Dynamical correlation functions of the transverse spin and energy density for the one-dimensional spin-1/2 Ising model with a transverse field*†

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Dynamical correlation functions for the transverse (along the direction of the field) spin and energy densities are calculated for the one-dimensional spin-½ Ising model with a transverse field $H=-\Gamma\sum_i S_i^x - J\sum_i S_i^z S_{i+1}^z$. Explicit results are obtained for $\langle\{S^x(q,\omega)S^x(-q)\}\rangle$, $\langle\{E(q,\omega), E(-q)\}\rangle$, and their Fourier transforms in the limits $T=\infty$ and $T=0$ and for the autocorrelation functions $\langle\{S_i^x,S_i^x(t)\}\rangle$ and $\langle\{E_i,E_i(t)\}\rangle$ in the same limits. The results are discussed with special attention given to the coupling of the transverse spin component and energy densities.

I. INTRODUCTION

The Ising model with a transverse field (IMTF) has been much studied lately because of its usefulness in describing phase transitions in a variety of systems.[1] The one-dimensional spin-$\frac{1}{2}$ IMTF is of special interest because it can be solved exactly.[2-4] The work on the one-dimensional lattice has been primarily concerned with thermodynamic properties. In this paper we will extend the analysis to dynamical properties, studying in particular the infinite-temperature limit of the transverse-spin and energy-density correlation functions.

Recently it has been pointed out that the presence of the transverse field leads to a coupling between the fluctuations in the transverse magnetization and the energy density.[5,6] This coupling gives rise to an energy-density term in the transverse-spin correlation function. Because of the special properties of the one-dimensional spin-$\frac{1}{2}$ IMTF, both the transverse-spin correlation function and the energy-density correlation function can be calculated exactly. Thus we are able to study the effects of this coupling directly without recourse to hydrodynamic arguments or computer simulation.[5,6]

The remainder of this paper is divided into four sections. In Sec. II we outline the calculation of the correlation functions, while in Sec. III we present explicit results for the transverse (along the direction of the field) spin and energy correlation functions in the limiting cases $T=0$ and $T=\infty$. Our results are discussed and compared with the predictions of a thermodynamic-hydrodynamic theory in Sec. IV. Section V summarizes our findings.

II. CALCULATION OF THE CORRELATION FUNCTIONS

A. Transformation to noninteracting fermions

The Hamiltonian for the IMTF may be written as (we shall follow the notation of Pfeuty[2] throughout this paper)

$$H=-\Gamma\sum_i S_i^x - J\sum_i S_i^z S_{i+1}^z . \tag{1}$$

We consider only the case of the cyclic chain in which case the second sum in the Hamiltonian (1) runs over the interval $1\leq i\leq N$ with $S_{N+1}^z=S_1^z$. By making the transformations[7]

$$a_i^\dagger = S_i^z + iS_i^y , \tag{2a}$$

$$a_i = S_i^z - iS_i^y , \tag{2b}$$

which imply

$$a_i^\dagger a_i = S_i^x + \tfrac{1}{2} , \tag{2c}$$

and

$$c_i = \exp\left(\pi i \sum_{j=1}^{i-1} a_j^\dagger a_j\right) a_i , \tag{3a}$$

$$c_i^\dagger = a_i^\dagger \exp\left(-\pi i \sum_{j=1}^{i-1} a_j^\dagger a_j\right), \tag{3b}$$

the Hamiltonian becomes

$$H=-\Gamma\sum_{i=1}^N (c_i^\dagger c_i - \tfrac{1}{2}) - \frac{J}{4}\sum_{i=1}^N (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) + \frac{J}{4}(c_N^\dagger - c_N)(c_1^\dagger + c_1)(e^{i\pi L}+1) , \tag{4}$$

where

$$L=\sum_{j=1}^N c_j^\dagger c_j = \sum_{j=1}^N (S_j^z + \tfrac{1}{2}) . \tag{5}$$

The operators c_i and $c_i^\dagger$ are fermion operators.

As in Pfeuty[2] and Lieb, Schultz, and Mattis,[7] we neglect the last term of Eq. (4) for large systems. The Hamiltonian (4) is then a quadratic form in fermion operators and may be diagonalized to

$$H=\Gamma\sum_k \Lambda_k(\eta_k^\dagger \eta_k - \tfrac{1}{2}) \tag{6}$$

by the transformation

$$\eta_k = \frac{1}{2}\sum_i [(\phi_{ki}+\psi_{ki})c_i + (\phi_{ki}-\psi_{ki})c_i^\dagger] . \tag{7}$$

Defining $\lambda = J/2\Gamma$, we find, for $\lambda \neq 1$,

$$\phi_{kj} = \begin{cases} (2/N)^{1/2} \sin kj\,, & k > 0 \\ (2/N)^{1/2} \cos kj\,, & k \leq 0 \end{cases} \tag{8}$$

$$\psi_{kj} = -\Lambda_k^{-1}[(1+\lambda \cos k)\phi_{kj} + (\lambda \sin k)\phi_{-kj}]\,, \tag{9}$$

with

$$\Lambda_k^2 = (1 + \lambda^2 + 2\lambda \cos k) \tag{10}$$

and

$$k = 2\pi m/N\,,$$

$$\begin{aligned} &m = -\tfrac{1}{2}N, \ldots, 0, \ldots, \tfrac{1}{2}N - 1\,, && N \text{ even} \\ &m = -\tfrac{1}{2}(N-1), \ldots, 0, \ldots, \tfrac{1}{2}(N-1), && N \text{ odd.} \end{aligned} \tag{11}$$

For $\lambda = 1$ and $m = -\frac{1}{2}N$,

$$\Lambda_k = 0, \quad \phi_{kj} = N^{-1/2}, \quad \psi_{kj} = \pm N^{-1/2}\,. \tag{12}$$

Transformation (6) can be inverted, giving

$$c_j = \frac{1}{2} \sum_k [(\phi_{kj} + \psi_{kj})\eta_k + (\phi_{kj} - \psi_{kj})\eta_k^\dagger]\,. \tag{13}$$

B. Dynamical correlation functions

We wish to calculate the spin-spin and energy-energy correlation functions

$$\langle\{S^x(-q), S^x(q,\omega)\}\rangle = \frac{1}{2\pi} \int e^{-i\omega t} \langle\{S^x(-q), S^x(q,t)\}\rangle\, dt \tag{14}$$

and

$$\langle\{E(-q), E(q,\omega)\}\rangle = \frac{1}{2\pi} \int e^{-i\omega t} \langle\{E(-q), E(q,t)\}\rangle\, dt\,, \tag{15}$$

where

$$S^x(q,t) = \sum_l e^{iql} S_l^x(t) \tag{16}$$

and

$$E(q,t) = \sum_l e^{iql} E_l(t)\,, \tag{17}$$

with the energy density defined as

$$E_l(t) = -\Gamma S_l^x(t) - \tfrac{1}{2} J[S_l^z(t) S_{l+1}^z(t) + S_{l-1}^z(t) S_l^z(t)]\,. \tag{18}$$

These are symmetrized correlation functions in which

$$\{A, B\} = \tfrac{1}{2}(AB + BA)\,. \tag{19}$$

From (14) and (15) we can obtain the time-dependent correlations $\langle\{S^x(-q), S^x(q,t)\}\rangle$ and $\langle\{E(-q), E(q,t)\}\rangle$ by means of Fourier transforms. We will also calculate the autocorrelation functions $\langle\{S_i^x, S_i^x(t)\}\rangle$ and $\langle\{E_i, E_i(t)\}\rangle$.

The various correlation functions involve the operators $S_j^z(t)$ and $S_j^x(t)$, which have the time dependence

$$S_j^\alpha(t) = e^{iHt} S_j^\alpha(0) e^{-iHt}\,, \quad \alpha = x, y\,. \tag{20}$$

(We have set $\hbar = 1$.) The time dependence is complicated because S_j^z and S_j^x do not commute with H. We avoid this difficulty by using the transformations (2), (3), and (7) to convert the above into operators involving $\eta_k(t)$ and $\eta_k^\dagger(t)$. The noninteracting fermion operators have the simple time dependence

$$\eta_k(t) = e^{iHt}\eta_k(0)e^{-iHt} = e^{-i\Gamma\Lambda_k t}\eta_k \tag{21}$$

$$\eta_k^\dagger(t) = e^{i\Gamma\Lambda_k t}\eta_k^\dagger\,. \tag{22}$$

The correlation functions are then expressed as sums of products of ϕ's and ψ's multiplied by correlation functions involving η_k's. The latter correlation functions can be easily evaluated using Wick's theorem as applied to statistical mechanics.[8,9] The contractions are defined by

$$\langle\eta_k^\dagger \eta_{k'}^\dagger\rangle = \langle\eta_k \eta_{k'}\rangle = 0\,, \tag{23a}$$

$$\langle\eta_k^\dagger \eta_{k'}\rangle = \delta_{kk'} f_k \equiv \delta_{kk'} \frac{1}{e^{\beta\Gamma\Lambda_k} + 1}\,, \tag{23b}$$

$$\langle\eta_k \eta_{k'}^\dagger\rangle = \delta_{kk'}(1 - f_k)\,. \tag{23c}$$

Since the intermediate steps are lengthy we report only the final results. The details of the calculation are given elsewhere.[10]

III. RESULTS

A. $J = 2\Gamma$, all q, $T = 0$, and $T = \infty$

For $J = 2\Gamma$ we have $\lambda = 1$ and $\Gamma = \Gamma_c = \frac{1}{2}J$. This is the field-strength ratio at which ordering can just take place at zero temperature. For $\lambda = 1$ a number of expressions simplify; we have

$$\psi_{kj} = \begin{cases} -(2/N)^{1/2} \sin k(j + \frac{1}{2})\,, & k > 0 \\ -(2/N)^{1/2} \cos k(j + \frac{1}{2})\,, & k \leq 0 \end{cases} \tag{24}$$

and

$$\Lambda_k = 2\cos\tfrac{1}{2}k\,. \tag{25}$$

For $T = \infty$, $\lambda = 1$, and defining $\hat{\omega} = \omega/\Gamma$, we find

$$\langle\{S^x(-q), S^x(q,\omega)\}\rangle = \frac{N}{4\pi}\frac{1}{\Gamma}\left(\frac{[(4\sin\frac{1}{4}q)^2 - \hat{\omega}^2]^{1/2}}{(4\sin\frac{1}{4}q)^2}\,\Theta(4\sin\tfrac{1}{4}q - \hat{\omega})\Theta(4\sin\tfrac{1}{4}q + \hat{\omega}) + \frac{[(4\cos\frac{1}{4}q)^2 - \hat{\omega}^2]^{1/2}}{(4\cos\frac{1}{4}q)^2} \times \Theta(4\cos\tfrac{1}{4}q - \hat{\omega})\Theta(4\cos\tfrac{1}{4}q + \hat{\omega})\right) \tag{26}$$

and

$$\langle\{E(-q), E(q,\omega)\}\rangle = \frac{\Gamma N}{8\pi}\left(\frac{[(4\sin\frac{1}{4}q)^2-\hat{\omega}^2]^{1/2}}{(4\sin\frac{1}{4}q)^2}(3+\cos q+4\cos\tfrac{1}{2}q)\Theta(4\sin\tfrac{1}{4}q-\hat{\omega})\Theta(4\sin\tfrac{1}{4}q+\hat{\omega}) + \frac{[(4\cos\frac{1}{4}q)^2-\hat{\omega}^2]^{1/2}}{(4\cos\frac{1}{4}q)^2}(3+\cos q-4\cos\tfrac{1}{2}q)\Theta(4\cos\tfrac{1}{4}q-\hat{\omega})\Theta(4\cos\tfrac{1}{4}q+\hat{\omega})\right), \quad (27)$$

where $\Theta(x)$ is the Heaviside function, which is defined as

$$\Theta(x) = \begin{cases} 1 & \text{if } x>0, \\ 0 & \text{if } x<0. \end{cases} \quad (28)$$

See Figs. 1 and 2. Equations (26) and (27) can be Fourier transformed using Eq. 1.3(8) of Ref. 11. We obtain

$$\langle\{S^x(-q), S^x(q,t)\}\rangle = \frac{N}{4}\left(\frac{J_1(4\Gamma t\sin\frac{1}{4}q)}{4\Gamma t\sin\frac{1}{4}q}+\frac{J_1(4\Gamma t\cos\frac{1}{4}q)}{4\Gamma t\cos\frac{1}{4}q}\right) \quad (29)$$

and

$$\langle\{E(-q), E(q,t)\}\rangle = \frac{\Gamma^2 N}{8}\left(\frac{J_1(4\Gamma t\sin\frac{1}{4}q)}{4\Gamma t\sin\frac{1}{4}q}(3+\cos q+4\cos\tfrac{1}{2}q) + \frac{J_1(4\Gamma t\cos\frac{1}{4}q)}{4\Gamma t\cos\frac{1}{4}q}(3+\cos q-4\cos\tfrac{1}{2}q)\right), \quad (30)$$

where $J_1(x)$ is the Bessel function of order one.

For $T=0$, $\lambda=1$, we find

$$\langle\{S^x(-q), S^x(q,\omega)\}\rangle = \frac{1}{\Gamma}\left(\frac{N}{\pi}\right)^2\delta(q)\delta(\hat{\omega}) + \frac{N}{2\pi}\frac{1}{\Gamma}\frac{[(4\cos\frac{1}{4}q)^2-\hat{\omega}^2]^{1/2}}{(4\cos\frac{1}{4}q)^2} \times\Theta(4\cos\tfrac{1}{4}q-\hat{\omega})\Theta(4\cos\tfrac{1}{4}q+\hat{\omega}) \quad (31)$$

and

$$\langle\{E(-q), E(q,\hat{\omega})\}\rangle = \frac{1}{\Gamma}\left(\frac{2\Gamma N}{\pi}\right)^2\delta(q)\delta(\hat{\omega}) + \frac{\Gamma N}{4\pi}\frac{[(4\cos\frac{1}{4}q)^2-\hat{\omega}^2]^{1/2}}{(4\cos\frac{1}{4}q)^2}(3+\cos q-4\cos\tfrac{1}{2}q) \times\Theta(4\cos\tfrac{1}{4}q-\hat{\omega})\Theta(4\cos\tfrac{1}{4}q+\hat{\omega}). \quad (32)$$

Note that

$$\langle S^x(q)\rangle_{T=0} = (N/\pi)\delta(q) \quad (33)$$

and

$$\langle E(q)\rangle_{T=0} = -(2\Gamma N/\pi)\delta(q), \quad (34)$$

the squares of which appear in the first terms in (31) and (32), respectively. See Figs. 3 and 4. Fourier transforming (31) and (32) we obtain

$$\langle\{S^x(-q), S^x(q,t)\}\rangle = \left(\frac{N}{\pi}\right)^2\delta(q) + \frac{N}{2}\frac{J_2(4\Gamma t\cos\frac{1}{4}q)}{4\Gamma t\cos\frac{1}{4}q} \quad (35)$$

and

$$\langle\{E(-q), E(q,t)\}\rangle = \left(\frac{N2\Gamma}{\pi}\right)^2\delta(q) + \frac{\Gamma^2 N}{4}\frac{J_1(4\Gamma t\cos\frac{1}{4}q)}{4\Gamma t\cos\frac{1}{4}q}(3+\cos q-4\cos\tfrac{1}{2}q). \quad (36)$$

The autocorrelation functions may be expressed in terms of Bessel and related functions (see Ref. 12). For $T=\infty$ we find

$$\langle\{S_i^x, S_i^x(t)\}\rangle = \tfrac{1}{4}\{[J_0(2\Gamma t)]^2+[J_1(2\Gamma t)]^2\} \quad (37)$$

and

$$\langle\{E_i, E_i(t)\}\rangle = \Gamma^2\left([J_0(2\Gamma t)]^2+[J_1(2\Gamma t)]^2 - \frac{J_0(2\Gamma t)J_1(2\Gamma t)}{2\Gamma t} - \frac{[J_1(2\Gamma t)]^2}{8(\Gamma t)^2}\right), \quad (38)$$

and for $T=0$ we find

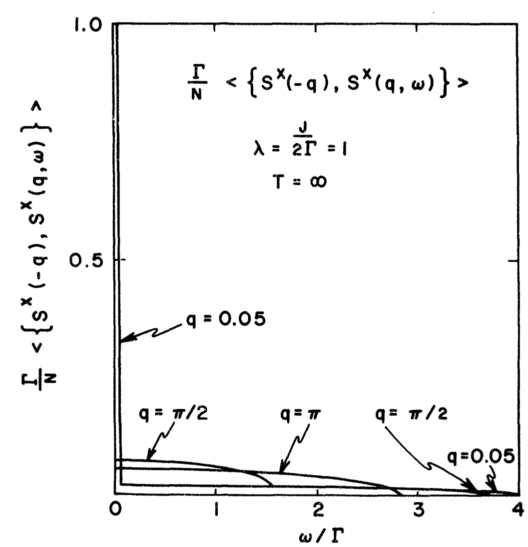

FIG. 1. $(\Gamma/N)\langle\{S^x(-q), S^x(q,\omega)\}\rangle$ vs ω/Γ at $T=\infty$, for $\lambda=J/2\Gamma=1$, Eq. (26).

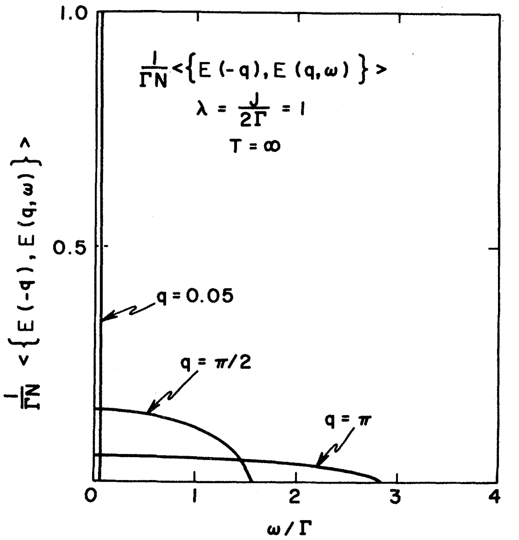

FIG. 2. $(1/\Gamma N)\langle\{E(-q),\ E(q,\omega)\}\rangle$ vs ω/Γ at $T=\infty$, for $\lambda=J/2\Gamma=1$, Eq. (27).

$$\langle\{S_i^x,\ S_i^x(t)\}\rangle = 1/\pi^2 + \tfrac{1}{4}\{[J_0(2\Gamma t)]^2 + [J_1(2\Gamma t)]^2 - [E_0(2\Gamma t)]^2 - [E_1(2\Gamma t)]^2\} \quad (39)$$

and

$$\begin{aligned}\langle\{E_i,\ E_i(t)\}\rangle = \frac{4\Gamma^2}{\pi^2} + \Gamma^2\Big([J_0(2\Gamma t)]^2 + [J_1(2\Gamma t)]^2 &- \frac{J_0(2\Gamma t)J_1(2\Gamma t)}{2\Gamma t} - \frac{[J_1(2\Gamma t)]^2}{2(2\Gamma t)^2} - [E_0(2\Gamma t)]^2 - [E_1(2\Gamma t)]^2 \\ &+ \frac{E_0(2\Gamma t)E_1(2\Gamma t)}{2\Gamma t} + \frac{[E_1(2\Gamma t)]^2}{2(2\Gamma t)^2} - \frac{3}{\pi}\frac{E_0(2\Gamma t)}{2\Gamma t} + \frac{1}{\pi}\frac{E_1(2\Gamma t)}{(2\Gamma t)^2} - \frac{2}{\pi}\frac{1}{(2\Gamma t)^2}\Big)\ . \end{aligned} \quad (40)$$

$J_n(z)$ is the Bessel function of nth order, which may be defined in integral form as

$$J_n(z) = \frac{1}{\pi}\int_0^\pi \cos(n\theta - z\sin\theta)\,d\theta \quad (41)$$

and $E_n(z)$ is the related Anger-Weber function, which is defined as

$$E_n(z) = \frac{1}{\pi}\int_0^\pi \sin(n\theta - z\sin\theta)\,d\theta\ . \quad (42)$$

B. $q=0$, all $\lambda=J/2\Gamma$, $T=0$, and $T=\infty$

For $T=\infty$ and small q, $\langle\{S^x(-q),\ S^x(q,\omega)\}\rangle$ has two terms, a narrow peak at $\omega=0$ which is due to the long-time asymptotic behavior of $\langle\{S^x(-q),\ S^x(q,t)\}\rangle$ and two quasiresonant peaks at plus and minus a finite frequency which are due to the rapidly decaying part of $\langle\{S^x(-q),\ S^x(q,t)\}\rangle$. For $\lambda=1$ the two quasiresonant peaks coalesce into one broad peak (see Fig. 1). For $q=0$, $T=\infty$, we find

$$\begin{aligned}\langle\{S^x(-q),\ S^x(q,\omega)\}\rangle_{q=0} &= \frac{1}{\Gamma}\frac{N}{16\pi}\frac{[4\lambda^2 - (\frac{1}{4}\hat{\omega}^2 - 1 - \lambda^2)^2]^{1/2}}{|\hat{\omega}|} \\ &\times[\Theta(\hat{\omega} - 2|1-\lambda|)\Theta(2(1+\lambda)-\hat{\omega}) + \Theta(\hat{\omega}+2(1+\lambda))\Theta(-2|1-\lambda| - \hat{\omega})] \\ &+\begin{Bmatrix}\frac{1}{4}N(1-\frac{1}{2}\lambda^2)\delta(\omega) & \text{for } \lambda<1 \\ \frac{1}{4}N[\frac{1}{2}\delta(\omega)] & \text{for } \lambda\geq 1\end{Bmatrix}\end{aligned} \quad (43)$$

and

$$\langle\{E(-q),\ E(q,\omega)\}\rangle_{q=0} = \tfrac{1}{4}N\Gamma^2(1+\lambda^2)\delta(\omega)\ . \quad (44)$$

For small but finite q the central peak acquires a finite width. This width is determined by the factor $\delta(\omega - \Gamma\Lambda_k + \Gamma\Lambda_{k+q}) + \delta(\omega + \Gamma\Lambda_k - \Gamma\Lambda_{k+q})$, which implies that for small q the term is nonzero only for $-\Gamma A q < \omega < \Gamma A q$, where A is the minimum of λ and 1. The behavior of the quasiresonant part of $\langle\{S^x(-q),\ S^x(q,\omega)\}\rangle_{q=0}$ [i.e., the part proportional to $\delta(\omega)$ has been subtracted out] for various values of λ is shown in Fig. 5.

For $T=0$ and $q=0$ we have

$$\begin{aligned}\langle\{S^x(-q),\ S^x(q,\omega)\}\rangle_{q=0} - \langle S^x(0)\rangle^2\delta(\omega) &= \frac{N}{8\pi}\frac{1}{\Gamma}\frac{[4\lambda^2 - (\frac{1}{4}\hat{\omega}^2 - \lambda^2 - 1)^2]^{1/2}}{|\hat{\omega}|} \\ &\times[\Theta(\hat{\omega} - 2|1-\lambda|)\Theta(2(1+\lambda)-\hat{\omega}) + \Theta(\hat{\omega}+2(1+\lambda))\Theta(-2|1-\lambda| - \hat{\omega})]\ ,\end{aligned} \quad (45)$$

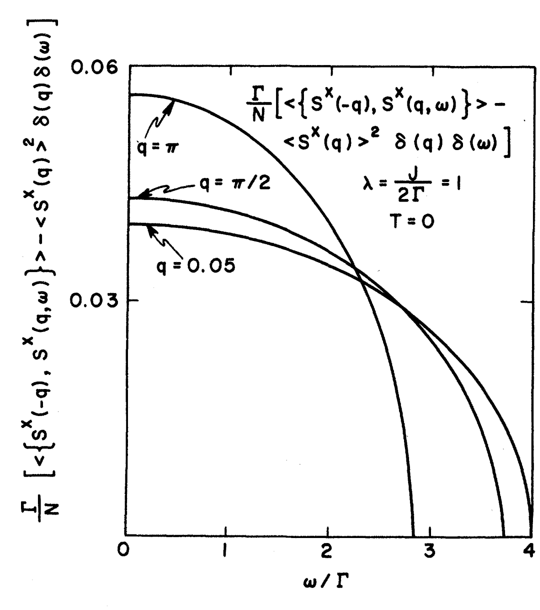

FIG. 3. $(\Gamma/N)[\langle\{S^x(-q),\ S^x(q,\omega)\}\rangle - \langle S^x(q)\rangle^2\delta(q)\delta(\omega)]$ vs ω/Γ at $T=0$, for $\lambda=J/2\Gamma=1$, Eq. (31).

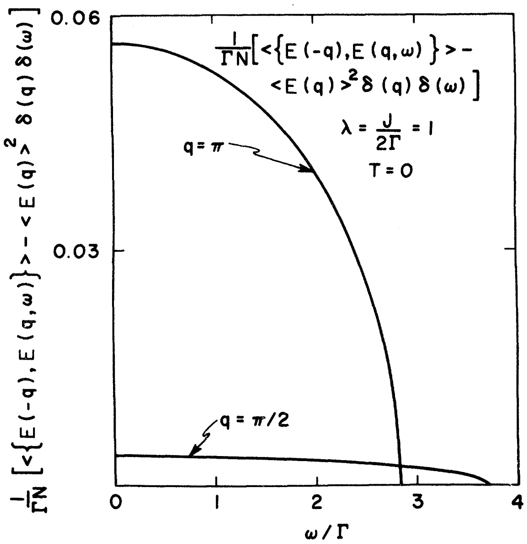

FIG. 4. $(1/\Gamma N)[\langle\{E(-q),\ E(q,\omega)\}\rangle - \langle E(q)\rangle^2\delta(q)\delta(\omega)]$ vs ω/Γ at $T=0$, for $\lambda=J/2\Gamma=1$, Eq. (32). (For $q=0$ the function is 0.)

where

$$\langle S^x(q)\rangle = \tfrac{1}{2}\,\delta(q)\sum_k \frac{1+\lambda\cos k}{\Lambda_k}$$

$$= \tfrac{1}{2}\,\delta(q)\,\frac{N}{2\pi}\int_{-\pi}^{\pi} dk\,\frac{1+\lambda\cos k}{(1+\lambda^2+2\lambda\cos k)^{1/2}}\ , \qquad (46)$$

and

$$\langle\{E(-q),\ E(q,\omega)\}\rangle_{q=0} - \langle E(0)\rangle^2\,\delta(\omega) = 0\ , \qquad (47)$$

where

$$\langle E(q)\rangle = -\frac{\Gamma}{2}\,\delta(q)\sum_k \Lambda_k = E_0\delta(q) \qquad (48)$$

and E_0 is the ground-state energy:

$$E_0 = -\frac{\Gamma}{2}\sum_k \Lambda_k = -\frac{N\Gamma}{4\pi}\int_{-\pi}^{\pi}(1+\lambda^2+2\lambda\cos k)^{1/2}\,dk\ . \qquad (49)$$

IV. DISCUSSION OF THE RESULTS

A. Energy-energy correlation functions

Expression (27) shows that as q becomes small the energy-density correlation function $\langle\{E(-q),\ E(q,\omega)\}\rangle$ at infinite temperature becomes peaked about $\omega=0$ with a broad low background. In the limit $q=0$ the peak becomes a δ function of ω and the background disappears. This behavior is shown in expression (44), which gives the correlation function for $q=0$ and arbitrary λ. The δ function for $q=0$ and the peaking for small q is due to the fact that the energy density for $q=0$ is the Hamiltonian operator and hence is a constant of motion, i.e.,

$$[E(q=0),H]=0\ , \qquad (50)$$

and so for $q=0$ and infinite temperature we can compute the correlation function $\langle\{E(-q),E(q,t)\}\rangle$ without making use of the fermion representation. We have

$$\langle\{E(0),E(0,t)\}\rangle = \langle\{E(0),\ e^{iHt}E(0)e^{-iHt}\}\rangle$$

$$= \langle\{E(0),E(0)\}\rangle$$

$$= \tfrac{1}{4}N\Gamma^2(\lambda^2+1)\ , \qquad (51)$$

which is constant in time, and so the frequency Fourier transformation yields expression (44) directly. By using the small-argument expansion of the Bessel functions

$$J_\nu(z) \sim \tfrac{1}{2}z\,\Gamma(\nu+1) \qquad (52)$$

we can see that expression (30) for the time correlation function $\langle\{E(-q),E(q,t)\}\rangle$ for $\lambda=1$ reduces in the limit $q=0$ to expression (51).

For small q and finite temperatures, the correlation function of the energy-density fluctuations $\langle\{E(-q),E(q,\omega)\}\rangle - \langle E(q)\rangle^2$ still has a peak about $\omega=0$ of the same width as at $T=\infty$, but reduced in intensity. Note that $\langle E(q)\rangle=0$ for $T=\infty$.

At zero temperature the intensity is equal to zero when $q=0$, and so the energy-density-fluctuation correlation function has a peak only for finite T, as shown in (32) and (47). That the correlation function equals zero at $T=0$ for $q=0$ can be explained by thermodynamic arguments. The specific heat of the system is equal to $(\langle E(q=0)^2\rangle - \langle E(q=0)\rangle^2)/kT^2$. Since specific heats vanish at zero tempera-

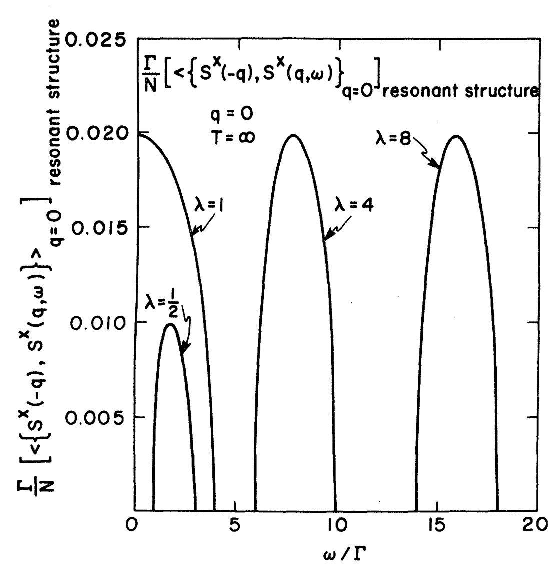

FIG. 5. Quasiresonant peaks of $(\Gamma/N)\langle\{S^x(-q),\ S^x(q,\omega)\}\rangle_{q=0}$ vs ω/Γ at $T=\infty$, for various values of $\lambda=J/2\Gamma$, Eq. (43).

ture, we must have $\langle E^2\rangle - \langle E\rangle^2 = 0$ at $T=0$.

Although the spectrum of the correlation function of the energy-density fluctuations is peaked about $\omega = 0$ for small values of q, this peaking is not due to diffusion since the asymptotic behavior is not of the form e^{-Dq^2t}. The absence of diffusion agrees with the fact that the IMTF for the spin-$\frac{1}{2}$ chain can be transformed to a system of noninteracting quasiparticles. Simple arguments in the kinetic theory of gases give the diffusion coefficient as being proportional to the mean free path. If the particles are noninteracting the mean free path is infinite, and so the diffusion constant is infinite. Thus in the case of noninteracting particles we would not expect diffusion.

On the other hand the chain with $S > \frac{1}{2}$ and the two- and three-dimensional IMTF with arbitrary spin do show diffusion.[10] This can be established from a calculation of the second and fourth moments of the energy-density correlation function, m_2^E and m_4^E. For the one-dimensional spin-$\frac{1}{2}$ IMTF we have $m_2^E \propto q^2$ and $m_4^E \propto q^4$, for small q. In contrast, for $S > \frac{1}{2}$ and for arbitrary S in two and three dimensions, $m_2^E \propto q^2$ and $m_4^E \propto q^2$. The q^4 dependence in m_4^E for the one-dimensional spin-$\frac{1}{2}$ IMTF reflects the fact that the thermal current operator, defined by $j^E = \lim_{q\to 0}(i/q)dE(q,t)/dt$ $[=\frac{1}{2}J\sum_n S_n^z(S_{n+1}^y - S_{n-1}^y)$, for one dimensional systems], is a constant of motion for this system, which is not the case in the other examples of the IMTF.

It happens then that the spin-$\frac{1}{2}$ chain, by virtue of the fact that it can be transformed to a system of noninteracting quasiparticles, has behavior which is quite different from the other cases. This is seen in the lack of diffusion for the energy density and will be seen in the form of the spin-spin correlation function.

B. Spin-correlation functions

We first will look at the spin-correlation functions in two limiting cases in which the correlation functions can be analyzed without making use of the fermion representation. If in the Hamiltonian

$$H = -\Gamma\sum_i S_i^x - J\sum_i S_i^z S_{i+1}^z \tag{1}$$

we set $J=0$ (i.e., $\lambda = 0$ in the fermion representation), H represents a system of independent spins; if we set $\Gamma = 0$ (i.e., $\lambda = \infty$), H is the Ising-model Hamiltonian.

In the case of the free spins we have

$$H = -\sum_i S_i^x , \tag{53}$$

so that the total x component of the spin is a constant of motion and we have

$$\langle\{S^x(q,t), S^x(-q)\}\rangle = \langle\{e^{iHt}S^x(q)e^{-iHt}, S^x(-q)\}\rangle$$

$$= \langle\{S^x(0), S^x(0)\}\rangle . \tag{54}$$

In the finite-temperature limit this equals $\frac{1}{3}NS(S+1) = \frac{1}{4}N$ which agrees with expression (43) for the spin-correlation function.

In the other limiting case (i.e., the Ising model) we have

$$H = -J\sum_i S_i^z S_{i+1}^z \tag{55}$$

and

$$S^x(q,t) = \sum_l e^{iql}e^{iHt}S_l^x e^{-iHt}$$

$$= \frac{1}{2}\sum_l e^{iql}S_l^+ e^{-Jt(S_{l+1}^z + S_{l-1}^z)} + S_l^- e^{+iJt(S_{l+1}^z + S_{l-1}^z)} , \tag{56}$$

where $S_l^+ = S_l^x + iS_l^y$ and $S_l^- = S_l^x - iS_l^y$, and where we have used

$$[S_i^z, S_j^\pm] = \pm\delta_{ij}S_i^\pm \tag{57}$$

and

$$e^A C e^{-A} = C + \frac{1}{1!}[A, C] + \frac{1}{2!}[A,[A,C]] + \frac{1}{3!}[A,[A,[A,C]]] + \cdots . \tag{58}$$

Hence for $T = \infty$ we have

$$\langle\{S^x(q=0), S^x(q=0,t)\}\rangle = \tfrac{1}{8}N(1+\cos Jt) , \tag{59}$$

where we have used the fact that at infinite temperatures spins on different sites are uncorrelated, together with the result

$$\langle e^{iJtS_l^z}\rangle_{T=\infty} = \tfrac{1}{2}e^{iJt1/2} + \tfrac{1}{2}e^{iJt(-1/2)} = \cos\tfrac{1}{2}Jt . \tag{60}$$

Fourier transforming (59), we obtain

$$\langle\{S^x(-q), S^x(q,\omega)\}\rangle_{q=0} = \tfrac{1}{8}N\,\delta(\omega) + \tfrac{1}{16}N[\delta(\omega+J) + \delta(\omega - J)] , \tag{61}$$

which agrees with expression (43) in the limit $\lambda \to \infty$. Expression (61) shows $\langle\{S^x(-q), S^x(q,\omega)\}\rangle$ as a function of ω to have δ function peaks at $\omega = 0$ and $\omega = \pm J$. The three-peak structure of $\langle\{S^x(-q), S^x(q,\omega)\}\rangle$ is a general feature for small q; the function is composed of two parts, quasiresonant peaks at plus and minus a finite frequency and a peak at $\omega = 0$ which is related to the energy-density correlation function. This can be seen in the expressions (26) and (43) and in Figs. 1 and 5. (For the case $\lambda = 1$ the two quasiresonant peaks coalesce into a broad background.)

Comparing expressions (26) and (27) and expressions (43) and (44) we see that the peaks about $\omega = 0$ for the energy-density and the spin-density correlation functions are the same function of ω which is multiplied by different functions of q. Thus for small q the spin correlation contains the energy-density correlation. Such coupling of the spin and energy densities is predicted by thermodynamic arguments.[13] These, together with the hydrodynamic approximation when applied to the simple cubic IMTF, lead to the expression[5]

$$\frac{\langle\{S^x(-q), S^x(q,\omega)\}\rangle}{\langle\{S^x(-q), S^x(q)\}\rangle} = \frac{\chi_T - \chi_S}{\chi_T}\,\frac{\Gamma_E(q)}{\pi[\omega^2 + \Gamma_E(q)^2]} + \frac{\chi_S}{\chi_T} f(\omega)\ , \tag{62}$$

where χ_T and χ_S are the isothermal and adiabatic susceptibilities in the x direction. The symbol $\Gamma_E(q)$ denotes the decay rate of the temperature fluctuations and is equal to $D_E q^2$, where D_E is the thermal diffusion constant. Also, $f(\omega)$ is a slowly varying function of q with a width (in frequency) $\gg \Gamma_E(q)$ and whose integral over the interval $(-\infty, \infty)$ is equal to unity.

We noted earlier that for the spin-$\frac{1}{2}$ chain there is no diffusion of the energy density, and so we should replace the Lorentzian appearing in expression (62) by the normalized energy-density correlation function. We also find for the spin-$\frac{1}{2}$ chain that the coefficient $(\chi_T - \chi_S)/\chi_T$ must be modified. Noting that, for $T=\infty$,

$$\langle S^z(-q)S^z(q)\rangle = \tfrac{1}{4}N$$

and

$$\langle E(-q)E(q)\rangle = \tfrac{1}{4}N\Gamma^2\left[\tfrac{1}{2}\lambda^2(1+\cos q)+1\right]$$

and using Eqs. (43) and (44) we find

$$\frac{[\langle\{S^x(-q), S^x(q,\omega)\}\rangle/\langle\{S^x(-q), S^x(q)\}\rangle]_{q=0,\text{peak}}}{[\langle\{E(-q), E(q,\omega)\}\rangle/\langle\{E(-q), E(q)\}]_{q=0}} = \begin{cases} 1-\frac{1}{2}\lambda^2, & \lambda<1 \\ \frac{1}{2}, & \lambda>1 \end{cases} \tag{63}$$

whereas we obtain for $T=\infty$

$$(\chi_T - \chi_S)/\chi_T = 1/(\lambda^2+1)\ , \tag{64}$$

which does not agree with the ratio predicted by thermodynamic arguments given in Eq. (63). This disagreement is related to the fact that the isolated, or Kubo, susceptibility χ_I for the spin-$\frac{1}{2}$ chain is not the same as the corresponding adiabatic susceptibility.[6] We calculate the isolated susceptibility as

$$\begin{aligned}\chi_I &= \text{Re}\chi_{\text{Kubo}}(q=0, \omega=0) \\ &= \beta P\int_{-\infty}^{\infty}\langle\{S^x(-q), S^x(q,\omega)\}\rangle_{q=0}\,d\omega \\ &= \begin{cases}\beta\frac{1}{4}N\frac{1}{2}\lambda^2, & \lambda<1 \\ \beta\frac{1}{4}N\frac{1}{2}, & \lambda>1\end{cases}\end{aligned} \tag{65}$$

where P denotes the principle value of the integral and where in the last line we have used Eq. (43). Thus we find

$$\frac{\chi_T-\chi_I}{\chi_T} = \begin{cases} 1-\frac{1}{2}\lambda^2, & \lambda<1 \\ \frac{1}{2}, & \lambda>1 \end{cases} \tag{66}$$

which is equal to the ratio of the normalized correlation functions as given in Eq. (63). So for the spin-$\frac{1}{2}$ chain we must replace χ_S by χ_I in the coefficient of the energy-density term. The question of which susceptibility, isolated or adiabatic, to use in calculating the energy-density contribution to the spin-density correlation function has arisen before[14]; however, for most systems the question is moot in that the isolated and adiabatic susceptibilities are the same. Wilcox[15] has derived bounds on the isothermal, adiabatic, and isolated susceptibilities,

$$0 \le \chi_I \le \chi_S \le \chi_T\ , \tag{67}$$

and has commented that it is not necessarily true that $\chi_S = \chi_I$ in the thermodynamic limit, as has been stated by others. Verbeek[16] and Siskens and Mazur[17] have shown that the isolated susceptibility equals the adiabatic susceptibility for ergodic systems. Mazur[18] has also shown that some systems are nonergodic; in particular, the systems described by the Hamiltonian

$$H = \sum_{j=1}^{N}\left[(1+\gamma)S_j^x S_{j+1}^x + (1-\gamma)S_j^y S_{j+1}^y - BS_j^z\right] \tag{68}$$

for a one dimensional chain of spin-$\frac{1}{2}$ are nonergodic. For $\gamma=1$ the above Hamiltonian reduces to (1), the IMTF. Thus the IMTF for a spin-$\frac{1}{2}$ chain is nonergodic, and so we have $\chi_I \ne \chi_S$; however, it is seen that $\chi_I \le \chi_S$.

For the spin-$\frac{1}{2}$-chain IMTF we can write an expression analogous to that given in (62); we write

$$\langle\{S^x(-q), S^x(q,\omega)\}\rangle = \langle\{S^x(-q), S^x(q)\}\rangle\left(\frac{\chi_T-\chi_I}{\chi_T}\,g(q,\omega) + \frac{\chi_I}{\chi_T}f(\omega)\right)\ , \tag{69}$$

where $g(q,\omega)$ is equal to $\langle\{E(-q), E(q,\omega)\}\rangle/\langle\{E(-q), E(q)\}\rangle$, and it is assumed that $|q| \ll 1$. $f(\omega)$ is the corresponding function of Eq. (62).

In fact Eq. (69) is a generalization of (62). For ergodic systems we can replace χ_I with χ_S in expression (69). If there is energy diffusion we can approximate the correlation function $\langle\{E(-q), E(q,\omega)\}\rangle/\langle\{E(-q), E(q)\}\rangle$ by the hydrodynamic form

$$g(q,\omega) = \Gamma_E(q)/\pi[\omega^2 + \Gamma_E(q)^2]\ , \tag{70}$$

where $\Gamma_E(q) = D_E q^2$, with D_E being the energy-diffusion constant. Making these two identifications we obtain Eq. (62) from (69).

The bifurcation of the spin-density correlation function as expressed in (69) for the spin-$\frac{1}{2}$ chain is then a general feature of the Hamiltonian and is independent of the hydrodynamic approximations.

V. SUMMARY

The IMTF for the spin $S=\frac{1}{2}$ chain can be solved exactly. It is hoped that results for this system will cast light on the dynamics of the three dimensional IMTF. The dynamics of the one dimensional chain will not be masked by approximations; however, the spin-$\frac{1}{2}$ chain does have some peculiarities which the other realizations of the IMTF do not have.

The energy-energy density correlation function spectrum for $q \approx 0$ shows a peaking about $\omega = 0$. For the spin-$\frac{1}{2}$ chain this behavior is nondiffusive, whereas for the other systems it is diffusive. The peaking about $\omega = 0$ is, however, a general feature of the IMTF.

The spin-spin correlation-function spectrum shows a three-peak structure for q small and $T = \infty$. This behavior which has been observed for the three-dimensional IMTF[19] and which has been shown to be due to the coupling of the energy and transverse spin densities[5] is now seen to be a general feature of the Hamiltonian and is not due to hydrodynamic approximations. For the spin-$\frac{1}{2}$ chain the energy density is not diffusive and $\chi_I \neq \chi_S$, and so the three-peak behavior is expressed as in (69). Expression (69) does reduce to the usual form (62) in the other cases.

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