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Time-dependent behavior of classical spin chains at infinite temperature

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An ultrafast, vectorized spin-dynamics method is used to study the time-dependent properties of classical XY and Heisenberg spin chains at infinite temperature. The decay of the energy-energy and spin-spin correlation functions is oscillatory for short times and at long times is consistent with classical diffusion, although the approach to the asymptotic behavior is extremely slow. We have also calculated $S(q,\omega)$ and find clear indication of spin-wave peaks in both models.

I. INTRODUCTION

Although the time-dependent behavior of magnetic spin systems has been investigated for several decades, relatively little has been learned about the properties of systems at infinite temperature. There are several important questions to be answered, including the nature of long-time correlations and the difference between classical and quantum behavior.[1,2] Much work in this area has concentrated on understanding the low-temperature properties and had neglected the high-temperature limit. Since many experiments[3] are carried out at relatively high temperature, this problem has more than purely theoretical significance. Time-dependent behavior has been studied theoretically using moment theories.[2] Windsor[4] first simulated Heisenberg spin chains with nearest-neighbor coupling J using a spin-dynamics method, and similar calculations were later made by Lurie, Huber, and Blume.[5] The first investigations of equivalent XY models of which we are aware were by Huber[6] and followed by Thomchick and Landau.[7] All of these simulations were performed over restricted periods of time $t \leq 10J^{-1}$ and for systems of modest size. Interest in this problem was recently rekindled when Müller[8] studied the classical Heisenberg model at infinite temperature using spin-dynamics simulations and concluded that anomalous diffusion was occurring. In this paper we present a reinvestigation of this problem as well as results for the XY model using 2 orders of magnitude more computing effort than used in Ref. 8. Indeed, our study shows that quite long simulations are needed to observe the true long-time properties.[9]

II. MODEL AND METHOD

We have studied spin chains of length $L=20\,000$ with a periodic boundary and with classical three-component spins (unit vectors) at each site. The spins interact with nearest neighbors only with the Hamiltonian

$$\mathcal{H}_H = -J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z) \tag{1}$$

for the Heisenberg model, and

$$\mathcal{H}_{XY} = -J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) \tag{2}$$

for the XY model. Equations of motion for each spin were obtained by evaluating the expression

$$\dot{\mathbf{S}}_i = \mathbf{S}_i \times \nabla_{\mathbf{S}_i} \mathcal{H} \ . \tag{3}$$

We used a vectorized, fourth-order predictor-corrector method on a Cyber 205 to integrate the equations of motion for each spin; the method is explained in more detail elsewhere.[10] Time-displaced, space-displaced correlation functions were determined, and the results for multiple chains were averaged together. Results from as many as 300 chains were averaged to produce the final estimates. The scattering function $S(q,\omega)$ was determined by calculating the space-time Fourier transform of the spin-spin correlation functions $c(r,t)$, where the resolution function factors used were $\delta r = 0.015$ and $\delta t = 0.02J$:

$$S(q,\omega) = \sqrt{2/\pi} \int_0^{t_{\max}} \sum_{r=-r_{\max}}^{r_{\max}} \cos(\omega t)\cos(qr)c(r,t)\exp[-\tfrac{1}{2}(r\,\delta r)^2]\exp[-\tfrac{1}{2}(t\,\delta t)^2]dt \ . \tag{4}$$

This process introduces a certain broadening in the scattering function which is equivalent to resolution broadening in experiments; but it also removes spurious wiggles produced by the "cutoffs" in our data. A review of the tests of the limitations in accuracy of the results is also presented in Ref. 10.

III. RESULTS

A. Heisenberg model

Data for the spin autocorrelation function and energy-energy correlation function are plotted in Fig. 1. In the

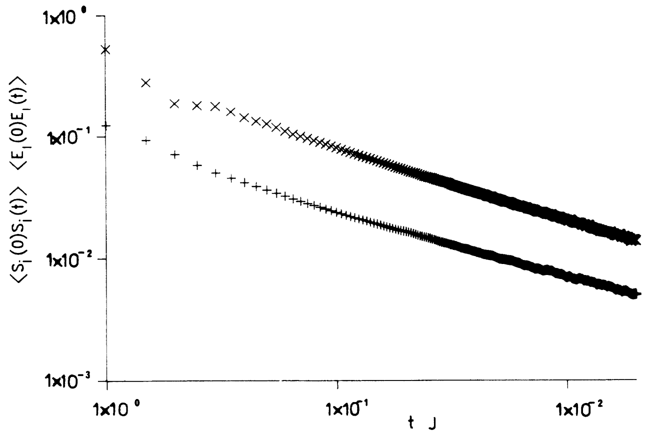

FIG. 1. Time dependence of the spin autocorrelation function (upper curve) and energy-energy correlation function (lower curve) for the classical Heisenberg chain at $T=\infty$. The solid lines have slope $\frac{1}{2}$.

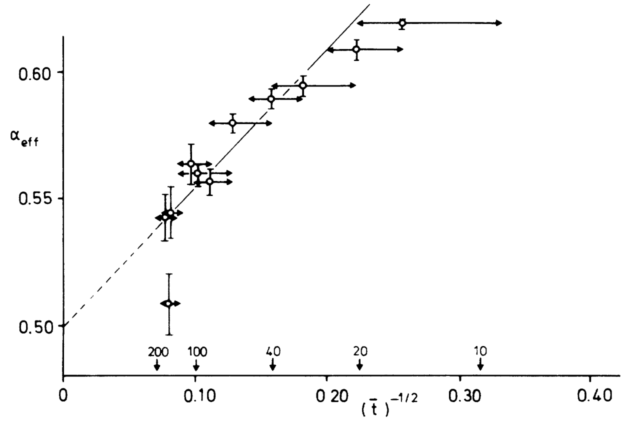

FIG. 2. Asymptotic behavior of the spin autocorrelation function for the classical Heisenberg chain at $T=\infty$. The open circles show the results of least-squares fits to simple power laws using data that are within the horizontal arrows; the vertical bars are error bars for these fits. The mean time for each fitting interval is $\bar{t}$. The dashed line shows a simple linear extrapolation to $t=\infty$.

early-time regime the spin autocorrelation function shows several gentle undulations which are far outside the statistical error of the data, but these have died out by a time of $10J^{-1}$. The decay is then almost simple power law, but the effective power of the decay continues to decrease very slowly until times well past $t=100J^{-1}$ (see Fig. 2). We have analyzed the data over restricted regions of time in the following way. Least-squares fits were made to a power-law decay of the form

$$\langle S_i(0)S_i(t)\rangle \propto t^{-\alpha} , \quad (5)$$

where an effective exponent α_{eff} is extracted for each time interval. In Fig. 2 we plot the resultant values as a func-

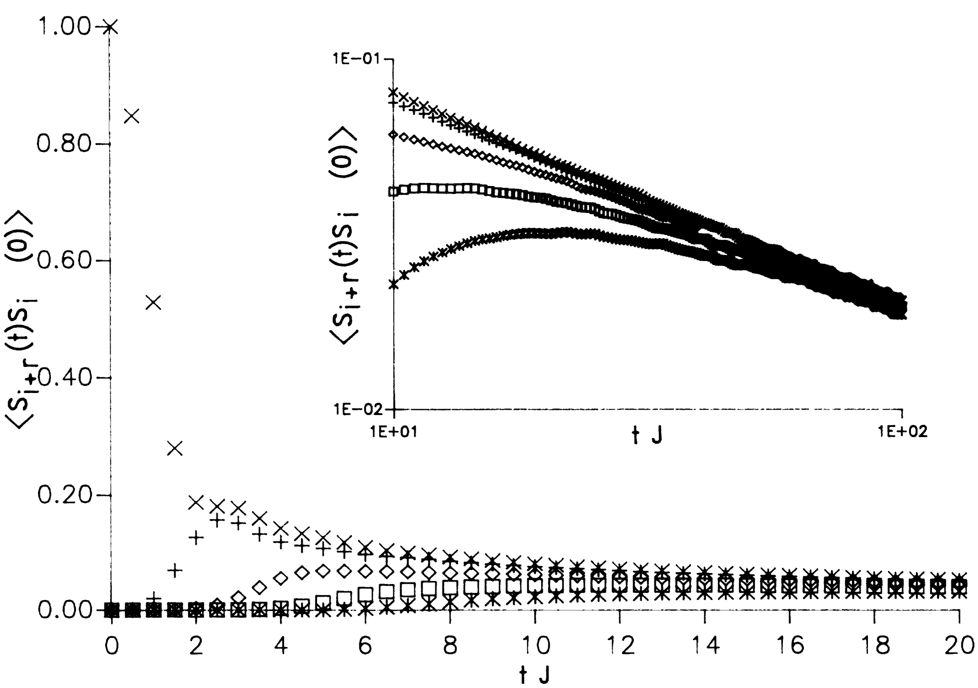

FIG. 3. Time dependence of the space-displaced spin-spin correlation functions for the classical Heisenberg chain at $T=\infty$. The inset shows the long-time behavior on a double logarithmic scale. The symbols denote the following: ($\times$) $r=0$, ($+$) $r=2$, ($\Diamond$) $r=4$, ($\Box$) $r=6$, and ($*$) $r=8$.

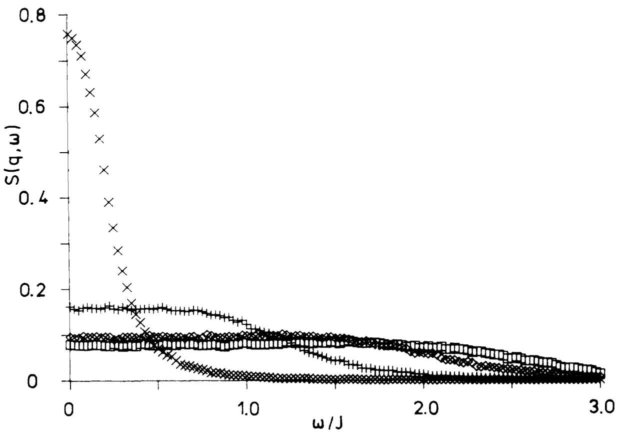

FIG. 4. Neutron-scattering function $S(q,\omega)$ for the classical Heisenberg chain at $T=\infty$. The symbols denote the following: ($\times$) $qa=\pi/8$, ($+$) $qa=3\pi/8$, ($\Diamond$) $qa=5\pi/8$, and ($\Box$) $qa=7\pi/8$.

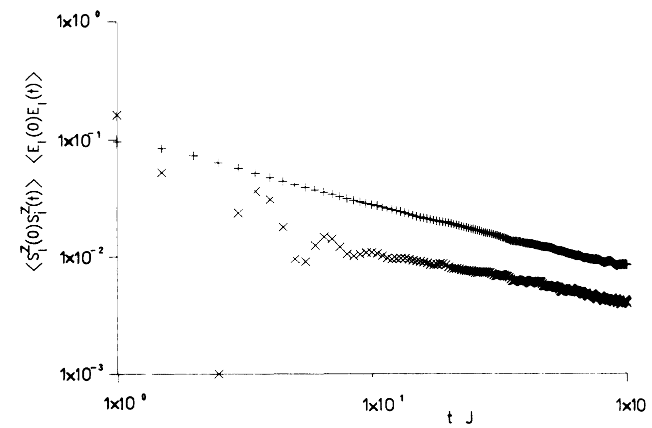

FIG. 6. Time dependence of the out-of-plane spin autocorrelation function (lower curve) and energy-energy correlation function (upper curve) for the classical XY chain at $T=\infty$.

tion of the mean time of the fitting interval. The open circles show the results of least-squares fits using data that are within the horizontal arrows; the vertical bars are error bars for these fits. The mean time for each fitting interval is $\bar{t}$. The dashed line shows a simple linear extrapolation to $t=\infty$. For very short times the effective exponent is well above 0.6, but it decreases *systematically* as the fitting interval is moved to longer times. At the very longest times the fitting is no longer robust; i.e., the answer depends on the explicit interval used, but the trend is still quite clear. The data can be convincingly extrapolated to $\alpha=\frac{1}{2}$, although it would also be possible, within the errors bars, to extrapolate to slightly larger

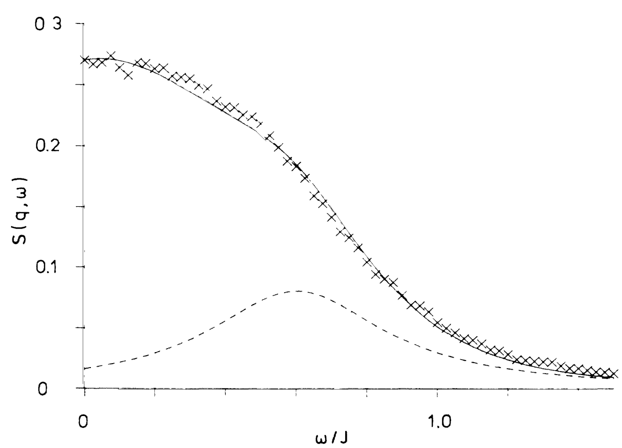

FIG. 5. Fit of $S(q,\omega)$ for $qa=2\pi/8$ to a Gaussian (diffusive) central peak and a Lorentzian spin-wave peak at $\omega=0.60J$. Note that both the "theoretical" functions have been convoluted with the "resolution function" appropriate for our spin-dynamics calculation as described in Sec. II. The dotted line is the Gaussian and the dashed line is the Lorentzian line shape, and the solid line is the sum of both.

values. The energy-energy correlation function also shows a relatively slow approach to the asymptotic behavior, but by a time of $40J^{-1}$ it is well described by a $t^{-1/2}$ decay all the way out to the maximum time of the study. Thus these data show that there is diffusion, as suggested by Müller,[8] but that it is *not* anomalous; moreover, the approach to the long-time behavior is extremely slow. This is a rather curious effect since Müller[11] showed that the asymptotic time regime is easily reached in linear Heisenberg models which included nonuniform exchange.

We have also examined the time dependence of space-displaced correlations. The various rounded peaks in the correlation functions have been explained in terms of the diffusion of information from spin to spin (or back again). We can see, however, from Fig. 3 that the long-time behavior of all the correlation functions is apparently the same, although the effective power is now smaller than $\frac{1}{2}$

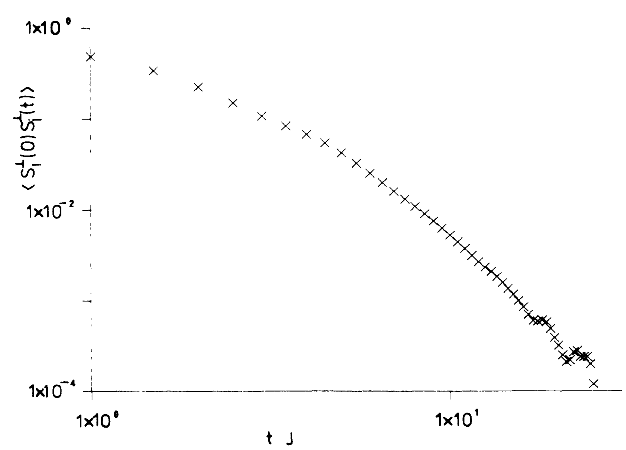

FIG. 7. Time dependence of the in-plane spin autocorrelation function for the classical XY chain at $T=\infty$.

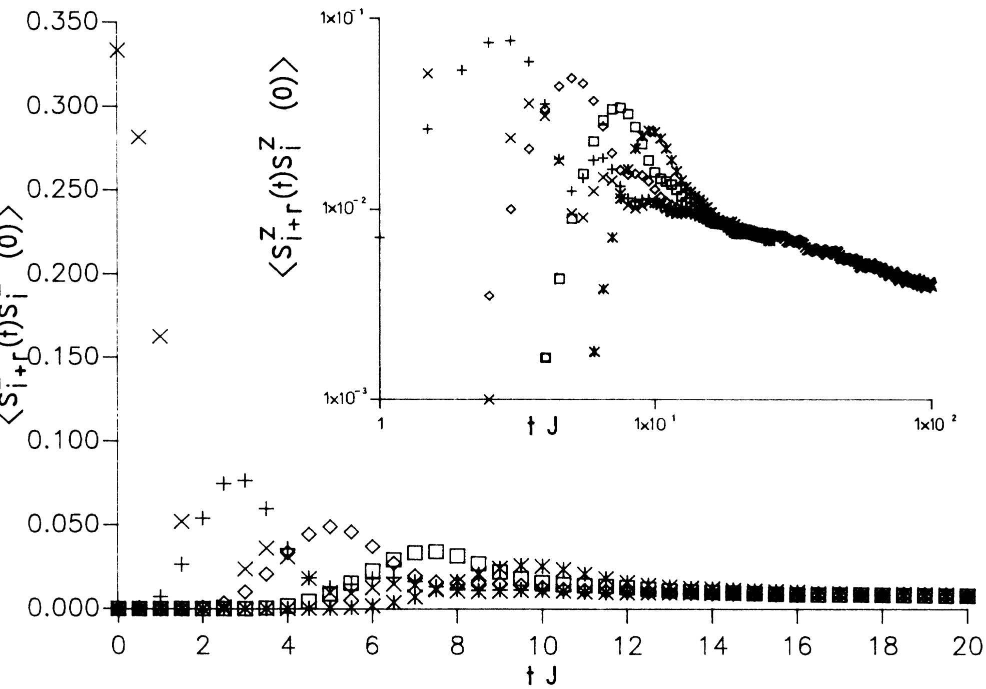

FIG. 8. Time dependence of the space-displaced spin-spin correlation functions for the classical XY chain at $T=\infty$. Same notation as in Fig. 3.

at short times.

The excitations in this system can be understood in a more direct way by examining $S(q,\omega)$, which we show in Fig. 4. The initial impression that one obtains from this figure is that there is a simple diffusive central peak which broadens as we move further out into the Brillouin zone. A diffusive peak should, however, be a simple Gaussian, and the data in Fig. 4 indicate that the peaks are far too square to be Gaussian. In Fig. 5 we show the result of an attempt to fit $S(q,\omega)$ to the sum of a Gaussian central peak and a Lorentzian spin-wave peak at nonzero frequency. The deviation of the overall line shape from a Gaussian is pronounced, but the inclusion of the spin-wave peak improves the comparison dramatically. Nonetheless, there are systematic differences that indicate that a simple Lorentzian line shape is inadequate for a truly quantitative analysis. Theoretical guidance is needed to determine the functional form of the spin-wave peak to be used in any further curve fitting.

B. *XY* model

Many of the qualitative features of the XY-model behavior parallel those of the Heisenberg model. The out-

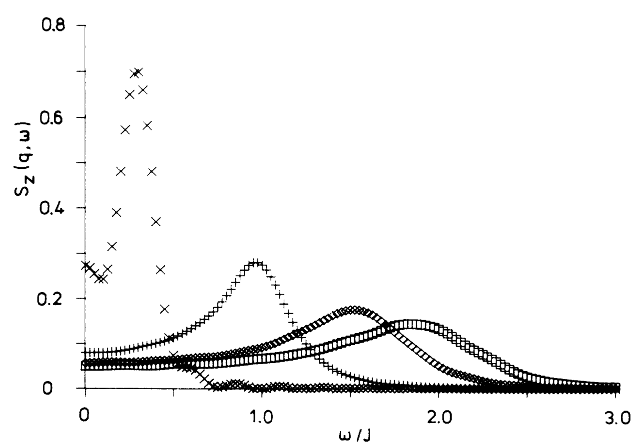

FIG. 9. $S_z(q,\omega)$ for the classical XY chain at $T=\infty$. Same notation as in Fig. 4.

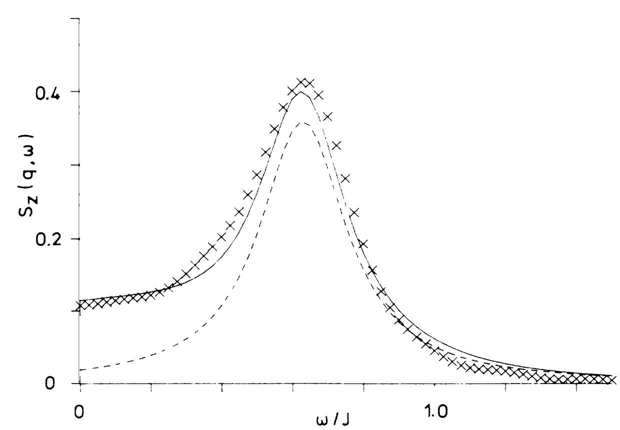

FIG. 10. Fit of $S_z(q,\omega)$ for $qa=2\pi/8$ to a Gaussian (diffusive) central peak and a Lorentzian spin-wave peak at $\omega=0.63J$. Both "theoretical" functions have been convoluted with the "resolution function" appropriate for our spin-dynamics method as described in Sec. II. Same notation as in Fig. 5.

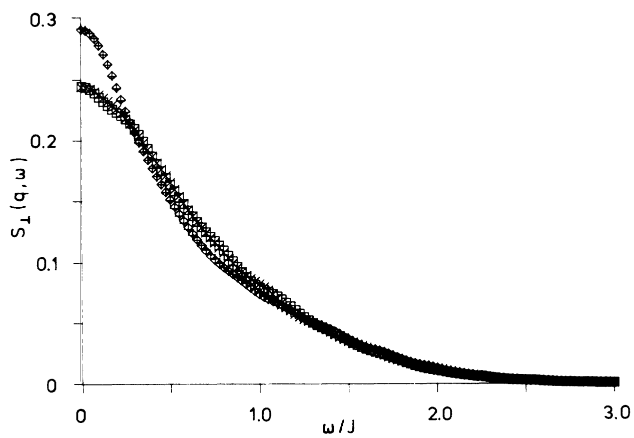

FIG. 11. $S_\perp(q,\omega)$ for the classical XY chain at $T=\infty$. Same notation as in Fig. 4.

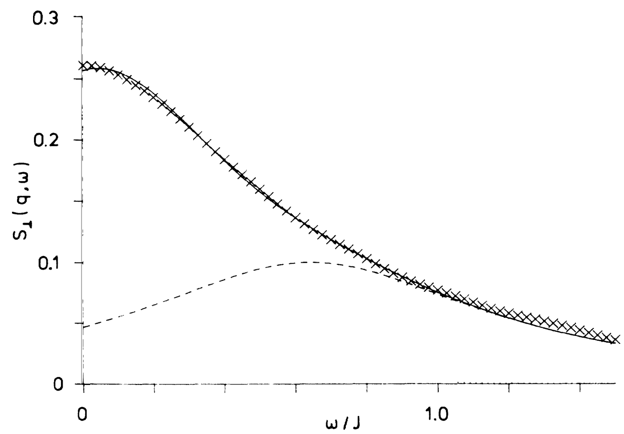

FIG. 12. Fit of $S_\perp(q,\omega)$ for $qa=2\pi/8$ to a Gaussian (diffusive) central peak and a Lorentzian spin-wave peak at $\omega=0.64$. Both "theoretical" functions have been convoluted with the "resolution function" appropriate for our spin-dynamics method as described in Sec. II. Same notation as in Fig. 5.

of-plane spin-spin and energy-energy correlation functions, shown in Fig. 6, show a clear $t^{-1/2}$ decay at long times, although the oscillations in the early-time spin-spin correlations are much more pronounced than they are in the Heisenberg model. In the "medium-time" regime the correlation function is fairly well described by a power law with an effective exponent that is less than $\frac{1}{2}$. The behavior of the in-plane spin-spin correlations is more difficult to understand. The correlations decay quite rapidly, and by a time of $25J^{-1}$ the statistical fluctuations begin to dominate (see Fig. 7). Spin-diffusion theory predicts an exponential decay for a spin-spin correlation function only if the corresponding magnetization is conserved. Therefore, we do not expect an exponential decay for this correlation function, and the decay is clearly not power law for times that we can follow. It is also not exponential or even Gaussian as has been found for the spin-$\frac{1}{2}$ case.[2] More distant-neighbor correlations show peaks at short times (see Fig. 8), with a separation in time which depends upon the spatial separation of the spins; at long times they are all consistent with a $t^{-1/2}$ behavior.

For the XY model, $S_z(q,\omega)$ shows very pronounced spin-wave peaks (see Fig. 9), in addition to a diffusive central peak. The positions of these peaks describe a dispersion curve which is softened moderately with respect to the $T=0$ curve. Here, too, fits to the sum of a Lorentzian and a Gaussian reproduce the features of the data moderately well (see Fig. 10), but remaining systematic differences can only be explained by using a more complicated line shape for the spin waves. For the in-plane component $S_\perp(q,\omega)$ (shown in Fig. 11), only a monotonic central peak appears. It also shows almost no q dependence. Nonetheless, this central peak is not Gaussian, but can be rather well described by the combination of a Gaussian central peak and a Lorentzian at some finite ω (Fig. 12).

IV. CONCLUSION

We have used high-resolution spin-dynamics simulations to probe the infinite-temperature time-dependent behavior of simple Heisenberg and XY chains. We find a somewhat surprising richness of behavior with very slow approach to the asymptotic behavior for some quantities and with spin-wave shoulders and peaks in $S(q,\omega)$. We know of no theoretical framework for describing these findings.

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