Reply to "Comment on 'Ground-state properties of a spin-1 antiferromagnetic chain' "

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We contrast, on the same figure, our phenomenological renormalization-group results on the $S=1$ Heisenberg-Ising antiferromagnetic chain with results that we have recently obtained for $S=\frac{1}{2}$ and $S=\frac{3}{2}$. The different behaviors of integer- and half-integer-spin chains are revealed very clearly. This confirms the conclusion of our Communication.

We really thank Bonner and Müller for their comment on the Communication "Ground-state properties of a spin-1 antiferromagnetic chain" by two of us (R.B. and R.J.).[1] They give us the opportunity, by replying to their remarks, to present here clear numerical evidence for the different behavior of integer- and half-integer-spin antiferromagnetic (AF) Heisenberg-Ising chains.

Bonner and Müller focus their criticisms on our extrapolation to $N\rightarrow\infty$ of $\lambda_c(N,N+2)$, the location of the crossings of the successive scaled gaps $NG_N(\lambda)$ between the two lowest states for $\lambda>1$. In our Communication we conclude that a transition occurs at a given λ_c different from $\lambda=1$ in the infinite N spin-1 chain. They argue that the same kind of extrapolation done in the spin-$\frac{1}{2}$ case yields also a transition at a given λ_c different than $\lambda=1$, while it is known that λ_c is rigorously equal to 1 in that case. To make the comparison between their analysis and our analysis more transparent and to let the reader judge for himself, we would like to present both results on the same figure. For that purpose we have performed a new series of calculations more complete and more precise than before. We have calculated $G_N(\lambda)$ for $S=\frac{1}{2}$, 1, and $\frac{3}{2}$, respectively, up to $N=16,12,10$ (our calculation for $S=\frac{1}{2}$ adds two points to the results by Bonner and Müller). Details of the present calculation have been reported recently.[2] Let us present here in Fig. 1 the results for $\lambda_c(N,N+2)$ just to clarify the point of controversy. We have dropped the trivial point corresponding to $N=2,4$ which does not depend on S $[\lambda_c(2,4)=1]$. Moreover, we have voluntarily not drawn any straight line going through more than two successive points. In the light of these results, we must say that the behavior of $\lambda_c(N,N+2)$ when N increases is drastically different for $S=\frac{1}{2}$ and $\frac{3}{2}$ than for $S=1$: while the points are decreasing for $S=\frac{1}{2}$ and $\frac{3}{2}$ they are increasing for $S=1$, up to the largest size for which we have been able to perform the calculation. Moreover, while the curvature is negative for $S=\frac{1}{2}$, and $S=\frac{3}{2}$, it is positive for $S=1$ (at least for $N>4$). We completely agree with Bonner and Müller that any extrapolation to $N\rightarrow\infty$ must be done carefully. However, we still believe that, while the points for $S=\frac{1}{2}$ seem to converge nicely to the exact value $\lambda_c=1$, the points for $S=1$ seem to converge to a value definitively larger than 1. The positive curvature that we observe here in our more precise results yields an extrapolated value, $\lambda_c\approx 1.22$,[3] even larger than the one reported in our paper. Obviously, we cannot exclude *a priori* that there could be some downturn in the $S=1$ curve for a characteristic size $N=N^*$ with $N^*\approx 20$ or 30 as Bonner and Müller suggested. This possibility, which already would have been very strange, when the $S=\frac{3}{2}$ results were not yet known, becomes even more doubtful now when looking at the $S=\frac{3}{2}$ results. How would one explain that N^* is so large for integer spins while it stays small for half-integer spins? With this type argument, any kind of finite-size scaling results could be invalidated!

Several other points have been raised by the authors of the Comment. One point concerns the location of the XY phase boundary, λ_{c_1}. Numerically, we found $\lambda_{c_1}\lesssim 0.1$ and we must say that the conclusion $\lambda_{c_1}=0$ was only a *suggestion* in our Communication. This conclusion is in apparent contradiction with the fact that an essential singularity occurs at $D=D_c\neq 0$ when a single ion anisotropy $\sum_i DS_i^{z^2}$ is added to the XY part $(\lambda=0)$.[4] This causes some problems when drawing the complete phase diagram in the (λ,D) plane, as it has been extensively discussed in a recent publication.[5] Another point concerns the possibility that at $\lambda=\lambda_{c_2}$, only one isolated excited state would join the

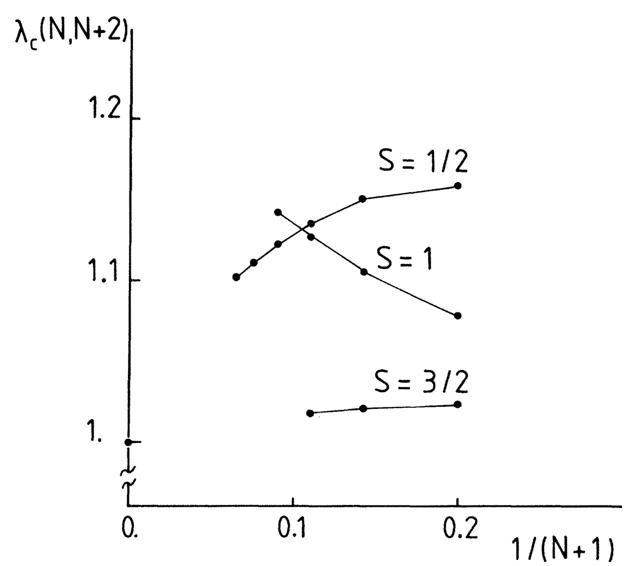

FIG. 1. Plot of $\lambda_c(N,N+2)$ vs $1/(N+1)$ for $S=\frac{1}{2}$, 1, $\frac{3}{2}$.

ground state, instead of a whole continuum of states. In that hypothesis, the correlation function would not show a power-law behavior at $\lambda = \lambda_{c_2}$ as we stated. We agree that we did not answer this point in (1) since only the behavior of the first excited state was reported. We have recently computed other excited states.[2] The next excited state goes through a minimum at $\lambda = \lambda_{\min}$ and for $S = 1$, $\lambda_{\min} \rightarrow 1.2$ when $N \rightarrow \infty$ (while $\lambda_{\min} \rightarrow 1$ for $S = \frac{1}{2}$) and the second gap at $\lambda_{\min}$ tends to zero.[2] This result shows that the first excited state is certainly not isolated. At last we would like to say that "universality" has no meaning unless it has been demonstrated. To our knowledge, nobody demonstrated that the ground-state properties of *quantum* spin chains would not depend on the size of the spin. Our results tend to show that such kind of universality does not occur in the case studied here.

[1]R. Botet and R. Jullien, Phys. Rev. B 27, 613 (1983).
[2]M. Kolb, R. Botet, and R. Jullien, J. Phys. A 16, L673 (1983).
[3]The error bars which we reported in our Communication ($\lambda_c = 1.18 \pm 0.01$) were slightly too optimistic.
[4]R. Jullien and P. Pfeuty, J. Phys. A 14, 3111 (1981).
[5]R. Botet, R. Jullien, and M. Kolb, Phys. Rev. B 28, 3914 (1983).