Comment on "Anomalous Spin Diffusion in Classical Heisenberg Magnets"

The time-dependent spin-autocorrelation function and the energy-energy correlation function at $k_B T = \infty$ for classical magnets are expected to show diffusive behavior characterized by power-law long-time tails of the form $t^{-\alpha}$, where $\alpha = d/2$ and d is the dimensionality of the lattice. In a recent Letter,[1] Müller reported the results of spin-dynamics computer simulations and concluded that the spin relaxation was diffusive, but with an exponent α in the long-time tail that was slightly greater than $d/2$ for $d=2,3$, and substantially larger, and $\alpha = 0.609 \pm 0.005$ for $d=1$. This exponent implies special behavior of the q-dependent correlation function in the limit that $q \to 0$, such as the occurrence of confluent singularities in their Laplace transforms, and is thus important to the general theoretical understanding of spin diffusion.

In this Comment we report new spin-dynamics simulations carried out to much longer times than those reported in Ref. 1. We used a fourth-order predictor-corrector method,[2] vectorized for the Cyber 205, to study chains of length $L = 20000$ for times out to $200J^{-1}$ (where J is the nearest-neighbor coupling constant) with a time increment $\Delta t = 0.005J^{-1}$. (The simulations in Ref. 1 were limited to times $t \le 40J^{-1}$.) Data for 400 such chains were averaged together before the time dependence was analyzed. For times up to $Jt \approx 40$ our data are consistent with those from Ref. 1; however, they show that the asymptotic time dependence is not reached until well beyond the longest time studied in Ref. 1. In Fig. 1 we plot both the autocorrelation and energy-energy correlation functions versus time. For short times, pronounced oscillations can be seen, but by $t = 10J^{-1}$ these have been damped out and the behavior is smooth. The effective power of the decay of the autocorrelation function is initially about 0.6, as observed by Müller, but decreases *very* slowly and approaches a value consistent with $\alpha = \frac{1}{2}$ although a larger value cannot be excluded. The energy-energy correlation qualitatively shows similar behavior but a clear asymptotic region with $\alpha = \frac{1}{2}$ is reached much sooner, i.e., for $t \gtrsim 60J^{-1}$. We do not understand why the nonasymptotic time regimes are so pronounced, particularly for the spin-autocorrelation function and it is clear that a substantial computer effort is needed to study spin diffusion at $T = \infty$.

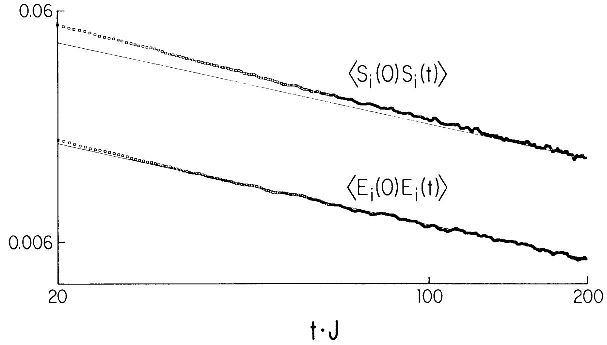

FIG. 1. Log-log plots of the spin-autocorrelation function $\langle \mathbf{S}_i(0)\cdot\mathbf{S}_i(t)\rangle$ (averaged over 400 configurations) and the energy-energy correlation function $\langle E_i(0)E_i(t)\rangle$ averaged over 310 configurations) as functions of time. The solid lines have a slope of $\frac{1}{2}$.

In conclusion, our data show that the determination of the long-time behavior of the spin-autocorrelation function is a subtle and difficult problem to treat computationally. We believe that these data suggest that there is no anomalous spin diffusion in $d=1$, and if this is indeed the case the much smaller discrepancies[1] in $d=2$ and $d=3$ are likely to be due to nonasymptotic behavior as well.

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