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 via a boson formalism involving a non-Hermitian potential. 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 α, which can be related to the helicity modulus and the uniform perpendicular susceptibility, diverges in the limit $d \to 2$, where d is the spatial dimensionality. One major 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 $S' = S$. Thus $d = 2$ (which is the case for the copper oxide antiferromagnets) is the lower critical dimension at which infrared divergences affect the dynamic response due to vacancies ($S' = 0$). To elucidate our results we consider the way the antiferromagnetic symmetry is broken when defects occur unequally on the two sublattices, and our results are consistent with previous general hydrodynamic arguments. We give detailed expressions for the actual spin susceptibility in terms of the boson response function. We also consider how defects affect the zero-point contribution to magnetization and density of states.

I. INTRODUCTION

The problem of impurities in a magnetic insulator was at the forefront of condensed matter research some 20 years ago.[1] This problem has recently been reexamined in response to the interest in the magnetic properties of systems like lanthanum cuprate,[2] which, when appropriately doped, give rise to high-temperature superconductors. Here our main objective is to study the effect of defects on a Heisenberg antiferromagnet at zero temperature. By a defect we mean the perturbation to the Hamiltonian caused by the introduction of an impurity which has a spin S' which may differ from that, S, of the host and whose coupling to the host, J', may also differ from that, J, between nearest neighbors in the pure host system. The perturbation associated with such a defect is limited to the impurity site and its shell of nearest neighbors.

The method to obtain the exact solution for a single defect of finite spatial extent was developed[3] in the late 1960s and was subsequently applied in great detail to treat the case of a low concentration of defects in a ferromagnet.[4,5] In some early works[6] the single-defect problem was expressed in terms of boson operators by using the Holstein-Primakoff transformation.[7] Although correct answers were obtained by this method, later work[8] using the equations of motion implied, as we shall see, that a better boson potential, patterned after the Dyson-Maleev potential[9,10] for spin–wave interactions, displays explicitly the fact that the scattering cross section vanishes in the long–wavelength limit.[9] The only slightly controversial point in this early work concerned the best way to project out the impurity site for the case of a vacancy. When the single–defect solution was extended to treat higher defect concentrations of vacant bonds[11] using an approximation equivalent[12] to the coherent potential approximation[13,14] (CPA), difficulties were encountered[12] due to spurious resonances on the vacancy sites. These difficulties were overcome[15] by introduction of a hard core potential on the impurity site, the effect of which was to move the spurious resonance to infinite energy.

To summarize these results, for a low concentration, x, of defects in a ferromagnet on a d–dimensional hypercubic lattice, the spin–wave energies are given by

$$E(\mathbf{q};x) = 2JSa^2q^2[1 - \alpha x + O(x^2)] \equiv D(x)a^2q^2 \quad (1.1a)$$

and, as we shall see, the scattering potential at long wavelength is of order $v(\mathbf{q},\mathbf{q}') \sim q^2$, which leads to the imaginary part of the energy, or the damping rate being given by[3–6,8,16]

$$\Gamma(\mathbf{q};x)/(2JS) = \beta x(aq)^{d+2}\,, \quad (1.1b)$$

where α and β are constants. (Both here and for the antiferromagnet we trivially extend previous results to arbitrary spatial dimension.) When applied to the vacancy case, the result in Eq. (1.1a) was shown to be closely related to that for the randomly diluted resistor network.[17,18] In fact, for the generic defect problem,

at long wavelength one may write[19–21] (in appropriate units)

$$E(\mathbf{q};x) \sim \frac{A(x)}{M(x)}q^2 \equiv D(x)q^2 , \tag{1.2}$$

where $M(x)$ is the magnetization (magnetic moment per unit volume) and $A(x)$ is the helicity modulus. Obviously, for small x we have

$$M(x) = M(0)[1 + (xS'/S) - x] . \tag{1.3}$$

The helicity modulus, $A(x)$, which measures the stiffness of the system to twisting the magnetic moment, is determined within linearized spin-wave theory by a set of equations which are isomorphic to those for the bulk conductivity $\Sigma^{(\mathrm{el})}$, of an analogous resistor network[17,21,22] in which the exchange interaction, J_b on the bond b is replaced by a conductance, $\sigma_b = J_b S_1 S_2$, where S_1 and S_2 are the spins which are connected by the bond b. Thus if we write

$$\Sigma^{(\mathrm{el})}(x) = \Sigma^{(\mathrm{el})}(x=0)[1 - \alpha' x + O(x^2)] , \tag{1.4}$$

then for the case of vacancy defects the coefficients of Eqs. (1.1a) and (1.4) are related by $\alpha = \alpha' - 1$. The most complete analysis of the effect of defects on the spin-wave spectrum of a ferromagnet was given by Izyumov[6] and Jones.[8] The behavior of $D(x)$ near the percolation threshold has been extensively studied by many analytic and numerical techniques.[23] Knowing the dependence of the damping on wave vector, Stinchcombe and Cristou[24] developed a scaling theory to describe the singular damping of spin waves in the vicinity of the percolation threshold.

The situation for defects in the antiferromagnetic Heisenberg (AFH) model is similar, but as we shall see, the results are not quite as definitive. In this case the properties of defects were of interest in view of the suggestions of Marshall[25] and of Lovesey[26] that the diffuse scattering due to zero-point motion should be observable in mixed magnetic crystals. At the same time Tonegawa[27] used a method equivalent to that of Koster and Slater[3] to give a detailed study, within linear spin–wave theory, of possible spin–wave bound states due to the presence of a single defect. Subsequently, the distribution of zero–point spin deviation near an impurity was studied in some detail by Solyom and Bergov.[28] Edwards and Jones[29] (EJ) used the spin-wave equations of motion to discuss the effect of vacancies on the elementary excitation spectrum, but instead of resumming perturbation theory, as in the Koster-Slater[3] approach, they worked only up to second order in the defect perturbation. Nevertheless, in principle, they should have obtained qualitatively correct results, as we will discuss later. They found that

$$E(\mathbf{q};x) = zJSaq[1 - \rho x + O(x^2)] \equiv c(x)q . \tag{1.5}$$

The later work of Kirkpatrick and Harris[21] (KH), using the Koster-Slater[3] approach, led to a result of the form of Eq. (1.5) but with a renormalized value of the constant ρ which is consistent with that one would predict on the basis of spin-wave hydrodynamics:[20]

$$c(x) = \sqrt{A(x)/\chi_\perp(x)} , \tag{1.6}$$

where $\chi_\perp(x)$ is the perpendicular susceptibility with respect to a uniform applied field. The helicity modulus, $A(x)$, measures the stiffness of the system with respect to twisting the staggered magnetic moment, and within linearized spin–wave theory is the same as for a ferromagnet on the same structure. Note that both Eqs. (1.2) and (1.6) express a dynamic quantity in terms of static elastic or density quantities. The results of EJ (Ref. 29) for $c(x)$ were consistent with Eq. (1.6) up to the order in perturbation theory to which they worked. Their result for the damping rate (in energy units) at low concentration of vacancies was

$$\Gamma(\mathbf{q};x) \sim x(aq)^{d+1} + O(x^2) . \tag{1.7}$$

Later, in the course of analytic and numerical work[30] to systems of experimental relevance, some results in conflict with Eq. (1.7) were found. For instance, it was found that in two dimensions the damping rate that became independent of $\mathbf{q}$ was the $q \to 0$ limit and was thus not negligible in comparison to $E(\mathbf{q};x)$ in this limit. Also a low-frequency divergence in the "constant" ρ in Eq. (1.5) was identified. (This divergence was implied by the results of EJ,[29] but they did not specifically consider applying their result to the case $d = 2$.) Also arguments[30] were given by Harris and Kirkpatrick (HK) that the perpendicular susceptibility was anomalous in the presence of dilution, due to the creation of local regions which had a net ferromagnetic moment. In fact, it is intuitively quite clear that vacancies for the antiferromagnet give rise to local fluctuating ferromagnetic regions which in turn amount to creation of a local gap as one would expect in a ferrimagnet having two sublattices of different spin. In the ferromagnet, there is no question of a local gap, as dilution does not change the symmetry, even locally. In the antiferromagnet, the symmetry between sublattices is only recovered on average: locally one has a ferrimagnet with one acoustic mode and one optical mode at long wavelength. From the work of HK it is therefore clear that the lower critical dimension for the zero-temperature dynamics of an antiferromagnet is two. An explicit result for the damping due to vacancies was given by HK, but the details of the calculation were perhaps too brief. In fact, earlier work[31] for the case of a vacancy defect also disagreed with the result of EJ (Ref. 29) in Eq. (1.7), but this work was not published. Furthermore, since the CPA, as used by Holcombe,[32] is exact in the low concentration limit, it implicitly contains the correct [i.e., Koster-Slater (Ref. 3)] solution for a single vacancy and therefore is also expected to disagree with Eq. (1.7). However since no analytic results for low concentration were given in Ref. 32, one cannot use this work to obtain the elementary excitation spectrum in the long-wavelength limit. Thus one is led to expect that the EJ result of Eq. (1.7) is incorrect.

Accordingly, here we treat in detail the case of a defect with arbitrary spin and coupling constant. Also, to

illustrate the importance of ferrimagnetic fluctuations we treat in detail the case where defects appear unequally on the two sublattices. Our results, where they overlap, do agree with those of KH and of Kumar.[31] We find that for defects, such as a vacancy, whose spin differs from that of the host,

$$\Gamma(\mathbf{q};x) = 2zJSx\beta_1(aq)^{d-1} + O(x^2), \quad S' \neq S, \quad (1.8a)$$

where for defects with spin equal to that of the host we find

$$\Gamma(\mathbf{q};x) = 2zJSx\beta_2(aq)^{d+1} + O(x^2), \quad S' = S\ , \quad (1.8b)$$

where β_1 and β_2 are constants. The physical reason for the difference between these two results is that in the case where the defect has the same spin as the host the antiferromagnetic symmetry is preserved within each unit cell, whereas in the latter case it is only preserved on the average. Since breaking the symmetry between sublattices leads to an optical mode, it is clear that the scattering must be stronger when $S' \neq S$ than when $S' = S$. Note that for vacancies in $d = 2$ the damping never becomes small in comparison to the frequency, so that antiferromagnetic magnons are not perfect elementary excitations in this case. A scaling theory for the damping near the percolation threshold was given by Stinchcombe and Christou,[33] but it was based on the results of EJ,[29] which, as we have said, we believe to be incorrect. In fact, recently an unpublished paper[34] has appeared in which a finite result for ρ in $d = 2$ was obtained, in contradiction to all the early work.

Just as for the ferromagnet, the vacancy limit for defects in an antiferromagnet is an interesting special case. As we shall see, there are several ways to obtain the vacancy case by suitably adjusting the parameters. One way, clearly, is to set the defect spin $S' = 0$. The equations of motion method, introduced by EJ (Ref. 29) and used by Jones[8] for the ferromagnet, amounts to this choice with $J' = J$. This choice is also equivalent to the treatment of Bulot *et al.*[35] In our opinion, and as discussed in detail previously,[15] the best way to treat vacancies is to set $S' = 0$ and $J' = \infty$ to project out any effects of the vacancy in the response functions. By so doing, we believe that we give here the first correct treatment for the spin response of antiferromagnets with a small concentration of defects.

This paper is organized as follows. In Sec. II we review briefly the calculation for the ferromagnet. We show that the previous equations of motion for spin operators can be reproduced by a convenient non-Hermitian boson Hamiltonian. In Sec. III we extend this method to treat the antiferromagnet with a low concentration of arbitrary local defects. Where they overlap our results agree with those of KH and Kumar.[31] In Sec. IV we discuss the results obtained in Sec. III in various limits. Here we consider vacancies and also unequal substitution on two antiferromagnetic sublattices. In Sec. V we briefly consider density of states a low energy and show that it is expressible in terms of the hydrodynamic parameters. Here we also consider the alteration in the zero-point motion due to defects. Finally, in Sec. VI we give briefly conclusions from this work.

II. FORMALISM: THE FERROMAGNET

In this section we will describe the formalism and discuss its application to defects in a ferromagnet, where the algebra is somewhat more transparent than in the case of interest, viz. the antiferromagnet which is treated in the next section. For operators A and B we define the retarded Green's functions by[30]

$$\langle\langle A(t);B(t')\rangle\rangle = -i\theta(t-t')\langle[A(t),B(t')]\rangle_T\ , \quad (2.1)$$

where $\langle\ \rangle_T$ denotes a Boltzmann average at temperature T. The temporal transform is given by

$$\langle\langle A;B\rangle\rangle_E = \int_{-\infty}^{\infty} e^{iE(t-t')/\hbar}\langle\langle A(t);B(t')\rangle\rangle dt \quad (2.2)$$

and obeys the equations of motion

$$E\langle\langle A;B\rangle\rangle_E = \langle\langle[A,H];B\rangle\rangle_E + \langle[A,B]\rangle_T\ . \quad (2.3)$$

The Hamiltonian we wish to treat is a spin-S Heisenberg magnet with defect sites:

$$H = H_0 + \sum_{\mathbf{R}} \epsilon(\mathbf{R})V(\mathbf{R})\ , \quad (2.4)$$

where ϵ is unity at defect sites, which are assumed not to be adjacent to one another and $\epsilon(\mathbf{R}) = 0$ otherwise. We take

$$H_0 = \pm J\sum_{\mathbf{R},\boldsymbol{\delta}} \mathbf{S}(\mathbf{R})\cdot\mathbf{S}(\mathbf{R}+\boldsymbol{\delta})\ , \quad (2.5)$$

where we take the positive sign for an antiferromagnet and the negative sign for the ferromagnet, and $\boldsymbol{\delta}$ is summed over nearest-neighbor vectors. The defect is allowed to have spin, S', different from that of the host, and to be coupled to its neighbors with an exchange constant J'. Thus for a defect at site $\mathbf{R}$ the defect perturbation is

$$V_{\mathbf{R}} = \mp 2\sum_{\boldsymbol{\delta}}[J'\mathbf{S}'(\mathbf{R}) - JS(\mathbf{R})]\cdot\mathbf{S}(\mathbf{R}+\boldsymbol{\delta})\ . \quad (2.6)$$

Throughout we will use lower case variables to indicate dimensionless (or reduced) versions of the counterparts in capitals. Thus we set $S'/S = s$ and $J'/J = j$.

As we shall see explicitly below, using linearized spin-wave theory we obtain a Hamiltonian which is quadratic in terms of boson operators. We are thus led to a scattering problem which we solve in the limit of a low concentration, x, of defects, using the Koster-Slater[3] approach. In that case the boson Green's function, when simultaneous scattering involving more than a single site are omitted, can be written in the form

$$G(\mathbf{R},\mathbf{R}';E) \equiv \langle\langle a_{\mathbf{R}}; a^{\dagger}_{\mathbf{R}'}\rangle\rangle_E = G^0(\mathbf{R},\mathbf{R}';E) + \sum_{\mathbf{R}'',\mathbf{r},\mathbf{r}'} \epsilon(\mathbf{R}'')G^0(\mathbf{R},\mathbf{R}''+\mathbf{r};E)T_{\mathbf{R}''}(\mathbf{r},\mathbf{r}')G^0(\mathbf{R}''+\mathbf{r}',\mathbf{R};E) , \tag{2.7}$$

where $T_{\mathbf{R}''}$ is the T matrix for a defect at site $\mathbf{R}''$. Here and below lower case position vectors such as $\mathbf{r}$ and $\mathbf{r}'$ are taken relative to the defect position, i.e., they assume the value 0 or any of the z nearest-neighbor vectors $\boldsymbol{\delta}$. Also

$$T_{\mathbf{R}}(\mathbf{r},\mathbf{r}';E) = V_{\mathbf{R}}(\mathbf{r},\mathbf{r}') + \sum_{\mathbf{r}'',\mathbf{r}'''} V_{\mathbf{R}}(\mathbf{r},\mathbf{r}'')G^0(\mathbf{r}'',\mathbf{r}''';E)T_{\mathbf{R}}(\mathbf{r}''',\mathbf{r}';E) , \tag{2.8}$$

which has a Fourier transform

$$T(\mathbf{q},\mathbf{q}';E) = \sum_{\mathbf{r},\mathbf{r}'} e^{i\mathbf{q}\cdot(\mathbf{R}+\mathbf{r})-i\mathbf{q}'\cdot(\mathbf{R}+\mathbf{r}')}T_{\mathbf{R}}(\mathbf{r},\mathbf{r}';E) . \tag{2.9}$$

To first order in x the Fourier transformed configurationally averaged Green's function is given by

$$\begin{aligned} G(\mathbf{q},E)^{-1} &= E - E_{\mathbf{q}} - xT(\mathbf{q},\mathbf{q};E) \\ &\equiv E - E_{\mathbf{q}} - \Sigma(\mathbf{q},E) , \end{aligned} \tag{2.10a}$$

or, in dimensionless terms with $g = 2JzSG$ and $\Sigma = 2JzS\sigma$

$$g(\mathbf{q},e) = e - e_{\mathbf{q}} - \sigma(\mathbf{q},e) . \tag{2.10b}$$

Furthermore, as we will discuss below, the configurationally averaged spin Green's function, $H(\mathbf{q},E)$, is related to the boson Green's function by[8]

$$H(\mathbf{q},E) = 2S[1 + x\Lambda(\mathbf{q},E)]G(\mathbf{q},E) , \tag{2.11}$$

where Λ is a vertex renormalization which, when properly chosen, is essentially constant in the vicinity of the spin-wave resonance at $E = E_{\mathbf{q}}$. In the above, G and T are scalars for the ferromagnet, but are 2×2 matrices for the antiferromagnet.[29,40]

We now describe the calculations for a ferromagnet within the boson formalism. The linearized Holstein–Primakoff transformation[7] for the defect–free host leads to the Hamiltonian (omitting the ground state energy)

$$H_0 = 2JS \sum_{\langle\mathbf{R}\mathbf{R}'\rangle} (a^{\dagger}_{\mathbf{R}} - a^{\dagger}_{\mathbf{R}'})(a_{\mathbf{R}} - a_{\mathbf{R}'}) = \sum_{\mathbf{q}} E_{\mathbf{q}} a^{\dagger}_{\mathbf{q}} a_{\mathbf{q}} , \tag{2.12}$$

where the sum is over pairs of nearest neighbors, $a^{\dagger}_{\mathbf{q}} = N^{-1/2}\sum_{\mathbf{R}} a^{\dagger}_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}}$, where N is the total number of sites, and

$$E_{\mathbf{q}} = 2JzS(1-\gamma_{\mathbf{q}}) \equiv 2JzSe_{\mathbf{q}} , \tag{2.13}$$

where $\gamma_{\mathbf{q}} = z^{-1}\sum_{\delta}\exp(i\mathbf{q}\cdot\boldsymbol{\delta})$. Then[5]

$$\frac{V(\mathbf{R})}{2JzS} = -\frac{1}{z}\sum_{\delta}(a^{\dagger}_{\mathbf{R}} - a^{\dagger}_{\mathbf{R}+\delta})(a_{\mathbf{R}} - a_{\mathbf{R}+\delta}) + ja^{\dagger}_{\mathbf{R}}a_{\mathbf{R}} + \frac{js}{z}\sum_{\delta} a^{\dagger}_{\mathbf{R}+\delta}a_{\mathbf{R}+\delta} - \frac{j\sqrt{s}}{z}\left[a^{\dagger}_{\mathbf{R}}\sum_{\delta} a_{\mathbf{R}+\delta} + \sum_{\delta} a^{\dagger}_{\mathbf{R}+\delta}a_{\mathbf{R}}\right] \equiv v_{\mathbf{R}} . \tag{2.14}$$

As noted by Jones,[8] this formulation, although correct, may not be the most convenient. It suffers from three drawbacks: (a) the scattering matrix element does not vanish in the zero wave vector limit,[4] (b) although the final results depend rationally on s, we see in Eq. (2.14) the appearance of $\sqrt{s}$, and (c) it does not lead to factorizable potentials. To avoid these undesirable features, we make a non-Hermitian transformation for operators on the defect site such that $a^{\dagger}_{\mathbf{R}}$ is replaced by $a^{\dagger}_{\mathbf{R}}\sqrt{s}$ and $a_{\mathbf{R}}$ is replaced by $a_{\mathbf{R}}/\sqrt{s}$. This replacement is motivated by the desire to map the equations of motion of the spin operators into those of the boson operators. In the famous problem of spin-wave interactions,[9] it has been shown that the equations of motion of spin wave can be reproduced by a non-Hermitian Hamiltonian (the so-called Dyson–Maleev Hamiltonian[9,10]) which leads to simpler results than that of the Hermitian Hamiltonian one obtains from the usual Holstein–Primakoff transformation. Of course, in constructing the full spin Green's function we must take proper account of this intermediate transformation. The resulting non-Hermitian Hamiltonian which we will discuss is written in terms of the same H_0 but now instead of Eq. (2.14) we have

$$\begin{aligned} \frac{V(\mathbf{R})}{2JzS} \equiv v_{\mathbf{R}} = \frac{1}{z}\sum_{\delta}(a^{\dagger}_{\mathbf{R}} - a^{\dagger}_{\mathbf{R}+\delta}) \\ \times[(j-1)a_{\mathbf{R}} + (1-js)a_{\mathbf{R}+\delta}] . \end{aligned} \tag{2.15a}$$

In wave-vector representation

$$\begin{aligned} v_{\mathbf{R}} = \frac{1}{Nz}\sum_{\mathbf{q},\mathbf{q}',\delta'} e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}(1-e^{-i\mathbf{q}\cdot\delta}) \\ \times[j-1-(js-1)e^{i\mathbf{q}'\cdot\delta}]a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}'} , \end{aligned} \tag{2.15b}$$

so that the scattering matrix element at long wavelength of order $v_{\mathbf{q},\mathbf{q}'} = je_{\mathbf{q}}(1-s)/N$, which vanishes in the limit

$q \to 0$. In contrast, in Eq. (2.14) $v_{\mathbf{q},\mathbf{q}'} = j(1-\sqrt{s}\gamma_{\mathbf{q}})(1-\sqrt{s}\gamma_{\mathbf{q}'})$, which becomes $j(1-\sqrt{s})^2 \neq 0$ for $q = q' = 0$.

We now introduce symmetry adapted coordinates.[4] The z nearest-neighbor vectors form a z-dimensional reducible representation of the point group of the hypercubic lattice which contains each irreducible representation, s, p, d, etc., at most once. The associated unitary transformation coefficients are denoted $U_\delta^{(\mu)}$ and their phases are chosen so that the $\phi^{(\mu)}$'s and $\psi^{(\mu)}$'s (introduced below) are real. For instance, the s-wave transformation coefficients are $U_\delta^{(s)} = 1/\sqrt{z}$. The only other symmetry of interest to us here is p-wave, for which $U_\delta^{(p,\alpha)} = i\delta_\alpha/(\sqrt{2}a)$, where α assumes any one of the Cartesian directions, x, y, z, etc. Thus we write $v_{\mathbf{R}} = \sum_\mu v_{\mathbf{R}}^\mu$, where

$$v_{\mathbf{R}}^{(\mu)} = \frac{1}{z}\sum_\delta U_\delta^{(\mu)\,*}(a_{\mathbf{R}}^\dagger - a_{\mathbf{R}+\delta}^\dagger) \times \sum_{\delta'} U_{\delta'}^{(\mu)}[(j-1)a_{\mathbf{R}} - (js-1)a_{\mathbf{R}+\delta'}] \tag{2.16a}$$

$$\equiv \frac{1}{Nz}\sum_{\mathbf{q},\mathbf{q}'} \phi^{(\mu)}(\mathbf{q})\psi^{(\mu)}(\mathbf{q}')e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}a_{\mathbf{q}}^\dagger a_{\mathbf{q}'}\,, \tag{2.16b}$$

where

$$\phi^{(\mu)}(\mathbf{q}) = \sum_\delta (1-e^{-i\mathbf{q}\cdot\delta})U_\delta^{(\mu)\,*} \tag{2.17a}$$

and

$$\psi^{(\mu)}(\mathbf{q}) = \sum_\delta [(j-1) - (js-1)e^{i\mathbf{q}\cdot\delta}]U_\delta^{(\mu)}\,. \tag{2.17b}$$

For s-wave symmetry we have

$$\phi^{(s)}(\mathbf{q}) = \sqrt{z}e_{\mathbf{q}} \tag{2.18a}$$

and

$$\psi^{(s)}(\mathbf{q}) = \sqrt{z}[j(1-s) + (js-1)e_{\mathbf{q}}]\,. \tag{2.18b}$$

For non-s-wave symmetry $\sum_\delta U_\delta^{(\mu)} = 0$ and we set

$$\phi^{(\mu)}(\mathbf{q}) = \psi^{(\mu)}(\mathbf{q})/(js-1) = -\sum_\delta e^{i\mathbf{q}\cdot\delta}U_\delta^{(\mu)}\,. \tag{2.19}$$

For instance, $\phi^{(p,x)}(\mathbf{q}) = \sqrt{2}\sin(q_x a)$.

We see from Eqs. (2.16a) and (2.16b) that for each symmetry label the potential is factorizable which is not the case for the s-wave potential arising out of the potential of Eq. (2.14). In this representation the T matrix, i.e., the solution to Eq. (2.8), is of the form of Eq. (2.9) with

$$T(\mathbf{q},\mathbf{q}';E) \equiv 2JzSt(\mathbf{q},\mathbf{q}';e) \equiv 2JzS\sum_\mu t^{(\mu)}(\mathbf{q},\mathbf{q}';e) \equiv 2JzS\sum_\mu \phi^{(\mu)}(\mathbf{q})t^{(\mu)}(e)\psi^{(\mu)}(\mathbf{q}')\,, \tag{2.20}$$

where

$$t^{(\mu)}(e) = \left(z - \frac{1}{N}\sum_{\mathbf{q}} \phi^{(\mu)}(\mathbf{q})\psi^{(\mu)}(\mathbf{q})(e-e_{\mathbf{q}})^{-1}\right)^{-1}. \tag{2.21}$$

For non-s-wave symmetry we get

$$t^{(\mu)}(\mathbf{q},\mathbf{q}';e) = \frac{\phi^{(\mu)}(\mathbf{q})\phi^{(\mu)}(\mathbf{q}')(js-1)}{z-(js-1)g^{(\mu)}(e)}\,, \tag{2.22}$$

where

$$g^{(\mu)}(e) = N^{-1}\sum_{\mathbf{q}} \phi^{(\mu)}(\mathbf{q})^2(e-e_{\mathbf{q}})^{-1}\,. \tag{2.23}$$

For s-wave symmetry evaluation of Eqs. (2.20) and (2.21) gives

$$t^{(s)}(\mathbf{q},\mathbf{q}';e) = \frac{e_{\mathbf{q}}}{\Delta(e)}[j(1-s) + (js-1)e_{\mathbf{q}'}]\,, \tag{2.24}$$

where

$$\Delta(e) = [j-e][1-eg_F(e)] + ejs[1+(1-e)g_F(e)]\,, \tag{2.25}$$

where $g_F(e) = N^{-1}\sum_{\mathbf{q}}(e-e_{\mathbf{q}})^{-1}$ is the local Green's function for the ferromagnet.

Next we consider the full frequency-dependent spin Green's function, $H(\mathbf{q},E)$, which we must express in terms of the boson Green's function. This we do by writing

$$H(\mathbf{R},\mathbf{R}';E) \equiv \langle\langle S^+(\mathbf{R}); S^-(\mathbf{R}')\rangle\rangle_E = (Jz)^{-1}[1+(s-1)\epsilon(\mathbf{R}')] \times \left[g^0(\mathbf{R},\mathbf{R}';E) + \sum_{\mathbf{R}'',\mathbf{r},\mathbf{r}'} \epsilon(\mathbf{R}'')g^0(\mathbf{R},\mathbf{R}''+\mathbf{r}'')t_{\mathbf{R}''}(\mathbf{r}'',\mathbf{r}''')g^0(\mathbf{R}''+\mathbf{r}''',\mathbf{R}')\right]. \tag{2.26}$$

This relation follows from the fact that $S^+(\mathbf{R}) = \sqrt{2S}a_{\mathbf{R}}$ and $S^-(\mathbf{R}) = s\sqrt{2S}a^\dagger_{\mathbf{R}}$. If $h(\mathbf{r},\mathbf{r}';e)$ denotes the configurationally averaged result for $JzH(\mathbf{r},\mathbf{r}';E)$, then correct to order x we have

$$h(\mathbf{q};e) = [1 + x\Lambda(\mathbf{q};e)]g(\mathbf{q},e) \ , \tag{2.27}$$

where

$$\Lambda(\mathbf{q},e) = (s-1) - \frac{e_{\mathbf{q}}}{\Delta(e)}(s-1)\{(js-1)[1-eg_F(e)] + j(s-1)g_F(e)\} \tag{2.28}$$

and, as we have seen, $g(\mathbf{q},e) = [e - e_{\mathbf{q}} - xt(\mathbf{q},\mathbf{q};e)]^{-1}$. As expected, these results reproduce exactly those obtained by Jones[8] using an equation-of-motion approach.

According to Eqs. (2.10a) and (2.10b) the excitation energy is given by

$$e_{\mathbf{q}}(x) = e_{\mathbf{q}} + \sigma(\mathbf{q};e_{\mathbf{q}}) \tag{2.29a}$$

$$\sim \hbar d(x)q^2 \ , \quad q \to 0 \ , \tag{2.29b}$$

where $\sigma(\mathbf{q},e) = \Sigma(\mathbf{q},E)/(2zJS)$. The p-wave contribution to $\sigma(\mathbf{q},e_{\mathbf{q}})$ at small q is

$$\sigma^{(p)}(\mathbf{q};e_{\mathbf{q}}) \sim x(a^2q^2/z)\sigma_p \ , \tag{2.30}$$

where

$$\sigma_p = \frac{2z(js-1)}{z-(js-1)g^{(p)}(0)} \ . \tag{2.31}$$

This p-wave result is identical to that required to calculate the macroscopic electrical conductivity, $\Sigma^{\rm el}$, for the analogous resistor network[17,21,22] in which nodes i and j are connected by a resistor of conductance $\sigma_{ij} = J_{ij}S_iS_j$. Consistent with this identification we see that $\sigma_p = 0$ for $js = 1$, even though j and s do not individually have to be unity. (When $js = 1$ there is no conductance defect.) In the dilute limit we have[17]

$$\frac{\Sigma^{\rm el}(x)}{\Sigma^{\rm el}(0)} = 1 + x\sigma_p \ . \tag{2.32}$$

A direct evaluation of Eq. (2.29a) yields[6,8]

$$\frac{d(x)}{d(0)} = 1 + x\sigma_p + x\sigma_s \ , \tag{2.33}$$

where

$$\sigma_s = \lim_{q\to 0} t^{(s)}(\mathbf{q},\mathbf{q};e_{\mathbf{q}})/e_{\mathbf{q}} \ . \tag{2.34}$$

In Eqs. (2.32) and (2.33) it suffices to evaluate the p-wave contribution at zero energy. Alternatively, we have the macroscopic relation[17,19–21]

$$\frac{d(x)}{d(0)} = \frac{\Sigma^{\rm el}(x)M(0)}{\Sigma^{\rm el}(0)M(x)} \ , \tag{2.35}$$

where $M(x)$ is the magnetization. Since $M(x)/M(0) = 1+x(s-1)$, Eq. (2.35) would predict that (a) for a defect coupled to the host we should find $\sigma_s = (1-s)$ and (b) for a vacancy $\sigma_s = 1$. Indeed one can explicitly verify these results.

Perhaps the biggest advantage of the non-Hermitian Hamiltonian is that because the scattering vanishes in the long-wavelength limit, it gives qualitatively correct results order by order in perturbation theory. In contrast, as noted by Callaway[4] and by Izyumov,[6] it is necessary to regroup perturbation theory when the representation of Eq. (2.14) is used. One grouping, of course, is to sum all contributions of order x, as Izyumov did[6] using the t–matrix. A less well–known scheme uses $1/z$ as an expansion parameter.[36] Nevertheless, the two Hamiltonians corresponding to the perturbations of Eqs. (2.14) and (2.15a) do give equivalent results, contrary to the implications of Ref. 15.

It is interesting to consider the vacancy limit. There are at least three ways to take this limit. First, one can set $j = 0$ and use the representation of Eq. (2.14) which has no hard core long–wavelength interaction in this case. In fact, for $j = 0$ the scattering matrix element is of order $v(\mathbf{q},\mathbf{q}') \sim e_{\mathbf{q}}e_{\mathbf{q}'}$. It would seem then, that s-wave scattering is unimportant for vacancies. However, in this representation the defect has a zero-frequency excitation, and the t matrix is of order[15] $t(\mathbf{q},\mathbf{q}';e) \sim e_{\mathbf{q}}e_{\mathbf{q}'}/e$. The Born series diverges at zero energy. However, on resonance (i.e., for $e = e_{\mathbf{q}}$), it does lead to correct results.[15] It is possible, but somewhat cumbersome, to project out the $e = 0$ excitation on the vacancy, for instance, by introducing a potential on the vacancy site.[15,34] If this is done by adding a potential on the defect site, it seems necessary to sum over all repeated scatterings to treat this hard core potential correctly. Use of the lowest-order Born approximation is then totally misleading.

The second choice to represent the vacancy limit is to set $s = 0$ and let j remain finite. The choice $j = 1$ corresponds to the equation-of-motion method used by Jones[8] and by Bulot *et al.*[35] Here again, the perturbation of Eq. (2.14) has nonzero scattering in the long-wavelength limit, so finite-order perturbation theory will lead to a gap in the excitation spectrum.[4,6,8] Use of the non-Hermitian potential of Eqs. (2.15a) and (2.15b) improves the situation in that successive orders in perturbation theory lead to a numerical renormalization of the effective interaction at long wavelength and are thus qualitatively unimportant. However, one sees from Eq. (2.25) that the t matrix has a pole at $e = j$ reflecting the decoupled excitation on the vacancy having this energy,[15] even when the equations of motion for spin operators are used. When the full spin Green's function of Eq. (2.27) is expanded to order x this pole vanishes: it is absent from the combination

$$\frac{t(\mathbf{q},\mathbf{q};e)}{(e-e_{\mathbf{q}})^2} + \frac{\Lambda(\mathbf{q},e)}{e-e_{\mathbf{q}}} \ . \tag{2.36}$$

However, the fact that each individual term in Eq. (2.36) has a pole at $e = j$ means that for the choice $s = 0$, $j = 1$ the form for the full spin Green's function given in Eq. (2.27) is not numerically reliable for energy near $e = j$. In fact, it is a check on the calculations that the expression

in Eq. (2.36) is independent of j, since the actual spin response cannot involve j when the defect has zero spin.

Finally the third and most satisfactory approach is to set $s = sj = j^{-1} = 0$. By setting $j = \infty$ we project out the decoupled excitation on the vacancy site in a way similar to that adopted in Ref. 15. Furthermore, this choice is clearly good if the constraints are not handled exactly, as is the case for the CPA.[15]

We now return to the case of a weakly coupled spin and see in a more detailed way how the vacancy result can be obtained from this limit. The only nonuniformity in the $j \to 0$ limit occurs in the s-wave t matrix, $t^{(s)}(\mathbf{q},\mathbf{q}';e)$. On resonance and when both j and $e_{\mathbf{q}}$ are both much less than unity, but $j - e_{\mathbf{q}}$ is not near zero, we have

$$\frac{t^{(s)}(\mathbf{q},\mathbf{q};e_{\mathbf{q}})}{e_{\mathbf{q}}} = \frac{j(1-s)-e_{\mathbf{q}}}{j-e_{\mathbf{q}}} . \tag{2.37}$$

Now we see how the $j \to 0$ limit works. For any nonzero j the $q \to 0$ limit gives $\sigma_s = 1 - s$, as expected for $j \neq 0$. But this result only applies for $e_{\mathbf{q}} \ll j$. For $j \ll e_{\mathbf{q}} \ll 1$, $t^{(s)}(\mathbf{q},\mathbf{q};e_{\mathbf{q}})/e_{\mathbf{q}} = 1$, as we would expect for a vacancy. [Recall the discussion following Eq. (2.35).] Even for arbitrarily weak coupling, as long as the frequency is sufficiently small, the defect spin can respond to the time-dependent field of its neighbors and Eq. (2.35) holds with $M(x) = M(0)[1+x(s-1)]$. In the "high-frequency" limit the weakly coupled defect cannot respond and the defect looks like a vacancy: in Eq. (2.35) we should set $M(x) = M_\infty$, with $M_\infty = M(0)(1-x)$. In the crossover regime there will be anomalous dispersion and accompanying damping when the spin wave resonates with the localized resonance. This scenario is illustrated in Fig. 1, where we plot $t^{(s)}(\mathbf{q},\mathbf{q};e_{\mathbf{q}})/e_{\mathbf{q}}$ [evaluated from Eq. (2.24)] versus $e_{\mathbf{q}}$ for a small value of j.

Finally we consider the damping of elementary excitations. The decay rate in dimensionless units, Γ, is related to the imaginary part of the self-energy on resonance: $\Gamma(\mathbf{q}) = \mathrm{Im}\sigma(\mathbf{q},e_{\mathbf{q}})$. To start we note that nonzero imaginary parts come exclusively from the Green's functions evaluated at $e = e_{\mathbf{q}} - i0^+$. There we have, for $e \to 0$,

$$\mathrm{Im}g_F(e-i0^+) = \left(\frac{a}{2\pi}\right)^d \int d^d\mathbf{q}\pi\delta(e-a^2q^2/z) = \frac{z}{2}\pi K_d(ze)^{\frac{d}{2}-1} \tag{2.38a}$$

and

$$\mathrm{Im}g_p(e-i0^+) = \left(\frac{a}{2\pi}\right)^d \int d^d\mathbf{q}\pi(2a^2q^2/d)\delta(e-a^2q^2/z) = \frac{z}{d}\pi K_d(ze)^{\frac{d}{2}} , \tag{2.38b}$$

where $K_d^{-1} = 2^{d-1}\pi^{d/2}\Gamma(d/2)$ is a phase space scale factor in d dimensions. We can neglect d-wave and higher angular momentum symmetry which give rise to even smaller contributions at long wavelength. Our evaluation of the self-energy leads to results in agreement with previous ones:[4-6,8,16]

$$\Gamma(\mathbf{q}) = K_d(ze_{\mathbf{q}})^{\frac{d}{2}+1} \times \left[\frac{\pi}{2z}(1-s)^2 + \frac{2\pi}{zd}\frac{(js-1)^2}{[1-(js-1)g_p(0)/z]^2}\right] . \tag{2.39}$$

We recall that an advantage of the non-Hermitian Hamiltonian is that the correct wave vector dependence of the self-energy is obtained even within lowest-order perturbation theory. Consider, for example, the case of defects, for which we may take $s = 0$. For this case a Born approximation indicates that the imaginary part of the s-wave contribution to the self-energy at this order is

$$\mathrm{Im}\sigma^{(s)}(\mathbf{q},e) \sim \int d\mathbf{q}'\delta(e_{\mathbf{q}} - e_{\mathbf{q}'})e_{\mathbf{q}}e_{\mathbf{q}'} \sim q^{d+2} , \tag{2.40}$$

and similarly for the p-wave contribution, both as in the exact result of Eq. (2.39). The alternative approach involving setting $j = 0$ is harder to interpret. From Eq. (2.14) one can establish that the s-wave scattering matrix element in this case is of order $e_{\mathbf{q}}e_{\mathbf{q}'}$, which indicates that in any finite order of perturbation theory this scattering is negligible in comparison to that from the p-wave potential. For instance, lowest-order perturbation theory with $j = 0$ gives

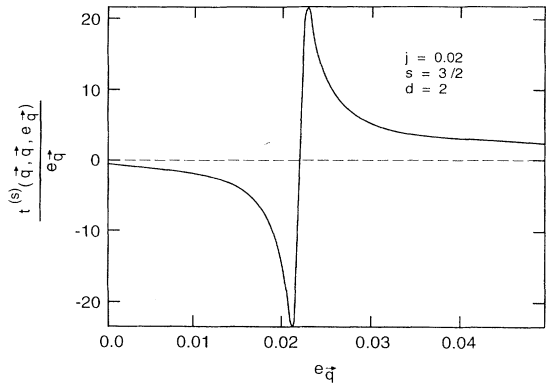

FIG. 1. The s-wave perturbation on the dispersion relation due to the defect for $j = 0.02$, $s = 3/2$, and $d = 2$. Here we plot $y \equiv t^{(s)}(\mathbf{q},\mathbf{q},e_{\mathbf{q}})/e_{\mathbf{q}}$ vs $e_{\mathbf{q}}$ for $\mathbf{q}$ along (1,0). To get $e_{\mathbf{q}}(x)$ use Eqs. (2.33) and (2.34). When the factor x is included [(to get $e_{\mathbf{q}}(x)$], the resonance is much less prominent than in this figure. Here we show the crossover from the low-frequency (hydrodynamic-like) regime in which all spins follow the motion to the high-frequency regime in which the defect spin cannot follow the motion. Effectively, in the low-frequency regime $M(x) = M(0)[1 + x(s-1)]$, in which case $y = 1 - s$. In the high-frequency regime $M(x) = M_\infty$. For infinitesimal j, $M_\infty = M(0)[1-x]$ or $y = 1$. We do not accurately reproduce this limit because j is not infinitesimal. The crossover occurs at a value of q such that $e_{\mathbf{q}} = j$. The extreme values of y are approximately $\pm(2j)^{-1}$ and occur for $e_{\mathbf{q}} = j \pm j^2 s$. Similar results obtain for the antiferromagnet when the vertical axis represents $\omega_{\mathbf{q}}/q$.

$$\mathrm{Im}\sigma(\mathbf{q},e)^{(2)} \sim \int d\mathbf{q}'\delta(e_{\mathbf{q}}-e_{\mathbf{q}'})(e_{\mathbf{q}}e_{\mathbf{q}'})^2 \sim q^{d+6} \ . \quad (2.41)$$

We use a superscript (n) to indicate the s-wave contribution from nth order perturbation theory. The zero energy excitation on the decoupled defect gives rise to a divergent perturbation series. In fact we find for $n \geq 2$

$$\mathrm{Im}\sigma(\mathbf{q},e)^{(n)} \sim (n-1)\int d\mathbf{q}'\delta(e_{\mathbf{q}}-e_{\mathbf{q}'}) \times[1+e_{\mathbf{q}}]^{n-2}(e_{\mathbf{q}}e_{\mathbf{q}'})^2 \sim q^{d+6} \ . \quad (2.42)$$

Summing this series reproduces the correct result of Eq. (2.39), but obviously this approach is rather opaque, compared to the one we prefer.

To summarize: we conclude that using the non-Hermitian Hamiltonian gives qualitatively correct results even in lowest Born approximation. To treat vacancies, one should take $s = sj = j^{-1} = 0$.

III. DEFECTS IN AN ANTIFERROMAGNET: RESULTS

In this section we will develop the calculation for the antiferromagnet with defects using the approaches which proved useful in the previous section for the ferromagnet. A detailed discussion of the results will be given in the next section.

The model we treat is an isotropic Heisenberg antiferromagnet with a low concentration of defect sites, each of which consist of a defect spin of magnitude S' coupled to its neighbors with exchange coupling J'. The corresponding host values are S and J and the notation in terms of reduced values introduced in the preceding section will be adopted here. We take the ground state of the pure system to consist of two interpenetrating hypercubic lattices. In the Néel ground state the A sublattice spins have $S^z_{\mathbf{R}} = +S$ and the B sublattice spins have $S^z_{\mathbf{R}} = -S$. As usual we introduce boson operators which create spin deviations: $a^\dagger_{\mathbf{R}}$ ($b^\dagger_{\mathbf{R}}$) creates an excitation on the site $\mathbf{R}$ in the A (B) sublattice. The Néel state is the boson vacuum.[37,38] For concreteness one may visualize a simple cubic or, in two dimensions, a square centered lattice. The unit cell is a d-dimensional hypercube of side a containing two sites and the Brillouin zone (over which all wave vector sums are carried) corresponds to this choice of unit cell, of course. For spins on the A sublattice we have

$$S^z_{\mathbf{R}} = S - a^\dagger_{\mathbf{R}}a_{\mathbf{R}}, \quad (3.1a)$$

$$S^+_{\mathbf{R}} = \sqrt{2S_{\mathbf{R}}}a_{\mathbf{R}}, \quad (3.1b)$$

$$S^-_{\mathbf{R}} = \sqrt{2S_{\mathbf{R}}}a^\dagger_{\mathbf{R}}, \quad (3.1c)$$

and for those on the B sublattice

$$S^z_{\mathbf{R}} = -S + b^\dagger_{\mathbf{R}}b_{\mathbf{R}}, \quad (3.2a)$$

$$S^+_{\mathbf{R}} = \sqrt{2S_{\mathbf{R}}}b^\dagger_{\mathbf{R}}, \quad (3.2b)$$

$$S^-_{\mathbf{R}} = \sqrt{2S_{\mathbf{R}}}b_{\mathbf{R}} \ , \quad (3.2c)$$

where $S_{\mathbf{R}}$ is the magnitude of the spin on site $\mathbf{R}$. The pure system is then described (neglecting spin-wave interactions) by the Hamiltonian

$$h_0 \equiv H_0/(2JzS) = \frac{1}{z}\sum_{\mathbf{R}\in A}\sum_{\delta}(a^\dagger_{\mathbf{R}} + b_{\mathbf{R}+\delta})(a_{\mathbf{R}} + b^\dagger_{\mathbf{R}+\delta}) \ . \quad (3.3)$$

Since we are not keeping track of the constant ground state energy, neither is it important, nor is it notationally convenient, nor will we keep track of the ordering of the operators. In terms of Fourier transforms,

$$h_0 = \sum_{\mathbf{q}}(a^\dagger_{\mathbf{q}}a_{\mathbf{q}} + b^\dagger_{\mathbf{q}}b_{\mathbf{q}} + \gamma_{\mathbf{q}}a^\dagger_{\mathbf{q}}b^\dagger_{-\mathbf{q}} + \gamma_{\mathbf{q}}a_{\mathbf{q}}b_{-\mathbf{q}}) \ . \quad (3.4)$$

This Hamiltonian is diagonalized by the transformation

$$a^\dagger_{\mathbf{q}} = l_{\mathbf{q}}\alpha^\dagger_{\mathbf{q}} - m_{\mathbf{q}}\beta_{-\mathbf{q}}, \quad (3.5a)$$

$$b_{-\mathbf{q}} = -m_{\mathbf{q}}\alpha^\dagger_{\mathbf{q}} + l_{\mathbf{q}}\beta_{-\mathbf{q}} \ , \quad (3.5b)$$

where

$$l_{\mathbf{q}} = \left(\frac{1+e_{\mathbf{q}}}{2e_{\mathbf{q}}}\right)^{1/2}, \qquad m_{\mathbf{q}} = \left(\frac{1-e_{\mathbf{q}}}{2e_{\mathbf{q}}}\right)^{1/2}, \quad (3.6)$$

where

$$e_{\mathbf{q}} = \sqrt{1-\gamma^2_{\mathbf{q}}} \ . \quad (3.7)$$

Then

$$h_0 = \sum_{\mathbf{q}}(\alpha^\dagger_{\mathbf{q}}\alpha_{\mathbf{q}} + \beta^\dagger_{\mathbf{q}}\beta_{\mathbf{q}})e_{\mathbf{q}} \ . \quad (3.8)$$

We introduce the boson Green's functions,[39,40]

$$g_{i,j}(\mathbf{q}) \equiv (2JzS)\langle\langle Q_i(\mathbf{q}); Q_j(\mathbf{q})^\dagger\rangle\rangle_E \ , \quad (3.9)$$

where $Q_1(\mathbf{q}) = \alpha_{\mathbf{q}}$ and $Q_2(\mathbf{q}) = \beta^\dagger_{-\mathbf{q}}$. The unperturbed Green's functions, indicated by superscript (0), are given as

$$\underline{g}^{(0)}(\mathbf{q};e) = \begin{pmatrix} \frac{1}{e-e_{\mathbf{q}}} & 0 \\ 0 & \frac{1}{-e-e_{\mathbf{q}}} \end{pmatrix} \ , \quad (3.10)$$

where $e = E/(2JzS)$.

Use of the above transformation to boson variables shows that for a defect on the A sublattice at site $\mathbf{R}$ the dimensionless defect perturbation is

$$v_{\mathbf{R}\in A} = -\frac{1}{z}\sum_{\delta}(a^\dagger_{\mathbf{R}} + b_{\mathbf{R}+\delta})(a_{\mathbf{R}} + b^\dagger_{\mathbf{R}+\delta}) + \frac{j}{z}\sum_{\delta}(a^\dagger_{\mathbf{R}} + \sqrt{s}b_{\mathbf{R}+\delta})(a_{\mathbf{R}} + \sqrt{s}b^\dagger_{\mathbf{R}+\delta}) \ . \quad (3.11)$$

As for the ferromagnet we now replace $a^\dagger_{\mathbf{R}}$ by $\sqrt{s}a^\dagger_{\mathbf{R}}$ and $a_{\mathbf{R}}$ by $a_{\mathbf{R}}/\sqrt{s}$. This transformation will lead to a perturbation with weak scattering in the long–wavelength limit. Thus all the transformations we are using retain Eqs. (3.1a) and (3.2a) but have

$$S^+_{\mathbf{R}} = \sqrt{2S}a_{\mathbf{R}} \ , \quad S^-_{\mathbf{R}} = s\sqrt{2S}a^\dagger_{\mathbf{R}} \tag{3.12a}$$

for defect spins on the A sublattice. For defect spins on the B sublattice we write

$$S^+_{\mathbf{R}} = \sqrt{2S}b^\dagger_{\mathbf{R}} \ , \quad S^-_{\mathbf{R}} = s\sqrt{2S}b_{\mathbf{R}} \ . \tag{3.12b}$$

For host spins Eqs. (3.1a)–(3.2c) continue to apply. Note that we chose versions of this nonunitary transformation such that the zero-wave vector Fourier component of boson operators corresponding to one component of spin (here S^-) is conserved. Then

$$v_{\mathbf{R}\in A} = \frac{1}{z}\sum_\delta (a^\dagger_{\mathbf{R}} + b_{\mathbf{R}+\delta})[(j-1)a_{\mathbf{R}} + (js-1)b^\dagger_{\mathbf{R}+\delta}] \ . \tag{3.13}$$

Again, in close analogy to the ferromagnet, we introduce symmetry adapted operators. The transformation coefficients U^μ_δ, where U is a unitary matrix, are exactly the same as for a ferromagnet on the same structure. If terms of the symmetry label μ, we have

$$v_{\mathbf{R}\in A} = \sum_\mu v^{(\mu)}_{\mathbf{R}\in A} \ , \tag{3.14}$$

where the perturbation of symmetry μ is

$$v^{(\mu)}_{\mathbf{R}\in A} = \frac{1}{z}\left(\sum_\delta (a^\dagger_{\mathbf{R}} + b_{\mathbf{R}+\delta})U^{(\mu)\,*}_\delta\right) \times \left(\sum_{\delta'}[(j-1)a_{\mathbf{R}} + (js-1)b^\dagger_{\mathbf{R}+\delta'}]U^{(\mu)}_{\delta'}\right) . \tag{3.15}$$

As before, the s-wave coefficients are $U^{(s)}_\delta = 1/\sqrt{z}$ and the p-wave coefficients are $U^{(p,\alpha)}_\delta = ic\delta_\alpha$, where α is x, y, etc., and c is a normalization constant, $c^2 = d/(z\delta^2)$.

Normally one solves the single-defect problem in a real-space representation in which all quantities are confined to the defect region. We find it simpler for the antiferromagnet, where there are inevitable algebraic subtleties involving the symmetry between sublattices, to work in terms of spatial Fourier components. Here the fact that the defect is localized reflects itself in the fact that the potential is the sum of a small number of separable potentials, each having different symmetry and each of rank one. For a defect on an A site, the s-wave perturbation in terms of Fourier transformed variables is

$$\begin{aligned} v^{(s)}_{\mathbf{R}\in A} &= \frac{1}{N}\sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}(a^\dagger_{\mathbf{q}} + \gamma_{\mathbf{q}}b_{-\mathbf{q}})[(j-1)a_{\mathbf{q}'} + (js-1)\gamma_{\mathbf{q}'}b^\dagger_{-\mathbf{q}'}] \\ &= \frac{1}{N}\sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}[\alpha^\dagger_{\mathbf{q}}(l_{\mathbf{q}} - \gamma_{\mathbf{q}}m_{\mathbf{q}}) + \beta_{-\mathbf{q}}(l_{\mathbf{q}}\gamma_{\mathbf{q}} - m_{\mathbf{q}})] \qquad (3.16) \\ &\qquad \times \{\alpha_{\mathbf{q}'}[l_{\mathbf{q}'}(j-1) - m_{\mathbf{q}'}\gamma_{\mathbf{q}'}(js-1)] + \beta^\dagger_{-\mathbf{q}'}[(js-1)l_{\mathbf{q}'}\gamma_{\mathbf{q}'} - m_{\mathbf{q}'}(j-1)]\} \qquad (3.17a) \\ &\equiv \frac{1}{N}\sum_{\mathbf{q},\mathbf{q}',i,j}\left[\underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}')\right]_{i,j} Q_i(\mathbf{q})^\dagger Q_j(\mathbf{q}') \ , \qquad (3.17b) \end{aligned}$$

where N is the number of sites in one sublattice, i.e., $N = \sum_{\mathbf{q}} 1$. Equation (3.17b) shows that the s-wave perturbation can be represented by a 2×2 matrix. From Eq. (3.17a) we see that this matrix is the outer product of a two-component column vector $|\eta(\mathbf{q})\rangle$ and a two–component row vector $\langle\xi(\mathbf{q}')|$:

$$\underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}') = |\eta(\mathbf{q})\rangle\langle\xi(\mathbf{q}')|e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}} \ , \tag{3.18}$$

where

$$|\eta(\mathbf{q})\rangle_1 = l_{\mathbf{q}} - \gamma_{\mathbf{q}}m_{\mathbf{q}} = l_{\mathbf{q}}e_{\mathbf{q}}, \tag{3.19a}$$

$$|\eta(\mathbf{q})\rangle_2 = l_{\mathbf{q}}\gamma_{\mathbf{q}} - m_{\mathbf{q}} = m_{\mathbf{q}}e_{\mathbf{q}}, \tag{3.19b}$$

$$\begin{aligned} \langle\xi(\mathbf{q})|_1 &= l_{\mathbf{q}}(j-1) - \gamma_{\mathbf{q}}m_{\mathbf{q}}(js-1) = l_{\mathbf{q}}[(js-1)e_{\mathbf{q}} - j(s-1)] &(3.19c)\\ &\equiv l_{\mathbf{q}}\phi_1(\mathbf{q}), &(3.19d) \end{aligned}$$

and

$$\begin{aligned} \langle\xi(\mathbf{q})|_2 &= l_{\mathbf{q}}\gamma_{\mathbf{q}}(js-1) - m_{\mathbf{q}}(j-1) = m_{\mathbf{q}}[(js-1)e_{\mathbf{q}} + j(s-1)] &(3.19e)\\ &\equiv m_{\mathbf{q}}\phi_2(\mathbf{q}) \ . &(3.19f) \end{aligned}$$

At long wavelength we have $l_{\mathbf{q}} \sim m_{\mathbf{q}} \sim e_{\mathbf{q}}^{-1/2}$. Thus at long wavelength the scattering matrix elements in Eq. (3.18) are of order

$$v^{(s)}(\mathbf{q},\mathbf{q}') \sim \sqrt{e_{\mathbf{q}}}\left[(js-1)\sqrt{e_{\mathbf{q}'}} \pm j(s-1)/\sqrt{e_{\mathbf{q}'}}\right] . \tag{3.20}$$

This result shows that the scattering is much larger for $s \neq 1$ than for $s = 1$, a fact which will be discussed in more detail in the next section.

Summing over all repeated s-wave scattering from a single defect on the A sublattice gives the s-wave part of the 2×2 (dimensionless) t matrix, $\underline{t}$, as

$$\underline{t}^{(s)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}') = \underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}') + \frac{1}{N}\sum_{\mathbf{q}''} \underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}'')\underline{g}^{(0)}(\mathbf{q}'')\underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q}'',\mathbf{q}')$$

$$+\frac{1}{N^2}\sum_{\mathbf{q}'',\mathbf{q}'''} \underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}'')\underline{g}^{(0)}(\mathbf{q}'')\underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q}'',\mathbf{q}''')\underline{g}^{(0)}(\mathbf{q}''')\underline{v}^{(s)}_{\mathbf{R}\in A}(\mathbf{q}''',\mathbf{q}') + \ldots \tag{3.21a}$$

$$= e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}|\eta(\mathbf{q})\rangle\langle\xi(\mathbf{q}')|\left(1 - \frac{1}{N}\sum_{\tau}\langle\xi(\tau)|\underline{g}^{(0)}(\tau)|\eta(\tau)\rangle\right)^{-1} \tag{3.21b}$$

$$= e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}|\eta(\mathbf{q})\rangle\langle\xi(\mathbf{q}')|/D(e) \tag{3.21c}$$

$$= e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}\frac{e_{\mathbf{q}}}{D(e)}\begin{bmatrix} l_{\mathbf{q}} \\ m_{\mathbf{q}} \end{bmatrix}\left[l_{\mathbf{q}'}\phi_1(\mathbf{q}')\,, m_{\mathbf{q}'}\phi_2(\mathbf{q}')\right] , \tag{3.21d}$$

where

$$D(e) = (j-e)[1 - e(1+e)g_0(e)] + ejs[1 + (1-e^2)g_0(e)] , \tag{3.22}$$

in agreement with KH and Tonegawa,[27] where

$$g_0(e) = N^{-1}\sum_{\mathbf{q}}(e^2 - e_{\mathbf{q}}^2)^{-1} . \tag{3.23}$$

In Eqs. (3.21a)–(3.21d) the two–sided Fourier transformation is defined similarly to Eq. (2.9). If the concentration of defect sites on the A sublattice is x_A, then the configurationally averaged Green's function has the self–energy (correct to first order in x) from such defects given by

$$\frac{1}{N}\left[\sum_{\mathbf{R}\in A}\epsilon(\mathbf{R})\underline{t}^{(s)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}')\right]_{\text{av}} \equiv x_A\delta_{\mathbf{q},\mathbf{q}'}\underline{\sigma}^{(s)}_A(\mathbf{q}) \tag{3.24a}$$

$$= x_A\delta_{\mathbf{q},\mathbf{q}'}|\eta(\mathbf{q})\rangle\langle\xi(\mathbf{q})|/D(e) \tag{3.24b}$$

$$= x_A\delta_{\mathbf{q},\mathbf{q}'}\frac{e_{\mathbf{q}}}{D(e)}\begin{bmatrix} l_{\mathbf{q}} \\ m_{\mathbf{q}} \end{bmatrix}[l_{\mathbf{q}}\phi_1(\mathbf{q})\,,\quad m_{\mathbf{q}}\phi_2(\mathbf{q})] . \tag{3.24c}$$

Note that the self-energy is thus subject to the same estimates as given in Eq. (3.20) for the potential.

Let us now construct the s-wave t matrix for a concentration, x_B, of defects on the B sublattice. One can see that the perturbation simply interchanges the role of a and $b^\dagger$ operators, or similarly, α and $\beta^\dagger$ operators. This same reasoning shows that this results in replacing $D(e)$ by $D(-e)$. So

$$\underline{t}^{(s)}_{\mathbf{R}\in B}(\mathbf{q},\mathbf{q}') = e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}\frac{e_{\mathbf{q}}}{D(-e)}\begin{bmatrix} m_{\mathbf{q}} \\ l_{\mathbf{q}} \end{bmatrix} \times [m_{\mathbf{q}'}\phi_2(\mathbf{q}')\,, l_{\mathbf{q}'}\phi_1(\mathbf{q}')] , \tag{3.25}$$

and, in analogy with Eq. (3.24c),

$$\underline{\sigma}^{(s)}_B(\mathbf{q}) = \frac{e_{\mathbf{q}}}{D(-e)}\begin{bmatrix} m_{\mathbf{q}} \\ l_{\mathbf{q}} \end{bmatrix}\ [m_{\mathbf{q}}\phi_2(\mathbf{q})\,,\ l_{\mathbf{q}}\phi_1(\mathbf{q})] . \tag{3.26}$$

The s-wave self-energy is the sum of the two contributions given in Eqs. (3.24c) and (3.26).

For non-s-wave scattering the calculations are simpler. We use the fact that for μ not s, $\sum_{\delta} U^{(\mu)}_{\delta} = 0$, as a result of which perturbations involving the defect site only appear in the s-wave scattering. For non-s-wave symmetry we have

$$v^{(\mu)}_{\mathbf{R}\in A} = \frac{js-1}{Nz}\sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}\phi^{(\mu)}(\mathbf{q})\phi^{(\mu)}(\mathbf{q}')(l_{\mathbf{q}}\beta^{\dagger}_{\mathbf{q}} - m_{\mathbf{q}}\alpha_{-\mathbf{q}})(l_{\mathbf{q}'}\beta_{\mathbf{q}'} - m_{\mathbf{q}'}\alpha^{\dagger}_{-\mathbf{q}'}) , \tag{3.27}$$

where $\phi^{(\mu)}(\mathbf{q})$ is defined in Eqs. (2.17a) and (2.17b). For a square-centered lattice $\phi^{(p,x)}(\mathbf{q}) = 2\sin(q_x a/2)\cos(q_y a/2)$ and for a body-centered-cubic lattice $\phi^{(p,x)}(\mathbf{q}) = \sqrt{8}\sin(q_x a/2)\cos(q_y a/2)\cos(q_z a/2)$. In matrix representation we have the analog of Eq. (3.18):

$$\underline{v}^{(\mu)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}') = |\rho(\mathbf{q})\rangle\langle\rho(\mathbf{q}')| , \tag{3.28}$$

where $|\rho(\mathbf{q})\rangle$ is the two–component vector $(m_{\mathbf{q}}, -l_{\mathbf{q}})$. Summing over repeated scatterings we find that

$$\underline{t}^{(\mu)}_{\mathbf{R}\in A}(\mathbf{q},\mathbf{q}') = e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}\frac{(js-1)\phi^{(\mu)}(\mathbf{q})\phi^{(\mu)}(\mathbf{q}')}{z-(1-e)(js-1)g^{(\mu)}(e)} \times \begin{bmatrix} m_{\mathbf{q}}m_{\mathbf{q}'} & -m_{\mathbf{q}}l_{\mathbf{q}'} \\ -l_{\mathbf{q}}m_{\mathbf{q}'} & l_{\mathbf{q}}l_{\mathbf{q}'} \end{bmatrix} , \tag{3.29a}$$

and after a configurational average

$$\underline{\sigma}^{(\mu)}_{A}(\mathbf{q}) = x_A\frac{(js-1)\phi^{(\mu)}(\mathbf{q})^2}{z-(1-e)(js-1)g^{(\mu)}(e)} \times \begin{bmatrix} m_{\mathbf{q}}^2 & -m_{\mathbf{q}}l_{\mathbf{q}} \\ -m_{\mathbf{q}}l_{\mathbf{q}} & l_{\mathbf{q}}^2 \end{bmatrix} , \tag{3.29b}$$

where

$$g^{(\mu)}(e) = \frac{1}{N}\sum_{\mathbf{q}}\frac{\phi^{(\mu)}(\mathbf{q})^2}{e^2-e_{\mathbf{q}}^2} . \tag{3.30}$$

At long wavelength the most important non-s-wave scattering is in the p-wave channel. Since $\phi^{(p)}(\mathbf{q}) \sim q$, we see that both the scattering potential $v^{(p)}$ and the p-wave self-energy are of order $\sqrt{qq'}$ at long wavelength. This scattering is comparable to that in the s-wave channel for $s = 1$. Likewise when the defect is on the B sublattice we obtain to first order in x

$$\underline{\sigma}^{(\mu)}_{B}(\mathbf{q}) = x_B\frac{(js-1)\phi^{(\mu)}(\mathbf{q})^2}{z-(1+e)(js-1)g^{(\mu)}(e)} \times \begin{bmatrix} l_{\mathbf{q}}^2 & -m_{\mathbf{q}}l_{\mathbf{q}} \\ -m_{\mathbf{q}}l_{\mathbf{q}} & m_{\mathbf{q}}^2 \end{bmatrix} . \tag{3.31}$$

Again the total contribution to the self-energy of symmetry μ is found as the sum of the contributions given in Eqs. (3.29b) and (3.31).

We summarize by collecting the results from Eqs. (3.24c), (3.26), (3.29b), and (3.31) to write the matrix elements of the self-energy for the configurationally averaged boson Green's function of Eq. (3.9) which is given in terms of the self-energy matrix σ as

$$\underline{g}(\mathbf{q},e) = [\underline{g}^{(0)}(\mathbf{q},e)^{-1} - \underline{\sigma}(\mathbf{q},e)]^{-1} , \tag{3.32}$$

where

$$\sigma_{\alpha,\alpha}(\mathbf{q},e) = \frac{x_A l_{\mathbf{q}}^2 e_{\mathbf{q}}}{D(e)}[(js-1)e_{\mathbf{q}} - j(s-1)] + \frac{x_B m_{\mathbf{q}}^2 e_{\mathbf{q}}}{D(-e)}[(js-1)e_{\mathbf{q}} + j(s-1)] + \sum_{\mu\neq s}(js-1)\phi^{(\mu)}(\mathbf{q})^2\left(\frac{x_A m_{\mathbf{q}}^2}{z-(1-e)(js-1)g^{(\mu)}(e)} + \frac{x_B l_{\mathbf{q}}^2}{z-(1+e)(js-1)g^{(\mu)}(e)}\right), \tag{3.33a}$$

$$\sigma_{\beta,\beta}(\mathbf{q},e) = \frac{x_B l_{\mathbf{q}}^2 e_{\mathbf{q}}}{D(-e)}[(js-1)e_{\mathbf{q}} - j(s-1)] + \frac{x_A m_{\mathbf{q}}^2 e_{\mathbf{q}}}{D(e)}[(js-1)e_{\mathbf{q}} + j(s-1)] + \sum_{\mu\neq s}(js-1)\phi^{(\mu)}(\mathbf{q})^2\left(\frac{x_A l_{\mathbf{q}}^2}{z-(1-e)(js-1)g^{(\mu)}(e)} + \frac{x_B m_{\mathbf{q}}^2}{z-(1+e)(js-1)g^{(\mu)}(e)}\right), \tag{3.33b}$$

$$\sigma_{\alpha,\beta}(\mathbf{q},e) = \frac{x_A l_{\mathbf{q}} m_{\mathbf{q}} e_{\mathbf{q}}}{D(e)}[(js-1)e_{\mathbf{q}} + j(s-1)] + \frac{x_B l_{\mathbf{q}} m_{\mathbf{q}} e_{\mathbf{q}}}{D(-e)}[(js-1)e_{\mathbf{q}} - j(s-1)] - \sum_{\mu\neq s}(js-1)\phi^{(\mu)}(\mathbf{q})^2 l_{\mathbf{q}} m_{\mathbf{q}}\left(\frac{x_A}{z-(1-e)(js-1)g^{(\mu)}(e)} + \frac{x_B}{z-(1+e)(js-1)g^{(\mu)}(e)}\right), \tag{3.33c}$$

$$\sigma_{\beta,\alpha}(\mathbf{q},e) = \frac{x_A l_{\mathbf{q}} m_{\mathbf{q}} e_{\mathbf{q}}}{D(e)}[(js-1)e_{\mathbf{q}} - j(s-1)] + \frac{x_B l_{\mathbf{q}} m_{\mathbf{q}} e_{\mathbf{q}}}{D(-e)}[(js-1)e_{\mathbf{q}} + j(s-1)] - \sum_{\mu\neq s}(js-1)\phi^{(\mu)}(\mathbf{q})^2 l_{\mathbf{q}} m_{\mathbf{q}}\left(\frac{x_A}{z-(1-e)(js-1)g^{(\mu)}(e)} + \frac{x_B}{z-(1+e)(js-1)g^{(\mu)}(e)}\right) , \tag{3.33d}$$

where $D(e)$ was given in Eq. (3.22). 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 $\sigma_{\alpha,\beta}(e) = \sigma_{\beta,\alpha}(-e)$.

In Appendix A it is shown that the spin Green's function is given by an expression similar to that in Eq. (2.27) for the ferromagnet. Using such a development we can express the spin susceptibility, which in dimensionless units is $\chi_{+-}(\mathbf{q},e) \equiv (Jz)\langle\langle S_+(\mathbf{q}); S_-(\mathbf{q})\rangle\rangle_e$, in terms of the matrix of Green's functions defined in Eq. (3.9) as

$$\chi_{+-}(\mathbf{q},e) = A(\mathbf{q},e)[1\ ,1]\underline{g}(\mathbf{q},e)\begin{bmatrix}1\\1\end{bmatrix} + B(\mathbf{q},e)[1\ ,1]\underline{g}(\mathbf{q},e)\begin{bmatrix}1\\-1\end{bmatrix}, \tag{3.34}$$

where

$$A(\mathbf{q},e) = \frac{1-\gamma_{\mathbf{q}}}{e_{\mathbf{q}}}\left[1+\frac{1}{2}(x_A+x_B)(s-1)\right] + (s-1)\frac{e_{\mathbf{q}}}{2}[x_A\tau(e)+x_B\tau(-e)] \tag{3.35a}$$

and

$$B(\mathbf{q},e) = \frac{(s-1)}{2}\{x_A - x_B + (1-\gamma_{\mathbf{q}})[x_A\tau(e) - x_B\tau(-e)]\}, \tag{3.35b}$$

where $\tau(e)$ is given in Eqs. (A16a)–(A17) of Appendix A. In the absence of defects ($x_A = x_B = 0$), the susceptibility has a wave vector-dependent amplitude which varies like $|\mathbf{q}-\mathbf{Q}|$ for $\mathbf{q}$ near a ferromagnetic wave vector $\mathbf{Q}$, and like $|\mathbf{q}-\mathbf{Q}|^{-1}$ near an antiferromagnetic Bragg wave vector $\mathbf{Q}$, in agreement with Refs. 20 and 40.

IV. DEFECTS IN AN ANTIFERROMAGNET: DISCUSSION

In this section we will discuss the results of the preceding section, as summarized in Eqs. (3.32) and ff, in various limiting cases and will compare them with previous developments. We thus give a comprehensive discussion of the response of the system to first order in the defect concentration, x. For this purpose we will mostly confine our attention to the long-wavelength limit. We distinguish three main cases: (I) $s = 1$, (II) $s \neq 1$, but $x_A = x_B$, and (III) $s \neq 1$ and $x_A \neq x_B$. Roughly speaking these cases represent the following physical situations. In case III the defects break the antiferromagnetic symmetry and we actually are dealing with a ferrimagnet (HK). In case II, we still have an antiferromagnet, but because $s \neq 1$, there are fluctuations in which locally ferrimagnetic regions can occur (HK). Case II for $s = 0$ describes the case of vacancies equally distributed on the two sublattices. To treat vacancies it is best to set $j = \infty$, to avoid spurious effects from decoupled excitations on the defect site at energy $e = j$. However, on resonance we would expect, in light of the results for the ferromagnet, that the results do not depend on j. Finally in case I, each unit cell has exactly zero ferromagnetic moment: there are no fluctuations towards ferrimagnetism. As we shall see, each of these three regimes is characterized by a distinctive long–wavelength behavior. In regime I the elementary excitations are weakly perturbed from those of the defect-free host. The same is true in regime II as long as the spatial dimensionality, d, is greater than 2. Therefore under these conditions the off-diagonal parts of the self-energy represent higher-order (in x) corrections and we may write the spin-wave energies in the presence of defects as

$$e^{\alpha}_{\mathbf{q}}(x_A,x_B) = e_{\mathbf{q}} + \sigma_{\alpha,\alpha}(\mathbf{q}, e_{\mathbf{q}} - i0^+), \tag{4.1a}$$

$$e^{\beta}_{\mathbf{q}}(x_A,x_B) = e_{\mathbf{q}} + \sigma_{\beta,\beta}(\mathbf{q}, -e_{\mathbf{q}} + i0^+), \tag{4.1b}$$

whose real part gives the perturbed energy and whose imaginary part, $\Gamma_{\mathbf{q}}$, gives the damping rate. For $x_A = x_B$ the antiferromagnetic symmetry is preserved and $e^{\alpha}_{\mathbf{q}}(x_A,x_B) = e^{\beta}_{\mathbf{q}}(x_A,x_B)$. However, for $d = 2$ and for $s \neq 1$, the decay rate remains a finite fraction of the frequency and the real part of the self-energy diverges in the low-frequency limit. Thus for $d = 2$ spin waves are strongly perturbed in regime II. Finally, in case III we need to consider the full self-energy matrix in order to describe ferrimagnetic spin waves which exist at long wavelengths. In the calculations which follow we consider a body–centered hypercubic lattice in d spatial dimensions.

In case I ($s = 1$), we have, at long wavelength,

$$\sigma_{\alpha,\alpha}(\mathbf{q},e) = \frac{j-1}{j}xe_{\mathbf{q}}\left(1+\frac{j-1}{j}e^2g_0(e)\right) + \left(\frac{x}{e_{\mathbf{q}}}\right)\frac{(j-1)\phi^{(p)}(\mathbf{q})^2}{z-(j-1)g^{(p)}(e)}, \tag{4.2}$$

where $x = (x_A + x_B)/2$ and $\phi^{(p)}(\mathbf{q})^2 = \sum_\rho \phi^{(p,\rho)}(\mathbf{q})^2$, where ρ is summed over components x, y, etc. [For future use, note that at long wavelengths $\phi^{(p)}(\mathbf{q})^2 \sim za^2q^2/4 \sim ze^2_{\mathbf{q}}$.] In writing Eq. (4.2) we used Eq. (3.6) for the transformation coefficients $l_{\mathbf{q}}$ and $m_{\mathbf{q}}$ and we dropped terms which lead to corrections at low energy or long wavelength. In this regime, then, for $q \to 0$,

$$\mathrm{Ree}_{\mathbf{q}}(x_A = x, x_B = x) \equiv \mathrm{Ree}_{\mathbf{q}}(x) = e_{\mathbf{q}}\left[1 + x\frac{j-1}{j} + x\frac{\phi^{(p)}(\mathbf{q})^2}{e^2_{\mathbf{q}}}\frac{j-1}{z-(j-1)g^{(p)}(0)}\right] \tag{4.3a}$$

$$\equiv e_{\mathbf{q}}(0)[1 - \rho x + O(x)^2]\,. \tag{4.3b}$$

From spin-wave hydrodynamics[18] or from an analysis[19,24] of the equations of motion at zero temperature neglecting spin–wave interactions, it is predicted that

$$\mathrm{Re}e_{\mathbf{q}}(x)^2 = \frac{\Sigma^{\mathrm{el}}(x)}{\Sigma^{\mathrm{el}}(0)}\frac{\chi_\perp(0)}{\chi_\perp(x)}e_{\mathbf{q}}(0)^2 , \tag{4.4a}$$

For small x this gives

$$\rho = -\frac{1}{2\Sigma^{\mathrm{el}}(0)}\frac{d\Sigma^{\mathrm{el}}(x)}{dx}\bigg|_{x=0} + \frac{1}{2\chi_\perp(0)}\frac{d\chi_\perp(x)}{dx} . \tag{4.4b}$$

In Appendix B it is verified that Eqs. (4.3a) and (4.3b) agree with Eq. (4.4b).[21,30] In Eqs. (4.3a) and (4.3b) it should be noted that $\phi^{(p)}(\mathbf{q})^2/e_{\mathbf{q}}^2$ is independent of $\mathbf{q}$ in the limit $q \to 0$, so that defects in regime I merely renormalize the spin–wave velocity. In Eqs. (4.3a) and (4.3b) we see a divergence in the limit $j \to 0$. This divergence reflects the divergence in $\chi_\perp$ when the coupling of a defect spin to the host becomes arbitrarily weak. But, as discussed for the ferromagnet (see Fig. 1), a crossover takes place for $e_{\mathbf{q}} \sim j$. Also from Eq. (4.2) we find

$$\mathrm{Im}e_{\mathbf{q}}(x) = x(j-1)^2 e_{\mathbf{q}}^3[\mathrm{Im}g_0(e_{\mathbf{q}})] \times\left[\frac{1}{j^2} + \frac{z^2}{d[z-(j-1)g^{(p)}(0)]^2}\right] , \tag{4.5}$$

where we used

$$\mathrm{Im}g^{(p)}(e) = \mathrm{Im}\frac{1}{N}\sum_{\mathbf{q}}\frac{\phi^{p,x}(\mathbf{q})^2}{(e-i0^+)^2-e_{\mathbf{q}}^2} \tag{4.6a}$$

$$= \mathrm{Im}\frac{1}{N}\sum_{\mathbf{q}}\frac{z\sin^2(q_x a/2)\cos^2(q_y/2)\ldots}{(e-i0^+)^2-e_{\mathbf{q}}^2}$$

$$= (ze^2/d)\mathrm{Im}g_0(e) . \tag{4.6b}$$

Also

$$\mathrm{Im}g_0(e) = 2\pi K_d(2e)^{d-2}\mathrm{sgn}(e) , \tag{4.6c}$$

where $\mathrm{sgn}(e) = e/|e|$. Thus Eq. (4.5) gives

$$\mathrm{Im}e_{\mathbf{q}}(x) = \frac{1}{4}x(j-1)^2\pi K_d(aq)^{d+1} \times\left[\frac{1}{j^2} + \frac{z^2}{d[z-(j-1)g^{(p)}(0)]^2}\right] . \tag{4.7}$$

This dependence on wave vector is clear from lowest-order perturbation theory: We saw in Eq. (3.20) that the scattering matrix element for $s = 1$ is of order $\sqrt{e_{\mathbf{q}}e_{\mathbf{q}'}}$. This leads to the estimate

$$\mathrm{Im}e_{\mathbf{q}} \sim \int d\mathbf{q}'\delta(e_{\mathbf{q}}-e_{\mathbf{q}'})e_{\mathbf{q}}e_{\mathbf{q}'} \sim q^{d+1} , \tag{4.8}$$

consistent with the complete result of Eq. (4.7).

Next we turn to case II, where $x_A = x_B = x$, but $s \neq 1$. There

$$\sigma_{\alpha,\alpha}(\mathbf{q},e) = xe_{\mathbf{q}}\frac{j-1}{j} - xe(s-1)\left(\frac{1}{j} - s + (1-s)g_0(e)\right) + \sum_{\mu\neq s}(js-1)\phi^{(\mu)}(\mathbf{q})^2\left(\frac{x_A m_{\mathbf{q}}^2}{z-(1-e)(js-1)g^{(\mu)}(e)} + \frac{x_B l_{\mathbf{q}}^2}{z-(1+e)(js-1)g^{(\mu)}(e)}\right) . \tag{4.9}$$

In this regime, therefore,

$$\mathrm{Re}e_{\mathbf{q}}(x) = e_{\mathbf{q}}\left[1 + x\frac{j-1}{j} + x(1-s)\left(\frac{1}{j}-s\right) + x(s-1)^2 g_0(0) + x\frac{\phi^{(p)}(\mathbf{q})^2}{e_{\mathbf{q}}^2}\frac{(js-1)}{z-(js-1)g^{(p)}(0)}\right] \tag{4.10}$$

and

$$\mathrm{Im}e_{\mathbf{q}}(x) = x(s-1)^2 e_{\mathbf{q}}\mathrm{Im}g_0(e_{\mathbf{q}}) \tag{4.11a}$$

$$= x(s-1)^2\pi K_d(aq)^{d-1} . \tag{4.11b}$$

Here we obtain a much larger damping rate than in the previous case because the spin fluctuations when $s \neq 1$ give rise to an anomaly in $\chi_\perp$. Also, for $d = 2$ we see a divergence in Eq. (4.10) [due to the presence of $g_0(0)$] whereas in case I there is no such divergence. We defer further discussion of the results in Eqs. (4.10)–(4.11b) until after treating case III, the results of which provide an explanation for the distinction between cases I and II.

We now proceed to case III, where $s \neq 1$ and $x_A \neq x_B$. To avoid undue algebra we will simplify this case by taking $js = 1$. This gets rid of the p-wave scattering and simplifies many of the expressions. For $js = 1$ we find

$$\sigma_{\alpha,\alpha}(\mathbf{q},e) = \frac{s-1}{2s^2D(e)D(-e)}\{x_B sD(e) - x_A sD(-e) - e_{\mathbf{q}}[x_A sD(-e) + x_B sD(e)]\}, \tag{4.12a}$$

$$\sigma_{\beta,\beta}(\mathbf{q},e) = \frac{s-1}{2s^2D(e)D(-e)}\{-x_B sD(e) + x_A sD(-e) - e_{\mathbf{q}}[x_A sD(-e) + x_B sD(e)]\}, \tag{4.12b}$$

$$\sigma_{\alpha,\beta}(\mathbf{q},e) = -\sigma_{\beta,\alpha}(\mathbf{q},e) = \frac{(s-1)\gamma_{\mathbf{q}}}{2s^2D(e)D(-e)}[x_A sD(-e) - x_B sD(e)] \,, \tag{4.12c}$$

where $sD(e) = 1+(s-1)e(1+e)g_0(e)$ for $js = 1$. The elementary excitations are given by the poles of the Green's function which occur at

$$[e - e_{\mathbf{q}} - \sigma_{\alpha,\alpha}(e)][-e - e_{\mathbf{q}} - \sigma_{\beta,\beta}(e)] - \sigma_{\alpha,\beta}(e)\sigma_{\beta,\alpha}(e) = 0 \,. \tag{4.13a}$$

Using the evaluations in Eqs. (4.12a)–(4.12c) we write this as

$$-e^2 + A_1 e + A_2 e_q^2 = 0 \,, \tag{4.13b}$$

where

$$A_1 = (x_B - x_A)(s-1)\left(\frac{x_B sD(e) - x_A sD(-e)}{s^2D(e)D(-e)(x_B - x_A)}\right), \tag{4.14a}$$

$$A_2 = \left(1 - \frac{x_A(s-1)}{sD(e)}\right)\left(1 - \frac{x_B(s-1)}{sD(-e)}\right) . \tag{4.14b}$$

We now analyze the situation at low energy. In that case, it suffices to keep terms in A_1 or A_2 up to order $eg_0(e)$. Then we get

$$-e^2[1 - 2x(s-1)^2 g_0(e)] - e(x_A - x_B)(s-1) + e_{\mathbf{q}}^2[1 - 2x(s-1) + (s-1)^2(x_A - x_B)eg_0(e)] = 0 \,. \tag{4.15}$$

We thereby get two roots. For the optical mode we do not calculate the damping. For it we find

$$e_{\mathrm{opt}}(\mathbf{q}) = (x_B - x_A)(s-1) + O(q^2) \,. \tag{4.16a}$$

For the acoustic mode we give both the dominant real and imaginary parts of the energy:

$$e_{\mathrm{ac}}(\mathbf{q}) = \frac{e_{\mathbf{q}}^2}{(x_A - x_B)(s-1)} + i\Gamma_{\mathbf{q}} \tag{4.16b}$$

with

$$\Gamma_{\mathbf{q}} = e^2 \mathrm{Im} g_0(e)\left[(s-1)^2(x_A - x_B) + \frac{2x(s-1)}{(x_A - x_B)}\right] . \tag{4.16c}$$

Here, in contrast to Rayleigh scattering in the ferromagnet [see Eq. (2.39)] with a low concentration of defects, we find an imaginary part of order $e^d \sim q^{2d}$, since $\mathrm{Im}g_0(e) \sim e^{d-2}$ and $e \sim q^2$. To recover the results for Rayleigh scattering in a ferromagnet, we no doubt have to work to higher order in the defect concentration x, since a ferromagnet involves coherent ordering of magnetic moments.

Finally, we should point out that our results in Eqs. (4.16a)-(4.16c) follow the expectations of Ref. 22 where the normal mode equation,

$$2Aq^2 + Me/(\hbar\gamma) + \chi_\perp[e/(\hbar\gamma)]^2 = 0 \,, \tag{4.17}$$

was obtained, where here γ denotes the gyromagnetic ratio of the spins, and A is the helicity modulus, which is proportional to the conductivity of the analog resistor network. Our result in Eq. (4.15) agrees with Eq. (4.17). To verify this use Eq. (B15) for $\chi_\perp$ and note that when $js = 1$, $A(x)/A(0) = 1$.

Now we return to a further discussion of the results for case II given in Eqs. (4.10)–(4.11b). Considering also Eq. (4.12a) we see that $\mathrm{Re}\sigma_{\alpha,\alpha}(\mathbf{q}, e_{\mathbf{q}})$ is of order $x_B - x_A$ at long wavelength. This indicates that unless $x_A = x_B$ scattering at long wavelength is large. This can be seen explicitly in Eq. (3.20): when $s \neq 1$ the scattering matrix element is of order $\sqrt{e_{\mathbf{q}}/e_{\mathbf{q}'}}$. An estimate analogous to that in Eq. (4.8) would give in this case

$$\mathrm{Im}e_{\mathbf{q}} \sim \int d\mathbf{q}'\delta(e_{\mathbf{q}} - e_{\mathbf{q}'}) \sim q^{d-1} \tag{4.18a}$$

and

$$\mathrm{Re}e_{\mathbf{q}} \sim \sqrt{e_{\mathbf{q}}/e_{\mathbf{q}}} = 1 \,. \tag{4.18b}$$

The strong scattering reflects the fact that when defects occur on only one sublattice, they give rise to an optical mode at nonzero frequency as given in Eq. (4.16a). This strong scattering has no analog in the ferromagnet. Nor does it happen in the antiferromagnet when $s = 1$.

But now we have to take account of the fact that in case II defects occur with equal probability on both sublattices. It is possible, and according to Eq. (4.12a) it does happen, that the real part of the energy shift has opposite signs for the two cases when the defect is on different sublattices. Thus the $\mathbf{q}$-independent energy shift, estimated in Eq. (4.18b), cancels out when $x_A = x_B$. In contrast, the scattering from incoherent scatterers cannot possibly cancel out. Thus the imaginary part of $e_{\mathbf{q}}$ is proportional to $(x_A + x_B)$, and the estimate of Eq. (4.18a) gives the correct dependence on wave vector. Furthermore, we see that for this case, ($s \neq 1$), only the s-wave scattering contributes, because the p-wave scattering gives a contribution to $\mathrm{Im}e_{\mathbf{q}}$ of order q^{d+1}. Another way of stating the physical difference between cases I ($S = S'$) and II ($S \neq S'$) is that in the former case the antiferromagnetic symmetry between sublattices is preserved in each unit cell, whereas in the latter case the antiferromagnetic symmetry is only preserved on the average. The fluctuations which locally destroy the antiferromagnetic sym-

metry tend to create a local gap which, when $x_A \neq x_B$, evolves into a true optical mode. This strong scattering only occurs when $S \neq S'$.

Finally, we should compare the present results with previously derived ones. We should emphasize that the result of EJ,[29] namely that $\mathrm{Im}e_{\mathbf{q}} \sim q^{d+1}$ was obtained only for the vacancy case, i.e., for $s = 0$, to which our result in Eqs. (4.11a) and (4.11b) applies. It is not clear why they got the result they did, because their formalism is closely related to ours, since it involves the equations of motion of spin operators directly. On the other hand, the later single-defect results of KH do agree with the present ones, where they overlap, i.e., for the vacancy case. There it was explicitly pointed out that there was a logarithmic divergence in ρ of Eq. (4.3b) for $d = 2$ for the vacancy case. We note that this divergence occurs when $s \neq 1$ and is identified with a divergence in the uniform susceptibility when $s \neq 1$. It seems that some recent work[34] is unaware of this divergence. In that reference numerical results for $d = 2$ are used to estimate ρ in Eq. (4.3b) to be approximately 3, whereas we know that the exact result corresponds to $\rho = \infty$. It has been suggested (KH) that this divergence results in an overdamped spin wave in the long-wavelength limit. A definitive analysis of the result of this divergence may require treating terms of higher order in x, which we do not consider here. We now know that for $d < 4$ the antiferromagnetically ordered phase is unstable[41] with respect to the application of an infinitesimal random field. In the present case this result applies because random dilution of an AFH in a uniform field gives rise to a random staggered field.[42] Within the low concentration expansion we only see this anomaly for $d = 2$. There seem not to be previous calculations of the damping due exclusively to a force constant defect, i.e., for our case I, where $s = 1$. There one has very weak scattering which is comparable to that in the ferromagnet and then one has $\mathrm{Im}e_{\mathbf{q}} \sim q^{d+1}$.

In the remainder of this section, we would like to remark on some extensions of our theory. We first point out that our result for the damping of spin wave due to vacancies also applies to the case of bond dilution. However, for bond dilution the calculations would be much more difficult. Consider a system with a concentration p of randomly removed bonds. To low order in p removing bonds does not remove a spin, so in low order results analogous to case I will be found. However, at order p^z one will begin to see the effects of removing a site, when all its z neighboring bonds happen to be removed. At this level, results characteristic of case II will appear. Thus, for bond dilution we expect the damping at small p to be of the form

$$\Gamma(q,p) \sim pC_1(p)q^{d+1} + \cdots + C_z p^z q^{d-1} , \tag{4.19}$$

where C_n is a constant. Therefore at small enough q, the q^{d-1} damping will dominate. Thus the q^{d-1} damping is a general feature for diluted AFH systems.

Secondly, based on our calculation, the dynamical scaling theory for the AFH system by Christou and Stinchcombe[33] (CS) has to be modified. The CS theory was based on the calculation by EJ (Ref. 29) which, as we have pointed out, incorrectly gives q^{d+1} damping. To apply our result to the scaling properties, we will use a simpler approach than that of CS. The dispersion relation for the antiferromagnetic case is

$$\omega(q) = c(x)q + i\gamma(x)q^{d-1} , \tag{4.20}$$

where $c(x)$ can be expressed as

$$c(x) = \sqrt{\frac{A(x)}{\chi_\perp(x)}} , \tag{4.21}$$

where $A(x)$ is the DC conductivity, and $\chi_\perp(x)$ the transverse susceptibility. Near the percolation threshold at x_c these scale as follows:

$$\begin{aligned} A(x) &\sim (x - x_c)^t \sim \xi^{-\frac{t}{\nu}} , \\ \chi_\perp(x) &\sim (x - x_c)^\tau \sim \xi^{\frac{\tau}{\nu}} , \end{aligned} \tag{4.22}$$

where ξ is the correlation length, and according to HK, τ can be expressed as $\tau = t - \beta - (d-2)\nu$. We then apply the dynamic scaling principle of Halperin and Hohenberg,[20] in order to get a relation consistent with (4.20). Thus, omitting amplitude factors we write

$$\omega(q) = q^z f(q\xi) = q^z(q^{1-z}\xi^{1-z} + iq^{d-1-z}\xi^{d-1-z}) . \tag{4.23}$$

Comparing this with Eqs. (4.20) and (4.21) we get

$$z = 1 + \frac{t+\tau}{2\nu} = 1 + \frac{2t - \beta - (d-2)\nu}{2\nu} , \tag{4.24}$$

so we find the same relation for z as did CS. The scaling for the damping rate is therefore found to be

$$\gamma(\xi) \sim \xi^{d-2-\frac{2t-\beta-(d-2)\nu}{2\nu}} . \tag{4.25a}$$

As in the CS paper, we can go further to write

$$\Gamma(q,\xi) \propto (x - x_c)^{-\mu} q^{d-1} , \tag{4.25b}$$

where $\mu = (d-2)\nu - 1/2[2t - \beta - (d-2)\nu]$ which differs from the CS result $\mu = d\nu - 1/2[2t - \beta - (d-2)\nu]$.

V. STATIC AND LOW-FREQUENCY PROPERTIES

In this section we will apply our results for the various low-frequency and static properties. First we consider the zero–point motion induced by the defect.

We first consider the total moment on the A sublattice, when there is a single defect located somewhere on the A sublattice. This quantity is given by

$$S_A^z = NS + (S' - S) - \sum_{\mathbf{R}} \langle a_{\mathbf{R}}^\dagger a_{\mathbf{R}} \rangle \tag{5.1a}$$

$$= NS + (S' - S) - \sum_{\mathbf{k}} [l_{\mathbf{k}}^2 \langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} \rangle + m_{\mathbf{k}}^2 \langle \beta_{-\mathbf{k}} \beta_{-\mathbf{k}}^\dagger \rangle - l_{\mathbf{k}} m_{\mathbf{k}} (\langle \alpha_{\mathbf{k}}^\dagger \beta_{-\mathbf{k}}^\dagger \rangle + \langle \beta_{-\mathbf{k}} \alpha_{\mathbf{k}} \rangle)] . \tag{5.1b}$$

We will separate this into various terms. First there are the terms which occur in the absence of defects. Then there is the static effect of the defect embodied in the term $S' - S$. Finally there are contributions due to modifications in the zero-point fluctuations due to the defect. To isolate such terms we write

$$\langle \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \rangle = \int_{-\infty}^{\infty} \frac{de}{\pi} \frac{1}{(e^{2JzSe/(kT)} - 1)} \mathrm{Im} g_{\alpha,\alpha}(\mathbf{k}, \mathbf{k}; e - i0^+) , \tag{5.2}$$

where T is the temperature, and we use

$$g_{\alpha,\alpha}(\mathbf{k}, \mathbf{k}, e) = \frac{1}{e - e_{\mathbf{k}}} + \left(\frac{1}{e - e_{\mathbf{k}}} \right)^2 t_{\alpha,\alpha}(\mathbf{k}, \mathbf{k}; e) . \tag{5.3}$$

Obviously, the contribution from the first term represents fluctuations in the absence of the defect, whereas the second is due to the presence of a single defect. In the zero-temperature limit, we have

$$\langle \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \rangle = - \int_{-\infty}^{0} \frac{de}{\pi} \mathrm{Im} g_{\alpha,\alpha}(\mathbf{k}, \mathbf{k}; e - i0^+) . \tag{5.4}$$

We denote the contribution to the zero-point motion due to fluctuations caused by the defect ΔS, so that $S_A^z = S_A^z(0) + S' - S - \Delta S$, where $S_A^z(0)$ is the value of S_A^z in the pure system. Then

$$\Delta S = -\frac{1}{N} \sum_{\mathbf{k}} \int_{-\infty - i0^+}^{-i0^+} \frac{de}{\pi} \mathrm{Im} \left[\frac{l_{\mathbf{k}}^2}{(e - e_{\mathbf{k}})^2} [\underline{\sigma}_A(\mathbf{k}; e)]_{\alpha,\alpha} + \frac{m_{\mathbf{k}}^2}{(e + e_{\mathbf{k}})^2} [\underline{\sigma}_A(\mathbf{k}; e)]_{\beta,\beta} + \frac{l_{\mathbf{k}} m_{\mathbf{k}}}{(e^2 - e_{\mathbf{k}}^2)} [\underline{\sigma}_A(\mathbf{k}; e)]_{\alpha,\beta} + \frac{l_{\mathbf{k}} m_{\mathbf{k}}}{(e^2 - e_{\mathbf{k}}^2)} [\underline{\sigma}_A(\mathbf{k}; e)]_{\beta,\alpha} \right] . \tag{5.5}$$

Here we noted that the diagonal (in wave vector) $\underline{t}$ matrix is given in terms of results written in Eqs. (3.33a)-(3.33d): $t_{\alpha,\alpha}(\mathbf{q}, \mathbf{q}, e) = \sigma_{\alpha,\alpha}(\mathbf{q}, e)$. Also, in Eq. (5.5) $\underline{\sigma}_A(\mathbf{k}; e)$ is the self-energy when the defect is on the A sublattice, whose symmetry-adapted components are given in Eqs. (3.24a)-(3.24c), (3.29a), and (3.29b). We decompose the contributions in Eq. (5.5) into those from s-wave scattering and non-s-wave scattering, indicated by a subscript. Thus we write the contribution involving s-wave scattering as

$$\Delta S_s = - \int_{-\infty - i0^+}^{-i0^+} \frac{1}{N} \sum_{\mathbf{k}} \mathrm{Im} \left[\frac{l_{\mathbf{k}}^4 \phi_1(\mathbf{k})}{(e - e_{\mathbf{k}})^2} + \frac{m_{\mathbf{k}}^4 \phi_2(\mathbf{k})}{(e + e_{\mathbf{k}})^2} + \frac{l_{\mathbf{k}}^2 m_{\mathbf{k}}^2 [\phi_1(\mathbf{k}) + \phi_2(\mathbf{k})]}{(e^2 - e_{\mathbf{k}}^2)} \right] \frac{e_{\mathbf{k}}}{D(e)} \frac{de}{\pi} \tag{5.6}$$

and that due to non-s-wave symmetry to be

$$\Delta S_{\mu} = - \int_{-\infty - i0^+}^{-i0^+} \frac{de}{\pi} \frac{1}{N} \sum_{\mathbf{k}} l_{\mathbf{k}}^2 m_{\mathbf{k}}^2 \times \mathrm{Im} \left[\frac{1}{(e - e_{\mathbf{k}})^2} + \frac{1}{(e + e_{\mathbf{k}})^2} - \frac{2}{(e^2 - e_{\mathbf{k}}^2)} \right] \frac{(js - 1)\phi^{(\mu)}(\mathbf{k})^2}{z - (1 - e)(js - 1) g^{(\mu)}(e)} , \quad \mu \neq s . \tag{5.7}$$

Thus

$$\Delta S_{\mu} = - \int_{-\infty - i0^+}^{-i0^+} \frac{de}{\pi} \mathrm{Im} \frac{1}{N} \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^2}{(e^2 - e_{\mathbf{k}}^2)^2} \frac{(js - 1)\phi^{(\mu)}(\mathbf{k})^2}{z - (1 - e)(js - 1) g^{(\mu)}(e)} , \quad \mu \neq s . \tag{5.8}$$

We should check the convergence of these expressions, as this will confirm the expected result that the lower dimension for the occurrence of long-range order in the presence of random dilution is $d_c = 1$. The integrals in Eqs. (5.6) and (5.8) are over the $(d + 1)$-dimensional manifold of momenta and frequency. Counting powers of momenta and frequency in the integrand of Eq. (5.6) yields three inverse powers. This result, taken at face value, would suggest a logarithmic divergence for $d = 2$. However, this apparently divergent term cancels out. To see this, we now consider the situation when the energy dependence of $D(e)$ is neglected. [The energy dependence of $D(e)$ would increase the power count we just made.] Also note that $\phi_1(\mathbf{k}) + \phi_2(\mathbf{k}) \sim e_{\mathbf{k}}$, so this term does not actually contribute in zeroth order in $e_{\mathbf{k}}$. Also the term in $(e - e_{\mathbf{k}})^{-2}$ has no imaginary part for negative e and therefore gives zero contribution. We are thus left with the term of order $m_{\mathbf{k}}^4$ in the integrand of Eq. (5.6) which yields

$$\mathrm{Im} \int_{-\infty - i0^+}^{-i0^+} \frac{de}{(e + e_{\mathbf{k}})^2} = -\mathrm{Im} \left[\frac{1}{e + e_{\mathbf{k}} - i0^+} \right]_{-\infty}^{0} = 0 . \tag{5.9}$$

So all the terms which appeared to lead to the divergence of ΔS for $d = 2$ actually vanish. Less dominant terms than those we just considered cause a divergence at $d = 1$.

We now analyze these expressions using the $1/z$ expansion.[36] Roughly speaking, this expansion is obtained by expanding momentum–dependent quantities in powers of $\gamma_{\mathbf{k}}$. To leading order in $1/z$ we drop the corrections of order unity to the denominator in the last factor of Eq. (5.8) and we set $e_{\mathbf{k}}^2 = 1 - \gamma_{\mathbf{k}}^2 \approx 1$. Also we use $N^{-1}\sum_{\mathbf{k}} \gamma_{\mathbf{k}}^2 = 1/z$ and

$$\sum_{\mu} \phi^{(\mu)}(\mathbf{k})^2 = 2z(1-\gamma_{\mathbf{k}}) \tag{5.10a}$$

so that

$$\sum_{\mu\neq s} \phi^{(\mu)}(\mathbf{k})^2 = z(1-\gamma_{\mathbf{k}}^2)\,. \tag{5.10b}$$

Thus to leading order in $1/z$ we have

$$\sum_{\mu\neq s} \Delta S_\mu = -\int_{-\infty-i0^+}^{-i0^+} \frac{de}{\pi}\frac{js-1}{z}\mathrm{Im}\frac{1}{(e+1)^2}\frac{1}{(e-1)^2}\,. \tag{5.11}$$

The integral is easily done using $\mathrm{Im}(x-i0^+)^{-1} = \pi\delta(x)$. Thus we have to leading order in $1/z$

$$\sum_{\mu\neq s} \Delta S_\mu = -\frac{js-1}{4z}\,. \tag{5.12}$$

Proceeding similarly, we have the s-wave contribution as

$$\Delta S_s = -\int_{-\infty-i0^+}^{-i0^+} \mathrm{Im}\frac{de}{\pi D(e)}\left[\frac{js-1}{N}\sum_{\mathbf{k}}\frac{(e+e_{\mathbf{k}}^2)^2}{(e^2-e_{\mathbf{k}}^2)^2} + \frac{j(1-s)}{N}\sum_{\mathbf{k}}\frac{(e+e_{\mathbf{k}}^2)(e+1)}{(e^2-e_{\mathbf{k}}^2)^2}\right]. \tag{5.13}$$

Here we have

$$\frac{js-1}{N}\sum_{\mathbf{k}}\frac{(e+e_{\mathbf{k}}^2)^2}{(e^2-e_{\mathbf{k}})^2} = \frac{js-1}{N}\sum_{\mathbf{k}}\frac{(e+1-\gamma_{\mathbf{k}}^2)^2}{(e^2-1+\gamma_{\mathbf{k}}^2)^2} \tag{5.14a}$$

$$\approx \frac{js-1}{(e-1)^2}\left[1-\frac{2}{z(e+1)}-\frac{2}{z(e^2-1)}\right] \tag{5.14b}$$

and

$$\frac{j(1-s)}{N}\sum_{\mathbf{k}}\frac{(e+e_{\mathbf{k}}^2)(e+1)}{(e^2-e_{\mathbf{k}}^2)^2} = \frac{j(1-s)(1+e)}{N}\sum_{\mathbf{k}}\frac{e+1-\gamma_{\mathbf{k}}^2}{(e^2-1+\gamma_{\mathbf{k}}^2)^2} \tag{5.15a}$$

$$= \frac{j(1-s)}{(e-1)^2}\left[1-\frac{1}{z(e+1)}-\frac{2}{z(e^2-1)}\right]. \tag{5.15b}$$

Also we need the $1/z$ expansion of $D(e)$. For this purpose we write

$$g_0(e) = \sum_{\mathbf{k}}\frac{1}{e^2-1+\gamma_{\mathbf{k}}^2} = \frac{1}{(e^2-1)} - \frac{1}{z(e^2-1)^2} + O(z^{-2})\,. \tag{5.16}$$

This result makes evident the nature of the $1/z$ expansion. The first term replaces the density of states (without defects) by two δ functions at $e = \pm 1$. Subsequent terms contain corrections which effectively give a finite width to the density of states. Using Eq. (5.16) we obtain the desired expansion:

$$D(e) = \frac{j-e}{1-e}\left[1+\frac{e}{z(1-e^2)}-\frac{ejs}{z(j-e)(1+e)}\right]. \tag{5.17}$$

Using these results we find that

$$\Delta S_s = -\frac{1}{4z}\left[\frac{j-1}{j+1}\left(1-\frac{2js}{j+1}\right)-\frac{2(js-1)}{j+1}\right]. \tag{5.18}$$

Combining Eqs. (5.12) and (5.18) we get the full result

$$\Delta S = -\frac{js(j-1)^2}{4z(j+1)^2}\,. \tag{5.19}$$

This shows that for vacancies ($s = 0$), the effect of zero-point defect fluctuations is of order $(1/z)^2$, at least, as was found some time ago by Kumar.[31]

Next we consider the dependence of the zero-point motion on distance from the defect. However, since this analysis is rather technical, it is relegated to Appendix C. There we obtain the result

$$\Delta S(\mathbf{r}) \sim r^{(-2d+1)} , \tag{5.20}$$

where we assume that the observation point a distance $\mathbf{r}$ ($r \gg a$) from the defect and the defect are both on the same sublattice. This analysis was done explicitly for vacancies, but it probably holds generally for the type of defects considered in this paper.

Next we study the density of states for spin deviations. For different applications one might consider different definitions of the density of states. Here we will evaluate

$$\rho(e) = \frac{1}{\pi}\sum_{\mathbf{k}} \mathrm{Im} g_{\alpha,\alpha}(\mathbf{k},\mathbf{k};e-i0^+) \tag{5.21}$$

for low energies. In fact what we should evaluate is the term linear in the concentration of defects, and we treat here only the case $x_a = x_B = x$. Thus we write

$$\rho(e) = \rho_0(e) + x\rho^{(1)}(e) . \tag{5.22}$$

Since defects contribute independently to $\rho^{(1)}$, we have

$$\rho^{(1)}(e) = \frac{1}{\pi}\sum_{\mathbf{k}} \mathrm{Im}\frac{1}{(e-e_{\mathbf{k}}-i0^+)^2}\sigma_{\alpha,\alpha}(\mathbf{k};e-i0^+)_{x_A=x_B=1} . \tag{5.23a}$$

We start with the s-wave contribution, which is denoted $\rho_s^{(1)}(e)$:

$$\rho_s^{(1)}(e) = \frac{1}{2\pi}\sum_{\mathbf{k}} \mathrm{Im}\left\{\frac{e_{\mathbf{k}}}{(e-e_{\mathbf{k}})^2}\left[\left(\frac{1}{D(e)}+\frac{1}{D(-e)}\right)[j(1-s)+(js-1)]\right.\right.$$
$$\left.\left.+\left(\frac{1}{D(e)}-\frac{1}{D(-e)}\right)\left(\frac{j(1-s)}{e_{\mathbf{k}}}+(js-1)e_{\mathbf{k}}\right)\right]_{e=e-i0^+}\right\} . \tag{5.23b}$$

If we write $e_{\mathbf{k}} = (e_{\mathbf{k}}-e)+e$, we can express the sums over $\mathbf{k}$ in terms of $g_0(e)$ and $f_0(e)$, where

$$f_0(e) = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{e-e_{\mathbf{k}}} . \tag{5.24}$$

To leading order in e we obtain

$$\pi\rho_s^{(1)}(e) = \frac{(1-j)}{j}\left(f_0(e)'' + e\frac{df_0(e)''}{de}\right) + e\left(\frac{(js-1)}{j}+(s-1)g_0(e)'\right)\left((1-s)\frac{df_0(e)''}{de}\right)$$
$$-eg_0(e)''\left(\frac{s-1}{j}\right)[(js-1)-j(1-s)df_0(e)'/de] , \tag{5.25}$$

where the prime indicates the real part and the double prime the imaginary part. Now, of course, $f_0(e)''$ is only nonzero for positive energy, e. But $g_0(e)''$ is an odd function of e, which for positive energy obeys

$$2eg_0(e)'' = f_0(e)'' . \tag{5.26a}$$

Also

$$df_0(e)'/de = g_0(e)' . \tag{5.26b}$$

For most applications we combine the positive and negative energy spectral weight:

$$\pi[\rho_s^{(1)}(e)-\rho_s^{(1)}(-e)] = \frac{(1-j)}{j}f_0(e)'' + e\frac{d[f_0(e)'']}{de}\left(\frac{s}{j}+s-1-s^2-(s-1)^2g_0(e)'\right) . \tag{5.27}$$

(Thermodynamic properties involve the negative of the spectral weight at negative energy.)

Next we include the non-s-wave contributions. For $\mu \neq s$, we have

$$\pi\rho_\mu^{(1)}(e) = \mathrm{Im}\left[\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{(e-e_{\mathbf{q}})^2}\{[\sigma_A^{(\mu)}(\mathbf{q};e)]_{\alpha,\alpha}+[\sigma_B^{(\mu)}(\mathbf{q};e)]_{\alpha,\alpha}\}\right]_{e=e-i0^+,x_A=x_B=1} . \tag{5.28}$$

For small e we may write this as

$$\pi\rho_\mu^{(1)}(e) = \mathrm{Im}\frac{1}{N}\sum_{\mathbf{q}}\frac{\phi^{(\mu)}(\mathbf{q})^2}{(e-e_{\mathbf{q}})^2}(l_{\mathbf{q}}^2+m_{\mathbf{q}}^2)\frac{(js-1)}{z-(js-1)g^{(\mu)}(e)} . \tag{5.29}$$

This can be written as the sum of two terms, the first taking the imaginary part of $(e-e_{\mathbf{q}})^2$, the second the imaginary part of $g^{(\mu)}(e)$. The second term can be dropped because it is of order $e^2 g_0(e)''$, as shown in Eqs. (4.6a), (4.6b), and(4.6c). So we have

$$\pi\rho_{\mu}^{(1)}(e) = \frac{js-1}{z-(js-1)g^{(\mu)}(0)'}\mathrm{Im}\frac{1}{N}\sum_{\mathbf{q}}\frac{\phi^{(\mu)}(\mathbf{q})^2}{e_{\mathbf{q}}(e-e_{\mathbf{q}})^2}\ . \tag{5.30}$$

The integrand only contributes an imaginary part for $e_{\mathbf{q}}$ near e. There $\phi^{(p)}(\mathbf{q})^2 = ze_{\mathbf{q}}^2$. Non-$p$-wave contributions can be neglected henceforth, since they are higher order in e. So

$$\pi\rho_{p}^{(1)}(e) = \frac{(js-1)}{z-(js-1)g^{(p)}(0)'}\frac{z}{N}\mathrm{Im}\sum_{\mathbf{q}}\frac{e_{\mathbf{q}}}{(e-e_{\mathbf{q}})^2} \tag{5.31a}$$

$$= -\frac{z(js-1)}{z-(js-1)g^{(p)}(0)'}\frac{d[ef_0(e)']}{de}\ . \tag{5.31b}$$

Thus in all we have

$$\pi[\rho^{(1)}(e)-\rho^{(1)}(-e)] = A_1 f_0(e)'' + A_2 e d f_0(e)''/de\ , \tag{5.32}$$

where

$$A_1 = \frac{(1-j)}{j} - \frac{z(js-1)}{z-(js-1)g^{(p)}(0)'}\ , \tag{5.33a}$$

$$A_2 = \frac{s}{j} + s - 1 - s^2 - (s-1)^2 g_0(e)' - \frac{z(js-1)}{z-(js-1)g_p(0)'}\ . \tag{5.33b}$$

Note that A_2 is identical with the constant ρ defined in Eq. (4.3b), and which is evaluated explicitly in Eq. (4.10).

We discuss briefly the meaning of this result. To order x we may write

$$\pi[\rho(e)-\rho(-e)] = (1+xA_1)f_0\left(\frac{e}{1+\rho x}\right)''\ , \tag{5.34}$$

where $1+\rho x$ to this order is $\sqrt{[A(x)\chi_{\perp}(0)]}/[\sqrt{[A(0)\chi_{\perp}(x)]}$. This result suggests that it is correct to view dilution as simply renormalizing the energy [as in Eq. (4.3b)] and the oscillator strength of the spin waves. However, this idea cannot be totally correct because there are contributions to the low–energy density of states from large q spin waves. An alternative way to obtain the above results is to consider the spectral weight for each value of $\mathbf{q}$ and sum over $\mathbf{q}$. In that approach the density of states for small e has contributions (a) from spin waves with $e_{\mathbf{q}} \approx e$ and (b) from spin waves with arbitrary $\mathbf{q}$. These latter contributions must be kept in order to obtain the result given in Eqs. (5.33a) and (5.33b). This observation suggests that to higher order in x the low-energy density of states may not be expressible in terms of the static magnetic elastic constants, as we were able to do at first order in x in Eq. (5.34).

In the following, we show briefly how one discusses the effect on local modes of mixing with extended states. This treatment will lead to shifts relative to the single-defect bound state energies as given for the antiferromagnet, for instance, by Tonegawa.[27] For simplicity, in the following example we consider the ferromagnetic case and suppose there exists only one local mode at frequency ω_l. Then the boson Green's function can be written

$$G(q,\omega) = \frac{1}{\omega-\omega_q - x\frac{\sigma(q,\omega)}{\omega-\omega_l}} \tag{5.35a}$$

$$= \frac{\omega-\omega_l}{(\omega-\omega_q)(\omega-\omega_l)-x\sigma(q,\omega)} \tag{5.35b}$$

which can be factorized as

$$G(q,\omega) = \frac{\omega-\omega_l}{(\omega-\omega_1)(\omega-\omega_2)}\ , \tag{5.36}$$

where $\lim_{q\to 0}\omega_1(q) = \text{const} \times q$ and $\omega_2 = \omega_l + xC(q)$. In this way we obtain the spin-wave pole discussed above and also the pole shifted away from the local excitation energy given by Tonegawa.[27]

VI. CONCLUSION

In this paper we have studied the quantum Heisenberg antiferromagnet in d spatial dimensions at zero temperature in the presence of defect sites. We have allowed the defects to have arbitrary spin and coupling constant to the neighbor host sites. We treat the low concentration limit, but for some applications we allow the concentration of defects x to be different on the two sublattices, A and B. Thus we do not necessarily require $x_A = x_B$. Of course, when $x_A \neq x_B$ we are dealing with a ferrimagnet.

Our principle results are as follows.

(1) Our treatment is sufficient to obtain dispersion relations for the case when $x_A \neq x_B$ which lead to a ferromagnetic acoustic mode and an optical mode, both of whose frequencies agree with the predictions of continuum theory. Also, the damping of the acoustic mode agrees with that obtained in a ferromagnet with a low concentration of vacancies.

(2) In the case when $x_A = x_B$ but the defect spin is different from that of the host, one has locally broken symmetry, so that one can view the modes as being locally those of a ferrimagnet. This indicates that the scattering is strong in this case. We find the scattering matrix element to be of order unity [for details see Eq. (3.20)] and consequently the damping of spin waves of wave vector $\mathbf{q}$ to be of order q^{d-1}, in agreement with a Golden Rule estimate.

(3) For the case when the defect spin is the same as that of the host, the scattering matrix element, given in Eq. (3.20), vanishes in the long-wavelength limit, and the damping is of order q^{d+1}. As long as $x_A = x_B$, the real part of the energy is given in agreement with continuum theory in terms of the perpendicular susceptibility, $\chi_\perp$, and the helicity modulus, A.

(4) We show that the local density of states is also related to the static elastic constants, $\chi_\perp$ and A. However, the density of states has non-negligible contributions even from large wave vectors.

(5) The total zero-point spin deviation attributable to the defect, ΔS, is shown to be finite for $d > 1$. To lowest order in $1/z$, where z is the coordination number, ΔS is found to be proportional to the spin on the defect site. For a vacancy, the fact that a spin is missing reduces the zero-point perturbation due to the missing S_+S_- terms, but the zero-point fluctuation is increased due to the decrease in the local excitation energy near the defect. A more accurate calculation would probably show that, in three dimensions, the zero-point motion scales with dilution as the mean field transition temperature.

(6) We find that the spin deviation field around a defect falls off as r^{-2d+1}, where r is the distance from the defect.

(7) Although we give no calculations, our formulation does enable one to calculate [via Eqs. (5.35a) and (5.35b)] the shift in the local mode energies due to interaction with the spin-wave continuum.

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APPENDIX A: VERTEX FUNCTION

In this appendix we relate the spin susceptibility to the boson Green's functions. We start by defining the matrix $\underline{H}$ by

$$\underline{H} = \frac{1}{2S}\begin{bmatrix} \langle\langle S^+_{\mathbf{r}\in A}; S^-_{\mathbf{r}'\in A}\rangle\rangle_e & \langle\langle S^+_{\mathbf{r}\in A}; S^-_{\mathbf{r}'\in B}\rangle\rangle_e \\ \langle\langle S^+_{\mathbf{r}\in B}; S^-_{\mathbf{r}'\in A}\rangle\rangle_e & \langle\langle S^+_{\mathbf{r}\in B}; S^-_{\mathbf{r}'\in B}\rangle\rangle_e \end{bmatrix} . \tag{A1}$$

In view of Eqs. (3.12a) and (3.12b) we write

$$S^+_{\mathbf{r}\in A} = \sqrt{2S}a_{\mathbf{r}}, \tag{A2a}$$

$$S^+_{\mathbf{r}\in B} = \sqrt{2S}b^\dagger_{\mathbf{r}}, \tag{A2b}$$

$$S^-_{\mathbf{r}\in A} = \sqrt{2S}a^\dagger_{\mathbf{r}}[1 + (s-1)\epsilon(\mathbf{r})], \tag{A2c}$$

$$S^-_{\mathbf{r}\in B} = \sqrt{2S}b_{\mathbf{r}}[1 + (s-1)\epsilon(\mathbf{r})] , \tag{A2d}$$

where $s = S'/S$ and $\epsilon(\mathbf{r})$ is unity if a defect is at site $\mathbf{r}$ and is zero otherwise. We define the analogous boson Green's functions by

$$\underline{G}(\mathbf{r},\mathbf{r}') = \begin{bmatrix} \langle\langle a_{\mathbf{r}\in A}; a^+_{\mathbf{r}'\in A}\rangle\rangle_e & \langle\langle a_{\mathbf{r}\in A}; b_{\mathbf{r}'\in B}\rangle\rangle_e \\ \langle\langle b^+_{\mathbf{r}\in B}; a^+_{\mathbf{r}'\in A}\rangle\rangle_e & \langle\langle b^+_{\mathbf{r}\in B}; b_{\mathbf{r}'\in B}\rangle\rangle_e \end{bmatrix} . \tag{A3}$$

Now use the t-matrix solution for the single-defect problem. Then

$$\underline{G}(\mathbf{r},\mathbf{r}') = \underline{G}^{(0)}(\mathbf{r},\mathbf{r}') + \sum_{\mathbf{R}} \epsilon(\mathbf{R}) \left[\underline{G}^{(0)}\underline{T}(\mathbf{R})\underline{G}^{(0)}\right](\mathbf{r},\mathbf{r}') , \tag{A4}$$

where $\underline{G}^{(0)}$ is the pure-system Green's function. Then

$$\underline{H}_{X,Y}(\mathbf{r},\mathbf{r}') = \left[\underline{G}^{(0)} + \sum_{\mathbf{R}} \epsilon(\mathbf{R})\underline{G}^{(0)}\underline{T}(\mathbf{R})\underline{G}^{(0)}\right]_{X,Y}(\mathbf{r},\mathbf{r}') \times [1 + (s-1)\epsilon(\mathbf{r}')] , \tag{A5}$$

where the subscripts X and Y assume the values 1 or A and 2 or B. After a configurational average this becomes, in Fourier transformed variables,

$$\underline{H}_{X,Y}(\boldsymbol{\lambda}) = [\underline{G}(\boldsymbol{\lambda})]_{X,Y}(\boldsymbol{\lambda})[1 + x_Y(s-1)] + x_Y(s-1)\frac{1}{N} \times \sum_{\mathbf{q}} \left[\underline{G}(\boldsymbol{\lambda})\underline{T}(Y;\boldsymbol{\lambda},\mathbf{q})\underline{G}^{(0)}(\mathbf{q})\right]_{X,Y} , \tag{A6}$$

where $\underline{T}(Y;\boldsymbol{\lambda},\mathbf{q})$ is the t-matrix when the defect is on sublattice Y. Thus

$$\underline{H}(\boldsymbol{\lambda}) = \underline{G}(\boldsymbol{\lambda})[\underline{I} + \underline{L}(\boldsymbol{\lambda})] , \tag{A7}$$

where $\underline{I}$ is the unit matrix and

$$\frac{[\underline{L}(\boldsymbol{\lambda})]_{X,Y}}{(s-1)x_Y} = \delta_{X,Y} + \frac{1}{N}\sum_{\mathbf{q}} \left[\underline{T}(Y;\boldsymbol{\lambda},\mathbf{q})\underline{G}^{(0)}(\mathbf{q})\right]_{X,Y} . \tag{A8}$$

From here on we drop the superscript (0) on $\underline{G}$. All subsequent Green's functions will be unperturbed ones.

Thus

$$[\underline{L}(\boldsymbol{\lambda})]_{X,A} = (s-1)x_A\delta_{X,A} + (s-1)\frac{x_A}{N}\sum_{\mathbf{q}}[\underline{T}(A;\boldsymbol{\lambda},\mathbf{q})\underline{G}(\mathbf{q})]_{X,A}\,, \tag{A9a}$$

$$[\underline{L}(\boldsymbol{\lambda})]_{X,B} = (s-1)x_B\delta_{X,B} + (s-1)\frac{x_B}{N}\sum_{\mathbf{q}}[\underline{T}(B;\boldsymbol{\lambda},\mathbf{q})\underline{G}(\mathbf{q})]_{X,B}\,. \tag{A9b}$$

We may think of $[\underline{L}]_{X,A}$ (or $[\underline{L}]_{X,B}$, respectively) as a two-component column vector which is the first (or second, respectively) column of the matrix $[\underline{L}]$.

It is important to understand the transformations between the A-B representation on the one hand and α-β on the other. We define the transformation which is used to express a and $b^\dagger$ in terms of α and $\beta^\dagger$:

$$\underline{U}(\boldsymbol{\lambda}) = \begin{bmatrix} l_{\boldsymbol{\lambda}} & -m_{\boldsymbol{\lambda}} \\ -m_{\boldsymbol{\lambda}} & l_{\boldsymbol{\lambda}} \end{bmatrix}. \tag{A10a}$$

Note that this matrix is symmetric, so we do not need to distinguish between it and its transpose. The inverse transformation is

$$\underline{U}(\boldsymbol{\lambda})^{-1} = \begin{bmatrix} l_{\boldsymbol{\lambda}} & m_{\boldsymbol{\lambda}} \\ m_{\boldsymbol{\lambda}} & l_{\boldsymbol{\lambda}} \end{bmatrix}. \tag{A10b}$$

If $\underline{g}$ denotes the matrix Green's function in the α-β representation, and $\underline{G}$ that in the A-B representation, then we have

$$\underline{g}(\boldsymbol{\lambda}) = \underline{U}(\boldsymbol{\lambda})^{-1}\underline{G}\underline{U}(\boldsymbol{\lambda})^{-1} \tag{A11a}$$

and

$$\underline{G}(\boldsymbol{\lambda}) = \underline{U}(\boldsymbol{\lambda})\underline{g}(\boldsymbol{\lambda})\underline{U}(\boldsymbol{\lambda})\,, \tag{A11b}$$

where

$$\underline{g}(\boldsymbol{\lambda}) = \begin{bmatrix} \frac{1}{e-e_{\boldsymbol{\lambda}}} & 0 \\ 0 & -\frac{1}{e+e_{\boldsymbol{\lambda}}} \end{bmatrix} \tag{A12a}$$

and

$$\underline{G}(\boldsymbol{\lambda}) = \begin{bmatrix} 1+e & -\gamma_{\boldsymbol{\lambda}} \\ -\gamma_{\boldsymbol{\lambda}} & 1-e \end{bmatrix}\frac{1}{e^2-e_{\boldsymbol{\lambda}}^2}\,. \tag{A12b}$$

Note that, on the other hand, the transformation properties of the potential are

$$\underline{V} = \underline{U}(\boldsymbol{\lambda})^{-1}\underline{v}\underline{U}(\boldsymbol{\lambda})^{-1} \tag{A13a}$$

and

$$\underline{v} = \underline{U}(\boldsymbol{\lambda})\underline{V}\underline{U}(\boldsymbol{\lambda})\,, \tag{A13b}$$

where $\underline{V}$ ($\underline{v}$) is the perturbation in the A-B (α-β) representation. For the pure system

$$\underline{V}(\boldsymbol{\lambda}) = \begin{bmatrix} 1 & \gamma_{\boldsymbol{\lambda}} \\ \gamma_{\boldsymbol{\lambda}} & 1 \end{bmatrix}, \tag{A14a}$$

$$\underline{v}(\boldsymbol{\lambda}) = \begin{bmatrix} e_{\boldsymbol{\lambda}} & 0 \\ 0 & e_{\boldsymbol{\lambda}} \end{bmatrix}, \tag{A14b}$$

$$\underline{t} = \underline{U}(\boldsymbol{\lambda})\underline{T}\underline{U}(\boldsymbol{\lambda})\,, \tag{A15}$$

where $\underline{T}$ ($\underline{t}$) is the configurationally averaged t-matrix in the A-B (α-β) representation.

Now

$$\frac{[\underline{L}]_{X,A}(\boldsymbol{\lambda})}{(s-1)x_A} = \delta_{X,A} + \frac{1}{N}\sum_{\mathbf{q}}[\underline{U}(\boldsymbol{\lambda})^{-1}\underline{t}(A;\boldsymbol{\lambda},\mathbf{q})\underline{U}(\mathbf{q})^{-1}\underline{U}(\mathbf{q})\underline{g}(\mathbf{q})\underline{U}(\mathbf{q})]_{X,A} \tag{A16a}$$

$$\equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{1}{N}\sum_{\mathbf{q}}[\underline{U}(\boldsymbol{\lambda})^{-1}\underline{t}(A;\boldsymbol{\lambda},\mathbf{q})\underline{g}(\mathbf{q})\underline{U}(\mathbf{q})]\begin{bmatrix} 1 \\ 0 \end{bmatrix}. \tag{A16b}$$

Similarly

$$\frac{[\underline{L}]_{X,B}(\boldsymbol{\lambda})}{(s-1)x_B} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \frac{1}{N}\sum_{\mathbf{q}}[\underline{U}(\boldsymbol{\lambda})^{-1}\underline{t}(B;\boldsymbol{\lambda},\mathbf{q})\underline{g}(\mathbf{q})\underline{U}(\mathbf{q})]\begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{A17}$$

Recall from Eqs. (3.19a)–(3.19f) that

$$\underline{t}(A,\boldsymbol{\lambda},\mathbf{q}) = \frac{e_{\boldsymbol{\lambda}}}{D(e)}\begin{bmatrix} l_{\boldsymbol{\lambda}} \\ m_{\boldsymbol{\lambda}} \end{bmatrix}\begin{bmatrix} l_{\mathbf{q}}\phi_1(\mathbf{q})\,, & m_{\mathbf{q}}\phi_2(\mathbf{q}) \end{bmatrix}, \tag{A18a}$$

$$\underline{t}(B,\boldsymbol{\lambda},\mathbf{q}) = \frac{e_{\boldsymbol{\lambda}}}{D(-e)}\begin{bmatrix} m_{\boldsymbol{\lambda}} \\ l_{\boldsymbol{\lambda}} \end{bmatrix}\begin{bmatrix} m_{\mathbf{q}}\phi_2(\mathbf{q})\,, & l_{\mathbf{q}}\phi_1(\mathbf{q}) \end{bmatrix}, \tag{A18b}$$

where $D(e)$ is given in Eq. (3.32).

To evaluate Eq. (A16b) note that

$$e_\lambda \underline{U}(\boldsymbol{\lambda})^{-1} \begin{bmatrix} l_\lambda \\ m_\lambda \end{bmatrix} = \begin{bmatrix} 1 \\ \gamma_\lambda \end{bmatrix} \tag{A19}$$

and to evaluate Eq. (A17) that

$$e_\lambda \underline{U}(\boldsymbol{\lambda})^{-1} \begin{bmatrix} m_\lambda \\ l_\lambda \end{bmatrix} = \begin{bmatrix} \gamma_\lambda \\ 1 \end{bmatrix} . \tag{A20}$$

Then we find that

$$\frac{[\underline{L}]_{X,A}(\boldsymbol{\lambda})}{(s-1)x_A} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \frac{K_+(e)}{D(e)} \begin{bmatrix} 1 \\ \gamma_\lambda \end{bmatrix} , \tag{A21a}$$

$$\frac{[\underline{L}]_{X,B}(\boldsymbol{\lambda})}{(s-1)x_B} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \frac{K_-(e)}{D(-e)} \begin{bmatrix} \gamma_\lambda \\ 1 \end{bmatrix} , \tag{A21b}$$

where

$$K_+(e) = \frac{1}{N} \sum_{\mathbf{q}} [\, l_{\mathbf{q}} \phi_1(\mathbf{q}) \,, \quad m_{\mathbf{q}} \phi_2(\mathbf{q}) \,] \left[\underline{g}^{(0)}(\mathbf{q}) \underline{U}(\mathbf{q}) \right] \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{A22}$$

and $K_-(e) = K_+(-e)$. Explicitly we have

$$K_+ = \frac{1}{N} \sum_{\mathbf{q}} \left[\frac{l_{\mathbf{q}}^2 \phi_1(\mathbf{q})}{e - e_{\mathbf{q}}} + \frac{m_{\mathbf{q}}^2 \phi_2(\mathbf{q})}{e + e_{\mathbf{q}}} \right] \tag{A23a}$$

$$= \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{e^2 - e_{\mathbf{q}}^2} \left[l_{\mathbf{q}}^2 \phi_1(\mathbf{q})(e + e_{\mathbf{q}}) + m_{\mathbf{q}}^2 \phi_2(\mathbf{q})(e - e_{\mathbf{q}}) \right] \tag{A23b}$$

$$= \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{e^2 - e_{\mathbf{q}}^2} \{ [j(1-s)[l_{\mathbf{q}}^2(e + e_{\mathbf{q}}) - m_{\mathbf{q}}^2(e - e_{\mathbf{q}})] + (js-1)e_{\mathbf{q}}[l_{\mathbf{q}}^2(e + e_{\mathbf{q}}) + m_{\mathbf{q}}^2(e - e_{\mathbf{q}})] \} \tag{A23c}$$

$$= \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{e^2 - e_{\mathbf{q}}^2} [j(1-s)(e+1) + (js-1)(e + e_{\mathbf{q}}^2)] \tag{A23d}$$

$$= \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{e^2 - e_{\mathbf{q}}^2} \{ (js-1)(e_{\mathbf{q}}^2 - e^2) + (1+e)[j(1-s) + e(js-1)] \} \tag{A23e}$$

$$= 1 - js + (1+e) g_0(e) [j(1-s) + e(js-1)] . \tag{A23f}$$

We can write the results in the form of Eq. (3.34) if we define

$$\tau(e) = \frac{K_+(e)}{D(e)} . \tag{A24}$$

APPENDIX B: HELICITY AND PERPENDICULAR SUSCEPTIBILITY

We will assume that the helicity for a ferromagnet is equivalent to the macroscopic conductivity, as expressed in Eq. (2.32). To evaluate this for a body–centered antiferromagnet, we will express the right-hand side of Eq. (2.32) and relate the result to the similar term in Eq. (4.11a). For a body-centered-cubic ferromagnet Eq. (2.32) gives

$$\frac{\Sigma^{\rm el}(x)}{\Sigma^{\rm el}(0)} = 1 + \frac{2xz(js-1)}{z - (js-1) g_F^p(0)} , \tag{B1}$$

where $g_F^p(0)$ is the p-wave Green's function for a ferromagnet. Recall that the symmetry-adapted function $\phi^{(\mu)}(\mathbf{q})$ is the same for both ferro- and antiferromagnets. We have

$$g_F^p(0) = \frac{1}{N} \sum_{\mathbf{q} \in \rm PZ} \frac{\phi^{(\mu)}(\mathbf{q})^2}{-1 + \gamma_{\mathbf{q}}} \tag{B2a}$$

$$= \frac{1}{N} \sum_{\mathbf{q} \in \rm AFZ} \left[\frac{\phi^{(\mu)}(\mathbf{q})^2}{-1 + \gamma_{\mathbf{q}}} + \frac{\phi^{(\mu)}(\mathbf{q})^2}{-1 - \gamma_{\mathbf{q}}} \right] , \tag{B2b}$$

where in Eq. (B2a) the sum is over the paramagnetic zone, whereas in Eq. (B2b) the sum is over the smaller antiferromagnetic zone (AFZ). The sum over the second antiferromagnetic zone, which is needed to reproduce the outer half of the paramagnetic zone, is obtained by noting that $\exp(i\mathbf{q} \cdot \boldsymbol{\delta}) = -\exp(i\mathbf{q}' \cdot \boldsymbol{\delta})$, where $\mathbf{q}'$ (in the first antiferromagnetic zone) is the value of $\mathbf{q}$ (in the second antiferromagnetic zone) modulo the antiferromagnetic re-

ciprocal lattice. Thus $\phi^{(\mu)}$ and γ change sign in going from a wave vector in the first antiferromagnetic zone to its equivalent in the second antiferromagnetic zone. Thus

$$g_F^p(0) = \frac{2}{N} \sum_{\mathbf{q}\in \mathrm{AFZ}} \frac{\phi^{(\mu)}(\mathbf{q})^2}{-1+\gamma_{\mathbf{q}}^2} \,. \tag{B2c}$$

Note that here $2/N$ is the number of $\mathbf{q}$ values in the AFZ. Thus, in the notation of Sec. III, this would be

$$g_{\mathrm{F}}^p(0) = \frac{1}{N} \sum_{\mathbf{q}} \frac{\phi^{(\mu)}(\mathbf{q})^2}{-e_{\mathbf{q}}^2} = g_{\mathrm{AF}}^p(0) \,, \tag{B3}$$

where $g_{\mathrm{AF}}^p(e)$ is the antiferromagnetic p-wave t matrix of Sec. III. Thus we may write

$$\frac{1}{\Sigma^{\mathrm{el}}(0)} \frac{d\Sigma^{\mathrm{el}}(x)}{dx} = \frac{2z(js-1)}{z-(js-1)g_{\mathrm{AF}}^p(0)} \,. \tag{B4}$$

For a body-centered hypercubic lattice in d spatial dimensions, one has

$$\gamma_{\mathbf{q}} \sim 1 - \frac{a^2q^2}{8} \tag{B5}$$

and

$$\phi^{p_x}(\mathbf{q}) = \sqrt{z}\sin(q_x a/2) \prod_{\beta=y,z,\ldots} \cos(q_\beta a/2) \sim \sqrt{z} a q_x/2 \,, \tag{B6}$$

so that

$$\phi^p(\mathbf{q})^2 = \sum_\beta \phi^{p_\beta}(\mathbf{q})^2 \sim z a^2 q^2/4 \sim z e_{\mathbf{q}}^2 \,, \tag{B7}$$

where β labels the d coordinate directions. Thus the last term in either Eqs. (4.3a) and (4.3b) or (4.10) inside the square brackets is

$$\frac{x}{2\Sigma^{\mathrm{el}}(0)} \frac{d\Sigma^{\mathrm{el}}(x)}{dx} \,. \tag{B8}$$

Next we evaluate the perpendicular susceptibility. The simplest way to do this is to consider the system in a small staggered field h_s whose purpose is to stabilize the antiferromagnetic ground state. The staggered field adds to h_0 in Eq. (3.4) the term $h_s \sum_{\mathbf{q}} (a_{\mathbf{q}}^\dagger a_{\mathbf{q}} + b_{\mathbf{q}}^\dagger b_{\mathbf{q}})$. The definition of the Green's function is such that $\chi_\perp = -\frac{1}{2}\lim_{h_s\to 0} \chi_{+-}(\mathbf{q}=0, e=0)$. In evaluating χ_{+-} we should first let $\mathbf{q}$ go to zero, then let h_s go to zero. In the presence of a staggered field, h_s, Eqs. (3.6) and (3.7) are revised:

$$l_{\mathbf{q}} = \left(\frac{1+h_s+e_{\mathbf{q}}}{2e_{\mathbf{q}}}\right)^{1/2}, \quad m_{\mathbf{q}} = \left(\frac{1+h_s-e_{\mathbf{q}}}{2e_{\mathbf{q}}}\right)^{1/2}, \tag{B9}$$

and

$$e_{\mathbf{q}} = \sqrt{(1+h_s)^2 - \gamma_{\mathbf{q}}^2} \,. \tag{B10}$$

Thus to leading order in h_s, $e_0^2 = 2h_s$ and $g_{\alpha,\alpha}^{(0)} = g_{\beta,\beta}^{(0)} = -e_0^{-1}$. Therefore from Eq. (3.34) we have that

$$\chi_\perp = -\frac{1}{2} A(0,0) \left[-\frac{2}{e_0} + \frac{1}{e_0^2} \sum_{\rho,\eta} \sigma_{\rho,\eta} \right] . \tag{B11}$$

Note also in Eqs. (3.35a) and (3.35b) that the quantity $(1-\gamma_{\mathbf{q}})/e_{\mathbf{q}}$ is actually $(l_{\mathbf{q}} - m_{\mathbf{q}})^2$. Using Eqs. (B9) and (B10) this quantity is $(1+h_s-\gamma_{\mathbf{q}})/e_{\mathbf{q}} \to \frac{1}{2}e_0$. Thus for $x_A = x_B = x$ we have

$$A(0,0) = (l_0 - m_0)^2[1 + x(s-1) + 2x(s-1)\tau(0)] \tag{B12a}$$

$$= \frac{1}{2}e_0^2 \left[1 + x(s-1) + 2\frac{x(s-1)}{j}[1 - js + jg_0(0)(1-s)] \right] . \tag{B12b}$$

Also

$$\sum_{\rho,\eta} \sigma_{\rho,\eta} = 2\frac{xe_0}{j}(j - 1 + js - 1) \,. \tag{B13}$$

Using the evaluations we have

$$\chi_\perp = \frac{1}{2}\left[1 + x(s-1) + 2x(s-1)\left(\frac{1}{j} - s + g_0(0)(1-s)\right)\right]\left[1 - x\left(1 + s - \frac{2}{j}\right)\right] . \tag{B14}$$

Thus

$$\frac{1}{2\chi_\perp(0)} \frac{d\chi_\perp(x)}{dx} = -g_0(0)(s-1)^2 + (s/j) + s - s^2 - 1 \,. \tag{B15}$$

This result agrees with Eq. (B.16) of KH when the anisotropies δ_A and δ_B are zero. In view of Eq. (B15) we see that Eqs. (4.3a), (4.3b), and (4.10) are all consistent with Eq. (4.4a).

APPENDIX C: ZERO-POINT DEVIATION

In this appendix we analyze how the zero-point deviation depends on the distance from the defect. For simplicity, we confine out attention to the case where the defect (located at $\mathbf{R}$) is on the same sublattice as the defect. We start from

$$g_{AA} = g^{(0)}_{AA} + \sum_{X,Y} g^{(0)}_{AX} t_{XY} g^{(0)}_{YA} \,, \tag{C1}$$

where X and Y are summed over the values A and B. Only the term involving the t matrix has a dependence on $\mathbf{r}$. Keeping only it, we have

$$g_{AA}(\mathbf{R}+\mathbf{r},\mathbf{R}+\mathbf{r}) = \frac{1}{N^2}\sum_{\mathbf{q},\boldsymbol{\lambda},\rho\sigma} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot(\mathbf{r}+\mathbf{R})}[l_{\mathbf{q}} g^{(0)}_{\alpha,\rho}(\mathbf{q}) - m_{\mathbf{q}} g^{(0)}_{\beta,\rho}(\mathbf{q})] t_{\rho,\sigma}(\mathbf{q},\boldsymbol{\lambda}) \left[l_{\boldsymbol{\lambda}} g^{(0)}_{\sigma,\alpha}(\boldsymbol{\lambda}) - m_{\boldsymbol{\lambda}} g^{(0)}_{\sigma,\alpha}(\boldsymbol{\lambda}) \right] . \tag{C2}$$

In matrix notation we have

$$[t(\mathbf{q},\boldsymbol{\lambda})] = e^{i(\boldsymbol{\lambda}-\mathbf{q})\cdot\mathbf{R}} \Bigg\{ \begin{bmatrix} l_{\mathbf{q}} \\ m_{\mathbf{q}} \end{bmatrix} \frac{e_{\mathbf{q}}}{D(e)} \left[\, l_{\boldsymbol{\lambda}}\phi_1(\boldsymbol{\lambda}),\ m_{\boldsymbol{\lambda}}\phi_2(\boldsymbol{\lambda}) \, \right]$$

$$+ \sum_{\mu\neq s} (js-1) \begin{bmatrix} m_{\mathbf{q}} \\ -l_{\mathbf{q}} \end{bmatrix} \frac{\phi^{(\mu)}(\mathbf{q})\phi^{(\mu)}(\boldsymbol{\lambda})}{D(e)} \left[\, m_{\boldsymbol{\lambda}},\ -l_{\boldsymbol{\lambda}} \, \right] \Bigg\} . \tag{C3}$$

Thus the terms which concern us are

$$g_{AA} = \frac{1}{N^2}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}} \, \mathrm{Im} \Bigg[\frac{e_{\mathbf{q}}}{D(e)} \left(\frac{l^2_{\mathbf{q}}}{e-e_{\mathbf{q}}} + \frac{m^2_{\mathbf{q}}}{e+e_{\mathbf{q}}} \right) \left(\frac{l^2_{\boldsymbol{\lambda}}\phi_1(\boldsymbol{\lambda})}{e-e_{\boldsymbol{\lambda}}} + \frac{m^2_{\boldsymbol{\lambda}}\phi_2(\boldsymbol{\lambda})}{e+e_{\boldsymbol{\lambda}}} \right)$$

$$+ \sum_{\mu\neq s} \left(\frac{2e_{\mathbf{q}} l_{\mathbf{q}} m_{\mathbf{q}} \phi^{(\mu)}(\mathbf{q})}{e^2-e^2_{\mathbf{q}}} \frac{2e_{\boldsymbol{\lambda}} l_{\boldsymbol{\lambda}} m_{\boldsymbol{\lambda}} \phi^{(\mu)}(\boldsymbol{\lambda})}{e^2-e^2_{\boldsymbol{\lambda}}} \frac{(js-1)}{D^{(\mu)}(e)} \right) \Bigg] \tag{C4}$$

in an obvious notation. Now for simplicity, we specialize to the case of vacancies, for which $\phi_1 = -\phi_2 = j$ and $D(e) = j[1-e(1+e)g_0(e)]$. Then

$$\langle a^\dagger_{\mathbf{R}+\mathbf{r}} a_{\mathbf{R}+\mathbf{r}} \rangle = - \int_{-\infty-i0^+}^{-i0^+} \frac{de}{\pi} \frac{1}{N^2} \sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}}$$

$$\times \mathrm{Im} \Bigg\{ \left[\frac{e_{\mathbf{q}}}{1-e(1+e)g_0(e)} \right] \left(\frac{l^2_{\mathbf{q}}}{e-e_{\mathbf{q}}} + \frac{m^2_{\mathbf{q}}}{e+e_{\mathbf{q}}} \right) \left(\frac{l^2_{\boldsymbol{\lambda}}}{e-e_{\boldsymbol{\lambda}}} - \frac{m^2_{\boldsymbol{\lambda}}}{e+e_{\boldsymbol{\lambda}}} \right)$$

$$- \sum_{\mu\neq s} \left(\frac{\gamma_{\mathbf{q}}\phi^{(\mu)}(\mathbf{q})}{e^2-e^2_{\mathbf{q}}} \frac{\gamma_{\boldsymbol{\lambda}}\phi^{(\mu)}(\boldsymbol{\lambda})}{e^2-e^2_{\boldsymbol{\lambda}}} \frac{1}{z+(1-e)g^{(\mu)}(e)} \right) \Bigg\} . \tag{C5}$$

One can analyze the non-s-wave contributions in Eq. (C5) by simple power counting estimates and one finds them to be of order R^{-2d+1}. However, keeping in mind Eq. (5.9), we have to be careful with any power counting argument for the s-wave contributions. To see the problem, replace $D(e)$ by a constant, in which case the integration over e can be done explicitly first. So we set

$$\frac{1}{1-e(1+e)g_0(e)} = 1 + \frac{e(1+e)g_0(e)}{1-e(1+e)g_0(e)} \,. \tag{C6}$$

Then

$$\langle a^\dagger_{\mathbf{R}+\mathbf{r}} a_{\mathbf{R}+\mathbf{r}} \rangle = T_1 + T_2 + T_3 \,, \tag{C7}$$

where

$$T_1 = - \int_{-\infty-i0^+}^{-i0^+} \frac{de}{\pi} \frac{1}{N^2} \sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}} e_{\mathbf{q}} \mathrm{Im} \left\{ \left(\frac{l^2_{\mathbf{q}}}{e-e_{\mathbf{q}}} + \frac{m^2_{\mathbf{q}}}{e+e_{\mathbf{q}}} \right) \left(\frac{l^2_{\boldsymbol{\lambda}}}{e-e_{\boldsymbol{\lambda}}} - \frac{m^2_{\boldsymbol{\lambda}}}{e+e_{\boldsymbol{\lambda}}} \right) \right\}, \tag{C8a}$$

$$T_2 = -\int_{-\infty-i0^+}^{-i0^+} \frac{de}{\pi}\frac{1}{N^2}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}}\mathrm{Im}\left\{\left[\frac{e_{\mathbf{q}}e(1+e)g_0(e)}{1-e(1+e)g_0(e)}\right]\left(\frac{l_{\mathbf{q}}^2}{e-e_{\mathbf{q}}}+\frac{m_{\mathbf{q}}^2}{e+e_{\mathbf{q}}}\right)\left(\frac{l_{\boldsymbol{\lambda}}^2}{e-e_{\boldsymbol{\lambda}}}-\frac{m_{\boldsymbol{\lambda}}^2}{e+e_{\boldsymbol{\lambda}}}\right)\right\}, \tag{C8b}$$

and

$$T_3 = \int_{-\infty-i0^+}^{-i0^+} \frac{de}{\pi}\frac{1}{N^2}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}}\mathrm{Im}\left\{\sum_{\mu\neq s}\left(\frac{\gamma_{\mathbf{q}}\phi^{(\mu)}(\mathbf{q})}{e^2-e_{\mathbf{q}}^2}\frac{\gamma_{\boldsymbol{\lambda}}\phi^{(\mu)}(\boldsymbol{\lambda})}{e^2-e_{\boldsymbol{\lambda}}^2}\frac{1}{z+(1-e)g^{(\mu)}(e)}\right)\right\}. \tag{C8c}$$

We have

$$T_1 = \frac{1}{N^2}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}} e_{\mathbf{q}}\left(\frac{m_{\mathbf{q}}^2 l_{\boldsymbol{\lambda}}^2}{e_{\mathbf{q}}+e_{\boldsymbol{\lambda}}}-\frac{l_{\mathbf{q}}^2 m_{\boldsymbol{\lambda}}^2}{e_{\mathbf{q}}+e_{\boldsymbol{\lambda}}}\right) \tag{C9a}$$

$$= \frac{1}{2N^2}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}}\frac{(e_{\boldsymbol{\lambda}}-e_{\mathbf{q}})}{e_{\boldsymbol{\lambda}}(e_{\mathbf{q}}+e_{\boldsymbol{\lambda}})} \tag{C9b}$$

$$= \frac{1}{2N^2}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}}\left(\frac{2}{(e_{\mathbf{q}}+e_{\boldsymbol{\lambda}})}-\frac{1}{e_{\boldsymbol{\lambda}}}\right) \tag{C9c}$$

$$= \frac{1}{N^2}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\mathbf{q}-\boldsymbol{\lambda})\cdot\mathbf{r}}\frac{1}{(e_{\mathbf{q}}+e_{\boldsymbol{\lambda}})}. \tag{C9d}$$

In going from Eq. (C9c) to (C9d) we dropped the completely local term, since we are only interested in the behavior at large r. Thus

$$T_1 = K(r/a)^{-2d+1}, \tag{C10}$$

where we find the constant K to be $1/(32\pi)$ for $d=2$ and $1/(16\pi^3)$ for $d=3$. Note the cancellation which led to the result of Eq. (C10) rather than a power law with exponent $-2d+3$. The same cancellation in T_2 makes it irrelevant. Actually we find

$$T_2 \sim r^{-3d+2}. \tag{C11}$$

Finally, we consider T_3 for simplicity for $d=2$. Then

$$T_3 = \frac{8}{FN^2}\int_{-\infty-i0^+}^{-i0^+}\frac{de}{\pi}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\boldsymbol{\lambda}-\mathbf{q})\cdot\mathbf{r}}\frac{\sin(\frac{1}{2}q_x a)\sin(\frac{1}{2}\lambda_x a)}{(e^2-e_{\mathbf{q}}^2)(e^2-e_{\boldsymbol{\lambda}}^2)}, \tag{C12}$$

where $F = z + g^{(p)}(0)$ and we have omitted corrections at finite wave vector in Eq. (C12). We have

$$T_3 = \frac{1}{4FN^2}\int_{-\infty-i0^+}^{-i0^+}\frac{de}{\pi}\sum_{\mathbf{q},\boldsymbol{\lambda}} e^{i(\boldsymbol{\lambda}-\mathbf{q})\cdot\mathbf{r}}\frac{a^2\mathbf{q}\cdot\boldsymbol{\lambda}}{e_{\mathbf{q}}e_{\boldsymbol{\lambda}}}\left(\frac{1}{e-e_{\mathbf{q}}}-\frac{1}{e+e_{\mathbf{q}}}\right)\left(\frac{1}{e-e_{\boldsymbol{\lambda}}}-\frac{1}{e+e_{\boldsymbol{\lambda}}}\right) \tag{C13a}$$

$$= \frac{a^4}{2F(2\pi)^4}\int d\mathbf{q}\int d\boldsymbol{\lambda} e^{i(\boldsymbol{\lambda}-\mathbf{q})\cdot\mathbf{r}}\frac{a^2\mathbf{q}\cdot\boldsymbol{\lambda}}{e_{\mathbf{q}}e_{\boldsymbol{\lambda}}}\frac{1}{e_{\mathbf{q}}+e_{\boldsymbol{\lambda}}} \tag{C13b}$$

$$= \frac{1}{32F\pi^4}\int\lambda d\lambda\int q dq\int_0^{2\pi}d\phi_q\int_0^{2\pi}d\phi_\lambda\cos\phi_q\cos\phi_\lambda\int_0^\infty dt e^{-t(q+\lambda)+i\lambda\cos\phi_\lambda(r/a)+iq\cos\phi_q(r/a)}. \tag{C13c}$$

It is easily shown that this integral gives a contribution of order $r^{-3} = r^{1-2d}$ which must be added to that of Eq. (C10) to get the full result.

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