# Time-dependent correlations for axially symmetric infinite-range spin Hamiltonians

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The time-correlation functions  $\langle \hat{s}_x(t)\hat{s}_y(0) \rangle$  and  $\langle \hat{s}_x(t)\hat{s}_y(0) \rangle$  are evaluated for an arbitrary infinite-range axially symmetric Hamiltonian with an arbitrary elementary spin. The behavior above the critical temperature as well as that for the three possible types of ordered phases (XY-like, intermediate, and Ising-like) is presented. Some physical consequences are discussed.

# I. INTRODUCTION

The anisotropic Heisenberg (AH) model was applied both in the theory of magnetism<sup>1</sup> and as a lattice model of a quantum fluid.<sup>2</sup> The need for higher-order terms in the spin operators was discussed by Zilsel<sup>3</sup> in an attempt to account for the complete phase diagram of liquid <sup>4</sup>He.

The dynamic properties of spin systems are described by means of the time- and temperature-dependent spin correlation functions which contain all the information concerning the energies of the "elementary excitations" and are closely related to the response functions of the system.

The dynamic properties of the XY model, which is a special case of the AH model, have been extensively studied.<sup>4,5</sup> Exact results for the spin correlation functions in the one-dimensional AH model were derived by Schneider and Stoll.<sup>6</sup>

The study of the dynamic properties of infinite-range anisotropic spin models was pioneered by Lee and coworkers<sup>7-10</sup> who evaluated the transverse time correlation function for the axially symmetric Heisenberg Hamiltonian with an elementary spin  $\sigma = \frac{1}{2}$ .

In order to obtain a more comprehensive view of the dynamical properties of infinite-range spin Hamiltonians, we propose to generalize the work of Lee and co-workers in three ways: (1) An arbitrary axially symmetric infinite-range spin Hamiltonian is considered. (2) An arbitrary elementary spin is allowed. (3) In addition to  $\langle \hat{S}_x(t)\hat{S}_x(0) \rangle$ , we evaluate  $\langle \hat{S}_x(t)\hat{S}_y(0) \rangle$ . Our study is based on the results we have recently obtained concerning the static properties of the generalized axially symmetric infinite-range spin Hamiltonian.<sup>11</sup>

The time-dependent correlation functions evaluated for infinite-range models have certain obvious limitations. These models lack a natural length scale which makes it impossible to account for spatial fluctuations. The spincorrelation functions obtained in these models are independent of the space coordinates so that their Fourier transforms (the form factors) are defined only for q = 0. Consequently, the elementary excitations obtained are dispersionless. At best, they represent the  $q \rightarrow 0$  limit of the realistic excitation spectrum corresponding to finite-range interactions. The fact that the form factors are evaluated only at q = 0 may give rise to difficulties in obtaining the static limit ( $q \rightarrow 0, \omega \rightarrow 0$ ) of the response functions.<sup>12</sup> In view of the extreme simplicity of the exact evaluation of the time-dependent spin correlation functions for infinite-range Hamiltonians, we feel that despite the above reservations it is worthwhile to examine the properties of these correlation functions and their relation to more accurate models.

### II. THE TIME-CORRELATION FUNCTIONS: GENERAL EXPRESSIONS

It will be convenient to use the "microscopic" spin operators  $\hat{s}_{\alpha}$  ( $\alpha = x, y, z$ ), which are related to the "macroscopic" spin operators  $\hat{S}_{\alpha} = \sum_{i=1}^{N} \hat{s}_{i\alpha}$  by  $\hat{s}_{\alpha} = \hat{S}_{\alpha}/N$ . These operators satisfy the slightly modified commutation relations

$$[\hat{s}_x, \hat{s}_v] = i \hat{s}_z / N$$
, etc.

We consider a system described by an arbitrary axially symmetric infinite-range spin Hamiltonian

$$\mathcal{H} = NH(\hat{s}^2, \hat{s}_z)$$

with an elementary spin  $\sigma$ . The static properties of this Hamiltonian were recently investigated.<sup>11</sup> The end result was that in addition to the high-temperature paramagnetic state there are three types of ordered (low-temperature) phases. In terms of the thermal averages  $s_z = \langle \hat{s}_z \rangle$  and  $s^2 = \langle \hat{s}^2 \rangle$ , these phases can be characterized as follows. (a) Ising type, for which  $|s_z| = s$ , and s is determined from the equation  $s = \sigma B_{\sigma}(-\beta \sigma dH/ds)$ , (b) intermediate type, for which  $s_z$  and s are determined from the coupled equations

$$\partial H/\partial s_z = 0$$

and

$$s = \sigma B_{\sigma}(-\beta\sigma \,\partial H/\partial s)$$

and (c) XY type, for which  $s_z = 0$  and

$$s = \sigma B_{\sigma}(-\beta\sigma\partial H/\partial s)$$
, and

$$\sigma B_{\sigma}(\sigma\mu) = (\sigma + \frac{1}{2}) \operatorname{coth}[(\sigma + \frac{1}{2})\mu] - \frac{1}{2} \operatorname{coth}(\mu/2)$$

is Brillouin's function.

We are interested in the time-correlation functions  $S_{\alpha\beta}(t) = \langle \hat{s}_{\alpha}(t) s_{\beta}(0) \rangle$ ,  $\alpha, \beta = x, y$ . As will be evident later, it is convenient to study the time dependence of  $\hat{s}_{+} = \hat{s}_{x} \pm i \hat{s}_{y}$ . In terms of these operators

$$S_{xx}(t) = [S_{+-}(t) + S_{-+}(t) + S_{++}(t) + S_{--}(t)]/4, \qquad (1)$$

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where  $S_{+-}(t) = \langle \hat{s}_{+}(t) \hat{s}_{-}(0) \rangle$ , etc. Similar relations hold for  $S_{yy}(t)$ ,  $S_{xy}(t)$ , and  $S_{yx}(t)$ .

The time dependence of  $\hat{s}_{\pm}$  is determined by their commutators with the Hamiltonian. The only terms in the Hamiltonian which do not commute with these operators are the terms containing  $\hat{s}_z$ . One can easily show that for an arbitrary function of  $\hat{s}_z$  the identity

$$\hat{s}_{\pm}f(\hat{s}_{z}) = f\left[\hat{s}_{z} \mp \frac{1}{N}\right]\hat{s}_{\pm}$$
$$= \left[\exp\left[\mp \frac{1}{N}\frac{\partial}{\partial\hat{s}_{z}}\right]f(\hat{s}_{z})\right]\hat{s}_{\pm}$$

is satisfied. It follows immediately that

$$\dot{\hat{s}}_{\pm} = i \left[ \hat{\mathscr{H}}, \hat{s}_{\pm} \right] = i \hat{F}_{\pm} (\hat{s}^2, \hat{s}_z) \hat{s}_{\pm} , \qquad (2)$$

where

$$\hat{F}_{\pm} = N \left[ 1 - \exp\left[ \pm \frac{1}{N} \frac{\partial}{\partial \hat{s}_z} \right] \right] \hat{H}(\hat{s}^2, \hat{s}_z) .$$
(3)

In the limit  $N \rightarrow \infty$  we obtain

$$\widehat{F}_{\pm} \simeq \pm \left[ \frac{\partial \widehat{H}}{\partial \widehat{s}_z} \right]_{\widehat{s}} - \frac{1}{2N} \left[ \frac{\partial^2 \widehat{H}}{\partial \widehat{s}_z^2} \right]_{\widehat{s}} + \cdots \qquad (4)$$

In the discussion of the XY and intermediate phases it will be important to note that the thermal average of the leading term in Eq. (4),  $\langle \partial \hat{H} / \partial \hat{s}_z \rangle$ , vanishes. From Eq. (2) it follows that

$$\hat{s}_{+}(t) = \exp[it\hat{F}_{+}(\hat{s}^{2},\hat{s}_{z})]\hat{s}_{+}(0)$$

and

$$\hat{s}_{-}(t) = \exp[it\hat{F}_{-}(\hat{s}^2,\hat{s}_{\tau})]\hat{s}_{-}(0)$$

Thus

$$\begin{split} S_{+-}(t) &= \langle \exp[it\hat{F}_{+}(\hat{s}^{2},\hat{s}_{z})]\hat{s}_{+}(0)\hat{s}_{-}(0)\rangle \\ &= \langle \exp[it\hat{F}_{+}(\hat{s}^{2},\hat{s}_{z})][\hat{s}^{2} - \hat{s}_{z}^{2} + (1/N)\hat{s}_{z}]\rangle , \\ S_{-+}(t) &= \langle \exp[it\hat{F}_{-}(\hat{s}^{2},\hat{s}_{z})][\hat{s}^{2} - \hat{s}_{z}^{2} - (1/N)\hat{s}_{z}]\rangle , \\ S_{++}(t) &= \langle \exp[itF_{+}(\hat{s}^{2},\hat{s}_{z})]\hat{s}_{+}^{2}(0)\rangle , \end{split}$$

a similar relation holding for  $S_{--}(t)$ .

Evaluating these correlation functions in a basis  $\{|s,s_z\rangle\}$  of eigenstates of the axially symmetric Hamiltonian, we observe that

$$S_{++}(t) = S_{--}(t) = 0$$
,

so that

$$S_{xx}(t) = S_{yy}(t) = [S_{+-}(t) + S_{-+}(t)]/4$$

and

$$S_{xy}(t) = -S_{yx}(t) = i[S_{+-}(t) - S_{-+}(t)]/4$$
.

For a Hamiltonian which is even in  $s_z$ , Eq. (3) implies that

$$\hat{F}_{\pm} = \hat{F}_e \pm \hat{F}_o$$

where  $F_e(F_o)$  contain the even (odd) terms in  $s_z$ . In this case

$$S_{xx}(t) = \frac{1}{2} [\langle \exp(it\hat{F}_e)\cos(t\hat{F}_o)(\hat{s}^2 - \hat{s}_z^2) \rangle + (i/N) \langle \exp(it\hat{F}_e)\sin(t\hat{F}_o)\hat{s}_z \rangle]$$

and

$$S_{xy}(t) = \frac{1}{2} \left[ -\langle \exp(it\hat{F}_e)\sin(t\hat{F}_o)(\hat{s}^2 - \hat{s}_z^2) \rangle + (i/N)\langle \exp(it\hat{F}_e)\cos(t\hat{F}_o)\hat{s}_z \rangle \right].$$

In the special case considered by Dekeyser and Lee,<sup>7</sup>  $\hat{H} = -J\hat{s}^2 + \lambda \hat{s}_z^2$ , we obtain  $\hat{F}_{\pm} = \lambda(\pm 2\hat{s}_z - 1/N)$  so that

$$\begin{split} S_{xx}(t) &= \frac{1}{2} \exp[-i(\lambda/N)t] [\langle \cos(2\lambda t \widehat{s}_{z})(\widehat{s}^{2} - \widehat{s}_{z}^{2}) \rangle \\ &+ (i/N) \langle \sin(2\lambda t \widehat{s}_{z}) \widehat{s}_{z} \rangle ], \end{split}$$

$$S_{xy}(t) = \frac{1}{2} \exp[-i(\lambda/N)t] [-\langle \sin(2\lambda t \hat{s}_{z})(\hat{s}^{2} - \hat{s}_{z}^{2}) \rangle + (i/N) \langle \cos(2\lambda t \hat{s}_{z}) \hat{s}_{z} \rangle ].$$

(8)

(7)

Equation (7) is in agreement with Eq. (30a) of Ref. 7.

In order to evaluate the correlation functions we have to consider the fluctuations of s and  $s_z$  around their equilibrium values,  $\bar{s}$  and  $\bar{s}_z$ . As these fluctuations are of order  $N^{-1/2}$  relative to the equilibrium values, we shall follow Dekeyser and Lee<sup>7</sup> and write  $s = \bar{s} + N^{-1/2}x$  and  $s_z = \bar{s}_z + N^{-1/2}z$  with x and z varying over appropriate ranges.

As is usually the case, the probability distribution may be considered as a sharp Gaussian centered at the equilibrium values. A slight modification of this statement is necessary for the behavior of  $s_z$  in the Ising-like phase, and will be considered in Sec. III C. In writing the appropriate expansions we shall use the notation

$$U_{ij} \equiv \frac{1}{i!j!} \frac{\partial^{(i+j)}U}{\partial s^i \partial s_z^j} \bigg|_{\overline{s},\overline{s}_z}$$

The degeneracy function for an arbitrary elementary spin  $\sigma$  can be written in the form<sup>13</sup>

$$\Omega = g_0(s) \exp[-NW(s)],$$

where

$$W = \mu s + \ln \sinh(\mu/2) - \ln \sinh[\mu(\sigma + \frac{1}{2})], \qquad (9)$$

and  $\mu$  is determined by the equation

$$s = \sigma B_{\sigma}(\sigma \mu) . \tag{10}$$

The preexponential factor  $g_0(s)$  is not relevant to the equilibrium properties and was therefore omitted in Ref. 13. It only affects the correlation functions above the critical temperature, because for small s this factor can be shown to be proportional to s, in the limit  $N \rightarrow \infty$ . In view of Eq. (9), the degeneracy function is, for arbitrary  $\sigma$ , an implicit function of s and only for  $\sigma = \frac{1}{2}$  an explicit expression can be obtained. This expression, up to normalization, is

(6)

(5)

$$\Omega = \frac{s}{2s+1} (1-4s^2)^{-1/2} \exp\{-\frac{1}{2}N[(1-2s)\ln(1-2s) + (1+2s)\ln(1+2s)]\}$$

and is in agreement with that used by Dekeyser and Lee,<sup>7</sup> apart from the preexponential factor  $(1-4s^2)^{-1/2}$ , which is always inconsequential.

The distribution function can be written in the form  $\exp[-NG(s,s_z)]/Z$  where

$$G(s,s_z) = W(s) + \beta H(s,s_z)$$
  
and

$$Z = \sum_{s,s_z} \exp[-NG(s,s_z)] \; .$$

Expanding in the fluctuations we obtain, for all but the Ising-type phase,

$$G \simeq \overline{G} + N^{-1} [W_2 x^2 + \beta (H_{20} x^2 + H_{11} xz + H_{02} z^2)], \quad (12)$$

where

$$W_2 = \frac{1}{2} \frac{\partial^2 W}{\partial s^2} \bigg|_{\overline{s}}.$$

From Eq. (9) it follows that  $\partial W / \partial s = \mu$  and

$$\frac{\partial^2 W}{\partial s^2} = \frac{\partial \mu}{\partial s} = \left(\frac{\partial s}{\partial \mu}\right)^{-1}$$
$$= \frac{1}{4 \sinh^2(\mu/2)} - \frac{(\sigma + \frac{1}{2})^2}{\sinh^2[(\sigma + \frac{1}{2})\mu]} . \quad (13)$$

To obtain  $\partial^2 W/\partial s^2$  as a function of s we substitute in Eq. (13) the value of  $\mu$  satisfying Eq. (10). The two asymptotic expressions

$$\frac{\partial^2 W}{\partial s^2} \simeq \begin{cases} \frac{3}{\sigma(\sigma+1)} , s \to 0 \\ \frac{1}{\sigma-s} , s \to \sigma \end{cases}$$

are easily obtained. The low-s limit remains fairly accurate up to  $s/\sigma \sim 0.1$ .

In order to expand  $F_{\pm}(s,s_z)$  in terms of the fluctuations we note that in the paramagnetic as well as in the XY and intermediate phases  $H_{01}=0$  so that the leading terms

(11) In the Ising case 
$$H_{01} \neq 0$$
, so that  
 $F_{\pm} \simeq \pm [H_{01} + N^{-1/2} (H_{11} x + H_{02} z)]$ .

in  $\partial H / \partial s_z$ , resulting in

 $F_{\pm} \simeq \pm N^{-1/2} (H_{11}x + H_{02}z)$ .

of order  $N^{-1}$  which may be neglected.

Inspection of Eqs. (14) and (15) indicates that in the limit  $N \rightarrow \infty$  only the Ising phase will exhibit a time dependence in the correlation functions  $S_{xx}(t)$  and  $S_{xy}(t)$ , while for the other phases these functions will be time independent.

(lowest order in N) are due to the fluctuations of s and  $s_z$ 

The second derivative term in Eq. (4) contributes a term

The expressions for the time-correlation functions, Eqs. (5), contain the factor  $s^2 - s_z^2 \pm s_z/N$ . The term  $s_z/N$  is only comparable with the  $s^2 - s_z^2$  term in the Ising case. In the paramagnetic case  $s^2 - s_z^2 \sim N^{-1}$  and  $s_z/N \sim N^{-3/2}$ ; in the XY and intermediate cases  $s^2 - s_z^2$  is independent of N while  $s_z/N$  is at most of order  $N^{-1}$ . Therefore, in all but the Ising case, in the limit  $N \rightarrow \infty$  we obtain  $S_{-+}(t) = S_{+-}(t)$  so that  $S_{xy}(t) = 0$ .

In the following section we evaluate the timecorrelation functions for the various phases possible, retaining the lowest-order *N*-dependent terms.

# III. THE TIME-CORRELATION FUNCTIONS IN THE EQUILIBRIUM PHASES

#### A. The paramagnetic phase

Above the critical temperature the average values  $\bar{s}$  and  $\bar{s}_z$  vanish. Therefore, the only terms in the Hamiltonian which contribute to Eq. (12) are those involving  $s^2$  and  $s_z^2$ . Thus, we can restrict the Hamiltonian to the form  $H = -J\hat{s}^2 + \lambda \hat{s}_z^2$  studied by Dekeyser and Lee,<sup>7</sup> without loss of generality.

For this case Eqs. (6), (11), and (12) yield

$$S_{xx}(t) = \frac{1}{2N} \exp[-i(\lambda/N)t](I_1 + iN^{-1/2}I_2)/Z ,$$

where

$$\begin{split} I_1 &= \int_0^\infty dx \, \int_{-x}^x dz \, x \, \exp(-\alpha x^2 - \beta \lambda z^2) \cos(2\lambda t N^{-1/2} z) (x^2 - z^2) \\ I_2 &= \int_0^\infty dx \, \int_{-x}^x dz \, x \, \exp(-\alpha x^2 - \beta \lambda z^2) \sin(2\lambda t N^{-1/2} z) z \, , \\ Z &= \int_0^\infty dx \, \int_{-x}^x dz \, x \, \exp(-\alpha x^2 - \beta \lambda z^2) \, , \end{split}$$

and

$$\alpha = \frac{3}{2\sigma(\sigma+1)} - \beta J \; .$$

Evaluating the integrals we obtain

$$S_{xx}(t) = \frac{1}{2N} \left[ \frac{1}{\frac{3}{2\sigma(\sigma+1)} - \beta J} + \frac{i\lambda t}{N\left[\frac{3}{2\sigma(\sigma+1)} - \beta J_z\right]} \right]$$
$$\times \exp\left[ -\lambda^2 t^2 / N\left[\frac{3}{2\sigma(\sigma+1)} - \beta J_z\right] \right], \quad (16)$$

(14)

(15)

where

 $J_z = J - \lambda$ .

This is the generalization to arbitrary  $\sigma$  of Eq. (36a) of Dekeyser and Lee.<sup>7</sup> In this range of temperatures Eq. (8)results in  $S_{xy}(t)=0$ , because  $s_z$  fluctuates symmetrically about  $\overline{s_z} = 0$ .

As one could have expected on the basis of the fact that the leading term in  $F_{\pm}$  [Eq. (4)] vanishes, in the thermodynamic limit  $(N \rightarrow \infty)$   $S_{xx}$  is time independent and Eq. (16) simply means that

$$\langle s_x^2 \rangle = [T/(T-T_x)]\sigma(\sigma+1)/3N$$

where  $T_x = 2J\sigma(\sigma+1)/3k$ . If  $\lambda < 0$ , i.e., the transition is into an XY-type phase,  $T_x$  is the critical temperature and  $\langle s_x^2 \rangle$  exhibits critical fluctuations which are identical with those of the usual mean-field results for the Heisenberg model. If  $\lambda > 0$ , i.e., the low-temperature phase is Isingtype, the critical fluctuations are present in  $\langle s_z^2 \rangle$  but not in  $\langle s_x^2 \rangle$ . The static susceptibility, being proportional to  $\langle s_x^2 \rangle$ , exhibits the Curie-Weiss behavior  $\chi \sim (T - T_x)^{-1}$ .

# B. XY and intermediate phases

Assuming that the equilibrium values  $\overline{s}$  and  $\overline{s}_z$ , for which G [Eq. (11)] is extremal, have been determined from the magnetization equation, we proceed to evaluate the correlation functions  $S_{xx}(t)$  and  $S_{xy}(t)$ . The coefficients appearing in Eqs. (12) and (14) are determined at  $\overline{s}$  and  $\overline{s}_{z}$ .

The expression to be evaluated is • •

- -

$$S_{+-}(t) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dz \exp[-(\alpha x^{2} + \beta H_{11}xz + \beta H_{02}z^{2})] \exp[itN^{-1/2}(H_{11}x + H_{02}z)][\bar{s}^{2} - \bar{s}_{z}^{2} + 2N^{-1/2}(\bar{s}x - \bar{s}_{z}z)] \\ \times \left[\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dz \exp[-(\alpha x^{2} + \beta H_{11}xz + \beta H_{02}z^{2})]\right]^{-1},$$

where

$$\alpha = W_2(\overline{s}) + \beta H_{20}(\overline{s}, \overline{s}_7) \; .$$

The integrals involved are straightforward, resulting in

$$S_{xx}(t) = S_{yy}(t) = \frac{1}{2}(\overline{s}^2 - \overline{s}_z^2) \exp\left[-\frac{t^2}{N}(G_{20}H_{02}^2 + G_{02}H_{11}^2 - G_{11}H_{11}H_{02})/(4G_{20}G_{02} - G_{11}^2)\right],$$

where

$$G_{20} = W_2 + \beta H_{20}$$
,  $G_{11} = \beta H_{11}$ ,  $G_{02} = \beta H_{02}$ .

Note that in the limit  $N \rightarrow \infty$ ,

$$S_{xx}(t) = S_{yy}(t) = (\bar{s}^2 - \bar{s}_z^2)/2$$

For the Dekeyser-Lee-type Hamiltonian,  $H = -J\hat{s}^2$  $+\lambda \hat{s}_{z}^{2}$ , with an arbitrary value of the elementary spin  $\sigma$ , we obtain

$$H_{02} = 2\lambda$$
,  $H_{11} = 0$ ,  
 $G_{20} = W_2 - \beta J$ ,  $G_{11} = 0$ 

and

$$G_{02}=\beta\lambda$$

Thus

$$S_{xx}(t) = \frac{1}{2} (\overline{s}^2 - \overline{s}_z^2) \exp(-\lambda t^2 / \beta N) ,$$

which agrees with the result obtained for  $\sigma = \frac{1}{2}$  in Ref. 7 [Eq. (41a)].

In order to interpret these results it is important to realize that in the XY and intermediate phases  $S_{xx}(t)$  and  $S_{xy}(t)$  have a longitudinal contribution, i.e., are not transverse correlation functions. The correlation function  $\langle \hat{s}_{z}(t)\hat{s}_{z}(0) \rangle$ , which is the transverse correlation function in the XY case, is rigorously time independent for the infinite-range Hamiltonian, because  $\hat{s}_z = -i[\hat{s}_z, \hat{H}] = 0$ . This situation is familiar with respect to the isotropic finite-range Heisenberg Hamiltonian.

In analogy with the isotropic Heisenberg Hamiltonian we expect the finite-range analog of our axially symmetric Hamiltonian to exhibit in the XY phase a branch of magnons with a dispersion law satisfying  $\lim_{q\to 0} \omega(q) = 0$ . An examination of the uniaxial Heisenberg model suggests that the dispersion law is of the form  $\omega(q) \propto |q| (q \rightarrow 0)$ with a coefficient which includes the anisotropy  $(J_z - J_x)$ . This result, which is to be contrasted with the quadratic dependence of  $\omega$  on q obtained for the isotropic case, is derived in the Appendix. The linear-dispersion law results in a  $\sim T^3$  dependence of the low-temperature magnetization and specific heat, instead of the  $\sim T^{3/2}$  dependence resulting from the spin-wave contribution in the isotropic case. An intermediate-type solution does not exist for the axially symmetric Heisenberg Hamiltonian, which makes it impossible to obtain a similar estimate of the low-q form of the dispersion law, in the simple way presented in the Appendix.

#### C. Ising-type phase

The Ising case  $(\bar{s}_z = \bar{s})$  has to be treated separately for the following three reasons.

(i) The fluctuations of s and  $s_z$  occur about the same average value so that the satisfaction of the condition  $s_z \leq s$  is nontrivial.

(ii) In the limit  $N \rightarrow \infty$ ,  $F_{\pm} = \pm H_{01}$  where  $H_{01} < 0$ , leading to a nonvanishing time dependence of the correlation functions.

(iii) A further consequence of the fact that  $H_{01} < 0$  is that the dependence of the Hamiltonian on  $s_z$  is expressed by means of the expansion

$$H(s,s_z) = H(s,s) + H_{01}(s_z - s) + \cdots$$
 (17)

In order to evaluate the time-correlation functions we note that as a consequence of Eq. (17) the distribution of the fluctuations of  $s_z$  is not Gaussian but rather given by  $\exp[-N\beta H_{01}(\bar{s}_z - s_z)]$  with  $\bar{s}_z = \bar{s}$  and  $s_z \le s = \bar{s} + N^{-1/2}x$ . Therefore, the typical fluctuations in  $s_z$  are of the order of magnitude of  $N^{-1}$ , unlike the typical Gaussian fluctuations, which are of order  $N^{-1/2}$ . Thus

$$Z \simeq \frac{g(\bar{s})}{2N\beta |H_{01}|} e^{-NG_0} \{ 2\pi / [W_2 + \beta (H_{20} + 2H_{11} + H_{02})] \}^{1/2} .$$

Using Eq. (18), we obtain

$$S_{+-}(t) = \frac{1}{Z} \int_0^{\sigma} ds \int_0^s ds_z g(s) \exp\{-N[W + \beta H + \beta H_{01}(s_z - s)]\} e^{itH_{01}} \left[2s(s - s_z) + \frac{1}{N}s\right]$$

(19)

which can be integrated straightforwardly to yield

$$S_{+-}(t) = \frac{\bar{s}}{N} e^{itH_{01}} \left[ 1 + \frac{2}{\beta |H_{01}|} \right].$$

Similarly,

$$S_{-+}(t) = \frac{\overline{s}}{N} e^{-itH_{01}} \left[ -1 + \frac{2}{\beta |H_{01}|} \right]$$

so that

$$S_{xx}(t) = \frac{\overline{s}}{2N} \left[ i \sin(tH_{01}) + \frac{2}{\beta |H_{01}|} \cos(tH_{01}) \right]$$

and

$$S_{xy}(t) = \frac{\overline{s}}{2N} \left[ \cos(tH_{01}) + \frac{2i}{\beta |H_{01}|} \sin(tH_{01}) \right]$$

For the system studied by Dekeyser and Lee,<sup>7</sup>

$$\widehat{H} = -J\widehat{s}^2 + \lambda \widehat{s}_z^2 \quad (\lambda < 0) , \quad H_{01} = 2\lambda \overline{s}$$

and

$$S_{xx}(t) = \frac{\overline{s}}{2N} \left[ \frac{1}{-\lambda\beta\overline{s}} \cos(2\lambda t\overline{s}) + i\sin(2\lambda t\overline{s}) \right]$$

which is in agreement with their Eq. (45).

The frequency  $\omega = |H_{01}|$  appearing in the spin correlation functions is the frequency of a magnon with an infinite wavelength (vanishing wave vector,  $\vec{q}$ ). Such a nonvanishing  $q \rightarrow 0$  limit corresponds to a branch of optical magnons. The energy gap  $\hbar\omega$  corresponds to the finite energy required for a rotation of the spin from the z axis to the xy plane. This frequency depends on  $\vec{s}$  and, therefore, on the temperature, and is thus a finite-

$$s^{2} - s_{z}^{2} + \frac{1}{N}s_{z} = (s + s_{z})(s - s_{z}) + \frac{1}{N}s_{z}$$
  

$$\simeq 2s(s - s_{z}) + \frac{1}{N}s, \qquad (18)$$

where terms of order  $N^{-2}$  were neglected.

This approach is equivalent to that of Dekeyser and Lee,<sup>7</sup> which involves the asymptotic properties of the Dawson integral.

The canonical partition function is obtained in the form  $-c^{\sigma} + c^{s}$ 

$$Z = \int_0^\infty ds \int_0^\infty ds_z g(s) \exp\{-N[W(s) + \beta H(s,s) + \beta H_{01}(s_z - s)]\}.$$

After integration with respect to  $s_z$ , we evaluate the integral over s using an expansion about  $\overline{s}$ , up to quadratic terms in the fluctuations, obtaining

temperature collective mode. It is analogous to the optical spin mode obtained in the study of ferromagnetic resonance, where it is due to a combination of the effects of the external magnetic field and the anisotropy of the dipole-dipole interaction.<sup>14</sup> In view of the similarity of Eq. (19) to the spin correlation function studied by Lee,<sup>5</sup> it is clear that all his results concerning the response functions can be transferred to the present context with the trivial replacement of his constant  $\omega_0$  with the temperature dependent  $|H_{01}|$ . In particular, this implies a resonative behavior of the dynamic magnetic susceptibility.

A treatment analogous to that used in the Appendix results in the present case in the low-q dispersion law  $\omega = \omega_0 + \alpha q^2$ . As a consequence of the nonvanishing value of  $\omega_0$  the magnetization and the specific heat will have a gaplike exponential behavior at low temperatures. Thus mean-field theory is a more valid approach in this extremely anisotropic case than for systems having a gapless spin-wave spectrum which corresponds to a brokensymmetry thermodynamic ground state.<sup>12,15</sup>

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#### APPENDIX

For the axially symmetric finite-range Heisenberg Hamiltonian

$$\begin{split} \widehat{\mathscr{H}} &= -\sum_{(i,j)} \left[ J_{\mathbf{x}}(\mid i-j \mid ) (\widehat{s}_{\mathbf{x}_i} \widehat{s}_{\mathbf{x}_j} + \widehat{s}_{\mathbf{y}_i} \widehat{s}_{\mathbf{y}_j}) \right. \\ &+ J_{\mathbf{z}}(\mid i-j \mid ) \widehat{s}_{\mathbf{z}_i} \widehat{s}_{\mathbf{z}_j} \right], \end{split}$$

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we derive the dispersion relation for finite-temperature magnons in the XY phase, following the procedure presented by White.<sup>16</sup>

The Fourier-transformed Hamiltonian is

$$\begin{split} \hat{\mathscr{H}} &= -\sum_{\vec{q}'} \left\{ J_x \left( \vec{-q}' \right) [ \hat{s}_x (\vec{q}') \hat{s}_x (-\vec{q}') + \hat{s}_y (\vec{q}') \hat{s}_y (-\vec{q}') ] \right. \\ &+ J_z (-\vec{q}') \hat{s}_z (\vec{q}') \hat{s}_z (-\vec{q}') \right\} \,. \end{split}$$

We assume that the magnetization is along the x axis. The equations of motion for the transverse components are

$$\hat{s}_{\alpha}(\vec{q}) = -i[\hat{s}_{\alpha}(\vec{q}), \hat{\mathcal{H}}], \ \alpha = y, z$$
.

Using the random-phase approximation and noting that

 $\langle \hat{s}_{z}(\vec{q}) \rangle \simeq \bar{s} \delta(\vec{q})$ 

(where  $\overline{s} = \overline{S}/N$ ,  $\overline{S}$  being the magnetization), we obtain

- <sup>1</sup>J. Als-Nielsen, O. W. Dietrich, W. Marshall, and P. A. Lindgard, Solid State Commun. 5, 607 (1967).
- <sup>2</sup>M. E. Fisher, Rep. Prog. Phys. **30**, 615 (1967), and references therein.
- <sup>3</sup>P. R. Zilsel, Phys. Rev. Lett. 15, 476 (1965).
- <sup>4</sup>R. V. Ditzian and D. D. Betts, Can. J. Phys. 50, 129 (1972), and references therein.
- <sup>5</sup>M. H. Lee, Phys. Rev. B 8, 3290 (1973).
- <sup>6</sup>T. Schneider and E. Stoll, Phys. Rev. Lett. 47, 377 (1981).
- <sup>7</sup>R. Dekeyser and M. H. Lee, Phys. Rev. B 19, 265 (1979).
- <sup>8</sup>I. M. Kim and M. H. Lee, Phys. Rev. B 24, 3961 (1981).
- <sup>9</sup>M. H. Lee, J. Math. Phys. 23, 464 (1982).
- <sup>10</sup>M. H. Lee, I. M. Kim, and R. Dekeyser, Phys. Rev. Lett. 52,

 $\dot{\hat{s}}_{y}(\vec{q}) = -2\bar{s}\left[J_{z}(\vec{q}) - J_{x}(0)\right]\hat{s}_{z}(\vec{q}) ,$  $\dot{\hat{s}}(\vec{d}) = -2\bar{s}\left[J_{z}(0) - J_{x}(0)\right]\hat{s}(\vec{d})$ 

$$s_z(\mathbf{q}) = -2s \left[ J_x(\mathbf{0}) - J_x(\mathbf{q}) \right] s_y(\mathbf{q})$$

A solution of the form

 $\hat{s}_{\alpha}(\vec{q},t) \propto \exp[i\omega(\vec{q})t]$ ,

where

$$\omega(\vec{q}) = 2\bar{s} \{ [J_x(0) - J_x(\vec{q})] [J_x(0) - J_z(\vec{q})] \}^{1/2}$$

is obtained.

In the limit  $\vec{q} \rightarrow 0$ , the dispersion relation becomes

$$\omega(\vec{q}) = 2\bar{s}[J_x(0) - J_z(0)]^{1/2} \left[ -\frac{\partial^2 J_x}{\partial q^2} \Big|_{q=0} \right] |\vec{q}| .$$

In the isotropic case  $J_x(\vec{q})=J_z(\vec{q})$  we obtain  $\omega(\vec{q})=2\bar{s}[J_x(0)-J_x(\vec{q})]$  which, for  $q \rightarrow 0$ , results in the familiar quadratic dispersion law.

1579 (1984).

- <sup>11</sup>G. F. Kventsel and J. Katriel, Phys. Rev. B 30, 2828 (1984).
- <sup>12</sup>D. Forster, *Hydrodynamic Fluctuations, Broken Symmetry* and Correlation Functions (Benjamin, Reading, Mass., 1975).
   <sup>13</sup>G. F. Kventsel and J. Katriel, J. Appl. Phys. 50, 1820 (1979).
- <sup>14</sup>N. N. Bogoliubov and S. V. Tyablikov, Dokl. Akad. Nauk SSSR 126, 53 (1959) [Sov. Phys.—Dokl. 4, 589 (1959)]; V. L. Bonch-Bruevich and S. V. Tyablikov, *The Green Function Method in Statistical Mechanics* (North-Holland, Amsterdam, 1962).
- <sup>15</sup>R. Brout, *Phase Transitions* (Benjamin, New York, 1965).
- <sup>16</sup>R. M. White, Quantum Theory of Magnetism (McGraw-Hill, New York, 1970), pp. 149–150.