Spin diffusion and relaxation in three-dimensional isotropic Heisenberg antiferromagnets

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A theory is proposed for kinetic effects in isotropic Heisenberg antiferromagnets at temperatures above the Néel point. The scaling behavior of the generalized coefficient of spin diffusion and relaxation constant in the paramagnetic phase is studied in terms of the approximation of interacting modes. It is shown that the kinetic coefficients in an antiferromagnetic system are singular in the fluctuation region. The corresponding critical indices for diffusion and relaxation processes are calculated. The scaling dimensionality of the kinetic coefficients agrees with the predictions of dynamic similarity theory and a renormalization group analysis. The proposed theory can be used to study the momentum and frequency dependence of the kinetic parameters, and to determine the form of the scaling functions. The role of nonlocal correlations and spin-fluid effects in magnetic systems is discussed. © *1997 American Institute of Physics.* [S1063-7761(97)02111-2]

1. INTRODUCTION

Recent heightened interest in the critical dynamics of antiferromagnetic materials[1–6] has been stimulated by active experimental and theoretical research on quasi-two-dimensional magnetic correlations in high-temperature superconductors, and on the anomalous magnetic properties of heavy-fermion compounds.[6–8] In particular, critical spin fluctuations have been invoked to explain the non-Fermi fluid behavior of the specific heat and resistance at low temperatures in the compounds[7,8] $CeCu_{6-x}Au_x$ and $Ce_{1-x}La_xRu_2Si_2$ near the concentration critical point. In addition, a proposed[9,10] spin-fluid approach to the Heisenberg model, based on introducing resonating valence bonds with Fermi statistics for excitations in the magnetic sublattice (spinons), may, in turn, also serve as a scenario for describing the behavior of cerium compounds with heavy fermions.[11,12] Here it turns out that critical spin fluctuations play an important role in the formation mechanism of a spin fluid. The behavior of the kinetic coefficients in this case can deviate substantially from that predicted by dynamic similarity theory.[13]

In this paper we develop a microscopic approach for studying the scaling behavior of the spin diffusion coefficient and the relaxation constant of an isotropic Heisenberg antiferromagnet in the fluctuation region above the Néel temperature. The scaling dimensionality of the kinetic coefficients in magnets was predicted by Halperin and Hohenberg,[14,15] who developed a hypothesis of scale invariance based on the idea that the values of the dynamic critical indices are conserved on both sides of the phase transition. Maleev then made a microscopic study of spin diffusion in the paramagnetic phase of ferromagnets.[16,17] He, in particular, established the approximations required to satisfy the requirements of the hypothesis of scale invariance, and studied the momentum and frequency dependence of the spin diffusion coefficient. The analogous problem for antiferromagnets will be examined in the present paper.

It is known[14] that in the neighborhood of a phase transition, two regions can be distinguished in the momentum-temperature plane: a hydrodynamic region determined by long-wavelength fluctuations in the ordering parameter $\mathbf{N}=\mathbf{N}_1-\mathbf{N}_2$, the difference in the moments of the sublattices, with characteristic wave vectors $q\xi\ll 1$, where $q=|\mathbf{k}-\mathbf{Q}|$ describes the deviation of the moment from the antiferromagnetic vector $\mathbf{Q}$ and ξ is the correlation length, and a critical region, with wave vectors $q\xi\gg 1$. Here the concept of a correlation length is related to the characteristic behavior of the ordering parameter $\mathbf{N}$. In an antiferromagnet, however, there is an additional conserved quantity, the vector $\mathbf{M}=\mathbf{M}_1+\mathbf{M}_2$, the sum of the moments of the sublattices. Nevertheless, we shall also refer to the long-wavelength fluctuation region for the vector $\mathbf{M}$, $k\xi\ll 1$, as hydrodynamic. In this paper we examine the behavior of the spin correlation functions in the paramagnetic phase and establish the relationship between the kinetic coefficients in the fluctuation region of the phase diagram.

In the hydrodynamic regime, the dynamics of the fluctuations in the magnetization have a diffusive character, i.e., the variation in the magnetic moment with time obeys the macroscopic van Hove diffusion equation:

$$\frac{\partial \mathbf{M}}{\partial t}=D_0\nabla^2\mathbf{M}, \tag{1}$$

where D_0 is the spin diffusion coefficient. This behavior of the fluctuations is related to the conservation of the magnetic moment; the operator corresponding to it commutes with the Hamiltonian.

A different pattern is observed in the critical region. The nonconservation of the ordering parameter determines the

relaxation character of the time variation in the vector **N**, i.e., the dynamics of this vector obey the relaxation equation:

$$\frac{\partial \mathbf{N}}{\partial t} = -\frac{\Gamma_0}{\chi}\mathbf{N}, \tag{2}$$

where χ is the susceptibility and the kinetic coefficient $\Gamma_0 > 0$. We note also that, in contrast to the diffusion equation (1), relaxation (2) can be uniform; the gradient corrections omitted from Eq. (2) are proportional to q^2 in this case. Although the average value of the magnetization vector **M** is zero on both sides of the phase transition point, fluctuations occur in the magnetization vector near the zero value. Unlike in a ferromagnet, however, the diffusion mode is not critical.

In the following we shall be interested in the dynamic susceptibility of a cubic Heisenberg antiferromagnet located in zero magnetic field above the Néel temperature:

$$H = -\sum_{\langle i,j\rangle} V_{ij}\mathbf{S}_i \cdot \mathbf{S}_j . \tag{3}$$

We also neglect dipole forces.[17]

The susceptibility is known to be related to the retarded spin Green function by the equation

$$\lambda(\mathbf{k},\omega) = (g\mu_0)^2 K^R_{SS}(\mathbf{k},\omega), \tag{4}$$

where g is the Landé g factor, μ_0 is the Bohr magneton, and

$$K^R_{SS}(\mathbf{k},\omega) = i\int_0^\infty dt\ e^{i\omega t}\langle [S^z_{\mathbf{k}}(t), S^z_{-\mathbf{k}}(0)]\rangle,$$

$$\mathbf{S}_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i}\mathbf{S}_i ,$$

$$\mathbf{M} = \langle \mathbf{S}_0\rangle, \quad \mathbf{N} = \langle \mathbf{S}_{\mathbf{Q}_{\mathbf{AFM}}}\rangle. \tag{5}$$

Proceeding from Eqs. (1) and (2), we can obtain the form of the correlation functions K^R in the diffusion

$$K^R_{SS}(\mathbf{k}\to\mathbf{0},\omega) = \mathscr{K}(\mathbf{k},\omega) = G_0(k)\ \frac{iDk^2}{\omega + iDk^2} \tag{6}$$

and relaxation regions

$$K^R_{SS}(\mathbf{q} = (\mathbf{k}-\mathbf{Q}) \to 0, \omega) = \mathscr{L}(\mathbf{q},\omega) = \frac{1}{-i\omega/\Gamma + G_0^{-1}(q)}. \tag{7}$$

Here G_0 is the static susceptibility.

In the fluctuation region $\tau = |T - T_c|/T_c \ll Gi$ (Gi is the Ginzburg number, which characterizes the limits of applicability of the Landau theory), when the fluctuations become large, the fluctuation dynamics obey the Halperin–Hohenberg similarity law, according to which the dynamic susceptibility χ and, therefore, the function K^R_{SS} can be expressed in terms of the scaling function F:

$$K^R_{SS}(\mathbf{k},\omega) = G_0(\mathbf{k})F\left(k\xi, \frac{\omega}{T_c\tau^{\nu z}}\right), \tag{8}$$

i.e., the dynamic index z which characterizes the energy scale of the critical fluctuations, $\omega \propto k^z$, can be related to a static index $\nu \approx 2/3$ which determines the variation in the correlation length, $\xi \propto \tau^{-\nu}$. For small deviations from the antiferromagnetic vector, the static susceptibility varies as $G_0(q) \propto \xi^{2-\eta}$. In the following discussion the Fisher index η, which characterizes the so-called anomalous dimensionality,[18] will be set equal to zero. This approximation is valid for three-dimensional systems.[18] It is necessary to introduce two scaling functions $\mathscr{F}_1$ and $\mathscr{F}_2$ to describe the fluctuation regions in an antiferromagnet:

$$\mathscr{K}(\mathbf{k},\omega) = G_0(\mathbf{k})\mathscr{F}_1\left(k\xi, \frac{\omega}{T_c\tau^{\nu z}}\right),$$

$$\mathscr{L}(\mathbf{q},\omega) = G_0(\mathbf{q})\mathscr{F}_2\left(q\xi, \frac{\omega}{T_c\tau^{\nu z}}\right). \tag{9}$$

Here, however, the kinetic coefficients D_0 and Γ_0 can, in turn, themselves be correlation lengths. Furthermore, as a renormalization group analysis shows,[14,19] the kinetic coefficients are singular in the fluctuation region of an antiferromagnet.

The theory developed in this paper is a variant of the interacting mode theory of Kawasaki.[20] We have tried to generalize the theory proposed by Maleev[16] for spin diffusion in ferromagnets to antiferromagnetic systems. In many regards, we follow the style and spirit of that paper. As noted before, our problem involves a study of the form of the scaling function F (see Eqs. (8) and (9)) and a determination of the frequency and momentum dependences of the kinetic coefficients in the fluctuation region, as well as establishing those approximations which must be made in a microscopic approach in order to satisfy the requirements of scaling invariance.

2. GENERALIZED KINETIC COEFFICIENTS

We therefore study the dynamic susceptibility of a cubic Heisenberg antiferromagnet located in zero magnetic field above the Néel temperature in the fluctuation region. Equations (6) and (7) can be rewritten in the more general form

$$K^R_{SS}(\mathbf{k},\omega) = \frac{i\gamma(\mathbf{k},\omega)}{\omega + iG_0^{-1}(\mathbf{k})\gamma(\mathbf{k},\omega)}, \tag{10}$$

while in the diffusion region

$$D_0 = \lim_{k\to 0}\lim_{\omega\to 0} k^{-2}\gamma(\mathbf{k},\omega)G_0^{-1}(\mathbf{k}), \tag{11}$$

and in the relaxation region the generalized kinetic coefficient $\gamma(\mathbf{k},\omega) = \Gamma(\mathbf{k},\omega)$. The limit of Eqs. (6) and (7) for $\mathbf{k}\to 0$ and $\omega\to 0$ depends strongly on the relationship between k and ω, similarly to the way it does in the theory of Fermi fluids.[21] In the following we shall be interested in the quasistatic limit, i.e. $k\to 0$ and $|\omega|/k^2 \to 0$.

As Maleev shows,[16] it is possible to go beyond the linear response theory and express the kinetic coefficients in terms of the Kubo function[22] of the operators S and $\dot{S}$ (the dot denotes differentiation with respect to time):

$$\gamma(\mathbf{k},\omega) = \frac{\Phi_{\dot{S}\dot{S}}(\mathbf{k},\omega)}{1 + G_0^{-1}(k)\Phi_{\dot{S}S}(\mathbf{k},\omega)}, \tag{12}$$

where

$$\Phi_{AB}(\mathbf{k},\omega)=\frac{1}{i\omega}\,[K^R_{AB}(\mathbf{k},\omega)-K^R_{AB}(\mathbf{k},0)],$$

$$K^R_{AB}(\mathbf{k},\omega)=i\int_0^\infty dt\; e^{i\omega t}\langle[A_{\mathbf{k}}(t),B_{-\mathbf{k}}(0)]\rangle.$$

Equation (12) is exact and accounts for the nonlinear nature of the relaxation forces. In the case of a purely exchange interaction in the long wavelength limit $\dot{S}_{\mathbf{k}}\sim k$, i.e., $\gamma=\Phi_{SS}(\mathbf{k},\omega)$, the denominator equals unity and Eq. (11) is the same as the result from the linear response theory. Generally speaking, however, the functions in the denominator cannot be neglected in a study of the frequency and momentum dependence of the kinetic coefficients.

It is easy to show that the retarded Green functions $K^R_{SS}(\mathbf{k},\omega)$, $K^R_{\dot{S}S}(\mathbf{k},\omega)$, and $K^R_{\dot{S}\dot{S}}(\mathbf{k},\omega)$ are related in the paramagnetic phase by simple formulas which follow from the dispersion relations:[23]

$$K^R_{SS}(\mathbf{k},\omega)=-i\omega K^R_{SS}(\mathbf{k},\omega),$$

$$K^R_{S\dot{S}}(\mathbf{k},\omega)=-K^R_{SS}(\mathbf{k},\omega)=i\omega K^R_{SS}(\mathbf{k},\omega),$$

$$\omega^2 K^R_{SS}(\mathbf{k},\omega)=[K^R_{\dot{S}\dot{S}}(\mathbf{k},\omega)-K^R_{\dot{S}\dot{S}}(\mathbf{k},0)]. \tag{13}$$

It is clear from these relations, in particular, that $K^R_{\dot{S}S}(\mathbf{k},\omega)$ is analogous to $K^R_{\dot{S}\dot{S}}(\mathbf{k},\omega)$ in its properties and symmetry.[16]

Combining Eqs. (11) and (13) with the equation of motion for the spin operators,

$$\dot{S}^\alpha_{\mathbf{k}}=-\frac{1}{\sqrt{N}}\sum_{\mathbf{p}}\,[V(\mathbf{p}+\mathbf{k})-V(\mathbf{p})]\epsilon_{\alpha\beta\gamma}S^\beta_{\mathbf{p}+\mathbf{k}}S^\gamma_{-\mathbf{p}} \tag{14}$$

(here $V(\mathbf{p})$ is the Fourier transform of the exchange integral) and transforming to ''imaginary'' time, we can obtain the relation between the Kubo functions and the correlators of the spin currents at the Matsubara frequencies:

$$K_{\dot{S}\dot{S}}(\mathbf{k},\omega_n)=\frac{(a^2T_c\alpha)^2}{6N}\int_0^{1/T}d\tau e^{i\omega_n\tau}\sum_{\mathbf{p}_1,\mathbf{p}_2}(\nabla V(\mathbf{p}_1)\mathbf{k})\times(\nabla V(\mathbf{p}_2)\mathbf{k})\times\langle T_\tau(S^\mu_{\mathbf{p}_1+\mathbf{k}}S^\rho_{-\mathbf{p}_1})_\tau(S^\mu_{-\mathbf{p}_2-\mathbf{k}}S^\rho_{\mathbf{p}_2})_0\rangle. \tag{15}$$

In retaining only the first gradients of the potentials, $\nabla V(\mathbf{p})\approx\mathbf{p}T_ca^2\alpha$, we limit ourselves to the lowest order terms in an expansion in ka, where a is the lattice constant; the constant $\alpha\approx1$. It will be clear from the following analysis that the corrections to the kinetic coefficients will be expressed in the form of series in powers of $k\xi$ and, since $\xi\gg a$, it is valid to neglect the higher derivatives of the exchange integral. Therefore, the problem of finding the kinetic coefficients has been reduced to calculating four-spin correlators with a current vertex. This problem can be solved by analytic continuation of the temperature diagrams with an upper semiaxis into the complex ω plane. A graphical expression for the current correlator is shown in Fig. 1.

The ''seed'' poles for the spin Green functions (6) and (7) lie on the imaginary axis, i.e., if we set up some fictitious quasiparticles to correspond to these poles, their energies will be purely imaginary. Introducing quasiparticles of this sort, e.g., ''diffusons'' and ''relaxons'', allows us to obtain closed expressions for the kinetic coefficients and to determine their scaling dimensionality.

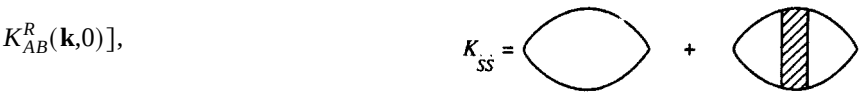

FIG. 1. Diagram series for the current correlator.

For the static susceptibility in the critical region we use the Ornstein–Zernike law:

$$G_0(\mathbf{q})=K^R_{SS}(\mathbf{q},0)=\frac{A}{T_c\tau^{2\nu}}\frac{1}{(q\xi)^2+1}, \tag{16}$$

where A is a constant ($A\sim1$) and $\tau\ll1$. In the diffusion region the static susceptibility has no singularities and $G_0\approx A/2T_c$.

The following sections are devoted to analyzing the diagram series for the spin current correlator in the fluctuation regions, finding the dynamic critical indices for the kinetic coefficients, and determining the momentum and frequency dependence of the spin diffusion coefficient and relaxation constant.

3. RELATIONSHIPS AMONG THE KINETIC COEFFICIENTS

To analyze the diagram series we introduce the concept of an irreducible self-energy part as a diagram which is continuous along one interaction line. Using the definition of γ and the properties of the functions K, we rewrite the expression for the generalized kinetic coefficient in terms of irreducible self-energy parts:

$$\gamma(\mathbf{k},\omega)=\frac{1}{i\omega}\left[\Sigma^R_{\dot{S}S}(\mathbf{k},\omega)-\Sigma^R_{\dot{S}\dot{S}}(\mathbf{k},0)+\frac{\mathscr{R}^R_{\dot{S}S}(\mathbf{k},\omega)\,\gamma(\mathbf{k},\omega)\,\mathscr{R}^R_{S\dot{S}}(\mathbf{k},\omega)}{-i\omega+G_0^{-1}(k)\,\gamma(\mathbf{k},\omega)}\right]\times\left[1+G_0^{-1}\frac{\mathscr{R}^R_{SS}(\mathbf{k},\omega)\,\gamma(\mathbf{k},\omega)}{i\omega(-i\omega+G_0^{-1}(k)\,\gamma(\mathbf{k},\omega))}\right]^{-1}. \tag{17}$$

Equation (17) can also be obtained by analyzing the diagram series for the spin current correlator,[16] as well as directly from the Larkin equation.[12,23] In the following we use the following notation:

$$K^R_{\dot{S}S}(\mathbf{k},\omega)=\mathscr{R}^R(\mathbf{k},\omega)K^R_{SS}(\mathbf{k},\omega);$$

and Σ^R_{AB} for the irreducible self-energy parts. The graphical expression for the irreducible part $\Sigma^R_{\dot{S}\dot{S}}$ corresponds to replacing a complete vertex in Fig. 1 by an irreducible vertex. Estimating $\mathscr{R}$ in self-consistent field theory[16,24] yields

$$\mathscr{R}\sim(k\xi)(ka)\ll(k\xi)^2. \tag{18}$$

In addition, its analytic properties imply that $\mathscr{R}^R\sim\omega$. We assume that the expression for $\mathscr{R}$ in the critical region also contains a term of order a/ξ in smallness, and for small ω we neglect this contribution. Thus, the generalized kinetic coef-

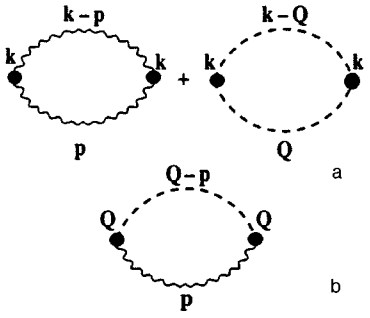

FIG. 2. Diagrams for the kinetic coefficients when two-particle intermediate states are included. A wavy line corresponds to the diffusion mode, a dashed line, to the relaxation mode. A dot denotes the vertex part of the static similarity theory.

ficient γ is defined only by the irreducible self-energy parts:

$$\gamma(\mathbf{k},\omega)=\frac{1}{i\omega}\,(\Sigma^R_{\dot S\dot S}(\mathbf{k},\omega)-\Sigma^R_{\dot S\dot S}(\mathbf{k},0)). \tag{19}$$

We now consider diagrams of a general form for the irreducible self-energy part Σ_{SS} at imaginary frequencies. These diagrams, in turn, can be classified in terms of the number of intermediate states. To begin with, we limit ourselves to diagrams with two-frequency intermediate states (Fig. 2a and b):

$$\begin{aligned}\Sigma^{(2)}_{\dot S\dot S}(\mathbf{k},i\omega)=&\frac{(T_c a^2\alpha)^2}{\sqrt{N}}\\ &\times T\sum_{\epsilon}\sum_{\mathbf{p}}\,(\mathbf{k}\Lambda^{(2)}(\mathbf{p},\mathbf{k},i\omega,i\epsilon,i(\omega-\epsilon)))\\ &\times(\mathbf{k}\Lambda^{(2)^\dagger}(\mathbf{p},\mathbf{k},i\epsilon,i(\omega-\epsilon),i\omega))\\ &\times K_{SS}(\mathbf{p},i\epsilon)K_{SS}(\mathbf{k}-\mathbf{p},i\omega-i\epsilon).\end{aligned} \tag{20}$$

In replacing the sum over the vectors $\mathbf{p}$ by an integral, we use $p\sim\xi^{-1}$ as an upper bound. Here the functions are integrated near the singularities (small $\mathbf{p}$ and $\mathbf{p}\sim\mathbf{q}+\mathbf{Q}$ in the neighborhood of the antiferromagnetic vector $\mathbf{Q}$).

The vertex parts Λ are analytic functions of all three frequencies, each of which has cuts along the real axis.[25] Vertex parts of this type have no other singularities in the complex ω planes.[25] Because of this property, the vertices can be resolved into a static part, which transforms into the vector vertex of static similarity theory, and a dynamic correction, which vanishes in the limit $\omega\to 0$. We now study the static part in more detail.

The static vertices in the diagrams (Fig. 2a) describe the long-wavelength processes of creating ''diffuson''–''diffuson'' and ''relaxon''–''relaxon'' pairs, i.e., identical modes interact. As we know, however, the static Green functions are independent of the direction of the momentum, i.e., diffuson and relaxon scattering processes contain the same vertex parts as do pair creation processes. This means that for these vertices, the Ward identity[18,21] holds (Fig. 3):

$$\Lambda^{(2)}(\mathbf{p},\mathbf{k},0)\sim\partial G_0^{-1}/\partial\mathbf{p}. \tag{21}$$

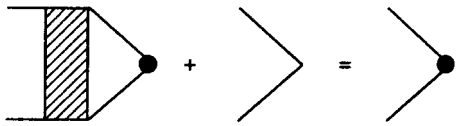

FIG. 3. The equations for a two-particle vertex part.

Here, in the second term the region of integration with respect to the momenta is concentrated near the points $\mathbf{p}\approx\mathbf{Q}$. The contribution of critical fluctuations to spin diffusion can be calculated by making the substitution $\mathbf{p}=\mathbf{q}+\mathbf{Q}$ and using the property $\partial G_0^{-1}/\partial\mathbf{p}=\partial G_0^{-1}/\partial\mathbf{q}$.

We now consider the diagram of Fig. 2b. Without loss of generality we can set the external momentum equal to the antiferromagnetic vector. In this case, we must consider two interacting modes of different kinds: a diffusion mode with short wave vectors and a relaxation mode with small deviations from the antiferromagnetism vector. Thus, the diagram of Fig. 2b describes ''diffuson''–''relaxon'' pair production. Thus, we cannot use the Ward identities for this vertex. However, the seed vertex (Fig. 3) has the scaling dimensionality

$$\Lambda_0^{(2)}(\mathbf{p},\mathbf{Q},0)\sim\partial V/\partial\mathbf{p}\sim\mathbf{p}.$$

It is also known that in the antiferromagnetic phase there is a doubling of the lattice, and the Brillouin zone of the ordered phase equals half the Brillouin zone of the disordered phase. This means that the points 0 and $\mathbf{Q}$ become equivalent in the antiferromagnetic phase. Given this fact, as well as the lack of a dependence on the direction of the momentum for the interacting modes, we may assume that rescattering by the static field does not change the scaling dimensionality of the static vertex at the antiferromagnetic vector, which can also be written in the form (21).[1)]

Continuing the diagrams shown in Fig. 2 analytically,[21] we obtain expressions for the kinetic coefficients:

$$\begin{aligned}D_0^{(2)}=&\widetilde{A}T_c\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\coth\left(\frac{\varepsilon}{2T}\right)\sum_{\mathbf{p}}\,(\nabla G_0^{-1}(\mathbf{p}))^2\\ &\times\Big[\mathrm{Im}\,\mathscr{K}(\mathbf{p},\varepsilon)\,\frac{\partial}{\partial\varepsilon}\,\mathrm{Im}\,\mathscr{K}(\mathbf{p}-\mathbf{k},\varepsilon)\\ &+\mathrm{Im}\,\mathscr{L}(\mathbf{p},\varepsilon)\,\frac{\partial}{\partial\varepsilon}\,\mathrm{Im}\,\mathscr{L}(\mathbf{p}-\mathbf{k},\varepsilon)\Big],\end{aligned} \tag{22}$$

and

$$\begin{aligned}\Gamma_0^{(2)}=&\widetilde{B}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\coth\left(\frac{\varepsilon}{2T}\right)\sum_{\mathbf{p}}\,(\nabla G_0^{-1}(\mathbf{p})\mathbf{Q})^2\\ &\times\Big[\mathrm{Im}\,\mathscr{K}(\mathbf{p},\varepsilon)\,\frac{\partial}{\partial\varepsilon}\,\mathrm{Im}\,\mathscr{L}(\mathbf{p}-\mathbf{q},\varepsilon)\\ &+\mathrm{Im}\,\mathscr{L}(\mathbf{p},\varepsilon)\,\frac{\partial}{\partial\varepsilon}\,\mathrm{Im}\,\mathscr{K}(\mathbf{p}-\mathbf{q},\varepsilon)\Big].\end{aligned} \tag{23}$$

Here the index (2) indicates that only processes with two-particle intermediate states have been taken into account. For a ferromagnet it is necessary to restrict ourselves to just the

first term in Eq. (22), since a single-mode regime is involved. Equations (22) and (23) can be rewritten in a somewhat different form. Setting $\mathbf{k}=0$ and $\mathbf{q}=0$ in the integrands and integrating by parts, we obtain

$$D_0^{(2)}=\frac{\widetilde{A}}{4}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\sinh^{-2}\left(\frac{\varepsilon}{2T}\right)\sum_{\mathbf{p}}(\nabla G_0^{-1}(\mathbf{p}))^2 \times[(\mathrm{Im}\,\mathscr{K}(\mathbf{p},\varepsilon))^2+(\mathrm{Im}\,\mathscr{L}(\mathbf{p},\varepsilon))^2] \tag{24}$$

and

$$\Gamma_0^{(2)}=\frac{\widetilde{B}}{2T_c}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\sinh^{-2}\left(\frac{\varepsilon}{2T}\right)\sum_{\mathbf{p}}(\nabla G_0^{-1}(\mathbf{p})\mathbf{Q})^2 \times\mathrm{Im}\,\mathscr{K}(\mathbf{p},\varepsilon)\mathrm{Im}\,\mathscr{L}(\mathbf{p},\varepsilon). \tag{25}$$

These expressions can be regarded as a generalization of the equations obtained by Maleev[16] from the unitarity condition for the self-energy parts to the case of two interacting modes.

The region for integrating by parts is concentrated near the singular points of the scaling functions (9). Here because of the ''critical retardation'' in the neighborhood of the phase transition points, the characteristic energies of the fluctuations satisfy the condition $\omega^*\ll T_c$, which makes it possible to retain only the first term of the expansion of the hyperbolic tangent (Eqs. (22) and (23)) or hyperbolic sine (Eqs. (24) and (25)). Evaluating the integrals with respect to the frequencies and momenta in Eqs. (22) and (24) and separating out the scaling dimensionality, we obtain a relationship between the spin diffusion coefficient and the relaxation constant:

$$D_0=b_1T_c^2a^4\left(\frac{\xi}{a}\right)^{-3}\frac{1}{D_0}+b_2T_ca^2\left(\frac{\xi}{a}\right)\frac{1}{\Gamma_0}. \tag{26}$$

Note that in order to obtain Eq. (26), it suffices to substitute the retarded Green spin functions in the form of Eqs. (6) and (7) into Eqs. (22) and (24). After integrating with respect to the frequency, the remaining integrals over the momenta contain only the static correlator G_0. The first term is determined by a two-diffuson intermediate state, and the second by a two-relaxon intermediate state.

The integrals in Eqs. (23) and (25) can be calculated in similar fashion. The relaxation constant Γ_0 and the spin diffusion coefficient are related by the equation

$$\Gamma_0=c_1\left(\frac{\xi}{a}\right)\frac{1}{\Gamma_0}+c_2\left(\frac{\xi}{a}\right)\frac{D_0/T_ca^2}{\Gamma_0^2}. \tag{27}$$

The coefficients $b_{1,2}$, $c_{1,2}\sim 1$ in Eqs. (26) and (27) depend on the form of the dynamic and static scaling functions, and in general cannot be calculated using this approach. Solving the closed system of algebraic equations (26) and (27) yields the following scaling dimensionality for the kinetic coefficients:[2)]

$$D_0/T_ca^2\propto\Gamma_0\propto(\xi/a)^{1/2}. \tag{28}$$

This sort of behavior is entirely consistent with that predicted by the dynamic scaling invariance hypothesis[14,15] and a renormalization group analysis.[15,19] Therefore, first, the kinetic coefficients for an antiferromagnet are singular in the fluctuation region, and second, spin diffusion is entirely determined by intermediate relaxation processes. The correction to the coefficient D_0 owing to self-diffusion is of smallness $\delta D_0/D_0\propto(\xi/a)^{-4}\propto\tau^{8/3}\ll 1$. That is, diffusion is not intrinsically a critical mode in an antiferromagnet. The dynamic critical index (see Eq. (8)) is $z=3/2$.

The simple physical considerations which will allow us to describe diffusion and relaxation in the fluctuation region are based on the idea that regions of size ξ with near ordering will develop as $T\to T_c$. In these regions the excitations are antiferromagnetic magnons with an acoustic dispersion character. Estimating the spin diffusion coefficient as $D_0\sim\xi^2/t_{\mathrm{diff}}$, where $t_{\mathrm{diff}}\sim\xi/c$ is the characteristic diffusion time and $c\sim\xi^{-1/2}$ is the ''sound'' speed,[14] we obtain $D_0\sim\xi^{1/2}$. Given the dynamic similarity hypothesis, according to which the dynamic critical index z, which determines the scale of the characteristic fluctuation energies, is invariant, we obtain $\Gamma_0\sim\xi^{1/2}$.

Despite the singularity of the kinetic coefficients, the relaxation time for the ordering parameter approaches infinity, which ensures the existence of macroscopic states corresponding to incomplete equilibrium.[27] The same applies to the characteristic spin diffusion times.

It should be noted that in introducing Eq. (26) we do not formally assume knowledge of the character of the excitations in the ordered phase. However, the conservation of the total moment and nonconservation of the ordering parameter actually determine the magnetic ordering properties in full.

4. FREQUENCY AND MOMENTUM DEPENDENCE OF THE KINETIC COEFFICIENTS

We shall now consider the generalized kinetic coefficients as functions of frequency and momentum. To do this we use the relationship between the retarded spin Green functions and the Kubo functions (see Eqs. (12) and (17)). Based on these equations, it is clear that the corrections associated with the frequency and momentum dependence of the kinetic coefficients are determined, first of all, by the frequency and momentum dependence of the irreducible self-energy parts, and second, by the nonlinear character of the relaxation forces. According to the estimate of Eq. (18), the momentum and frequency dependence of the kinetic coefficients can be studied in terms of the linear response theory, i.e., the nonlinearity of the relaxation forces can be neglected.

Let us first investigate the static renormalization of the kinetic coefficients. Equations (22) and (23) transform to the usual series expansion of the functions in the powers $(k\xi)^{2n}$ and $(q\xi)^{2n}$ from the static theory:

$$D^{(2)}(\mathbf{k},0)=D_0(0,0)[1+\alpha'(k\xi)^2+\ldots],$$

$$\Gamma^{(2)}(\mathbf{q},0)=\Gamma_0(0,0)[1+\beta'(q\xi)^2+\ldots].$$

This expansion is related to the existence of singularities in the correlators of the static theory at the points $k_i=-n^2\xi^{-2}$ (Ref. 26), where n is an integer. The coefficients α' and β' depend only on the form of the static correlation function.

We now proceed to analyze the energy dependence of the kinetic coefficients. Using Eq. (19), we obtain the following expressions for the real and imaginary parts of $\gamma(\mathbf{k},\omega)$:

$$\text{Re } \gamma(\mathbf{k},\omega)=\frac{\text{Im } \Sigma^R_{\dot S\dot S}(\mathbf{k},\omega)}{\omega},$$

$$\text{Im } \gamma(\mathbf{k},\omega)=-\frac{\text{Re } \Sigma^R_{\dot S\dot S}(\mathbf{k},\omega)-\text{Re } \Sigma^R_{\dot S\dot S}(\mathbf{k},0)}{\omega}. \tag{29}$$

Since Im γ is an odd function of ω and Re γ is an even function of ω, the regular expansion of the kinetic coefficients in powers of the frequency begins with ω^2.

We introduce an effective generalized kinetic coefficient γ^* according to the definition

$$\gamma^*=\frac{\dfrac{\partial}{\partial\omega}\,\text{Im } \Sigma^R_{\dot S\dot S}(\mathbf{k},\omega)\big|_{\omega=0}}{1+G_0^{-1}(\mathbf{k})\,\dfrac{\partial}{\partial\omega}\,\text{Re } \Sigma^R_{\dot S\dot S}(\mathbf{k},\omega)\big|_{\omega=0}}. \tag{30}$$

This expression for the effective generalized kinetic coefficient is analogous to the definition of effective mass in the theory of quantum liquids. The role of the Z factor is played by the renormalization constant on the mass shell:

$$Z=\frac{1}{1+G_0^{-1}(\mathbf{k})\,\dfrac{\partial}{\partial\omega}\,\text{Re } \Sigma^R_{\dot S\dot S}(\mathbf{k},\omega)\big|_{\omega=0}}.$$

Calculations of Z in the hydrodynamic and critical regions yield the following expressions for the renormalization constant:

$$Z(k\to 0)=\frac{1}{1+\epsilon'(k\xi)^2},$$

$$Z(q\to 0)=\frac{1}{1+\delta'+\delta''(q\xi)^2}, \tag{31}$$

where the constants ϵ', $\delta'\ll 1$ can also be expressed in terms of integrals of the static correlator G_0.

Extending the definition (30) to small but nonzero ω, we obtain an expansion for the real generalized spin diffusion coefficient D^* and the relaxation constant Γ^*:[3)]

$$D^{(2)*}(\mathbf{k},\omega)=D_0(0,0)[1+\alpha'(k\xi)^2+\alpha''_{k\xi}(\omega/\omega^*)^2+\ldots],$$

$$\Gamma^{(2)*}(\mathbf{q},\omega)=\Gamma_0(0,0)[\beta+\beta'(q\xi)^2+\beta''_{k\xi}(\omega/\omega^*)^2+\ldots]. \tag{32}$$

Here it must be noted that we do not claim to describe the behavior of the kinetic coefficients in the region $\omega\sim\omega^*$, $k,q\sim\xi^{-1}$. This range of frequencies and energies can scarcely be subject to detailed analysis at the present time. We therefore neglect the irregular corrections to the kinetic coefficients resulting from the generation in the higher orders of perturbation theory of an infinite sequence of poles in the retarded spin Green function, which contract to the real axis and cover the pole that produced them. We shall also not discuss the phenomena associated with the loss of a pole through a cut, etc.[16,17] All these corrections are small in the region of $\mathbf{k}$ and ω of interest to us and can be discarded.

We now consider the effect of the diagrams with many-particle ($m>2$) intermediate states. As noted above, we are only interested in the regular contribution:

$$\frac{\text{Im } \Sigma^{R(m)}_{\dot S\dot S}}{\omega}\sim(ka)^2\sum_{\mathbf{p}_1}\ldots\sum_{\mathbf{p}_m}\Lambda^{(m)}(\mathbf{k},\mathbf{p}_1,\ldots,\mathbf{p}_m)$$

$$\times\Lambda^{(m)\dagger}(\mathbf{k},\mathbf{p}_1,\ldots,\mathbf{p}_m)\,\delta(\mathbf{p}_1+\ldots p_m-\mathbf{k})\,\frac{1}{\pi^{m-1}}$$

$$\times\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\frac{d\varepsilon_1\ldots d\varepsilon_m\,\text{Im } K^R_{SS}(\mathbf{p}_1,\varepsilon_1)\ldots\text{Im } K^R_{SS}(\mathbf{p}_m,\varepsilon_m)}{\varepsilon_1\ldots\varepsilon_m}$$

$$\times\delta(\varepsilon_1+\ldots+\varepsilon_m-\omega), \tag{33}$$

where the functions K describe both the ''diffusons'' and the ''relaxons,'' and the integrals with respect to frequency are taken near the singular points of the scaling function. For $m=2$, Eq. (33) transforms into Eqs. (24) and (25).

As $k\to 0$, there are generalizations of Ward's identity[16] for the vertex parts $\Lambda^{(m)}$ analogous to Eq. (21), as a result of which the vertex can be expressed in terms of a sum of derivatives of the ordinary m-particle vertices of the static similarity theory. Using the ''dimensionality'' estimate for static vertices,[26] according to which $\Gamma_m\propto p^{3-m/2}$, in the limit $k\to 0$ we see that replacing the diagrams with two-particle intermediate states in the creation channel for ''diffusons'' and ''relaxons'' by diagrams with m-particle intermediate states does not change the scaling dimensionality of the irreducible self-energy parts. As for the behavior of the vertex parts at the antiferromagnetic vector, here the arguments advanced for diagrams with two-particle intermediate states are also valid. Thus, considering intermediate states with more than two particles does not change the scaling dimensionality of the kinetic coefficients, but only affects the values of the constants, which in any event cannot be calculated using the approach described here. The same can be said of the corrections associated with the energy dependence of the vertex parts.[16]

In conclusion, we note that the corrections associated with the frequency and momentum dependence of the kinetic coefficients can be investigated experimentally using neutron scattering, for which the scattering cross section is determined by the quantity $\text{Im } K^R_{SS}(\mathbf{k},\omega)/\omega$, where the imaginary part of the retarded spin Green function satisfies Eqs. (6) and (7) with the coefficients (32).

5. CONCLUSION

In this paper we have studied the scaling behavior of the generalized kinetic coefficients in a three-dimensional Heisenberg antiferromagnet. By means of an analysis based on a modified version of the interacting mode theory, we have found approximations in a microscopic approach for satisfying the requirements of the scaling invariance hypothesis. Specifically, it has been shown that in order to determine the scaling dimensionality of the kinetic coefficients, is sufficient to limit ourselves to processes with two-particle intermediate states, with the vertex parts being given by static similarity theory.

The regular frequency and momentum dependence of the spin diffusion coefficient and relaxation constant have been determined in a pole approximation. We have introduced the concept of effective kinetic coefficients, analogous to the definition of effective mass in the theory of quantum liquids. Including the renormalizations associated with multiple scattering of ''diffusons'' and ''relaxons'' has made it possible to write explicit series expressions for the scaling function in the frequency and momentum range $\omega \ll \omega^*$ and $k,q \ll \xi^{-1}$.

The static and dynamic similarity laws, as well as the assumed existence of just two modes (two singularities at low frequencies owing to the existence of the hydrodynamic and critical regimes), underlie the results obtained in this paper. The existence of diffusion and relaxation in an antiferromagnetic system is, in turn, related to the existence of a conserved quantity in the Heisenberg model and to the nonconservation of the ordering parameter in this model. Thus, all the formulas depend only to a small extent on the specific features of Heisenberg antiferromagnets and will be valid for any system with a nonconserved ordering parameter when an additional integral of the motion exists.

In more complicated physical systems, such as heavy Fermion compounds with integral filling of the f-shell (compounds based on Ce are an example of such materials) in the Kondo lattice model, for which the Heisenberg spin interaction is mediated by indirect exchange via conduction electrons, there may be a substantial deviation from the scaling behavior of Heisenberg magnets owing to the existence of additional modes that interact with paramagnons. Modes of this sort can develop, for example, as a result of spin-liquid correlations, which inhibit growth of the magnetic correlation length. In other words, a test for the existence of spin-liquid correlations may be to measure the generalized kinetic coefficients by neutron scattering. Other objects to which the methods described in this paper may be applied include systems with nearly zero or even negative temperatures of antiferromagnetic ordering,[6,28,29] anisotropic ferri-, and antiferrimagnets, and systems with dipole interactions.

The study of the kinetic coefficients near the Néel temperature carried out in this paper shows that diagram techniques for describing kinetic effects in antiferromagnets have many advantages over existing methods[14,15,20] and can be used to analyze unrenormalizable Hamiltonians, as well as for problems with nonlocal interacting modes.

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[1)]Recall that the anomalous dimensionality index (Fisher index) is assumed equal to zero.

[2)]In a ferromagnet, the spin diffusion coefficient is not a singular function: $D_0/T_c a^2 \propto (\xi/a)^{-1/2}$.

[3)]$\omega^* \sim T_c \tau^{\nu z}$ is the characteristic energy of the fluctuations, with $z = 3/2$.

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