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Low-temperature properties of quantum antiferromagnetic chains with alternating spins $S = 1$ and $S = 1/2$

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Abstract. We study the low-temperature properties of $S = 1$ and $S = 1/2$ alternating spin chains with antiferromagnetic nearest-neighbour 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 using perturbation theory in terms of 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 describes the present system well. We conclude that the quantum ferrimagnetic chain exhibits both ferromagnetic and antiferromagnetic aspects.

1. 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, on the basis of analytical methods and various numerical approaches, it has become well accepted that the integer-spin chain is massive, whereas the half-odd-integer-spin chain is massless. This also stimulated several attempts to investigate the quantum behaviour of chains consisting of two types of spin. An integrable model of this type was constructed by de Vega and Woynarovich [2], which allows us to guess the essential consequences of chains being composed of spins of different magnitudes S. Recently, several authors [3, 4] discussed in detail such a chain composed of spins $S = 1$ and $S = 1/2$ 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

$$\mathcal{H} = J \sum_{i=1}^{L} \left[(\boldsymbol{S}_i \cdot \boldsymbol{s}_i)_\lambda + (\boldsymbol{s}_i \cdot \boldsymbol{S}_{i+1})_\lambda \right] \tag{1}$$

where $(\boldsymbol{S}_i \cdot \boldsymbol{s}_j)_\lambda = \lambda(S_i^x s_j^x + S_i^y s_j^y) + S_i^z s_j^z$, with $\boldsymbol{S}_i$ and $\boldsymbol{s}_i$ 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 the properties of the ground state and of the low-lying excited states by spin-wave theory, series expansion with regard to the Ising anisotropy λ, and a quantum Monte Carlo (QMC) method.

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Basic predictions for the low-lying level structure can be made by applying the Lieb–Mattis theorem [6] and the Goldstone theorem [7]. First we consider the ordering of the energy levels. The A sublattice is defined by the $S = 1$ sites (the maximum spin is $S_A = L$), and the B sublattice is defined by the spin-1/2 sites (the maximum spin is $S_B = L/2$). The Hamiltonian (1) consists of intersublattice interactions only, which allows us to apply the results of [6] to our system. The energy levels order in the following manner:

$$E(S+1) > E(S) \qquad \text{for all } S \geqslant \mathcal{S}$$
$$E(S) > E(\mathcal{S}) \qquad \text{for } S < \mathcal{S}.$$

Here $\mathcal{S} = |S_A - S_B|$ denotes the total spin of the ground state, which takes the value $\mathcal{S} = L - L/2 = L/2$ in our case. Therefore the ground-state degeneracy is $L + 1$. Although the ground states have finite spin $\mathcal{S}$, the following points show a contrast with the usual behaviour of ferromagnets:

(i) the ground-state degeneracy of a ferromagnet is larger by a macroscopic amount;

(ii) 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 [7] 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 for calculating 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.

2. 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 $g = 2$. We start from the fully ordered state with $S^z_{tot} = M = L/2$, and use the following spin operators in the two sublattices in the lowest order in $1/S$:

$$\text{sublattice A: } S^z_n = gS - a^\dagger_n a_n \qquad S^+_n = \sqrt{2gS}\,a_n \tag{2}$$
$$\text{sublattice B: } s^z_n = -S + b^\dagger_n b_n \qquad s^+_n = \sqrt{2S}\,b^\dagger_n. \tag{3}$$

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

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

where $a_n^\dagger = L^{-1/2}\sum_k \mathrm{e}^{\mathrm{i}k(n-1/4)}a_k^\dagger$ and $b_n^\dagger = L^{-1/2}\sum_k \mathrm{e}^{-\mathrm{i}k(n+1/4)}b_k^\dagger$. Here k is given as $k = 2\pi m/Na, m = -L/2+1,\ldots,L/2$, with a the lattice constant. We set a to unity in the following. The Hamiltonian is straightforwardly diagonalized to

$$H_{SWT} = E_0 + 2SJ\sum_k(\omega_k^- \alpha_k^\dagger\alpha_k + \omega_k^+\beta_k^\dagger\beta_k) \tag{5}$$

where

$$\omega_k^\pm = \frac{1}{2}\left(\sqrt{(g+1)^2 - 4g\cos^2(k/2)} \pm (g-1)\right) \tag{6}$$

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

and where the eigenvectors are determined by

$$\alpha_k^\dagger = \cosh(\eta_k)a_k^\dagger + \sinh(\eta_k)b_k \qquad \beta_k^\dagger = \sinh(\eta_k)a_k + \cosh(\eta_k)b_k^\dagger \tag{8}$$

$$\tanh(2\eta_k) = \frac{2\sqrt{g}}{1+g}\cos(k/2). \tag{9}$$

The results from the spin-wave theory contain both ferromagnetic and antiferromagnetic aspects. In the ferromagnetic branch (ω_k^-) we obtain a gapless spin wave for which $M = L/2-1$. For small values of the wave vector the dispersion is

$$\omega_k^- = \frac{g}{4(g-1)}k^2 + \cdots.$$

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 $g = 2, S = \frac{1}{2}$. This result will be compared to the result of the QMC calculation to be presented in the next section. If we choose the spins such that the spin magnitudes 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

$$\langle M_A\rangle_{g.s.} = L - \sum_{n=1}^{L} a_n^\dagger a_n = L(1-\tau) \tag{10}$$

$$\tau = \frac{1}{\pi}\int_0^\pi \mathrm{d}k\ \sinh^2(\eta_k) \approx 0.305. \tag{11}$$

Notice that the one-dimensional ferrimagnet has a finite spin reduction τ. 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 1D).

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

$$E_0/J = -\frac{5}{2}L + \frac{L}{2\pi}\int_0^\pi \mathrm{d}k\ \sqrt{9 - 8\cos^2(k/2)} \approx -1.4365L \qquad \left(S = \frac{1}{2}, g = 2\right). \tag{12}$$

Furthermore, we studied the ground-state correlation functions for two sites with $S = 1$ for the ground state with magnetization $L/2$, and obtained the following results:

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

$$\langle S_n^+ S_{n+r}^- \rangle \propto \sqrt{f(r)} \tag{14}$$

$$f(r) = \frac{1}{L^2} \sum_{k,q} \mathrm{e}^{\mathrm{i}\,2qr} \sinh^2(\eta_k) \cosh^2(\eta_{k+q}). \tag{15}$$

The asymptotic behaviour for the function $f(r)$ is calculated by taking the continuum limit for the sum in equation (15). We observe asymptotical exponential decay with a correlation length ξ, $\xi^{-1} = 2\ln(2)$. So for the intrasublattice distance $r \geqslant 2$, the 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 that this is a qualitatively correct picture.

As a conclusion to this section, we discuss the case of strong alternation, a limit which naturally reproduces the scenario as given above. If we introduce J, the strength of the interaction between the sites $2n$ and $2n+1$, and δJ, that between the 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 as

$$|0\rangle = |\mathrm{D}_+\rangle_1 |\mathrm{D}_+\rangle_2 \cdots |\mathrm{D}_+\rangle_L$$

$$(\boldsymbol{S}_n + \boldsymbol{s}_n)^2 |\mathrm{D}_+\rangle_n = \frac{1}{2}\left(\frac{1}{2}+1\right)|\mathrm{D}_+\rangle_n \qquad (S_n^z + s_n^z)|\mathrm{D}_+\rangle_n = \frac{1}{2}|\mathrm{D}_+\rangle_n$$

$$|\mathrm{D}_+\rangle = \frac{1}{\sqrt{3}}(|0,+1/2\rangle - \sqrt{2}|+1,-1/2\rangle).$$

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

$$|q\rangle = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} \mathrm{e}^{\mathrm{i}qn} |\mathrm{D}_+\rangle_1 \cdots |\mathrm{D}_-\rangle_n \cdots |\mathrm{D}_+\rangle_L. \tag{16}$$

The dispersion up to the first order in δ is $\omega(q) = (4/9)\delta(1-\cos(q)) + \mathcal{O}(\delta^2)$. 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 $S_{tot}^z = L/2+1$. Again we discuss the case of strong alternation, and end up with

$$|q\rangle = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} \mathrm{e}^{\mathrm{i}qn} |\mathrm{D}_+\rangle_1 \cdots |\mathrm{Q}_3\rangle_n \cdots |\mathrm{D}_+\rangle_L. \tag{17}$$

Here $|\mathrm{Q}_3\rangle$ denotes the quartet with magnetization 3/2. The first-order dispersion is $\omega(q) = 3/2 + \delta(7/18 - (2/3)\cos(q)) + \mathcal{O}(\delta^2)$, and is gapped.

3. Numerical results

3.1. A brief account of the numerical procedure

In the following we employ a quantum Monte Carlo method based on the Suzuki–Trotter decomposition [9] of checkerboard type [10]. Raw data are taken for a set of Trotter

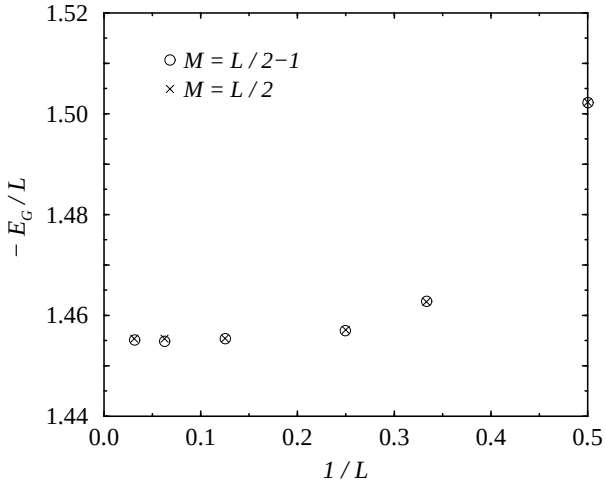

Figure 1. Size dependences of the ground-state energy in the subspaces with $M = L/2$ and $M = L/2 - 1$.

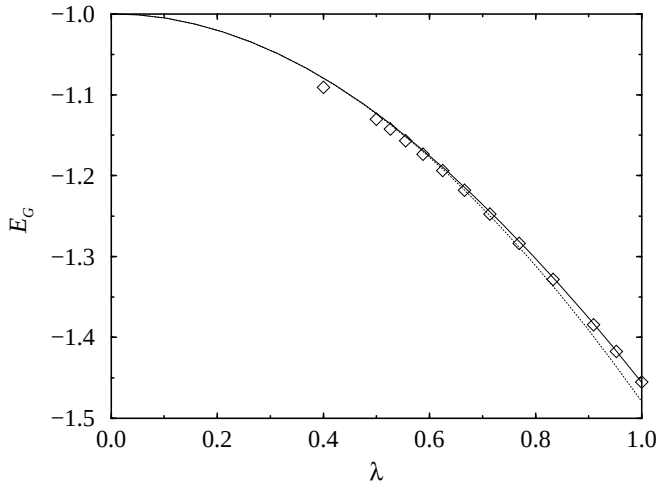

Figure 2. Dependences of the ground-state energy on the Ising anisotropy λ obtained by a QMC method (◊), and fourth-order (dotted line) and eighth-order (solid line) perturbation theory.

numbers n, and are extrapolated to the $n \to \infty$ limit with the parabolic fitting formula. We carry out all of 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 account in the numerical procedure. On the other hand, global flips along the Trotter direction—which are fluctuations of the total magnetization—are not included, in order to retain a good description of the ground-state properties. The quantum Monte Carlo algorithm used 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 for successfully extracting the lowest-energy-state

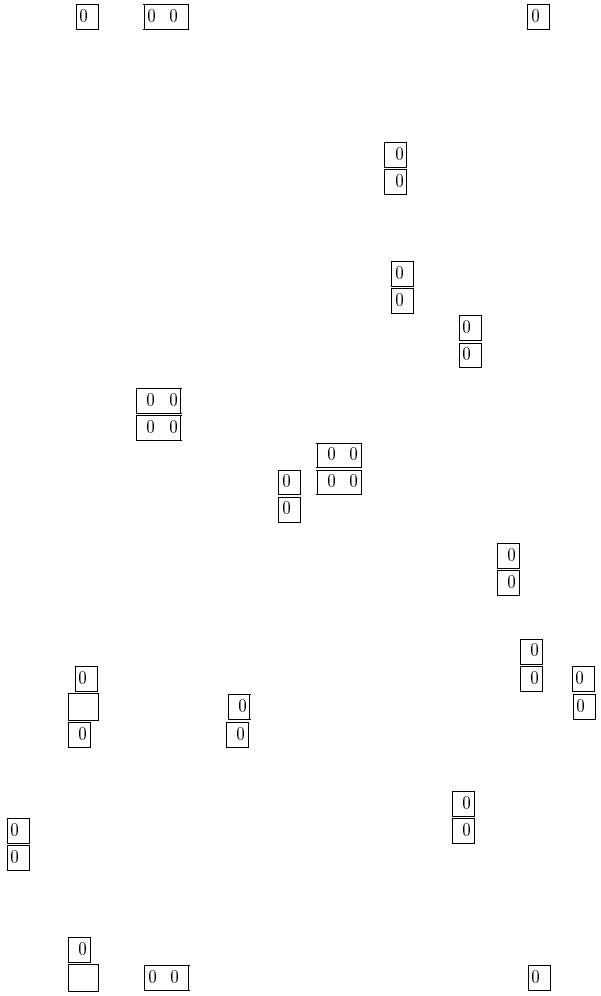

Figure 3. A snapshot of the transformed two-dimensional Ising system, where the horizontal and the vertical lines denote the chain and the Trotter directions corresponding to space and time, respectively, and '↑', '↑', '0', '↓', and '↓' denote the spin projections $+1$, $+1/2$, 0, $-1/2$, -1.

properties. Here we show the data obtained for $k_{\mathrm{B}}T/J = 0.02$. The data precision is almost four digits for the energy, and two digits for the spin correlations.

3.2. The low-energy structure

In figure 1 we plot the lowest energies per unit cell in the subspaces for which $M = \sum_i (S_i^z + s_i^z) = L/2, L/2 - 1$ as a function of L. The coincidence of the sets of data is simply a numerical demonstration of the above-mentioned Lieb–Mattis theorem—that is, the $(L/2)$-multiplet structure of the ground state. The rapid convergence to the long-chain limit suggests a rather small correlation length in this system, which will actually be observed in the following. Within the present numerical precision, the ground-state energy in the thermodynamic limit is estimated as $E_{\mathrm{G}} = -1.455 \pm 0.001$. As we have observed in figure 1, even the ground-state energy of the $L = 16$ chain is already close to the thermodynamic

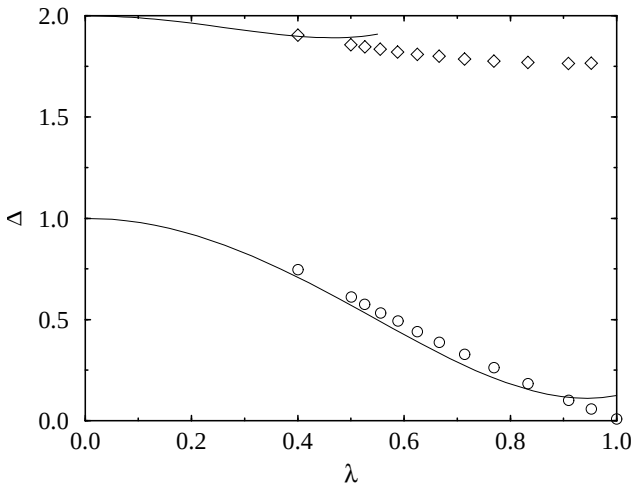

Figure 4. Dependences of the excitation gaps $E_G(L/2-1)-E_G(L/2)$ (◯) and $E_G(L/2+1)-E_G(L/2)$ (◇) on the Ising anisotropy obtained by a QMC method, where the results within the fourth-order perturbation treatment are also shown (solid lines).

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 applied to the Ising anisotropy λ. We compare in figure 2 the quantum Monte Carlo estimated ground-state energies and the corresponding perturbation theory result:

$$-E_G/L = 1 + \frac{\lambda^2}{2} - \frac{\lambda^4}{48} - 0.051\,36\,\lambda^6 + 0.028\,09\,\lambda^8 + \mathcal{O}(\lambda^{10}) \tag{18}$$

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

(a) two-site fluctuation: $1, -1/2, 1, -1/2, \underbrace{0, 1/2}, 1, -1/2, 1, -1/2, \ldots$

(b) three-site fluctuation: $1, -1/2, 1, \underbrace{1/2, -1, 1/2}, 1, -1/2, 1, -1/2, \ldots$

(c) four-site fluctuation: $1, -1/2, \underbrace{0, 1/2, 0, 1/2}, 1, -1/2, 1, -1/2, \ldots.$

We note that the formation energy of the defects of type (c) is not twice as much as that of the defects of type (a), and therefore they should be distinguished. On the basis on these fluctuations, we are led to discuss microscopic quantum fluctuations at the isotropic point ($\lambda = 1$). We present in figure 3 a QMC snapshot from which we can extract an 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 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 describe well the $M = L/2$ ground state.

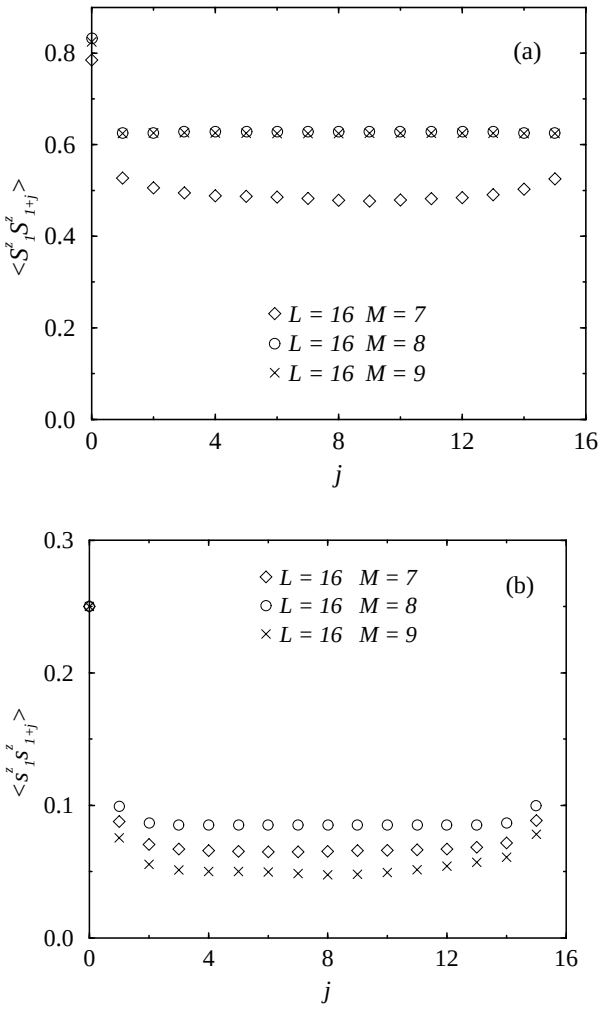

Figure 5. The ground-state spin correlations between spins $S = 1$ (a) and between spins $S = 1/2$ (b) in the subspaces with $M = L/2$, $L/2 - 1$, and $L/2 + 1$, for $L = 16$.

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 figure 4. The perturbation result gives reasonable results up to $\lambda \approx 0.8$. A comparison of these 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 figure 4. Here the validity for the fourth-order expansion only holds up to $\lambda \approx 0.4$. From the QMC calculation we obtain a gap of $\Delta/J = 1.767 \pm 0.003$. Here a somewhat larger uncertainty, rather than that for the ground-state energy, mainly arises from the Monte Carlo estimate in the subspace with $M = L/2 + 1$. 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 spin-1–spin-1/2 system results in an enhancement of the gap. From figure 4 we observe that the pure Ising energy of $2J$ is just lowered by a small amount when moving to the isotropic point.

3.3. Spin correlations

We show in figure 5 the spin-correlation functions for 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 $M = L/2 + 1$ as in the case of spin-1, and vice versa in the case of spin-1/2. This is readily understood on 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 $S = \frac{1}{2}$ sublattices, respectively. Those excitations are expected to reduce the ferromagnetic correlations between spins with $S = 1$ and spins with $S = \frac{1}{2}$. 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, figure 5 is still useful because it suggests to a certain extent the thermodynamic limit spin correlations in the subspaces with magnons of finite density.

In the above sense, let us now concentrate on the subspace with $M = L/2$. 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 a decay of the correlations that an estimate of the correlation length is beyond the present numerical precision. However, careful observation of figure 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 equation (15) for both sublattices. We further point out that the Monte Carlo calculation gives the spin reduction τ as $\tau \simeq 0.21$, which is somewhat smaller than the spin-wave theory result. Therefore the spin-wave theory cannot quantitatively describe the quantum fluctuations.

4. Conclusion

We have calculated ground-state properties and low-lying excited states for an alternating ferrimagnetic spin chain with spins $S = 1$ and $S = \frac{1}{2}$. The ground state is a spin $S = L/2$ multiplet. The model consists of a ferromagnetic and an antiferromagnetic branch corresponding to magnetizations $M < L/2$ and $M > L/2$, respectively. The ferromagnetic branch has gapless excitations with dispersions $\omega \propto k^2, k \to 0$, 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 (the square of the spin reduction) plus strong exponential decay, and therefore both branches show long-range order. The manifestation of quantum behaviour lies in the following points:

(i) the gap for the $M = L/2 + 1$ excitation is enhanced compared to that of the spin-wave theory;

(ii) the $L/2$ ground state deviates from the Néel state owing to quantum fluctuations; and

(iii) there is an indication that the correlation length is larger in the $S = 1/2$ sublattice than in the $S = 1$ sublattice.

In order to study the mechanism for the gap formation in detail we have to investigate the perturbation theory to higher order. This investigation is under way, as is the construction of matrix product states as variational ground states 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 figure 3. Therefore the system exhibits a tendency towards weak ferromagnetism similar to the one discussed by Niggemann and Zittartz [13] in $S = 3/2$ chains with matrix product ground states.

Acknowledgments

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