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Low temperature magnetization and the excitation spectrum of antiferromagnetic quantum Heisenberg rings LARRY ENGELHARDT, MARSHALL LUBAN, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011 — We have performed quantum Monte Carlo calculations to obtain the low temperature magnetization and differential susceptibility for finite, antiferromagnetic Heisenberg rings of intrinsic spins $s = 1/2, 1, 3/2, 2, 5/2, 3, 7/2$. From these data we have determined the level-crossing fields as well as the dependence of the minimal excitation energies on the total spin quantum number S. For large intrinsic spins ($s \geq 3/2$) we find that the data exhibit scaling behavior, approaching the classical limit proportional to $s^{-1.05}$. Since this limit is approached so slowly, even $s = 7/2$ spins are distinctly non-classical. We have also found for large s that as the number of spins N increases, the energy gap between the ground state and the first excited state approaches zero proportional to $1/N^{\alpha}$, where $\alpha \approx 0.76$ for $s = 3/2$ and $\alpha \approx 0.84$ for $s = 5/2$. Finally, we demonstrate the usefulness of our results by examining the Fe_{12} molecular ring, leading to a new, more accurate estimate of the exchange constant for this system than has been obtained heretofore.

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