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# The Heisenberg Antiferromagnet With a Low Concentration of Static Defects

## Abstract

The static and dynamic response associated with a low concentration,  $x$ , of static defects in a Heisenberg antiferromagnet at zero temperature is analyzed within linearized spin-wave theory. We obtain the dispersion relation for long-wavelength spin waves in the form  $\omega(q) = c(x)q + i\gamma(x)q^\tau$ . Our results for  $c(x)$  agree with previous work, and in particular give  $c(x) = c(0)[1 + \alpha x + O(x^2)]$  where the coefficient  $\alpha$ , which can be related to the helicity modulus and the uniform perpendicular susceptibility, diverges in the limit  $d \rightarrow 2$ , where  $d$  is the spatial dimensionality. One major new result is that  $\tau = d - 1$  for defects whose spin,  $S'$ , is different from that ( $S$ ) of the host lattice and  $\tau = d + 1$  when  $S' = S$ .

## Disciplines

Physics | Quantum Physics

# The Heisenberg antiferromagnet with a low concentration of static defects

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The static and dynamic response associated with a low concentration,  $x$ , of static defects in a Heisenberg antiferromagnet at zero temperature is analyzed within linearized spin-wave theory. We obtain the dispersion relation for long-wavelength spin waves in the form  $\omega(\mathbf{q}) = c(x)q + i\gamma(x)q^\tau$ . Our results for  $c(x)$  agree with previous work, and in particular give  $c(x) = c(0)[1 + \alpha x + O(x^2)]$  where the coefficient  $\alpha$ , which can be related to the helicity modulus and the uniform perpendicular susceptibility, diverges in the limit  $d \rightarrow 2$ , where  $d$  is the spatial dimensionality. One major new result is that  $\tau = d - 1$  for defects whose spin,  $S'$ , is different from that ( $S$ ) of the host lattice and  $\tau = d + 1$  when  $S' = S$ .

The transition from a magnetic insulator, through doping, to a nonmagnetic superconductor is familiar in the high- $T_c$  materials like lanthanum cuprate.<sup>1</sup> It is interesting to understand how impurities in such a system eventually destroy the magnetic long-range order and induce the transition to superconducting phase. Here we treat the simpler problem of a low concentration of static defects at zero temperature. Our model is a Heisenberg spin system with spin  $S$  and nearest neighbor coupling constant  $J$ , and the defects have spin  $S'$  and a coupling constant  $J'$ . The Hamiltonian of such a system can be written as

$$H = \sum_{\mathbf{R}, \delta} \mathbf{S}(\mathbf{R}) \cdot \mathbf{S}(\mathbf{R} + \delta) + \sum_{\mathbf{R}} \epsilon(\mathbf{R}) V(\mathbf{R})$$

$$\equiv H_0 + \sum_{\mathbf{R}} \epsilon(\mathbf{R}) V(\mathbf{R}), \quad (1)$$

where  $\delta$  is summed over nearest-neighbor vectors and  $\epsilon(\mathbf{R})$  is unity at defect sites, which are assumed not to be adjacent to one another and  $\epsilon(\mathbf{R}) = 0$  otherwise. For a defect at site  $\mathbf{R}$  we have

$$V(\mathbf{R}) = \sum_{\delta} (J'S'(\mathbf{R}) - JS(\mathbf{R})) \cdot \mathbf{S}(\mathbf{R} + \delta). \quad (2)$$

Throughout we use dimensionless parameters, such as  $s \equiv S'/S$ , and  $j \equiv J'/J$ . We introduce boson operators in the usual way. For spins on the  $A$  sublattice we set  $S_{\mathbf{R}}^z = S - a_{\mathbf{R}}^+ a_{\mathbf{R}}^-$ ;  $S_{\mathbf{R}}^+ = \sqrt{2S} a_{\mathbf{R}}^-$ ;  $S_{\mathbf{R}}^- = \sqrt{2S} a_{\mathbf{R}}^+$ . For the  $B$  sublattice we have  $S_{\mathbf{R}}^z = -S + b_{\mathbf{R}}^+ b_{\mathbf{R}}^-$ ;  $S_{\mathbf{R}}^+ = \sqrt{2S} b_{\mathbf{R}}^+$ ;  $S_{\mathbf{R}}^- = \sqrt{2S} b_{\mathbf{R}}^-$ . Within linear spin-wave theory, the Hamiltonian of the pure system is

$$h_0 \equiv H_0 / (2JzS)$$

$$= z^{-1} \sum_{\mathbf{R} \in A} \sum_{\delta} (a_{\mathbf{R}}^+ + b_{\mathbf{R}+\delta}) (a_{\mathbf{R}} + b_{\mathbf{R}+\delta}^+). \quad (3)$$

In terms of Fourier transforms

$$h_0 = \sum_{\mathbf{q}} (a_{\mathbf{q}}^+ a_{\mathbf{q}} + b_{\mathbf{q}}^+ b_{\mathbf{q}} + \gamma_{\mathbf{q}} a_{\mathbf{q}}^+ b_{-\mathbf{q}}^+ + \gamma_{\mathbf{q}} a_{\mathbf{q}} b_{-\mathbf{q}}), \quad (4)$$

where  $\gamma_{\mathbf{q}} = z^{-1} \sum_{\delta} \exp(i\mathbf{q} \cdot \delta)$ . This Hamiltonian can be diagonalized by a Bogoliubov transformation

$$a_{\mathbf{q}}^+ = l_{\mathbf{q}} \alpha_{\mathbf{q}}^+ - m_{\mathbf{q}} \beta_{-\mathbf{q}}$$

$$b_{-\mathbf{q}} = -m_{\mathbf{q}} \alpha_{\mathbf{q}}^+ + l_{\mathbf{q}} \beta_{-\mathbf{q}} \quad (5)$$

where

$$l_{\mathbf{q}} = \sqrt{(1 + e_{\mathbf{q}}) / (2e_{\mathbf{q}})}$$

and

$$m_{\mathbf{q}} = \sqrt{(1 - e_{\mathbf{q}}) / (2e_{\mathbf{q}})}.$$

Then

$$h_0 = \sum_{\mathbf{q}} e_{\mathbf{q}} (\alpha_{\mathbf{q}}^+ \alpha_{\mathbf{q}} + \beta_{\mathbf{q}}^+ \beta_{\mathbf{q}}), \quad (6)$$

where  $e_{\mathbf{q}} = \sqrt{1 - \gamma_{\mathbf{q}}^2}$  in the usual notation.

The Green's function for the pure system,<sup>2</sup> indicated by superscript (0), is given by the diagonal matrix:  $g^{(0)}(\mathbf{q}, e)_{\alpha, \alpha} = (e - e_{\mathbf{q}})^{-1}$  and  $g^{(0)}(\mathbf{q}, e)_{\beta, \beta} = (-e - e_{\mathbf{q}})^{-1}$ , where  $e = E / (2JzS)$ . The perturbation from a defect on the  $A$  sublattice at site  $\mathbf{R}$  is

$$v_{\mathbf{R} \in A} = -z^{-1} \sum_{\delta} (a_{\mathbf{R}}^+ + b_{\mathbf{R}+\delta}) (a_{\mathbf{R}} + b_{\mathbf{R}}^+)$$

$$+ jz^{-1} \sum_{\delta} (a_{\mathbf{R}}^+ + \sqrt{s} b_{\mathbf{R}+\delta}) (a_{\mathbf{R}} + \sqrt{s} b_{\mathbf{R}+\delta}^+). \quad (7)$$

Now we use a non-Hermitian transformation for the operators on site  $\mathbf{R}$ , i.e., we replace  $a_{\mathbf{R}}^+$  by  $\sqrt{s} a_{\mathbf{R}}^+$  and  $a_{\mathbf{R}}$  by  $a_{\mathbf{R}} / \sqrt{s}$ . This transformation leads to the following perturbation with weak scattering in the long-wavelength limit:

$$v_{\mathbf{R} \in A} = z^{-1} \sum_{\delta} (a_{\mathbf{R}}^+ + b_{\mathbf{R}+\delta})$$

$$\times [(j-1)a_{\mathbf{R}} + (js-1)b_{\mathbf{R}+\delta}^+]. \quad (8)$$

The potential is decomposed in the well-known way<sup>3</sup> into components which each transform according to an irreducible representation of the point group. Thus we have  $s, p, d$ , etc., potentials and the corresponding Green's functions,  $g^{(\mu)}(e)$  with symmetry labels,  $\mu$ . The contribution to the self-energy matrix from a single defect on the  $A$  sublattice is obtained by summing over repeated scatterings from that defect.<sup>4</sup> This is done independently for each symmetry channel in the usual way. In addition, one performs the same operations when the defect is on the  $B$  sublattice.

That calculation can be trivialized by using the symmetry operations which carry one sublattice into another: interchanging  $l_q$  and  $m_q$  and inverting the sign of the energy,  $e$ . The complete details of this calculation will be given elsewhere.<sup>5</sup> The total self-energy matrix is the superposition of contributions from all symmetry labels. To get the self-energy matrix for the configurationally averaged Green's function we average over all possible positions for

the defect, assuming a uniform concentration  $x_A$  of defects on the  $A$  sublattice and  $x_B$  on the  $B$  sublattice. Then the matrix Green's function correct to first order in the concentration of defects is

$$g(\mathbf{q}, e) = [g^{(0)}(\mathbf{q}, e)^{-1} - \sigma(\mathbf{q}, e)]^{-1}, \quad (9)$$

where the matrix  $\sigma(\mathbf{q}, e)$  is the following:

$$\sigma_{\alpha, \alpha}(\mathbf{q}, e) = \frac{x_A l_q^2 e_q}{D(e)} [(js-1)e_q - j(s-1)] + \frac{x_B m_q^2 e_q}{D(-e)} [(js-1)e_q + j(s-1)] + \sum_{\mu \neq s} (js-1) \phi^\mu(\mathbf{q})^2 \left( \frac{x_A m_q^2}{z - (1-e)(js-1)g^\mu(e)} + \frac{x_B l_q^2}{z - (1+e)(js-1)g^\mu(e)} \right), \quad (10a)$$

$$\sigma_{\alpha, \beta}(\mathbf{q}, e) = \frac{x_A l_q m_q e_q}{D(e)} [(js-1)e_q + j(s-1)] + \frac{x_B l_q m_q e_q}{D(-e)} [(js-1)e_q - j(s-1)] - \sum_{\mu \neq s} (js-1) \phi^\mu(\mathbf{q})^2 l_q m_q \left( \frac{x_A}{z - (1-e)(js-1)g^\mu(e)} + \frac{x_B}{z - (1+e)(js-1)g^\mu(e)} \right), \quad (10b)$$

and the other elements of the self-energy matrix are found by

$$\sigma_{\beta, \beta}(\mathbf{q}, e; x_A, x_B) = \sigma_{\alpha, \alpha}(\mathbf{q}, -e; x_B, x_A), \quad (11a)$$

$$\sigma_{\beta, \alpha}(\mathbf{q}, e; x_A, x_B) = \sigma_{\alpha, \beta}(\mathbf{q}, -e; x_B, x_A). \quad (11b)$$

Here  $\phi^\mu$  is a form factor for symmetry label  $\mu$  as defined in Ref. 6,

$$g^\mu = N^{-1} \sum_{\mathbf{q}} \phi^\mu(\mathbf{q})^2 (e^2 - e_q^2)^{-1}, \quad (12a)$$

and

$$D(e) = (j-e)[1 - e(1+e)g_0(e)] + ejs[1 + (1-e^2)g_0(e)] \quad (12b)$$

with

$$g_0(e) = N^{-1} \sum_{\mathbf{q}} (e^2 - e_q^2)^{-1}. \quad (13)$$

Note that only when  $x_A = x_B$  is the symmetry between the two sublattices preserved. In that case the above results satisfy the relations  $\sigma_{\alpha, \alpha}(e) = \sigma_{\beta, \beta}(-e)$  and  $\sigma_{\alpha, \beta}(e) = \sigma_{\beta, \alpha}(-e)$ .

We now discuss the implications of these results. First, of all, if one expresses the defect perturbation of Eq. (8) in Fourier components one finds a scattering matrix element  $v(\mathbf{k}, \mathbf{k}')$  which is of order

$$v(\mathbf{k}, \mathbf{k}') \sim (l_{\mathbf{k}} - m_{\mathbf{k}})((j-1)(l_{\mathbf{k}} - m_{\mathbf{k}}) + j(s-1)m_{\mathbf{k}}) \quad (14a)$$

$$\sim (j-1)\sqrt{kk'} + j(s-1)\sqrt{k/k'}. \quad (14b)$$

This indicates that for  $s=1$  the scattering is of order  $\sqrt{kk'}$ , whereas for  $s \neq 1$ , it is larger, of order  $\sqrt{k/k'}$ . Thus

we are led to consider three regimes: (I)  $s=1$ , (II)  $s \neq 1$ , but  $x_A = x_B$ , and (III)  $s \neq 1$  and  $x_A \neq x_B$ . In the first two regimes, the symmetry of the mode structure is preserved and consistent with previous work<sup>7,8</sup> the spin-wave energy is given by

$$e_q(x) = e_q + \sigma_{\alpha, \alpha}(\mathbf{q}, e_q - i0^+). \quad (15)$$

Then, for  $x_A \neq x_B$ , we find

$$Re_q(x) = e_q(1 + \alpha x), \quad (16a)$$

where

$$\alpha = \frac{j-1}{j} + (s-1)^2 g_0(0) + \frac{\phi^{(p)}(\mathbf{q})^2}{e_q^2} \frac{(js-1)}{z - (js-1)g^{(p)}(0)}, \quad (16b)$$

This result agrees with the prediction of hydrodynamics<sup>9,8</sup> that  $e_q = cq$ , with  $c(x) = \sqrt{A(x)/\chi_1(x)}$ , where  $A(x)$  is the helicity (proportional to the conductivity of an associated resistor network<sup>10</sup>) and  $\chi_1$  is the perpendicular susceptibility. For case III, one must actually diagonalize the Green's function matrix to find its poles which give the elementary excitations. Thus we set  $\Delta(\mathbf{q}, e) = 0$ , where

$$\Delta(\mathbf{q}, e) = [-e - e_q - \sigma_{\beta, \beta}(\mathbf{q}, e)][e - e_q - \sigma_{\alpha, \alpha}(\mathbf{q}, e)] - \sigma_{\alpha, \beta}(\mathbf{q}, e)\sigma_{\beta, \alpha}(\mathbf{q}, e). \quad (17)$$

In this way we find the expected result,<sup>8</sup> namely that this ferrimagnetic system has an acoustic branch with  $e_q \sim [A(x)/M]q^2$ , where  $M \sim (x_A - x_B)$  is the net magnetization, and an optical branch whose energy is proportional to  $M$ . It is obvious that such a result is caused by the breaking of symmetry between sublattices. Formally, such a result is expected for a case when the scattering matrix

element (for  $k \sim k'$ ) is of order unity in the long wavelength limit. In this context, one views the case  $x_A = x_B$  (with  $s \neq 1$ ) as being special in that, for this case the optical mode energy averages to zero on large scales. In this language one has strong scattering if  $s \neq 1$ , but the scattering potential fluctuates in sign according to the fluctuations in  $(s - 1)(x_A - x_B)$ . Of course, when  $s = 1$  the scattering is much weaker, because then even locally there is no tendency to form an optical mode. Thus vacancy ( $s = 0$ ) scattering is strong. In fact, for two spatial dimensions, the renormalization factor  $\alpha$  of Eq. (16) is infinite, due to the divergent term,  $g_0(0)$ . This result is due to the fact that  $\chi_1$  is divergent for the random two-dimensional system.

These considerations also indicate the nature of the results for the damping, which is found as the imaginary part of  $e_q$  given in Eq. (15). For case I,  $s = 1$ , we find

$$\Gamma_q \equiv F e_q \sim q^{(d+1)}, \quad (18)$$

as one would estimate for a scattering matrix element of order  $\sqrt{kk'}$  from Eq. (14). On the other hand, for regime II,  $s \neq 1$ , the scattering matrix element is of order unity and we find

$$\Gamma_q \sim q^{(d-1)}. \quad (19)$$

As we have said, one can understand the difference between these two results either formally, by looking at Eq. (14b), or physically by the following argument. If all the defects were on one sublattice, we obviously obtain an optical mode. Averaging over defects can average the gap to zero energy, but the decay rate from incoherent scatterers always adds. Thus for  $s \neq 1$ , the energy is of order  $(x_A - x_B) + O(q)$  while the damping is of order  $(x_A + x_B)q^{d-1}$ . It is worth noting that there is no such effect for ferromagnets, since there is no locally broken symmetry. Finally, we remark that our results for the damping contradict some previous work,<sup>7</sup> but do agree with the unpublished work of Kumar<sup>10</sup> and that results implied by Ref. 8. The reason for the discrepancy with Ref. 7 is not understood. However, from our results we revise the scaling theory of Christou and Stinchcombe (CS)<sup>11</sup> which was based on the work of Ref. 7, which we believe to be incorrect. To do this, we first write down the dispersion as

$$\omega(q) = c(x)q + i\gamma(x)q^{d-1}, \quad (20)$$

and following Harris and Kirkpatrick (HK)<sup>8</sup> one has<sup>9</sup>

$$c(x) = \sqrt{A(x)/\chi_1(x)}, \quad (21)$$

where  $A(x)$  is the dc conductivity, and  $\chi_1(x)$  is the transverse susceptibility, which scale near the percolation threshold at  $x_c$  as

$$\begin{aligned} A(x) &\sim (x - x_c)^t \sim \xi^{-t/\nu} \\ \chi_1(x) &\sim (x - x_c)^\tau \sim \xi^{\tau/\nu}, \end{aligned} \quad (22)$$

where  $\xi$  is the correlation length, and according to HK,  $\tau$  can be expressed as  $\tau = t - \beta - (d - 2)\nu$ . We then apply the dynamic scaling principle of Halperin and Hohenberg,<sup>8</sup> in order to get a relation consistent with Eq. (20). We have

$$\omega(q) = q^z f(q\xi) \equiv q^z (q^{1-z}\xi^{1-z} + iq^{d-1-z}\xi^{d-1-z}). \quad (23)$$

Thus from Eqs. (21) and (22) we get

$$z = 1 + \frac{t + \tau}{2\nu} = 1 + \frac{2t - \beta - (d - 2)\nu}{2\nu}, \quad (24)$$

in agreement with CS. The scaling for the damping rate is therefore easy to get, we find

$$\gamma(\xi) \sim \xi^{d-2 - [2t - \beta - (d - 2)\nu]/(2\nu)}. \quad (25)$$

As was done in CS paper, we can go further to write

$$\Gamma(q, \xi) \propto (x - x_c)^{-\mu} q^{d-1}, \quad (26)$$

where  $\mu = (d - 2)\nu - [2t - \beta - (d - 2)\nu]/2$  which differs from the CS result  $\mu = d\nu - [2t - \beta - (d - 2)\nu]/2$ .

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