Low Temperature Properties of Quantum Antiferromagnetic Chains with Alternating Spins $S = 1$ and $1/2$

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Abstract

We study the low-temperature properties of $S = 1$ and $1/2$ alternating spin chains with antiferromagnetic nearest-neighbor exchange couplings using analytical techniques as well as a quantum Monte Carlo method. The spin-wave approach predicts two different low-lying excitations, which are gapped and gapless, respectively. The structure of low-lying levels is also discussed by perturbation theory in the strength of the Ising anisotropy. These analytical findings are compared with the results of quantum Monte Carlo calculations and it turns out that spin-wave theory well describes the present system. We conclude that the quantum ferrimagnetic chain exhibits both ferromagnetic and antiferromagnetic aspects.

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I. INTRODUCTION

The low temperature properties of low-dimensional quantum antiferromagnets have been of great interest for many years, in particular since Haldane [1] made the prediction that integer-spin and half-odd-integer-spin Heisenberg antiferromagnetic chains should behave very differently. Now, with the help of analytical methods and various numerical approaches, it is well accepted that the integer-spin chain is massive, whereas the half-odd-integer-spin chain is massless. This stimulated also several attempts to investigate the quantum behaviour of chains consisting of two types of spins. An integrable model of this type was constructed by de Vega and Woynarovich [2], which allows us to guess the essential consequences of chains with spins of different length $S$. Recently, several authors [3,4] discussed in detail such a chain with spins $S = 1$ and $1/2$ as the simplest case. However, these integrable models usually include complicated interactions and very little is known about the pure Heisenberg model which is supposed to describe real ferrimagnetic compounds [5].

In the following we therefore study the $S = 1$ and $1/2$ Heisenberg antiferromagnetic chain defined by the Hamiltonian (1)

$$\mathcal{H} = J \sum_{i=1}^{L} \left[ (S_i \cdot s_i)_{\lambda} + (s_i \cdot S_{i+1})_{\lambda} \right] ,$$

where $(S_i \cdot s_j)_{\lambda} = \lambda (S_i^x s_j^x + S_i^y s_j^y) + S_i^z s_j^z$ with $S_i$ and $s_i$ being the $S = 1$ and $S = 1/2$ spin operators, respectively, and $L$ is the number of unit cells. We adopt periodic boundary conditions and investigate ground-state properties as well as the low-lying excited states spin-wave theory as well as series expansions with regard to the Ising anisotropy $\lambda$ and a quantum Monte Carlo (QMC) method.

Basic predictions on the low lying level structure can be made by applying the Lieb-Mattis-Theorem [3] and the Goldstone-Theorem [7]. First we consider the ordering of the energy levels. The $A$ sublattice is defined by the $S = 1$ sites (maximum spin is $S_A = L$), the $B$ sublattice is defined by the spin-1/2 sites (maximum spin is $S_A = L$). The Hamiltonian (1) consists of intersublattice interactions only, which allows us to apply [3] to our system.
The energy levels order in the following manner:

\[ E(S + 1) > E(S) \quad \text{for all } S \geq S \]

\[ E(S) > E(S') \quad \text{for } S < S' \]

Here \( S = |S_A - S_B| \) denotes the total spin of the ground state which takes the value \( S = L - L/2 = L/2 \) in our case. Therefore the ground-state degeneracy is \( L + 1 \). Although the ground states have finite spin \( S \) the following points are in contrast to the usually ferromagnet:

- The ground-state degeneracy of the ferromagnet is larger by a macroscopic amount.
- Due to quantum fluctuations the ground state deviates from the ferrimagnetic Néel state, \( |+1, -1/2, +1, -1/2, \ldots \rangle \).

Because each of the ground states of the chain breaks the rotational symmetry of the Hamiltonian, we can apply the Goldstone-Theorem [1] to predict a gapless excitation. For magnetizations lower than \( L/2 \) the ferrimagnet is comparable to a ferromagnet and therefore this gapless excitation should belong to a branch of excitations of ferromagnetic character.

The paper is organized as follows: In the second section we present the spin-wave approach to calculate the dispersion relations as well as the ground-state energy and the ground-state correlation functions. In the following section we study the low-temperature properties employing a QMC method. The numerical data will be compared to the results of the first section and to perturbation calculations. Conclusions will be given in the final section.

**II. SPIN WAVE THEORY**

In this section the spin wave theory (see e.g. [8]) is applied to our system in the large \( S \) limit. For this purpose the odd sites are assigned spins \( gS \) and the even sites spins \( S \). To discuss the case of our Hamiltonian [1] we use \( g = 2 \) large \( S \) limit. We start from the fully ordered state with \( S_{\text{tot}}^z = M = L/2 \) and use the following spin operators in the two sublattices in the lowest order in \( 1/S \):

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sublattice A: \[ S_n^z = gS - a_n^\dagger a_n, \quad S_n^+ = \sqrt{2gS}a_n, \] (2)

sublattice B: \[ s_n^z = -S + b_n^\dagger b_n, \quad s_n^- = \sqrt{2S}b_n^\dagger, \] (3)

Here \( a_n^\dagger, b_n^\dagger \) are Bose operators. We expect the spin wave theory to give qualitatively correct results for the following reason: In the classical antiferromagnet the two Neel states become disconnected by the transformation (2,3) since the action of the transverse Hamiltonian on one of the two Neel states does not lead to the other Néel state. However, it is known that domain wall excitations, namely excitations connecting the two Neel states, are very important for the spin-1/2 antiferromagnet. Spin wave theory is wrong for the spin-1/2 antiferromagnet since domain wall excitations cannot be taken into account. In the spin 1-1/2 system the two Néel states are disconnected in principle because they belong to subspaces with different magnetization. Thus a classical ground state including quantum fluctuations should be qualitatively correct.

In the limit \( S \to \infty \) the interaction terms in the Bose Hamiltonian become negligible and we end up with the following expression for the Hamiltonian, bilinear in the Bose operators,

\[ H_{SW} = -2gS^2 JL + 2SJ \sum_k \left[ gb_k^\dagger b_k + a_k^\dagger a_k + \sqrt{g} \cos(k)(a_k^\dagger b_k^\dagger + a_k b_k) \right], \] (4)

where \( a_n^\dagger = L^{-1/2} \sum_k e^{i k n} a_k^\dagger \) and \( b_n^\dagger = L^{-1/2} \sum_k e^{-i k n} b_k^\dagger \). The Hamiltonian is straightforwardly diagonalized into

\[ H_{SWT} = E_0 + 2SJ \sum_k \left( \omega_k^- \alpha_k^\dagger \alpha_k + \omega_k^+ \beta_k^\dagger \beta_k \right), \] (5)

\[ \omega_k^\pm = \frac{1}{2} \left( \sqrt{(g+1)^2 - 4g \cos^2(k)} \pm (g-1) \right), \] (6)

\[ E_0 = JS \sum_k \left[ \sqrt{(1+g)^2 - 4g \cos^2(k)} - (1+g) \right] - gJS^2 N, \] (7)

where the eigenvectors are determined by

\[ \alpha_k^\dagger = \cosh(\eta_k) a_k^\dagger + \sinh(\eta_k) b_k, \quad \beta_k^\dagger = \sinh(\eta_k) a_k + \cosh(\eta_k) b_k^\dagger, \] (8)

\[ \tanh(2\eta_k) = \frac{2\sqrt{g}}{1+g} \cos(k). \] (9)

The results of the spin wave theory contain both ferromagnetic and antiferromagnetic aspects: In the ferromagnetic branch (\( \omega_k^- \)) we obtain a gapless spin wave with \( M = L/2 - 1 \).
For small values of the wave vector the dispersion is \( \omega_k = g/(g-1) \ k^2 + \ldots \). The quadratic behaviour with wave vector \( k \) indicates the ferromagnetic character of this mode.

The antiferromagnetic spin wave with \( M = L/2 + 1 \) is gapped. The magnitude of the gap is exactly \( J \) when we put \( g = 2, S = 1/2 \). This result will be compared to the result of the QMC calculation to be presented in the next section. If we chose the spins such that the spin lengths in the different sublattices are equal, i.e. \( g \to 1 \) the gap of the antiferromagnetic branch vanishes. Another interesting feature is the ground-state sublattice magnetization as defined by

\[
\langle M_A \rangle_{\text{g.s.}} = L - \sum_{n=1}^{L} a_n^\dagger a_n = L(1 - \tau) \quad (10)
\]

\[
\tau = \frac{1}{\pi} \int_0^\infty dk \sinh^2(\eta_k) \approx 0.305 . \quad (11)
\]

Notice that the one dimensional ferrimagnet has a finite spin reduction \( \tau \). This is due to the factor \( 2\sqrt{2}/3 < 1 \), obtained for \( g = 2 \) in relation (9). In the usual antiferromagnet the corresponding factor is 1 and leads to a diverging spin reduction (in 1 D).

The ground-state energy per unit cell in the spin wave approach is obtained as

\[
E_0/J = -\frac{5}{2} L + \frac{L}{2\pi} \int_0^\pi dk \sqrt{9 - 8 \cos^2(k)} \approx -1.4365 L \quad (S = 1/2, \ g = 2). \quad (12)
\]

Further we studied the ground-state correlation functions between two sites with \( S = 1 \) for the ground state with magnetization \( L/2 \) and obtained the following results:

\[
\langle S_n^z S_{n+r}^z \rangle = (1 - \tau)^2 + f(r) \quad (13)
\]

\[
\langle S_n^+ S_{n+r}^- \rangle \propto \sqrt{f(r)} \quad (14)
\]

\[
f(r) = \frac{1}{L^2} \sum_{k,q} e^{i2qr} \sinh^2(\eta_k) \cosh^2(\eta_{k+q}) \quad (15)
\]

The asymptotic behaviour for the function \( f(r) \) is calculated by taking the continuum limit for the sum in eq.(15). We observe asymptotical exponential decay with a correlation length \( \xi, \xi^{-1} = 2 \ln(2) \). So for the intrasublattice distance \( r \geq 2 \) correlations have decayed and the square of the spin reduction \( (1 - \tau)^2 \) remains. From comparison with the QMC results it will be shown later this is a qualitatively correct picture.
As conclusion of this section we discuss the case of strong alternation, a limit which naturally reproduces the scenario as given above. If we introduce the interaction strength $J$ between sites $(2n)$ and $(2n+1)$ and $\delta J$ between sites $(2n-1)$ and $(2n)$ the Lieb-Mattis-Theorem and the Goldstone-Theorem still hold. The $M = L/2$ ground state in the dimerized limit $\delta = 0$ can be written down as

$$|0\rangle = |D_+\rangle_1|D_+\rangle_2 \ldots |D_+\rangle_L$$

$$(\vec{S}_n + \vec{s}_n)^2|D_+\rangle_n = \frac{1}{2}(\frac{1}{2} + 1)|D_+\rangle_n$$

$$(S^z_n + s^z_n)|D_+\rangle_n = \frac{1}{2}|D_+\rangle_n$$

$$|D_+\rangle = \frac{1}{\sqrt{3}}(|0\rangle, + 1/2) - \sqrt{2}|1, - 1/2)$$

For values $\delta \ll 1$ the system behaves like a $S = 1/2$ ferromagnet with the dublets $(D_+, D_-)$ being the effective spin $S_{\text{eff}} = 1/2$. A first order perturbation calculation in the alternation parameter $\delta$ leads to a ground-state energy of $E_0 = -L(1 + 1/9) + O(\delta^2)$. Now a ferromagnetic spin wave can be constructed within the dublet subspace

$$|q\rangle = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{iqn}|D_+\rangle_1|D_-\rangle_n \ldots |D_+\rangle_L$$

The dispersion up to the first order in $\delta$ is $\omega(q) = 4/9\lambda(1 - \cos(q)) + O(\delta^2)$. It is gapless and proportional to $q^2$ for small wavevectors as one would expect.

In addition to the ferromagnetic excitations we can construct antiferromagnetic spin waves, i.e. spin waves with $S^z_{\text{tot}} = L/2 + 1$. Again we discuss the case of strong alternation and end up with

$$|q\rangle = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{iqn}|D_+\rangle_1|Q_3\rangle_n \ldots |D_+\rangle_L$$

Here $|Q_3\rangle$ denotes the quartet with magnetization 3/2. The first order dispersion is $\omega(q) = 3/2 + \lambda(7/18 - 2/3 \cos(q)) + O(\delta^2)$ and is gapped.

**III. NUMERICAL RESULTS**
A. Brief Account on the Numerical Procedure

In the following we employ a quantum Monte Carlo method based on the Suzuki-Trotter decomposition \([9]\) of checker-board type \([10]\). Raw data are taken for a set of Trotter numbers \(n\) and are extrapolated to the \(n \to \infty\) limit with the parabolic fitting formula. We carry out all the calculations in certain subspaces with a fixed value of the total magnetization. Since we treat the chains with periodic boundary conditions, not only the Monte Carlo flips of local type but also the global flips along the chain direction are taken into the numerical procedure. On the other hand, global flips along the Trotter direction, which mean fluctuations of the total magnetization, are not included in order to well describe the ground-state properties. The quantum Monte Carlo algorithm to update the spin configuration is detailed elsewhere \([11]\). We have confirmed that almost the same results are obtained at two temperatures, \(k_B T/J = 0.04, 0.02\), and thus we regard these temperatures as low enough to successfully extract the lowest-energy-state properties. Here we show the data taken at \(k_B T/J = 0.02\). The data precision is almost four digits for the energy, and two digits for the spin correlations.

B. Low-Energy Structure

In Fig.1 we plot the lowest energies per unit cell in the subspaces with \(M = \sum_i (S_i^z + s_i^z) = L/2, L/2 - 1\) as a function of \(L\). The coincidence between both sets of data is nothing but the numerical demonstration of the above mentioned Lieb-Mattis theorem, that is, the \(L/2\)-multiplet structure of the ground state. The rapid convergence into the long-chain limit suggests a rather small correlation length in this system, which will be actually observed in the following. Within the present numerical precision, the ground-state energy in the thermodynamic limit is estimated as \(E_G = -1.455 \pm 0.001\). As we have observed in Fig.4, even the ground-state energy of the \(L = 16\) chain is already close to the thermodynamic-limit value. Thus we have plotted the quantum Monte Carlo data for \(L = 16\).
Although the quantum Monte Carlo data as presented above are already conclusive in themselves, we present an additional argument based on perturbation theory in the Ising anisotropy $\lambda$. We compare in Fig. 2 the quantum Monte-Carlo estimated ground-state energies and the corresponding perturbation-theory result

$$-E_G/L = 1 + \frac{\lambda^2}{2} - \frac{\lambda^4}{48} - 0.05136\lambda^6 + 0.02809\lambda^8 + \mathcal{O}(\lambda^{10}),$$

as a function of $\lambda$. We find a fairly good agreement between the eighth-order perturbation result and the QMC calculation. What should be emphasized is that fourth order calculation shows good agreement with the correct result. This fact gives us an idea on the spin configuration in the $M = L/2$ ground state. All the fluctuations introduced within the fourth order are essentially classified into the following three types:

(a) 2-sites fluctuation : $1, -1/2, 1, -1/2, 0, 1/2, 1, -1/2, 1, -1/2, \cdots$

(b) 3-sites fluctuation : $1, -1/2, 1, 1/2, -1/2, 1, -1/2, 1, -1/2, \cdots$

(c) 4-sites fluctuation : $1, -1/2, 0, 1/2, 0, 1/2, 1, -1/2, 1, -1/2, \cdots$

We note that the formation energy of the defect (c) is not twice as much as that of (a) and therefore they should be distinguished. Based on these fluctuations we are led to discuss microscopic quantum fluctuations at the isotropic point $(\lambda = 1)$. We present in Fig. 3 a QMC snapshot from which we can extract the image of quantum fluctuations to a certain extent. Here we show the snapshot at $k_B T/J = 0.02$ for $\lambda = 1.0$, $L = 32$, and $n = 20$, where the horizontal and vertical lines denote the chain and the Trotter directions corresponding to space and time, respectively. We find out everywhere local defects breaking the Néel Order, whereas they are all identified with the above-mentioned fluctuations. Thus we expect the fourth order calculation to well describe the the $M = L/2$ ground state.

Next we discuss the lowest excited states for the ferromagnetic and the antiferromagnetic branches. In the subspace with $M = L/2 - 1$ we construct a magnon for $\lambda = 0$ by flipping a spin-1: $S^z = 1 \rightarrow S^z = 0$. Expanding this state and taking the limit $k \rightarrow 0$ we obtain the lowest mode in this subspace. Such an expansion up to the fourth order is compared
with $E_G(L/2 - 1) - E_G(L/2)$ from the QMC calculation in Fig. 4. The perturbation result gives reasonable results up to $\lambda \approx 0.8$. A comparison between them suggests that the $k = 0$ magnon condenses into the ground state with $M = L/2 - 1$ at the isotropic point.

The antiferromagnetic magnon is constructed by flipping a spin-$1/2$ up. Again the perturbation result and the QMC data for $E_G(L/2 + 1) - E_G(L/2)$ are illustrated in Fig. 4. Here the validity for the fourth order expansion only reaches up to $\lambda \approx 0.4$. From the QMC calculation we obtain a gap of $\Delta/J = 1.767 \pm 0.003$. Here somewhat larger uncertainty, rather than one for the ground-state energy, mainly comes from the Monte Carlo estimate in the subspace of $M = L/2 + 1$. This value is much bigger than the prediction of the spin wave theory $\Delta = J$.

We conclude this section by pointing out that the quantum behaviour of the 1-1/2 system results in an enhancement of the gap. From Fig. 4 we observe that the pure Ising energy of $2J$ is just lowered by a small amount when moving to the isotropic point.

C. Spin Correlations

We show in Fig. 5 the spin correlation functions between the spins of the same type for the lowest-energy states in the subspaces with $M = L/2 - 1, L/2, L/2 + 1$. We note that the self correlation of spin-1 deviates from $2/3$ because of the multiplet structure of the ground state. In comparison with the spin correlations for $M = L/2$, those for $M = L/2 - 1$ are significantly reduced rather than those for $M = L/2 + 1$ in the case of spin-1, and vice versa in the case of spin-1/2. This is well understood considering that the ferromagnetic and the antiferromagnetic magnons, which exist in the subspaces with $M = L/2 - 1$ and $M = L/2 + 1$, originate from the spin flips in the $S = 1$ and the $S = 1/2$ sublattices, respectively. Those excitations are expected to reduce the ferromagnetic correlations between spins with $S = 1$ and spins with $S = 1/2$. We note that in the thermodynamic limit, both spin correlations for $M = L/2 - 1$ and $M = L/2 + 1$ should coincide with those for $M = L/2$. Nevertheless, Fig. 5 is still useful because it suggest to a certain extent the thermodynamic-limit spin correlations.
in the subspaces with magnons of finite density.

In the above sense, now let us concentrate ourselves on the subspace with \( L/2 \). We have already confirmed that the spin wave theory gives the asymptotic exponential decay of the spin correlations, where the correlation length is estimated to be less than unity. We here observe so rapid decay of the correlations that an estimate of the correlation length is beyond the present numerical precision. However, careful observation of Fig.5 shows us that the correlations between spins \( S = \frac{1}{2} \) are a little bit less rapid than those between spins \( S = 1 \). Spin wave theory cannot reproduce this feature because the decay is determined by the function \( f(r) \) in eq.\((15)\) for both sublattices. We further point out that the Monte Carlo calculation gives the spin reduction \( \tau \) as \( \tau \approx 0.21 \), which is somewhat smaller than the spin-wave-theory result. Therefore the spin-wave-theory cannot quantitatively describe the quantum fluctuations.

IV. CONCLUSION

We have calculated ground-state properties and low-lying excited states for an alternating ferrimagnetic spin chain with spins \( S = 1 \) and \( \frac{1}{2} \). The ground state is a spin \( S = L/2 \) multiplet. The model consist of a ferromagnetic and an antiferromagnetic branch corresponding to magnetizations \( M < L/2 \) and \( M > L/2 \), respectivly. The ferromagnetic branch has gapless excitations with dispersions \( \omega \propto k^2 \), \( k \ll \pi \) according to spin wave theory. The antiferromagnetic branch with \( M = L/2 + 1 \) shows a gapped spin wave with \( \Delta/J = 1.767 \pm 0.003 \). Both branches have longitudinal correlation functions consisting of a constant (square of spin reduction) plus strong exponential decay and therefore both branches show long range order. The manifestation of quantum behaviour shows up in the following points

- the gap for the \( M = L/2 + 1 \) excitation is enhanced compared to the spin wave theory.
- the \( L/2 \) ground state deviates from the Néel state owing to quantum fluctuations.
- there is an indication for the correlation length to be larger in the \( S = 1/2 \) than \( S = 1 \).
In order to study the mechanism for the gap formation in detail we have to investigate the perturbation theory to higher order. This is under investigation as well as the construction of matrix product states as variational ground state for $M = L/2$ [12]. The construction of these matrices can be based on the fact that unit cells with magnetization $-3/2$ show up rather rarely in Fig.3. Therefore the system exhibits a tendency to weak ferromagnetism similar to the one discussed by Niggemann and Zittartz [13] in $S = 3/2$ chains with matrix product ground states.

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FIGURES

FIG. 1. Size dependences of the ground-state energy in the subspaces with $M = L/2$ and $M = L/2 - 1$

FIG. 2. Dependences of the ground-state energy on the Ising anisotropy $\lambda$ obtained by a QMC method ($\bigtriangleup$), and 4-th-order (dotted line) and 8-th-order (solid line) perturbation theory.

FIG. 3. A snapshot of the transformed two-dimensional Ising system, where the horizontal and the vertical lines denote the chain and the Trotter directions corresponding to space and time, respectively, and ‘#’, ‘+’, ‘0’, ‘-’, and ‘=’ denote the spin projections $+1$, $+1/2$, $0$, $-1/2$, $-1$.

FIG. 4. Dependences of the excitation gaps $E_G(L/2 - 1) - E_G(L/2)$ ($\bigcirc$) and $E_G(L/2 + 1) - E_G(L/2)$ ($\bigtriangleup$) on the Ising anisotropy obtained by a QMC method, where the results within the 4-th-order perturbation treatment are also shown (solid lines).

FIG. 5. The ground-state spin correlations between spins $S = 1$ (a) and between spins $S = 1/2$ (b) in the subspaces of $M = L/2, L/2 - 1$ and $L/2 + 1$ for $L = 16$. 13
$M = \frac{L}{2} - 1$

$M = \frac{L}{2}$
\[ \left\langle S^z_i S^z_{i+j} \right\rangle \]

- $L = 16$  $M = 7$
- $L = 16$  $M = 8$
- $L = 16$  $M = 9$
\[ \langle S^z_1 S^z_{1+j} \rangle \]

Graph showing the relationship between \( j \) and \( \langle S^z_1 S^z_{1+j} \rangle \) with different markers for various \( L \) and \( M \) values:
- \( L = 16 \) and \( M = 7 \) (diamonds)
- \( L = 16 \) and \( M = 8 \) (circles)
- \( L = 16 \) and \( M = 9 \) (crosses)

The graph includes the following annotations:
- \( L = 16 \) and \( M = 7 \)
- \( L = 16 \) and \( M = 8 \)
- \( L = 16 \) and \( M = 9 \)