg ladder. These models are depicted in figure 1.



**Figure 1.** Different dimerization patterns in two- and three-leg spin ladders: (*a*) and (*c*) are staggered, (*b*) and (*d*) are columnar. Thicker lines correspond to a coupling constant  $J_{i,\ell} = 1 + \gamma$  and thinner ones to  $J_{i,\ell} = 1 - \gamma$ .

# 3. Results

The natural extension of the TOP as defined in [30] to systems with many legs is as follows:

$$z_{\ell}^{1} := \langle \psi_{0} | \exp\left\{\frac{2\pi i}{N} \sum_{j=1}^{N} j S_{j}^{z}\right\} | \psi_{0} \rangle, \qquad (3)$$

where each operator now includes the contribution coming from each leg of the ladder  $S_i = \sum_{\ell} S_i(\ell)$ .

It is worth recalling that, despite the TOP is in general a complex number, it has been proved [30] that, both using open and periodic boundary conditions, the imaginary part of this parameter decays to zero as the total size N increases.

Much like the string-order parameter (SOP), the TOP is a non-local parameter since it involves non-local measurements. However, unlike the SOP, the success of the TOP relies on the  $2\pi$  twist carried out between both ends of the system. This fact makes it unclear how will the DMRG perform when measuring it. This is in sharp contrast with the SOP case, which can be accurately measured using only a representative subsystem within the bulk of the whole system.

#### 3.1. Spin chains

Due to this uncertainty and as a first check, we have reproduced the quantum Monte Carlo results for one-dimensional dimerized chains [30] using DMRG-adapted methods. Figure 2 shows the TOP computed for these chains using periodic boundary conditions. To compute these values the number of DMRG sweeps was set to three, the number of retained states of the density matrix was m = 200 and the Lanczos tolerance equal to  $10^{-10}$ . The discarded weight of the eigenstates of the density matrix will range throughout the computations in this paper from  $10^{-6}$  in the worst cases to values around  $10^{-9}$  in the vast majority of the runs.



Figure 2. DMRG computation of the TOP for different one-dimensional Heisenberg chains with alternated bonds. The size of the chains is L = 64 and periodic boundary conditions have been used.

With these parameters, the results obtained using the DMRG and quantum Monte Carlo agree almost identically. In order to go a bit further and obtain better estimates of these critical points, using DMRG it is more convenient to use open chains. Figure 3 represents the TOP computed using open boundary conditions and different sizes of the chains. The largest size L = 150 was computed performing four DMRG sweeps, m = 300 and the tolerance equal to  $10^{-9}$ , the less demanding case L = 80 required two sweeps, m = 120 and the tolerance equal to  $10^{-8}$ . The critical points of each chain are those where the TOP is zero. Looking at the different graphs two observations are in order: on one hand we see that the location of the critical points is overestimated in the case of periodic boundary conditions compared to the case of open chains. On the other hand, the values of the critical points computed with open boundary conditions are in good agreement with the values of these points computed in the thermodynamic limit in other works [30]. In fact, from figure 3 and the curves with L = 150 we see that for the S = 1 chain we obtain  $\gamma_c = 0.254$ , for S = 3/2,  $\gamma_c = 0.426$ . The case with S = 2 has two critical points at  $\gamma_c = 0.184$  and  $\gamma_c = 0.522$ . These values can be respectively compared with the previously computed  $\gamma_c = 0.25997(3)$ ,  $\gamma_c = 0.43131(7)$ ,  $\gamma_{\rm c} = 0.1866(7), 0.5500(1).$ 

Regarding the critical point  $\gamma_c = 0$  in the cases with S = 1/2 and S = 3/2, we observe that the TOP unambiguously goes to zero using periodic boundary conditions. With open boundary conditions, however, the TOP is still far from zero even with L = 150, moreover its value does not decrease noticeably from L = 80 to L = 150. In view of these results we do not expect that the TOP will decay to zero with increasing sizes, since L = 150 is by far a large size to capture the bulk physics of these systems. Note that this fact, although surprising, is not in contradiction with the established knowledge, namely the Lieb–Schultz–Mattis theorem is not applicable here because open boundary conditions break translation invariance. On the other hand, the ability of the twisted-order parameter to detect phase transitions between valence bond solids relies on the fact that it changes the sign according to the exact nature of the VBS in question, but nothing has been stated about its continuity at a critical point. Therefore this observed behavior seems to be an unexpected difference between open and periodic boundary conditions.



**Figure 3.** TOP computed in various Heisenberg chains with alternated bonds and different spin values: (*a*) S = 1/2, (*b*) S = 1, (*c*) S = 3/2, (*d*) S = 2. Computations using open boundary conditions properly capture the location of the critical points as we increase the size of the system, however the convergence of the TOP toward zero at the particular point  $\gamma_c = 0$  in the graphs (*a*) and (*c*) is very slow and makes a difference between both types of boundary conditions.

# 3.2. Spin ladders

In the rest of this section we will measure the TOP in the models described previously in section 2 in order to test whether or not it can also be successfully applied to non-strictly one-dimensional cases.



**Figure 4.** TOP computed in ladders with columnar and staggering dimerization. The constant J' has a fixed value equal to J' = -5 in the two- and three-leg ladder with columnar dimerization and J' = 1 in the two and three leg with staggered dimerization. Periodic boundary conditions have been used. The size of the two-leg ladders is  $L = 2 \times 60$ , and  $L = 3 \times 60$  for the three-leg ladders.

**Table 1.** Location of some critical points of different dimerized ladders. The identification of each ladder is done by means of the number of legs: two or three, and the dimerization pattern: staggered or columnar. We provide the values obtained with the TOP and the corresponding ones computed directly looking at the vanishing of the gap. References where these last values have been obtained from are given in the text.

Ladder	J'	ТОР	Other
3, Stagg.	1.0	$\gamma_{\rm c} = 0.001, -0.542, 0.536$	$\gamma_{\rm c} = 0, \pm 0.527$
3, Col.	-5.0	$\gamma_{\rm c} = 0.005, -0.372, 0.368$	$\gamma_c = 0, \pm 0.335$
2, Stagg.	1.0	$\gamma_{\rm c} = -0.38, 0.38$	$\gamma_{\rm c} = \pm 0.34$
2, Col.	-5.0	$\gamma_{\rm c} = -0.212, 0.211$	$\gamma_{\rm c} = \pm 0.196$

We saw in the previous section that some differences related to the continuity of the TOP may appear between open boundary conditions and periodic boundary conditions. Moreover, as was discussed in section 2, our models are invariant with periodic boundary conditions under sign reversal of the dimerization strength. This means that for a given computed critical point, say  $\gamma_c$ , there must exist another one equal to  $-\gamma_c$ . The difference in the value of these opposite points will then give us a hint about the truncation error of our DMRG computations. For these reasons we will use periodic boundary conditions in this section.

In figure 4 we have computed the TOP on each one of the critical ladders described in the previous section. To run the DMRG we have set m = 340, the tolerance equal to  $10^{-9}$  and performed three sweeps. For each one of the ladders we have used an arbitrary value of the constant J'. The critical lines of these models have been obtained by other techniques in [10, 12, 13]. Since we are using periodic boundary conditions we are constrained to use smaller sizes than those considered in the references and hence no exact agreement is expected. With this consideration in mind, the location of the critical points in figure 4, that is, the points where the TOP is zero, is in good agreement with those of the references, as comes out from table 1.

Remember that a valence bond solid in a system of spin *S* can be denoted generally as (m, n)-VBS where m + n = 2S. The sign of the TOP is related to the nature of the VBS phase. From its definition it can be seen that its sign is given by a factor  $(-1)^k$ , where *k* is the number of isolated spins at the end of the chain. More explicitly, k = m if the number of sites is odd and k = n if it is even.

The TOP itself may result insufficient to characterize a general (m, n)-VBS state. We see however in figure 4 that the sign of the TOP is coherent with the phase diagram of these models obtained in other works by means of the SOP. That is, in the cases of the two- and three-leg ladders with columnar dimerization the TOP is negative from  $\gamma = 0$  up to the corresponding critical values  $\gamma_c$  where the TOP is zero, and then the TOP is positive all the way to  $\gamma = 1$ . On the other hand, the behavior of the TOP with the two- and three-leg ladders with staggered dimerization is the contrary. Since our computations have been all done using an even number of sites per leg, the sign of the TOP agrees with the characterization of the phases of each model done by means of the generalized SOP in [12, 13]. That is, moving from  $\gamma = 0$  to  $\gamma = 1$  the two-leg ladder with columnar dimerization moves from a (1, 1)-VBS to a (2, 0)-VBS while the three-leg ladder with columnar dimerization moves from a (2, 1)-VBS to a (3, 0)-VBS. In these cases k = 1 and the sign of the TOP is negative in the first phases, and k = 0 and the sign of the TOP is positive in the second phases. In the case of the three-leg ladder with staggered dimerization we move from a (1, 2)-VBS to a (2, 1)-VBS and again the sign of the TOP is correct according to the value of k. We have no information on the VBS phases found in the two-leg ladder with staggered dimerization. In this particular case the information derived from the TOP does not allow us to uniquely determine each phase. That is, there is only one possible state that corresponds with a negative value of the TOP, namely a (1, 1)-VBS. In the case of a positive value of the TOP we have however two possible states: a (2, 0)-VBS or a (0, 2)-VBS.

## 4. Conclusions

The results shown in the previous section reveal that the DMRG algorithm is well suited to compute the twisted-order parameter even with open boundary conditions. We have applied TOP parameter to four different spin ladder systems and estimated the location of their critical points. We find agreement with other DMRG calculations which compute the vanishing of the gap directly. We have checked that the TOP computation is not only restricted to strictly one-dimensional systems but it also works in two- and three-leg ladders. This holds true despite that the LSM theorem based on the twist operator only works for ladders with an odd number of legs and  $S = \frac{1}{2}$  spins. In this sense, the twisted-order parameter serves as a suitable and complementary tool to the string-order parameter in the characterization of quantum phases in dimerized spin systems.

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