Investigation of the magnetic properties of chains with alternating ferro- and antiferromagnetic exchange interactions in the Heisenberg model with spin $S=1/2$

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The quantum Monte Carlo method is used to calculate the susceptibility and pairwise spin-spin correlation functions of chains with alternating ferro (K)- and antiferromagnetic (J)-exchange interactions within the Heisenberg model with spin $S=1/2$. From the susceptibility, the energy gap between the ground state and excited triplet states is determined for arbitrary ratios K/J. The value of the gap coincides with the Haldane gap for spin $S=1$ when $K/J>1.25$.
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The magnetic properties of one-dimensional antiferromagnetic chains are of interest both from an experimental[1,2] and from a theoretical point of view.[3] A question of fundamental interest is Haldane's hypothesis[4] regarding the qualitative difference between the ground states of antiferromagnets having integer and half-integer values of the spin: for half-integer spins there exist gapless magnetic excitations,[4] while for integer spins there is a gap in the excitation spectrum,[5,6] which was later observed experimentally.[7] For $S=1$ spins, values of the gap $g=0.41049$ and correlation radius $\xi=6.2$ have been determined by various methods: analytically, using perturbation theory,[8] by Monte Carlo,[9] and by exact diagonalization for small chains.[10]

Let us consider an antiferromagnetic chain consisting of coupled dimers. Then we can obtain a Haldane gap by alternating ferro- and antiferromagnetic interactions on a chain of spins with $S=1/2$. In the limit of strong ferromagnetic coupling ($K\to\infty$), the dimers are in the lowest triplet state, and the chain of spins with $S=1/2$ can be reduced to an effective antiferromagnetic chain with spins $S=1$. In the other limiting case ($K\to 0$), a gas of antiferromagnetic dimers is realized which also exhibits an energy gap between the singlet and triplet state, equal to the value of the antiferromagnetic exchange.

The question of magnetic behavior of chains and the value of the gap for arbitrary ratios of the exchange constants K/J remains open. In this paper we solve the problem as formulated by the quantum Monte Carlo method in the Heisenberg model with spin $S=1/2$. The Hamiltonian has the form

$$H=-2J\sum_{i=1}^{N/2} S_{2i-1}S_{2i}-2K\sum_{i=1}^{N/2} S_{2i}S_{2i+1}-h\sum_{i=1}^{N} S_i,$$

where $J<0$, $K>0$ are the ferro- and antiferromagnetic interactions respectively, N is the number of spins in the chain, and h is an external magnetic field.

A detailed description of the quantum Monte Carlo method, using the Trotter equation and corresponding expressions for computing the susceptibility, heat capacity, and pairwise spin-spin correlation functions, was presented in a previous paper.[11] In our Monte Carlo calculations, periodic boundary conditions were used along the Trotter direction (m) and along the chain. The number of spins in a chain was $L=200$, with $m=16$, 32, and 64. The number of Monte Carlo steps for one spin varied from $M=6000$ to 20000. One step was determined by the rotation of all the spins on a lattice of size $L\times 2m$. The mean-square errors for the energy and susceptibility were ~ 1 and $\sim 6\%$ respectively. The systematic error arising from the finite Trotter number, which takes into account the noncommutative nature of the operators, was proportional to $\sim 1/(mT)^2$.

The heat capacity, susceptibility, and spin correlation functions for an isotropic antiferromagnetic chain are in good agreement with known exact calculations and were given in Ref. 11. The magnetic susceptibility of a chain with alternating exchange interactions equals zero as $T\to 0$. Figure 1 shows the temperature dependence of the susceptibility for certain values of the ratio of exchange constants K/J and Trotter numbers. As the ferromagnetic coupling increases, the maximum in the susceptibility increases as well, and at low temperatures $T/J<1$ it is well described by the relation $\chi(T)=A\exp(-g/T)$, where g is the value of the gap between the ground and excited triplet states. The inset to Fig. 1 shows the susceptibility plotted on a logarithmic scale versus the inverse value of the temperature for various values of m. It is clear from Fig. 1 that quantum effects are correctly taken into account for these Trotter numbers, and within the limits of error for the susceptibility they are well described by a linear dependence.

The magnitude of the energy gap decreases with increasing ferromagnetic exchange, and for $K/J>1.25$ it is practically independent of the value of K (Fig. 2). It is probably the computed value of K for ferromagnetic coupling that is critical. Thus, the spin-spin correlation functions between nearest neighbors and next-to-nearest neighbors is negative for the whole temperature range when $K/J<1.25$, while for $K/J>1.25$ there is a certain temperature at which $\langle S^z(0)S^z(r=1)\rangle$ changes sign from negative to positive, as shown in Fig. 3. Probably this is caused by removing the

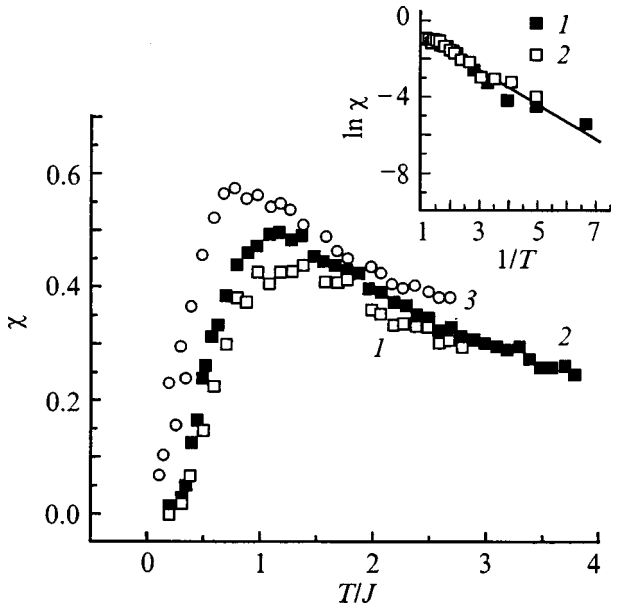

FIG. 1. Temperature dependence of the magnetic susceptibility of a chain with alternating ferro- and antiferromagnetic exchange constants when $K/J=-0.25$ (*1*), 1 (*2*), 3 (*3*). The inset shows the logarithm of the susceptibility plotted versus $1/T$ for $K/J=1$, $m=64$ (*1*), 32 (*2*).

degeneracy between the three multiplets of the ferromagnetic dimer with $S^z=\pm 1$ and 0, due to the antiferromagnetic interaction between them. With increasing J/K, the splitting between these multiplets increases. Thus, a one-dimensional

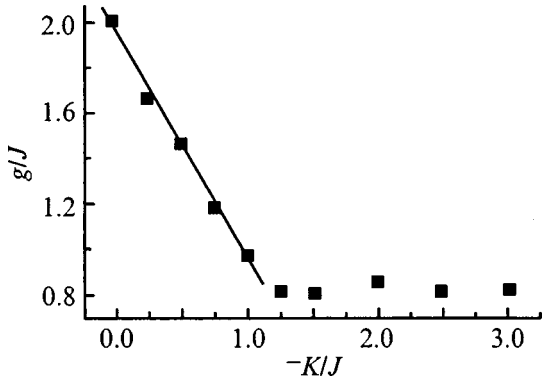

FIG. 2. Dependence of the energy gap between the ground and excited triplet states on the ratio of exchange constants K/J.

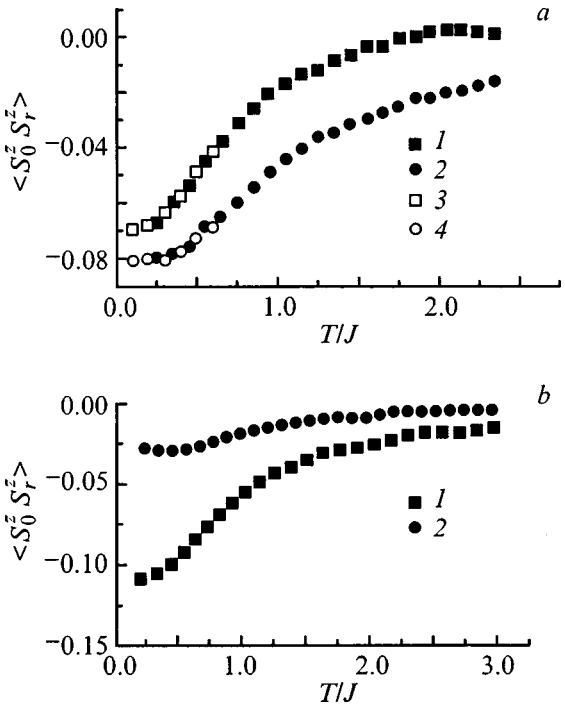

FIG. 3. Temperature dependence of the spin-spin correlation function for $K/J=-2$ (a), -0.5 (b), at distances $r/a=1$ (*1,3*), $r/a=2$ (*2,4*), $m=32$ (*1,2*), $m=64$ (*3,4*).

chain with alternating ferro- and antiferromagnetic exchanges has a gap in the energy of spin triplet excitations, whose value does not depend on the value of the ferromagnetic exchange for $K/J>1.25$, and equals the value of the Haldane gap when $S=1$.

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