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# Time-dependent correlation functions of the classical one-dimensional $XY$ model at infinite temperature*

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Computer calculations of the time-dependent spin and energy correlation functions of the classical one-dimensional $XY$ model at infinite temperature are reported. Plots of $\langle S_z^i S_z^i(t)\rangle$, $\langle S_z^i S_z^{i+1}(t)\rangle$, $\langle \epsilon^i \epsilon^i(t)\rangle$, and $(1/2)[\langle S_x^i S_x^i(t)\rangle + \langle S_y^i S_y^i(t)\rangle]$ out to times $Jt = 9$ are given ($\epsilon^i$ is the energy-density operator and $\hbar J$ is the exchange integral). Comparison is made with the exact results for the spin-1/2 $XY$ model. After an appropriate scaling of the exchange integral and normalization to the classical value at $t = 0$ the values of the spin-1/2 functions are close to the values of their classical counterparts for times up to $Jt \approx 4$.

## I. INTRODUCTION

Among spin systems the one-dimensional $XY$ model with $S = \frac{1}{2}$ falls into a special category in that many of its time-dependent correlation functions can be computed exactly. For $S > \frac{1}{2}$ and, in particular, in the classical limit, exact calculations are not possible and recourse has to be made to analyses based on approximate kinetic equations, moments, etc. The special character of the spin-$\frac{1}{2}$ system is a direct consequence of the fact that its Hamiltonian can be transformed into a Hamiltonian of an assembly of noninteracting fermions.[1,2] The evolution of the correlation functions in time reflects the nondissipative dephasing of the components of the wave packet characterizing the state of the system at $t = 0$. In contrast, the dissipative behavior associated with chains having $S > \frac{1}{2}$ leads to an irreversible dynamics.

In view of the fundamental differences in the behavior of dissipative and nondissipative systems, it is of interest to compare the time development of the correlation functions for $S = \frac{1}{2}$ and $S > \frac{1}{2}$. In this paper we report the results of a study where experimentally determined correlation functions for the classical chain are compared with the corresponding functions for the spin-$\frac{1}{2}$ chain. The experimental results were obtained by integrating the equations of motion of a chain of 4000 spins with initial conditions corresponding to infinite temperature and then computing the correlation functions by direct averaging over the array. Since the analysis is virtually identical to that carried out by Lurie, Huber, and Blume in their study of the dynamics of the classical Heisenberg chain,[3] we will not discuss the numerical work in great detail.

## II. COMPARISON

The Hamiltonian of the $XY$ model takes the form

$$H = \hbar J \sum_i (S_x^i S_x^{i+1} + S_y^i S_y^{i+1}) , \tag{1}$$

where the $S_\alpha^i$ denote components of the spin associated with the $i$th site. We have evaluated the correlation functions $\langle S_z^i S_z^i(t)\rangle$, $\langle S_z^i S_z^{i+1}(t)\rangle$, $\frac{1}{2}[\langle S_x^i S_x^i(t)\rangle + \langle S_y^i S_y^i(t)\rangle]$, and $\langle \epsilon^i \epsilon^i(t)\rangle$, where the angular brackets denote an average at infinite temperature. The symbol $\epsilon^i$ refers to the dimensionless energy-density operator

$$\epsilon^i = \tfrac{1}{2}(S_x^i S_x^{i+1} + S_y^i S_y^{i+1} + S_x^i S_x^{i-1} + S_y^i S_y^{i-1}) . \tag{2}$$

In the numerical studies of the classical chain the $\vec{S}^i$ were taken to be unit vectors and the integration was carried out to times $Jt = 9$. Beyond this point the cumulative effect of the round-off errors in the numerical analysis begins to be significant.

In order to compare the time evolution of the classical and spin-$\frac{1}{2}$ systems, it is convenient to scale the corresponding exchange integrals. This is done by the relation

$$J_{1/2}(\tfrac{1}{2})(\tfrac{1}{2} + 1)^{1/2} = J , \tag{3a}$$

or

$$J_{1/2} = (2/\sqrt{3}) J , \tag{3b}$$

where $\hbar J$ is the exchange integral for the classical chain and $\hbar J_{1/2}$ is the exchange integral for the spin-$\frac{1}{2}$ chain. At infinite temperature such a scaling has the effect of ensuring that the first and second derivatives of the normalized correlation functions $\langle S_\alpha^i S_\alpha^i(t)\rangle / \langle S_\alpha^2\rangle$, evaluated at $t = 0$, have the same value for both systems.

In the infinite temperature limit it is found that[4]

$$\langle S_z^i S_z^{i+n}\rangle = \tfrac{1}{4} J_n^2(J_{1/2} t) \tag{4}$$

for $S = \frac{1}{2}$, where $J_n(x)$ is the Bessel function of the first kind of order $n$. The function $\langle \epsilon^i \epsilon^i(t)\rangle$ can also be computed for this system. At infinite temperature we have[5]

$$\langle \epsilon^i \epsilon^i(t)\rangle = \tfrac{1}{16} [J_0^2(J_{1/2} t) + 2 J_1^2(J_{1/2} t) - J_0(J_{1/2} t) J_2(J_{1/2} t)] . \tag{5}$$

In Figs. 1, 2, and 3 our numerical results for

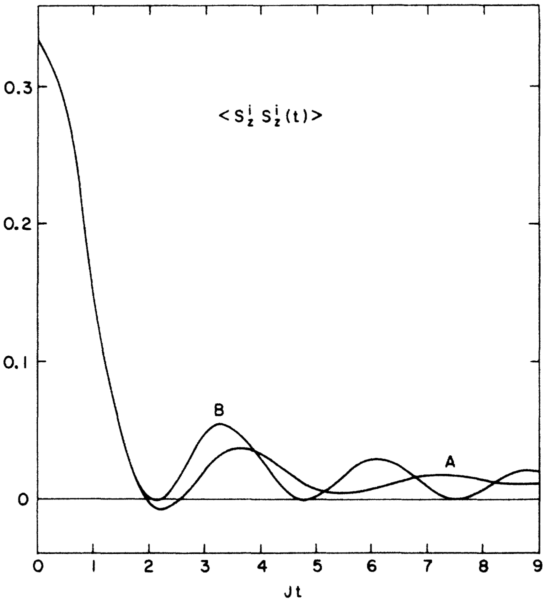

FIG. 1. $\langle S_z^i S_z^i(t)\rangle$. Curve A is the result for the classical chain of unit spins. Curve B is the scaled result for the spin-$\frac{1}{2}$ chain, $\frac{1}{3}J_0^2(2Jt/\sqrt{3})$.

the classical functions $\langle S_z^i S_z^i(t)\rangle$, $\langle S_z^i S_z^{i+1}(t)\rangle$, and $\langle \epsilon^i \epsilon^i(t)\rangle$, are labeled curve *A*. The curves are the average of data from three computer runs each with a different initial configuration. In these figures curve *B* is the corresponding result for the spin-$\frac{1}{2}$ chain with $J_{1/2}=(2/\sqrt{3})J$, normalized to agree with the classical value at $t=0$. In Fig. 4 we have plotted our values for the classical transverse function $\frac{1}{2}[\langle S_x^i S_x^i(t)\rangle + \langle S_y^i S_y^i(t)\rangle]$.

## III. DISCUSSION

Perhaps the most remarkable feature of our results is the striking similarity in the behavior of the correlation functions for the spin-$\frac{1}{2}$ and classical systems. It should be noted that our choice for $J_{1/2}$ and the normalization ensures that curves *A* and *B* will coincide for short times, $Jt \ll 1$. However, the close correspondence out to times $Jt \approx 4$ was unexpected. In particular, in the classical chain, the first minima of $\langle S_z^i S_z^i(t)\rangle$ and $\langle S_z^i S_z^{i+1}(t)\rangle$ fall almost exactly on the minima of the spin-$\frac{1}{2}$ functions. At longer times the minima in the classical functions become less pronounced and are out of phase with the spin-$\frac{1}{2}$ minima.

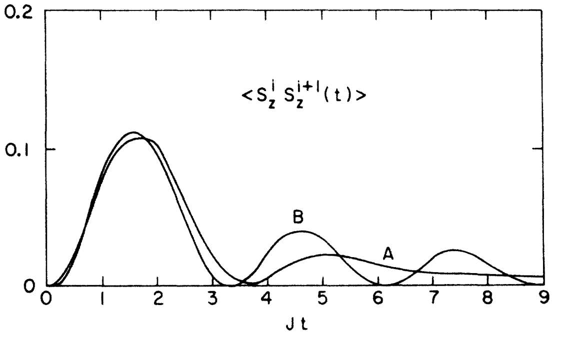

FIG. 2. $\langle S_z^i S_z^{i+1}(t)\rangle$. Curve A is the result for the classical chain of unit spins. Curve B is the scaled result for the spin-$\frac{1}{2}$ chain $\frac{1}{3}J_1^2(2Jt/\sqrt{3})$.

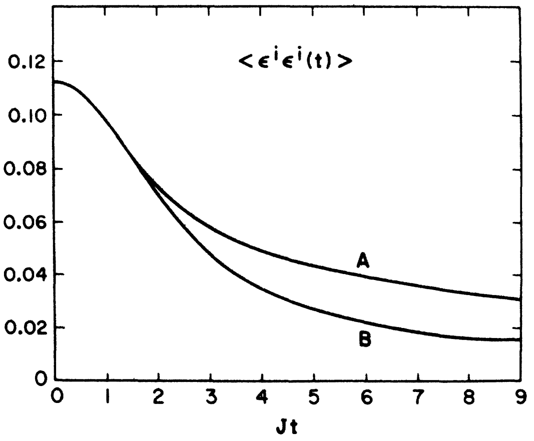

FIG. 3. $\langle \epsilon^i \epsilon^i(t)\rangle$. Curve A is the result for the classical chain of unit spins. Curve B is the scaled result for the spin-$\frac{1}{2}$ chain, $\frac{1}{9}[J_0^2(2Jt/\sqrt{3})+2J_1^2(2Jt/\sqrt{3})-J_0(2Jt/\sqrt{3})J_2(2Jt/\sqrt{3})]$.

In contrast to the longitudinal spin functions, $\langle \epsilon^i \epsilon^i(t)\rangle$ and $\frac{1}{2}[\langle S_x^i S_x^i(t)\rangle + \langle S_y^i S_y^i(t)\rangle]$ do not oscillate but decay smoothly toward zero. The similarity

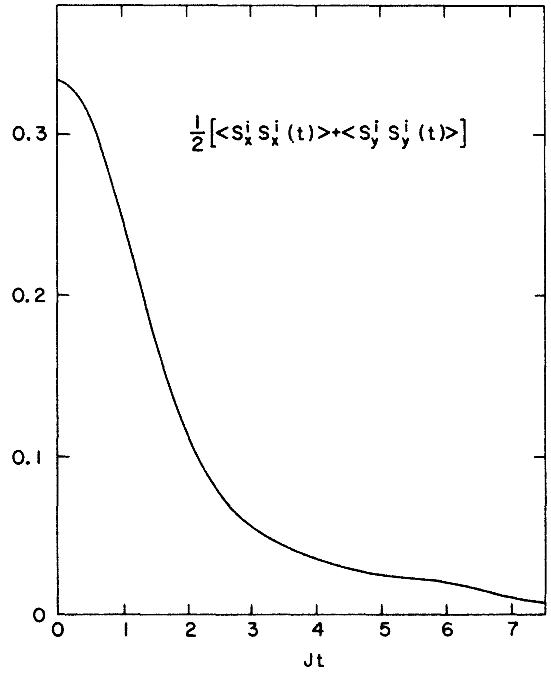

FIG. 4. $\frac{1}{2}[\langle S_x^i S_x^i(t)\rangle + \langle S_y^i S_y^i(t)\rangle]$. Classical chain of unit spins.

between curves $A$ and $B$ in Figs. 1–3 leads us to speculate that the transverse autocorrelation function for the spin-$\frac{1}{2}$ chain will behave similarly to its classical counterpart shown in Fig. 4.

Finally we must emphasize that we anticipate qualitative differences in the behavior of the classical and spin-$\frac{1}{2}$ correlation functions at long times. In the classical system we expect diffusive (i.e., $t^{-1/2}$) decay to dominate the asymptotic behavior of $\langle S_z^i S_z^{i+n}(t)\rangle$ and $\langle \epsilon^i \epsilon^i(t)\rangle$ since the variables $\sum_i S_z^i$ and $\sum_i \epsilon^i$ are constants of the motion. In contrast, the corresponding spin-$\frac{1}{2}$ functions fall off as $t^{-1}$.

*Note added in proof.* Recent calculations by A. Sur (private communication) have indicated that in the infinite-temperature limit $\langle S_x^i S_x^i(t)\rangle$ for the one-dimensional spin-$\frac{1}{2}$ $XY$ model has essentially Gaussian behavior. He has found that the first sixteen moments of the Fourier transform of $\langle S_x^i S_x^i(t)\rangle$ are identical to the corresponding moments of the Fourier transform of $\frac{1}{4}\exp[-\frac{1}{4} \times (J_{1/2}\,t)^2]$.

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[5] This result can be obtained by integration over $k$ and $\omega$ of the function $(a/32\pi)[1+\cos(ka)]\cos(\omega t)F_E(k,\omega)$, where $F_E(k,\omega)$ is given by Huber and Semura [D. L. Huber and J. S. Semura, Phys. Rev. 182, 602 (1969); Ref. 8] and $a$ is the lattice parameter.