PHYSICAL REVIEW VOLUME 178, NUMBER 2 10 FEBRUARY 1969

Frequency-Dependent Self-Correlation Function for the Heisenberg Spin System in One Dimension

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(Received 23 September 1968)

The exact numerical calculations by Carboni and Richards for $\langle S_1^z(t)S_1^z(0)\rangle_{(\omega)}$ in a one-dimensional Heisenberg system of $S=\frac{1}{2}$ spins at elevated temperatures are compared with the predictions of a simple, two-parameter Gaussian representation of the generalized diffusivity. The parameters of the diffusivity are completely determined by the known second and fourth frequency moments, and the procedure is free of arbitrary parameters. The results of the calculation are found to be in good agreement with Carboni and Richards. The calculation is also carried out for $S>\frac{1}{2}$, and it is found that with the increase in the magnitude of spin, $\langle S_1^z(t)S_1^z(0)\rangle_{(\omega)}$ gradually loses its characteristic hump and approaches a shape roughly similar to the one which would result from the use of an appropriate Lorentzian for the function $\langle S_f^z(t)S_g^z(0)\rangle_{(k,\omega)}$.

I. INTRODUCTION

RECENTLY Carboni and Richards[1] have performed exact numerical calculations for the time-dependent self-correlation $\langle S_1^z(t)S_1^z(0)\rangle\equiv\phi(t)$ for finite linear chains with periodic boundary conditions containing up to 10 spins (with $S=\frac{1}{2}$) coupled by nearest-neighbor Heisenberg exchange interaction (in contact with a heat and angular momentum bath at temperature $T\rightarrow\infty$). Following the example of Bonner and Fisher,[2] who, after computing *equal-time* correlations for finite linear chains, extrapolated them to the case $N=\infty$ with excellent resultant accuracy, Carboni and Richards have made a plausible extrapolation to the thermodynamic limit $N=\infty$. Their results have the surprising feature (see the histogram in Fig. 1) that the frequency Fourier-transform of the self-correlation $\phi(\omega)$ has a steep rise as $\omega\rightarrow 0$. Moreover, $\phi(\omega)$ clearly has neither the Gaussian form, in contradiction to the requirements of the classic theory of Kubo and Tomita,[3] nor is the shape entirely Lorentzian.

Very recently Fernandez and Gersch[4] (FG) have noted that if the Fourier transform $\langle S_1^z(t)S_0^z(0)\rangle_{(k,\omega)}\equiv f_k(\omega)$ is assumed to possess a Lorentzian structure for small k and ω, the steep rise of the transform $\phi(\omega)$ can be qualitatively explained. Moreover, in analogy with the work of Collins and Marshall[5] (for three-dimensional Heisenberg spin systems), FG propose that the line shape $f_k(\omega)$ be taken to be a Gaussian for k close to the Brillouin zone boundary.

This qualitative picture is then developed into a quantitative representation of the line shape $f_k(\omega)$ by an arbitrary choice of the weighting factors $W_n^\pm(k)=[J(0)]^{2n+1}\pm[J(k)]^{2n+1}/2[J(0)]^{2n+1}$, where the upper sign refers to the Lorentzian and the lower to the Gaussian weighting factor [note the limiting requirements $W_n^\pm(k=0)=1$, 0 and $W_n^\pm(k=\text{zone boundary})=0$, 1]. With some further arbitrary choices for the numerical coefficients of the Gaussian, FG have been able to get a "satisfactory" agreement with the extrapolated exact numerical calculations of Ref. 1.

In view of the somewhat *ad hoc* nature of the FG procedure for constructing the line shape $f_k(\omega)$, and the consequent arbitrariness of the choice of the weighting factors $W_n^\pm(k)$ [note that $W_n^\pm(k)$, for all integral $n\geq 0$ would still satisfy the limiting requirements mentioned earlier] as well as the actual numerical

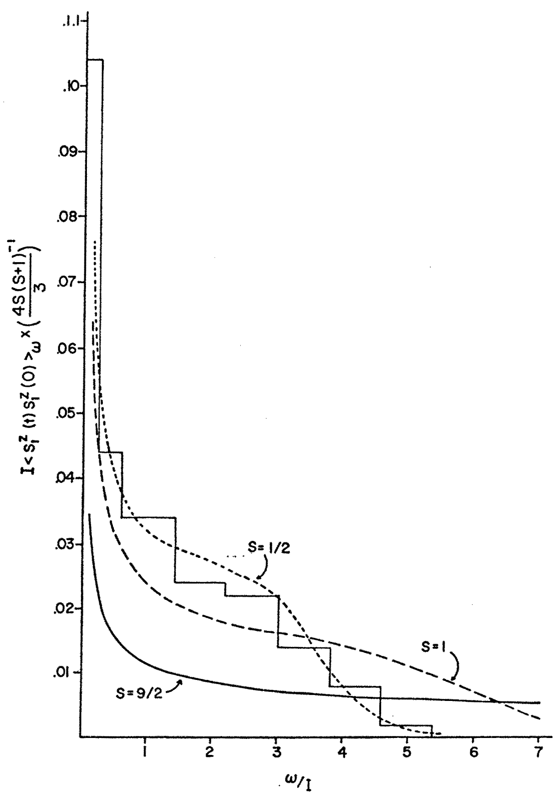

FIG. 1. Plot of $\langle S_1^z(t)S_1^z(0)\rangle_{(\omega)}[4S(S+1)/3]^{-1}$ versus (ω/I). The histogram shows the exact numerical results of Carboni and Richards for spin $\frac{1}{2}$. The other curves are the results of the present analysis for spins $\frac{1}{2}$, 1, and $\frac{9}{2}$.

* Supported by National Science Foundation predoctoral traineeship.
[1] F. Carboni and P. M. Richard, J. App. Phys. **39**, 967 (1968).
[2] J. C. Bonner and M. E. Fisher, Phys. Rev. **135**, A640 (1964).
[3] R. Kubo and K. Tomita, J. Phys. Soc. Japan **9**, 888 (1954).
[4] J. F. Fernandez and H. A. Gersch, Phys. Rev. **172**, 341 (1968).
[5] M. F. Collins and W. Marshall, Proc. Phys. Soc. (London) **92**, 390 (1967).

coefficients of the Gaussian, and to a lesser extent the Lorentzian, in the present work it is intended to proceed from a well-defined procedure. This procedure is a logical extension of the ideas of Martin, Bennett, Kadanoff, and Tahir-Kheli[6,7] for three-dimensional spin systems and can be thought to be in the same spirit as the recent work of Martin and Yip on diffusion in simple liquids.[8]

The crucial assumption in this treatment is the two-parameter Gaussian representation of the frequency-wave-dependent diffusivity. This representation accurately preserves the sum rule $\phi(0)=\frac{1}{3}S(S+1)$ as well as the second and the fourth frequency moments known from the work of Collins and Marshall[5] and moreover, does not contain any arbitrary adjustable parameters. The results for $S=\frac{1}{2}$ are in satisfactory agreement with the "exact" numerical results[1] (see Figs. 1 and 2).

We have also carried out the evaluation of $\phi(\omega)$ for $S>\frac{1}{2}$ and we find that with the increase in the magnitude of S, the function $\phi(\omega)$ gradually loses its hump and approaches a shape similar to the one which would result from the use of an appropriate Lorentzian for the line shape $f_k(\omega)$. It should be interesting to compare the results for $S\to\infty$ (which are nearly the same as those for $S=\frac{9}{2}$ given in Fig. 1) with the corresponding "exact" ones for the classical Heisenberg spin system.[9]

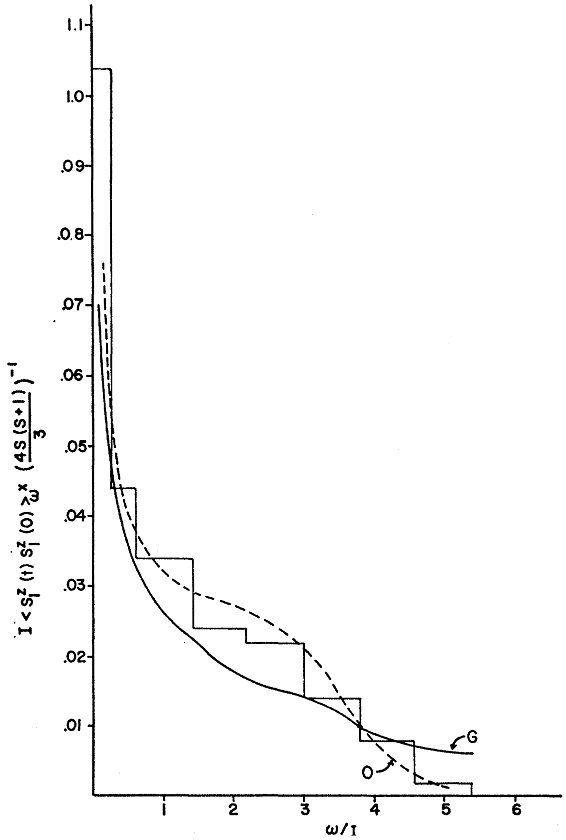

FIG. 2. The spin-$\frac{1}{2}$ results for $\langle S_1{}^z(t)S_1{}^z(0)\rangle_{(\omega)}[4S(S+1)/3]^{-1}$ versus (ω/I). The full curve G shows the Fernandez-Gersch's results, the histogram the exact numerical results of Carboni and Richards, and the dotted curve the results of the present calculation. Note that the agreement of our results with the exact ones seems to be better than that of Fernandez and Gersch for all ω and in particular for $\omega\geq 5I$.

II. FORMALISM

For an infinite one-dimensional array of spins S, the Heisenberg Hamiltonian has the form

$$H=-\sum_{f_1,f_2} I(f_1f_2)\mathbf{S}_{f_1}\cdot\mathbf{S}_{f_2}, \tag{2.1}$$

where the exchange integral between positions f_1 and f_2, $I(f_1,f_2)$, is assumed to be restricted only to the nearest neighbors, i.e.,

$$I(f_1f_2)=I,\ \text{when } f_1 \text{ and } f_2 \text{ are nearest neighbors} \\ =0,\ \text{otherwise.} \tag{2.2a}$$

It is convenient to define the spectral function $F_k(\omega)$ as

$$\langle[S_{f_1}{}^z(t),S_{f_2}{}^z(t')]\rangle=\left(\frac{1}{2\pi}\right)\int_{-\pi}^{+\pi}dk\ e^{ik(f_1-f_2)} \times\int_{-\infty}^{+\infty}F_k(\omega)e^{-i\omega(t-t')}d\omega, \tag{2.2b}$$

and, therefore,

$$\langle S_{f_2}{}^z(t')S_{f_1}{}^z(t)\rangle=\left(\frac{1}{2\pi}\right)\int_{-\pi}^{+\pi}dk\ e^{ik(f_1-f_2)} \times\int_{-\infty}^{+\infty}\frac{F_k(\omega)}{(e^{\beta\omega}-1)}e^{-i\omega(t-t')}d\omega, \tag{2.2c}$$

(the unit of length being the nearest-neighbor distance), where as usual the pointed brackets denote a statistical average over a canonical ensemble and where the time dependence of the spin operators is in the Heisenberg picture. The retarded Green's function,

$$M_{f_1,f_2}(t,t')=-i\Theta(t-t')\langle[S_{f_1}{}^z(t),S_{f_2}{}^z(t')]\rangle \tag{2.3}$$

then has the usual spectral representation

$$M_k(Z)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{F_k(\omega)}{Z-\omega}d\omega, \tag{2.4}$$

[6] H. S. Bennett and P. C. Martin, Phys. Rev. **138**, A608 (1965); L. P. Kadanoff and P. C. Martin, Ann. Phys. (N. Y.) **24**, 419 (1963).

[7] R. A. Tahir-Kheli, Phys. Rev. **159**, 439 (1967); (J. Appl. Phys. to be published); H. S. Bennett, Phys. Rev. **174**, 629 (1968).

[8] P. C. Martin and S. Yip, Phys. Rev. **170**, 151 (1968).

[9] In this connection it should be noted that in the limit $S\to\infty$, the statistical mechanics of the classical Heisenberg model (CHM) coincides with that of the quantum-mechanical Heisenberg spin system (QHM). On the other hand, the CHM for finite spin [see, e.g., C. G. Windsor, Proc. Phys. Soc. (London) **91**, 353 (1967)] cannot be directly compared with the $S\to\infty$ limit of the QHM being discussed in the present work. A possible identification—of somewhat dubious value—of the finite-spin cases of the CHM and the QHM could be achieved by replacing in the CHM the magnitude of the spin vector S with its quantum-mechanical counterpart $[S(S+1)]^{1/2}$.

where $\mathrm{Im}Z>0$ and $M_k(Z)$ is the analytic extension of the Fourier transform $M_k(E)$

$$M_{f_1,f_2}(t,t')=\frac{1}{2\pi}\int_{-\pi}^{+\pi}dk\, e^{ik(f_1-f_2)}\times\int_{-\infty}^{+\infty}M_k(E)e^{-iE(t-t')}dE. \quad (2.5)$$

Following Kadanoff and Martin,[6] it is convenient to define the frequency-wave-dependent diffusivity $D_k(\omega)$ as follows:

$$\left[1-\frac{M_k(Z)}{M_k(0)}\right]^{-1}=1-\frac{k^2}{\pi}\int_{-\infty}^{+\infty}\frac{D_k(\omega)}{Z^2-\omega^2}d\omega. \quad (2.6)$$

Now using Eq. (2.4), the relationship between the spectral function $F_k(\omega)$ and the diffusivity may be readily established

$$F_k(\omega)=-2M_k(0)\omega k^2D_k(\omega)\left\{\omega^2\left[1-\frac{k^2}{\pi}P\int_{-\infty}^{+\infty}\frac{d\omega' D_k(\omega')}{\omega^2-\omega'^2}\right]^2+[k^2D_k(\omega)]^2\right\}^{-1}, \quad (2.7)$$

where $M_k(0)$ is related to the wave-dependent susceptibility $\chi(k)$ by

$$\chi(k)=\beta\sum_f e^{-ikf}\int_0^1 d\lambda\,\langle S_0^z(0)e^{-\beta\lambda H}S_f^z(0)e^{+\beta\lambda H}\rangle$$
$$=-2\pi M_k(0). \quad (2.8)$$

In the limit $\beta\to 0$, the dominant term of $\chi(k)$ is readily calculated

$$\lim_{\beta\to 0}[\chi(k)]=\beta\tfrac{1}{3}S(S+1), \quad (2.9)$$

and, therefore, Eq. (2.7) becomes

$$\lim_{T\to\infty}\left[\frac{F_k(\omega)}{\beta\omega}\right]=\left[\frac{S(S+1)}{3\pi}\right]k^2D_k(\omega)\left\{\omega^2\left[1-\frac{k^2}{\pi}P\int_{-\infty}^{+\infty}\frac{d\omega' D_k(\omega')}{\omega^2-\omega'^2}\right]^2+[k^2D_k(\omega)]^2\right\}^{-1}. \quad (2.10)$$

The left-hand side of Eq. (2.10) is what we called the line shape $f_k(\omega)$ in Sec. I [To see this, expand the factor $(e^{\beta\omega}-1)^{-1}$ in the integrand of Eq. (2.2c), retaining the dominant term, $1/\beta\omega$].

Before we conclude this section, we need to notice that using Eq. (2.4) in the left-hand side of Eq. (2.6), expanding both sides in inverse powers of $(1/Z)$ for large $\mathrm{Re}(Z)$ and comparing coefficients of equal powers of $(1/Z)$ on either side, we readily get the following relationships which will be needed later:

$$k^2D_k^{(0)}=F_k^{(2)}, \quad (2.11)$$
$$k^2D_k^{(2)}+k^4[D_k^{(0)}]^2=F_k^{(4)},$$

where

$$D_k^{(n)}=\frac{1}{\pi}\int_{-\infty}^{+\infty}D_k(\omega)\omega^n d\omega,$$
$$F_k^{(n)}=[-2\pi M_k(0)]^{-1}\int_{-\infty}^{+\infty}F_k(\omega)\omega^{n-1}d\omega,$$
$$n=0,\,1,\,2,\,\cdots. \quad (2.12)$$

III. GAUSSIAN DIFFUSIVITY AND RESULTS

The formal development of Sec. II is exact. It is, however, clear that the introductoin of the diffusivity $D_k(\omega)$ does not by itself guarantee any revealing information about the spectral function $F_k(\omega)$. Rather, Eq. (2.10) merely reexpresses the function $F_k(\omega)$ in terms of another, as yet unknown but possibly quite well-behaved, function $D_k(\omega)$.

The essential statement of the treatments of Refs. 6–8 is that a phenomenological representation of the well-behaved function $D_k(\omega)$ is hopefully a less hazardous assumption than one which makes statements about the rather singular function $F_k(\omega)$ itself. In any case, we shall for the present assume that this viewpoint has merit. The results of the present work will hopefully justify it *a posteriori*.

The second and the fourth frequency moments of the function $F_k(\omega)$ are known in the limit of infinite temperatures.[5] In the present notation for spin S these moments are

$$F_k^{(2)}=(8/3)[S(S+1)]I[J(0)-J(k)],$$
$$F_k^{(4)}=32[\tfrac{1}{3}S(S+1)]^2I^2[J(0)-J(k)]\times[7J(0)-3J(k)-(4+[3/2S(S+1)])I], \quad (3.1)$$

where

$$J(k)=2I\cos k. \quad (3.2)$$

These two moments uniquely determine the moments $D_k^{(0)}$ and $D_k^{(2)}$ of the diffusivity [see Eqs. (2.11) and (2.12)].

In analogy with the Refs. 6–8, we shall assume a two parameter Guassian representation for the diffusivity, i.e.,

$$D_k(\omega)\sim\Delta(k)\Gamma(k)e^{-\omega^2\Gamma^2(k)}, \quad (3.3)$$

where the normalization and collision parameters $\Delta(k)$ and $\Gamma(k)$ are readily related to the known moments $F_k^{(2)}$ and $F_k^{(4)}$ via $D_k^{(0)}$ and $D_k^{(2)}$, i.e.,

$$\Delta(k)=(\sqrt{\pi})D_k^{(0)}=(\sqrt{\pi})[F_k^{(2)}/k^2],$$
$$\Gamma(k)=\left[\frac{D_k^{(0)}}{2D_k^{(2)}}\right]^{1/2}=\left[\frac{F_k^{(2)}}{2[F_k^{(4)}-(F_k^{(2)})^2]}\right]^{1/2}. \quad (3.4)$$

We emphasize that the above representation for the diffusivity conserves the frequency moments $F_k^{(0)}$ through $F_k^{(4)}$. Here, of course, $F_k^{(0)}$ is the sum rule

$$F_k^{(0)}=1,$$

$F_k^{(1)}$ and $F_k^{(3)}$ are identically zero because of the antisymmetry $F_k(\omega)=-F_k(-\omega)$, and the moments $F_k^{(2)}$ and $F_k^{(4)}$ are automatically preserved because of the particular choice (3.4).

After introducing the two parameter Gaussian representation (3.3) with the moment conserving choice of Eq. (3.4) into the right-hand side of Eq. (2.10), we have numerically carried out the k sum, i.e.,

$$\frac{1}{2\pi}\int_{-\pi}^{+\pi}dk\left[\frac{F_k(\omega)}{\beta\omega}\right]=\lim_{\beta\to 0}[\langle S_1^z(t)S_1^z(0)\rangle_{(\omega)}], \quad (3.5)$$

for various values of spin S. The results for $S=\frac{1}{2}$, $\frac{3}{2}$, and $\frac{9}{2}$ are plotted in Figs. 1 and 2 along with those given by the numerical calculations of Carboni and Richards and the recent results of Fernandez and Gersch.

IV. CONCLUSIONS

The results of the present analysis provide an interesting check on the adequacy of the two parameter Gaussian description of the frequency-wave-dependent diffusivity. The relatively reasonable agreement of the present results suggests that while in principle the diffusivity could possibly be highly peaked in certain regions of the frequency-wave-vector space, for the case of a one-dimensional Heisenberg spin system at elevated temperatures, a simple two parameter Gaussian representation of this function *does seem to be an adequate approximation*. Moreover, such a representation is free from any arbitrariness of choice and preserves all the known frquency moments.

Note added in proof. We have recently noticed that when the results displayed in Fig. 1 are expressed as a plot of $I'\phi'(\omega)$ versus ω', the curves are almost spin-independent, i.e., the spread between the $S=\frac{1}{2}$ and $S=\infty$ is only a few percent. Here $\phi'(\omega)=\phi(\omega)y^{-2}$, $I'=Iy$, $\omega'=(\omega/I')$, and $y=[S(S+1)]^{\frac{1}{2}}$.

ACKNOWLEDGMENT

We are greatly indebted to the Temple University Computer Center for generous allotment of computer time on their CDC-6400.