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Spin-wave theory of critical dynamics in one- and two-dimensional Heisenberg models: Failure of the dynamic-scaling hypothesis and the mode-coupling theory

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The usual spin-wave theory, when applied to the calculation of rotationally invariant averages in the Heisenberg model, permits exact calculation of static and dynamical correlation functions in one dimension. The results are also believed to be exact in two dimensions, although this has not been shown rigorously here. The one-dimensional ferromagnet in the hydrodynamic regime and the two-dimensional ferromagnet at all wave vectors do not satisfy the dynamical scaling hypothesis. There is no characteristic exponent in these cases. The present results contradict the prediction of the mode-coupling theory.

It is shown here that a self-contained spin-wave theory exists for the Heisenberg model in one and two dimensions that permits the calculation of the equilibrium correlation functions and the dynamical response in a simple way. The method is an extension of the usual spin-wave theory to the case that the order parameter vanishes but there is still well-developed local order. One may calculate correlation functions of operators that are combined in rotationally invariant quantities involving spins located within a distance much less than a coherence length, obtaining the leading term in a temperature expansion, or expansion in $1/S$, exactly. The method reproduces both the exactly known static correlations and the exact results for the leading term in the temperature expansion of the generalized spin current damping rate[1] for the classical nearest-neighbor Heisenberg chain, and permits the extension of these results to two-dimensional systems, more general interactions, and quantum systems where exact results for static correlations have not been previously available. We use it here to calculate the static and dynamic pair correlations for the classical ferromagnet in two dimensions and the dynamical response of the ferromagnetic chain, when $q \ll \kappa$. ($\tilde{\kappa}$ is the inverse coherence length.)

We find that there are severe violations of the dynamical scaling hypothesis in both cases.[2] In the one-dimensional chain a characteristic frequency that is hypothesized to vary as $(\kappa a)^2$ actually varies as $(\kappa a)^2|\ln\kappa a|$, where κ is the inverse coherence length. In two dimensions, the characteristic frequency varies as $(\ln\kappa a)^{-2}$, rather than $(\kappa a)^2$. The situation in two dimensions is particularly interesting in that the theory makes clear that the decay of the longest-wavelength spin fluctuations involves modes distributed uniformly throughout the zone, in contrast to the assumption underlying the mode-coupling theory.[3] Indeed, the mode-coupling theory predicts, incorrectly, that scaling is satisfied for the one-dimensional Heisenberg model, and gives violations of scaling in two dimensions that do not agree with the results for the Heisenberg model. We note that these are first examples of the mode-coupling theory giving incorrect dynamical exponents (there really are no exponents in the two cases mentioned), as opposed to incorrect spectral functions.

We shall not comment further on the extension of the theory to quantum systems, other than to point out that it can be done in a straightforward manner.[4]

I. SPIN-WAVE THEORY—STATIC RESPONSE

The spin-wave theory used here is essentially a classical version of the Holstein-Primakoff theory. We expand the longitudinal spin vector

$$S_i^z=(S^2-S_i^-S_i^+)^{1/2}\simeq S-\tfrac{1}{2}S_i^-S_i^+/S \quad , \tag{1}$$

where $S_i^{\pm}=S_i^x\pm iS_i^y$.

The method is generally regarded as inapplicable in one and two dimensions because when one calculates $\langle S_i^-S_i^+\rangle$ one finds that it diverges, as indeed it must, since $\langle S_i^z\rangle=0$, and is not close to S.[1] We shall not use the method to calculate averages such as S_i^z, which are not rotationally invariant. For a quantity such as S_i^z, the probability of large scale deviations from the z axis is large, and the linearization Eq. (1) impermissible. However, to calculate a rotationally invariant quantity such as $\vec{S}_i\cdot\vec{S}_j$, we need only the conditional distribution for $\vec{S}_j$ given $\vec{S}_i$, and as long as $\kappa|\vec{r}_i-\vec{r}_j|\ll 1$, only small deviations of $\vec{S}_j$ from the direction given by $\vec{S}_i$ are probable. The linearization will be valid, if we choose for S_i^z the direction of $\vec{S}_i$. Since the average does not depend upon the direction of $\vec{S}_i$, the full average is equal to the conditional average. For the ferromagnet

$$\vec{S}_i\cdot\vec{S}_j \cong S^2 - \tfrac{1}{2}(S_i^- S_i^+ + S_j^- S_j^+) + \tfrac{1}{2}(S_i^- S_j^+ + S_j^- S_i^+) \quad , \tag{2}$$

or in terms of $\vec{S}_q = N^{-1/2}\sum e^{i\vec{q}\cdot\vec{r}_i}\vec{S}_i$

$$\vec{S}_{q_1}\cdot\vec{S}_{q_2} = N\delta_{q_1}\delta_{q_2}S^2 - \tfrac{1}{2}(\delta_{q_1}+\delta_{q_2})\sum\delta(q_1+q_2-q_1'-q_2')S_{q_1'}^- S_{q_2'}^+ + \tfrac{1}{2}(S_{q_1}^- S_{q_2}^+ + S_{q_2}^- S_{q_1}^+) \quad , \tag{3}$$

Eq. (3) has only operational significance, since some of the spins involved in the transform are further apart than a coherence length. It is to be understood as having meaning in sums that restrict the distance between sites to distances such that Eq. (2) is valid. The Hamiltonian is such a sum. For calculating the conditional distribution of a group of spins, given that a particular site in the group is aligned along some axis we take as the z axis, we can use the approximation

$$e^{-\beta H} = \exp \tfrac{1}{2}\beta\sum J_q \vec{S}_q\cdot\vec{S}_{-q}$$
$$\simeq \exp -\tfrac{1}{2}\beta\sum(J_0-J_q)S_q^- S_{-q}^+ + \tfrac{1}{2}\beta N J_0 S^2 \quad . \tag{4}$$

The approximations (2)–(4) yield

$$\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle = NS^2\delta_q - \delta\sum_{qq'} 2kT(J_0-J_{q'})^{-1} + 2kT(J_0-J_q)^{-1} \quad . \tag{5}$$

The sum is divergent in one or two dimensions, but Eq. (5) can only be strictly valid for each q (rather than in the sense of a formal expression for calculating averages for fixed site separation), when $q >> \kappa$, where it should be compared with the exact result for the nearest-neighbor chain, for small values of T[5]

$$\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle_{\text{exact}} = 2kT[J(\kappa a)^2 + J_0 - J_q]^{-1} \tag{6}$$
$$J_q = 2J\cos qa \quad ,$$

a is the lattice spacing and $\kappa a = kT/JS^2$. For this system, we have from Eq. (5), with $na = |\vec{r}_i - \vec{r}_j|$

$$\langle\vec{S}_i\cdot\vec{S}_j\rangle = N^{-1}\sum\cos qna\,\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle$$
$$= S^2 - kT/J\sum(1-\cos qna)(1-\cos qa)^{-1}$$
$$= S^2(1-n\kappa a) \quad . \tag{7}$$

The exact result, from Eq. (6) is $S^2(1-\kappa a)^n$. Thus for $n\kappa a << 1$, the leading term in an expansion in $(n\kappa a)$ is given correctly. Higher-order correlations are also given correctly in the same sense. For

$$\delta\vec{S}_i\cdot\vec{S}_j \equiv \vec{S}_i\cdot\vec{S}_j - \langle\vec{S}_i\cdot\vec{S}_j\rangle \quad ,$$

we find

$$\langle(\delta\vec{S}_i\cdot\vec{S}_j)^2\rangle = S^4(n\kappa a)^2 \quad , \tag{8}$$

which agrees with the exact solution for $n\kappa a << 1$.[1]

It is $\langle(\delta\vec{S}_i\cdot\vec{S}_j)^2\rangle^{1/2}$ which is the smallness parameter in the spin-wave expansion, not $\langle S_i^- S_i^+\rangle$, when there is no long-range order.

The prediction of the spin-wave theory for the correlation functions of the 2D Heisenberg model, is, for nearest-neighbor interactions of equal strength J in both directions, on a square lattice, with $n_x a = |\vec{r}_{i,x} - \vec{r}_{j,x}|$, etc.,

$$\langle\vec{S}_i\cdot\vec{S}_j\rangle = S^2 - \frac{kTN^{-1}}{J}\sum\frac{1-\cos(q_x n_x a + q_y n_y a)}{(2-\cos q_x a - \cos q_y a)} \quad . \tag{9}$$

The preceding heuristic arguments do not of course prove that Eq. (9) is correct. The theory is expected to work better in two dimensions than in one dimension, however. When $n_x = n_y = n$ the result (9) is particularly simple and is

$$\langle\vec{S}_i\cdot\vec{S}_j\rangle = S^2 - \frac{kT}{\pi J}\sum_{n'=0}^{n-1}(n'+\tfrac{1}{2})^{-1} \quad . \tag{10}$$

II. SPIN-WAVE THEORY—DYNAMICAL RESPONSE

If one attempts to do a straightforward perturbation theory to calculate dynamical quantities such as spin-wave linewidths, one runs immediately into divergence difficulties.[6] These can be avoided by using the projection operator[7] identities to reduce the problem to the calculation of dynamical response functions that may be evaluated from the lowest-order harmonic theory. One can show that the correlation function $\Sigma_q(z)$ can be represented in terms of the frequency- and wave-factor-dependent spin current damping rate $\gamma_q(z)$ as

$$\Sigma_q(z) \equiv \int_0^\infty e^{izt}\langle\vec{S}_q(t)\cdot\vec{S}_{-q}(0)\rangle dt$$
$$= i\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle\{z - \omega_q^2/[z+\gamma_q(z)]\}^{-1} \quad , \tag{11}$$

ω_q^2 is the exact second moment, $\langle\dot{\vec{S}}_q\cdot\dot{\vec{S}}_{-q}\rangle/\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle$. To calculate ω_q^2 for $q < \kappa$, requires knowledge of $\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle$ for $q < \kappa$, and so falls outside the range of the theory, in that Eq. (6) not Eq. (5) must be used. The theory is only self-contained for $q > \kappa$ in general. We expect this can be remedied by including higher-order terms in the perturbation series. For the moment, one can calculate for $q < \tilde{\kappa}$ if the susceptibility is known by other means.

$\gamma_q(t)$, where $\gamma_q(z)=\int_0^\infty e^{izt}\gamma_q(t)\,dt$, is given exactly by[6]

$$\gamma_q(t)=i\sum\Gamma(q_1q_2q_3)\Gamma(q_1'q_2'q_3')\langle\vec{S}_{q_1}(t)\delta\vec{S}_{q_2}(t)\cdot\vec{S}_{q_3}(t)\cdot\vec{S}'_{q_1}\delta\vec{S}_{q_2'}\cdot\vec{S}_{q_3'}\rangle/\langle\dot{\vec{S}}_q\cdot\dot{\vec{S}}_{-q}\rangle\ , \tag{12}$$

where

$$\Gamma(q_1q_2q_3)=\tfrac{1}{2}[(J_{q_1+q_2}-J_{q_3})(J_{q_1}-J_{q_2})+(J_{q_1+q_3}-J_{q_2})(J_{q_1}-J_{q_3})]\delta(q-q_1-q_2-q_3)\ .$$

There are actually projection operators involved in Eq. (12), but as has been shown in Ref. 7, these produce only higher-order corrections (in T) to the terms we will calculate. The essential reason for this is that by subtracting the average part of $\vec{S}_{q_1}\cdot\vec{S}_{q_3}$ we have eliminated most of $\vec{S}_{q_1}\delta\vec{S}_{q_2}\cdot\vec{S}_{q_3}$ that has a projection along $\vec{S}_q$, and that projection is now of order T.

At this point, in Ref. 7, it was necessary to resort to the exact calculations of the correlation functions for the classical chain, and equations of motion for $\delta\vec{S}_{q_1}\cdot\vec{S}_{q_2}(t)$ that could be shown to be exact at $T=0$, to evaluate the expressions in Eq. (12). We have already seen, that to lowest order in the temperature, the initial value of rotationally invariant averages such as those appearing in Eq. (12) could be calculated exactly from the spin-wave theory. It is also true that the approximation (3), together with the time dependence appropriate for a free spin wave,

$$S_q^{\pm}(t)=e^{\pm i\omega_q t}S_q^{\pm}\ , \tag{13}$$

where $\omega_q=S(J_0-J_q)$, leads to the exact $T=0$ equation of motion for $\delta\vec{S}_{q_1}\cdot\vec{S}_{q_2}(t)$. (This is true in the antiferromagnet as well, with the appropriate expressions for ω_q.) Consequently, Eqs. (13), (12), and (3) allow one to determine approximations for $\gamma_q(t)$ that will be correct to leading order in the temperature. $\gamma_q(t)$ can be expanded as

$$\gamma_q(t)=JS\frac{kT}{JS^2}\left[\gamma_{q,1}(t)+\frac{kT}{JS^2}\gamma_{q,2}(t)+\cdots\right]\ . \tag{14}$$

The rigorous definition of the terms in Eq. (14) is obtained by observing that the moments of $\gamma_q(t)$ for any order $2n$, i.e., the $2n$th term in the Taylor series expansion, depends on the average of spins a finite distance apart and can be expanded as a Taylor series in the temperature. Resumming terms to all order in n for a particular order of the temperature leads to $\gamma_{q,1}(t)$, $\gamma_{q,2}(t)$, etc. We note from Eq. (8) and the Schwartz inequality[7] that each factor of $\delta\vec{S}_{q_1}\cdot\vec{S}_{q_2}$ that appears in an average introduces a factor of kT/JS^2, and one may show that $\langle\dot{\vec{S}}_q\cdot\dot{\vec{S}}_{-q}\rangle$ is also proportional to kT/JS^2, so that the leading term in a temperature expansion of Eq. (12) is proportional to T, as indicated in Eq. (14). We also note that the relation between the coherence length and the temperature is quite different in one and two dimensions. In one dimension $kT/JS^2=\kappa a$, whereas in two dimension $kT/JS^2\propto|\ln\kappa a|^{-1}$.

The leading term in Eq. (14) is obtained by replacing $\vec{S}_{q_1}(t)\cdot\vec{S}_{q_1'}$ by $NS^2\delta_{q_1}\delta_{q_2'}$ in Eq. (12), and we obtain the expression for $\gamma_{q_1'}(t)$

$$(JS)^2\frac{kT}{JS^2}\gamma_{q,1}(t)=iS^2N^{-1}\sum\Gamma(0,q_1q_2)\Gamma(0,q_1'q_2')\langle\delta\vec{S}_{q_1}(t)\cdot\vec{S}_{q_2}(t)\delta\vec{S}_{q_1'}\cdot\vec{S}_{q_2'}\rangle/\langle\dot{\vec{S}}_q\cdot\dot{\vec{S}}_{-q}\rangle\ . \tag{15}$$

For arbitrary q, $\gamma_{q,2}$ is quite complicated, and contains contributions, arising from the higher-order terms in the time evolution of $S_q^{\pm}$ that have been neglected in Eq. (13), as well as contributions from the projection operators that have been neglected. For $q=0$, since as we shall see, $\gamma_{0,1}(t)\equiv 0$, there are no contributions of the first kind, and it may be shown that there are also no contributions of the second kind.[7] We can therefore evaluate $\gamma_{0,2}(t)$ from the harmonic theory,

$$(JS)^2\frac{kT}{JS^2}\gamma_{0,2}(t)=N^{-2}\sum\Gamma(q_1q_2q_3)\Gamma(q_1'q_2'q_3')\langle\delta\vec{S}_{q_1}(t)\cdot\vec{S}_{q_1'}\delta\vec{S}_{q_2}(t)\cdot\vec{S}_{q_3}(t)\delta\vec{S}_{q_1'}\cdot\vec{S}_{q_2'}\rangle/\langle\dot{\vec{S}}_q\cdot\dot{\vec{S}}_{-q}\rangle\ , \tag{16}$$

where Eq. (3) is used to express $\delta\vec{S}_{q_1}\cdot\vec{S}_{q_2}$ in terms of $S_{q_i}^{\pm}$, and Eq. (14) is used for the time dependence. It is straightforward now to evaluate $\gamma_{q,1}$ and $\gamma_{0,2}$, in both one and two dimensions.

We note that the first use of the notion of local order in a dynamical calculation appears to be the work of McLean and Blume.[8] Berezhinsky and Blank,[9] and others,[10] have incorporated this notion into the calculation of static correlations, where it is the basis of renormalization group calculations[11–14] near two dimensions. Using the identity $\langle A\dot{B}\rangle=kT\langle[A,B]\rangle$ one may show that

$$\langle\dot{\vec{S}}_q\cdot\dot{\vec{S}}_{-q}\rangle=2kT\sum_{q'}(J_{q'}-J_{q-q'})\langle\vec{S}_{q'}\cdot\vec{S}_{-q'}\rangle\ , \tag{17}$$

and we have for nearest-neighbor interactions $J_q = 2J\cos q$,

$$\langle \dot{S}_q \cdot \dot{S}_{-q} \rangle = 4JkT(1-\cos qa)\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle \simeq 4JS^2kT(1-\cos qa) \quad . \tag{18}$$

The numerator in Eq. (15), using Eqs. (3) and (12)

$$iS^2N^{-1}\sum[\Gamma(0,0,q)-\Gamma(0,q_1,q_2)][\Gamma(0,0,q)-\Gamma(0,q_1'q_2')]\langle \delta S^-_{q_1}S^+_{q_2}\delta S^-_{q_1'}S^+_{q_2'}\rangle e^{i(\omega_{q_2}-\omega_{q_1})t} \quad . \tag{19}$$

Using Eq. (4) to evaluate the average and the explicit expression for Γ, we have

$$i(kT)^2S^2N^{-1}\sum[(J_0-J_q)^2-(J_{q_1}-J_{q_2})^2]^2(J_0-J_{q_1})^{-1}(J_0-J_{q_2})^{-1}\cos(\omega_{q_1}-\omega_{q_2})t\,\delta(q-q_1-q_2) \quad . \tag{20}$$

For nearest-neighbor interactions, this reduces to

$$16(JSkT)^2\sin^4\tfrac{1}{2}qN^{-1}\sum_{q'}(\cos\tfrac{1}{2}q+\cos q')^2\cos[4JS\sin(\tfrac{1}{2}q)\sin q't] \quad . \tag{21}$$

Utilizing Eq. (18), we have, setting $a=1$ henceforth

$$(JS)^2\frac{kT}{JS^2}\gamma_{q,1}(t) = i2JkT\sin^2\tfrac{1}{2}qN^{-1}\sum_{q'}(\cos\tfrac{1}{2}q+\cos q')^2\cos(4JS\sin\tfrac{1}{2}q\sin q't) \quad , \tag{22}$$

which vanishes at $q=0$ as predicted. The right-hand side may be expressed in terms of Bessel functions, and we have

$$\gamma_{q,1}(t) = i8\sin^2\tfrac{1}{2}q[J_1(\tau)/\tau + J_0(\tau)\cos^2\tfrac{1}{2}q] \quad , \tag{23}$$

where $\tau = 4JS\sin q/2t$. Equation (23) agrees with the results obtained previously by other methods, and is the exact result for $\gamma_{q',1}(t)$.[7] It is in fact this agreement that serves to justify the spin-wave theory for the dynamics, as we have not yet attempted to justify the validity of the spin-wave theory from within the theory itself. The arguments presented at the outset, coupled with the correct prediction of results known to be exact from more complicated arguments, seem strong enough grounds to extend the theory to calculations where there are no other results to compare with.

III. ONE-DIMENSIONAL FERROMAGNET

One such region is the ferromagnet in one dimension for $q < \kappa$, where the leading term in the temperature expansion $\gamma_{q,1}(t)$, because of the q dependence is not in fact the dominant term, but is supplanted by $\gamma_{q,2}(t)$.

As already mentioned, it is only in the limit that $q \to 0$ that $\gamma_{q,2}(t)$ can be calculated readily from the lowest-order theory. This is, however, the most interesting limit since it allows us to calculate the diffusion coefficient.

The long wavelengths $q \ll \pi/a$ are the significant ones in the sum in Eq. (16) for our purposes, and we will evaluate the matrix elements for this case. Using Eqs. (3) and (4) the definition of Γ, $\langle \dot{\vec{S}}_q \cdot \dot{\vec{S}}_{-q}\rangle = 2J^2S^4(\kappa a)(qa)^2$ we find

$$\lim_{\kappa a\to 0}\gamma_0(t) = 2J^2S^{-4}(\kappa a)^{-1}a^6N^{-2}\sum q_1^2q_2^2q_3^2[\langle S^-_{q_1}(t)S^+_{-q_1}\rangle + \langle S^+_{q_1}(t)S^-_{-q_1}\rangle]$$
$$\times \langle S^-_{q_2}(t)S^+_{-q_2}\rangle\langle S^+_{q_3}(t)S^-_{-q_3}\rangle\delta(q_1+q_2+q_3) \quad . \tag{24}$$

Utilizing Eqs. (5) and (13), we find for the limiting spin current damping

$$\gamma_0''(\omega) = JS(\kappa a)^2\gamma_{0,2}''(\omega) = \pi 16J^2S^2(\kappa a)^2N^{-2}\sum[\delta(\omega-\omega_{q_1}-\omega_{q_2}+\omega_{q_3})+\delta(\omega+\omega_{q_1}-\omega_{q_2}+\omega_{q_3})]\delta(q_1+q_2+q_3) \quad . \tag{25}$$

With the quadratic approximation for the spin-wave frequencies, $\omega_q = JS(qa)^2$, one sees that the integral is logarithmically divergent at small q, for small ω. This result demonstrates that the expansion (14) is breaking down, and $\gamma''_{0,2}(0)$ which our procedure calculates accurately, is not finite. This implies already that the dynamical scaling hypothesis is violated in this system.

From Eq. (11) and $\omega_q^2 = JS(\kappa a)^2(qa)^2$ for $q \ll \kappa$, the characteristic decay frequency for long-wavelength modes is $JS(\kappa a)^2(qa)^2/\gamma''_0(\omega=0)$. The dynamical scaling hypothesis requires that this frequency scale with κ as some characteristic power of κ, for fixed values of the ratio q/κ. Since the spin-wave frequency is proportional to $q^2 = \kappa^2(q/\kappa)^2$, this characteristic exponent $z = 2$. Consequently $\gamma''_0(\omega=0)$, which we can write as $\gamma''_0(t=0)\tau_c$, thus defining τ_c, must be proportional to $(\kappa a)^2$. Since $\gamma''_0(t=0)$ is proportional to $(\kappa a)^2$, τ_c must be finite and independent of κ for small κ if the hypothesis is to hold. In fact, as we have seen, this is not the case. To see what actually happens to $\gamma''_0(\omega)$ requires going beyond the lowest-order spin-wave theory. The lowest-order contribution from a renormalized theory presumably corresponds to replacing the correlation functions in Eq. (24) by their exact values. The time dependence at long wavelengths $q_1 q_2 q_3 < \kappa$ would have to be calculated self-consistently. This is not necessary to obtain the behavior of the divergence in the relaxation time of $\gamma_0(t)$. The divergence is present even if one includes only those modes in the intermediate states for which $|q_1, q_2, q_3| > \rho\kappa$, $\rho \gg 1$. The time dependence of these modes contains a damping[1] $JS(\tilde{\kappa}a)(qa)$ and the static correlations are given accurately by Eq. (5). We find then

$$\gamma''_0(0) > 16JS(\kappa a)^2\left(\frac{2\pi}{a}\right)^2 a^{-2}\int_{|q_1|>\rho\kappa,\,|q_2|>\rho\kappa} dq_1 dq_2 \frac{\kappa(|q_1|+|q_2|+|q_1+q_2|)}{4q_1^2q_1^2+\kappa^2(|q_1|+|q_2|+|q_1+q_2|)^2} \;. \tag{26}$$

The integral in Eq. (17) is $\propto |\ln(\kappa a)|$ and hence $\gamma''_0(0) \propto JS(\kappa a)^2 |\ln\kappa a|^{-1}$. The characteristic decay rate for the modes with $q \ll \kappa$ is therefore $\propto (qa)^2 \times |\ln\kappa a|^{-1}$. One easily convinces oneself that if one assumes diffusive behavior for $q < \kappa$, with $D \propto |\ln(\kappa a)|^{-1}$, that the hydrodynamic modes also contribute a term $\propto |\ln(\kappa a)|$. Furthermore, the same logarithmic behavior has been obtained by a different method, which essentially cuts off the divergence by replacing the equilibrium averages of pairs of spins given by the spin-wave theory Eq. (5), by the exact value Eq. (6).[7] In this case, the coefficient of the logarithm is rather easy to calculate. We show in Fig. 1 a comparison of that result with the numerical simulations of Heller.[15] What is being plotted is the characteristic relaxation time for spin diffusion divided by $(\kappa a)^2$. If scaling were valid, this would be a constant. The logarithmic dependence is very clear, and remarkably the coefficient is in agreement with that calculated in Ref. 7.

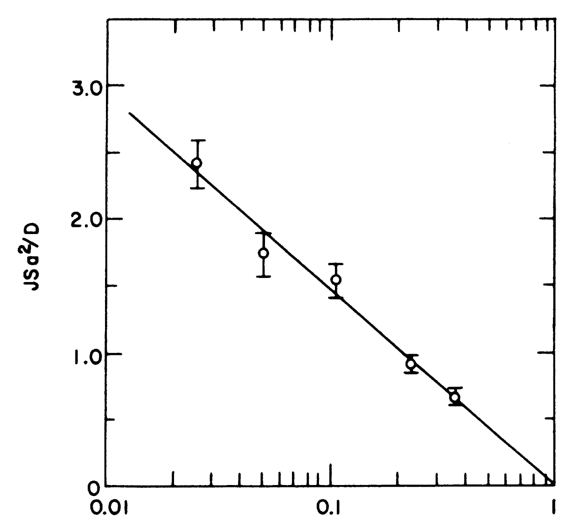

FIG. 1. Comparison of the value of the characteristic time, for the spin current damping function $\gamma_q(t)$ with the results of computer simulations of Heller. The coefficient of the logarithmic dependence on temperature is uncertain and depends upon the assumptions made in cutting off the divergence. The coefficient shown is due to the procedure of Ref. 7.

IV. TWO-DIMENSIONAL FERROMAGNET

In two dimensions calculations that employ a spin-wave theory to calculate the generators of the renormalization group[12] have shown that there is no transition in the two-dimensional Heisenberg model for any temperature, although the coherence length diverges as $T \to 0$. The physical situation at low temperatures and short distances is therefore analogous to the situation in one dimension.

Equations (17) and (19) are valid here as well; the summations over wave vector being taken in two dimensions. We will consider again the nearest-neighbor model with equal exchange strength in both directions on the square lattice.

We find for the leading term

$$\lim_{T\to 0}\gamma_q(t) = i2(kT)JN^{-1}\sum \frac{[q^4-(q_1^2-q_2^2)^2]^2}{q^2q_1^2q_2^2}\cos JS(q_1^2-q_2^2)t\,\delta(q-q_1-q_2) \ , \tag{27}$$

from which we obtain

$$\lim_{T\to 0}\gamma_q''(\omega) = \pi kTJN^{-1}\sum \frac{[q^4-(q_1^2-q_2^2)^2]^2}{q^2q_1^2q_2^2}[\delta(\omega - JS(q_1^2-q_2^2)) + \delta(\omega + JS(q_1^2-q_2^2))]\delta(q-q_1-q_2) \ , \tag{28}$$

which, with a change of variables, reduces to

$$\lim_{T\to 0}\gamma_q''(\omega) = \frac{\pi kTJ}{q^2}\left[q^4 - \left(\frac{\omega}{JS}\right)^2\right]^2 N^{-1}\sum \frac{[\delta(\omega - 2JS\vec{q}\cdot\vec{q}^{\,1}) + \delta(\omega + 2JS\vec{q}\cdot\vec{q}^{\,1})]}{(\vec{q}/2+\vec{q}^{\,1})^2(\vec{q}/2-\vec{q}^{\,1})^2} \ . \tag{29}$$

Choosing the q_x axis along the direction of q and doing the q_x integration

$$\gamma_q''(\omega) = \frac{2\pi kTJ}{q^2}\left[q^4 - \left(\frac{\omega}{JS}\right)^2\right]^2 \frac{1}{2JSq}\frac{1}{(2\pi)^2}\int dq_y \left(\frac{[q^4-(\omega/JS)^2]^2}{16q^4} + \frac{[q^4+(\omega/JS)^2]}{2q^2}q_y^2 + q_y^4\right)^{-1} \ . \tag{30}$$

We are particularly interested in $\gamma_q''(\omega_q)$; i.e., $\omega/JS = q^2$. At this value, the integral is divergent for small q_y. Near this value, the dominant term in the integral is due to small values of q_y, and we can neglect q_y^4 in evaluating it. We then obtain

$$\gamma_{q,1}''(\omega) = \tfrac{1}{2}|\omega^2 - (JSq^2)^2|/JSq^2 \ , \tag{31}$$

and the result is valid when $|q^2 - |\omega/JS||q^{-1} << 1$. If the spin-wave frequency were not shifted, the damping $(kT/S)\gamma_{q,1}''(\omega_q)$ would vanish. In fact, there is a shift linear in the temperature due both to the real part of γ_q and the shift in the second moment, and so the damping at the corrected spin-wave frequency is proportional to $JSq^2(kT/JS^2)^2$. Since $\gamma_{q,2}(\omega)$ is independent of q for small q, the damping arising from the second term in the series Eq. (13) dominates the contribution from the first, and $\gamma_q(\omega)$ may be approximated by $JS(kT/JS^2)^2\gamma_{q,2}(\omega)$.

It suffices to evaluate $\gamma_{q,2}(\omega)$ at $q=0$ and $\omega=0$ since it turns out to vary continuously in both variables, and it is therefore the limiting value that determines the spin-wave lifetimes as $q\to 0$, and the spin diffusion coefficient. Using Eqs. (3), (4), and (12), the definition of Γ, we find for $q\to 0$

$$\lim_{T\to 0}\gamma_q(t) = \frac{J^3a^6}{4kTS^2q^2}\sum(\vec{q}\cdot\vec{q}_2q_3^2 + \vec{q}\cdot\vec{q}_3q_2^2)(\vec{q}\cdot\vec{q}_2'q_3'^2 + \vec{q}\cdot\vec{q}_3'q_2'^2)$$
$$\times\langle[S_{q_1}^-(t)S_{q_1'}^+ + S_{q_1}^+(t)S_{q_1'}^-]\delta(S_{q_2}^-(t)S_{q_3}^+(t))\delta(S_{q_2'}^-S_{q_3'}^+)\rangle\delta(\vec{q}_1+\vec{q}_2+\vec{q}_3)\delta(\vec{q}_1'+\vec{q}_2'+\vec{q}_3') \ . \tag{32}$$

At $\omega=0$,

$$\lim_{T\to 0}\gamma_q''(0) = \frac{4(kT)^2\pi}{S^2q^2}\sum\frac{(\vec{q}\cdot\vec{q}_2q_3^2 + \vec{q}\cdot\vec{q}_3q_2^2)^2}{q_1^2q_2^2q_3^2}\delta(\omega_{q_1}+\omega_{q_2}-\omega_{q_3})\delta(\vec{q}_1+\vec{q}_2+\vec{q}_3) \ . \tag{33}$$

The integral is convergent, and upon eliminating the δ functions and doing the angular integrations, we find that it reduces to

$$\lim_{T\to 0}\gamma_0''(0) = (JS)\left(\frac{kT}{JS^2}\right)^2\frac{a^2}{2\pi}\int_0^{q^*}\int_{q_2}^{q^*}(q_3^2-q_2^2)^{-1/2}q_3\,dq_3\,dq_2 \ . \tag{34}$$

The dominant contribution to the integral actually comes from large wave vectors, and in fact the upper cutoff, q^*, determines the value of the integral. To evaluate it exactly requires that the long-wavelength approximation not be used, but we can conclude that $\lim_{T\to 0}\gamma_0''(0) = AJS(kT/JS^2)^2$, with A of order unity, and lattice dependent. To summarize then,

$$\lim_{T\to 0}\gamma_q''(\omega) = AJS\left(\frac{kT}{JS^2}\right)^2[1+O(q^2)] \ , \tag{35}$$

for ω close to the spin-wave frequency; i.e.,

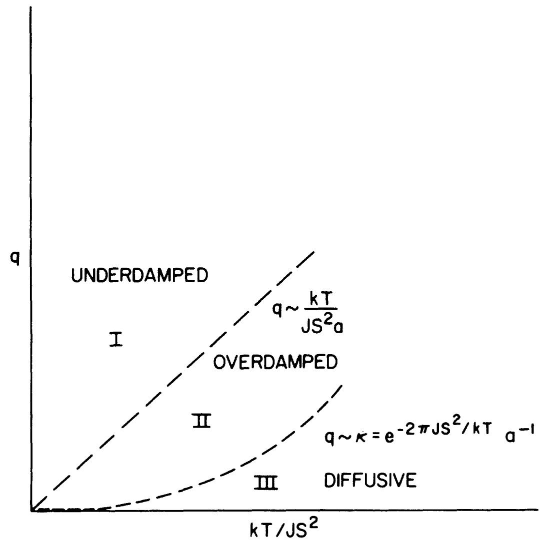

FIG. 2. Schematic diagram of the various regions of $q\kappa$ plane for which the dynamics are qualitatively different. Region I: Frequency $\sim JSq^2$, damping $\sim JS(kT/JS^2)^2$. Region II: Linewidth $\sim JSq^4/(kT/JS^2)^2$. Region III: Linewidth $\sim Dq^2, D \propto (kT/JS^2)^{-2} e^{-4\pi JS^2/kT}$.

$|\omega - JSq^2|/q \ll 1$, where the $O(q^2)$ term contains small corrections due to $\gamma_{q,1}(\omega)$, as well as finite q and ω corrections to the value of $\gamma_0''(0)$ that we have calculated.

This result contradicts the dynamical scaling hypothesis. Inasmuch as the spin-wave frequencies are $\omega_q = JS(qa)^2$ the spin waves will be well defined when $q \gg kT/JS^2a$, with a linewidth $\frac{1}{2}\gamma_0''(0)$ and overdamped when $q \ll kT/JS^2a$. The evidence from the renormalization group calculations is that the inverse coherence length $\kappa a \propto e^{-2\pi JS^2/kT}$. The linewidth evidently does not scale as $(\kappa a)^2 f(q/\kappa)$. Using the renormalization group[14] results for the susceptibility to calculate ω_q^2, we find that the region of overdamped spin waves having essentially Lorentzian line shapes with a width $2JSq^4/\gamma_0''(0)$ when $q \gg \kappa$, goes over to a diffusive regime with a diffusion coefficient $D \propto \gamma_0''(0)^{-1} \exp -4\pi JS^2/kT$, when $q \ll \kappa$. The situation is shown graphically in Fig. 2.

V. COMPARISON WITH MODE-COUPLING THEORY

The violations of scaling discussed here contradict the prediction of the mode-coupling theory, in both one and two dimensions, and in fact, the mode-coupling theory is really not valid for the Heisenberg model in one and two dimensions. This has been discussed extensively for the case of one dimension,[16] and we will limit ourselves here to a comparison of the characteristic exponents for the diffusion coefficient, estimated from the lowest-order calculation. If we express the correlation function as[16]

$$q^{(z)} = i\langle S_q S_{-q}\rangle [z - \phi_q(z)]^{-1} \ , \tag{36}$$

then if we assume that as $q \to 0$, $\omega \to 0$, $\phi_q(z) \to -iDq^2$, the mode-coupling result for D is given by

$$D^2 = \lim_{q\to 0} q^{-2} \sum \{ (J_{\vec q'} - J_{\vec q - \vec q'})^2 \times \rho_{\vec q'} \rho_{\vec q - \vec q'} / \rho_q [\vec q'^2 + (\vec q - \vec q')^2]^{-1} \} \ , \tag{37}$$

where ρ_q is the normalized static correlation function

$$\rho_q = \langle \vec S_q \cdot \vec S_{-q} \rangle / N^{-1} \sum_q \langle \vec S_q \cdot \vec S_{-q} \rangle \ . \tag{38}$$

In one dimension

$$\rho_q = \frac{2\tilde\kappa}{\tilde\kappa^2 + q^2} \ , \tag{39}$$

and we have

$$D^2 \propto \kappa^3 \int \frac{dq' q'^2}{(\tilde\kappa^2 + q'^2)[\tilde\kappa^2 + (q-q')^2][q'^2 + (q-q')^2]} \propto \kappa^0 \ . \tag{40}$$

Then D would be a constant in the mode-coupling theory. This corresponds to $\gamma_0''(0)$ being proportional to κ^2, but as we have seen, it is actually proportional to $\kappa^2|\ln\kappa|$ and D actually vanishes as $|\ln\kappa|^{-1}$. In two dimensions, for small q

$$\rho_q = \frac{2\ln\kappa}{\tilde\kappa^2 + q^2} \ . \tag{41}$$

This result follows from the dynamical spherical model theory as well as from renormalization group calculations.[14] κ and the temperature are related by $kT \propto \ln\kappa$. We have then

$$D^2 \sim q^{-2}\kappa^2 \ln\kappa \int \frac{(\vec q \cdot \vec q')^2}{(\vec q^2)^2 + (\vec q - \vec q')^2} \times \frac{1}{\kappa^2 + q'^2} \frac{1}{\kappa^2 + (q-q')^2} d\vec q' \tag{42}$$

As $q \to 0$

$$D^2 \propto \ln\kappa \ . \tag{43}$$

We have then the rather interesting result that $D \propto (\ln\kappa)^{1/2}$. The prediction of the mode-coupling theory is therefore in disagreement with the prediction of the dynamical scaling hypothesis, which requires, since $z=2$, that $D \propto \tilde\kappa^0$, as well as in disagreement with the results for the Heisenberg model, in which $D \propto \tilde\kappa^2(\ln\tilde\kappa)^2$. The disagreement in this situation is about as severe as it could be, since the mode-coupling theory predicts the diffusion coefficient diverges at $T=0$, the scaling hypothesis predicts it should be a constant, and the actual result for the Heisenberg model is that it vanishes.

The proper interpretation of these results requires that one observe that the mode-coupling theory is actually the exact result, term by term in an expansion of $\phi_q(z)$ in renormalized skeleton diagrams, for the dynamical spherical model, that is, for a model with the same equations of motion as the Heisenberg model but with the fixed length constraint for the spins replaced by the requirement that the average length of the spins be fixed. Relaxing this constraint eliminates the well-defined spin waves characteristic of the Heisenberg model in one and two dimensions, as may be seen in Ref. 16. In one dimension, the singularity in the two spin-wave density of states leads to the scaling violations in both the ferromagnet and the antiferromagnet. This is particularly clear in the derivation employed in Ref. 7 for the ferromagnet, while in the present work the scaling violation appears as due to a singularity in the three spin-wave density of states. The point is the same in either case. If the spin waves were not well defined at $T=0$, there would be no such singularities, and no scaling violations. In one dimension, then, it is clear that the relaxation of the constraint is an essential difference between the Heisenberg and dynamical spherical models, we should not expect the results of the two models to agree, and hence, the mode-coupling theory is not applicable to the Heisenberg model. That the Heisenberg model should violate the scaling hypothesis is also a consequence of the singularity in the density of states. It leads to long-time tails $(t^{-1/2})$ in the decay of the spin current damping rate correlation function that are not anticipated in the intuition underlying the scaling hypothesis.

In two dimensions it is again the difference in the fluctuation spectrum at $T=0$ that is the essential difference between the dynamical spherical model and the Heisenberg model, and there is, therefore, no reason to expect the mode-coupling calculation to be applicable. As we have seen there are contributions to the spin current damping rate from wave vectors throughout the zone, in the Heisenberg model, even for $q=0$ and again, one of the essential intuitive arguments underlying the dynamical scaling hypothesis, the notion that the critical modes interact predominantly with themselves, the effect of short-wavelength fluctuations being unimportant, is violated.

It is rather interesting that the dynamical spherical model also does not appear to satisfy the dynamical scaling hypothesis in two dimensions, even though the previous objection is not applicable here, since it is indeed the long-wavelength modes that are significant in the integral defining D^2. This result has been obtained by a rather cavalier treatment of the lowest-order diagram (the same treatment usually applied in three dimensions), and it is possible that a more careful treatment of the model will eliminate this feature. We think that will probably not be the case, that the scaling violation is a real feature of the model, and that it is tied up with the nonanalytic relation between the scaling length and the temperature.

We note that Trimper[6] has argued that dynamical scaling holds in $2+\epsilon$ dimensions. He shows that ω_q^2 scales correctly, using Nattermann's[14] expressions for $\langle \vec{S}_q \cdot \vec{S}_{-q} \rangle$. However, this does not suffice, since one must also show that the damping scales properly, which as we have seen, it does not do in two dimensions.

Note that one cannot argue this difficulty away by asserting that the damping is irrelevant in the renormalization group sense, since its value is much larger than the value it would have if scaling held, i.e., $(\ln \kappa a)^2 \gg (\kappa a)^2$, and in fact, the boundary $q \simeq \kappa$ determines only the region in which the diffusive behavior changes over to an overdamped mode whose width is proportional to q^4 (see Fig. 2).

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