$\sigma = d$ we would expect log terms to appear in $\mu - \mu_c$ and in $h(\mathbf{r})$, as they do in the spherical model. For the value $\sigma = \tilde{s}$, similar complexity could also appear because of the possible confluence of the $V$ and $R_c$ terms at this value.

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# Spin Correlations in the Heisenberg Linear Chain at Infinite Temperature*

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This paper is concerned with the nonmonotonic frequency dependence of $S(k,\omega)$, the wave-number–frequency transform of the time-dependent spin-spin correlation functions for a one-dimensional Heisenberg magnet at infinite temperature, as calculated by Carboni and Richards. It is argued that this nonmonotonic feature of $S(k,\omega)$ is a one-dimensional effect, and supporting evidence is presented via a phenomenological calculation of $S(k,\omega)$, utilizing the equivalence of the Heisenberg chain with a fermion system.

## I. INTRODUCTION

THIS paper deals with the frequency–wave-vector Fourier transform $S(k,\omega)$ of the paramagnetic spin-spin correlation function for a one-dimensional Heisenberg spin-$\frac{1}{2}$ system. This spectral function $S(k,\omega)$ has been computed exactly numerically for a large set of $k$, $\omega$ values by Carboni and Richards[1] (CR), and their results are shown in Fig. 1. Considering the sparsity of exact results for interacting systems, these CR results are valuable guideposts for testing the various phenomenological theories introduced to study spin dynamics in the paramagnetic region of insulating magnets, and several papers devoted to such comparisons have appeared.[2]

We are here concerned with one feature of $S(k,\omega)$ found by CR which is strikingly different from predictions of working theories of three-dimensional systems, namely, the nonmonotonic behavior of $S$ as a function of $\omega$ for $k > 2\pi/9$, which is evident in Fig. 1. Practically useful theories for three-dimensional systems[3] predict a Gaussian in $\omega$ dependence of $S$ at large $k$ and at elevated temperature, and such behavior fits experimental data on neutron scattering[4] and magnetic resonance.[5] One therefore suspects that the nonmonotonic behavior found by CR is a peculiarity of one-dimensional systems, and considering that the system is at infinite temperature, its only relevant feature is the density of states for the periodic chain. Inspection of $S(k,\omega)$ for the one-dimensional $x$-$y$ model, exactly soluble as a system of noninteracting fermions, supports this guess. As shown in Fig. 2, $S(k,\omega)$ for the $x$-$y$ model (derived in Sec. II) has infinities at the cutoff frequency $\omega_{\max}$, and these are due to a behavior of the one-dimensional density of states which is analogous to the infinity in phonon density of states for a linear chain.

In the fermion language, $S(k,\omega)$ is the spectral function for the particle density-density correlation function. To get to the one-dimensional $x$-$y$-$z$ model treated by CR from the $x$-$y$ model requires the addition to the latter of the $z$ spin interactions, and these spin interactions play the role of fermion two-body interactions. We conjecture that the major effect of such fermion interactions is to introduce lifetimes for the Fermi quasiparticles, and we work out $S(k,\omega)$ based on a naive phenomenological treatment of lifetimes. The resulting $S(k,\omega)$, expressible in closed form, and depicted as dashed lines in Fig. 1 reproduces quite well the nonmonotonic character of the CR results in the region $k > 2\pi/9$, where the agreement should be best. We take this agreement to indicate the correctness of the approach, and conclude that the nonmonotonic behavior of $S(k,\omega)$ as found by CR is a feature of their results peculiar to one-dimensional systems.

## II. $S(k,\omega)$ FOR $x$-$y$ MODEL

The Hamiltonian for this model[6] is given by

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

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[1] F. Carboni and P. M. Richards, Phys. Rev. **177**, 889 (1969).
[2] J. F. Fernandez and H. A. Gersch, Phys. Rev. **172**, 341 (1968); R. A. Tahir-Kheli and D. G. McFadden, *ibid.* **182**, 604 (1969).
[3] P. G. de Gennes, J. Phys. Chem. Solids **4**, 223 (1958).
[4] M. F. Collins and R. Nathans, J. Appl. Phys. **36**, 1092 (1965).
[5] A. J. Henderson and R. N. Rogers, Phys. Rev. **152**, 218 (1966).

[6] The $x$-$y$ model was introduced by E. Lieb, T. Schulz, and D. Mattis, Ann. Phys. (N. Y.) **16**, 407 (1961); S. Katsura, Phys. Rev. **127**, 1508 (1962).

where $S_i$ is the spin operator at the $i$th lattice site, and we consider only the case for spin $\frac{1}{2}$. In Ref. 6 it is shown how this Hamiltonian can be rewritten in terms of fermion operators as

$$\mathcal{H}=\sum_{k_1} \epsilon_{k_1} a_{k_1}{}^{\dagger} a_{k_1}\,, \tag{2}$$

with $\epsilon_k=-2J\cos k$. The connection between the density of fermions and the $z$ component of spin both at the $j$th site is expressed by

$$S_j{}^z=\tfrac{1}{2}-a_j{}^{\dagger}a_j\,.$$

Thus in the ground state, for which $\langle S_j{}^z\rangle=S=\frac{1}{2}$, there are no fermions in the system. At infinite temperatures, or in the absence of an external magnetic field at finite temperatures, the expectation value of the $z$ spin at any site is zero, so that we have a medium-density fermion

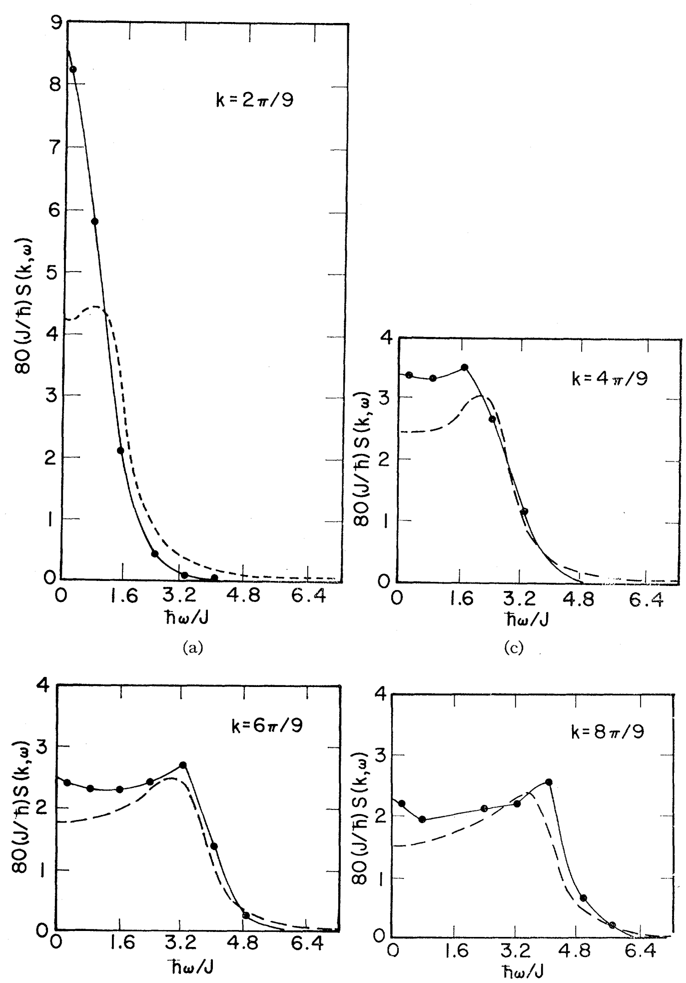


FIG. 1. Wave-vector–frequency transform $S(k,\omega)$ of the time-dependent two spin correlation functions for a Heisenberg linear chain versus frequency for wave-vector values $2n\pi/9$, $n=1, 2, 3, 4$. The solid curves are the computer results of CR, while the dashed curves are given by Eq. (13).

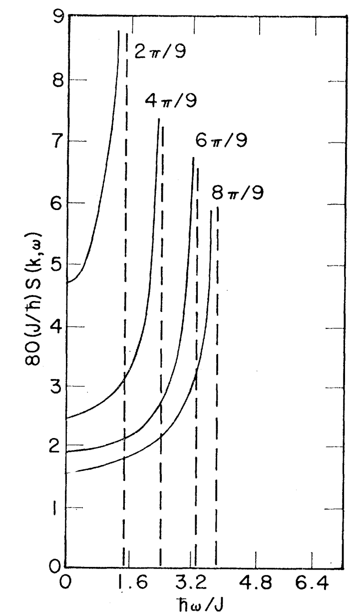


FIG. 2. Wave-vector–frequency transform $S(k,\omega)$ of the time-dependent two spin correlation functions for the $x$-$y$ model versus frequency for wave-vector values $2n\pi/9$, $n=1, 2, 3, 4$.

system $\langle a_j{}^{\dagger}a_j\rangle=\frac{1}{2}$, characterized by a total number of fermions equal to $\frac{1}{2}$ the number of spin sites. Equation (2) indicates we have a lattice gas of noninteracting fermions each with the energy $\epsilon_k$. The expectation value for the number of fermions in each single-particle momentum state, $\langle a_k{}^{\dagger}a_k\rangle$ is equal to $\frac{1}{2}$. The spectral function $S(k,\omega)$ is defined by

$$S(k,\omega)=\sum_j e^{ikj}\int_{-\infty}^{\infty}\frac{d}{2\pi}\,e^{i\omega t}\langle S_0{}^z(t)S_j{}^z(0)\rangle\,. \tag{3}$$

In the fermion representation, $S(k,\omega)$ becomes

$$S(k,\omega)=(N)^{-1}\langle\rho_{-k}(t)\rho_k(0)\rangle_\omega\,, \tag{4}$$

where

$$\rho_k=\sum a_{k_1}{}^{\dagger}a_{k_1+k}\,,$$

the subscript $\omega$ standing for the time Fourier transform. For our system of noninteracting fermions, the density fluctuations have the simple time dependence corresponding to propagation of free particle-hole pairs, and $S(k,\omega)$ becomes

$$S(k,\omega)=(4N)^{-1}\sum_{k_1}\delta(\omega+\epsilon_{k_1}-\epsilon_{k_1+k})\,. \tag{5}$$

The factor $\frac{1}{4}$ in Eq. (5) is the proper normalization required by the infinite temperature sum rule

$$\int_{-\infty}^{\infty} S(k,\omega)\;d\omega=\langle(S_j{}^z)^2\rangle=\tfrac{1}{4}\,.$$

To evaluate $S(k,\omega)$, convert the sum in Eq. (5) to an integral, and make the substitution of variables

$$P=\omega+\epsilon_{k_1}-\epsilon_{k_1+k}$$
$$=\omega+4J\sin\tfrac{1}{2}k\sin(k_1+\tfrac{1}{2}k). \quad (6)$$

Then

$$S(k,\omega)=(8\pi)^{-1}(dk_1/dP)_{P=0}$$
$$=(4\pi)^{-1}[(4J\sin\tfrac{1}{2}k)^2-\omega^2]^{-1/2}. \quad (7)$$

Equation (7), which has been obtained previously by several investigators,[7] is plotted as a function of $\omega$ for several $k$ values in Fig. 2. Each curve goes to infinity at $\omega_{\max}=4J\sin\frac{1}{2}k$. According to Eq. (7), this is the point at which the density of available single particle-hole Fermi states becomes infinite. Pictorially, the particle and hole run at the same velocity at $\omega_{\max}$. This particular feature is attributable to the one-dimensional periodicity of the single-particle energies. For example, if the single-particle energies were given by a non-periodic form, say, $\epsilon=k^2/2m$, we would find $S(k,\omega)=m/2\pi k$ in one dimension. On the other hand, work on phonon densities has shown that wave-vector periodicity of energies produce much weakened singularities in density of states in two- and three-dimensional systems,[8] so periodicity plays a smaller role in introducing structure into $S(k,\omega)$ in these cases. In addition, the fermion Hamiltonian for the higher dimensions contains interactions which oscillate in sign, reminiscent of random impurities or force constants in harmonic lattices, and their effect should be to wash out the weak singularities induced by periodicity.

## III. $S(k,\omega)$ FOR $x$-$y$-$z$ MODEL

To describe the one-dimensional isotropic Heisenberg magnet, we must add to the Hamiltonian of Eq. (1) the $z$-$z$ spin interaction term, which plays the role of an interaction potential. Written in terms of Fermi operators this interaction represents an attractive potential energy between nearest neighbors, to be added to the kinetic-energy–like term coming from the $x$-$x$ and $y$-$y$ interactions.

The addition of the potential-energy term to the Hamiltonian produces correlations between positions of the fermions, not contained in Eq. (5). We will neglect these correlations, keeping the form of Eq. (5) but allowing for the effect of interactions in altering the single-particle energies $\epsilon_k$ and introducing finite lifetimes for the Fermi quasiparticles. The periodicity in $k$ space of the interaction potential along with the equal occupation of every available single-particle state ($\langle a_k^\dagger a_k\rangle=\frac{1}{2}$) at infinite temperature results in zero energy shift in the single-particle energies in the Hartree-Fock approximation, leaving only the effect of lifetimes in altering $S(k,\omega)$. One expects the changes in $S(k,\omega)$ to be relatively small for the large $k$ values, and more drastic for the smaller $k$ values. This expectation follows from considerations of the second and fourth moments of $S(k,\omega)$ for the $x$-$y$ and $x$-$y$-$z$ models, where the moments are defined by

$$\langle\omega^n\rangle=\int_{-\infty}^{\infty}\omega^n S(k,\omega)\,d\omega\Big/\left(\int_{-\infty}^{\infty}S(k,\omega)\,d\omega\right). \quad (8)$$

The moments at infinite temperature for the $x$-$y$ model are easily calculated from Eq. (7) to be

$$\langle\omega^2\rangle=4J^2(1-\cos k),$$
$$\langle\omega^4\rangle=96J^4\sin^4\tfrac{1}{2}k. \quad (9)$$

For the $x$-$y$-$z$ model, the moments, first calculated by de Gennes,[3] are

$$\langle\omega^2\rangle=4J^2(1-\cos k),$$
$$\langle\omega^4\rangle=8J^4(1-\cos k)(4-3\cos k). \quad (10)$$

Now comparison of Eqs. (9) and (10) shows that the second moments are identical, for all $k$, while the fourth moments become almost equal only in the limit of largest $k$, $k=\pi$. For small $k$, expanding the relevant expression for $\langle\omega^4\rangle$ yields the expressions

$$x\text{-}y\text{ model: }\langle\omega^4\rangle\to 6J^4k^4,$$
$$x\text{-}y\text{-}z\text{ model: }\langle\omega^4\rangle\to 4J^4k^2+6J^4k^4, \quad (11)$$

showing that $\langle\omega^4\rangle$ is much larger for small $k$ values in the $x$-$y$-$z$ model. These comparisons imply that the $z$-$z$ interactions do not drastically change $S(k,\omega)$ for large $k$ values whereas a large modification in $S(k,\omega)$ is produced by these interactions at small $k$ values. These characteristics are consistent with the general notion that small $k$ values correspond to large distances between spins in the chain, and for such large distances the interactions introduced by the potential-energy term cause a diffusion of the fermions which gets represented in $S(k,\omega)$ by a Lorentzian function, with its characteristic greatly increased fourth moment.

We are also led to expect that the introduction of finite lifetimes for the fermions will go far toward reproducing $S(k,\omega)$ for the $x$-$y$-$z$ model. Comparison of $S(k,\omega)$ for the $x$-$y$ model, Fig. 2, with the CR results for the $x$-$y$-$z$ model, Fig. 1, shows that the major difference at large $k$ values is the removal of the infinity at $\omega_{\max}$ characteristic of the $x$-$y$ model and its replacement by a broadened response such as one might expect from the introduction of finite lifetimes.

To test this, we next calculate $S(k,\omega)$ under the assumption that the major effect of interactions is to introduce a lifetime $(\Gamma)^{-1}$ for the single-particle states appearing in Eq. (5). Neglecting any wave-vector

[7] Th. Niemeijer, Physica **36**, 377 (1967); R. Liem and R. B. Griffiths (private communication); S. Katsura, T. Horiguchi, and M. Suzuki (unpublished).

[8] L. Van Hove, Phys. Rev. **89**, 1189 (1953).

dependence of $\Gamma$, we can calculate $S(k,\omega)$ replacing Eq. (5) by

$$S(k,\omega)=\frac{\Gamma}{8\pi^2}\int_0^{2\pi}\frac{dk'}{(\omega+\epsilon_{k'}-\epsilon_{k'+k})^2+\Gamma^2}. \quad (12)$$

In the limit $\Gamma\to 0$, $\Gamma/(x^2+\Gamma^2)\to\pi\delta(x)$ so we recapture Eq. (5) for infinite lifetime fermions. The integral in Eq. (12) is easy to evaluate in closed form. The result is

$$4\pi CS(k,\omega)=[A+(A^2+B^2)^{1/2}]^{1/2}, \quad (13)$$

where

$$A=[C^2-(\omega^2-\Gamma^2)]/2DC^2,$$

$$B=\omega\Gamma/2DC^2, \quad (14)$$

$$D=\left(\frac{C^2-(\omega^2-\Gamma^2)}{C^2}\right)^2+\left(\frac{2\omega\Gamma}{C^2}\right)^2,$$

and

$$C=4J\sin\tfrac{1}{2}k.$$

To estimate $\Gamma$, we make the following naive argument.[9] The velocity of a fermion is $v=\partial\epsilon/\partial p=2Ja\sin ka$, and the mean speed $\langle|v|\rangle$ is $2Ja\langle|\sin ka|\rangle=4Ja/\pi$, since every single-particle level is occupied with the same probability. The mean distance between fermions is equal to $2a$, twice the lattice spacing, since there are twice as many lattice sites as particles. Then the inverse time between collisions, which we may identify as the probability per second for a transition, is given by $4Ja/2\pi a\cong 0.636\,J$. This implies a value for $\Gamma$ in Eq. (13) of $0.636\,J$.

In Fig. 1 we plot $S(k,\omega)$ as given by Eq. (13) for $\Gamma=0.6\,J$, which actually yields the best fit to the CR calculations. Inspection of these figures shows that the introduction of fixed momentum-independent lifetimes reproduces quite well the qualitative aspects of computer results for the $x$-$y$-$z$ model. However, in general, the behavior at small $\omega$ values is not correctly given, and in addition, the lifetime broadened $S(k,\omega)$ has a long tail extending to large $\omega$ values, whereas the CR results are characterized by a sharp cutoff in $\omega$.

Some improvement in our predictions could be made by modifying $S(k,\omega)$ through the requirement that it yield the correct second and fourth moments of $\omega$. The major effect of such constraints would be to introduce a high-frequency cutoff for $S$, thus removing the long tail now present. Such embellishments have the disadvantage that a closed form expression for $S(k,\omega)$ is no longer possible. Although the required computer studies might form the basis for a more quantitative comparison with the CR results, they will not change the conclusion that the nonmonotonic behavior of $S(k,\omega)$ is a one-dimensional effect.

[9] Calculation of the single-particle lifetime in the first Born approximation yields zero lifetime, coming from an unrealistic overassessment of scattering cross section for the special case when the two fermions being scattered travel at the same velocity. If this difficulty is overcome by using decaying states, a self-consistent equation for the lifetime results, whose approximate solution is not materially different from the value for $\Gamma$ arrived at by the simple argument given here.