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Series expansion analysis of a tetrahedral cluster spin chain

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Abstract. Using analytical series expansion by continuous unitary transformations we study the magnetic properties of a frustrated tetrahedral spin-$\frac{1}{2}$ chain. Starting from the limit of isolated tetrahedra we analyze the evolution of the ground state energy and the elementary triplet dispersion as a function of the inter-tetrahedral coupling. The quantum phase diagram is evaluated and is shown to incorporate a singlet product, a dimer, and a Haldane phase. Comparison of our results with those from several other techniques, such as density matrix renormalization group, exact diagonalization, bond-operator theory and other numerical series expansion are provided and convincing agreement is found.

PACS. 75.10.Jm Quantized spin models – 75.50.Ee Antiferromagnetics – 02.30.Mv Approximations and expansions

1 Introduction

Geometric frustration is an important aspect of magnetism. In particular, magnets on triangular or tetrahedral lattices have been of recent interest because of their potentially exotic phases [1]. Introducing spatially inhomogeneous exchange couplings in geometrically frustrated spin systems is an additional issue since it can lead to quantum phase transitions between such exotic phases. In this context, and motivated by various transition metal compounds [2–4], models of one-, two- and three-dimensional (1, 2 and 3D) networks of frustrated spin-1/2 tetrahedra, with variable inter-tetrahedral exchange couplings, have been investigated recently [2,3,5–12]. In 1D, the effect of inter-tetrahedral coupling has been analyzed using bond-boson mean field theory (MFT), exact diagonalization (ED) [13] and effective Hamiltonians [14]. In 3D, molecular field theories [5,6] and numerical(analytical) series expansions (SE) up to 4th(2nd) order have been carried out [15]. Rich quantum phase diagrams with several competing states were observed in all cases.

The SE technique used in reference [15] would allow for considerably higher orders to be evaluated if applied to a 1D situation therefore improving the earlier analysis of the 1D tetrahedral chains. Such analysis has not been done up to now. Therefore it is the primary aim of this work to perform high order analytic SE expansion. Moreover high order SE for the 1D case will also allow for a closer comparison with results obtained by other means.

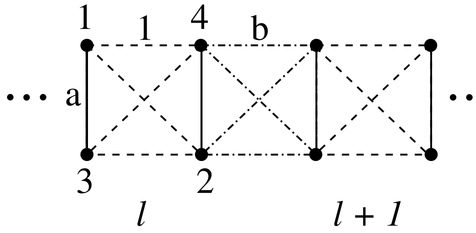

Fig. 1. Tetrahedral cluster-chain. The unit cell, labelled with l, contains spin-1/2 moments $\mathbf{s}_{i\,l}$ at vertices $i = 1, \ldots, 4$ (solid circles). All couplings are in units of J_1 (dashed lines).

To set the scene, we briefly repeat some facts on the tetrahedral spin-1/2 chain, shown in Figure 1, which we will investigate, and which were introduced in references [13,14]. The tetrahedra correspond to the sites 1–4 with couplings J_1 and $J_2 = aJ_1$. Inter-tetrahedral exchange occurs through $J_3 = bJ_1$. The Hilbert space of a single tetrahedron is listed in Table 1. The Hamiltonian of the chain can be written in terms of the total edge-spin operators $\mathbf{P}_{1(2),l} = \mathbf{s}_{1(4),l} + \mathbf{s}_{3(2),l}$, where $\mathbf{s}_{i,l}$ denotes a spin-1/2 at vertex i on the tetrahedron at site l

$$\frac{H}{J_1} = \sum_{l=1}^{L/2} \left[\mathbf{P}_{1,l}\mathbf{P}_{2,l} + \frac{a}{2}\left(\mathbf{P}_{1,l}^2 + \mathbf{P}_{2,l}^2 - 3\right) + b\mathbf{P}_{2,l}\mathbf{P}_{1,l+1} \right]. \tag{1}$$

L is the number of rungs, i.e. sites coupled by $J_2 = aJ_1$.

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Table 1. Eigenstates of a single tetrahedron: singlets ($\mathcal{S}_1, \mathcal{S}_2$); triplets ($\mathcal{T}_1, \mathcal{T}_{2,3}$) and Quintet ($\mathcal{Q}$). Each state is labelled by the $P_{1,2}$ edge-spin quantum numbers and the energy E/J_1. Site index l suppressed.

	P_1	P_2	E/J_1
$\mathcal{S}_1$	1	1	$-2 + a/2$
$\mathcal{S}_2$	0	0	$-3a/2$
$\mathcal{T}_1$	1	1	$-1 + a/2$
$\mathcal{T}_{2,3}$	0,1	1,0	$-a/2$
$\mathcal{Q}$	1	1	$1 + a/2$

The Hamiltonian commutes with the edge spin, i.e. $[H, \mathbf{P}^2_{i(=1,2),l}] = 0;\ \forall\, l, i = 1, 2$. Hence, the Hilbert space decomposes into sectors of fixed distributions of locally conserved edge-spin eigenvalues $P_{i,l}$, each corresponding to a sequence of spin-1 chain-segments ($P_{i,l} = 1$) intermitted by chain-segments of *localized* singlets ($P_{i,l} = 0$). It has been shown in reference [13] that the ground state of equation (1) occurs only within the homogeneous sector of purely $\mathcal{S}_2$ states or in the $P_{i,l} = 1$, $\forall i, l$ sector. Keeping b fixed and for $a \to \infty$, the ground state must result from local $\mathcal{S}_2$ type of states. This is a trivial, decoupled *singlet product* phase with singlets on each rung. The ground state energy per tetrahedron in this phase is independent of b and it is given by: $e_{g\,\mathcal{S}_2} = -3a/2$. In the opposite limit $a \to 0$ the ground state is in the $P_{i,l} = 1$, $\forall i, l$ sector.

For $P_{i,l} = 1$, $\forall i, l$ the tetrahedral chain is equivalent to that of a dimerized spin-1 chain with L sites

$$\frac{H}{J_1} = \sum_{l=1}^{L} [\mathbf{S}_{2l-1}\mathbf{S}_{2l} + b\mathbf{S}_{2l}\mathbf{S}_{2l+1}] + \frac{a}{4}L, \tag{2}$$

where the edge-spin operators $\mathbf{P}_{1,l} = \mathbf{S}_{2l-1}$ and $\mathbf{P}_{2,l} = \mathbf{S}_{2l}$ have been relabelled in terms of spin-1 operators $\mathbf{S}_l$. The dimerized spin-1 chain is known to have a second order quantum phase transition at $b = b_c$ between a *dimer phase* ($b < b_c$) and the *Haldane phase* ($b > b_c$), as first pointed out by Affleck and Haldane [16,17]. The a-dependence in equation (2) is reduced to a constant term and then it has no influence on the location of the transition. We will analyze the transition in Section 4 by SE in terms of b and compare our results with those obtained from other methods.

2 Series expansion by continuous unitary transformation

The Hamiltonian of the tetrahedral chain (Eq. (1)) can be written as

$$\frac{H}{J_1} = H_0 + aT_{a\,0} + b\sum_{n=-N}^{N} T_{b\,n}. \tag{3}$$

H_0 is the sum over local tetrahedral Hamiltonians at $a = 0$. Their spectra consist of four equidistant energy levels $E/J_1 = -2, -1, 0, 1$ (see Tab. 1). With these levels we associate a number q_l of local energy *quanta* $q_l = 0, \ldots, 3$. Together with $P_{1,2}$, this characterizes the basis. H_0 has an equidistant ladder spectrum labelled by $Q = \sum_l q_l$. $Q = 0$ refers to the *unperturbed* ground state of H_0: $|0\rangle \equiv |\mathcal{S}_{1,1} \ldots \mathcal{S}_{1,L/2}\rangle$, i.e. an $\mathcal{S}_1$ singlet product. The $Q = 1$ sector of H_0 consists of linear combinations of local $\mathcal{T}_{1,j}$ triplet excitations $|t_j\rangle \equiv |\mathcal{S}_{1,1} \ldots \mathcal{T}_{1,j} \ldots \mathcal{S}_{1,L/2}\rangle$, with a $\mathcal{T}_{1,j}$ triplet on the tetrahedron at site j. $T_{a\,0}$ refers to the sum over the local terms proportional to a in equation (1). By construction, this term is diagonal in the basis of H_0. The third term in equation (3) refers to the inter-tetrahedral coupling via b. The operators $T_{b\,n}$ non-locally create (destroy) $n \geq (<)\, 0$ quanta within the ladder spectrum of H_0. For our model $N \leq N_{max} \equiv 6$, in principle. Explicit calculation of the T_{bn}, however, shows that $N \leq 4$ [18]. By a shift of 1/2 of the unit cell, equation (1) is symmetric under $(J_1, a, b) \to (J_1 b, a/b, 1/b)$. Therefore, to cover the parameter space $a, b \in [0, \infty]$ is sufficient to consider the range $a \in [0, \infty]$ and $b \in [0, 1]$.

It has been shown [19–21] that models of type equation (3) allow for high-order SE using a continuous unitary transformation generated by the flow equation method of Wegner [22]. Adapted to our case, the mapping of equation (3) onto the unitarily rotated effective Hamiltonian H_{eff} reads [19,21]

$$H_{\text{eff}} = H_0 + aT_{a\,0} + \sum_{n=1}^{\infty} b^n \sum_{\substack{|\mathbf{m}|\,=\,n\\ M(\mathbf{m})=0}} C(\mathbf{m})\, T_{b\,m_1} T_{b\,m_2} \ldots T_{b\,m_n}, \tag{4}$$

where $\mathbf{m} = (m_1, \ldots, m_n)$ is an $n = |\mathbf{m}|$-tuple of integers, each in a range of $m_i \in \{0, \pm 1, \ldots, \pm N\}$ and $M(\mathbf{m}) \equiv \sum_{i=1}^{n} m_i$. A main advantage of this method is that, in contrast to H of equation (3), H_{eff} is constructed to *conserve* the total number of quanta Q at each order n, allowing for easy access to several quantities using the bare eigenstates of H_0 (see [15]).

3 Ground state energy and triplet dispersion

Now we discuss results for the ground state energy E_g and the triplet dispersion $\omega(k)$ in the dimer phase as obtained from SE with respect to the inter-tetrahedral coupling b. Q-conservation leads to

$$E_g = \langle 0|H_{\text{eff}}|0\rangle, \tag{5}$$

where $|0\rangle = |\mathcal{S}_{1,1} \ldots \mathcal{S}_{1,L/2}\rangle$ and H_{eff} is the effective Hamiltonian given by equation (4). Wrap-around of graphs up to length n will not occur if this matrix element is evaluated on chains with $n+1$ tetrahedral clusters and periodic boundary conditions (PBC). This is required by linked-cluster theorem [23] and leads to SE's valid to $O(n)$ in the thermodynamic limit, i.e. for infinite-sized systems.

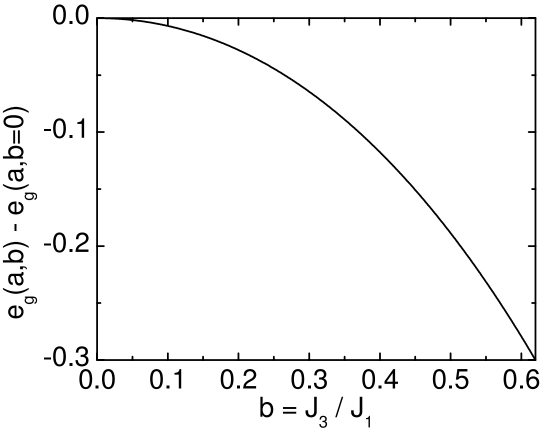

Fig. 2. Ground state energy per tetrahedron $e_g(a, b) - e_g(a, b = 0)$ versus b in the dimer phase.

We have evaluated E_g up to $O(8)$. The ground state energy per tetrahedron e_g in the dimer phase reads

$$e_g(a,b) = -2 + \frac{a}{2} - \frac{2\,b^2}{3} - \frac{b^3}{6} + \frac{b^4}{108} - \frac{67\,b^5}{1620} - \frac{53273\,b^6}{1749600} + \frac{27311519\,b^7}{5038848000} - \frac{414299313497\,b^8}{17459608320000}. \quad (6)$$

The first two terms in equation (6) correspond to the non interacting energy of the $\mathcal{S}_1$ state as in Table 1. For $a = 0$ equation (6) is also a SE of the ground state energy per dimer of the dimerized spin-1 chain. To our knowledge, equation (6) has not been published previously. Figure 2 depicts the ground state energy, which is a monotonously decreasing function of the inter-tetrahedral coupling b. We find that plots of $e_g(a, b)$ to $O(7)$ and $O(8)$, as well as the different Padé approximants [24], are indistinguishable on the scale of Figure 2, which provides an estimate of the convergence. Using $e_g(a, b)$ we will discuss the first order critical line $b_c(a_c)$ for the dimer-to-singlet transition in Section 4. Trivially, the non-interacting critical point is $b_c(1) = 0$ (Tab. 1).

To calculate the triplet dispersion we have to consider the subspace of exactly one $\mathcal{T}_{1,j}$−type of excitation: $|t_j\rangle = |\mathcal{S}_{1,1} \dots \mathcal{T}_{1,j} \dots \mathcal{S}_{1,L/2}\rangle$, i.e. one-triplet $\mathcal{T}_{1,j}$ on a tetrahedron at site j. Q conservation implies that H_{eff} can only translate the triplets $|t_j\rangle$, i.e. $H_{\text{eff}}|t_j\rangle = \sum_i c_i |t_{j+i}\rangle$. Diagonalization in momentum space leads to the triplet dispersion

$$\omega(k) \equiv \langle t_k | H_{\text{eff}} | t_k \rangle - E_g = c_0 - E_g + \sum_{j=1}^{\infty} 2c_j \cos(kj). \quad (7)$$

We have evaluated the coefficients c_i up to $O(8)$. To our knowledge, an analytic expression for the triplet dispersion of a dimerized spin-1 chain has not been obtained previously. This result is displayed explicitly in equation (A-1) in Appendix A. Our calculation to $O(8)$ significantly extends earlier SE to $O(4)$, obtained in reference [15] for a 3D generalization of the 1D tetrahedral chain.

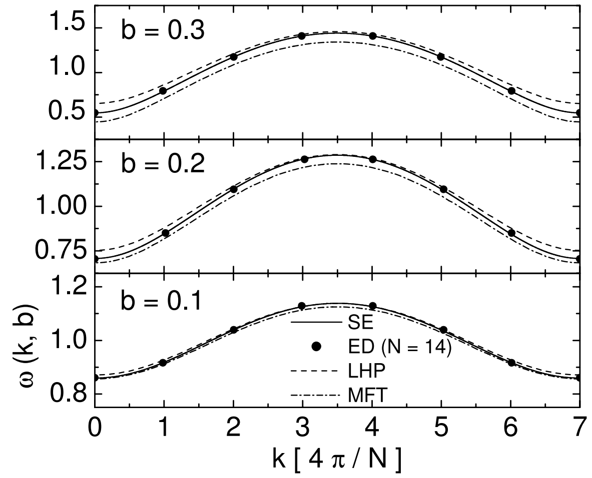

Fig. 3. Elementary triplet dispersion in the spin-1 dimer phase for $b = 0.1, 02$ and 0.3. Solid line: SE from equation (A-1). Dash-dotted line, dashed line, and solid dots: MFT, LHP approximation, and ED from [13]. A tendency to close the gap $\Delta \equiv \omega(k = 0, b)$ can be observed as b increases.

In Figure 3 we compare our SE results for $\omega(k, b)$ with findings from ED on dimerized spin-1 chains [13], as well as bond-operator MFT and a linearized Holstein-Primakoff (LHP) approach [13]. While it is clear from this figure that at $b \ll 1$ all methods agree very well, it is also obvious that, upon increasing b, SE and ED agree best. This is consistent with the fact that the MFT and LHP are approximations which are strictly valid only in the limit of vanishing inter-tetrahedral coupling [13]. The quality of these approximations at finite b remains uncontrolled. Figure 3 also shows that there is a tendency of the gap to close at $k = 0$ as b increases. This signals the transition to the Haldane phase and will be analyzed in detail in Section 4.

4 Quantum phase transitions

In this Section we consider the critical points of our model. Figure 4 summarizes the phase diagram of the tetrahedral cluster spin chain as determined from the present SE and other methods [13,14]. It displays the singlet product, dimer and Haldane phases. These regions are separated by a first order critical line between the dimerized spin-1 chain sector and the singlet product phase, as well as the second order critical line between the dimer and the Haldane phases.

We start by studying the dimer-to-singlet transition. The solid line represents our evaluation of the critical line $b_c(a_c)$ using SE. It has been obtained by solving $e_g(a, b) - e_{g\,\mathcal{S}_2} = 0$, where $e_{g\,\mathcal{S}_2} = -3a/2$ is the exact

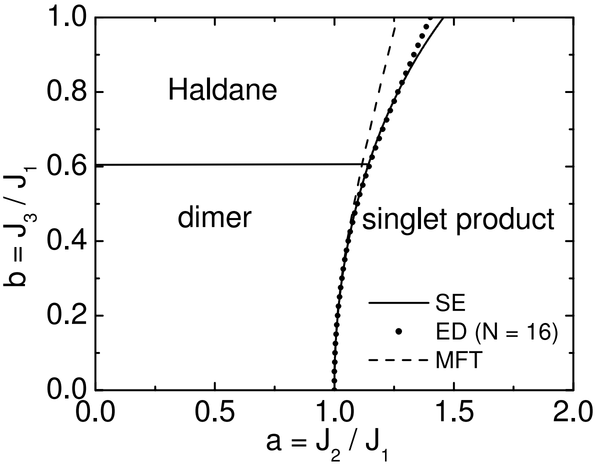

Fig. 4. Quantum phase diagram of the tetrahedral cluster chain. Solid: first order dimer-to-singlet critical line $b_c(a_c)$ obtained from SE. Dashed and dots: $b_c(a_c)$ from MFT and ED in the dimerized spin-1 sector for $N = 16$ sites and PBC (Ref. [13]). Horizontal solid line at $b_c \in [0.610, 0.613]$: second order dimer-to-Haldane transition obtained by Dlog-Padé analysis of the triplet-gap closure of equation (A-1). (See also Fig. 5.)

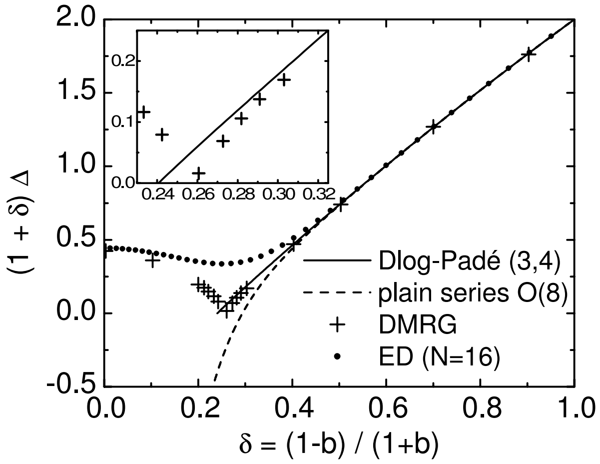

Fig. 5. Dashed and solid lines: plain $O(8)$ SE (Eq. (A-1)), and its integrated Dlog-Padé $(3, 4)$ approximant, for the one-triplet gap $\Delta \equiv \omega(k = 0, b)$. Axes have been scaled to allow for a comparison with other methods. Dots: ED on $N = 16$ sites with PBC in the dimerized spin-1 sector [13]. Crosses: DMRG results from [26]. Inset: zoom of the transition region.

ground state energy of the singlet-product phase, for $b(a)$. Obviously, there is an excellent agreement with ED results [13,25] (dotted line in Fig. 4). This is true even for b-values beyond the dimer-Haldane transition, where the SE is not expected to be valid anymore. I.e. the ground state energy of the Haldane phase differs only little from that of an adiabatically continued dimer phase.

While the accuracy of approximate bond-operator approaches, eg. MFT [13], is hard to asses, it is interesting to see from Figure 4 that SE and ED agree very well with the latter approach at least up to $b \approx 0.5$, which gives an estimation of the range of validity of the MFT calculation.

We now turn to the dimer-Haldane transition, which has been studied by many authors. The first analysis was carried out by Affleck and Haldane [16,17], by mapping onto the O(3) nonlinear $\sigma-$model (NLSM) for $S \gg 1$. They showed that the topological angle θ is given by $\theta = 2\pi S(1-\delta)$, where $\delta = (1-b)/(1+b)$, and that the system is gapless when θ/π is integer. Therefore, for $S = 1$ a gapless point was predicted at $b_c = 1/3(\delta_c = 1/2)$, which is not expected to be quantitative correct since $1/S$-corrections may play a role and have not been analyzed.

Numerically, the dimer-Haldane transition was studied employing Density Matrix Renormalization Group (DMRG) [26,27], Quantum Monte Carlo (QMC) [28,29], and ED techniques [13,30,31]. These methods agree on a critical point at $b_c(\delta_c) \simeq 0.6(0.25)$. SE by a method different from the continuous unitary transformation was also applied to the dimerized spin-1 chain [32,33]. From SE reference [32], $b_c \in [0.56, 0.64]$ was obtained from the second moment of the equal time structure factor in the ground state. From SE reference [33], $b_c \in [0.608, 0.616]$ was reported from an $O(8)$ SE of the triplet gap. These SE approaches, however, did not give analytic results for the triplet gap and dispersion, or for the coefficients of the series expansion. One of the main advantages of our SE approach is that it provides such results, i.e. equation (A-1).

Figure 5 shows the integrated $(3, 4)$-Dlog-Padé approximant for the triplet gap from our SE at $O(8)$. As from equation (A-1), the gap is located at $k = 0, \pi$. The axes have been scaled to allow for a comparison with two other approaches, i.e. ED on $N = 16$ sites with PBC in the dimerized spin-1 chain sector [13] and DMRG results from reference [26]. The last two cover the complete range of $b(\delta) \in [0, 1]([1, 0])$. For $b(\delta) \lesssim 0.4(\gtrsim 0.4)$, there is a very good agreement among all three approaches displayed. For greater (smaller) values of $b(\delta)$ finite size effects become evident in the ED data. The results from the SE, however, remain very close to the DMRG over the complete range of inter-tetrahedral couplings, up until the critical point. From the inset of Figure 5 one can observe that the SE slightly over(under) estimates the critical value of $b_c(\delta_c)$ as compared to the findings of DMRG. In fact, performing standard Dlog-Padé error analysis [24], by evaluating the scatter of the critical point $b_c(\delta_c)$ obtained from different approximants, we get $b_c(\delta_c) \in [0.610, 0.613](\in [0.239, 0.241])$, whereas DMRG gives $b_c(\delta_c) \in [0.59, 0.61]$ $(\in [0.24, 0.26])$ [26]. The small difference may be due to non analytic corrections to a plain power-law behavior of Δ. Indeed, the gap has been claimed to close as $\Delta \sim (\lambda)^{\frac{2}{3}}/|\log\lambda|^{\frac{1}{2}}$, with $\lambda = |b - b_c|/b_c$, in the vicinity of the critical point [30,34]. In case of such logarithmic corrections, deviations as those shown in the inset of Figure 5 are likely to occur due to the asymptotic behavior of the series very close to the critical point. Further evidence for the relevance of logarithmic corrections stems from the critical exponent of $\nu \in [0.96, 0.98]$ which we extract from the Dlog-Padé approximant which, as can be seen also from Figure 5, varies almost linearly with $b(\delta)$

close to the critical point. This is at variance with extrapolation of ED data, which predicts a critical *effective* exponent $\nu \in [0.7, 0.8]$ ($\Delta \sim \lambda^{\nu}$) [30], and with the onset of additional curvature which can be observed in the DMRG results close to $b_c(\delta_c)$ in the inset of Figure 5. This issue should be addressed in future studies.

5 Conclusions

To summarize, we have studied zero temperature properties of a tetrahedral cluster spin chain using an analytical series expansion technique based on Wegner's flow equation method. Starting from the limit of isolated tetrahedra, we have obtained results for the ground state energy and the dispersion of the elementary one-triplet excitations within the dimer phase to $O(8)$ in the inter-tetrahedral couplings. The ground state energy has been used to determine a first order quantum critical line which separates a dimerized spin-1 chain sector from a singlet product phase. The second order critical line of the dimer-to-Haldane phase transition was obtained by analyzing the closure of the triplet gap. Very good agreement was found with the previous results from ED, DMRG, QMC and other SE techniques.

Finally, we note that the continuous unitary transformation also allows for the evaluation of two-particle properties and spectral functions [35]. These quantities could be of interest at the critical lines and should be considered in future work.

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Appendix A

In this appendix we give an analytic expression for the triplet dispersion $\omega(k,b)$ in the dimerized spin-1 chain phase up to $O(b^8)$

$$
\begin{aligned}
\omega(k,b) = \Bigg(& 1 + \frac{8\,b^2}{27} + \frac{19\,b^3}{27} - \frac{571\,b^4}{972} + \frac{183943\,b^5}{233280} \\
& - \frac{391390595851\,b^6}{380936908800} + \frac{913820919969227\,b^7}{511979205427200} \\
& - \frac{1495255820258178144 6149\,b^8}{38318571650993356800000}\Bigg) \\
+ \Bigg(& -\frac{4\,b}{3} - \frac{2\,b^2}{3} + \frac{26\,b^3}{27} - \frac{29\,b^4}{54} + \frac{145237\,b^5}{98415} \\
& - \frac{4087919\,b^6}{1959552} + \frac{10916063988776383\,b^7}{2879883030528000} \\
& - \frac{362386906595826940 67\,b^8}{4838203491287040000}\Bigg) \cos(k) \\
+ \Bigg(& -\frac{4\,b^2}{9} - \frac{2\,b^3}{9} - \frac{7285\,b^4}{34992} + \frac{912407\,b^5}{699840} \\
& - \frac{18113617135\,b^6}{10158317568} + \frac{485683037077901\,b^7}{142216445952000} \\
& - \frac{1300945425233619173 09\,b^8}{199057515070095360 00}\Bigg) \cos(2k) \\
+ \Bigg(& -\frac{8\,b^3}{27} - \frac{32\,b^4}{81} + \frac{1558441\,b^5}{3149280} \\
& - \frac{135853999\,b^6}{220449600} + \frac{53288026128863\,b^7}{21332466892800} \\
& - \frac{735512137634711051\,b^8}{140794281492480000}\Bigg) \cos(3k) \\
+ \Bigg(& -\frac{20\,b^4}{81} - \frac{268\,b^5}{729} - \frac{22011727\,b^6}{94478400} \\
& + \frac{5321414051\,b^7}{3429216000} - \frac{1053001348140670001\,b^8}{403183624273920000}\Bigg) \cos(4k) \\
+ \Bigg(& -\frac{56\,b^5}{243} - \frac{3068\,b^6}{6561} + \frac{2345836457\,b^7}{25509168000} \\
& - \frac{190707195454693\,b^8}{349985784960000}\Bigg) \cos(5k) \\
+ \Bigg(& -\frac{56\,b^6}{243} - \frac{32332\,b^7}{59049} - \frac{813174250853\,b^8}{2295825120000}\Bigg) \cos(6k) \\
+ \Bigg(& -\frac{176\,b^7}{729} - \frac{360560\,b^8}{531441}\Bigg) \cos(7k) - \frac{572\,b^8}{2187} \cos(8k).
\end{aligned}
\tag{A-1}
$$

Interestingly, the leading order contribution of each harmonic of this series agrees with that obtained from bond-operator MFT [13]. There, $\omega^{MFT}(k,b) = (1 + 2\epsilon_k)^{1/2}$, with $\epsilon_k = -\frac{4}{3} b \cos k$. We have observed the same relation to be true also between SE [21] and the MFT technique of reference [13] for the dimerized spin-1/2 chain.

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