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Dynamics of Heisenberg ferromagnets at low temperature

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The dynamical correlation function $G_{\mathbf{r}}(t)\equiv\langle \mathbf{S}_{\mathbf{r}}(t)\cdot\mathbf{S}_0(0)\rangle$ and dynamical structure factor $S_{\mathbf{q}}(\omega)$ are calculated by the modified spin-wave theory for the low-dimensional quantum Heisenberg ferromagnets at low temperature. We use the Dyson-Maleev transformation, ideal spin-wave states, and the rotational averaging. $S_{\mathbf{q}}(\omega)$ satisfies the dynamic scaling relation. The explicit form of the scaling function is obtained. The classical limit of our results is compared with a molecular-dynamics calculation. The agreement is surprisingly good.

Low-dimensional Heisenberg ferromagnets have attracted much experimental and theoretical interest because they relate to quasi-low-dimensional magnets and ^{3}He atoms adsorbed on a solid surface.[1] At present we understand the static properties of these systems. They have no long-range order at finite temperature. The correlation function decays exponentially and correlation length is proportional to $1/T$ for 1D and $\exp(\alpha/T)$ for 2D. But for dynamical properties we do not know as much. As these systems have strong short-range order, they may have a sloppy spin-wave mode.

In recent papers[2] we proposed the modified spin-wave theory for these systems. Approximations of the same kind for 3D systems had been done by several authors.[3] Static properties such as free energy and instantaneous two-point functions were calculated. These agreed very well with numerical results of Bethe ansatz equations[4,5] and Monte Carlo calculations[6] at low temperatures. Modified spin-wave theory is characterized by the following: (i) the mean-field theory for ideal spin-wave states; (ii) the chemical potential for the spin wave is determined so that $\langle S_i^z\rangle=0$; (iii) the rotational averaging for rotationally asymmetric physical quantities. On the contrary, the orthodox spin-wave theory[7] is the perturbation expansion by $1/S$. The chemical potential is the uniform external magnetic field. Physical quantities are calculated in a finite field. To get the zero-field result one takes the limit of the infinite system and after that the limit of the zero field. Rotational averaging cannot be taken because the field breaks the symmetry.

In the following we will set $\hbar=k_B=1$. The Hamiltonian is

$$H=-J\sum_{\langle ij\rangle}S_i\cdot S_j \ . \tag{1}$$

We assume exchange coupling between nearest neighbors, a periodic lattice with N spins, and a periodic boundary condition. The two-point function $\langle S_i^\alpha(t)S_j^\beta(0)\rangle$ $(\alpha,\beta=x,y,z)$ is the basic quantity for the dynamics of this system. As this system is rotationally symmetric in spin space and translationally symmetric in lattice space, we have

$$\langle S_i^\alpha(t)S_j^\beta(0)\rangle=\tfrac{1}{3}\delta_{\alpha\beta}G_{\mathbf{r}_i-\mathbf{r}_j}(t)\ ,$$

$$G_{\mathbf{r}}(t)\equiv\langle \mathbf{S}_{\mathbf{r}}(t)\cdot\mathbf{S}_0(0)\rangle\ .$$

In our experience the direct calculation of the left-hand side (lhs) by the modified spin-wave theory is dangerous because it is asymmetric for rotation in spin space. Our density matrix breaks the rotational symmetry. So this theory gives poor results for rotationally asymmetric quantities. Then we try to calculate the symmetric quantity $G_{\mathbf{r}}(t)$. We define its Fourier transforms as

$$S_{\mathbf{q}}(t)\equiv N^{-1}\sum_{\mathbf{r}}G_{\mathbf{r}}(t)e^{-i\mathbf{q}\cdot\mathbf{r}}\ ,$$

$$S_{\mathbf{q}}(\omega)\equiv\frac{1}{2\pi}\int_{-\infty}^{\infty}S_{\mathbf{q}}(t)e^{-i\omega t}dt\ .$$

We call $S_{\mathbf{q}}(\omega)$ a dynamic structure factor. We write $S_{\mathbf{q}}(t=0)$ as $S_{\mathbf{q}}$, which is called the static structure factor. If we know all eigenstates and eigenvalues of H, $S_{\mathbf{q}}(\omega)$ is written as follows:

$$S_{\mathbf{q}}(\omega)=\sum_{I,F}P(I)\delta(\omega-E_F+E_I)\big(\tfrac{1}{2}\langle I|S^{+}_{-\mathbf{q}}|F\rangle\langle F|S^{-}_{\mathbf{q}}|I\rangle+\tfrac{1}{2}\langle I|S^{-}_{-\mathbf{q}}|F\rangle\langle F|S^{+}_{\mathbf{q}}|I\rangle+\langle I|S^{z}_{-\mathbf{q}}|F\rangle\langle F|S^{z}_{\mathbf{q}}|I\rangle\big)\ . \tag{2}$$

Here $S^{\pm,z}_{\mathbf{q}}\equiv N^{-1/2}\sum_l e^{-i\mathbf{q}\cdot\mathbf{r}_l}S_l^{\pm,z}$, $S_l^{\pm}\equiv S_l^x\pm iS_l^y$. $|I\rangle$ and $|F\rangle$ are eigenstates of H. E_I and E_F are their eigenvalues. $P(I)$ is the probability of state I. We use the Dyson-Maleev transformation[8]

$$S_l^-=a_l^\dagger,\quad S_l^+=(2S-a_l^\dagger a_l)a_l,\quad S_l^z=S-a_l^\dagger a_l\ . \tag{3}$$

As Bose operator a_l is defined on the lattice, its Fourier transform is defined on the first Brillouin zone $a_{\mathbf{k}}\equiv\sqrt{1/N}\sum_l\exp(i\mathbf{k}\cdot\mathbf{r}_l)a_l$. The Hamiltonian (1) becomes

$$H=-\frac{Jz}{2}\left[NS^2-2S\sum_{\mathbf{k}}(1-\gamma_{\mathbf{k}})a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+N^{-1}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}(\gamma_{\mathbf{q}}-\gamma_{\mathbf{k}+\mathbf{q}})a_{\mathbf{k}+\mathbf{q}}^{\dagger}a_{\mathbf{k}'-\mathbf{q}}^{\dagger}a_{\mathbf{k}'}a_{\mathbf{k}}\right],\quad \gamma_{\mathbf{q}}\equiv z^{-1}\sum_{\delta}e^{i\mathbf{q}\cdot\delta}\,. \tag{4}$$

Here z is the number of nearest neighbors and the δ's are vectors to the near neighbors. We assume that the eigenstates of H are approximated by ideal spin-wave states:

$$|\{n_{\mathbf{k}}\}\rangle=\prod_{\mathbf{k}}(n_{\mathbf{k}}!)^{-1/2}(a_{\mathbf{k}}^{\dagger})^{n_{\mathbf{k}}}|0\rangle\,. \tag{5}$$

$|0\rangle$ is the ferromagnetic ground state where all spins are in the z direction. The expectation value of (4) is

$$E=-\frac{NJz}{2}\left[S^2-2SN^{-1}\sum_{\mathbf{k}}(1-\gamma_{\mathbf{k}})n_{\mathbf{k}}+N^{-2}\sum_{\mathbf{k},\mathbf{p}}(1-\gamma_{\mathbf{k}}-\gamma_{\mathbf{p}}+\gamma_{\mathbf{k}-\mathbf{p}})[n_{\mathbf{k}}n_{\mathbf{p}}-\tfrac{1}{2}\delta_{\mathbf{k},\mathbf{p}}(n_{\mathbf{k}}^2+n_{\mathbf{k}})]\right]\,. \tag{6}$$

We assign an eigenstate by N quantum numbers $\{n_{\mathbf{k}}\}$. The thermal average of $n_{\mathbf{k}}^2$ is

$$\langle n_{\mathbf{k}}^2\rangle=2\bar{n}_{\mathbf{k}}^2+\bar{n}_{\mathbf{k}},\quad \bar{n}_{\mathbf{k}}\equiv\langle n_{\mathbf{k}}\rangle\,. \tag{7}$$

The free energy

$$F=-\tfrac{1}{2}NJz\left[S-\sum_{\mathbf{k}}(1-\gamma_{\mathbf{k}})\bar{n}_{\mathbf{k}}\right]^2-T\sum_{\mathbf{k}}[(1+\bar{n}_{\mathbf{k}})\ln(1+\bar{n}_{\mathbf{k}})-\bar{n}_{\mathbf{k}}\ln\bar{n}_{\mathbf{k}}]$$

should be minimized under the zero magnetization condition. So we get

$$S=\frac{1}{N}\sum_{\mathbf{k}}\bar{n}_{\mathbf{k}},\quad S'=\frac{1}{N}\sum_{\mathbf{k}}\gamma_{\mathbf{k}}\bar{n}_{\mathbf{k}},\quad \bar{n}_{\mathbf{k}}=\frac{1}{\exp(\varepsilon_{\mathbf{k}}/T)-1}\,,$$
$$\varepsilon_{\mathbf{k}}=JzS'(1-\gamma_{\mathbf{k}})-\mu\,. \tag{8}$$

Parameters S' and μ are determined by these self-consistent equations.

The Fourier transforms of the spin operators in (3) are written as follows:

$$S_{\mathbf{q}}^{-}=a_{\mathbf{q}}^{\dagger},\quad S_{\mathbf{q}}^{+}=2Sa_{-\mathbf{q}}-\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}'}a_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}\,,$$
$$S_{\mathbf{q}}^{z}=N^{1/2}S\delta_{\mathbf{q},0}-N^{-1/2}\sum_{\mathbf{k}}a_{\mathbf{k}+\mathbf{q}}^{\dagger}a_{\mathbf{k}}\,.$$

Consider the term $\langle I|S_{-\mathbf{q}}^{+}|F\rangle\langle F|S_{\mathbf{q}}^{-}|I\rangle$ in Eq. (2). If $\langle F|S_{\mathbf{q}}^{-}|I\rangle\neq0$, $|F\rangle$ should be $(n_{\mathbf{q}}+1)^{-1/2}a_{\mathbf{q}}^{\dagger}|I\rangle$. Then this term is

$$2S(n_q+1)+N^{-1}\left[n_{\mathbf{q}}^2+n_{\mathbf{q}}-\sum_{\mathbf{k}}2(n_{\mathbf{q}}+1)n_{\mathbf{k}}\right]\,.$$

The thermal average of this term is zero, because of (7) and (8). For the second term of (2), $|F\rangle$ should be $n_{-\mathbf{q}}^{-1/2}a_{-\mathbf{q}}|I\rangle$. Then it is

$$2Sn_{-\mathbf{q}}+N^{-1}(n_{-\mathbf{q}}^2+n_{-\mathbf{q}}-\textstyle\sum_{\mathbf{k}}2n_{-\mathbf{q}}n_{\mathbf{k}})$$

and the thermal average also vanishes. For the third term of (2), $|F\rangle$'s should be

$$[(n_{\mathbf{k}+\mathbf{q}}+1)n_{\mathbf{k}}]^{-1/2}a_{\mathbf{k}+\mathbf{q}}^{\dagger}a_{\mathbf{k}}|I\rangle$$

and

$$\langle I|S_{-\mathbf{q}}^{z}|F\rangle\langle F|S_{\mathbf{q}}^{z}|I\rangle=N^{-1}(n_{\mathbf{k}+\mathbf{q}}+1)n_{\mathbf{k}}\,,$$

$$E_F-E_I=e_{\mathbf{k}+\mathbf{q}}-e_{\mathbf{k}}+N^{-1}Jz(1-\gamma_{\mathbf{k}+\mathbf{q}}-\gamma_{\mathbf{k}}+\gamma_{\mathbf{q}})\,,$$

$$e_{\mathbf{k}}\equiv Jz\left[S(1-\gamma_{\mathbf{k}})-N^{-1}\sum_{p}(1-\gamma_{\mathbf{k}}-\gamma_{\mathbf{p}}+\gamma_{\mathbf{k}-\mathbf{p}})n_{\mathbf{p}}\right]-\mu\,.$$

The average of $e_{\mathbf{k}}$ is $\varepsilon_{\mathbf{k}}$ in Eq. (8). Neglecting the term $O(N^{-1})$ and taking thermal averages we have

$$S_{\mathbf{q}}(\omega)=\frac{1}{N}\sum_{\mathbf{k}}\bar{n}_{\mathbf{k}}\bar{n}_{\mathbf{k}+\mathbf{q}}^{+}\delta(\omega+\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}}),\quad \bar{n}_{\mathbf{k}}^{+}\equiv\bar{n}_{\mathbf{k}}+1\,. \tag{9}$$

The Fourier transform of this gives the two-point function $G_r(t)$:

$$G_{\mathbf{r}}(t)=\left[\frac{1}{2N}\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}(\bar{n}_{\mathbf{k}}^{+}e^{i\varepsilon_{\mathbf{k}}t}+\bar{n}_{\mathbf{k}}e^{-i\varepsilon_{\mathbf{k}}t})\right]^2-\left[\frac{1}{2N}\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}(\bar{n}_{\mathbf{k}}^{+}e^{i\varepsilon_{\mathbf{k}}t}-\bar{n}_{\mathbf{k}}e^{-i\varepsilon_{\mathbf{k}}t})\right]^2\,. \tag{10}$$

Equation (9) predicts that $S_{\mathbf{q}}(\omega)$ is always zero at $\omega>2JzS$. As $\bar{n}_{\mathbf{k}}^{+}=\exp(\varepsilon_{\mathbf{k}}/T)\bar{n}_{\mathbf{k}}$, it satisfies the detailed balance condition $S_{\mathbf{q}}(\omega)=e^{\omega/T}S_{\mathbf{q}}(-\omega)$. Equation (10) at $t=0$ gives

$$G_{\mathbf{r}}(0)=\left[N^{-1}\sum_{\mathbf{q}}\bar{n}_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}\right]^2+S\delta_{\mathbf{r}0}\,.$$

This instantaneous two-point function coincides with that in Ref. 2.

At $T=0$ we have $\bar{n}_{\mathbf{k}}=NS\delta_{\mathbf{k}0}$, $\mu=0$, $S'=S$. Then Eq. (9) gives

$$S_{\mathbf{q}}(\omega)=S\delta(\omega-JSz(1-\gamma_{\mathbf{q}}))\,.$$

This means that $S_{\mathbf{q}}(\omega)$ has the δ-function peak at the spin-wave energy.

We can show that Eq. (9) satisfies the dynamic scaling law[9] at low temperature and low momentum. At $k^2\ll T/(JS')$ Eqs. (8) give

$$\tilde{n}_k \simeq \tilde{n}_k^+ \simeq T/\varepsilon_k ,$$

$$\varepsilon_k \simeq JS'[k^2+(2\xi)^{-2}] ,$$

$$\xi = \tfrac{1}{2}\sqrt{JS'/-\mu} .$$

Here ξ is the correlation length. From the investigation of static properties in Refs. 2 we know that $\xi = JS^2/T$ for a 1D and $(JS/T)^{1/2}\exp(2\pi JS^2/T)$ for a 2D square lattice ferromagnet. The sum in Eq. (9) is replaced by an integral:

$$S_q(\omega) = T^2 \int \frac{d^dk}{(2\pi)^d} \frac{\delta(\omega+\varepsilon_k-\varepsilon_{k+q})}{\varepsilon_k\varepsilon_{k+q}} . \tag{11}$$

(i) Linear chain: From the δ function we get

$$k = \tfrac{1}{2}[\omega/(JS'q)-q] .$$

Then Eq. (11) becomes

$$\frac{4}{\pi}\left[\frac{T\xi}{JS'}\right]^2 \frac{\tau}{q} \frac{1}{\{1+[\omega\tau/(q\xi)-q\xi]^2\}\{1+[\omega\tau/(q\xi)+q\xi]^2\}}, \quad \tau \equiv \frac{\xi^2}{JS'} .$$

This means the existence of characteristic time τ. We get the dynamic scaling relation

$$S_q(\omega) = S_q \tau \Phi(q\xi, \omega\tau) , \tag{12}$$

with

$$S_q = \left[\frac{T\xi}{JS'}\right]^2 \frac{2\xi}{1+(q\xi)^2} ,$$

$$\Phi(x,y) = \frac{2}{\pi} \frac{1+x^2}{x[1+(y/x-x)^2][1+(y/x+x)^2]} .$$

(ii) Square lattice: We set $\mathbf{q}=(q,0)$, $q \geq 0$. From the δ function in (11) we have

$$k_x = \tfrac{1}{2}[\omega/(JS'q)-q] .$$

Integrating with respect to k_y we get $S_q(\omega)$:

$$\frac{1}{4\pi q\xi\omega}\left[\frac{T\xi}{JS'}\right]^2 \left\{ \left[1+\left[\frac{\omega\tau}{q\xi}-q\xi\right]^2\right]^{-1/2} - \left[1+\left[\frac{\omega\tau}{q\xi}+q\xi\right]^2\right]^{-1/2} \right\}.$$

Then in this case we have dynamic scaling relation (12) with

$$S_q = \frac{1}{\pi}\left[\frac{T\xi}{JS'}\right]^2 \frac{\ln\{[1+(\xi q)^2]^{1/2}+\xi q\}}{\xi q[1+(\xi q)^2]^{1/2}}, \quad \Phi(x,y)$$

$$= \frac{(1+x^2)^{1/2}}{4y\ln[(1+x^2)^{1/2}+x]} \left[\frac{1}{[1+(y/x-x)^2]^{1/2}} - \frac{1}{[1+(y/x+x)^2]^{1/2}} \right] .$$

Thus we find that the dynamic scaling law stands for our dynamic structure factor and that the characteristic time τ is given by

$$\xi^2/(JS') = (-4\mu)^{-1}$$

for both 1D and 2D ferromagnets. In the case $q\xi \gg 1$, $S_q(\omega)$ has a sloppy spin-wave peak at $\omega \simeq \pm JS'q^2$. The width is $q\xi/\tau$. Behaviors of the scaling function Φ are shown in Fig. 1.

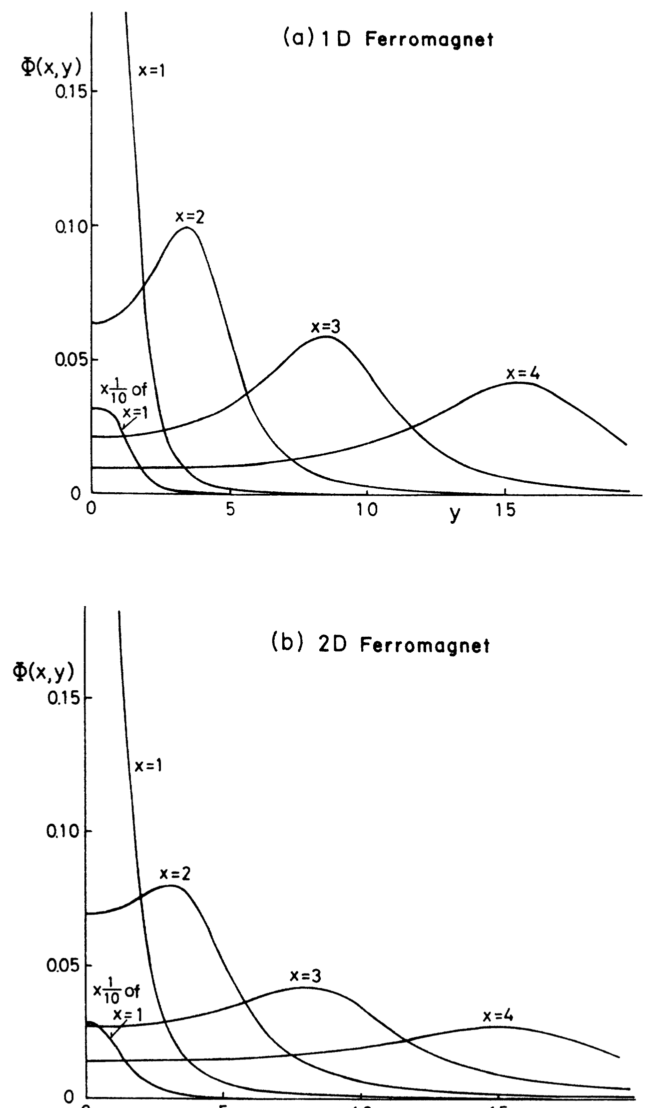

FIG. 1. Scaling functions $\Phi(x,y)$ of the Heisenberg ferromagnets for 1D (a) and 2D (b). At $x=0$, Φ become a δ function. At $x \gg 1$, Φ have the quasi-spin-wave peaks.

Next we consider the classical limit $S \rightarrow \infty$. We set $\mathbf{s}=\mathbf{S}/S$ and $J_0 = JS^2$; then the Hamiltonian and equation of motion become

$$H = -J_0 \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j, \quad \frac{d}{du}\mathbf{s}_i = -J_0 \sum_j \mathbf{s}_i \times \mathbf{s}_j , \tag{13}$$

where we define scaled time $u \equiv t/S$. We can define the classical correlation function

$$g_{\mathbf{r}}(u) \equiv \langle \mathbf{s}_{\mathbf{r}}(u) \cdot \mathbf{s}_0(0) \rangle ,$$

and its Fourier transform is

$$s_{\mathbf{q}}(\nu) \equiv (2\pi N)^{-1} \sum_{\mathbf{r}} \int g_{\mathbf{r}}(u) e^{-i(\nu u + \mathbf{q}\cdot\mathbf{r})} du .$$

These functions are calculated by following relations:

$$g_{\mathbf{r}}(u) = S^{-2} G_{\mathbf{r}}(uS), \quad s_{\mathbf{q}}(\nu) = S^{-2} S_{\mathbf{q}}(\nu/S) .$$

The limit $S \rightarrow \infty$ is taken at $JS \ll T \ll JS^2$. From Eq. (8) $\tilde{n}_{\mathbf{k}}$ becomes

$$\tilde{n}_{\mathbf{k}} \simeq \tilde{n}_{\mathbf{k}}^{+} = ST/h_{\mathbf{k}}, \quad h_{\mathbf{k}} \equiv J_0 x [z(1-\gamma_{\mathbf{k}}) + v] ,$$

where $x \equiv S'/S$, $v \equiv -\mu S/(J_0 x)$. Self-consistent equations for x and v are

$$1 = \frac{T}{N} \sum_{\mathbf{k}} \frac{1}{h_{\mathbf{k}}}, \quad x = \frac{T}{N} \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}}{h_{\mathbf{k}}} . \tag{14}$$

The dynamical correlation function (9) and the two-point function (10) become

$$s_{\mathbf{q}}(\nu) = \frac{T^2}{N} \sum_{\mathbf{k}} \frac{\delta(\nu - h_{\mathbf{k}+\mathbf{q}} + h_{\mathbf{k}})}{h_{\mathbf{k}} h_{\mathbf{k}+\mathbf{q}}} ,$$

$$g_{\mathbf{r}}(u) = \left[\frac{T}{N} \right]^2 \left[\left[\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \frac{\cos(h_{\mathbf{k}} u)}{h_{\mathbf{k}}} \right]^2 + \left[\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} \frac{\sin(h_{\mathbf{k}} u)}{h_{\mathbf{k}}} \right]^2 \right] . \tag{15}$$

In Fig. 2 we compare these formulas and the results of molecular-dynamics calculations of the 1D classical Heisenberg ferromagnet at $T = 0.1 J_0$. $g_0(u)$ and $g_8(u)$ are calculated for the $N = 16$ ring. The initial configuration of classical spins at a certain temperature T is obtained by Monte Carlo calculation. The equation of motion (13) is solved numerically by the Runge-Kutta method. The correlation function $g_{\mathbf{r}}(u)$ is calculated. By changing the initial conditions about 500 times, we take the average of the correlation functions. Details of the numerical methods were given in Ref. 10. The agreement is surprisingly good.

Several years ago Reiter *et al.*[11] argued that the dynamic scaling law is not valid for 1D Heisenberg ferromagnets. They calculated moments of $S_{\mathbf{q}}(\omega)$ by orthodox spin-wave theory. But their calculations are based on very short time and short distance behavior of the two-point function. So calculations of $S_{\mathbf{q}}(\omega)$ at very small q and ω by the moment method are not reliable.

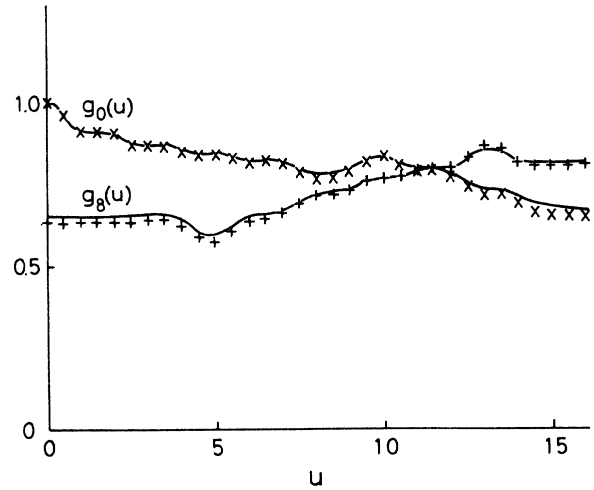

FIG. 2. Autocorrelation function $g_0(u)$ and $g_8(u)$ (eighth neighbor correlation function) for 1D classical Heisenberg ferromagnet with $N = 16$ and $T = 0.1 J_0$. ×'s and +'s are the results of our spin-wave formula (15) and the solid lines are the results of molecular dynamics. Equations (14) are solved numerically and we get $v = 0.007\,596\,8$ at $T = 0.1 J_0$. The agreement is very good.

In this paper we calculate $S_{\mathbf{q}}(\omega)$ of the 1D and 2D Heisenberg ferromagnets assuming that eigenstates are approximated by ideal spin-wave states. Using the Dyson-Maleev transformation[8] and mean-field approximation we give a very natural derivation of the dynamical structure factor. We show that our results satisfy the dynamic scaling relations (12) (Ref. 9) at low temperature. The characteristic time τ satisfies $\tau = \xi^2/(JS')$. We obtain the explicit form of the scaling function $\Phi(x,y)$. This system has a transition point at zero temperature. So scaling properties are different from the usual finite T_c phase transitions. We take the classical limit ($S \rightarrow \infty$) and compare with the results of the molecular dynamics of the classical Heisenberg model.[10] The accordance is quite good.

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