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Breakdown of Hydrodynamics in the Classical ID Heisenberg Model

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Extensive spin-dynamics simulations have been performed to study the dynamical behavior of the classical Heisenberg chain at infinite temperatures and long wavelengths. We find that the energy and spin show distinctly different dynamics in the isotropic system. The energy correlation function follows the classical diffusion theory prediction, namely, it decays exponentially with q^2t. In contrast, the spin correlation function is found to decay exponentially as $q^{2.12}t\ln t$, implying a logarithmically divergent diffusion constant and the failure of the usual hydrodynamic assumptions.

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The investigation of the time-dependent behavior of low-dimensional magnetic systems has significantly increased over the past years [1,2]. Theoretically, both analytical tools [3,4] and computer simulations [5–16] have been widely used. In particular, Müller [11] analyzed in some detail the time dependence of the spin autocorrelation function of the classical Heisenberg model for dimensionalities $d=1$, 2, and 3 at infinite temperatures and observed a power-law long-time tail whose exponent deviated from the classical diffusion theory prediction: $\alpha_d=d/2$. For $d=1$ Müller found the largest deviation $\alpha_1\simeq 0.57$. The deviations persisted to a lesser degree for higher dimensions. These findings were strongly challenged by Gerling and Landau [13], who carried out an extensive simulation for the spin autocorrelation function to much longer times and found that the slope of the spin autocorrelation in a log-log plot showed a tendency to decrease for increasing times. They conclude there is no anomalous diffusion in $d=1$ much less in higher dimensions and that the asymptotic behavior for the autocorrelation function is only reached at very long times. Subsequently Jian-Min Liu *et al.* [16] suggested that the computational error in the numerical integration of the equations of motion affects the long-time decay of the autocorrelation causing a crossover from anomalous spin diffusion $(\alpha>\frac{1}{2})$ to classical spin diffusion at some characteristic time that depends on the accuracy of the numerical integration. In the present work we give a much more detailed analysis of this problem by simulating the q-dependent energy and spin correlations as well as the respective current-current correlations. The picture that emerges is that although the energy diffusion shows a classical diffusive behavior, surprisingly, the spin diffusion shows a nonclassical behavior that is manifested in all measured quantities. In particular the asymptotic behavior of the autocorrelation is of the form $C_0(t)\sim(t\ln t)^{-1/2.12}$ (we show later in the paper that this functional form explains the results of [11,16] and those of [13]). There is thus a breakdown of the usual hydrodynamic assumptions as originally suggested by Bloembergen [17] and van Hove [18]. We find no evidence of anomalous behavior in two dimensions.

The system is described by the Hamiltonian

$$H=J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{1}$$

where $\mathbf{S}_i$ are the three-dimensional classical vectors with $|\mathbf{S}_i|=1$. The exchange coupling between neighbors can be either ferromagnetic $(J<0)$ or antiferromagnetic $(J>0)$. The sum $\langle ij\rangle$ is over all nearest-neighbor pairs. The equation of motion for each spin resulting from the Hamiltonian (1) is

$$d\mathbf{S}_i/dt=-J\mathbf{S}_i\times(\mathbf{S}_{i-1}+\mathbf{S}_{i+1})\,. \tag{2}$$

This equation implies that both the total spin $\mathbf{S}=\sum_i\mathbf{S}_i$ and the energy of the system are conserved quantities. The spin-correlation function $C_s(q,t)=\langle\mathbf{S}(q,t)\cdot\mathbf{S}(-q,0)\rangle$ can be shown to satisfy exactly the equation [19]

$$\partial C_s(q,t)/\partial t=-\int_0^t\Phi(q,t-x)C_s(q,x)dx\,, \tag{3}$$

where the memory function $\Phi(q,t)$ [20] is, for small q,

$$\Phi(q,t)=q^2\langle\mathbf{j}_s(q,t)\cdot\mathbf{j}_s(q,0)\rangle/\langle\mathbf{S}(q,0)\cdot\mathbf{S}(-q,0)\rangle\,. \tag{4}$$

$\mathbf{j}_s(q,t)=\sum_j e^{iqR_j}J[\mathbf{S}_j(t)\times\mathbf{S}_{j+1}(t)]$ is the total spin current, which is not conserved. It usually assumed that $\Phi(q,t)$ decays on some microscopic scale $(\sim J^{-1})$ while $C_s(q,t)$ must decay on a time scale that is arbitrarily long as $q\to 0$. In this case for sufficiently small q

$$\partial C_s(q,t)/\partial t=-D_sq^2C_s(q,t)\,, \tag{5}$$

where $D_s=\int_0^\infty\langle\mathbf{j}_s(0,t)\cdot\mathbf{j}_s(0,0)\rangle dt$ is the spin diffusion constant at infinite temperature. As a consequence of Eq. (5) the spin-correlation function $C_s(q,t)$ behaves asymptotically for small q and long times as

$$C_s(q,t)=e^{-D_sq^2t}\,. \tag{6}$$

By Fourier transforming Eq. (6) we find that the spaceand time-displaced correlation function $C_r(t)=\langle \mathbf{S}_i(0) \cdot \mathbf{S}_{i+r}(t)\rangle$ takes the form

$$C_r(t)=\frac{1}{(4\pi D_s t)^{1/2}}e^{-r^2/4\pi D_s t} \tag{7}$$

in the limit of large times. The same discussion applies for the total energy leading to an analog asymptotic behavior for the energy correlation functions.

The computer simulation in this work was performed on a chain with N spins and periodic boundary conditions imposed. A random spin configuration was used as an initial condition for the spin dynamics calculations. The time evolution of coupled nonlinear equations of motion (2) was obtained by using a fourth-order fixed-step Runge-Kutta integration procedure. The sizes of the chains used ranged between 200 and 800 sites. The simulation presented no detectable finite-size effects. The integration step used in the Runge-Kutta integration was $\delta t=10^{-2}/J$. Runs with integration steps 10 times smaller showed no significant difference. For each randomly generated configuration the vector $\mathbf{S}(q,t)=\sum_j e^{iqR_j}\mathbf{S}_j(t)$ was stored as a function of time. The integration was performed up to times of $t=200J^{-1}$. The spin and energy correlations were calculated and averaged over many samples. The number of samples ranged between 2000 and 15000 depending on the lattice size. Since there is no controversy about the nature of diffusion for the energy, we shall mention the main results without presenting the data. The energy-correlation function $C_e(q,t)$ shows a distinct diffusive behavior with an exponential dependence in time. For the autocorrelation function we find the expected power-law decay $(t^{-1/2})$. The energy current-current correlation function does in fact decay to a negligible value in times of order J. In contrast Fig. 1(a) shows that the spin-correlation function does not scale as q^2t. Indeed, we find that the spin current-current correlation function, for $q=0$, has a t^{-1} dependence for large t as seen in Fig. 2, and the integral in Eq. (5) does not converge at all. This suggests, as is verified in Fig. 1(b), that the correct long-time dependence for $C_s(q,t)$ is $t\ln t$. In addition to that the spin-correlation function does not scale with the wave vector as q^2 but as $q^{2.12\pm0.02}$ [Fig. 1(b)] implying a $(t\ln t)^{-1/(2.12\pm0.02)}$ decay for the spin autocorrelation as depicted in Fig. 3. The uncertainty in the exponent was estimated by plotting the data for various exponents as in Fig. 1(b) and observing what values gave a clear violation of the scaling relation. The functional form of the spin autocorrelation found here explains the results of [11,16] and those of [13] thereby eliminating the controversy. The slope of the spin autocorrelation function (in a log-log plot) is given by $-[1+1/\ln(t)]/2.12$ which for $t\sim100$ is -0.57. That is exactly the result $C_0(t)\sim t^{-0.57}$ found in [11,16]. On the other hand, the slope decreases for increasing times confirming the results of [13]. The slope, however, does not reach the value 1/2 predicted in [13] but the value

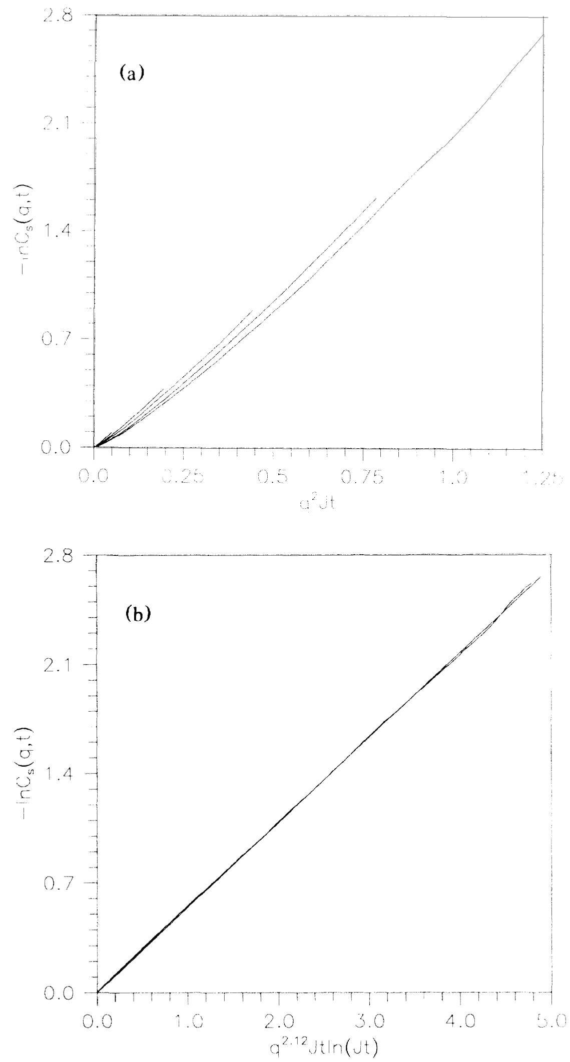

FIG. 1. (a) The logarithm of the spin-correlation function $C_s(q,t)$ for the 1D classical Heisenberg model at infinite temperature plotted against q^2t for various values of q ranging from $\pi/200$ (upper curve) to $5\pi/200$ (lower curve). The lines represent the simulation done in a lattice with 400 spins averaged over 15000 random initial conditions. (b) Same data as in (a) now plotted as a function of $q^{2.12}t\ln t$. The straight line is the fit using $C_s(q,t)=\exp(-0.543q^{2.12}t\ln t)$.

1/2.12. We should also point out that a scaling of the form $C_s(q,t)=\exp[-0.537q^2(1+0.1\ln q)t\ln t]$ fits the data as well as the form shown in Fig. 1(b). The anomalous q dependence is presumably due to a sensitive dependence of the long-time behavior of $\mathbf{j}_s(q,t)$ on q as $q\to0$ although we have not yet investigated this in detail.

Anomalous properties in low-dimensional systems ($d \le 2$) are known to occur in models for incompressible fluids [21]. The result there may be readily understood in terms of mode-coupling theory [22], but that is not the case for the present system, where mode coupling predicts

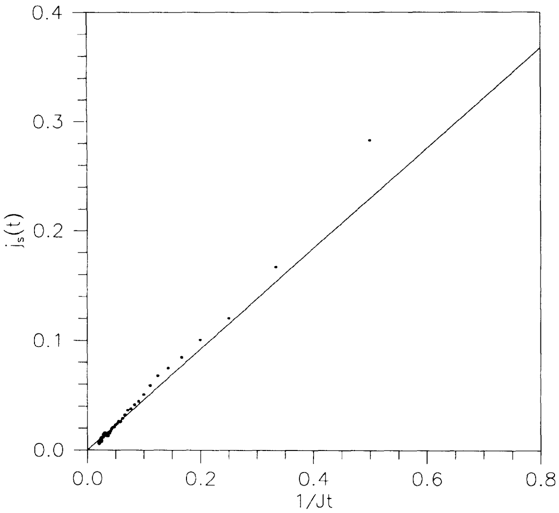

FIG. 2. The spin current-current correlation function plotted against the inverse of time. The slope of the straight line is 0.46. Here we used a lattice with 100 spins and averaged over 160000 random initial conditions.

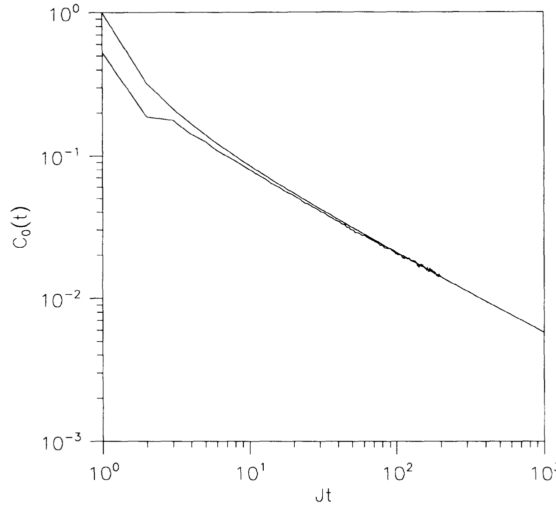

FIG. 3. The autocorrelation function $C_0(t) = \langle \mathbf{S}_i(0) \cdot \mathbf{S}_i(t) \rangle$ vs time. The wiggly line is the simulation result. The continuous line is the autocorrelation obtained by direct integration of the fitted equation given in Fig. 1(b). The simulation was performed as described in Fig. 1(a). The deviation at short times is to be expected since we have used the asymptotic value of $C_s(q,t)$ in calculating $C_0(t)$.

diffusive behavior. Similar computer simulations performed in the dynamical spherical model for infinite temperatures and long wavelengths also show that the spin-correlation function does not follow the expected classical diffusive behavior, although the exponents are different. The leading term in an expansion of $\Phi(q,t)$ in powers of $C_s(q,t)$ for this model is precisely the mode-coupling approximation [23], so that the nonhydrodynamical behavior must arise from vertex corrections. We have also extended the result for finite temperatures, and find that the anomalous long-wavelength dynamics persist, with exponents that vary with temperature in a distinctive way for the ferromagnet and antiferromagnet. The results will be reported elsewhere. The presence of a single-ion interaction of the form $D\sum_i (S_i^z)^2$ in Eq. (1) will break the rotational symmetry of the Hamiltonian. Numerical simulations show that the asymptotic behavior of $C_z(q,t) = \langle S_z(q,t) S_z(-q,0) \rangle$ follows the classical spin diffusion theory so isotropy is essential for the nonhydrodynamical behavior to occur. Physical realization of the phenomena in magnetic systems seems to be present in the 1D $S = \frac{5}{2}$ Heisenberg antiferromagnet TMMC [11], although we have not yet reanalyzed the data with the functional form of $C_s(q,t)$ suggested here.

In conclusion, we have performed extensive numerical simulations of the dynamics of the 1D Heisenberg model. The results show that the nature of diffusion for the energy and spin are very different in the isotropic model. The energy decay follows the classical prediction, namely, the energy-correlation function decays exponentially with $q^2 t$ implying a power-law decay ($t^{-1/2}$) for the energy autocorrelation function. On the other hand, the spin-correlation function decays exponentially with $q^{2.12} t \ln t$ leading to a decay of the form $(t \ln t)^{-1/2.12}$ for the spin autocorrelation function; this is consistent with the fact that the spin current-current correlation function at $q=0$ has a t^{-1} dependence implying a logarithmically divergent diffusion coefficient.

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