Series Expansion Analysis of a Frustrated Four-Spin-Tube

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We study the magnetism of a frustrated four-leg spin-1/2 ladder with transverse periodic boundary conditions: the frustrated four-spin tube (FFST). Using a combination of series expansion (SE), based on the continuous unitary transformation method and density-matrix renormalization group (DMRG) we analyze the ground-state, the one-, and the two-particle excitations in the regime of strong rung-coupling. We find several marked differences of the FFST with respect to standard two-leg ladders. First we show that frustration destabilizes the spin-gap phase of the FFST which is adiabatically connected to the limit of decoupled rung singlets, leading to a first order quantum phase transition at finite inter-rung coupling. Second, we show that apart from the well-known triplon branch of spin-ladders, the FFST sustains additional elementary excitations, including a singlon, and additional triplons. Finally we find, that in the two-particle sector the FFST exhibits collective (anti)bound states similar to two-leg ladders, however with a different ordering of the spin-quantum numbers. We show that frustration has significant impact on the FFST leading to a flattening of the ground-state energy landscape, a mass-enhancement of the excitations, and to a relative enhancement of the (anti)binding strength. Where possible we use DMRG to benchmark the findings from our SE calculations, showing excellent agreement.

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I. INTRODUCTION

Ever since it has been realized that there are 'surprises' on the way from one- to two-dimensional quantum magnets, spin ladder structures have attracted an enormous interest. Two-leg ladders, such as Sr$_11_{-x}$Ca$_x$Cu$_2$xO$_{4+2}$, have been under intense scrutiny mainly because of the potential interplay between their spin-gaped ground state and the occurrence of superconductivity, N-leg ladders with $N > 2$ are of particular relevance, not only because they allow for a generalized test of Haldane’s conjecture, but also because new, tube-like lattice structures can be realized if periodic transverse boundary conditions apply, such as in [(CuCl$_2$tachH)$_3$Cl]Cl$_2$ and CsCrF$_7$ with $N = 3$, Cu$_2$Cl$_4$D$_8$C$_4$SO$_4$ with $N = 4$, and Na$_2$V$_3$O$_{11}$ with $N = 9$. For $N = 3$, magnetic frustration surfaces as an additional ingredient, already for tubes with only nearest neighbor exchange, leading to a rich variety of phenomena not present in two-leg ladders.

Experimentally, the four-spin tube Cu$_2$Cl$_4$D$_8$C$_4$SO$_4$ has been suggested to display frustrating antiferromagnetic next-nearest neighbor exchange. Theoretically, unfrustrated four-spin tubes have been considered in two seminal papers, both, in the weak and the strong rung-coupling limit. Magnetic frustration, however, has not been considered in these studies. Therefore, in this work, we perform a first analysis of a frustrated four-spin tube (FFST)

$$H = \sum_{lm} j_{lm} S_l \cdot S_m ,$$

with a lattice structure and exchange couplings $j_{lm}$ as shown in Fig 1. Spin-1/2 moments are located on the solid circles and all couplings, $j_0, j_1$ and $j_2$ are antiferromagnetic (we set $j_0 = 1$ hereafter). This FFST is simpler than the one proposed for Cu$_2$Cl$_4$D$_8$C$_4$SO$_4$, where only part of the surface squares experience diagonal exchange, and the leg-couplings seem to be in-equivalent. Apart its relation to existing materials, the FFST is of interest as a 1D variant of the anisotropic triangular lattice on the torus with four site circumference, i.e. cutting the tube longitudinally one obtains an anisotropic triangular lattice strip.

For $j_{1,2} \ll 1$, the FFST resembles a chain of weakly coupled four-spin plaquettes each of which displays a singly degenerate singlet ground state, separated by a gap of $j_0 = 1$ from the first excited triplet. Therefore perturbation theory in $j_{1,2}$ applies. Motivated by this we investigate the FFST by series expansion (SE) in $j_{1,2}$. Moreover, we corroborate our approach and gauge our SE results by employing density-matrix renormalization group (DMRG) calculations. The structure of the paper is as follows. In section II we clarify the region of applicabil-
II. COUPLED PLAQUETTE REGIME

Proper application of SE hinges on the adiabatic renormalization of the bare starting state in terms of the coupling constants. In case of intervening second order quantum phase transitions, the SE can be used directly to limit its range of applicability in terms of diverging susceptibilities or vanishing elementary excitation gaps. In case of a discontinuous or first order transitions, SE based on a single bare ground state fails to signal any transition. To put our SE on firm grounds a-priori, we therefore search for potential first-order quantum phase transitions of the FFST at small $j_{1,2}$.  

To this end, it is instructive to first consider the classical phase diagram of the FFST. We allow the spin structure to be a spiral, which, due to $SU(2)$ symmetry can be considered to be planar $S = S(\cos(Q_x r), \sin(Q_x r), 0)$ with $r = l_x R_x + l_y R_y$, where $R_{x,y} = (1, 0), (0, 1), l_x \in \mathbb{N}$, and $l_y = \{1, \ldots, 4\}$. The transverse pitch vector $Q_y$ has to be discretized according to $\{(0, 1, 2, 3)\pi/2\}$. The ground state energy is $e_g = \cos(Q_y) + j_1 \cos(Q_x) + j_2 \cos(Q_x + Q_y)$. From this, four classical phases result, shown in Fig. 1.

III. SERIES EXPANSION METHOD

The main focus of this work is on SE in terms of $j_1$ and $j_2$, starting from the limit of isolated plaquettes. To this end we decompose the Hamiltonian of the FFST into $H = H_0 + V$.
Table I: Spectrum of the single plaquette. It consists of four equidistant energy levels $E_n = q_n - 2$ labeled by the quantum number $q_n = 0, \ldots, 3$, the total spin $S$, and its $z$-component $S_z$. The last column enumerates the states.

| State $q_n$, $E_n$, $S$, $S_z$, Idx |
|-----------------------------|
| $|s_0\rangle$ | 0 | -2 | 0 | 0 |
| $t^x_{1/2}$ | 1 | -1 | 1 | -1.01 | 1.23 |
| $|s_1\rangle$ | 2 | 0 | 0 | 0 |
| $t^y_{1/2}$ | 1 | 1 | 1 | -1.01 | 5.67 |
| $t^z_{1/2}$ | 2 | 0 | 1 | -1.01 | 8.910 |
| $|s_2\rangle$ | 3 | 1 | 2 | -2 | 11, ..., 15 |

where $h_{0,n}$ is the plaquette Hamiltonian at site $n$

$$h_{0,n} = [S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_4 + S_4 \cdot S_1]_n$$

and the perturbation $V = V_1 + V_2$ is given by

$$V_1 = j_1 \sum_{n} S_{i,n} \cdot S_{i,n+1},$$
$$V_2 = j_2 \sum_{n} (S_{i,n} \cdot S_{i,n+1} + S_{i,n+1} \cdot S_{i,n}) + S_{3,n} \cdot S_{3,n+1} + S_{4,n} \cdot S_{4,n+1}.$$ 

The eigenstates of an isolated plaquette consist of four equidistant energy levels $E_n = q_n - 2$, labeled by the quantum number $q_n = 0, \ldots, 3$, and can be classified according to the total and the $z$-component of the plaquette spin $S_n = \sum_{i=1}^{4} S_{i,n}$. Table I lists that the ground state is a singlet, the first excited state at $q_n = 1$ is a triplet, the $q_n = 2$ sector is composed of a singlet and two triplets, and for $q_n = 3$ one quintet remains.

In turn, $H_0$ displays an equidistant spectrum, labeled by $Q = \sum_n q_n$. At $V = 0$, the $Q = 0$ sector refers to the unperturbed singlet ground state $|0\rangle = \otimes_n |s_0\rangle$ composed of $q_n = 0$ singlets on all plaquettes. The $Q = 1$ sector comprises single $|t^z_{1/2}\rangle$ triplets inserted into $|0\rangle$ at site $m$. The $Q \geq 2$ sectors are of multi-particle nature. The perturbation $V$ can be rewritten as $V = \sum_{i=1}^{2} j_i \sum_{n=1}^{N} T^i_{n}$, where $T^i_{n}$ represent raising ($n > 0$) or lowering ($n < 0$) operators within the spectrum of $H_0$. For the FFST we find $N = 4$.

It has been shown quite generally, that models with the preceding type of spectrum allow for SE through a continuous unitary transformation (CUT) using the flow equation method of Wegner. The basic idea is to transform $H$ onto an effective Hamiltonian $H_{eff}$ which is block-diagonal in the quantum number $Q$. This transformation can be achieved exactly order-by-order in $j_{1,2}$ leading to

$$H_{eff} = H_0 + \sum_{n,0 \leq m \leq n} C_{n,m} j_{1}^{n-m} j_{2}^{m}.$$ 

Figure 3: Ground state energy per site $e_0$ versus $j_1$ and $j_2$, showing a monotonously decreasing behavior in the parameter range shown. Along the line of maximum frustration $j_1 = j_2$, the energy gain is smallest.

where the $C_{n,m}$ are weighted products of the $T^i_{m}$ operators which conserve the $Q$-number and have their weights determined by recursive differential equations, see [18] for details. Due to $Q$-number conservation several observables can be accessed directly from $H_{eff}$ in terms of a SE in $j_{1,2}$. For systems with coupled spin-plaquette CUT SE has been used for one[20], two[21,22] and three[23] dimensions.

IV. RESULTS

In this Section we present our findings from SE up to $Q = 2$, sectioning the discussion according to A. the ground-state energy, B. the one-, and C. the two-particle excitations. To assess the quality of the SE we complement our analysis by DMRG calculations for selected cases.

A. Ground State Energy

First we consider the ground state energy $E_0$. $Q$-conservation leads to

$$E_0 = \langle 0 | H_{eff} | 0 \rangle,$$

where $|0\rangle$ is the unperturbed ground state.

Evaluating this matrix element on chains with periodic boundary conditions (PBC) of a length $L$, sufficient not to allow for wrap-around of graphs with length $N$, i.e. $L = N + 1$, one can obtain analytic SEs which are valid to $O(N)$ with respect to eqn. [6] in the thermodynamic limit. Evaluating the ground state energy per spin $e_0 = E_0/(4L)$ up to $O(7)$ we get

$$e_0 = \frac{1}{2} - \frac{17j_1^2}{96} + \frac{17j_2^2}{96} + \frac{j_1 j_2}{3} - \frac{25j_1^3}{384} + \frac{25j_2^3}{384} + \frac{j_1^3}{16} + \frac{j_2^3}{16} + \frac{1919j_1^4}{196768} + \frac{1919j_2^4}{196768} + \frac{313j_1^5}{1728} + \frac{313j_2^5}{1728} + \frac{15457j_1^6}{48384} + \frac{1510499j_2^6}{27095040} + \frac{39353j_1^7}{27095040} + \frac{39353j_2^7}{188160}$$
Here, the first term corresponds to the bare energy per spin listed in Table I. Since the FFST can be mapped onto an identical FFST with \( j_1 \leftrightarrow j_2 \) by a \( \pi/2 \)-twist of the plaquettes around the tube, one expects that 
\[ e_0(j_1,j_2) = e_0(j_2,j_1), \]
which is obviously fulfilled. Figure 3 shows \( e_0(0 \leq j_1 \leq 1, 0 \leq j_2 \leq 1) \) to be monotonously decreasing with \( j_{1,2} \). Along the line \( j_1 = j_2 \), the energy gain is smallest. Speaking differently, along its maximally frustrated direction in parameter space the energy landscape is flattest.

In Fig. 4(a) we assess the accuracy of eqn. (4) in several ways. First, in panel (a) we compare \( e_0 \) with DMRG calculations along \( j_{2,0} = 0 \) where we expect no first-order transition. The DMRG results have been obtained for \( L = 30 \) and \( m = 300 \). Obviously the agreement between SE and DMRG is very good for \( j_1 \lesssim 0.75 \). In panel (b) we display a similar comparison along \( j_1 = j_2 \). Here the SE agrees very well with DMRG to even larger values of \( j_{1,2} \), however only up to the first-order transition discussed in Section II. Third, in panel (a) we also include three DlogPadé approximants to eqn. (7). For the FFST however, and for \( Q = 2 \), \( S = 0.1 \) and up to \( O(7) \), we find that all matrix elements of \( H_{\text{eff}} \) inducing such decay vanish identically. This feature can be traced back to the \( C_4 \) symmetry of the tube. In fact, we obtain that changing e.g. the exchange couplings \( j_1 \) into \( j_1' \neq j_1 \) on one of the legs, renders the one-particle \( Q = 2 \) states unstable against decay. In summary, for each momentum \( k \) the \( Q = 2 \) spectrum contains three genuine one-particle levels with \( S = 0, 1 \), all of which are degenerate in \( m \). For the remaining two-particle states with \( Q = 2 \) we refer to the next section.

For the rest of this section we label the one-particle states by \( |i\rangle Q,S_n \), where \( i \) refers to the plaquette’s site and \( S_n \) is the total spin, where the index \( n \) is only due to the fact that for \( Q = 2 \) there are two \( S = 1 \) states, say, \( n = a, b \). Spin-\( z \) quantum numbers \( m \) are discarded because of \( SU(2) \) invariance. Due to \( Q \)-conservation and \( SU(2) \) invariance the effect of \( H_{\text{eff}} \) on \( |i\rangle Q,S_n \) is limited to

\[
H_{\text{eff}}|i\rangle Q,S_n = \sum_{i,S_m=S_n} t_{Q,S_n,S_m} |j+i\rangle Q,S_m,
\]

where \( t_{Q,S_n,S_m} \) is an effective hopping matrix element between \( |i\rangle Q,S_n \) and \( |j+i\rangle Q,S_m \).
which implies a shift in real space, and potentially a mixing of states of equal $S$ with identical $Q$. The hopping amplitudes $t_{ij}^Q S_n, S_m$ do not depend on $j$ due to translation invariance. Therefore, by Fourier transformation $|k\rangle^Q S_n = 1/\sqrt{E} \sum_j \exp(-i\,k\,j)|j\rangle^Q S_n$ we get the dispersion from

$$E_{Q,S_n, S_m}^{1\text{pt}}(k) = \langle Q, S_n | H_{\text{eff}} | k \rangle^Q S_m - E_0 \delta_{S_n, S_m},$$

$$= t_0^{Q,S_n, S_m} + 2 \sum_i t_i^{Q,S_n, S_m} g(i,k),$$  \hspace{1cm} (9)

where, obviously $t_i^{Q,S_n, S_m} = t_i^{Q,S_n, S_m}$. However for $S_n \neq S_m$, i.e. for the two $Q = 2, S = 1$ states, we find $t_i^{Q,S_n, S_m} = -t_i^{Q, S_n, S_m}$. In turn, $g(x)$ is $\cos[i \sin(x)]$ for $S_n$-off-diagonal transitions.

To obtain hopping amplitudes valid to $O(N)$, in the thermodynamic limit, the $t_i^{Q,S_n, S_m}$ and the ground state energy $E_0 = \langle 0 | H_{\text{eff}} | 0 \rangle$ in eqn. (4) have to be evaluated on clusters with open boundary conditions (OBC), large enough to incorporate $N$-th order graphs for hopping processes of distance $\pi$. Depending on $i$, these clusters are of either of length $N$ or $N+1$. We have calculated analytic expressions for $E_{Q,S_n, S_m}^{1\text{pt}}(k)$ to $O(7)$ in $j_{1,2}$.

For $(Q,S) \neq (2,1)$ eqn. (4) is already diagonal in $S_n$, $S_m$ with eigenvalues $E_{Q,S_n}^{1\text{pt}}(k) \equiv E_{Q,S_n}^{1\text{pt}}(k)$. Only for $(Q,S) = (2,1)$ eqn. (4) displays a $2 \times 2$-matrix structure, referring to $n = a, b$, with eigenvalues $E_{Q,1a}^{1\text{pt}}(k)$ and $E_{Q,1b}^{1\text{pt}}(k)$.

In Fig. 5 we show the one-particle dispersions for selected values of $j_{1,2}$. This figure displays only bare SE results and no Padé extrapolations. Several comments are in order. First, the figure does not only display $E_{Q,S_n}^{1\text{pt}}(k)$ for all $S$ and $Q \leq 2$, but for curiosity also the quintet with $Q = 3$, assuming that the latter does not decay into multi-particle states - which we have not checked.

As for the ground state energy, since exchanging $j_1 \leftrightarrow j_2$ maps the FFST onto an equivalent one by a $\pi/2$-twist there are related symmetries of the one-particle dispersions. These respect the additional fact, that the single-particle states on the bare plaquette are the eigenstates of a four-site spin-1/2 chain with PBC, which carry one out of four momenta $k_{n,\pm} = n\pi/2$ with $n = 0, 1, 2, 3$ transverse to the FFST. In turn, exchanging $j_1 \leftrightarrow j_2$ maps the one-particle dispersions onto identical ones up to a shift of the Brillouin zone by one out of $k_{n,\pm}$, and may also exchange the dispersion branches for the degenerate bare $Q, S = 2, 1$ states. We have checked this to be fulfilled by all $E_{Q,S_n}^{1\text{pt}}(k)$. E.g., for $(Q,S) = (1,1)$ we have $E_{Q,1a}^{1\text{pt}}(k, j_1, j_2) = E_{Q,1a}^{1\text{pt}}(k + \pi, j_1', j_2')$ and for $(Q,S) = (2,1)$ we have $E_{Q,1a}^{1\text{pt}}(k, j_1, j_2) = E_{Q,1a}^{1\text{pt}}(k + \pi/2, j_2, j_1'$). Additionally $E_{Q,1a}^{1\text{pt}}(k, j_1, j_2)$ are degenerate at $j_2 = 0$.

Considering the elementary triplet dispersion $E_{1,1}^{1\text{pt}}(k)$ at $j_2 = 0$, we observe a zone-boundary gap in Fig. 5 (a) which decreases as $j_1$ increases, see panel (b). For four-leg ladders without frustration, i.e. $j_2 = 0$, the analytic expression for the gap we get is

$$E_{1,1}^{1\text{pt}}(\pi, j_1, 0) = 1 - \frac{4}{3} j_1 + \frac{41}{108} j_1^2 + \frac{349}{1296} j_1^3$$

$$- \frac{4596401}{39191040} j_1^4 - \frac{169497997}{4702924800} j_1^5$$

$$- \frac{68984713639377}{2986549364992000} j_1^6$$

$$- \frac{843016345498432721}{45156565918790400000} j_1^7, \hspace{1cm} (10)$$

which, in passing, improves earlier SE to $O(4)$ on unfrustrated four-leg ladder by three orders. The dispersion $E_{1,1}^{1\text{pt}}(k)$ shows rather strong oscillations in panel (b). These are not related to convergence issues of the SE, but are robust features of hopping to more than only nearest-neighbors.

Increasing $j_2$ from zero, at fixed $j_1$, as from Fig. 5 (a) to (c) the bandwidth of $E_{1,1}^{1\text{pt}}(k)$ is reduced. On the line of maximum frustration, i.e. at $j_1 = j_2$ in panel (d), it is only very small, albeit not exactly zero, namely $O(j_1^2)$. A similar tendency can be observed in all other $(Q,S)$ sectors, yet less pronounced.

To assess the quality of the SE, we have also calculated the elementary $(Q, S) = (1, 1)$ gap by DMRG. The results are shown by the large crosses at the zone-boundaries in Fig. 5. As is obvious, the agreement is very good in all four panels. This is particularly noteworthy for panel (b), corroborating the preceding statement, that the oscillations...
Table II: \( Q = 2 \) states from the bare plaquette. \( C_{1n,1m-n}^{Sm} = (1n, 1m - n|Sm) \) are Clebsch-Gordan coefficients.

The existence of such collective states is know for simpler 1D quantum magnets, such as chains and two-leg ladders. Here we show that similar states exist also on the FFST. To this end we evaluate the two-particle spectrum following ideas developed for dimer-SE of two-particle irreducible two-particle interactions at \( Q = 2 \). The real-space representations of all \( Q = 2 \) states with proper spin quantum numbers \( S, m \) are listed in table [1]. Here the genuine two-particle states are labeled by \( |i, j S, m) \), where \( i, j \) refers to sites on the 1D lattice and \( S, m \) to total spin, and spin-\( z \) quantum numbers. As discussed in the preceding section the one- and two-particle excitations at \( Q = 2 \) do not mix. Therefore we focus on the genuine two-particle excitations hereafter.

Because of translational invariance the two-particle states can be classified according to a center-of-mass momentum \( q \) and a relative distance \( d \)

\[
|q, d)^{Sm} = \frac{1}{\sqrt{L}} \sum_r e^{iq(r+d/2)} |r, r + d)^{Sm} \tag{11}
\]

These states have an exchange parity \( P = (-1)^S \) for \( d \rightarrow -d \), i.e. \( |q, -d)^{Sm} = P|q, d)^{Sm} \). The effective Hamiltonian, eqn. [1], will mix states at different \( d \). The two-particle spectrum is obtained from the sum of the one- and two-particle irreducible Hamiltonians (see appendix [VII] and appendix [VII]), labeled by \( H_1 \) and \( H_2 \), with analytic matrix elements calculated by SE from the states of eqn. [11]. We have evaluated these matrix elements to \( O(6) \).

In Fig. [a] we show the two-particle spectrum \( \rho_S(q, \omega) = \sum_p \delta(\omega - E^{2pt}_{2S,m}(q, p)) \) at fixed total momentum \( q \) and spin \( S, m \), summed over the relative momentum \( p \), where \( E^{2pt}_{2S,m}(q, p) \) are the two-particle eigenenergies. We choose \( (j_1, j_2) = (0.6, 0.4) \) and \( q \approx \pi \) as an example. To analyze the effects of the interaction we consider \( E^{2pt}_{2S,m}(q, p) \) at various levels of approximation. First, we set the irreducible two-particle interactions \( H_2 \) to zero - i.e. no ‘actual’ interactions occur. The corresponding spectrum is shown in Fig. [b] for \( S = 0 \) and \( S = 1 \). These spectra are indistinguishable on the scale of this plot. The van-Hove singularities are related to the extrema of the one-particle dispersion in the \( (Q, S) = (1, 1) \) sector as in Fig. [5]. Even though the irreducible one-particle interaction \( H_1 \) will act only on one of the two particles, this does not imply, that the spectra in Fig. [a] are identical to the convoluted bare spectra of two single \( |t_0^{S\pm}) \)-particles at fixed total momentum \( q \) and finite \( L \). This is due to the hard-core constraint which forbids double occupation of plaquettes by \( |t_0^{S\pm}) \)-particles. This constraint is encoded in the matrix elements of \( H_1 \) when acting on the two particle sector. Since there are \( L \) double occupancies within \( L^2 \) two-particle states, their removal amounts to a \( 1/L \) effect on the integrated spectral weight at fixed to-
At fixed total and relative momentum, this effect will be quantitatively identical for two-particle states of identical exchange parity \((-\\)\)\(3\). For this reason Figs. (a) and (b) contain only \(S = 0\) and 1 states. Figure (b) depicts the difference between the bare spectra and that obtained from \(H_j\) for \(S = 0\) and \(S = 1\) for \(L = 200\). Clearly the integrated spectral weight for both values of \(S\) is finite but of order very small. Figure (a) shows that no (anti-)bound state arises in the two-particle sector solely due to the hard-core repulsion.

Next we consider the complete \(Q = 2\) spectrum in Fig. (c) for \(S = 1, 2\) and 3, including the irreducible two-particle interaction \(H_2\). The latter is spin-dependent and longer-ranged. This figure clearly demonstrates a main point of this section, i.e. the occurrence of three split-off (anti-bound) states (above) below the continuum depending on their spin. Apart from that, and similar to the hard-core constraint \(H_2\) leads to an \(O(1/L)\) redistribution within the two-particle continuum. The total momentum \(q\) in Fig. (a) has been chosen, such as to evidence the (anti)-bound states clearly. Depending on \(q\) they can approach and also merge with the continuum.

A qualitative understanding of binding versus anti-binding of the collective two-particle states can be obtained from considering the diagonal matrix elements \(S^m(q, d)\) of two particles versus their relative distance \(d\) at fixed total momentum \(q\). This matrix element is \(\propto \delta_{S,S'}\delta_{m,m'}\) and independent of \(m\). It is shown in Fig. (b) for \(S = 1\) identical to that of Fig. (a). This figure demonstrates that the irreducible two-body interactions are very rapidly decaying as a function of the relative distance of the particles (note the scaling of the matrix elements by \(10^{d-1}\) on the y-axis). Second, and for both total momenta depicted, the interactions for \(S = 1\) are attractive, while those for \(S = 0, 2\) are repulsive. This is consistent with binding versus anti-binding of the collective states in Fig. (a) Yet, one should keep in mind the matrix elements \(S^m(q, d)\) which are off-diagonal in \(d', d\). We have not tested if these invalidate the simplified argument given here. Finally, we emphasize, that the ordering of anti-bound versus bound states on the FFST is different from that on plain two-leg ladders. In the latter case two-particle singlets also form bound states with a binding energy larger than that of the two-particle triplets.

In Fig. (a) we show the dispersion of all one and two-particle states from the \(Q = 1\) and \(Q = 2\) sector as a function of total momentum for two sets of \(j_{1,2}\), obtained by SE, together with DMRG results for one and two-particle states at the zone-boundary(center). This figure is another main result of our paper and summarizes several aspects. First, the spectrum is very rich and consists of various discrete states and three superimposed two-particle continua. This should be contrasted against plain two-leg ladders, which show a less involved low-energy spectrum. Some of the discrete states are
genuine one-particle states and some are collective two-particle states. For the parameters depicted, the collective two-particle states are clearly visible only close to the zone boundary. The potential existence of critical parameters $j_{1,2}$ or wave-vectors $q^* \in (\mathbb{Z}^2)_{\text{BCS}}$ for which the collective states merge with the continua is unclear at present. The $Q = 2$ one-particle states are contained almost completely within the spectral range of the continua and split off from the latter only in a range of $q$ similar to the collective states. This situation is also very different from two-leg spin-ladders in which the states which split off from the continuum close to the zone boundary are collective (anti)-bound states only. From an experimental point of view this may pose a challenge on discriminating between such genuine one-particle and collective two-particle states. Finally, the effects of frustration are clearly visible only close to the zone boundary. The apparent ’two-curve’ structure is due to an oscillation of the error.

To conclude this section we provide some measure of convergence of the SE for the two-particle continuum in Fig. 9. This figure shows the relative change in energy of all two-particle states at a fixed total momentum versus their energy when switching from an $O(6)$ to an $O(7)$ evaluation of the matrix elements of $H_{1,2}$. For this we confine ourselves to $S = 0$. As is obvious, the changes are completely negligible and fully justify the use of $O(6)$ SE for the two-particle states. We note in passing, that $O(7)$ SE will not only lead to longer-range irreducible one-particle hoppings, but also increase the range of the irreducible two-particle interactions in Fig. 4 retaining however the rapid decay with distance depicted there.

V. CONCLUSIONS

To summarize, we have studied the strong rung-coupling regime of the frustrated four-spin tube. Remarkably, this spin model displays several twists with respect to conventional two-leg spin ladders. It allows for frustration induced quantum-phase transitions into phases other than the plaquette singlet phase. The nature of these phases remains to be explored. The structure of the excitations is both richer, and different as compared to two-leg ladders, including a reordering of two-particle (anti)bound states and additional elementary excitation modes, some of which can be made to decay by reducing the symmetry of the FFST. Finally geometric frustration on the FFST introduces a control parameter allowing for almost localization of excitations and a flattening of the energy landscape. As compared to potential material realizations of the FFST in Cu$_2$Cl$_2$-D$_2$C$_2$SO$_4$, several extensions have to be considered in the future. These comprise e.g. reducing the $C_4$-symmetry and considering the weak rung-coupling limit.

VI. ACKNOWLEDGMENTS

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VII. EFFECTIVE HAMILTONIAN MATRIX IN THE Q = 2 SECTOR

In this appendix we list some of the details necessary to evaluate the two-particle matrix elements by SE. First, we refer to the parity of the states in eqn. (11). Because of this we may confine ourselves to $d > 0$ ($d = 0$, i.e. $|r, r\rangle^{S_{\text{nn}}}$ is forbidden). The matrix elements of the one(two)-particle irreducible Hamiltonian $H_{1/2}$ are obtained by subtracting the one(two)-particle reducible contributions from the matrix elements of $H_{\text{eff}}^{30,32}$.

$$t_{0,n} = t_{n,0} = \langle n|H_1|0\rangle = \langle n|H_{\text{eff}} - H_0|0\rangle$$

$$t_{d|n,d'} = \langle n, n + d'|H_2|0, d\rangle = \langle n, n + d'|H_{\text{eff}} - H_1 - H_0|0, d\rangle$$

$$a_{d|n,d'}^{\text{cl}} = \delta_{0,n} \delta_{d,d'} E_0^{\text{cl}} - \delta_{d,n} \delta_{d,d'} E_0^{\text{cl}} - \delta_{d,n} \delta_{d,d'} E_0^{\text{cl}}$$
\[ \delta_{0,n}l_{n,d}^{cl} - P\delta_{d,n}l_{n,d}^{cl} - P\delta_{0,n+d}l_{n,d}^{cl} \]

Here \( a_{0,n}^{cl} = \langle n| H_{i,j} | 0 \rangle \), \( a_{d,n}^{cl} = \langle n, n + d'| H_{i,j} | 0, 0 \rangle \), and \( cl \) refers to the cluster on which these matrix elements are evaluated. For \( t_{0,n} \) and \( t_{d,n,d'} \) to be size consistent, the cluster has to be the largest linked cluster for a given one- and two-particle state in real space at a given order \( N \) of the SE. The \( d_{0,n}^{cl} \) in eqn. (13) refers to \( t_{0,n} \) evaluated on the same linked cluster `cl' as the \( a_{d,n}^{cl} \) corresponding to a given \( t_{d,n,d'} \) and \( E_{0}^{cl} = \langle 0| H_{0} | 0 \rangle \) is the ground state energy of that cluster. The two-particle state results from the eigensystem of

\[
S \langle q, d'| H_{i,j} - H_{0} | q, d \rangle S = S \langle q, d'| H_{2} + H_{1} | q, d \rangle S
\]

which, due to translational and spin-rotational invariance is diagonal in \( q, S \) and \( m \) and is independent of \( m \). For each \( (q, S, m) \) the two matrices on the left of eqn. (14) are hermitian with, matrix-indices \((d', d)\). Thus, for the remainder we may consider only \( d' \leq d \). We begin with \( h_{2,d,d} = S \langle q, d'| H_{2} | q, d \rangle S \). Because a linked cluster can have at most \( N + 1 \) sites, \( h_{2,d,d} = 0 \) for \( d', d > N \). I.e. \( h_{2,d,d} \) is an \( N \times N \) matrix. The action of \( H_{2} \) is

\[
H_{2}|q, d\rangle = \frac{1}{\sqrt{L}} \sum_{r} e^{i(r+d'2/2)} \times \sum_{\text{max}(n+d', d-n) \leq N} t_{d,n,d'} |r + n, r + n + d'\rangle S
\]

\[
= \sum_{\text{max}(n+d', d-n) \leq N} t_{d,n,d'} e^{i(q(r-d'/2)2-n)} |q, d\rangle S
\]

(15)

where \( n \) must be restricted to \( \text{max}(n + d', d - n) \leq N \), because of the sites \((0, d, n + d')\) to reside within a linked cluster at order \( N \). I.e. \( n \) is confined to the interval \( d - N < n \leq N - d' \), which has its midpoint at \( n_m = (d - d')/2 \)

\[
H_{2}|q, d\rangle = \sum_{\text{max}(n+d', d-n) \leq N} t_{d,(d-d')/2,d'} + \sum_{\text{max}(n+d', d-n) \leq N} 2t_{d,n,d'} \cos[\sqrt{q} (d - d'2 - n)] |q, d'\rangle S
\]

(16)

where \( t_{d,n,d'} = t_{d,(d-d')/2,d'} \) has been used, which refers to reflection symmetry of the two-particle matrix element about the midpoint, and the addends with matrix elements \( t_{d,(d-d')/2,d} \) occurs only if \( n_m = (d - d')/2 \) is \( \mathbb{Z} \).

Next, we apply \( H_{1} \) to a two-particle state. This will only shift one of the particles, i.e.

\[
H_{1}|q, d\rangle = \sum_{\text{max}(n+d', d-n) \leq N} t_{d,n,d'} (e^{-i\sqrt{q}/2} + e^{i\sqrt{q}/2})
\]

\[
\times \frac{1}{\sqrt{L}} \sum_{r} e^{i(r+(d-n)/2)} |r + n, r + d - n)\rangle S
\]

For each \( q, H_{1} \) connects states \( d \) and \( |d - n\rangle \), \( \forall - N \leq n \leq N \). This is equivalent to a band-matrix of width \( 2N + 1 \). For \( d \geq N \), the non-zero content of the columns of this matrix is independent of \( d \), for \( 1 \leq d < N \) this is not so. The latter relates to the exclusion of on-site double-occupation.

For reference we explicitly display one specific low-order matrix element \( S \langle q, d' | H_{1} + H_{2} | q, d \rangle S \) from eqns. (13) (16), (17), namely \( d' = d = 1 \), \( N = 4 \) and \( S = 0 \). Figure 10 relates to the two-particle irreducible matrix element from \( H_{2} \), and depicts all \( t_{d,n,d'} \) on their respective clusters including a label for reducing contributions to be evaluated according to eqns. (12) (13). These are \( E_{0}^{cl}, t_{0,0}, t_{1,1}^{cl} \) for \( n = 0 \) and \( t_{cl}^{cl} \) for \( n = 1 \) for this particular matrix element. Note that on finite clusters \( t_{0}^{cl} \) and \( t_{1}^{cl} \) are not necessarily identical. The one-particle irreducible matrix element from \( H_{1} \) is straightforward. The complete matrix element reads

\[
0 \langle q, 1 | H_{1} + H_{2} | q, 1 \rangle = 0 + \frac{j_{2}}{6} + \frac{431 j_{1}^{2}}{432} + \frac{5827 j_{1}^{3}}{15552}
\]

Figure 10: Linked clusters with size \( l_{i} \) and with initial (halve circles) and final (wedges) two-particle states for all addend in eqn. (15) at order \( N = 4 \) and for \( d = d' = 1 \). (1R labels (ir)reducible graphs.

\[
= \sum_{-N \leq n \leq N, n \neq d} 2t_{0,n}^{cl} \cos(\frac{nq}{2}) \text{sgn}(d - n) S \langle q, |d - n\rangle S
\]

(17)
Finally, in the $Q = 2$ sector the single-particle states $|t_{1i}^1\rangle$, $|t_{2i}^2\rangle$, and $|s_{1i}\rangle$ need to be considered. Any one-particle irreducible Hamiltonian matrix element between the two- and one-particle states for $Q = 2$ is zero due to orthogonality. Two-particle irreducible contributions require matrix elements of the form

$$\langle q', d'| H_{eff} | q, d \rangle$$

where $|q\rangle^{Sm} = \sum_r e^{iqr} |r\rangle^{Sm} / \sqrt{L}$ is a one-particle state of spin quantum numbers $S, m$ with $Q = 2$. This implies a decay of $Q = 2$ single-particle states into $Q = 2$ two-particle states. Up to the order that we have performed the SE, we have not observed such decay. In turn the Hamiltonian matrix in the $Q = 2$ sector of the four-tube is already diagonal w.r.t. the particle number.