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Ground-state long-range order in quasi-one-dimensional Heisenberg quantum antiferromagnets: high-order coupled-cluster calculations

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Abstract. We investigate the ground-state magnetic long-range order of quasi-one-dimensional quantum Heisenberg antiferromagnets for spin quantum numbers $s = 1/2$ and $s = 1$. We use the coupled cluster method to calculate the sublattice magnetization and its dependence on the inter-chain coupling $J_\perp$. We find that for the unfrustrated spin-1/2 system, an infinitesimal inter-chain coupling is sufficient to stabilize magnetic long-range order, in agreement with results obtained by other methods. For $s = 1$, we find that a finite inter-chain coupling is necessary to stabilize magnetic long-range order. Furthermore, we consider a quasi one-dimensional spin-1/2 system, where a frustrating next-nearest neighbor in-chain coupling is included. We find that for stronger frustration as well, a finite inter-chain coupling is necessary to have magnetic long-range order in the ground state, and that the strength of the inter-chain coupling necessary to establish magnetic long-range order is related to the size of the spin gap of the isolated chain.

PACS. 75.10.Jm Quantized spin models – 75.10.Pq Spin chain models – 75.50.Ee Antiferromagnetics

1 Introduction

Low-dimensional quantum antiferromagnets have attracted much attention as model systems where strong quantum fluctuations may destroy magnetic long-range order in the ground state (GS) [1]. In particular, the one-dimensional (1d) quantum Heisenberg antiferromagnet (HAFM) does not exhibit magnetic long-range order (LRO). In addition, there is a basic difference between half-integer and integer antiferromagnetic Heisenberg chains [2]. While the 1d HAFM with half-integer spin quantum number exhibits a gapless excitation spectrum and a power-law decay of spin-spin correlations, a faster exponential decay of spin-spin correlations — accompanied by a finite excitation gap Δ (spin gap) — is observed for integer-spin 1d HAFM. However, it is known that for the 1d spin-half HAFM a frustrated next-nearest neighbor exchange coupling may also open an excitation gap (for a more detailed discussion of 1d spin systems, see [3]). For the formation of magnetic LRO in HAFM, the transition to two-dimensional (2d) lattices is crucial. The HAFM on 2d bipartite lattices exhibits magnetic LRO at zero temperature and only competing interactions may destroy LRO (for a more detailed discussion of 2d spin systems, see [4,5]). In real materials we are often faced with the situation that the nearest-neighbor in-chain coupling J_1 is dominant but an inter-chain coupling $J_\perp$ is also present. A very weak inter-chain coupling even seems to be a rare exception, see e.g. reference [6]. Therefore, the study of quasi 1d quantum HAFM's, i.e. systems where the in-chain couplings are larger than the inter-chain couplings, are — on one hand — of basic interest in connection with the dimensional crossover from one dimensions to two, and on the other hand, of interest for the interpretation of experiments. The quasi 1d spin-1/2 HAFM has been studied in several papers [7–15] in recent years. A main focus of these studies has been on the estimation of the critical inter-chain coupling $J_\perp^c$ where the transition between the phase with magnetic LRO and the magnetically disordered phase takes place. The answers given in the literature to this question are contradictory and not completely conclusive. While some papers find indications for a finite $J_\perp^c$ [8–10], others find $J_\perp^c = 0$ [7,11–15] which seems to be more plausible, given that the GS of the 1d spin-1/2 HAFM is not gapped. In particular, data obtained by the quantum Monte Carlo method (QMC) [11,14,15], which is precise for unfrustrated spin models, strongly support the result $J_\perp^c = 0$. The behaviour of the quasi 1d spin-1 HAFM might be different from its spin-1/2 counterpart, but is less studied so far. Indeed, the existing studies of the spin-1 case find indications for a finite $J_\perp^c$ [7,14–18] which can be attributed to the spin gap between the singlet GS and the

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magnetic excitations. In reference [7] a lower bound of $J_\perp^c$ was estimated as $J_\perp^c \geq 0.025 J_1$, whereas an upper bound $J_\perp^c \leq 0.1892 J_1$ was given in reference [18]. Recent QMC calculations [14,15,17] yield $J_\perp^c \approx 0.043$–$0.044 J_1$, which is only about 10% of the Haldane gap Δ.

To get experimental input for the theoretical work, materials with a quasi 1d behavior and a small coupling ratio between inter- and in-chain exchange are needed. Experimentally, materials such as Sr_2CuO_3, Ca_2CuO_3 [19,20], $Sr_2V_3O_9$ [21], $BaCu_2Si_2O_7$ [22], $Sr_2Cu(PO_4)_2$, $Ba_2Cu(PO_4)_2$ [23] are quite good examples of quasi 1d spin-1/2 antiferromagnets with "not-too-large" interchain coupling. The spin-1/2 antiferromagnet showing the most perfect 1d behavior so far is $SrCu(PO_4)_2$ [6]; this material has the smallest ratio $k_B T_N/J_1 \sim 6 \times 10^{-4}$ between the Néel temperature T_N and the in-chain coupling J_1. All of the above-mentioned materials show magnetic LRO below T_N, although their coupling ratio is remarkably small. Contrary to the spin-1/2 materials in some quasi-1d spin-1 antiferromagnets such as $Ni(C_2H_8N_2)_2NO_2(ClO_4)$ [24,25] and other Ni-compounds, see reference [24], no Néel LRO has been observed as measured down to very low temperatures.

Another interesting system is the 1d spin-1/2 HAFM with frustrated second neighbor interaction $J_2 > 0$. At $J_2 = 0.2411 J_1$ [26] a transition to a dimerized state with a spin gap and an exponential decay of the spin-spin correlation occurs. Hence, for $J_2 > 0.2411 J_1$ the effect of the inter-chain coupling on the GS behavior may be different from the case with $J_2 < 0.2411 J_1$. This problem has not been discussed in detail in the literature so far.

In the present paper we apply the coupled cluster method (CCM) [27,28] to study the GS LRO of quasi 1d HAFM with spin quantum numbers $s = 1/2$ and $s = 1$. This approach is a universal and powerful method of quantum many-body theory. Though the CCM is a fairly new method in the field of quantum spin systems, in recent years it has been developed to higher levels of approximation which allows its application to quantum spin systems with more and more success (for recent reviews, see Refs. [29,30]). In particular, the CCM has the advantage that it can be applied to frustrated quantum spin systems with arbitrary dimensions. Though, concerning the precision of the results, the CCM at the present level of approximation probably cannot compete with the QMC, it allows to find new results for frustrated systems, for which the QMC fails due to the so-called sign problem. On the other hand, the comparison of CCM results with QMC data for the unfrustrated models can be considered as a benchmark test of the CCM and is therefore of interest from an applied method point of view.

The Hamiltonian of the quasi 1d frustrated HAFM is written as

$$H = \sum_n \sum_i \left(J_1 \mathbf{s}_{i,n} \cdot \mathbf{s}_{i+1,n} + J_2 \mathbf{s}_{i,n} \cdot \mathbf{s}_{i+2,n} \right) + \sum_i \sum_n J_\perp \mathbf{s}_{i,n} \cdot \mathbf{s}_{i,n+1}. \quad (1)$$

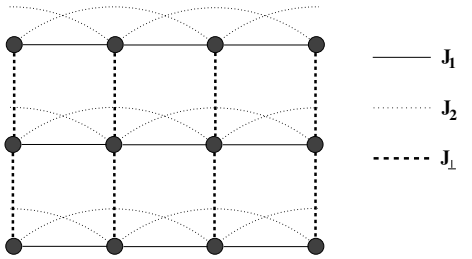

Fig. 1. Illustration of the quasi one-dimensional HAFM with the in-chain nearest-neighbor bonds J_1, the frustrating in-chain next-nearest neighbor bonds J_2, and the inter-chain bonds $J_\perp$, cf. the Hamiltonian (1). All bonds are antiferromagnetic.

The index n labels the chains and i the lattice sites within a chain n. The model is illustrated in Figure 1. While for spin quantum number $s = 1$ we consider only the model without frustration ($J_2 = 0$), for $s = 1/2$, we will discuss both cases, $J_2 = 0$ and $J_2 > 0$.

2 The coupled cluster method (CCM)

In this section, the CCM formalism will first briefly be outlined. For further details the interested reader is referred to references [29–39]. The starting point for the CCM calculation is the choice of a normalized reference or model state $|\Phi\rangle$, together with a set of (mutually commuting) multi-configurational creation operators $\{C_L^+\}$ and the corresponding set of their Hermitian adjoints $\{C_L\}$,

$$\langle \Phi | C_L^+ = 0 = C_L | \Phi \rangle \quad \forall L \neq 0, \quad C_0^+ \equiv 1 \quad (2)$$

$$[C_L^+, C_J^+] = 0 = [C_L, C_J]. \quad (3)$$

The operators C_L^+ (C_L) are defined over a complete set of many-body configurations denoted by the set-indices $\{L\}$. For the set $\{|\Phi\rangle, C_L^+\}$ the CCM parametrization of the exact ket and bra GS eigenvectors $|\Psi\rangle$ and $\langle\tilde{\Psi}|$ of our many-body system are given by

$$|\Psi\rangle = e^S |\Phi\rangle \ , \ S = \sum_{L \neq 0} a_L C_L^+ \quad (4)$$

$$\langle\tilde{\Psi}| = \langle\Phi|\tilde{S} e^{-S} \ , \ \tilde{S} = 1 + \sum_{L \neq 0} \tilde{a}_L C_L. \quad (5)$$

The CCM correlation operators, S and $\tilde{S}$, contain the correlation coefficients, a_L and $\tilde{a}_L$, which have to be calculated. Once these values are known, all the GS properties of the many-body system can be derived from them. To find the GS correlation coefficients a_L and $\tilde{a}_L$, we simply require that the expectation value $\bar{H} = \langle\tilde{\Psi}|H|\Psi\rangle$ (GS energy) is a minimum with respect to the entire set $\{a_L, \tilde{a}_L\}$, which leads to the GS CCM ket-state and bra-state equations

$$\langle \Phi | C_L^- e^{-S} H e^S | \Phi \rangle = 0 \ ; \ \forall L \neq 0 \quad (6)$$

$$\langle \Phi | \tilde{S} e^{-S} [H, C_L^+] e^S | \Phi \rangle = 0 \ ; \ \forall L \neq 0. \quad (7)$$

For the spin systems considered herein, we choose the Néel state with spins aligned in the z-direction as the reference state. The reasoning behind this choice is evident for the unfrustrated case [32], since the Néel state is the classical GS for $J_2 = 0$. For the $s = 1/2$ case, the frustrated model (i.e. $J_2 > 0$) is considered below as well. Note that the classical GS is an incommensurate spiral state for $J_2 > 0.25J_1$. However, the quantum GS for $J_\perp = 0$ does not exhibit spiral ordering for values of J_2 less than $J_2 \sim 0.5J_1$, but it is rather a collinear state. [30,41–43] Hence, the Néel state is an appropriate reference state for $0 < J_2 \lesssim 0.5J_1$ as well [30].

To treat each side equivalently, we perform a rotation of the local axis of the up spins, such that all spins in the reference state lign in the negative z-direction. In this new set of local spin coordinates the reference state and the corresponding creation operators C_L^+ are given by

$$|\hat{\Phi}\rangle = |\downarrow\downarrow\downarrow\downarrow\cdots\rangle\ ;\ C_L^+ = \hat{s}_i^+\ ,\ \hat{s}_i^+\hat{s}_j^+\ ,\ \hat{s}_i^+\hat{s}_j^+\hat{s}_k^+\ ,\ \ldots, \quad (8)$$

where the indices $i, j, k, ...$ denote arbitrary lattice sites. For the discussion of the GS Néel LRO, we have to calculate the order parameter (sublattice magnetization) M, which is given within the CCM scheme by

$$M = -\frac{1}{N}\langle\tilde{\Psi}|\sum_{i=1}^{N}\hat{s}_i^z|\Psi\rangle. \quad (9)$$

The CCM formalism becomes exact if we take into account all possible multispin configurations for the correlation operators S and $\tilde{S}$. However, in general, this is impossible to do in practice for a many-body quantum system. It is therefore necessary to use approximation schemes in order to truncate the expansions of S and $\tilde{S}$ in equations (4, 5) in any practical calculation. A very general approximation scheme is the so-called SUBn-m approximation. In this approximation, all correlations in the correlation operators S and $\tilde{S}$ are taken into account, as long as they span a range of no more than m contiguous sites and contain only n or fewer spins. In most cases, however, the SUBn-n scheme is used (i.e., with $n = m$), and in these cases, it is referred to as the LSUBn scheme (for spin-1/2 systems). To find all the different (i.e. fundamental) configurations entering S and $\tilde{S}$ for a given level of SUBn-n approximation, we use the lattice symmetries.

Although there is no theory available for how the results of the SUBn-n approximations scale with n, there is nevertheless a great deal of experience in how to extrapolate the raw CCM SUBn-n data properly to $n \to \infty$ [30–33,36,38,39]. The best results for the extrapolation of the order parameter are obtained if the poor SUB2-2 data are omitted. Previously, for systems showing an order-disorder quantum phase transition [30,36,38], a leading "power-law" extrapolation for the order parameter

$$M(n) = a_0 + a_1\left(\frac{1}{n}\right)^{a_2}, \quad (10)$$

has been used successfully to determine the phase transition points. In equation (10) the leading exponent a_2 is determined directly from the SUBn-n data. Alternatively, as has been discussed recently in reference [39], an extrapolation scheme with a fixed exponent but including an additional power in $1/n$, i.e.

$$M(n) = b_0 + \left(\frac{1}{n}\right)^{1/2}\left(b_1 + b_2\frac{1}{n}\right), \quad (11)$$

can also be used to find the phase transition point. The extrapolation of the order parameter is illustrated in Figure 2 for one particular data set - namely, for the unfrustrated $s = 1/2$ chain with zero inter-chain coupling, i.e. at the expected critical point. Note that when using the extrapolation of equation (10), the exponent a_2 for the considered data set is $a_2 = 0.414$, which is a value not far from the fixed leading exponent $1/2$ used in equation (11). Below, we will use both extrapolation formulas to determine the critical inter-chain coupling $J_\perp^c$, which will naturally yield slightly different values for $J_\perp^c$. We will use this difference as an estimation of the reliability of our results.

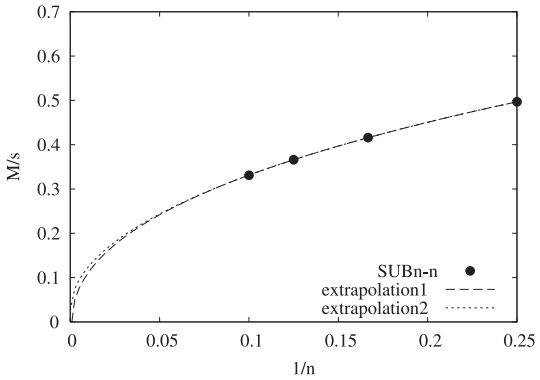

Fig. 2. Extrapolation of the GS order parameter (sublattice magnetization) M scaled by the spin quantum number s for the pure unfrustrated $s = 1/2$ chain (i.e. $J_\perp = 0$ and $J_2 = 0$). The two methods of extrapolation corresponding to equations (10) and (11) are indicated by "extrapolation1" and "extrapolation2", respectively.

Using parallel processing [35,40] we are able to use the CCM up to the SUB10-10 approximation for the spin-1/2 system, and up to the SUB8-8 approximation for the spin-1 system, which corresponds to the solution of more than 10^4 coupled nonlinear equations.

3 Results

The results for the dependence of the order parameter M scaled by the spin quantum number s on the inter-chain coupling $J_\perp$ are shown in Figures 3–5. In those figures, we show the raw CCM SUBn-n data used for the extrapolation, as well as the results for the extrapolation $n \to \infty$, cf. Section 2.

For the unfrustrated quasi 1d HAFM with $s = 1/2$ we find that for $J_1 \geq J_\perp \gtrsim 0.2J_1$, the variation of the order parameter M with $J_\perp$ is small, see Figure 3. Only for $J_\perp < 0.2J_1$ is the sublattice magnetization significantly

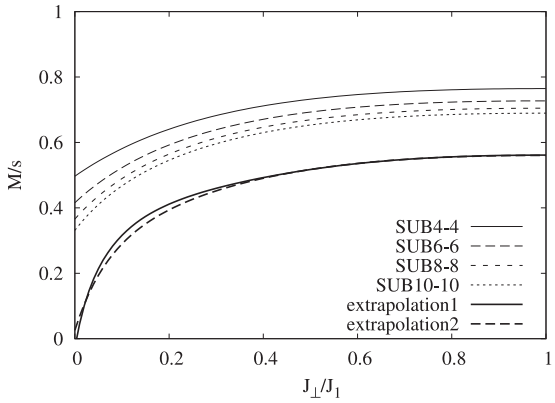

Fig. 3. The dependence of the GS order parameter (sublattice magnetization) M scaled by the spin quantum number s on the inter-chain coupling $J_\perp$ for the unfrustrated $s = 1/2$ quasi 1d HAFM. The two methods of extrapolation corresponding to equations (10) and (11) are indicated by "extrapolation1" and "extrapolation2", respectively.

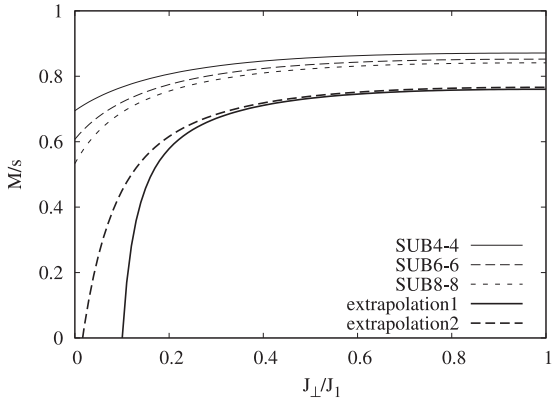

Fig. 4. The dependence of the GS order parameter (sublattice magnetization) M scaled by the spin quantum number s on the inter-chain coupling $J_\perp$ for the unfrustrated $s = 1$ quasi 1d HAFM. The two methods of extrapolation corresponding to equations (10) and (11) are indicated by "extrapolation1" and "extrapolation2", respectively.

diminished. As demonstrated in Figure 3, it is evident that both extrapolation schemes lead to similar results. Using the extrapolation formula equation (10), we obtain the critical inter-chain coupling $J_\perp^c \sim 0.003J_1$ at which the Néel LRO disappears . On the other hand, the extrapolation based on equation (11) leads to a finite but very small order parameter $M \approx 0.01$. These results are consistent with the conclusion that for the unfrustrated spin-1/2 system, an infinitesimally small inter-chain coupling is sufficient to stabilize antiferromagnetic LRO. This statement supports the findings of references [7,11–14] and are related to the gapless GS of the strictly 1d $s = 1/2$ HAFM.

Next, we consider the unfrustrated $s = 1$ HAFM. Here the number of fundamental configurations in the CCM SUBn-n approximation is much larger than for $s = 1/2$, and we are able to present CCM data up to $n = 8$. Hence, the extrapolation for $s = 1$ is expected to be less reliable

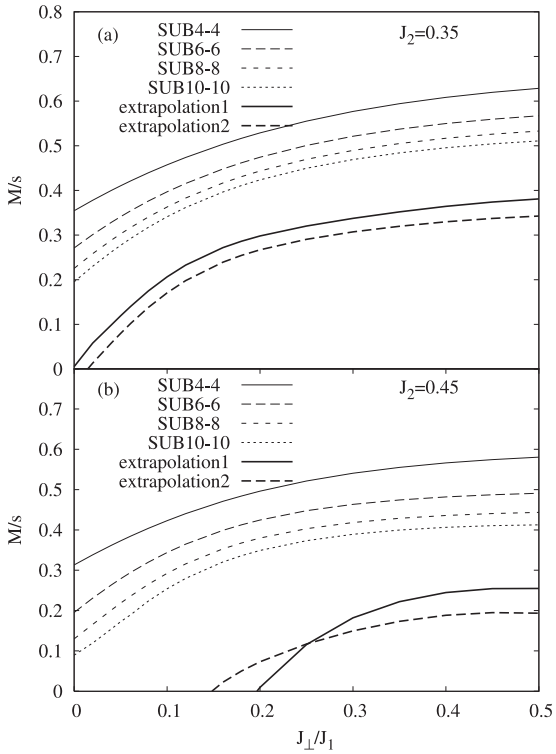

Fig. 5. The GS order parameter (sublattice magnetization) M scaled by the spin quantum number s in dependence on the inter-chain coupling $J_\perp$ for the frustrated $s = 1/2$ quasi 1d HAFM. The two variants of extrapolation according to equations (10) and (11) are indicated by "extrapolation1" and "extrapolation2", respectively. (a) $J_2 = 0.35J_1$; (b) $J_2 = 0.45J_1$.

than for $s = 1/2$, for which CCM data up to $n = 10$ are available. Again, for $J_1 \geq J_\perp \gtrsim 0.2J_1$, the variation of M with $J_\perp$ is small, see Figure 4. However, M/s is significantly larger than as calculated for $s = 1/2$, indicating the decrease of quantum fluctuations in the square-lattice HAFM with increasing spin quantum number s. A strong reduction of the order parameter occurs for $J_\perp \sim 0.2J_1$. Finally, M vanishes at a critical value $J_\perp^c > 0$, i.e. a finite inter-chain coupling is necessary to stabilize GS Néel LRO. However, both extrapolation schemes lead to different numerical values for $J_\perp^c$, namely $J_\perp^c \sim 0.1J_1$ using equation (10) but $J_\perp^c \sim 0.02J_2$ using equation (11). Both values differ by approximately a factor of 2 from the QMC results [14,15,17] $J_\perp^c \approx 0.043$–$0.044J_1$. This difference gives an indication of the accuracy of the CCM including SUBn-n data up to $n = 8$.

Next, we consider the frustrated quasi 1d $s = 1/2$ HAFM for which QMC calculations are not possible. The classical GS for $J_2 > 0.25J_1$ is an incommensurate spiral state independent of the value of $J_\perp$. In contrast to the classical model, for the strictly 1d problem ($J_\perp = 0$) the quantum GS does not exhibit spiral correlations for $0.25J_1 < J_2 \lesssim 0.5J_1$ [30,41–43], but is gapped with a spin gap Δ strongly varying with J_2 [42,44]. However, in presence of an appreciable inter-chain coupling $J_\perp$, spiral correlations may appear in the quantum model as

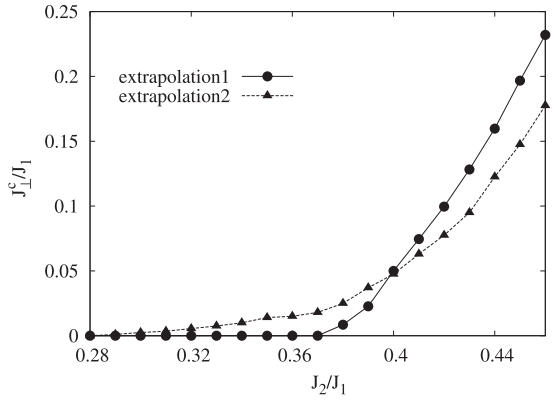

Fig. 6. The critical inter-layer coupling $J_\perp^c$ in dependence on the frustration parameter J_2 for the frustrated $s = 1/2$ quasi 1d HAFM. The two variants of extrapolation according to equations (10) and (11) are indicated by "extrapolation1" and "extrapolation2", respectively.

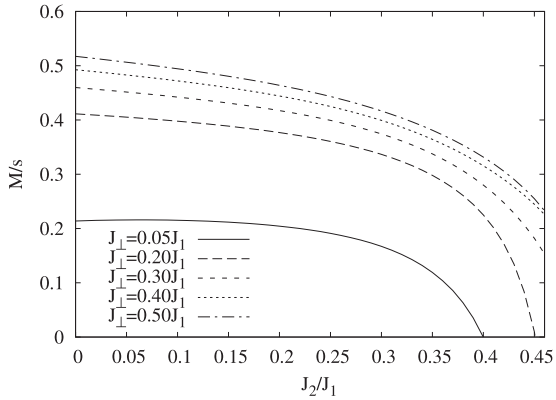

Fig. 7. The GS order parameter (sublattice magnetization) M scaled by the spin quantum number s for the frustrated $s = 1/2$ quasi 1d HAFM in dependence on the frustration parameter J_2 and for various strengths of the inter-chain coupling $J_\perp$.

well [30,45]. Therefore, we restrict our calculations to $J_\perp < 0.5J_1$ and to $J_2 \leq 0.46J_1$, where the CCM works well when based on a collinear reference state. The spin gap Δ of the 1d problem ($J_\perp = 0$) was found to be very small for $J_2 < 0.4J_1$, but Δ increases rapidly between $0.4J_1 < J_2 < 0.5J_2$ [42,44].

The results for M/s versus $J_\perp$ for $J_2 = 0.35J_1$ and $J_2 = 0.45J_2$ are shown in Figure 5. For $J_2 = 0.35J_1$ the critical inter-chain coupling is $J_\perp^c \sim 0$ when using the extrapolation equation (10) and is $J_\perp^c \sim 0.014J_1$ when using the extrapolation equation (11). Knowing that for $J_2 = 0.35J_1$ and $J_\perp = 0$, the spin gap should be finite [26] but very small [42,44], a zero or small $J_\perp^c$ is reasonable. On the other hand, for $J_2 = 0.45J_1$, where the spin gap for $J_\perp = 0$ is $\Delta \sim 0.13J_1$ [42,44] we already obtain quite a large value of $J_\perp^c \sim 0.20J_1$ using the extrapolation of equation (10) and $J_\perp^c \sim 0.15J_1$ using the extrapolation of equation (11)). Interestingly, the ratio $J_\perp^c/\Delta$ is seems to be larger than for the unfrustrated $s = 1$ HAFM. The variation of $J_\perp^c$ with J_2 is shown in Figure 6. Both extrapolation schemes yield qualitatively similar results. The variation of $J_\perp^c$ with J_2 is quite similar to the variation of the spin gap with J_2 [42,44]. However, we observe a monotonic increase of the ratio $R = J_\perp^c/\Delta$ from $R \sim 0.8$ to $R \sim 1.6$ in the region $0.4J_1 \leq J_2 \leq 0.46J_2$.

The variation of the order parameter M/s with frustration is illustrated in Figure 7, where for the sake of clarity, only the data obtained using an extrapolation scheme equation (10) are shown. As expected, frustration weakens the magnetic order and M becomes smaller with increasing J_2. Obviously, for fixed but not too large inter-chain coupling $J_\perp$, a quantum phase transition between Néel LRO and a magnetically disordered phase can be driven by frustration. However, In similarity to recent findings for the quasi-2d $J_1 - J_2$ model [38], it is likely that for stronger inter-chain coupling no magnetically disordered phase appears.

Let us finally mention that the quantum phase transition in the frustrated model is interesting from a more general point of view. For $0.2411J_1 < J_2 \lesssim 0.5J_1$, the model exhibits two ground state phases, each breaking different symmetries, namely (i) the rotationally invariant, spontaneously dimerized phase for zero (or small) $J_\perp$ breaking the translational symmetry of the lattice, and (ii) the Néel phase, breaking the spin rotational symmetry. A continuous transition between the dimerized phase and the Néel ordered phase is prohibited within the Landau theory [46]. Hence three different scenarios are possible. First, that there is a (small) disordered featureless spin-liquid phase between the dimerized and the Néel phase; second, that there is a first order transition between the dimerized and the Néel phase, and, third and most interesting, that the above-described transition is a candidate for a deconfined quantum critical point [46]. This question cannot be answered within the current approach but deserves further consideration.

To summarize, we find that the transition from the non-magnetic 1d GS to the magnetically ordered 2d GS in quasi 1d quantum HAFM's can be well described by the CCM if higher orders of approximation are used. Our results indicate that this transition, driven by the inter-chain coupling $J_\perp$, is related to the excitation gap of the strictly 1d HAFM, i.e. at $J_\perp = 0$. If the 1d quantum GS is gapless, most likely the magnetic LRO sets in immediately when $J_\perp$ is switched on, whereas for gapped GS's, a finite $J_\perp$ is necessary to establish magnetic LRO in the GS.

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