The phase diagram of the anisotropic
Spin-1 Heisenberg Chain

A. L. Malvezzi and F. C. Alcaraz
Departamento de Física
Universidade Federal de São Carlos
13565-905, São Carlos, SP, Brasil

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In 1983, Haldane conjectured that the isotropic antiferromagnetic spin-S Heisenberg chain has a gap or not depending if the spin is an integer or half-integer\cite{Haldane1}. This conjecture is today well established \cite{Haldane2, Haldane3}. In the case where an exchange z-anisotropy is present the situation is less clear and the location of the point where the massive Haldane phase appears is still controversial even for the spin 1 case. The Hamiltonian in this last case is the spin-1 XXZ chain

$$\mathcal{H} = \sum_{j=1}^{L} \left( S^x_j S^x_{j+1} + S^y_j S^y_{j+1} + \lambda S^z_j S^z_{j+1} \right)$$ \quad (1)

where $S^x_j$, $S^y_j$ and $S^z_j$ are the spin 1 operators.

From finite-size studies (for lattices sizes up to $L = 14$) and by exploring the results of conformal invariance\cite{Alcaraz1} Alcaraz and Moreo\cite{Alcaraz2} conjectured that for $\lambda < \lambda_c = 0$ the Hamiltonian (1) is in a massless X-Y phase with critical fluctuations governed by a conformal field theory with central charge $c = 1$. Moreover in the critical phase ($-1 \leq \lambda \leq 0$) the dimensions of operators $x^{(b)}_{n,m}$, $x^{(s)}_{n}$ governing the correlation functions in the bulk and in the surface are given by\cite{Alcaraz2}

$$x^{(b)}_{n,m} = n^2 x_p + \frac{m^2}{4x_p}, \quad x^{(s)}_{n} = 2x_p n^2$$ \quad (2)

where

$$x_p = \frac{\pi - \cos^{-1}(\lambda)}{4\pi}, \quad n, m = 0, \pm 1, \pm 2, \ldots$$ \quad (3)

The Haldane phase is expected to appear when the operator $x^{(b)}_{0,1} = \frac{1}{4x_p} = \frac{\pi}{\pi - \cos^{-1}(\lambda)}$ becomes relevant, which according to eqs. (2) and (3) occurs at $\lambda = \lambda_c = 0$. This fact explains\cite{Alcaraz2} some exact degeneracies appearing in the spectra of (1) with free ends and is corroborated by the results of ref. \cite{Alcaraz3}.

More recently Yajima and Takahashi\cite{Yajima1} by calculating the spectra of (1) for lattice sizes up to $L = 16$ concluded that the Haldane phase should starts at $\lambda = \lambda_c = 0.068 \pm 0.003$. Since this result destroy the conjecture (2) we decide to make a more precise calculation of $\lambda_c$ by using the density matrix renormalization group (DMRG) introduced by White\cite{White1}, which enable us to make spectral calculations in much larger lattice sizes. The direct way to estimate $\lambda_c$ would be by a direct mass gap evaluation of (1) in a periodic chain. However our results shows that for $\lambda \approx 0$ the finite-size gaps are very small (the transition at $\lambda_c$ should be of Kosterlitz-Thouless type) and it is
very difficult to decide if the point $\lambda = 0.065$ (the worse estimative against the conjecture (2)) is in a massive phase or not. Another way to estimate $\lambda_c$ is by calculating the exponents $\eta_z$, governing the correlation $\langle S^z_i S^z_{i+r}(r) \rangle \sim r^{-\eta_z}$. The critical phase disappears when $\eta_z$ reaches the value $2 \eta^{(b)}_{1,0} = 1/4$ or the surface exponent $x^{(s)}_1$ reaches the value $1/4$.

Since the DMRG is much more precise for spectral calculations in open chains we calculate $x^{(s)}_1$ in order to estimate $\lambda_c$. This is done by using the finite-size relations coming from the conformal invariance of the infinite system [4]. The exponent $x^{(s)}_{(1)}$ is obtained by extrapolating ($L \to \infty$) the sequence

$$x^{(s)}_1(L) = \frac{E^1_n(\lambda, L) - E^0_n(\lambda, L)}{E^0_2(\lambda, L) - E^0_1(\lambda, L)}, \quad (4)$$

where $E^n_j(\lambda, L)$ is the $j^{th}$ energy in the sector where $\sum S^z_i = n$ of the Hamiltonian ($\mathbb{H}$) with free ends.

In table 1 we show for the special cases $\lambda = 0$ and $\lambda = 0.065$ the estimated values for $x^{(s)}_1(L)$ for lattices up to $L = 48$. In our DMRG calculations we keep $k = 50$ and $80$ states in the truncated Hilbert space [8]. A good estimator for the errors is $1 - P_k$, where $P_k$ is the trace of the truncated density matrix. The values in table 1 were obtained by taking $P_k \to 1$.

At $\lambda = \lambda_c$, the operator $x^{(b)}_{0,1}$, which corrects the finite size scaling [4], should be marginal and logarithmic corrections in the sequence (4) are expected. In fig. 1 we show the data of table 1, at $\lambda = 0$, together with a mean square fit in the form

$$x^{(s)}_1(L) = \frac{1}{4} + a (\ln L)^b, \quad (5)$$

showing a good numerical fit. A similar polynomial fit, which would be the case if $\lambda_c > 0$, although possible shows larger deviations. On the other hand the data of table 1 at $\lambda = 0.065$ are not well fitted by (5). As we can see from table 1 the data at $\lambda = 0.065$ clear indicate a limiting value $x^{(s)}_1(\infty)$ bigger than $1/4$. In order to see this more clearly we calculated at $\lambda = 0.065$ this estimator for $L = 60$ sites and obtain $x^{(s)}_1(60) = 0.25023$, which indicates that $\lambda = 0.065$ is already a point in the Haldane phase.

In conclusion, our results indicate that, in agreement with the conjecture (2), the Haldane phase appears for $\lambda > \lambda_c = 0$, and the logarithmic corrections appearing at this point explains the numerical controversial in earlier numerical calculations.
Acknowledgments

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Figure Caption

Fig. 1 - The data of table 1 together with the mean square fit (continuum curve).

Table Caption

Table 1 - Finite size estimatives of $x_1^*$, obtained from eqs. (4) for $\lambda = 0$ and $\lambda = 0.065$. 

Table 1

| $L$ | $\lambda = 0.0$      | $\lambda = 0.065$   |
|-----|----------------------|----------------------|
| 8   | 0.236462774          | 0.246639580          |
| 16  | 0.237501420          | 0.247661670          |
| 24  | 0.237964476          | 0.248398065          |
| 32  | 0.238271248          | 0.248954979          |
| 40  | 0.238500913          | 0.249401545          |
| 48  | 0.238685182          | 0.249774106          |