

**Massive spinons in  $S = 1/2$  spin chains: Spinon-pair operator representation**

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Spinons are among the generic excitations in one-dimensional spin systems; they can be massless or massive. The quantitative description of massive spinons poses a considerable challenge in spite of various variational approaches. We show that a representation in terms of hopping and Bogoliubov spinon processes, which we call “spinon-pair” operators, and their combination is possible. We refer to such a representation as second quantized form. Neglecting terms which change the number of spinons yields the variational results. Treating the bilinear and quartic terms by continuous unitary transformations leads to considerably improved results. Thus, we provide the proof of principle that systems displaying massive spinons as elementary excitations can be treated in second quantization based on spinon-pair representation.

DOI: [10.1103/PhysRevB.95.155136](https://doi.org/10.1103/PhysRevB.95.155136)**I. INTRODUCTION**

Quantum magnets constitute a flourishing field of research. In particular, the search for unconventional excitations and their quantitative understanding represents an important issue of current interest.

The elementary excitations which are known best are spin waves or magnons. They appear as massless Goldstone bosons in long-ranged ordered magnets such as ferromagnets or antiferromagnets. Their effect on the total spin of the system is integer; i.e., they change the total magnetization or the sublattice magnetization by one  $\hbar$  [1,2]. Henceforth, we set Planck’s constant to unity for the sake of simplicity. Another class of integer excitations is triplons, i.e., gapped dressed particles with  $S = 1$  as they appear in valence bond solids, for instance in all models resulting from coupling spin dimers of  $S = 1/2$  in one dimension (see, e.g., Refs. [3–6]), in two dimensions (see, e.g., Refs. [3,7–9]), and in three dimensions (see, e.g., Refs. [10–14]).

But in particular in low-dimensional systems, fractionalization may occur. This means that the integer excitations decompose into several, mostly two, fractional excitations. The famous example is the  $S = 1/2$  spinons in the nearest-neighbor Heisenberg chain [15–18] with the Hamiltonian

$$H := J_1 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}, \quad (1)$$

where  $\mathbf{S}_i$  defines the spin  $S = 1/2$  operator at site  $i$  and the sum runs over the sites of a chain. The couplings  $J_1$  and  $J_2$  control the interaction strengths between nearest-neighbor (NN) and next-nearest-neighbor (NNN) sites, respectively. The NN case is given by  $J_2 = 0$ . For later use, we define the relative coupling  $\alpha := J_2/J_1$  which is a measure of the degree of frustration.

Another analytically solvable case of massless spinons is realized in the Haldane-Shastry model [19,20]. The Hamiltonian of this model is related to the one in Eq. (1), but for certain long-range couplings  $J_n$ . The concept of massless spinons is used to develop effective or approximate descriptions of a multitude of systems, even if the microscopic Hamiltonian does not match

perfectly [21], but it can provide a starting point for perturbative inclusion of interchain couplings [22–24]. Clearly, massless spinons represent an intensive field of research.

In addition, current research addresses massive spinons, i.e., spinons of which the creation requires a finite amount of energy. In one dimension, strongly frustrated chains such as given by the Hamiltonian (1) for  $\alpha \gtrsim 0.241$  display such elementary excitations [25–27]. Four-spin and six-spin interaction terms can be considered as well [28,29] which lead to spontaneous dimerization even without frustration. In two dimensions, systems such as kagome lattices are prone to be governed by fractional massive spinons [30–34]. Even in three dimensions, fractionalization takes place leading to magnetic monopoles [35–37]. But these occur in highly anisotropic spin models which marks an important difference to the spinons mentioned above in one and two dimensions.

Given the great interest in spinons and the fact that massive spinons are less well understood than their massless counterparts we study massive spinons in the present article. We start from the description introduced by Shastry and Sutherland [25] in a second quantized form. Conceptually, we extend the description of Shastry and Sutherland to general chains. As a proof of principle we will consider the frustrated spin chain in (1) for arbitrary frustration  $\alpha$ . We do not attempt to define the creation or annihilation of single spinons. Instead, we introduce spinon-pair operators which denote bilinear processes involving spinons, i.e., hopping of spinons or pairwise creation or annihilation of them. In addition, we keep track of the interactions of two spinons and of the decay of one spinon into three. We show that it is indeed possible to systematically define the Hamiltonian in terms of spinon pairs.

In a second step, we analyze the obtained second quantized Hamiltonian by continuous unitary transformations to extract the physical relevant properties. The processes changing the number of spinons are rotated away in this fashion. But their renormalizing effects on the physical properties are retained, at least on the level of our approximations. The physical properties comprise the effective spinon dispersion and the value of the spin gap in particular. In this way, we show that a second quantized description of massive spinons is possible on the proof-of-principle level.

The results obtained are considerably improved over the variational results. This illustrates the potential behind the

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idea to formulate microscopic Hamiltonian in terms of their elementary excitations. Of course, this route requires knowing what these quantities are. Often, however, this is the case. Thus, we believe that the approach pursued here can be transferred to many other physical systems as well.

The article proceeds as follows. In Sec. II we introduce a complete spinon basis for the subspaces with total spin  $S_t = 0$ ,  $S_t = \frac{1}{2}$ , and  $S_t = 1$ . Subsequently, in Sec. III the states in this basis are orthonormalized. This allows us to introduce spinon-pair operators for second quantization in Sec. IV. This formalism is applied to the frustrated Heisenberg chain with nearest-neighbor and next-nearest-neighbor interactions in Sec. V. The employed method of continuous unitary transformations is introduced in Sec. VI while the final results are presented in Sec. VII. The conclusions and the outlook terminate the paper in Sec. VIII.

## II. SPINON BASIS

Here we introduce a basis for spinon states in chains consisting of localized spins  $S = 1/2$ . We distinguish between vacua and states with various numbers of spinons. This does not imply that the vacua are ground states of the spin chains studied finally. The first aim of this section and the subsequent two sections is to express the Hamiltonian in terms of spinons. Then a continuous unitary transformation is applied to obtain quantitative results.

For a chain with an even number of sites, the 0-spinon state (spinon vacuum) is defined such that each spin at a site forms a singlet with its neighboring site. For a chain of length  $L$ , the 0-spinon state is given by

$$|0\rangle := \bigotimes_{n=-L/4}^{L/4-1} [2n, 2n+1] = |\dots \bullet \blacktriangleright \bullet \blacktriangleright \bullet \blacktriangleright \bullet \blacktriangleright \dots\rangle \quad (2)$$

where

$$[i, i+d] := |\bullet \blacktriangleright \bullet\rangle_{i, i+d} := \frac{1}{\sqrt{2}} (|\uparrow\rangle_i |\downarrow\rangle_{i+d} - |\downarrow\rangle_i |\uparrow\rangle_{i+d}) \quad (3)$$

depicts the singlet state between lattice positions  $i$  and  $i+d$ . The states  $|\uparrow\rangle_i$  and  $|\downarrow\rangle_i$  are eigenvectors of the  $S_i^z$  operator with eigenvalues  $+1/2$  and  $-1/2$ , respectively. Planck's constant is set to unity.

For the periodic boundary condition (PBC) there are two vacua which differ by a translation by one site. For the open boundary condition (OBC) these two states constitute the vacuum and a 2-spinon state with spinons at both boundary points. The spinon vacuum for the OBC is a product of singlet; it is the same as the well-known Majumdar-Ghosh (MG) state which represents the exact ground state of the  $J_1$ - $J_2$  Heisenberg chain, see Eq. (1), for  $J_2 = J_1/2 > 0$  [38,39]. This spinon vacuum can also be seen as a short-ranged "resonating valence-bond" (RVB) state [40,41] defined on a chain. Although spinons as spin- $\frac{1}{2}$  quasiparticles always appear in pairs for given even chain size, understanding the dynamics of a single spinon is necessary to describe deconfined spinon pairs [25]. This parallels fermionic systems with a fixed number of particles.

A spinon is defined as the domain-wall separating two possible vacua [25]. The 1-spinon state  $|\phi_i^\sigma\rangle$  with the spin index  $\sigma = \uparrow, \downarrow$  is given by

$$\begin{aligned} |\phi_i^\uparrow\rangle &:= \dots \otimes [i-2, i-1] \otimes \uparrow_i \otimes [i+1, i+2] \otimes \dots \\ &=: |\dots \bullet \blacktriangleright \bullet \blacktriangleright \uparrow_i \bullet \blacktriangleright \bullet \blacktriangleright \dots\rangle. \end{aligned} \quad (4)$$

and similarly for  $|\phi_i^\downarrow\rangle$ . For the OBC, the spinon can exist only on the odd or on the even sublattice, but for the PBC it can be on either of them. The 1-spinon states are not orthonormal displaying the overlap [42]

$$\langle \phi_i^\sigma | \phi_j^{\sigma'} \rangle = \delta_{\sigma, \sigma'} \left(-\frac{1}{2}\right)^{\frac{|i-j|}{2}}, \quad (i-j) \in \text{even}, \quad (5)$$

and zero for  $(i-j)$  odd in the limit  $L \rightarrow \infty$ .

The 2-spinon sector is spanned by singlet and triplet states. The singlet 2-spinon state  $|\phi_{i, i+d}^s\rangle$  with  $d \geq 3$  reads

$$|\phi_{i, i+d}^s\rangle := |\dots \bullet \blacktriangleright \bullet \blacktriangleright \dots \bullet \blacktriangleright \bullet \blacktriangleright \dots\rangle. \quad (6)$$

We notice that  $|\phi_{i, i+1}^s\rangle = |0\rangle$  and hence the singlet 2-spinon state with  $d=1$  is not defined because it is the vacuum state. In addition, there exists no 2-spinon state with even distance  $d$ .

Similarly, the triplet 2-spinon state  $|\phi_{i, i+d}^{t,p}\rangle$  with  $d \geq 1$  and the flavor  $p = x, y, z$  is given by

$$|\phi_{i, i+d}^{t,p}\rangle := |\dots \bullet \blacktriangleright \bullet \overset{p}{\curvearrowright} \bullet \blacktriangleright \bullet \blacktriangleright \dots\rangle, \quad (7)$$

where

$$\begin{aligned} |\bullet \overset{p}{\curvearrowright} \bullet\rangle_{j, j+d} &:= \begin{cases} \frac{1}{\sqrt{2}} (|\downarrow\rangle_j |\downarrow\rangle_{j+d} - |\uparrow\rangle_j |\uparrow\rangle_{j+d}), & p = x \\ \frac{i}{\sqrt{2}} (|\uparrow\rangle_j |\uparrow\rangle_{j+d} + |\downarrow\rangle_j |\downarrow\rangle_{j+d}), & p = y \\ \frac{1}{\sqrt{2}} (|\uparrow\rangle_j |\downarrow\rangle_{j+d} + |\downarrow\rangle_j |\uparrow\rangle_{j+d}), & p = z \end{cases} \\ &=: \{j, j+d\}_p \end{aligned} \quad (8)$$

denotes a triplet bond with the flavor  $p$  between sites  $j$  and  $j+d$  [3].

The overlap between the spinon vacuum (2) and the singlet 2-spinon state (6) is given by

$$\langle 0 | \phi_{i, i+d}^s \rangle = \left(-\frac{1}{2}\right)^{\frac{d-1}{2}}. \quad (9)$$

We also have the following overlap between singlet 2-spinon states:

$$\langle \phi_{j, j+d_2}^s | \phi_{i, i+d_1}^s \rangle = \begin{cases} \left(-\frac{1}{2}\right)^{\frac{d_1+d_2}{2}-1}, & n > d_1, \\ \left(-\frac{1}{2}\right)^{\frac{d_2-d_1}{2}+n}, & d_1 - d_2 \leq n < d_1, \\ \left(-\frac{1}{2}\right)^{\frac{d_1-d_2}{2}}, & n \leq d_1 - d_2, \end{cases} \quad (10)$$

where  $n := j - i \geq 0$ . For triplet 2-spinon states, the same relation holds, except that for  $n > d_1$  the result is zero.

How can we construct states which contain more than two spinons? In this paper, we focus on the subspaces with the total spin  $S_{\text{tot}} = 0$  ( $L$  even),  $S_{\text{tot}} = \frac{1}{2}$  ( $L$  odd), and  $S_{\text{tot}} = 1$  ( $L$  even). For these cases, we show that a complete spinon basis can be systematically constructed. The systematic construction is important for the second quantization process that we want to introduce in the sequel.

By introducing longer ranged singlets in the spinon vacuum we create various states with total spin zero. But these states are not all linearly independent. This is so because “crossed” singlets can be expressed in terms of “nested” singlets and “distinct” singlets according to

$$|\text{crossed}\rangle = |\text{nested}\rangle + |\text{distinct}\rangle. \quad (11)$$

This relation is valid for two arbitrary singlet bonds on arbitrary sites in the sequence of the chain. By recursive application of Eq. (11) any crossed singlet can be reexpressed in terms of nested and distinct singlets. One can choose any two groups from the three groups “distinct,” “nested,” and “crossed” singlets to have a complete basis spanning the  $S_{\text{tot}} = 0$  Hilbert space. Here, we adopt singlets of the type “distinct” and “nested” as they are already used in the definition of the 0-spinon and 2-spinon states. Thus, this choice appears to be the most suitable to define spinon-pair operators. We notice that the states with crossed singlets do not necessarily contain a well-defined number of spinons.

Similar to the case of the  $S_{\text{tot}} = 0$  subspace, by introducing singlet spinon pairs above 1-spinon states we can construct 3-spinon, 5-spinon, and higher spinon states with the total spin  $S_{\text{tot}} = \frac{1}{2}$ . The relation

$$|\text{crossed}\rangle = |\text{distinct}\rangle + |\text{nested}\rangle \quad (12)$$

makes the basis of all such states overcomplete. The positions in (12) are assumed to be arbitrary ones along the chain. Any state with a nested spinon can be expanded in terms of states in which the spinon is either before or beyond the singlet bond. In order to avoid overcounting, we restrict the  $S_{\text{tot}} = \frac{1}{2}$  subspace such that no single spinon occurs inside a singlet bond.

The states with  $S_{\text{tot}} = 1$  can be generated by replacing one of the singlet bonds of a state in the  $S_{\text{tot}} = 0$  subspace by a triplet bond. The identity

$$|\text{crossed}\rangle = |\text{nested}\rangle + |\text{distinct}\rangle \quad (13)$$

together with Eq. (11) justifies why no crossed bond needs to be considered in the  $S_{\text{tot}} = 1$  subspace. In Eq. (13) we omitted the flavor label  $p$  from the triplet bonds because the relation is valid for any fixed value of  $p$ . In addition to (13), we find

$$|\text{crossed}\rangle = |\text{distinct}\rangle + |\text{nested}\rangle + |\text{crossed}\rangle, \quad (14)$$

which is a relation between distinct and nested singlet and triplet bonds. We notice that (13) and (14) are two independent equations. By recursive application of Eq. (14) one can eliminate all nested triplet bonds. This means that in the

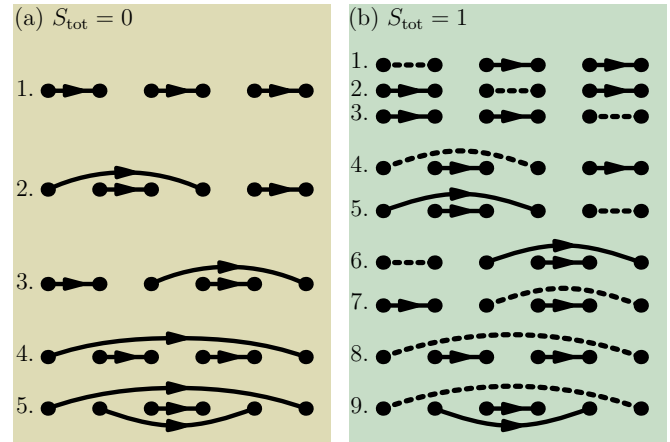


FIG. 1. The spinon states with (a)  $S_{\text{tot}} = 0$  and (b)  $S_{\text{tot}} = 1$  on a 6-site cluster. Each triplet bond (dashed line) can have the flavor  $p = x, y, z$ . The  $S_{\text{tot}} = 1$  states are constructed from  $S_{\text{tot}} = 0$  states by replacing one singlet bond with a triplet bond; no nested triplet bond is allowed as explained in the main text.

construction of  $S_{\text{tot}} = 1$  subspace, no nested triplet bond needs to be considered. Alternatively, one may decide to use Eq. (14) to consider only nearest-neighbor (NN) triplet bonds in the  $S_{\text{tot}} = 1$  subspace. But this leads to an overcomplete basis for the  $S_{\text{tot}} = 1$  sector and further restriction is required which would complicate the subsequent treatment.

This can be seen by inspecting the states on a 6-site cluster. In Fig. 1 we represent the  $S_{\text{tot}} = 0$  and the  $S_{\text{tot}} = 1$  spinon states of a 6-site cluster. One can also check that 14 spinon states with  $S_{\text{tot}} = 0$  and 28 ( $\times 3$ ) spinon states with  $S_{\text{tot}} = 1$  on an 8-site cluster can be successfully generated spanning the respective Hilbert subspaces.

### III. ORTHONORMALIZATION

The spinon basis introduced in the previous section is complete, but not orthonormal. In this section, we orthonormalize the spinon basis so that the basis can be used to define second quantized operators in the following.

We fix the vacuum as it is defined in Eq. (2). To make the 1-spinon states orthonormal to each other we employ the ansatz

$$|\Phi_i^\sigma\rangle = \alpha_1 |\phi_i^\sigma\rangle + \alpha_2 |\phi_{i-2}^\sigma\rangle \quad (15)$$

and determine the coefficients  $\alpha_1$  and  $\alpha_2$  such that  $\langle \Phi_i^\sigma | \Phi_j^{\sigma'} \rangle = \delta_{i,j} \delta_{\sigma,\sigma'}$  holds. The ansatz (15) for the orthonormal 1-spinon states is not unique but we did not find a simpler one; i.e., we think there is no other ansatz involving fewer sites. Using Eq. (5), we find two solutions

$$|\Phi_i^{\sigma,r}\rangle = \frac{1}{\sqrt{3}} (2 |\phi_i^\sigma\rangle + |\phi_{i+2}^\sigma\rangle), \quad (16a)$$

$$|\Phi_i^{\sigma,l}\rangle = \frac{1}{\sqrt{3}} (2 |\phi_i^\sigma\rangle - |\phi_{i-2}^\sigma\rangle), \quad (16b)$$

which we call orthonormal “right” and “left” 1-spinon states, respectively, and denote by the appropriate superscripts r or l.

One can choose any of these two solutions to form an orthonormal spinon basis [43]. We stress that in the orthonormal 1-spinon state the spinon is not localized at a single lattice site, but it has an extension of two lattice spacings to the right,  $|\Phi_i^{\sigma,t}\rangle$ , or to the left,  $|\Phi_i^{\sigma,l}\rangle$ . In the following, we use the 1-spinon state “left” and drop the index  $l$  to lighten the notation:  $|\Phi_i^\sigma\rangle := |\Phi_i^{\sigma,l}\rangle$ .

The orthonormal many-spinon states with larger distances between the spinons are constructed from the direct product of orthonormal 1-spinon states. Since each orthonormal spinon extends over two sites, this construction fails if the distance between spinons is 1. In this case the state is “distorted” and we need to perform an explicit orthonormalization to define it properly. The orthonormal singlet and triplet 2-spinon states for  $d \geq 3$  are given by

$$\begin{aligned} |\Phi_{i,i+d}^s\rangle &:= \sum_{\sigma\sigma'} \chi_{\sigma\sigma'}^s |\Phi_i^\sigma\rangle \otimes |\Phi_{i+d}^{\sigma'}\rangle \\ &= \frac{1}{3} (4 |\phi_{i,i+d}^s\rangle + 2 |\phi_{i-2,i+d}^s\rangle + 2 |\phi_{i,i+d-2}^s\rangle \\ &\quad + |\phi_{i-2,i+d-2}^s\rangle), \end{aligned} \quad (17a)$$

$$\begin{aligned} |\Phi_{i,i+d}^{t,p}\rangle &:= \sum_{\sigma\sigma'} \chi_{\sigma\sigma'}^{t,p} |\Phi_i^\sigma\rangle \otimes |\Phi_{i+d}^{\sigma'}\rangle \\ &= \frac{1}{3} (4 |\phi_{i,i+d}^{t,p}\rangle + 2 |\phi_{i-2,i+d}^{t,p}\rangle + 2 |\phi_{i,i+d-2}^{t,p}\rangle \\ &\quad + |\phi_{i-2,i+d-2}^{t,p}\rangle), \end{aligned} \quad (17b)$$

where  $\chi_{\sigma\sigma'}^s$  and  $\chi_{\sigma\sigma'}^{t,p}$  are the Clebsch-Gordan coefficients for singlet and triplet states. The orthonormal triplet state with  $d = 1$  is such a distorted state. To construct it, we start from

$$|\Phi_{i,i+1}^{t,p}\rangle := \frac{1}{N} (\alpha_1 |\phi_{i,i+1}^{t,p}\rangle + \alpha_2 |\phi_{i-2,i+1}^{t,p}\rangle + |\phi_{i-2,i-1}^{t,p}\rangle). \quad (18)$$

This ansatz is motivated by the extension of each orthonormal spinon by two sites to the left. Requiring that (18) is orthonormal to the triplet 2-spinon states leads to the nontrivial equations

$$\langle \Phi_{i-d+1,i+1}^{t,p} | \Phi_{i,i+1}^{t,p} \rangle = 0 \implies 2\alpha_1 - 3\alpha_2 = 0, \quad (19a)$$

$$\langle \Phi_{i-d-1,i-1}^{t,p} | \Phi_{i,i+1}^{t,p} \rangle = 0 \implies \alpha_2 - 2 = 0, \quad (19b)$$

with  $d \geq 3$ , and a normalization condition for  $N$ . One obtains

$$|\Phi_{i,i+1}^{t,p}\rangle = \frac{1}{\sqrt{6}} (3 |\phi_{i,i+1}^{t,p}\rangle + 2 |\phi_{i-2,i+1}^{t,p}\rangle + |\phi_{i-2,i-1}^{t,p}\rangle). \quad (20)$$

The orthonormal 3-spinon states are reported in Appendix A. We notice that the orthonormal  $n$ -spinon states can always be constructed from states with the same or a smaller number of spinons.

The many-spinon states constructed from the direct product of orthonormal 1-spinon states are not fully orthogonal. Some finite overlaps occur in the 3 and higher spinon subspaces. A finite overlap occurs if the positions of orthonormal spinons match. For instance, in the 3-spinon sector we find

$$\langle \Phi_i^\sigma \Phi_{i+n,i+n+d}^s | \Phi_{i,i+n}^s \Phi_{i+n+d}^\sigma \rangle = -\frac{1}{2}, \quad n \geq 3. \quad (21)$$

There is no such overlap in the 1-spinon and 2-spinon subspaces because after fixing the positions of the spinons there is only one possibility to form states with specific total spin and flavor. But in the 3-spinon subspace there are two possibilities; see the bra and the ket states in (21). This finite overlap is not a serious issue because subspaces with different numbers of spinons are mutually orthogonal. But to define the proper interactions in second quantization one has to carefully take the finite overlaps into account; see Appendix D.

All spinon states can be expanded in orthonormal states. For the 1-spinon state (4) and the singlet 2-spinon state (6) we find

$$|\phi_i^\sigma\rangle = \frac{\sqrt{3}}{2} \sum_{m \geq 0} \left(-\frac{1}{2}\right)^{\frac{m}{2}} |\Phi_{i-m}^\sigma\rangle, \quad (22a)$$

$$|\phi_{i,i+d}^s\rangle = -\frac{1}{2} |\phi_{i,i+d-2}^s\rangle + \frac{3}{4} \sum_{m \geq 0} \left(-\frac{1}{2}\right)^{\frac{m}{2}} |\Phi_{i-m,i+d}^s\rangle, \quad (22b)$$

with  $m$  even. These relations are obtained by reversing Eqs. (16b) and (17a). Equation (22b) is to be used in a recursive way starting from  $d = 3$ . We notice that  $|\phi_{i,i+1}^s\rangle := |0\rangle$ . A local spinon state represented in terms of orthonormal states becomes extended over the whole chain with a prefactor decreasing exponentially for increasing distance. Generally, in the expansion of an  $m$ -spinon state orthonormal states appear with  $m$  or fewer spinons.

## IV. SPINON-PAIR OPERATORS

### A. Definition

Any attempt to define single spinon creation or annihilation operators runs into severe problems. Typically, one has to work in a larger Hilbert space, for instance enlarge it artificially, and complement the description by a severe constraint so that the accessible Hilbert space is again the physical one [44].

In the present article, we want to follow a different route. We refrain from defining a single creation or annihilation event, but define spinon operators for pairs of spinons in a rather straightforward manner. No severe constraints are required to deal with the physical Hilbert space because creation and annihilation of spinons always happen in pairs. Spinon hopping does not alter the number of spinons so that it can also be expressed by a second quantized operator which addresses the hopping process as a whole.

There is an important point that has to be clarified before defining the spinon-pair operators. Considering a segment of the chain, there can be two local vacua  $|0_{i,i+d}\rangle$  and  $|\tilde{0}_{i,i+d}\rangle$  given by

$$|0_{i,i+d}\rangle := \left| \bullet \bullet \bullet \cdots \bullet \bullet \bullet \right\rangle_{i,i+d}, \quad (23a)$$

$$|\tilde{0}_{i,i+d}\rangle := \left| \bullet \bullet \bullet \cdots \bullet \bullet \bullet \right\rangle_{i,i+d}. \quad (23b)$$

Creation of two spinons at positions  $i$  and  $i+d$  from  $|0_{i,i+d}\rangle$  changes the state on the chain between sites  $i$  and  $i+d$ . However, a two-spinon creation from  $|\tilde{0}_{i,i+d}\rangle$  corresponds to a change in the state of the chain *before* site  $i$  and *beyond* site



$i + d$ . We call  $|0_{i,i+d}\rangle$  the “right” local vacuum and  $|\tilde{0}_{i,i+d}\rangle$  the “wrong” local vacuum.

The singlet operator  $\mathcal{S}_{i,i+d}^\dagger$  with  $d \geq 3$  is defined to create two orthonormal spinons at sites  $i$  and  $i + d$  with total spin zero if the state on the chain between sites  $i$  and  $i + d$  is the right local vacuum  $|0_{i,i+d}\rangle$ . This operator can be expressed as

$$\mathcal{S}_{i,i+d}^\dagger : |0_{i,i+d}\rangle \longrightarrow \left| \begin{array}{c} \curvearrowright \\ \circ \bullet \cdots \bullet \circ \\ \curvearrowleft \end{array} \right\rangle_{i,i+d} \quad (24)$$

where the states before  $i$  and beyond  $i + d$  are supposed to be arbitrary; they are not changed. The orthonormal spinons at positions  $i$  and  $i + d$  are indicated by empty circles. The result of  $\mathcal{S}_{i,i+d}^\dagger$  is zero if there is *any* other state different than  $|0_{i,i+d}\rangle$  between sites  $i$  and  $i + d$ . Hence, the singlet operator is defined only over odd distances  $d$ . We define  $\mathcal{S}_{i,i+1}^\dagger := 0$ .

Depending on the state on the chain sites  $i - 2, i - 1, i + 1$ , and  $i + 2$ , namely if they are occupied by spinons or not, the final state is distorted or not, as defined above. It is apparent from this definition that the singlet operator  $\mathcal{S}_{i,i+d}^\dagger$  is a string operator of which the action depends on the state between sites  $i - 2$  to  $i + d + 2$ . Moreover, we notice that there is no need to introduce additional operators to create distorted states at small distances. Each state from the  $S_{\text{tot}} = 0$  ( $S_{\text{tot}} = \frac{1}{2}$ ) subspace can be generated by applying the singlet operators on the spinon vacuum (a 1-spinon state).

The order of singlet operators does not matter in the creation of distinct singlets. However, to create nested singlets one has to start from the outermost singlet. This implies that two creation (annihilation) singlet operators do not necessarily commute.

We define the triplet operator  $\mathcal{T}_{i,i+d}^{p\dagger}$  with  $d \geq 1$  which creates a triplet bond with flavor  $p$  between sites  $i$  and  $i + d$  from the right local vacuum  $|0_{i,i+d}\rangle$ . Similarly to the singlet operator, the result is zero if there is any state different than  $|0_{i,i+d}\rangle$  between  $i$  and  $i + d$ . In addition, the result is zero if the action of the triplet operator leads to the creation of a nested triplet bond. This means that the application of the triplet operator depends on the state on the whole chain and not only on the state between sites  $i$  and  $i + d$ . This global feature of the triplet operator limits its general applicability. However, one can approximate it by its leading local contribution. The term “leading” refers to an expansion in terms with nonzero action on an increasing number of spinons.

First, we notice that  $\mathcal{T}_{i,i+d}^{p\dagger}$  with  $i$  odd (or even, depending on how we label the chain sites) always leads to creation of nested triplet bonds and hence it is zero. The action of  $\mathcal{T}_{i,i+d}^{p\dagger}$  with  $i$  even can still lead to nested triplet bonds, but this requires at least four spinons (two nested singlets) in the system. Hence the leading contribution of the triplet operator can be described by the local action

$$\mathcal{T}_{i,i+d}^{p\dagger} : |0_{i,i+d}\rangle \longrightarrow \left| \begin{array}{c} \overset{p}{\curvearrowright} \\ \circ \bullet \cdots \bullet \circ \\ \curvearrowleft \end{array} \right\rangle_{i,i+d} \quad (25)$$

for  $i$  even and zero for  $i$  odd. In this argument, we suppose arbitrary states on the chain before site  $i$  and beyond site  $i + d$ . The whole  $S_{\text{tot}} = 1$  subspace can be generated by applying the singlet (24) and the triplet (25) operators to the vacuum. There

will be some redundant states, i.e., some overcounting occurs. But this will only happen where at least 6 spinons are present due to the approximation (25). Hence we accept this degree of overcounting because it matters only on the hexatic level of operators. At low densities of spinons it is irrelevant.

The hopping operator  $\mathcal{H}_{i,i+d}^{\sigma\sigma'}$  annihilates an orthonormal spinon with spin  $\sigma$  at position  $i$  and creates an orthonormal spinon with spin  $\sigma'$  at position  $i + d$  if there is the right local vacuum between  $i + 1$  and  $i + d$ ; otherwise the result is zero. This restricts the hopping distance  $d$  to even values. One notices that the crossing of spinons is prohibited; i.e., the result is zero if there is any spinon between sites  $i$  and  $i + d$ . We obtain

$$\mathcal{H}_{i,i+d}^{\uparrow\uparrow} : \left| \begin{array}{c} \uparrow \\ \circ \bullet \cdots \bullet \circ \\ \downarrow \end{array} \right\rangle_{i,i+d} \longrightarrow \left| \begin{array}{c} \bullet \cdots \bullet \\ \circ \bullet \cdots \bullet \circ \\ \uparrow \end{array} \right\rangle_{i,i+d} \quad (26)$$

and similarly for other values  $\sigma$  and  $\sigma'$ .

Instead of introducing hopping operators  $\mathcal{H}_{i,i+d}^{\sigma\sigma'}$  with specific spin indices  $\sigma$  and  $\sigma'$  it turns out to be more convenient to define

$$\mathcal{H}_{j,j+d} := \mathcal{H}_{j,j+d}^{\uparrow\uparrow} + \mathcal{H}_{j,j+d}^{\downarrow\downarrow}, \quad (27a)$$

$$\mathcal{H}_{j,j+d}^x := \mathcal{H}_{j,j+d}^{\uparrow\downarrow} + \mathcal{H}_{j,j+d}^{\downarrow\uparrow}, \quad (27b)$$

$$\mathcal{H}_{j,j+d}^y := i(\mathcal{H}_{j,j+d}^{\downarrow\downarrow} - \mathcal{H}_{j,j+d}^{\uparrow\uparrow}), \quad (27c)$$

$$\mathcal{H}_{j,j+d}^z := \mathcal{H}_{j,j+d}^{\uparrow\uparrow} - \mathcal{H}_{j,j+d}^{\downarrow\downarrow}. \quad (27d)$$

Note that in an SU(2)-invariant model no hopping with spin flips such as  $\mathcal{H}_{j,j+d}^{\uparrow\downarrow}$  will occur. But even in such model, the hopping operators with spin flips appear in products of intermediate calculations; see below.

The action of the neutral hopping operator (27a) on a singlet (triplet) bond is always a singlet (triplet) bond. The flavor hopping operators  $\mathcal{H}_{j,j+d}^p$  with  $p = x, y, z$  acting on a singlet bond change it into a triplet bond with flavor  $p$  and vice versa. We note that the action of the neutral hopping operator  $\mathcal{H}_{j,j+d}$  only depends on the state between sites  $j$  and  $j + d$ . The actions of the flavor hopping operators depend on the state on the whole chains because they could replace a nested singlet bond with a triplet bond which is not allowed.

We call the singlet operators, the triplet operators, and the hopping operators bilinear although they are basically string operators. We do so because by analogy to a fermionic or bosonic Hamiltonian. The key property is that they are characterized by their action at two sites on the chain.

The quartic interactions are given by the normal-ordered product of two bilinear operators. To describe spinon interactions up to the quartic level in an SU(2)-symmetric Hamiltonian only the singlet operators, the triplet operators, and the neutral hopping operators are required. The polarized hopping operators can only appear on higher levels of interactions or in the intermediate steps of the calculations, for instance, as the results of commutators.

## B. Algebra

The next point to address is the commutation of different spinon-pair operators. Explicitly, we are interested in the normal-ordered form of  $[\mathcal{S}^\dagger, \mathcal{H}]$ ,  $[\mathcal{S}^\dagger, \mathcal{S}]$ ,  $[\mathcal{S}^\dagger, \mathcal{S}^\dagger]$ ,  $[\mathcal{S}^\dagger, \mathcal{T}]$ , and

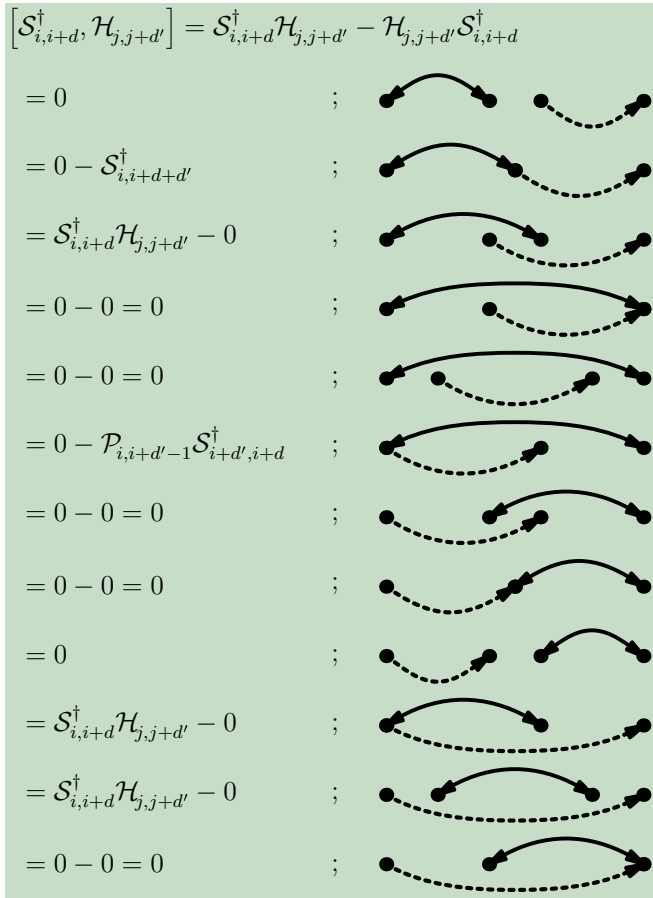


FIG. 2. Analysis of the commutator  $[\mathcal{S}_{i,i+d}^\dagger, \mathcal{H}_{j,j+d'}]$  in different cases. The double-headed arrow creates two spinons at the two ends ( $i$  and  $i+d$ ) and denotes the singlet operator  $\mathcal{S}_{i,i+d}^\dagger$ . The hopping operator  $\mathcal{H}_{j,j+d'}$  is shown by a dashed arrow indicating that a spinon hops from site  $j$  to  $j+d'$ .

$[\mathcal{H}, \mathcal{H}]$ . By normal-ordering we mean that we sort the effect of the commutators according to the number of spinons needed for the term to become active, i.e., to have a nontrivial effect. The commutators are calculated by inspecting their effects on arbitrary states.

Let us start with the commutator  $[\mathcal{S}_{i,i+d}^\dagger, \mathcal{H}_{j,j+d'}]$ . We restrict  $d'$  to positive values; negative values will be discussed below. Different cases are schematically distinguished in Fig. 2. The singlet operator  $\mathcal{S}_{i,i+d}^\dagger$  in this figure is represented by a double-headed arrow; two spinons are created at the two tips,  $i$  and  $i+d$ . The hopping operator  $\mathcal{H}_{j,j+d'}$  is depicted by a dashed arrow which specifies the hopping process from  $j$  to  $j+d'$ .

If  $j < i$  and  $j+d' \leq i+d$  or if  $j > i+d$  the result will be zero considering the properties of the singlet operators and the hopping operators. The result will be also zero if  $i < j, j+d' \leq i+d$ . If  $j < i+d$  and  $j+d' > i+d$ , the second part of the commutator vanishes and we obtain  $[\mathcal{S}_{i,i+d}^\dagger, \mathcal{H}_{j,j+d'}] = \mathcal{S}_{i,i+d}^\dagger \mathcal{H}_{j,j+d'}$ . For  $j = i+d$ , the first part vanishes  $\mathcal{S}_{i,i+d}^\dagger \mathcal{H}_{j,j+d'} = 0$  and the commutator

equals  $-\mathcal{S}_{i,i+d+d'}^\dagger$ . Finally, if  $j = i$  and  $j+d' < i+d$ , the commutator simplifies to  $-\mathcal{P}_{i,i+d'-1} \mathcal{S}_{i+d',i+d}^\dagger$ .

The projection operator  $\mathcal{P}_{i,i+d}$  is defined to be identity if there is the right local vacuum (23a) between sites  $i$  and  $i+d$  and zero otherwise. We define  $\mathcal{P}_{i,i-1} := 1$ . Combining everything, we obtain

$$\begin{aligned}
 [\mathcal{S}_{i,i+d}^\dagger, \mathcal{H}_{j,j+d'}] &= -\mathcal{S}_{i,i+d+d'}^\dagger \delta_{i+d,j} \\
 &\quad - \mathcal{P}_{i,i+d'-1} \mathcal{S}_{i+d',i+d}^\dagger \theta(d-d') \delta_{i,j} \\
 &\quad + \mathcal{S}_{i,i+d}^\dagger \mathcal{H}_{j,j+d'} \\
 &\quad \times \theta(i+d-j) \theta(j+d'-i-d),
 \end{aligned} \tag{28}$$

where the step function  $\theta(x)$  is 1 for  $x > 0$  and zero for  $x \leq 0$ .

It is instructive to compare Eq. (28) to its counterpart for hard-core bosons. For the hard-core boson  $b_i^{(\dagger)}$  acting on site  $i$  one has

$$\begin{aligned}
 [b_i^\dagger b_{i+d}^\dagger, b_{j+d'}^\dagger b_j] &= -b_i^\dagger b_{i+d+d'}^\dagger (1 - b_{i+d}^\dagger b_{i+d}) \delta_{i+d,j} \\
 &\quad - (1 - b_i^\dagger b_i) b_{i+d}^\dagger b_{i+d}^\dagger \delta_{i,j} \\
 &\quad + b_i^\dagger b_{i+d}^\dagger b_{j+d'}^\dagger b_j (\delta_{i+d,j} + \delta_{i,j}),
 \end{aligned} \tag{29}$$

where the local projection operator  $(1 - b_i^\dagger b_i)$  guarantees that site  $i$  is empty. We compare the right-hand side of the two Eqs. (28) and (29) term by term. The first term in Eq. (28) is similar to the one of (29) except that the projection operator is absorbed in the definition of the singlet operator because it occurs between sites  $i$  and  $i+d+d'$ . The local projection operator  $(1 - b_i^\dagger b_i)$  in the second term of (29) is replaced by  $\mathcal{P}_{i,i+d'-1}$  in (28). In addition, the step function  $\theta(d-d')$  in the second term of (28) reflects the fact that spinons cannot cross each other while bosons can. The step functions in the third term of (28) instead of the local delta functions in (29) also stem from the fact that spinons cannot pass each other on the chain.

Similarly, the commutator  $[\mathcal{S}_{i,i+d}^\dagger, \mathcal{H}_{j+d',j}]$  is analyzed with  $d' \geq 0$  leading to

$$\begin{aligned}
 [\mathcal{S}_{i,i+d}^\dagger, \mathcal{H}_{j+d',j}] &= -\mathcal{S}_{i-d',i+d}^\dagger \delta_{i,j+d'} \\
 &\quad - \mathcal{S}_{i,i+d-d'}^\dagger \mathcal{P}_{i+d-d'+1,i+d} \theta(d-d') \\
 &\quad \times \delta_{i+d,j+d'} \\
 &\quad + \mathcal{S}_{i,i+d}^\dagger \mathcal{H}_{j+d',j} \theta(i-j) \theta(j+d'-i).
 \end{aligned} \tag{30}$$

The commutator of creation and annihilation singlet operators is given by

$$\begin{aligned}
 [\mathcal{S}_{i,i+d}^\dagger, \mathcal{S}_{j,j+d'}] &= -\mathcal{P}_{i,i+d} \delta_{i,j} \delta_{d,d'} \\
 &\quad + \frac{1}{2} (\mathcal{H}_{i+d+d',i} \delta_{j,i+d} + \mathcal{H}_{i-d',i+d} \delta_{j,i-d'}) \\
 &\quad + \mathcal{S}_{i,i+d}^\dagger \mathcal{S}_{j,j+d'} \theta(i+d-j) \theta(j+d'-i).
 \end{aligned} \tag{31}$$

The leading contribution of this commutator is the projection operator  $\mathcal{P}_{i,i+d}$  which would reduce to the identity if the operators were normal fermions or bosons. The prefactor  $\frac{1}{2}$  in the second line results from the normalization of singlet states.

One can also check that the commutator between the creation singlet operator and the annihilation triplet operator reads

$$\begin{aligned} [\mathcal{S}_{i,i+d}^\dagger, \mathcal{T}_{j,j+d'}^p] &= \frac{1}{2} (\delta_{i,j+d'} \mathcal{H}_{i-d',i+d}^p - \delta_{j,i+d} \mathcal{H}_{i+d+d',i}^p) \\ &+ \mathcal{S}_{i,i+d}^\dagger \mathcal{T}_{j,j+d'}^p \theta(i+d-j) \theta(j+d'-i). \end{aligned} \quad (32)$$

Other useful commutators are provided in Appendix B.

### C. Projection operator

In practical calculation, the projection operator has to be expressed in terms of the singlet operators, the triplet operators, and the hopping operators. The projection operator  $\mathcal{P}_{i,i+d}$  is zero if there is a spinon at or between sites  $i$  and  $i+d$ .

In addition, the projection returns zero if there is the wrong local vacuum (23b) between  $i$  and  $i+d$ . The former property can be simply captured by

$$\prod_{j=i}^{i+d} (1 - \mathcal{H}_{j,j}), \quad (33)$$

which vanishes if there exists a spinon at or between  $i$  and  $i+d$ . The latter property, however, which requires distinguishing between the right (23a) and the wrong (23b) local vacua, is not a local feature. This makes it difficult to find a representation for the projection operator.

Nevertheless, the projection operator never appears alone in our calculations. It either occurs in a sum over chain sites or it is multiplied with other operators; see the following. In these cases, one can find the leading contributions of the expression by applying it to the first subspaces containing only a few spinons.

We start with the operator  $\mathcal{P}_d := \sum_i \mathcal{P}_{i,i+d}$  where the sum  $i$  runs over the chain sites. To find the leading contributions of  $\mathcal{P}_d$  we consider the ansatz

$$\mathcal{P}_d = C_0 \sum_i \mathbb{1} + C_1 \sum_i \mathcal{H}_{i,i} + \sum_i \sum_{d'} C_2(d') \left( \mathcal{S}_{i,i+d'}^\dagger \mathcal{S}_{i,i+d'} + \sum_{p=x,y,z} \mathcal{T}_{i,i+d'}^{p\dagger} \mathcal{T}_{i,i+d'}^p \right) + \dots, \quad (34)$$

where “...” stands for 3 and higher spinon interaction terms. The prefactor  $C_0$  is determined by applying the relation (34) to the spinon vacuum. We obtain  $\langle 0 | \mathcal{P}_d | 0 \rangle = \frac{1}{2}$  which yields  $C_0 = \frac{1}{2}$ . To calculate the prefactor  $C_1$  one needs to apply  $\mathcal{P}_d$  to the 1-spinon state. We have  $\langle \Phi_i^\sigma | \mathcal{P}_d | \Phi_i^\sigma \rangle = (\frac{1}{2} - \frac{d}{2})$  which leads to  $C_1 = -\frac{d}{2}$ . To find the interaction potential  $C_2(d')$ , one needs to compute  $\langle \Phi_{i,i+d'}^s | \mathcal{P}_d | \Phi_{i,i+d'}^s \rangle$ . We identify  $C_2(d') = \frac{d-d'}{2}$  for  $d' \leq d$  and zero otherwise. Therefore, the final result reads

$$\mathcal{P}_d = \frac{1}{2} \sum_i \mathbb{1} - \frac{d}{2} \sum_i \mathcal{H}_{i,i} + \sum_i \sum_{d' \leq d} \frac{d-d'}{2} \left( \mathcal{S}_{i,i+d'}^\dagger \mathcal{S}_{i,i+d'} + \sum_{p=x,y,z} \mathcal{T}_{i,i+d'}^{p\dagger} \mathcal{T}_{i,i+d'}^p \right) + \dots. \quad (35)$$

It is remarkable that the prefactor of the spinon density operator  $\mathcal{H}_{i,i}$  is proportional to the distance  $d$ . The two-spinon interaction potential in  $\mathcal{P}_d$  decreases linearly with increasing distance between the spinons and vanishes at the maximum distance  $d$ .

The product of the projection operator and the singlet operator also appears in the commutators; see for example Eqs. (28) and (30). We consider  $\mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \mathcal{P}_{i,i+d}$ . Here and in the following we use the subscripts “e” and “o” to indicate even and odd numbers. We observe that

$$\mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \mathcal{P}_{i,i+d} | 0 \rangle = \mathcal{S}_{i+d_e, i+d_e+d'}^\dagger | 0 \rangle \quad (36)$$

because the singlet operator guarantees the existence of the right local vacuum between  $i$  and  $i+d$ . To study the effect of the product on 1-spinon states we distinguish three cases: (i)  $d_e \geq 0$  and  $d_e + d' \geq d$ , (ii)  $d_e \geq 0$  and  $d_e + d' < d$ , and (iii)  $d_e < 0$ . We analyze case (i) explicitly; the other cases can be treated in the same way.

The action of  $\mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \mathcal{P}_{i,i+d}$  on the 1-spinon state  $|\Phi_j^\sigma\rangle$  is given by

$$\begin{aligned} \mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \mathcal{P}_{i,i+d} |\Phi_j^\sigma\rangle &= [1 - \theta(j-i+1) \theta(i+d_e-j)] \\ &\times \mathcal{S}_{i+d_e, i+d_e+d'}^\dagger |\Phi_j^\sigma\rangle. \end{aligned} \quad (37)$$

We notice that even for  $i+d < j < i+d_e$  the result is zero because for  $(j-i)$  odd the wrong local vacuum appears between  $i$  and  $i+d$  and for  $(j-i)$  even the wrong local vacuum appears between  $i+d_e$  and  $i+d_e+d'$ . Therefore, we obtain

$$\begin{aligned} \mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \mathcal{P}_{i,i+d} &= \mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \left( 1 - \sum_{n_o=1}^{d_e-1} \mathcal{H}_{i+n_o, i+n_o} \right. \\ &\left. + \dots \right), \{d_e \geq 0 \text{ and } d_e + d' \geq d\}, \end{aligned} \quad (38)$$

where “...” involves 2 and higher spinon interactions which we neglect. The sum over  $n_o$  is limited to odd numbers because

for even numbers the wrong local vacuum occurs between  $i + d_e$  and  $i + d_e + d'$  and the vanishing is guaranteed by the application of the singlet operator  $\mathcal{S}_{i+d_e, i+d_e+d'}$ .

One can analyze cases (ii) and (iii) to obtain relations analogous to (38). Combining the three equations and after some simplifications we obtain

$$\mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \mathcal{P}_{i, i+d} = \mathcal{S}_{i+d_e, i+d_e+d'}^\dagger \left[ 1 - \sum_{n_e} \mathcal{H}_{i+n_e, i+n_e} \theta(d - n_e) \theta(n_e - d_e - d') - \sum_{n_o} \mathcal{H}_{i+n_o, i+n_o} \theta(d_e - n_o) \theta(n_o) + \dots \right], \quad (39)$$

which is valid up to quartic level in spinon creation and annihilation operators.

We also inspect the product of the neutral hopping operator with the projection operator:  $\mathcal{P}_{i+d_e+n, i+d_e+n+d} \mathcal{H}_{i, i+d_e}$  where  $n$  is odd for  $n > 0$  and even for  $n < 0$ . The expression can be analyzed by applying it to the 1- and 2-spinon sectors similarly to the above discussion. The final result reads

$$\begin{aligned} & \mathcal{P}_{i+d_e+n, i+d_e+n+d} \mathcal{H}_{i, i+d_e} \\ &= \theta(n) \left[ \mathcal{H}_{i, i+d_e} - \sum_{m_o \geq 1} \theta(m_o + d_e) \theta(n + d - m_o) \left( \mathcal{S}_{i+d_e, i+d_e+m_o}^\dagger \mathcal{S}_{i, i+d_e+m_o} + \sum_{p=x, y, z} \mathcal{T}_{i+d_e, i+d_e+m_o}^{p\dagger} \mathcal{T}_{i, i+d_e+m_o}^p \right) \right] \\ &+ \theta(-n - d) \left[ \mathcal{H}_{i, i+d_e} - \sum_{m_o \geq 1} \theta(m_o + d_e) \theta(-n - d_e - m_o) \left( \mathcal{S}_{i-m_o, i+d_e}^\dagger \mathcal{S}_{i-m_o, i} + \sum_{p=x, y, z} \mathcal{T}_{i-m_o, i+d_e}^{p\dagger} \mathcal{T}_{i-m_o, i}^p \right) \right] + \dots, \quad (40) \end{aligned}$$

where 3 and higher spinon interaction terms are ignored.

Before closing this section, we state that the product of two neutral hopping operators is not a valid representation for 2-spinon interactions. In fact, 2-spinon interactions are always described in terms of singlet and triplet operators. Wherever the product of two neutral hopping operators appears in the calculations it has been expanded in terms of hopping operators, singlet operators, and triplet operators as we did above in the expansion of the projection operator. Further useful expansions can be found in Appendix C.

## V. FRUSTRATED HEISENBERG CHAIN

As an example of the application of the spinon-pair operator representation we study the frustrated Heisenberg chain. Its Hamiltonian has been given in Eq. (1). For a chain with an even number of sites, the exact ground state

at  $\alpha = \frac{1}{2}$ , known as Majumar-Ghosh point, is given by the fully dimerized state (2) [38,39]. Upon decreasing the degree of frustration below  $\alpha = \frac{1}{2}$  the spontaneously dimerized phase undergoes a second-order phase transition to a Mott insulator with quasi-long-range magnetic order (spin liquid) at  $\alpha_c = 0.241167$  [45,46]. In both the dimerized and the spin liquid phases, the elementary excitations (quasiparticles) are known to be spinons [15,25]. The minimum of the spinon dispersion for chains with an odd number of sites moves from commensurate to incommensurate momenta beyond the Lifshitz point  $\alpha_l = 0.538(1)$  [47]. For systems with an even number of sites, the Lifshitz point takes place at smaller frustration  $\alpha_l = 0.52036(6)$  [48].

To express the Hamiltonian (1) in terms of spinon-pair operators, we start from the following general ansatz:

$$\begin{aligned} H &= \mathcal{A}_{0:0} H_{0:0} + \mathcal{A}_{1:1}(0) H_{1:1}(0) + \sum_{d_e \geq 2} \mathcal{A}_{1:1}(d_e) H_{1:1}(d_e) + \sum_{d_o \geq 3} \mathcal{A}_{2:0}(d_o) [H_{2:0}(d_o) + \text{H.c.}] \\ &+ \sum_{d_o \geq 3} \sum_{d_e} \sum_n \mathcal{A}_{3:1}(d_e, n, d_o) [H_{3:1}(d_e, n, d_o) + \text{H.c.}] + \sum_{d_o \geq 3} \sum_{d'_o \geq 3} \sum_{d_e} \mathcal{A}_{2:2}^s(d_o, d_e, d'_o) H_{2:2}^s(d_o, d_e, d'_o) \\ &+ \sum_{d_o \geq 3} \sum_{d'_o \geq 3} \sum_{d_e} \mathcal{A}_{2:2}^t(d_o, d_e, d'_o) H_{2:2}^t(d_o, d_e, d'_o) + \dots, \quad (41) \end{aligned}$$

where we defined

$$H_{0:0} := \sum_i \mathbb{1}, \quad (42a)$$

$$H_{1:1}(0) := \sum_i \mathcal{H}_{i,i}, \quad (42b)$$



$$H_{1:1}(d_e) := \sum_i \mathcal{H}_{i,i+d_e} + \text{H.c.}, \quad d_e \geq 2, \quad (42c)$$

$$H_{2:0}(d_o) := \sum_i \mathcal{S}_{i,i+d_o}^\dagger, \quad (42d)$$

$$H_{3:1}(d_e, n, d_o) := \sum_i \mathcal{S}_{i+d_e+n, i+d_e+n+d_o}^\dagger \mathcal{H}_{i,i+d_e}, \quad (42e)$$

$$H_{2:2}^s(d_o, d_e, d'_o) := \sum_i \mathcal{S}_{i+d_e, i+d_e+d'_o}^\dagger \mathcal{S}_{i,i+d_o}, \quad (42f)$$

$$H_{2:2}^t(d_o, d_e, d'_o) := \sum_i \sum_{p=x,y,z} \mathcal{T}_{i+d_e, i+d_e+d'_o}^{\dagger p} \mathcal{T}_{i,i+d_o}^p. \quad (42g)$$

The “...” in Eq. (41) denotes 3 and higher spinon interactions which may occur. But we neglect such contributions here; i.e., we develop an approach which is valid for low densities of spinons, but which may fail in regimes where their density is higher.

The variable  $n$  in the third line of Eq. (41) takes odd values if  $n > 0$  and takes even values if  $n < -d_o$ . We notice that  $H_{3:1}(d_e, n, d_o) = 0$  for  $-d_o \leq n \leq 0$ . The term  $H_{p:q}$  in Eqs. (42) is bilinear if  $p + q = 2$  and it is quartic if  $p + q = 4$ .

The so far unknown prefactors  $\mathcal{A}$  in the ansatz (41) are determined from the matrix elements of the Hamiltonian calculated in the orthonormal basis. The following relations are useful to analyze the action of (1) on spinon states:

$$\left( \mathcal{S}_{(1,x)} \cdot \mathcal{S}_{(2,y)} \mp \frac{1}{4} \right) \left| \begin{array}{ccc} \bullet & \bullet & \bullet \\ (1,l) & (1,r) & (2,l) \end{array} \right\rangle = \pm \frac{1}{2} \left| \begin{array}{ccc} \bullet & \bullet & \bullet \\ (1,l) & (1,r) & (2,l) \end{array} \right\rangle \quad (43a)$$

$$\left( \mathcal{S}_{(1,x)} \cdot \mathcal{S}_{(2)} \mp \frac{1}{4} \right) \left| \begin{array}{ccc} \bullet & \bullet & \uparrow \\ (1,l) & (1,r) & (2) \end{array} \right\rangle = \pm \frac{1}{2} \left| \begin{array}{ccc} \bullet & \bullet & \uparrow \\ (1,l) & (1,r) & (2) \end{array} \right\rangle \quad (43b)$$

where  $x, y \in \{l, r\}$  and accordingly the spin operators  $\mathcal{S}_{(1,x)}$  and  $\mathcal{S}_{(2,y)}$  act on the lattice positions in the ket states in (43). The upper sign in Eq. (43a) holds if  $x$  and  $y$  are different and the lower sign holds if they are the same. In Eq. (43b), the upper sign holds for  $x = r$  and the lower sign for  $x = l$ . In addition to Eqs. (22), we use the following expansions for the 3-spinon states:

$$|\phi_i^\sigma \phi_{i+n, i+n+d}^s\rangle = \frac{\sqrt{3}}{2} \left(-\frac{1}{2}\right)^{\frac{d-1}{2}} \sum_{m_e \geq 0} \left(-\frac{1}{2}\right)^{\frac{m_e}{2}} |\Phi_{i-m_e}^\sigma\rangle + \frac{\sqrt{3}}{2} \left(-\frac{1}{2}\right)^{\frac{n+1}{2}} \sum_{m_e \geq 0}^{d-3} \left(-\frac{1}{2}\right)^{\frac{m_e}{2}} |\Phi_{i+n+d-m_e}^\sigma\rangle + \dots, \quad (44a)$$

$$|\phi_{i,i+d}^s \phi_{i+d+n}^\sigma\rangle = \frac{\sqrt{3}}{2} \left(-\frac{1}{2}\right)^{\frac{n+1}{2}} \sum_{m_e \geq 0} \left(-\frac{1}{2}\right)^{\frac{m_e}{2}} |\Phi_{i-m_e}^\sigma\rangle + \frac{\sqrt{3}}{2} \left(-\frac{1}{2}\right)^{\frac{d-1}{2}} \sum_{m_e \geq 0}^{n-1} \left(-\frac{1}{2}\right)^{\frac{m_e}{2}} |\Phi_{i+n+d-m_e}^\sigma\rangle + \dots, \quad (44b)$$

where “...” stands for orthonormal 3-spinon states.

The prefactors  $\mathcal{A}_{0:0}$  and  $\mathcal{A}_{2:0}(d)$  can be computed by applying the Hamiltonian (1) to the vacuum (2) and comparing the result with the application of the ansatz (41) to the vacuum. In this way, we obtain

$$\frac{H}{J_1} |0\rangle = -\frac{3L}{8} |0\rangle + \frac{\tilde{\alpha}}{2} \sum_{i \in \text{even}} \left( \frac{1}{2} |0\rangle + |\phi_{i,i+3}^s\rangle \right) = -\frac{3L}{8} |0\rangle + \frac{3\tilde{\alpha}}{2} \sum_{d_o \geq 3} \sum_{i \in \text{even}} \left(-\frac{1}{2}\right)^{\frac{d_o+1}{2}} |\Phi_{i,i+d_o}^s\rangle, \quad (45)$$

where  $\tilde{\alpha} := 1 - 2\alpha$ . The second equality is derived using Eq. (22b) for  $d = 3$ . The sum over  $i$  runs over the even sites supposing that the first lattice site in the spinon vacuum (2) is even. For the other degenerate vacuum one sums over the odd sites. We should not, however, restrict the sum over  $i$  in Eq. (42d) to even (or odd) values only. Note that both kinds of vacuum can be present on distinct pieces of the chain, separated by a spinon or any odd number of spinons as domain walls.

Thus it is important to keep the processes creating nested singlets. From Eq. (45), we identify

$$\mathcal{A}_{0:0} = -\frac{3}{8} J_1, \quad (46a)$$

$$\mathcal{A}_{2:0}(d) = \frac{3\tilde{\alpha}}{2} \left(-\frac{1}{2}\right)^{\frac{d+1}{2}} J_1. \quad (46b)$$

This result shows that the spin Hamiltonian (1) is not fully local represented in spinon-pair operators. But the Bogoliubov prefactors (46b) decrease exponentially upon increasing the distance  $d$ . Moreover, we see that there is no term linking the 0-spinon state to 4-spinon states. Such terms appear upon inclusion of longer-range (beyond NNN sites) spin-spin interactions in (1). At the MG point  $\alpha = \frac{1}{2}$ , all the Bogoliubov terms vanish indicating that the spinon vacuum (2) is an exact state of the system as known previously [39].

To compute the hopping prefactors  $\mathcal{A}_{1,1}(d)$  we apply the Hamiltonian (1) to the 1-spinon state  $|\Phi_i^\sigma\rangle$  and compare it with the action of the ansatz (41) on the same state. Some lengthy calculations yield

$$\begin{aligned} \frac{H}{J_1} |\Phi_i^\sigma\rangle = & + \left( -\frac{3}{8}L + \frac{5+2\tilde{\alpha}}{8} \right) |\Phi_i^\sigma\rangle \\ & + \left( \frac{2+\tilde{\alpha}}{8} \right) (|\Phi_{i+2}^\sigma\rangle + |\Phi_{i-2}^\sigma\rangle) \\ & - \frac{3\tilde{\alpha}}{4} \sum_{d_e \geq 4} \left( -\frac{1}{2} \right)^{\frac{d_e}{2}} (|\Phi_{i+d_e}^\sigma\rangle + |\Phi_{i-d_e}^\sigma\rangle) \\ & + \dots, \end{aligned} \quad (47)$$

where “...” denotes the 3-spinon contributions orthonormal to the 1-spinon subspace which we neglect. To derive this relation we employed Eqs. (44) for  $d = 3$ . No term linking the 1-spinon to the 5-spinon sector is produced. After subtracting the contribution  $\mathcal{A}_{0,0}$ , the hopping prefactors read

$$\mathcal{A}_{1,1}(0) = \frac{5+2\tilde{\alpha}}{8} J_1, \quad (48a)$$

$$\mathcal{A}_{1,1}(2) = \frac{2+\tilde{\alpha}}{8} J_1, \quad (48b)$$

$$\mathcal{A}_{1,1}(d_e) = -\frac{3\tilde{\alpha}}{4} \left( -\frac{1}{2} \right)^{\frac{d_e}{2}} J_1, \quad d_e \geq 4. \quad (48c)$$

At the MG point,  $\tilde{\alpha} = 0$ , only hopping over two sites is present. However, there are long-range hopping processes present away from the MG point. The hopping prefactors decay exponentially with distance.

It is more cumbersome to calculate the interaction coefficients  $\mathcal{A}_{3,1}$ ,  $\mathcal{A}_{2,2}^s$ , and  $\mathcal{A}_{2,2}^t$  analytically. The linked cluster expansion theorem allows us to determine the irreducible matrix elements  $\mathcal{A}$  in Eq. (41) on finite but large enough clusters, in the thermodynamic limit. We refer the reader to Ref. [49] for details. We notice that the interaction coefficients can be computed exactly on finite clusters due to the locality of the spin Hamiltonian (1).

We implemented a program to compute the Hamiltonian matrix elements between orthonormal spinon states. In the choice of the size of the cluster, one must keep in mind that each orthonormal spinon is extended over two sites to the left. Careful attention is also required in identifying the interaction coefficients  $\mathcal{A}_{3,1}$  because of the finite overlap (21) between orthonormal 3-spinon states. The interaction coefficients are calculated and reported in Appendix D. Even at the MG point the spin Hamiltonian (1) is not local in the spinon-pair operator

representation, but the nonlocal terms fall off quickly with distance.

## VI. CONTINUOUS UNITARY TRANSFORMATIONS

We use continuous unitary transformations (CUTs) to analyze the Hamiltonian (41). We briefly introduce the CUT method of which the first versions were suggested over 20 years ago [50]. The CUT method maps a given initial Hamiltonian  $H$  to a final effective one by a unitary transformation which is parametrized by an auxiliary parameter  $\ell$  [51]. The transformation is such that at  $\ell = 0$  the transformed Hamiltonian  $H(\ell)$  equals the initial Hamiltonian  $H$  and at  $\ell = \infty$  the desired effective Hamiltonian is reached. The Hamiltonian during the flow is given by

$$\partial_\ell H(\ell) = [\eta(\ell), H(\ell)] \quad (49)$$

which is called the flow equation. The anti-Hermitian operator  $\eta(\ell)$ , called generator, determines the essence of the transformation. One can use the Wegner generator [50], the particle-conserving (pc) generator [5,52,53], or various reduced generators [54] to fully or partially rotate away the off-diagonal elements.

By writing the initial Hamiltonian in a quasiparticle (QP) representation and eliminating the terms which change the number of QPs in the system, one can map a many-particle problem to a few-particle problem using the CUT method. There are different approximations to truncate the flow equation (49) so that this systems of differential equations is closed. One may achieve perturbative [5,55] or renormalized effective Hamiltonians [55,56]. The method is applied to describe systems with elementary excitations such as triplons with spin  $S = 1$  [57], magnons [58], electrons and holes [59,60], and so on.

In the following, we employ the pc generator and keep the transformed Hamiltonian  $H(\ell)$  terms which are at most quartic. This truncation can be justified by two arguments. The first argument refers to the density of spinons because the hexatic terms need at least three spinons to become active. Thus at low concentrations of spinons the bilinear terms acting on single spinons and the quartic terms acting on pairs of spinons are the most important ones. The second argument refers to the scaling of the terms. For fermionic and bosonic systems in one dimension it is known that the bilinear and the quartic terms have the lowest scaling dimension [58,61]. If the bilinear terms are without mass term they are of equal scaling dimension, hence of equal importance. Hexatic and higher terms are irrelevant in the scaling sense.

In the bilinear approximation, the terms (42a) to (42d) define the operator basis. In the quartic approximation, we consider the terms (42a) to (42f). For technical simplicity, we neglect to include the triplet 2-spinon interaction (42g) because its treatment in the present formalism breaks the translational symmetry of the lattice. Such a translational symmetry breaking is expected since we have implicitly chosen one of the two degenerate vacua. One notices that no term linking the 0-spinon sector to the 4-spinon sector

appears during the flow because the pc generator preserves the band-diagonal structure of the initial Hamiltonian [5,53].

To determine the set of flow equations we need to calculate the commutators between the operators of the basis (42) [55]. The necessary relations for the commutators up to quartic level are provided in Sec. IV and in Appendices B and C. While the flow equations up to bilinear level can be easily obtained it is a very tedious task to obtain the quartic contributions. This motivates us to implement a program for subsequent applications.

To integrate the derived flow equations we limit the range of processes in real space such that the distance between initial spinons, the distance between final spinons, and the maximum distance between initial and final spinons is not larger than a maximum distance,  $d_{\max}$ . The flow equations are integrated numerically with the initial conditions (46), (48), (D9), and (D10).

## VII. RESULTS

Before presenting the CUT results let us consider the simplest approximation, i.e., neglecting all off-diagonal terms, i.e., all terms which change the number of spinons in (41). This approximation is expected to be most accurate at and near the MG point where the Bogoliubov terms (46b) vanish. But we stress that it is an approximation even at the MG point because terms exist which link the 1-spinon states to the 3-spinons states.

The approximate 1-spinon dispersion neglecting all spinon-number-changing terms reads

$$\begin{aligned} \omega(k) &= \mathcal{A}_{1;1}(0) + 2 \sum_{d_e=2} \mathcal{A}_{1;1}(d_e) \cos(d_e k) \\ &= \frac{\alpha}{4} [5 + 4 \cos(2k)] J_1 + \tilde{\alpha} \left[ \frac{3}{8} + \frac{4 + 5 \cos(2k)}{5 + 4 \cos(2k)} \right] J_1, \end{aligned} \quad (50)$$

based on Eqs. (48). This simple approximation recovers the variational results obtained by Brehmer *et al.* [27,62]. The formalism presented in this article allows us to systematically improve these variational results by rotating away the off-diagonal elements using the CUT or by other approaches.

We define the spin gap  $\Delta_s$  as twice the minimum energy of the spinon dispersion. Thus, the spin gap equals the minimum of the 2-spinon continuum. We notice that the spinons are asymptotically free although they cannot pass each other. The spin gap  $\Delta_s$  versus the frustration degree  $\alpha$  is depicted in Fig. 3. The variational result (50) and the CUT results in the bilinear and quartic approximation for different maximum distances,  $d_{\max}$ , are shown. The density-matrix renormalization group (DMRG) results by Chitra *et al.* [63] and by White and Affleck [64] are included for comparison.

Figure 3 shows that the spurious transition point predicted by the variational result at  $\alpha \approx 0.87$  is shifted in CUT on bilinear level to  $\alpha \approx 1.47$  making the spontaneously dimerized phase more stable as expected from the DMRG results. Both the variational result and the result from bilinear CUT vanish almost linearly at  $\alpha \approx 0.43$ . They do not show evidence of the exponentially slow vanishing gap at the Berezinskii-Kosterlitz-Thouless (BKT) transition at  $\alpha \approx 0.241$ .

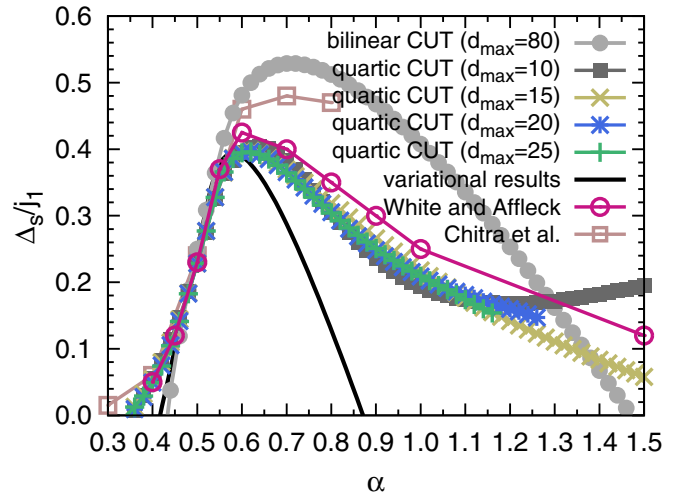


FIG. 3. The spin gap  $\Delta_s$  versus the frustration  $\alpha$ . The various CUT truncation schemes are compared to the variational results by Brehmer *et al.* [27] and to the DMRG results by Chitra *et al.* [63] and White and Affleck [64].

The CUT results on the quartic level in Fig. 3 nicely capture the qualitative behavior of the spin gap predicted by White and Affleck [64]. The agreement between the two approaches is quantitative near the MG point. Lack of convergence of the flow equations prevents us from reaching beyond  $\alpha = 1.26$  for  $d_{\max} = 20$  and beyond  $\alpha = 1.14$  for  $d_{\max} = 25$ . The CUT on the quartic level predicts the transition to the quasi-long-range spin liquid phase at  $\alpha \approx 0.34$ . This value is larger than the established critical value  $\alpha_c \approx 0.241$ . We believe that this deviation is due to the very slow vanishing of the spin gap near the BKT transition point [65] which is only detectable if extremely long-range processes are kept track of reliably. Based on large-scale DMRG results [65] the value of the spin gap at  $\alpha = 0.34$  is only about  $0.004 J_1$  which is too small to be detected in our approach.

We denote by  $k^*$  the momentum at which the minimum of the spinon dispersion occurs. For weak frustration it occurs at  $\pi/2$ . Figure 4 denotes the deviation  $(\frac{\pi}{2} - k^*)$  versus the frustration  $\alpha$ . The minimum of the spinon dispersion moves from  $k = \frac{\pi}{2}$  to an incommensurate value beyond the Lifshitz transition point  $\alpha_l$ . We find  $\alpha_l = 0.539$  for  $d_{\max} = 20$  and  $\alpha_l = 0.540$  for  $d_{\max} = 25$  and  $d_{\max} = 30$ . This finding agrees quantitatively with the DMRG prediction  $\alpha_l = 0.538(1)$  by Deschner and Sørensen [47]. However, it is difficult to capture the behavior of  $k^*$  for  $\alpha > 0.538(1)$  by DMRG due to a plethora of level crossings [47]. We expect  $(\frac{\pi}{2} - k^*) \rightarrow \frac{\pi}{4}$  in the limit  $\alpha \rightarrow \infty$  because the system approaches weakly coupled penetrating Heisenberg chains with lattice constant  $2a$  so that the minimum occurs for  $a = 1$  at  $\frac{\pi}{4}$ .

In Fig. 5 we plot the low-energy spectrum of the  $J_1$ - $J_2$  Heisenberg model (1) with (a) an odd and (b) an even number of sites. The value of the frustration  $\alpha$  is set to 0.8. Figure 5(a) shows the 1-spinon dispersion and the 3-spinon continuum while Fig. 5(b) shows the 2-spinon continuum. We used the spinon dispersion for  $d_{\max} = 30$  to construct the 2- and the 3-spinon continua relying on energy and

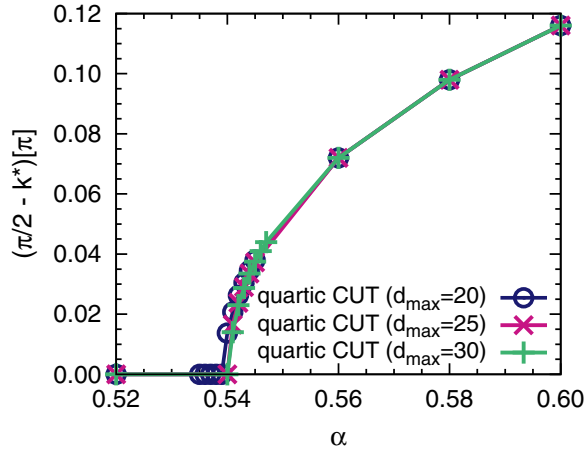


FIG. 4. The momentum  $(\frac{\pi}{2} - k^*)$  versus the frustration  $\alpha$ ;  $k^*$  is the momentum at which the minimum of the spinon dispersion is located.

momentum conservation. The numerical results for  $d_{\max} = 25$  are essentially the same. The 1-spinon dispersions obtained from different values of  $d_{\max}$  deviate noticeably only inside the 3-spinon continuum where a clear distinction between 1-spinon and 3-spinon states is not possible. One can extend the CUT approach to describe the decay of the 1-spinon dispersion into the 3-spinon continuum in Fig. 5(a) [54].

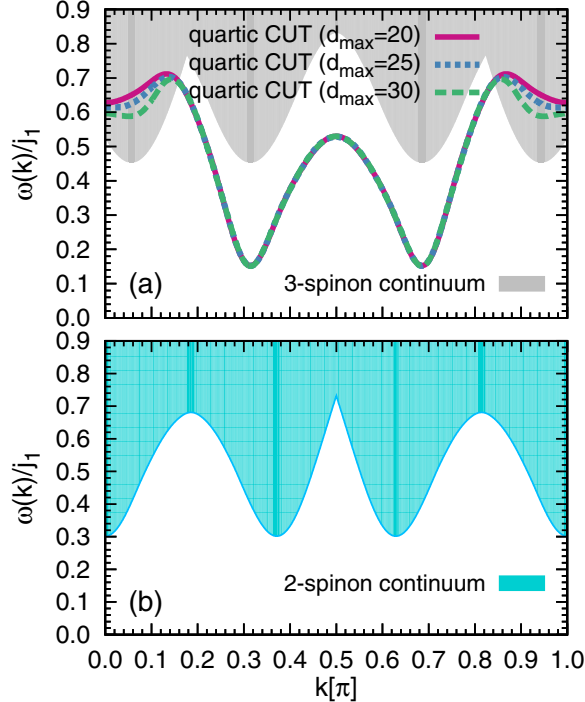


FIG. 5. The low-energy spectrum of the  $J_1$ - $J_2$  Heisenberg model (1) with (a) an odd and (b) an even number of sites at frustration  $\alpha = 0.8$ . Panel (a) displays the 1-spinon dispersion and the 3-spinon continuum and panel (b) denotes the 2-spinon continuum. The continua are constructed by energy and momentum conservation from the spinon dispersion with  $d_{\max} = 30$ . The results for  $d_{\max} = 25$  are the same within the linewidth.

But such an analysis is beyond the scope of the present article.

We recall that the triplet 2-spinon interactions (42g) are neglected in the present treatment. These terms are present even in the initial Hamiltonian, see Eq. (D11), and could make the CUT results on the quartic level even more accurate.

## VIII. CONCLUSIONS AND OUTLOOK

The aim of the present paper was to provide the proof of principle that models in terms of massive spinons can be formulated for a generic Hamiltonian, not only at special points such as the Majumdar-Ghosh point. This aim has been successfully realized. The formulation can be achieved in second quantization in the sense that the resulting effective Hamiltonian also applies to finite densities of spinons. The asset of such a formulation is that the subsequent treatment can employ all methods known for such problems.

We have constructed an orthonormal spinon basis and introduced string spinon-pair operators which can capture the fractional nature of the spinon excitation and describe different spinon processes. By applying the spinon-pair operators on the spinon vacuum (1-spinon states) one can fully construct the  $S = 0$  and the  $S = 1$  Hilbert spaces of an even (odd) size lattice. This enables us to write spin Hamiltonians in spinon-pair representation in second quantization. Our representation is valid for low densities of spinons because it takes processes involving single spinons and pairs of them exactly into account. Only on the level of three or more spinons are the processes neglected.

Here we used continuous unitary transformations to analyze the second quantized Hamiltonians obtained in the first step. We showed that processes which change the number of spinons can be systematically treated by this approach. They can be eliminated (“rotated away”) while their renormalization of the properties of the elementary spinons is kept. In this way, we obtained results for the spinon dispersion including gap and incommensurability for the frustrated spin chain in a wide range of frustration, i.e., not only for the Majumdar-Ghosh point where the next-nearest-neighbor interaction takes half the value of the nearest-neighbor interaction. The results are significantly improved over a purely variational treatment. This illustrates the potential of the pursued approach.

Further research to establish effective models in terms of their elementary excitations is called for. One promising route of research consists in passing from treatments in real space to treatments in momentum space. Another current challenge is to transfer the presented ideas from one to higher dimensions.

## ACKNOWLEDGMENTS

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**APPENDIX A: ORTHONORMAL 3-SPINON STATES**

The orthonormal  $S_{\text{tot}} = \frac{1}{2}$  3-spinon states  $|\Phi_i^\sigma \Phi_{i+d_1, i+d_1+d_2}^s\rangle$  and  $|\Phi_{i, i+d_2}^s \Phi_{i+d_1+d_2}^\sigma\rangle$  for  $d_1 \geq 3$  are given by

$$|\Phi_i^\sigma \Phi_{i+d_1, i+d_1+d_2}^s\rangle = |\Phi_i^\sigma\rangle \otimes |\Phi_{i+d_1, i+d_1+d_2}^s\rangle, \quad (\text{A1a})$$

$$|\Phi_{i, i+d_2}^s \Phi_{i+d_1+d_2}^\sigma\rangle = |\Phi_{i, i+d_2}^s\rangle \otimes |\Phi_{i+d_1+d_2}^\sigma\rangle, \quad (\text{A1b})$$

where the orthonormal 1-spinon state  $|\Phi_i^\sigma\rangle$  is defined by Eq. (16b) and the orthonormal singlet 2-spinon state  $|\Phi_{i, i+d}^s\rangle$  by Eq. (17a). If  $d_1 = 1$ , the orthonormal 3-spinon states

$$|\Phi_i^\sigma \Phi_{i+1, i+1+d}^s\rangle = \left| \dots \text{---} \overset{\uparrow}{\circ} \text{---} \overset{\circ}{\circ} \text{---} \dots \text{---} \overset{\circ}{\circ} \text{---} \overset{\circ}{\circ} \text{---} \dots \right\rangle \quad (\text{A2a})$$

and

$$|\Phi_{i, i+d}^s \Phi_{i+d+1}^\sigma\rangle = \left| \dots \text{---} \overset{\circ}{\circ} \text{---} \dots \text{---} \overset{\circ}{\circ} \text{---} \overset{\uparrow}{\circ} \text{---} \dots \right\rangle \quad (\text{A2b})$$

are distorted. The empty circles indicate orthonormal spinons. We require orthonormality to derive these states. It is a subtle issue to identify the initial form of the distorted 3-spinon states. But it can be found in a systematic way. Each orthonormal spinon in Eqs. (A2) has an extension of two sites to the left. This implies that 7 sites of the lattice are involved overall in 3-spinon states; see the dashed boxes in Eqs. (A2). On these 7 sites there are 12 states with  $S_{\text{tot}} = \frac{1}{2}$ . If  $d > 3$  in Eqs. (A2), 2 of these 12 states are 5-spinon states which do not contribute to the orthonormal 3-spinon states. We expect the same relation to be valid also for  $d = 3$ . Hence, we arrive at the following ansatz with 10 parameters for the distorted 3-spinon states:

$$\begin{aligned} |\Phi_i^\sigma \Phi_{i+1, i+d+1}^s\rangle = & \frac{1}{N_1} \left( |\phi_i^\sigma \phi_{i+1, i+d+1}^s\rangle + \alpha_1 |\phi_i^\sigma \phi_{i+1, i+d-1}^s\rangle + \alpha_2 |\phi_{i-2}^\sigma \phi_{i+1, i+d+1}^s\rangle + \alpha_3 |\phi_{i-2}^\sigma \phi_{i+1, i+d-1}^s\rangle \right. \\ & + \alpha_4 |\phi_{i-2}^\sigma \phi_{i-1, i+d+1}^s\rangle + \alpha_5 |\phi_{i-2}^\sigma \phi_{i-1, i+d-1}^s\rangle + \alpha_6 |\phi_{i+d+1}^\sigma\rangle + \alpha_7 |\phi_{i+d-1}^\sigma\rangle \\ & \left. + \alpha_8 |\phi_{i-2, i+1}^s \phi_{i+d+1}^\sigma\rangle + \alpha_9 |\phi_{i-2, i+1}^s \phi_{i+d-1}^\sigma\rangle \right), \end{aligned} \quad (\text{A3a})$$

$$\begin{aligned} |\Phi_{i, i+d}^s \Phi_{i+d+1}^\sigma\rangle = & \frac{1}{N_2} \left( |\phi_{i, i+d}^s \phi_{i+d+1}^\sigma\rangle + \beta_1 |\phi_{i-2, i+d}^s \phi_{i+d+1}^\sigma\rangle + \beta_2 |\phi_{i, i+d-2}^s \phi_{i+d+1}^\sigma\rangle + \beta_3 |\phi_{i-2, i+d-2}^s \phi_{i+d+1}^\sigma\rangle \right. \\ & + \beta_4 |\phi_{i, i+d-2}^s \phi_{i+d-1}^\sigma\rangle + \beta_5 |\phi_{i-2, i+d-2}^s \phi_{i+d-1}^\sigma\rangle + \beta_6 |\phi_i^\sigma\rangle + \beta_7 |\phi_{i-2}^\sigma\rangle \\ & \left. + \beta_8 |\phi_i^s \phi_{i+d-2, i+d}^s\rangle + \beta_9 |\phi_{i-2}^s \phi_{i+d-2, i+d}^s\rangle \right). \end{aligned} \quad (\text{A3b})$$

The unknown prefactors are determined in an orthonormalization process similar to the Gram-Schmidt algorithm. We start with the state  $d = 3$  in Eq. (A3a) and make it orthogonal to the 1-spinon states (16b) and to the 3-spinon states (A1). It is too tedious a task to calculate the overlaps by hand. Hence we implemented a C++ program for this purpose. In this way, we obtained the eight independent equations

$$\langle \Phi_{i-2}^\sigma | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies -4\alpha_1 - 4\alpha_2 + 8\alpha_3 + 2\alpha_4 - 4\alpha_5 - 1\alpha_6 + 2\alpha_7 + 2\alpha_8 - 4\alpha_9 + 2 = 0, \quad (\text{A4a})$$

$$\langle \Phi_i^\sigma | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies +4\alpha_1 + 1\alpha_6 - 2\alpha_7 - 2 = 0, \quad (\text{A4b})$$

$$\langle \Phi_{i+2}^\sigma | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies +1\alpha_4 - 2\alpha_5 - 2\alpha_6 + 4\alpha_7 + 1\alpha_8 - 2\alpha_9 = 0, \quad (\text{A4c})$$

$$\langle \Phi_{i+4}^\sigma | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies +1\alpha_2 - 2\alpha_4 + 4\alpha_6 - 2\alpha_8 - 2 = 0, \quad (\text{A4d})$$

$$\langle \Phi_{i-4}^\sigma \Phi_{i-1, i+2}^s | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies +3\alpha_4 - 6\alpha_5 - 1\alpha_8 + 2\alpha_9 = 0, \quad (\text{A4e})$$

$$\langle \Phi_{i-2}^\sigma \Phi_{i+1, i+4}^s | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies +2\alpha_2 - 1\alpha_8 - 1 = 0, \quad (\text{A4f})$$

$$\langle \Phi_{i-4}^\sigma \Phi_{i-1, i+4}^s | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies +1\alpha_2 - 2\alpha_4 = 0, \quad (\text{A4g})$$

$$\langle \Phi_{i-2, i+1}^s \Phi_{i+4}^\sigma | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle = 0 \implies +1\alpha_2 - 2\alpha_8 = 0. \quad (\text{A4h})$$

Fulfilling the single equation (A4a) is sufficient to make the state  $|\Phi_i^\sigma \Phi_{i+1, i+4}^s\rangle$  orthogonal to all 1-spinon states  $|\Phi_j^\sigma\rangle$  with  $j \leq i-2$ . The 1-spinon states  $|\Phi_j^\sigma\rangle$  with  $j \geq i+6$  are trivially orthogonal to  $|\Phi_i^\sigma \Phi_{i+1, i+4}^s\rangle$  leading to no condition for the prefactors  $\alpha_1 \dots \alpha_9$ . The overlaps  $\langle \Phi_{i-1-d}^\sigma \Phi_{i-1, i+2}^s | \Phi_i^\sigma \Phi_{i+1, i+4}^s \rangle$  for  $d = 3, 5, \dots$  all vanish based on Eq. (A4e). Similarly each of the Eqs. (A4f), (A4g), and (A4h) orthogonalize the distorted state  $|\Phi_i^\sigma \Phi_{i+1, i+4}^s\rangle$  to a class of orthonormal 3-spinon states.



From Eqs. (A4) we find

$$\alpha_1 = \frac{4}{9} + \frac{\alpha_9}{3}, \alpha_2 = \frac{2}{3}, \alpha_3 = \frac{2}{9} + \frac{2\alpha_9}{3}, \alpha_4 = \frac{1}{3}, \alpha_5 = \frac{1}{9} + \frac{\alpha_9}{3}, \alpha_6 = \frac{2}{3}, \alpha_7 = \frac{2}{9} + \frac{2\alpha_9}{3}, \alpha_8 = \frac{1}{3}, \quad (\text{A5})$$

where  $\alpha_9$  is left undetermined. In addition to the relations (A5), the orthogonalization process of the distorted state (A3a) with  $d = 5$  requires satisfying

$$\langle \Phi_{i-2,i+1}^s \Phi_{i+4}^\sigma | \Phi_i^\sigma \Phi_{i+1,i+6}^s \rangle = +1\alpha_2 - 2\alpha_3 - 2\alpha_8 + 4\alpha_9 = 0 \quad (\text{A6})$$

leading to

$$\alpha_9 = \frac{1}{6}, N_1 = \frac{\sqrt{3}}{2\sqrt{2}}, \quad (\text{A7})$$

where  $N_1$  is the normalizing prefactor. We checked that the states (A3a) for different  $i$  and  $d$  are also orthogonal.

The prefactors  $\beta_1 \cdots \beta_9$  in Eq. (A3b) can be computed similarly. We orthogonalize the distorted state (A3b) to the 1-spinon state (16b) and to the 3-spinon states (A1) and (A3a). For  $d = 3$ , this yields the eight independent equations

$$\langle \Phi_{i-2}^\sigma | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies -4\beta_1 - 1\beta_2 + 2\beta_3 + 2\beta_4 - 4\beta_5 - 4\beta_6 + 8\beta_7 + 2\beta_8 - 4\beta_9 + 2 = 0, \quad (\text{A8a})$$

$$\langle \Phi_i^\sigma | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies +1\beta_2 - 2\beta_4 + 4\beta_6 - 2\beta_8 - 2 = 0, \quad (\text{A8b})$$

$$\langle \Phi_{i+2}^\sigma | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies -2\beta_2 + 1\beta_3 + 4\beta_4 - 2\beta_5 = 0, \quad (\text{A8c})$$

$$\langle \Phi_{i+4}^\sigma | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies +1\beta_1 + 4\beta_2 - 2\beta_3 - 2\beta_8 + 1\beta_9 - 2 = 0, \quad (\text{A8d})$$

$$\langle \Phi_{i-2,i+1}^s \Phi_{i+4}^\sigma | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies -1\beta_1 + 2\beta_3 - 1\beta_9 = 0, \quad (\text{A8e})$$

$$\langle \Phi_{i-4}^\sigma \Phi_{i-1,i+2}^s | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies +1\beta_3 - 2\beta_5 = 0, \quad (\text{A8f})$$

$$\langle \Phi_{i-2}^\sigma \Phi_{i+1,i+4}^s | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies +3\beta_3 + 3\beta_8 - 6\beta_9 - 1 = 0, \quad (\text{A8g})$$

$$\langle \Phi_{i-4}^\sigma \Phi_{i-1,i+4}^s | \Phi_{i,i+3}^s \Phi_{i+4}^\sigma \rangle = 0 \implies +1\beta_1 - 3\beta_9 = 0, \quad (\text{A8h})$$

leading to

$$\beta_1 = 3\beta_9, \beta_2 = \frac{2}{3}, \beta_3 = 2\beta_9, \beta_4 = \frac{1}{3}, \beta_5 = \beta_9, \beta_6 = \frac{2}{3}, \beta_7 = 2\beta_9, \beta_8 = \frac{1}{3}. \quad (\text{A9})$$

The prefactor  $\beta_9$  remains unspecified.

The orthogonalization process for the state (A3b) with  $d = 5$  leads to the same results as (A9). However, one still needs to orthogonalize the distorted states (A3b) for different  $i$  and  $d$ . We find the equation

$$\langle \Phi_{i,i+5}^s \Phi_{i+6}^\sigma | \Phi_{i+2,i+5}^s \Phi_{i+6}^\sigma \rangle = 0 \implies +18\beta_9^2 - 15\beta_9 + 2 = 0, \quad (\text{A10})$$

where we used the relations (A9). This gives us the two solutions  $\beta_9 = \frac{1}{6}$  and  $\frac{2}{3}$ . We choose the solution  $\beta_9 = \frac{1}{6}$  as it indicates that the spinon at position  $i$  is of type *left*. The other solution  $\beta_9 = \frac{2}{3}$  corresponds to a spinon of type *right* at  $i - 2$ . Hence, we obtain

$$\begin{aligned} \alpha_1 = \beta_1 = \frac{1}{2}, \alpha_2 = \beta_2 = \frac{2}{3}, \alpha_3 = \beta_3 = \frac{1}{3}, \alpha_4 = \beta_4 = \frac{1}{3}, \alpha_5 = \beta_5 = \frac{1}{6}, \alpha_6 = \beta_6 = \frac{2}{3}, \\ \alpha_7 = \beta_7 = \frac{1}{3}, \alpha_8 = \beta_8 = \frac{1}{3}, \alpha_9 = \beta_9 = \frac{1}{6}, N_1 = N_2 = \frac{\sqrt{3}}{2\sqrt{2}}. \end{aligned} \quad (\text{A11})$$

This concludes the construction of the distorted orthonormal 3-spinon states (A3a) and (A3b).

## APPENDIX B: COMMUTATORS

The commutators between two neutral hopping operators are given by

$$\begin{aligned} [\mathcal{H}_{i,i+d}, \mathcal{H}_{j,j+d'}] = & (\delta_{i,j+d'} \mathcal{H}_{i-d',i+d} - \delta_{j,i+d} \mathcal{H}_{i,i+d+d'}) + (\delta_{i+d,j-1} + \delta_{i-1,j+d'}) (\mathcal{H}_{i,i+d} \mathcal{H}_{j,j+d'} - \mathcal{H}_{j,j+d'} \mathcal{H}_{i,i+d}) \\ & + \left( \theta(j-i)\theta(i+d-j)\theta(j+d'-i-d) \mathcal{H}_{i,i+d} \mathcal{H}_{j,j+d'} - \left\{ \begin{array}{l} i \rightarrow j \\ d \rightarrow d' \end{array} \right\} \right), \end{aligned} \quad (\text{B1a})$$

$$\begin{aligned}
 [\mathcal{H}_{i+d,i}, \mathcal{H}_{j,j+d'}] &= \delta_{i+d,j+d'} [\theta(d-d'+1) \mathcal{P}_{i+d-d'+1,i+d} + \theta(d'-d) \mathcal{P}_{i+1,i+d}] \mathcal{H}_{i+d-d',i} \\
 &\quad - \delta_{i,j} [\theta(d'-d+1) \mathcal{P}_{i,i+d-1} + \theta(d-d') \mathcal{P}_{i,i+d-1}] \mathcal{H}_{i+d,i+d'}
 \end{aligned} \tag{B1b}$$

with  $d$  and  $d'$  positive. We defined  $\mathcal{P}_{i,i-1} = 1$ . If the hopping operator brings two spinons in the singlet state to nearest-neighbor sites the result is zero. This explains why the second contribution in Eq. (B1a) can lead to a finite value. These commutators are required only up to bilinear level due to the approximation that we employ in this paper. Hence, Eqs. (B1) simplify to

$$[\mathcal{H}_{i,i+d}, \mathcal{H}_{j,j+d'}] = (\delta_{i,j+d'} \mathcal{H}_{i-d',i+d} - \delta_{j,i+d} \mathcal{H}_{i,i+d+d'}) + \dots \tag{B2}$$

with  $d' \geq 0$  and arbitrary  $d$ . Hermitian conjugation yields the commutator for  $d' \leq 0$ .

Two creation singlet operators do not necessarily commute; we find

$$[\mathcal{S}_{i,i+d}^\dagger, \mathcal{S}_{j,j+d'}^\dagger] = \mathcal{S}_{i,i+d}^\dagger \mathcal{S}_{j,j+d'}^\dagger \theta(i-j) \theta(j+d'-i-d) - \mathcal{S}_{j,j+d'}^\dagger \mathcal{S}_{i,i+d}^\dagger \theta(j-i) \theta(i+d-j-d'). \tag{B3}$$

This reflects the fact that in the creation of nested singlets the order of the singlet operators matters.

### APPENDIX C: EXPANSION OF PRODUCTS OF HOPPING OPERATORS

The product of two neutral hopping operators can be expanded as

$$\begin{aligned}
 \mathcal{H}_{i+n,i+n+d'} \mathcal{H}_{i,i+d} &= \delta_{n,d} \left[ \mathcal{H}_{i,i+d+d'} - \sum_{m_0 \geq 1} \theta(-m_0+d) \theta(m_0-d-d') \left( \mathcal{S}_{i+d+d',i+m_0+2}^\dagger \mathcal{S}_{i,i+m_0+2} + \sum_{p=x,y,z} \mathcal{T}_{i+d+d',i+m_0}^{p\dagger} \mathcal{T}_{i,i+m_0}^p \right) \right. \\
 &\quad \left. - \sum_{m_0 \geq 1} \theta(-m_0-d) \theta(m_0+d+d') \left( \mathcal{S}_{i-m_0-2,i+d+d'}^\dagger \mathcal{S}_{i-m_0-2,i} + \sum_{p=x,y,z} \mathcal{T}_{i-m_0,i+d+d'}^{p\dagger} \mathcal{T}_{i-m_0,i}^p \right) \right] \\
 &\quad + \theta(+n-2) \theta(n-d-2) \theta(n+d'-d-2) \mathcal{S}_{i+d,i+n+d'}^\dagger \mathcal{S}_{i,i+n} + \theta(+n) \theta(n-d) \theta(n+d'-d) \\
 &\quad \times \sum_{p=x,y,z} \mathcal{T}_{i+d,i+n+d'}^{p\dagger} \mathcal{T}_{i,i+n}^p + \theta(-n-2) \theta(d-n-2) \theta(d-n-d'-2) \mathcal{S}_{i+n+d',i+d}^\dagger \mathcal{S}_{i+n,i} \\
 &\quad + \theta(-n) \theta(d-n) \theta(d-n-d') \sum_{p=x,y,z} \mathcal{T}_{i+n+d',i+d}^{p\dagger} \mathcal{T}_{i+n,i}^p + \dots,
 \end{aligned} \tag{C1}$$

where 3 and higher spinon interactions are neglected.

### APPENDIX D: INTERACTION COEFFICIENTS

In order to compute the interaction coefficients  $\mathcal{A}_{3;1}$  one has to take into account the possible overlap (21) between orthonormal 3-spinon states. For each  $S_{\text{tot}} = \frac{1}{2}$  orthonormal 3-spinon state  $|\Phi_i^\sigma \Phi_{i+n,i+n+d}^s\rangle$  we define a dual state given by

$$|\Phi_i^\sigma \Phi_{i+n,i+n+d}^s\rangle^{(d)} := \begin{cases} |\Phi_{i,i+n}^\sigma \Phi_{i+n+d}^s\rangle, & \text{if } n > 0, \\ |\Phi_{i+n}^\sigma \Phi_{i+n+d,i}^s\rangle, & \text{if } n < -d. \end{cases} \tag{D1}$$

Each orthonormal 3-spinon state is orthogonal to all other states except to its dual state. The overlap is given by

$$\langle \Phi_i^\sigma \Phi_{i+n,i+n+d}^s | \Phi_i^\sigma \Phi_{i+n,i+n+d}^s \rangle^{(d)} = -\frac{1}{2}. \tag{D2}$$

We notice that there is no such finite overlap for the distorted 3-spinon states (A3). Hence they do not have a dual state.

We define the Hamiltonian matrix element

$$\mathcal{C}_{3;1}(d_e, n, d_0) := \langle \Phi_{i+d_e}^\sigma \Phi_{i+d_e+n,i+d_e+n+d_0}^s | H | \Phi_i^\sigma \rangle \tag{D3}$$

and its corresponding dual

$$\mathcal{C}_{3;1}^{(d)}(d_e, n, d_0) := {}^{(d)} \langle \Phi_{i+d_e}^\sigma \Phi_{i+d_e+n,i+d_e+n+d_0}^s | H | \Phi_i^\sigma \rangle. \tag{D4}$$

One has the relation

$$\mathcal{C}_{3;1}^{(d)}(d_e, n, d_0) = \begin{cases} \mathcal{C}_{3;1}(d_e+n+d_0, -n-d_0, n), & \text{if } n > 0, \\ \mathcal{C}_{3;1}(d_e+n, d_0, -n-d_0), & \text{if } n+d_0 < 0. \end{cases} \tag{D5}$$

Similarly, we define the dual of the interaction coefficient  $\mathcal{A}_{3:1}(d_e, n, d_o)$  as

$$\mathcal{A}_{3:1}^{(d)}(d_e, n, d_o) := \begin{cases} \mathcal{A}_{3:1}(d_e + n + d_o, -n - d_o, n), & \text{if } n > 0, \\ \mathcal{A}_{3:1}(d_e + n, d_o, -n - d_o), & \text{if } n + d_o < 0, \end{cases} \quad (\text{D6})$$

which links to the 1-spinon state  $|\Phi_i^\sigma\rangle$  to  $|\Phi_{i+d_e}^\sigma \Phi_{i+d_e+n, i+d_e+n+d_o}^s\rangle^{(d)}$ .

Using the relation (41), the Hamiltonian matrix elements  $\mathcal{C}_{3:1}(d_e, n, d_o)$  and  $\mathcal{C}_{3:1}^{(d)}(d_e, n, d_o)$  are given by

$$\mathcal{C}_{3:1}(d_e, n, d_o) = \mathcal{A}_{3:1}(d_e, n, d_o) - \frac{1}{2}\mathcal{A}_{3:1}^{(d)}(d_e, n, d_o) + \delta_{n,0}\mathcal{A}_{2:0}(d_o) - \frac{1}{2}\delta_{n+d_o, -d_e}\mathcal{A}_{2:0}(n) - \frac{1}{2}\delta_{n, -d_e}\mathcal{A}_{2:0}(-n - d_o), \quad (\text{D7a})$$

$$\mathcal{C}_{3:1}^{(d)}(d_e, n, d_o) = \mathcal{A}_{3:1}^{(d)}(d_e, n, d_o) - \frac{1}{2}\mathcal{A}_{3:1}(d_e, n, d_o) - \frac{1}{2}\delta_{n,0}\mathcal{A}_{2:0}(d_o) + \delta_{n+d_o, -d_e}\mathcal{A}_{2:0}(n) + \delta_{n, -d_e}\mathcal{A}_{2:0}(-n - d_o), \quad (\text{D7b})$$

where we supposed  $\mathcal{A}_{2:0}(d) = 0$  if  $d$  is even or if  $d < 3$ . In addition, we assumed  $n > 1$  or  $n + d_o < -1$  which means that the final state is not distorted. From Eqs. (D7) we find

$$\mathcal{A}_{3:1}(d_e, n, d_o) = \frac{4}{3}\mathcal{C}_{3:1}(d_e, n, d_o) + \frac{2}{3}\mathcal{C}_{3:1}^{(d)}(d_e, n, d_o) - \delta_{d_e,0}\mathcal{A}_{2:0}(d_o), \quad \{n > 1 \text{ or } n < -1 - d_o\}. \quad (\text{D8a})$$

For the case in which the final state is distorted, the interaction coefficient is given by

$$\mathcal{A}_{3:1}(d_e, n, d_o) = \mathcal{C}_{3:1}(d_e, n, d_o) - \delta_{d_e,0}\mathcal{A}_{2:0}(d_o), \quad \{n = 1 \text{ or } n + d_o = -1\}. \quad (\text{D8b})$$

Equations (D8) help to determine the interaction coefficients  $\mathcal{A}_{3:1}(d_e, n, d_o)$  from the Hamiltonian matrix elements and the Bogoliubov prefactors. Since  $\mathcal{H}_{3:1}(d_e, n, d_o)$  is cluster additive, we can compute  $\mathcal{A}_{3:1}(d_e, n, d_o)$  for each specific  $d_e, n$ , and  $d_o$  on finite clusters of sufficient size [49]. Comparing coefficients, we arrive at the analytical, compact form

$$\mathcal{A}_{3:1}(d_e, 1, d_o) = \frac{\sqrt{2}}{12}\delta_{d_o,3}[(3\alpha - 1)\delta_{d_e, -4} + 2\alpha\delta_{d_e, -2}] + \left(-\frac{1}{2}\right)^{\frac{(d_o+3)}{2}} [(3 - 2\sqrt{2})\delta_{d_e,0} - \sqrt{2}\delta_{d_e, -2}](1 - 2\alpha), \quad (\text{D9a})$$

$$\mathcal{A}_{3:1}(d_e, n, 3) = \left(-\frac{1}{2}\right)^{\frac{(n+3)}{2}} \left(\frac{6\alpha - 2}{3}\delta_{-d_e, n+3} + \frac{3 - 2\alpha}{3}\delta_{-d_e, n+1} + \frac{1 - 2\alpha}{2}\delta_{-d_e, n-1}\right), \quad n = 3, 5, \dots, \quad (\text{D9b})$$

$$\mathcal{A}_{3:1}(d_e, n, d_o) = \left(-\frac{1}{2}\right)^{\frac{(n+d_o)}{2}} \left(\delta_{-d_e, n+1} + \frac{1}{2}\delta_{-d_e, n-1}\right)(1 - 2\alpha), \quad n = 3, 5, \dots, \quad d_o = 5, 7, \dots, \quad (\text{D9c})$$

$$\mathcal{A}_{3:1}(d_e, -d_o - 1, d_o) = \left(-\frac{1}{2}\right)^{\frac{(d_o+3)}{2}} \left[\frac{6 - 3\sqrt{2}}{2}(1 - 2\alpha)\delta_{d_e,0} - \frac{\sqrt{2}}{2}\delta_{d_e,0} - 2\sqrt{2}\alpha\delta_{d_e,2}\right], \quad (\text{D9d})$$

$$\mathcal{A}_{3:1}(d_e, -d_o - 3, d_o) = \left(-\frac{1}{2}\right)^{\frac{(d_o+3)}{2}} \left[\frac{3\alpha - 1}{3}\delta_{d_e,0} + \frac{3 - 2\alpha}{6}\delta_{d_e,2} + (1 - 2\alpha)\delta_{d_e,4}\right], \quad (\text{D9e})$$

$$\mathcal{A}_{3:1}(d_e, n, d_o) = \left(-\frac{1}{2}\right)^{\frac{(d_e+d_o+1)}{2}} \left(\frac{1}{2}\delta_{d_e+1, -n-d_o} - 2\delta_{d_e-1, -n-d_o}\right)(1 - 2\alpha), \quad n = -d_o - 5, -d_o - 7, \dots \quad (\text{D9f})$$

The interaction coefficients  $\mathcal{A}_{2:2}^s(d_o, d_e, d'_o)$  and  $\mathcal{A}_{2:2}^t(d_o, d_e, d'_o)$  for specific  $d_o, d_e$ , and  $d'_o$  can also be calculated on finite clusters [49]. From the analysis of the coefficients we deduce

$$\mathcal{A}_{2:2}^s(d_o, d_e, 3) = \frac{5 - 7\tilde{\alpha}}{24}\delta_{d_o,3}\delta_{d_e,0} + \left(-\frac{1}{2}\right)^{\frac{d_o+3}{2}} \left[\delta_{d_o-3, d_e}(1 - 3\tilde{\alpha}) - \delta_{d_o-1, d_e}\left(1 + \frac{\tilde{\alpha}}{2}\right)\right], \quad (\text{D10a})$$

$$\mathcal{A}_{2:2}^s(d_o, d_e, d'_o) = -\frac{3\tilde{\alpha}}{2}\left(-\frac{1}{2}\right)^{\frac{d_o+d'_o}{2}}\delta_{d_o-1, d_e}, \quad d'_o = 5, 7, \dots, \quad (\text{D10b})$$

where we supposed  $d_e \geq 0$ .

The triplet channel interactions are given by

$$\begin{aligned} \mathcal{A}'_{2:2}(d_o, 0, d'_o) = & \left( \frac{23\alpha - 10 + 4\sqrt{6}(1 - 2\alpha)}{6} \right) \delta_{d_o,1} \delta_{d'_o,1} + \frac{\alpha}{2} \left( \frac{4\sqrt{6}}{9} - 1 \right) (\delta_{d_o,1} \delta_{d'_o,3} + \delta_{d_o,3} \delta_{d'_o,1}) + \frac{(\alpha - 1)}{18} \delta_{d_o,3} \delta_{d'_o,3} \\ & + \frac{(1 - 2\alpha)}{2} \left( \frac{4\sqrt{6}}{3} - 3 \right) \left( -\frac{1}{2} \right)^{\frac{d_o+d'_o}{2}} (\delta_{d_o,1} + \delta_{d'_o,1}), \end{aligned} \quad (\text{D11a})$$

$$\begin{aligned} \mathcal{A}'_{2:2}(d_o, d_e, 1) = & + \frac{(2 - \sqrt{6})\alpha}{6} \delta_{d_o,1} \delta_{d_e,2} + \frac{\alpha}{2} \left( \frac{4\sqrt{6}}{9} - 1 \right) \delta_{d_o,3} \delta_{d_e,2} - \frac{\sqrt{6}\alpha}{3} \left( -\frac{1}{2} \right)^{\frac{d_e}{2}} \delta_{d_o+1, d_e} \\ & + \left( \frac{3(1 - 2\alpha)}{4} + \frac{(3\alpha - 2)\sqrt{6}}{6} \right) \left( -\frac{1}{2} \right)^{\frac{d_e}{2}} \delta_{d_o-1, d_e}, \quad d_e \geq 2, \end{aligned} \quad (\text{D11b})$$

$$\begin{aligned} \mathcal{A}'_{2:2}(d_o, d_e, 3) = & + \left( -\frac{1}{2} \right)^{\frac{d_e}{2}+2} \left[ (1 - 2\alpha) \delta_{d_o+1, d_e} + \frac{3 - 2\alpha}{6} \delta_{d_o-1, d_e} + \frac{3\alpha - 1}{3} \delta_{d_o-3, d_e} \right] \\ & + \delta_{d_o,1} \delta_{d_e,2} \frac{3 - \sqrt{6}}{24} (1 - 2\alpha), \quad d_e \geq 2, \end{aligned} \quad (\text{D11c})$$

$$\mathcal{A}'_{2:2}(d_o, d_e, d'_o) = \frac{(1 - 2\alpha)}{2} \left( -\frac{1}{2} \right)^{\frac{d_o+d'_o}{2}} \left( \delta_{d_o-1, d_e} - \delta_{d_o+1, d_e} + \frac{3 - \sqrt{6}}{3} \delta_{d_o,1} \delta_{d_e,2} \right), \quad d_e \geq 2, \quad d'_o \geq 5. \quad (\text{D11d})$$

The prefactors  $\mathcal{A}'_{2:2}(d_o, d_e, d'_o)$  and  $\mathcal{A}_{2:2}(d_o, d_e, d'_o)$  with  $d_e < 0$  can be calculated from the symmetry relation

$$\mathcal{A}_{2:2}(d_o, d_e, d'_o) = \mathcal{A}_{2:2}(d'_o, -d_e, d_o). \quad (\text{D12})$$

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