Comment on "Ground-State Energy of Heisenberg Antiferromagnet for Spins $s=\frac{1}{2}$ and $s=1$ in $d=1$ and 2 Dimensions"

In a recent Letter, Mattis and Pan[1] used a real-space renormalization-group (RSRG) technique to estimate the ground-state energy of Heisenberg antiferromagnets of spin $\frac{1}{2}$ and 1 in both one and two dimensions. In this Comment, I point out an error in their calculations for the case of spin $\frac{1}{2}$ on a square lattice. This error invalidates their proof of antiferromagnetic long-range order for this case.

The first-order[2] RSRG that Mattis and Pan used provides a strict variational upper bound e_+ to the ground-state energy e_0. Unfortunately, this bound is usually quite loose (for example, the bound is more than 10% too high for the one-dimensional spin-$\frac{1}{2}$ Heisenberg model using 3-spin clusters.) One would expect that in the two-dimensional case, surface effects would be larger than in one dimension and that the bound would be even looser, so Mattis and Pan's extremely tight upper bound of $e_+ = -0.67228$ is very surprising, as they point out.

I had independently performed the same calculation[3] that Mattis and Pan describe on 3×3 clusters and arrived at different results. To reconfirm my calculation, I used two independent and well-tested computer programs. My results, using Mattis and Pan's notation and units, are $E_0(3) = -4.7493273$, $\Lambda^2 = 0.5067635$, and $e_+ = -0.5591886$. This upper bound is quite loose, as expected. Note that $\Lambda^2 < 1$, so Mattis and Pan's proof of long-range order is invalidated.

It should be recalled that a similar calculation has been performed on the spin-$\frac{1}{2}$ Heisenberg model on the triangular lattice using 7-spin clusters.[4] There, the RSRG again provides the strict, but loose, upper bound of $e_+ = -0.45506$ J, which should be compared with the more recent bound of $e_+ \approx -0.5367$ J found by Huse and Elser.[5]

RSRG calculations can provide significantly more accurate estimates when the calculation is taken to higher order in a perturbation expansion which uses the interblock interaction as a perturbation parameter.[2] The calculations can also be improved by retaining more levels at each truncation of the basis. I will report at more length on improved RSRG calculations for quantum antiferromagnets in the future.[6]

I thank Professor P. W. Anderson for his continuing advice and support. I acknowledge the financial support of AT&T Bell Laboratories. I thank D. A. Huse and V. Elser for many useful conversations, and the theory department at Murray Hill for their hospitality.

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Received 29 July 1988
PACS numbers: 75.10.Jm

[1]D. C. Mattis and C. Y. Pan, Phys. Rev. Lett. **61**, 463 (1988).

[2]See H. P. van de Braak *et al.*, Physica (Amsterdam) **87A**, 354 (1977), and J. E. Hirsch and G. F. Mazenko, Phys. Rev. B **19**, 2656 (1979), for explanations of higher-order RSRG calculations.

[3]A very clear introduction to quantum RSRG calculations, applied to Heisenberg-Ising chains, is given by J. M. Rabin, Phys. Rev. B **21**, 2027 (1980).

[4]H. P. van de Braak, W. J. Caspers, and M. W. M. Willemse, Phys. Lett. **67A**, 147 (1978).

[5]D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).

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