

Mattis and Pan Reply: After several independent calculations failed to confirm our published¹ numbers on the ground-state energy of the $s = \frac{1}{2}$ antiferromagnet in two dimensions, we checked our computer programs and found some deplorable errors introduced in proceeding from one dimension to two. The new numbers for $s = \frac{1}{2}$ are the following: $E_0(3) = -4.7493273$, $\lambda_1^2 = (0.4582)^2 = 0.2100$, and $\lambda_2^2 = (-0.2946)^2 = 0.0868$ resulting in $e_0 = 0.5592$, a much less satisfactory ground-state energy per spin than before, and $\Lambda^2 = 0.51$. (These numbers correct the first line of Table I in our paper which now agrees with the calculation of Yedidia as presented in his preceding Comment,² and with the identical results of von der Linden.³) This value of $\Lambda^2 < 1$ fails indeed to prove long-range order (LRO) for $s = \frac{1}{2}$, which becomes once again an open question.

Our calculation for $s = 1$ was not subject to this unfortunate programming error, and so the numbers for $s = 1$ quoted in the table stand intact. Nevertheless, we missed an obvious feature which Lin⁴ kindly pointed out to us (too late, unfortunately, to include in the published manuscript), and which the readers will wish to note, viz., for $s = 1$ the total renormalization-group energy per site, $e_0 = -1.907$, is not as good as that of the far simpler Ising-Néel state, $e_0 = -2.0$, a state which, incidentally, exhibits perfect LRO! We recall that real-space renormalization group was unable to prove this, although the calculated $\Lambda^2 = 0.9136$ came to within 10% of doing so.

Thus, far from yielding fortuitously excellent results as we believed, the real-space renormalization-group method which we used in our paper seems to converge as slowly in two dimensions as it did in one, and the conclusions which can be derived from 3×3 clusters are totally inadequate. This is unfortunate, as the calculation of Λ for clusters of the next allowed size, 5×5 , is just at the threshold of possibility, and for 7×7 , outside the realm of possibility with present-day computing technology.⁵ However, it remains interesting, and important, to determine whether LRO exists.

Following the discovery and correction of our programming error, we extended the $s = \frac{1}{2}$ calculation to the anisotropic Heisenberg antiferromagnet. If $J_x = J_y = 1$ and $J_z \geq 1$, then evidently $\Lambda_z \geq \Lambda_x = \Lambda_y$. If J_z is

sufficiently large, the transverse interactions are minor perturbations on an Ising-Néel antiferromagnet, and ground-state LRO necessarily sets in [as manifested by $\Lambda_z^2(J_z) \geq 1$ at large J_z]. Also, $\Lambda_z^2(J_z) < 1$ in the "x-y" phase, $J_z < 1$. Thus, if there is no LRO at the isotropy point $J_z = 1$, $\Lambda_z^2(J_z)$ must be discontinuous there [i.e., $\Lambda_z^2(1+\delta) \neq \Lambda_z^2(1-\delta)$ for $\delta \rightarrow 0$]. Conversely, if $\Lambda_z^2(J_z) = 1$ and $d[\Lambda_z^2(J_z)]/dJ_z < \infty$ at $J_z = 1$, we can safely infer the existence of LRO at the isotropy point.

Our new calculations for 3×3 clusters show $\Lambda_z^2(J_z) \geq 1$ for $J_z \geq 1.23$. We have extended this calculation to 5×5 clusters using a variational approach. The resulting threshold for LRO drops, and it is now $J_z \geq 1.13$. The curves show no hint of discontinuity over a wide range of J_z . Although these preliminary results are inconclusive, we are hopeful that the question of LRO in the isotropic antiferromagnet can ultimately be settled in this manner, and are therefore proceeding with a rigorous calculation for the 5×5 , and ultimately, when data storage problems are resolved, for the 7×7 clusters.

The authors are grateful to Dr. H.-Q. Lin for verifying some of his results, and for helpful comments.

Daniel C. Mattis

Physics Department
University of Utah
Salt Lake City, Utah 84112

C. Y. Pan

Physics Department
Utah State University
Logan, Utah 84322

Received 12 September 1988

PACS numbers: 75.10.Jm

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

²J. S. Yedidia, preceding Comment [Phys. Rev. Lett. **61**, 2278 (1988)].

³Wolfgang von der Linden, private communication.

⁴H.-Q. Lin, private communication.

⁵It should be noted that calculation of Λ requires more knowledge of the ground-state correlations than is obtained from conventional Monte Carlo calculations.