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Numerical study of antiferromagnetic Heisenberg-Ising chains for spin s=1/2

Djalma Medeiros and G. G. Cabrera
Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas (UNICAMP), Caixa Postal 6165, Campinas 13.081, São Paulo, Brasil

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Abstract The Heisenberg-Ising Hamiltonian has been exactly solved using the Lanczos method, for chain of up to N = 28 spins. In the whole anisotropic region, the mass gap displays a dominant exponential behavior with size. The extrapolated ground state is doubly degenerate, and presents long-range order with dominant components of the Néel type. Quantum fluctuations become more important as long as the anisotropy is reduced, leading to a disordered singlet ground state for the infinite system at the isotropic point.

Low-dimensional magnetism is a fascinating subject. Experimentally, quasi-one dimensional magnetic systems can be obtained in crystals where the magnetic ions are arranged in chains, with weak interchain interactions[1]. From the theoretical point of view, the Heisenberg antiferromagnetic chain is one of the simplest models that presents non trivial many-body effects, where quantum fluctuations play an important role[2]. The exact solution via Bethe ansatz[3] is very intricate, and closed analytic results have been obtained only in particular cases or within approximate schemes[4].

Concerning finite chains, Bethe ansatz methods lead to coupled transcendental equations which are extremely difficult to handle in a neat analytical way. Some asymptotic estimates of finite-size corrections can be made for finite, but large sizes[5]. In most instances numerical investigations are necessary, either for direct calculations or for testing approximate analytic solutions.

In this contribution we present numerical computations for the ***mass gap*** of the Heisenberg-Ising antiferromagnetic chain for spin s=1/2. We also study the

structure of the ground-state wave function. Our calculation was based on the Lanczos method[6], N = 28 being the largest size computed. Results show that the gap closes exponentially with size in the asymptotic limit of large N, but power-law corrections become increasingly important as long as we go in the direction of the isotropic regime. In the thermodynamic limit ($N \to \infty$), the ground state is doubly degenerate, and the system displays long-range order. Its nature is essentially Néel-like, but quantum fluctuations reduce the magnetic moment as function of the anisotropy. At the isotropic point, the ground state is a singlet and the system becomes disordered. In this latter case, finite-size effects become 1ogarithmic[7], making it difficult to do extrapolations based on finite-size scaling. However, combining theoretical arguments and proper handling of numerical data, one can get correct insights on the behavior of the infinite chain[8].

In our calculation we used the following Hamiltonian:

$$H = J \sum_m [S_x(m)S_x(m+1) + \alpha\{S_x(m)S_x(m+1) + S_y(m)S_y(m+1)\}], \qquad (1)$$

where J > 0 is the exchange constant and $S_x(m)$, $S_y(m)$, and $S_z(m)$ are the spin operators for s=1/2 at site m. Anisotropy effects are taken into account through the α parameter. In (1), we have assumed periodir boundary condition and have calculated even values of N.

A fundamental step in our calculation is the exact diagonalization of the Hamiltonian. This method is the most reliable, since it is free of the rounding errors which are characteristic of the stocastic methods. For large matrices, the Lanczos method[6] appears as an efficient technique, whose attractive feature is that the lowest eigenvalues and corresponding eigenvectors are obtained in an iterative way. Convergence is optimized if the trial state, which starts the Lanczos process, contains the full synimetry of the solution. In our case, the ground and first excited levels are contained within the manifold of total $S_z = 0$. Taking also ínto account translatíonal and time inversion symmetries, a sizable reduction of computer memory is attained. Concerning CPU time, quick search and storage of states is efficiently implemented via the *hashing* technique[g].

Numerical extrapolations were done using the VBS algorithm[10]. Excellent agreement is found with the analytic result by Orbach[3] for the energy of the ground state of the infinite chain, in the whole region $0 \leq a \leq 1$. Within our numerical accuracy, splitting G_N between the two low-lying levels (mass gap) vanishes for $N \to \infty$. A main issue in finite-size calculations is the knowledge of how the mass gap scales with size. If the gap closes exponentially with N, the ground state of the infinite system is doubly degenerate, while the $G_N \sim 1/N$ dependence is characteristic of the quasi-continuum spectrum.

As a working hypothesis, we have assumed an asymptotic mass gap dependence with size of the form:

$$G_N = AN^{-\beta} \exp(-\sigma N), \tag{2}$$

where the coefficient a is a-dependent, $a = \sigma(\alpha)$. The scaling law given by eq. (2) includes in a mixed form exponential and power-law corrections. Size-dependent quantities $\sigma(N, a)$ and $\beta(N, a)$ are obtained from three successive sets of numerical data, and the corresponding sequences can be used to extrapolate the coefficient σ and the exponent β of eq. (2). Results are shown in Table 1, where extrapolated values for a are compared with theoretical predictions[5]. There is an excellent agreement, indicating that the gap closes exponentially in the whole anisotropic region, and therefore the ground state is a doublet. As regards to β, our finite-size estimates are within the limits predicted by theory, but strong size effects make extrapolations uncertain.

In the range $0 \leq a < 1$, the ground state displays long-range order and can be pictured as a linear quantum superposition of components contained in the manifold of $S_z = 0$ [2]. Néel states are the dominant components and their weights increase with the anisotropy. Other contributions to the ground-state wave function, in hierarchical order, include configurations obtained from the Néel states by flipping pairs of neighboring spins (one pair, two pairs, and so on, in linear combinations with translational symmetry). Their relative weights increase when going from the Ising regime to the isotropic point, thus reducing the net magnetic moment. To illustrate the above effect, we show in Table 2 simulation results for

weights of the three most important components of the normalized ground state as functions of a , for N = 24 spins.

In figure 1 we display the correlation function for the most distant spins in the chain, $\omega(N/2) = < S_z(m)S_z(m + N/2) >$, also for $N = 24$. $\omega(N/2)$ extrapolates to the square of the staggered magnetization M, in the limit N $\rightarrow \infty$. Our results are compared with the exact formula by Baxter for the infinite chain[11]. Finite-size effects appear when the bulk correlation length ξ is of the order of the size of the system. As is apparent from the figure, this happens near the critical point. In the strong anisotropic regime our simulation is free from size corrections and reproduces the analytic result already with fairly small chains.

Table 1 – The coefficient σ as a function of the a parameter (for N = 28 and extrapolated values), compared with theoretical ones (Ref. 5). Strong exponential behavior for α=0.1 requires extremely precise computations for large sizes, and the extrapolation was done with N = 24 as the maximum size. Around α=0.7, a crossover of finite-size corrections makes difficult extrapolations within the sizes used (see Ref. 8).

α	$\sigma(N = 28)$	o (Extrap.)	o (Theor.)
0.1	–	0.8083	0.8085
0.2	0.4717	0.4727	0.4732
0.3	0.2874	0.2888	0.2893
0.4	0.1692	0.1714	0.1719
0.5	0.0887	0.0935	0.0944
0.6	0.0363	0.0441	0.0448
0.7	0.0115	0.0099	0.0162
0.8	0.0031	0.0023	0.0032
0.9	0.0009	0.0004	0.0001

In summary, an exponential dependence with size for the mass gap has been numerically obtained, in agreement with theoretical predictions. Our simulatiori shows that the ground state for the infinite chain is doubly degenerate and displays long-range order in the whole axially anisotropic region, with dominant components of the Néei type. At the isotropic point the sçaled mass gap NG_N converges logarithmically to a constant, indicating tha the ground state is a singlet without long-range order[8].

Table 2 – Weights for different components of the ground-state wave packet as function of a, for N = 24. P_N refers to the Néel states, while P_1 and P_2 refer to configurations obtained from the Néel states with one and two flipped pairs, respectively. Numbers in front label the corresponding multiplicity.

α	$2 \times P_N$	$48 \times P_1$	$48 \times P_2$
0.1	0.94184	0.05623	0.00056
0.2	0.78761	0.18526	0.00722
0.3	0.58625	0.30258	0.02541
0.4	0.38799	0.34413	0.04937
0.5	0.22645	0.30122	0.06436
0.6	0.12105	0.22030	0.06336
0.7	0.06580	0.15255	0.05409
0.8	0.03888	0.10867	0.04450
0.9	0.02515	0.08134	0.03684
1.0	0.01754	0.06376	0.03106

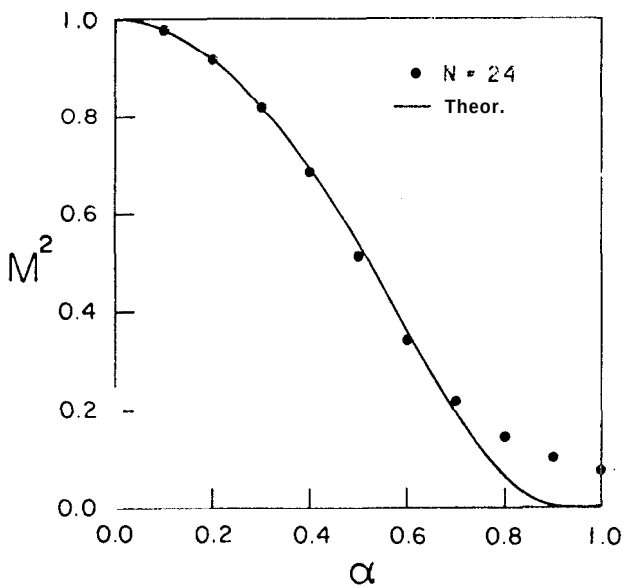

Fig. 1 – Correlation function $\omega(N/2) = < S_z(m) S_z(m+N/2) >$, for $N = 24$. The limit of $\omega(N/2)$, for $N \to \infty$, yields the square of the staggered magnetization M. Simulation data are compared with exact resiilts (Ref. *11*).

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Resumo

Cadeias finitas foram resolvidas exatamente usando o método de Lanczos, até $N = 28$ spins, para o Hamiltoniano de Heisenberg-Ising. Em toda a região anisotrópica, o gap de massa mostra um comportamento exponencial dominante com o tamanho. O estado fundamental extrapolado é duplamente degenerado, *e* apresenta ordem de longo alcance com componentes dominantes do tipo Néel.

Flutuações quânticas tornam-se mais importantes à medida que a anisotropia é reduzida, levando a um estado fundamental singleto desordenado para o sistema infinito no ponto isotrópico.