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

Daniel C. Mattis
Physics Department, University of Utah, Salt Lake City, Utah 84112
(Received 17 July 1984)

Botet and Jullien [Phys. Rev. B **27**, 613 (1983)] and Botet, Jullien, and Kolb [Phys. Rev. B **28**, 3914 (1983)] performed a finite-size scaling analysis of the spin-1 antiferromagnetic Heisenberg-Ising chain. Their work was criticized by Bonner and Müller [Phys. Rev. B **29**, 5216 (1984)] on the grounds that a similar analysis for spin $\frac{1}{2}$ yields misleading results. In the present work, we show that the plane-rotator version of spin-1 chain has some features similar to that obtained by Botet *et al*, although, unfortunately, our model can be solved analytically only over a restricted set of the parameters, and thus does not unambiguously confirm their results. The need for further studies is emphasized.

There have been a number of solutions of the spin-1 linear chain antiferromagnet, with or without crystal-field anisotropy, and the results to date are confusing.

The latest controversy centers about recent studies by Botet, Jullien, and Kolb.[1] Following upon qualitative suggestions by Haldane,[2] these authors set out to demonstrate "experimentally" by finite-size scaling methods, some of the differences between integer-spin systems and those of half-odd integer spins. Indeed, some of their results *are* truly unusual, and differ from well-known properties[3] of analogous $s=\frac{1}{2}$ spin chains. For example, they find at the isotropic antiferromagnetic ($\lambda=1$) point that the excitation spectrum has a finite gap. This energy gap disappears when the anisotropy parameter $D\lesssim-\frac{1}{4}$, or at $D=1$ precisely. A number of other properties also appear unusual, and undoubtedly motivated Bonner and Müller[4] to reexamine the method of calculation.

In their Comment on the work of Botet, Jullien, and Kolb, Bonner and Müller[4] stated that their application of the same finite-size scaling techniques to the $s=\frac{1}{2}$ chain also led to unusual, and incorrect, results and therefore the method should be considered suspect, for short chains at least. In their reply, Botet, Jullien, and Kolb[5] (BJK) indicated that the convergence of integer-spin chains might differ from that of half-odd–integer-spin chains, and showed some similarities between $s=\frac{1}{2}$ and $s=\frac{3}{2}$, as distinguished from $s=1$. At the present time, the situation may be said to be unsettled with respect to these questions.

In the present Comment, we introduce a modified, plane-rotator-like model of integer spin. This we can solve approximately, but analytically on the parameter lines $D=\lambda\geqslant0$, and also $\lambda=0$, $0<D$. Other values of D,λ cannot be examined simply by our methods, although they might be amenable to more sophisticated analyses. Our conclusions are that an energy gap does exist for $D=\lambda>2$, and for $\lambda=0$, $D>1$. For $D=\lambda\leqslant2$, and for $\lambda=0$, $0<D\leqslant1$, the energy gap vanishes and the correlations decay algebraically. The line $D=\lambda$ appears to be special; there, decoupling of the chain into two interpenetrating, but noninteracting, chains occurs. It would certainly be interesting to see whether this also appears in the model studied by BJK.

Consider the spin-1 Hamiltonian on the linear chain $1\leqslant n\leqslant N$,

$$H=\sum_n[S_n^xS_{n+1}^x+S_n^yS_{n+1}^y+\lambda S_n^zS_{n+1}^z+D(S_n^z)^2]$$
$$=\sum_n[\tfrac{1}{2}(S_n^+S_{N+1}^-+\text{H.c.})+\lambda S_n^zS_{n+1}^z+D(S_n^z)^2]\ , \qquad (1)$$

where $S_n^z=-1,0,1$ and the matrix elements of $S^{\pm}$ include $\sqrt{2}$. If D is sufficiently large, we can enlarge the Hilbert space to include higher integer values of S_n^z without appreciably affecting the results, provided the matrix elements connecting to the unphysical states, arising from $S^{\pm}$, are not too big. Suppose we introduce the continuous angular variables θ_n, and replace

$$\frac{1}{\sqrt{2}}S_n^+\text{ by }e^{i\theta_n},\quad \frac{1}{\sqrt{2}}S_n^-\text{ by }e^{-i\theta_n}\ . \qquad (2a)$$

Then the conjugate variables p_n must be the (discrete) operators

$$\frac{1}{i}\frac{\partial}{\partial\theta_n}\equiv p_n=0,\ \pm1,\ \ldots \qquad (2b)$$

replacing S_n^z. We have thus motivated our modified spin-1 model. It is *defined* by the following Hamiltonian:

$$H=\sum_n^N[2\cos(\theta_n-\theta_{n+1})+\lambda p_np_{n+1}+Dp_n^2]\ . \qquad (3)$$

We now perform a duality transformation

$$\theta_{n+1}-\theta_n\to\frac{1}{i}\frac{\partial}{\partial x_{n+1}},\quad p_{n+1}\to x_{n+1}-x_n\ . \qquad (4)$$

The x_n's are discrete (integers). On the line $D=\lambda$, (3) now simplifies to the following:

$$H=\sum_n^N(e^{\partial/\partial x_n}+e^{-\partial/\partial x_n})+\tfrac{1}{2}D\sum_n^N(x_{n+1}-x_{n-1})^2$$
$$=\sum_{m=1}^{N/2}(e^{\partial/\partial x_{2m}}+e^{-\partial/\partial x_{2m}})+\tfrac{1}{2}D\sum_{m=1}^{N/2}(x_{2m}-x_{2m-2})^2+\sum_{m=1}^{N/2}(e^{\partial/\partial x_{2m+1}}+e^{-\partial/\partial x_{2m+1}})+\tfrac{1}{2}D\sum_{m=1}^{N/2}(x_{2m+1}-x_{2m-1})^2\ . \qquad (5)$$

The Hamiltonian has separated into two interlacing parts: that on the even-numbered "particles" and that on the odd-numbered ones. We can treat either one of them, or the case $\lambda=0$, $D>0$ by the same method that we now illustrate.

We concentrate first on the coefficient of D. Replacing x_{2m} by $(x_{2m}-2m)$, we find $x_{2m}-x_{2m-2}$ is replaced by

$$\Delta x_m \equiv (x_{2m}-x_{2m-2}-2) \ . \tag{6}$$

Next, defining u_m by

$$\Delta x_m^2 \equiv u_m + \Delta x_m \ , \tag{7}$$

we obtain

$$\tfrac{1}{2}D \sum_m^{N/2} \Delta x_m^2 = \tfrac{1}{2}D \sum_m^{N/2} u_m + (x_N - x_2 - N) \ . \tag{8}$$

We make the term in parentheses vanish in the thermodynamic limit by requiring $\langle \Delta x_m - 2\rangle = 0$, i.e., by *requiring* that the density of even-subscripted particles be exactly $\frac{1}{2}$. This becomes a strict requirement if we realize that u_m is "large" at $\Delta x_m \le 0$ $[u_m(0)=6]$, and thus only $\Delta x_m = 1$ $[u_m(1)=2]$, $\Delta x_m = 2$ $[u_m(2)=0]$, and $\Delta x_m = 3$ $[u_m(3)=0]$ can have significant amplitudes in the state vectors, assuming the potentials at $\Delta x_m \le 0$ are replaced by a "hard wall" boundary condition. (We have already discussed this procedure elsewhere[6] in connection with the solution of the transfer matrix in the plane-rotator model, and the conjugate problems of surface roughening.) The hard wall and the density $\frac{1}{2}$ suggest that a replacement of the even-subscripted Hamiltonian by a spin-$\frac{1}{2}$ linear antiferromagnet would be advantageous. In terms of spin-$\frac{1}{2}$ operators $\sigma_m^{\pm}$ and σ_m^z,

$$\tfrac{1}{2}Du_m \leftrightarrow D[\sigma_m^z \sigma_{m-1}^z + \tfrac{1}{4}]$$

and

$$\exp(\partial/\partial x_m) \leftrightarrow \sigma_m^+ \sigma_{m-1}^- \ . \tag{9}$$

Thus,

$$H_{\text{even}} = 2 \sum_m [\tfrac{1}{2}(\sigma_m^+ \sigma_{m-1}^- + \text{H.c.}) + \tfrac{1}{2}D(\sigma_m^z \sigma_{m-1}^z + \tfrac{1}{4})] \ . \tag{10}$$

The properties of this $s=\frac{1}{2}$ chain are known.[3,4] In particular, the critical point is at $D_c = 2$, corresponding to an essential singularity. For $D \le 2$ the spectrum is gapless. For $D>2$ an energy gap given by $\Delta \approx A \exp(-B/\sqrt{D-2})$ opens up, with A,B being known constants, a law also satisfied in the Kosterlitz-Thouless model where the $S=1$ model also plays an interesting role.[6]

The odd-numbered subchain yields identical results; thus, the system breaks up into two interpenetrating, identical, noninteracting $s=\frac{1}{2}$ chains on the $\lambda = D$ line.

On the $\lambda=0$ line, the reduction of (3) leads to just one Hamiltonian, identical to what we have already studied, with, however, D replacing $\frac{1}{2}D$. Thus, for $\lambda=0$ we find $D_c = 1$.

We are unable to solve the model when $D=0$, and so cannot confirm that $\lambda_c = 1$ in that case, at the isotropy point of Eq. (1). The reason is not merely technical—it seems that (3) does not have a finite ground state when $D=0$, without a formal cutoff on the $|p_n|$'s being imposed additionally.

Because our model, Eq. (3), differs in some essentials from the original, Eq. (1), it should not be surprising if the numerical value of some critical constants differs. The feature—the decoupling of the spectrum into two disjoint spectra on the line $D=\lambda$—may be a feature of both, however, and may indicate a singular line in the phase diagram. The search for such a "trajectory" would be a worthwhile numerical goal, in our estimation.

This work was supported through Grant No. DMR 81-06223 of the National Science Foundation. I am grateful to S. Rudin for bringing the details of this controversy to my attention.

[1]R. Botet, R. Jullien, and M. Kolb, Phys. Rev. B **28**, 3914 (1983); R. Botet and R. Jullien, *ibid.* **27**, 613 (1983).
[2]F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).
[3]See, e.g., J. D. Johnson, S. Krinsky, and B. M. McCoy, Phys. Rev. A **8**, 2526 (1973).
[4]J. C. Bonner and G. Müller, Phys. Rev. B **29**, 5216 (1984).
[5]R. Botet, R. Jullien, and M. Kolb, Phys. Rev. B **29**, 5222 (1984).
[6]D. C. Mattis, Phys. Lett. **104A**, 357 (1984).