Spin-$\frac{1}{2}$ Heisenberg antiferromagnet with anisotropic nearest- and next-nearest-neighbor coupling

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A modified Lanczos method has been used to study the ground-state properties of a frustrated one-dimensional anisotropic Heisenberg antiferromagnet. The ground-state energy as well as all two-particle spin-spin correlation functions are obtained for a 16-site lattice. Both the relative couplings and anisotropies for nearest and next-nearest neighbors are varied.

I. INTRODUCTION

One-dimensional magnetic systems have been the focus of serious attention since the early 1960's when the exact solutions to a number of quantum spin-chain problems were obtained. The excellent agreement achieved in some cases, both qualitatively and quantitatively, between theory and experiment has pointed up the relevance of these systems to our understanding of real quasi-one-dimensional magnets. In particular, the compound $[C_6H_{11}NH_3]CuBr_3$ has been studied extensively[1] as has the linear chain magnetic insulator $CoCl_2(2H_2O)$ which may be interpreted in terms of one-dimensional spin-$\frac{1}{2}$ anisotropic Heisenberg model with a nearest-neighbor exchange interaction. The case of alternating spin chains is also of interest to physicists. This problem was originally studied by chemists to explain the properties of certain organic free radicals.[2] More recent applications have been to copper nitrate[3,4] and copper bromide imidazole[5] as well as the members of a family of organometallic complexes, insulating relatives of the organic conductor TTF-TCNQ. These include the TTF bisdithiolenes [TTF BDT(M), where M = Cu or Au]. There are many other quasi-one-dimensional materials which are known to exhibit either ferromagnetic or antiferromagnetic properties. Interpretation of neutron-scattering experiments has yielded evidence that dichlorobispyridine copper $[CuCl_2 2N(C_5D_5)]$ behaves as an isotropic spin-$\frac{1}{2}$ Heisenberg quantum antiferromagnet while $CsCoCl_3$ (and $CsCoBr_3$), on the one hand, and Cs_2CoCl_4, on the other, represent spin-$\frac{1}{2}$ Heisenberg antiferromagnets of the XXZ type, displaying high anisotropy into the Ising-like and planarlike regimes, respectively.[5] More recently the discovery of high-T_c superconductors has reignited interest in systems of low dimensionality. In particular, the extraordinary magnetic properties both of the normal and superconducting states has brought quantum spin systems to the fore. One major area requiring further study is the nature of the ground state. The spin-$\frac{1}{2}$ Heisenberg model has been studied as a model for the ground state by a number of authors on a variety of lattices.[6,7,8] A fully disordered resonating-valence-bond (RVB) state has been proposed by Anderson as candidate for the two-dimensional ground state. However, recent numerical studies of the antiferromagnetic Heisenberg model which have included frustration by considering next-nearest-neighbor interactions point to an ordered ground state of the Néel variety.

In one dimension, various ground-state properties for the isotropic nearest-neighbor case have been calculated in the exact $N \rightarrow \infty$ limit.[9–13] This case has also been studied by Borysowicz, Kaplan, and Horsch[14] who calculated the correlation function for rings of up to 16 spins by the Lanczos method; by Betsuyaku and Yokota[15] who made the same calculation for rings of from 10 to 20 spins using the projector method and by Gagliano *et al.*,[16] who calculated the ground-state energy and correlation function for rings of up to 24 sites using a modified Lanczos method. The isotropic case with next nearest-neighbor interactions has been examined by Majumdar and Ghosh[17] who calculated the ground-state energy for linear chains of up to 10 particles. For this same case Tonegawa and Harada[18] calculated several ground-state properties, including the energy and correlation function for a railroad trestle lattice of up to 20 sites.

For the anisotropic case Lagos and Cabrera[19] have looked at the ground-state energy for nearest-neighbor interactions only using a coherent-state solution, and Gottlieb *et al.*[20] have made the same calculation for a frustrated system by the addition of a next-nearest-neighbor interaction.

In this paper we extend the work of Gagliano *et al.*[16] by applying the modified Lanczos method to the case of a spin-$\frac{1}{2}$ antiferromagnet Heisenberg system with the addition of anisotropic first- and second-nearest-neighbor exchange interactions. We consider a ring of 16 sites with periodic boundary conditions. The behavior of the ground-state energy per site and all spin-spin correlation functions are studied. Variations in both anisotropy parameters as well as the nearest-neighbor and next-nearest-neighbor exchange ratios are considered.

The paper is organized as follows: In Sec. II, we define the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg Hamiltonian and outline the modified Lanczos method. In Sec. III, we present our results and compare with previous work. In Sec. IV, we offer our final comments.

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II. METHOD

The Hamiltonian for a one-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet with anisotropic first- and second-nearest-neighbor exchange interactions is given by

$$H=J_1\sum_{i=1}^{N}[S_i^+S_{i+1}^-+S_i^-S_{i+1}^++2\rho_N S_i^zS_{i+1}^z]+J_2\sum_{i=1}^{N}[S_i^+S_{i+2}^-+S_i^-S_{i+2}^++2\rho_{\rm NN}S_i^zS_{i+2}^z]\ , \quad (1)$$

where J_1 and J_2 are the first- and second-nearest-neighbor coupling; ρ_N and $\rho_{\rm NN}$ are the corresponding anisotropy parameters. In the following we define the relative coupling $j\equiv J_2/J_1$ and relative anisotropy $\lambda\equiv\rho_{\rm NN}/\rho_N$. $\bar{S}_i$ is the spin-$\frac{1}{2}$ operator at the ith site and $S_i^{\pm}$ are the spin raising and lowering operators defined by $S_i^{\pm}\equiv S_i^x\pm iS_i^y$. We assume a ring of N (even) sites, and consider periodic boundary conditions with $\bar{S}_{N+i}=\bar{S}_i$. In this study we consider both interactions to be antiferromagnetic ($J_1>0$, $J_2\geq 0$), thus competing with each other, and that the anisotropy is of the Heisenberg XY type ($0\leq\lambda\leq 1$).

Our method of calculation is a modification of the Lanczos tridiagonalization method. The Lanczos equations are generated by operations with the Hamiltonian on a normalized initial trial vector, Ψ_0, which has a nonzero overlap with the true ground state Φ_0 of the system. This operation yields a set of equations which we require to be in tridiagonal form:

$$H|\Psi_i\rangle=m_{i,i-1}|\Psi_{i-1}\rangle+m_{i,i}|\Psi_i\rangle+m_{i,i+1}|\Psi_{i+1}\rangle\ . \quad (2)$$

Solving the resulting simultaneous equations gives the energy of the system to any degree of approximation desired.

In the modified Lanczos scheme of Gagliano *et al.*,[16] we only consider a (2×2) representation of H given by the basis

$$H|\Psi_0\rangle=m_{00}|\Psi_0\rangle+m_{01}|\Psi_1\rangle\ , \quad (3)$$

$$H|\Psi_1\rangle=m_{10}|\Psi_0\rangle+m_{11}|\Psi_1\rangle\ . \quad (4)$$

Then,

$$|\Psi_1\rangle=\frac{1}{m_{01}}[H-m_{00}]|\Psi_0\rangle \quad (5)$$

and

$$m_{00}=\langle\Psi_0|H|\Psi_0\rangle\equiv\langle H\rangle \quad (6)$$

with

$$m_{01}=m_{10}=[\langle H^2\rangle-\langle H\rangle^2]^{1/2}\equiv b\ , \quad (7)$$

$$m_{11}=\frac{1}{m_{10}^2}[\langle H^3\rangle-2\langle H\rangle\langle H^2\rangle+\langle H\rangle^3]=\frac{1}{b^2}[\langle H^3\rangle-3\langle H\rangle\langle H^2\rangle+2\langle H\rangle^3]+\frac{\langle H\rangle}{b^2}[\langle H^2\rangle-\langle H\rangle^2]\equiv 2bf+\langle H\rangle\ . \quad (8)$$

Diagonalizing the matrix obtained from Eq. (3) yields

$$\epsilon_1=\langle H\rangle+\alpha b \quad (9)$$

as the lowest eigenvalue, and

$$\hat{\Psi}_0=\frac{1}{(1+\alpha^2)^{1/2}}[\Psi_0+\alpha\Psi_1] \quad (10)$$

as its corresponding eigenvector, with $\alpha\equiv f-(f^2+1)^{1/2}$. Obviously ϵ_1 and ψ_0 are better approximations of the ground-state energy and wave function than $\epsilon_0\equiv\langle H\rangle$ and ψ_0. Further improvements can be made by interaction; ψ_0 is now taken to be the trial wave function and a new lowest eigenvalue, ϵ_2, and eigenvector, ψ_0, are generated. ψ_0 is then taken as the next trial wave function and so on. Each interaction generates a better estimate of the ground-state energy and wave function of H. Since we confine ourselves to the case where $J_1>0$ and $J_2\geq 0$, we have chosen our initial trial wave function to be the ordered Néel state (with $S_z=0$ in accordance with the ground-state theorems of Lieb and Mattis[21]). Thus, the ground-state energy is given by the lowest eigenvalue of the matrix for $S_z=0$.

III. RESULTS

The majority of theoretical and computer simulation studies of purely exchange coupled magnets focus on results for antiferromagnets because of the experimental data available for the nearly ideal one-dimensional magnet TMMC.[18,22,23] In this section we discuss the numerical results for both the ground-state energy and all two-spin correlation functions for the 16-site Heisenberg antiferromagnetic lattice. Comparisons are then made with other works in the appropriate parameter ranges.

In Fig. 1, we have plotted the ground-state energy per site as a function of the relative coupling j, for various values of the relative anisotropy $\lambda=0$, 0.25, 0.50, 0.75,and 1.00. In the isotropic limit, $\lambda=1$, our results agree with those of Tonegawa and Harada[18] and with Ono.[24]

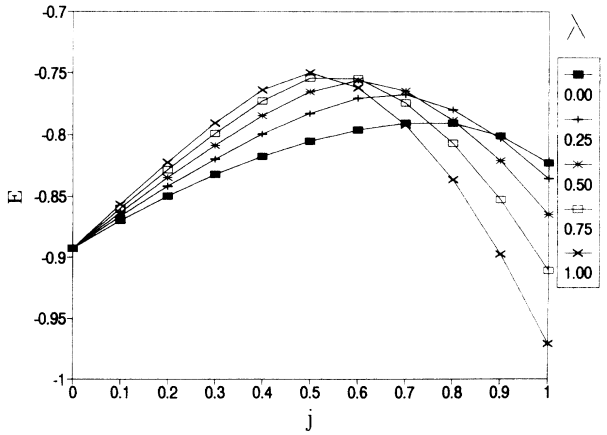

FIG. 1. Ground-state energy $E_0/(NJ_1)$ as a function of the relative coupling $j=J_2/J_1$ for various values of the anisotropy ratio $\lambda=\rho_N/\rho_{\rm NN}$ and $N=16$.

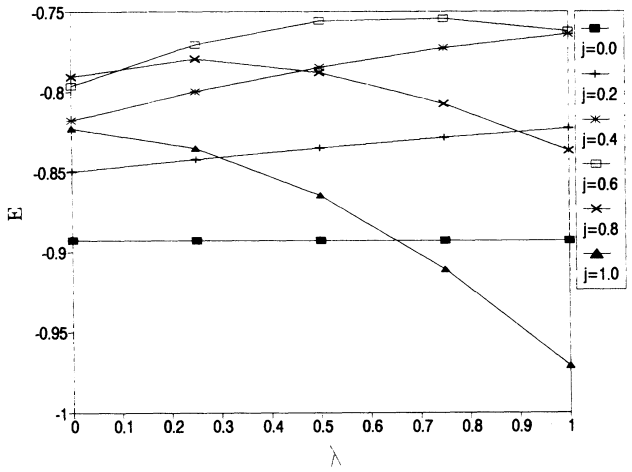

FIG. 2. Ground-state energy $E_0/(NJ_1)$ as a function of the anisotropy ratio with $j=J_2/J_1=0$, 0.2, 0.4, 0.8, 1.0, and $N=16$.

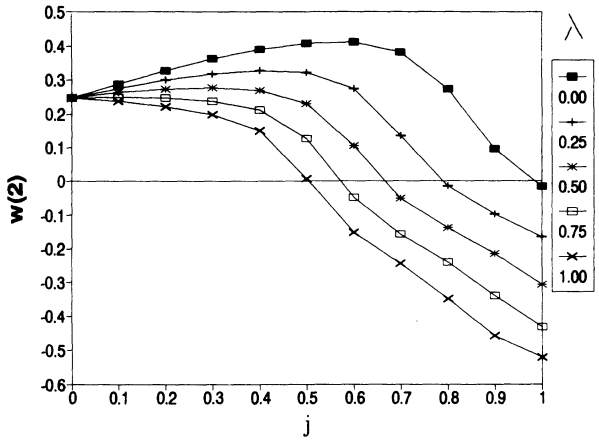

FIG. 4. Plot of the second-neighbor two-spin correlation function $\omega(2)$ vs j for selected values of λ. The point $\lambda=0$, $j=0$ agrees with the results of Hulthen.

Furthermore, for $j=0$, $\lambda=0$ we appear to be in exact agreement with Hulthen's exact value $(1-4\ln 2)J_1/2=-0.886\,294J_1$. In accordance with Ref. 18 we note that the energy increases monotonically for $j<0.5$, and has a more complicated structure for $j>0.5$. Of particular curiosity is the curve for $\lambda=0$ which represents a nearest-neighbor XYZ model coupled with a next-nearest-neighbor XY model.

In Fig. 2, the ground-state energy per site is plotted as a function of the relative anisotropy λ for various values of the relative coupling $j=0$, 0.2, 0.4, 0.6, 0.8, and 1.0. We see that for those values of $j<0.5$, the ground-state energy increases monotonically while for $j>0.5$ there is a complicated λ dependence resulting in a crossing of levels.

The two-spin correlation function $\omega(l,N)$, which is associated with Néel order, is defined by

$$\omega(l,N)=\langle\Psi_0(N)|S_l^zS_{l+1}^z|\Psi_0(N)\rangle\ . \tag{11}$$

In Figs. 3 and 4 we have plotted the correlation functions

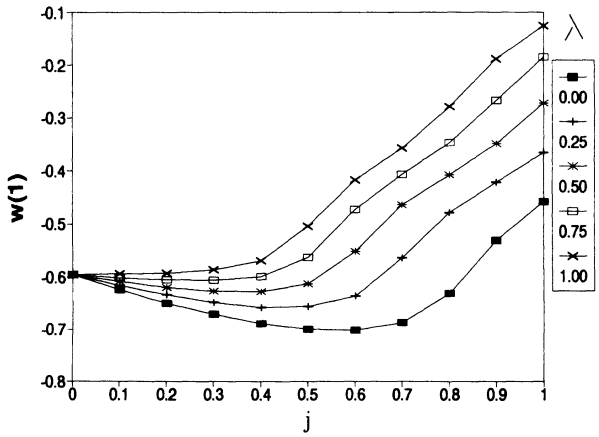

FIG. 3. Plot of the first-neighbor two-spin correlation function $\omega(1)$ vs j for selected values of λ. The point $\lambda=0$, $j=0$ agrees with Bethe.

$\omega(1)$, $\omega(2)$ for $N=16$, as a function of the relative coupling j for values of relative anisotropy $\lambda=0$, 0.25, 0.5, 0.75, 1.0. Once again in the isotropic limit $\lambda=1$ our results agree with those of Tonegawa and Harada.[18] For $j=0$, $\lambda=0$, we reproduce the recent results of Betsuyalsu and Yokota[15] as well as the early work of Bethe[10] and Hulthen.[11] Some exact results are known for the limiting behavior of $\omega(l,N)$ as $N\rightarrow\infty=-0.147\,716$, since it is related to the exact limit ground-state energy determined by Hulthen[11] $[\omega(1;\infty)=E_0(\infty)/6J_1]$. More recently Takahashi[25] has calculated exactly $\omega(2;\infty)$ to obtain $\omega(2;\infty)=0.060\,680$. The data presented in this study using a truncated Lanczos basis for a 16-site lattice compare favorably with these exact results. Luther and Peschel[26] have determined analytically that the correlation function $\omega(1;\infty)$ is asymptotically given by $\omega(1;\infty)\sim(-1)^l A/l$, where A is the unknown constant. This would then imply the absence of long-range order in one dimension since

$$\omega_{\mathrm{LRO}}=\lim_{l\rightarrow\infty}|\omega(l;\infty)|\rightarrow 0\ ,$$

where ω_{LRO} is the long-range-order parameter. Although we have not explicitly extrapolated our results to the $N\rightarrow\infty$ limit, we conclude that the data presented here are consistent with Luther and Peschel, based on our agreement with other published work in the appropriate parameter ranges.

IV. CONCLUSIONS

Using a modified Lanczos method we have studied the ground-state properties of the one-dimensional antiferromagnetic Heisenberg model with anisotropic coupling between nearest and next-nearest neighbors. We have presented our results for the ground-state energy and for all two-particle correlation functions for the 16-site ring. Our results are in exact agreement, in the appropriate regions of parameter space,with previous works. Recently Gottlieb *et al.*[20] have calculated the ground-state energy

only for the same system studied here. However, their representation of the Hamiltonian and the regions of parameter space which they have studied make comparisons with our work intractable. In the spirit of Ref. 12, we have chosen a 2×2 truncation of the modified Lanczos equations. Higher-order truncations would accelerate the rate of convergence to the true ground-state with the price to pay an enormous increase in (symbolic) algebraic manipulation.

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