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IMPURITY ATOMS IN A FERROMAGNETIC CRYSTAL

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A general solution is given for the problem of vibrations of the spin system of a ferromagnetic crystal containing an impurity atom. It is shown that the one-particle Green's function for such a crystal satisfies the Dyson equation and can therefore be expressed simply in terms of the corresponding Green's function for the ideal crystal. The general theory is applied to the problem of inelastic magnetic scattering of slow neutrons in a crystal with a magnetic impurity. it is shown that the energy distribution of the scattered neutrons shows peaks corresponding to definite types of local magnetic vibrations of the perturbed crystal.

1. INTRODUCTION

I. Lifshitz[1] has treated a special class of perturbations, acting on a system with a continuous energy spectrum, which are characterized not by being small in the usual sense of perturbation theory, but by their local character. He showed that in such a perturbed system there may be, in addition to the continuous spectrum, individual discrete levels. This theory is beautifully suited for describing the state of a crystal in which one of the atoms is replaced by an atom of another sort.

Lifshitz himself applied his theory[2] to the analysis of the vibration spectrum of a crystal containing an impurity atom (and this same problem was later investigated in detail by various authors[3-6]), but it was clear that a similar treatment could be given for other branches of the spectrum of excitations of the crystal. Thus, Koster and Slater[7] treated the influence of an impurity on the spectrum of conduction electrons in a metal, and recently Wolfram and Calloway[8] have discussed the problem of the spectrum of spin waves in a ferromagnetic crystal containing a magnetic impurity.

Our purpose here is to give a complete solution of the problem of a ferromagnetic crystal with an impurity, i.e., to determine not only the spectrum of spin vibrations of the crystal but to find the correlation function, thus making it possible to give a description of a variety of questions associated with such a system. We found it convenient to use the Green's function method, but unlike Wolfram and Calloway,[8] we have started from the Green's function describing the crystal with the impurity and expressed it in terms of the Green's function for the ideal crystal.

The next three sections give the necessary mathematical tools for solving various problems concerning the properties of the system. In Sec. 5 we apply the theory to calculate the cross section for inelastic magnetic scattering of slow neutrons by such a crystal; our purpose is to examine the possibility of detecting magnetic oscillations from scattering data. For the case of the phonon spectrum of crystals this problem was solved by Kagan and Iosilevskiĭ.[4]

2. GREEN'S FUNCTION FOR A FERROMAGNETIC CRYSTAL WITH AN IMPURITY ATOM

Consider a ferromagnetic crystal consisting of atoms of one kind, having spin S and with the exchange integral between nearest neighbors $J > 0$. Suppose that one of the atoms is replaced by another with spin S' and with a different exchange coupling to its nearest neighbors, characterized by the exchange integral $J' > 0$. Since $J' > 0$, in the ground state the spin of the embedded atom should be parallel to the direction of spin ordering of the crystal. Our problem is now to determine the spectrum of vibrations of the spin system of such a crystal with one impurity and to calculate the spin correlation functions between different sites.

We shall start from the usual Dirac expression for the exchange Hamiltonian, which is conveniently written for our case in the form

$$H = -J\sum_{n}\sum_{\Delta}\mathbf{S}_n\mathbf{S}_{n+\Delta} + 2J\sum_{\Delta}\mathbf{S}_1\mathbf{S}_{1+\Delta} - 2J'\sum_{\Delta}\mathbf{S}_1'\mathbf{S}_{1+\Delta}. \qquad (2.1)$$

The subscript n runs over all the sites, and Δ over all nearest neighbors; the impurity site is labelled 1; S_1' is the spin operator for the impurity site.

Expression (2.1) is written so that the first term describes the exchange interaction in the ideal crystal without the impurity; the first two terms together give the exchange interaction in a crystal where there is no magnetic atom at site 1; the third term is the exchange energy of the impurity atom with all the other atoms. (We have used the nearest neighbor approximation throughout.)

Restricting ourselves to the spin wave approximation, we go over in (2.1) from spin operators to the Bose operators a_n and a_n^+ for the spin deviations, according to the relations[9]

$$S_n^+ = (2S)^{1/2}a_n, \quad S^- = (2S)^{1/2}a_n^+, \quad S_n^z = S - a_n^+a_n;$$
$$S_1'^+ = (2S')^{1/2}a_1, \quad S_1'^- = (2S')^{1/2}a_1^+, \quad S_1'^z = S' - a_1^+a_1. \tag{2.2}$$

To within an additive constant the Hamiltonian (2.1) is then a quadratic form in the system of operators a_n and a_n^+, which can in general be brought to diagonal form by a canonical transformation, so that one can separate out the elementary excitations of the spin system. It is more convenient, however, to use the Green's function method, since it allows us immediately to find not only the spectrum of excitations, but also the probabilities of spin deviations at different sites.

For example, consider the one-particle retarded Green's function $G_{nm}(t - t')$, defining it as follows:[10]

$$G_{nm}(t-t') = -i\theta(t-t')\langle[a_n(t), a_m^+(t')]\rangle, \tag{2.3}$$

where $a_n(t)$ is the operator a_n in the Heisenberg representation with the Hamiltonian (2.1), $\langle\ldots\rangle$ denotes a statistical average over a Gibbs ensemble with the Hamiltonian (2.1) at temperature T, $[\ldots, \ldots]$ denotes a commutator,

$$\theta(t-t') = \begin{cases} 1, & t > t' \\ 0, & t < t' \end{cases}$$

The correlation function for the spin deviation operators at two sites is given simply in terms of the Green's function:

$$\langle a_m^+(t')a_n(t)\rangle = \lim \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\operatorname{Im} G_{nm}(E - i\mathscr{E})}{e^{E/kT} - 1} e^{-iE(t-t')}\,dE, \tag{2.4}$$

where $\mathscr{E} = 0^+$, $G_{nm}(E)$ is the Fourier component of the function $G_{nm}(t - t')$ with respect to $t - t'$:

$$G_{nm}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} G_{nm}(E)\,e^{-iE(t-t')}\,dE. \tag{2.5}$$

It is not difficult to show that the Green's function in the energy representation $G_{nm}(E)$ (we shall denote it simply by G_{nm}) is subjected to the equation

$$\begin{aligned} EG_{nm} = \delta_{nm} &+ 2JS\sum_\Delta (G_{nm} - G_{n+\Delta, m}) \\ &- 2JS\sum_\Delta (\delta_{n,1} - \delta_{n,1+\Delta})(G_{1m} - G_{1+\Delta, m}) \\ &+ 2J'\sum_\Delta \{[SG_{1m} - (SS')^{1/2}G_{1+\Delta, m}]\,\delta_{n,1} \\ &+ [S'G_{1+\Delta, m} - (SS')^{1/2}G_{1m}]\,\delta_{n,1+\Delta}\}, \end{aligned} \tag{2.6}$$

where δ_{nm} is the Kronecker delta. For $S = S'$ and $J = J'$, (2.6) becomes the equation for the Green's function of the ideal ferromagnetic crystal:

$$EG^0_{nm} = \delta_{nm} + 2JS\sum_\Delta (G^0_{nm} - G^0_{n+\Delta, m}), \tag{2.7}$$

whose solution is given as a Fourier series:

$$G^0_{nm} = \frac{1}{N}\sum_{\mathbf{k}} G^0(\mathbf{k})\,e^{i\mathbf{k}(\mathbf{n}-\mathbf{m})} = \frac{1}{N}\sum_{\mathbf{k}} \frac{e^{i\mathbf{k}(\mathbf{n}-\mathbf{m})}}{E - \mathscr{E}_{\mathbf{k}}}, \tag{2.8}$$

where $\mathscr{E}_{\mathbf{k}}$ is the energy of a spin wave in the ideal crystal:

$$\mathscr{E}_{\mathbf{k}} = 2JS\Big(z - \sum_{\mathbf{k}} e^{i\mathbf{k}\Delta}\Big), \tag{2.9}$$

and z is the number of nearest neighbors.

We look for a solution of (2.6) corresponding to the crystal with impurity in the form

$$G_{nm} = \sum_{p=1}^{N} A_{np}G^0_{pm}. \tag{2.10}$$

Substituting (2.10) in (2.6) and using Eq. (2.7), we find the equation which A_{np} must satisfy:

$$\sum_p (G^{0-1})_{np}A_{pm} = (G^{0-1})_{nm} + \sum_p V_{np}A_{pm}, \tag{2.11}$$

where we have introduced the matrix of coefficients

$$\begin{aligned} V_{np} = 2JS\Big(&\varepsilon z\delta_{n,1}\delta_{p,1} - \gamma\delta_{n,1}\sum_\Delta \delta_{p,1+\Delta} \\ &- \gamma\sum_\Delta \delta_{n,1+\Delta}\,\delta_{p,1} + \rho\sum_\Delta \delta_{n,1+\Delta}\,\delta_{p,1+\Delta}\Big) \end{aligned} \tag{2.12}$$

and have used the abbreviations (as in[8])

$$\varepsilon = (J' - J)/J, \quad \sigma' = S'/S, \quad \gamma = (\sigma')^{1/2}(1 + \varepsilon) - 1,$$
$$\rho = \sigma' - 1 + \varepsilon\sigma'. \tag{2.13}$$

Equation (2.11) can be written in symbolic form as follows:

$$G^{0-1}A = G^{0-1} + VA,$$

from which we get

$$A = (1 - G^0V)^{-1}. \tag{2.14}$$

Substituting this result in the symbolic form of (2.10), $G = AG^0$, we get the expression for the Green's function of the crystal with the impurity:

$$G = \frac{1}{1 - G^0V}G^0. \tag{2.15}$$

It is useful to note another form of (2.15):

$$G = G^0 + G^0 V G. \tag{2.16}$$

The perturbation operator V, whose matrix elements in the coordinate representation are given by (2.12), can be written in matrix form as

$$V = 2JS \begin{pmatrix} \varepsilon z & -\gamma & -\gamma \ldots & -\gamma \\ -\gamma & \rho & 0 \ldots & 0 \\ -\gamma & 0 & \rho \ldots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ -\gamma & 0 & 0 \ldots & \rho \end{pmatrix}. \tag{2.17}$$

In this matrix the rows and columns label the sites occupied by the impurity and its nearest neighbors, so that the matrix (2.17) is (z + 1) by (z + 1). But since the matrix V acts on the matrices G^0 and G, which are N by N, we have to insert zeros beyond the block that is (z + 1) by (z + 1).

Expression (2.15) gives the exact solution of the system (2.6). The latter is exact within the framework of the spin wave approximation as soon as we restrict ourselves to nearest neighbors. If we do not make this approximation, the exact expression for the Green's function of the crystal with impurity will still be given by (2.15), but the matrix V is no longer the cut-off form (2.17), and contains interaction terms with particles in the second coordination sphere, etc. Thus, using the exact equation (2.16), which is completely equivalent to (2.15), we see that the Green's function for the crystal with impurity satisfies the Dyson equation, in which V can be taken in any approximation corresponding to including the interactions of the impurity with any number of coordination spheres. Since the problem can be worked out completely only if the matrix V is cut off sufficiently, we are forced to use "perturbation theory." In contrast to standard perturbation theory, the smallness of the perturbation here simply means a sufficiently rapid drop of the interaction of the impurity atom with the crystal as the distance increases. I. Lifshitz[1] first called attention to this characteristic of the problem with local perturbations.

3. POLE SPECTRUM AND DENSITY OF STATES

To find the vibration spectrum of the crystal spin system, we use the pole of the Green's function G, given by (2.15). We write this expression in matrix form:

$$G_{nm} = \sum_{p=1}^{N} \left(\frac{1}{1 - G^0 V} \right)_{np} G^0_{pm}. \tag{3.1}$$

The matrix elements of the reciprocal matrix that appears in (3.1) can be expressed in terms of the algebraic complements C_{pn} of the matrix $(1 - G^0V)$:

$$\left(\frac{1}{1 - G^0 V} \right)_{np} = \frac{C_{pn}}{D} = \frac{(-1)^{p+n} \operatorname{Minor} \{(1 - G^0 V)_{pn}\}}{D}, \tag{3.2}$$

$$D = \det |1 - G^0 V|. \tag{3.3}$$

Since the matrix V is truncated to dimensions (z + 1) by (z + 1), the matrix $(1 - G^0V)$ has a simple structure: the first z + 1 columns are completely filled, the other places along the main diagonal contain 1, and all other elements are 0. Consequently the determinant D has dimension (z + 1) × (z + 1). Using the expression for V in the form (2.17), one can show that for a simple cubic lattice (to which we restrict our consideration), D is factorable:[8]

$$D = D(s) D^3(p) D^2(d); \tag{3.4}$$

$$\begin{aligned} D(s) = {} & [1 - (2JS)(\varepsilon z G_{11}{}^0 - \gamma z G_{12}{}^0)] \\ & \times \left[1 + (2JS) \left(z\gamma G_{12}{}^0 - \rho \sum_{i=2}^{z+1} G_{i2}{}^0 \right) \right] \\ & + z(2JS)^2 \left(\varepsilon z G_{12}{}^0 - \gamma \sum_{i=2}^{z+1} G_{i2}{}^0 \right) (\gamma G_{11}{}^0 - \rho G_{12}{}^0), \end{aligned} \tag{3.5}$$

$$D(p) = 1 - (2JS) \rho (G_{11}{}^0 - G_{23}{}^0), \tag{3.6}$$

$$D(d) = 1 - (2JS) \rho (G_{11}{}^0 + G_{23}{}^0 - 2G_{24}{}^0). \tag{3.7}$$

Because of (3.1) and (3.2), it is clear that the poles of the Green's function G are determined not only by the poles of the Green's function G^0 for the ideal crystal, but also by the zeros of the determinant D. The last condition determines the spectrum of so-called local vibrations of the spin system, which were studied by Wolfram and Calloway.[8] From (3.4), we see that there are three types of local levels, corresponding to the zeros of the separate factors D(s), D(p) and D(d). We call the corresponding vibrations s-, p-, and d-type vibrations. The reason for this nomenclature is that the symmetry of the spin deviations at the impurity site and its neighbors coincides in these vibrations with the symmetry of s-, p- and d-wave functions in the cubic crystal.

We shall now determine the density of states g(E) for the vibrations of the spin system of a ferromagnetic crystal with an impurity. For this we must use the general relation expressing the density of states in terms of the one-particle Green's function ($\mathscr{E} = 0^+$):

$$g(E) = \frac{1}{\pi N} \operatorname{Im} \operatorname{Sp} G(E - i\mathscr{E}). \tag{3.8}$$

It is convenient to use the following representation for the Green's function:

$$G = G^0 + G^0 V \frac{1}{1 - G^0 V} G^0, \qquad (3.9)$$

which is obtained by combining (2.15) and (2.16). Using (3.2), we write

$$\frac{1}{N} \operatorname{Sp} G(E) \equiv \frac{1}{N} \sum_n G_{nn} = G_0{}^0 + \frac{1}{ND} \sum_{nlpm} G_{nl}{}^0 V_{lp} C_{mp} G^0_{mn}, \qquad (3.10)$$

where $G_0^0 \equiv G_{nn}^0$ is independent of n.

The last term in this expression is easily transformed using the relations

$$\frac{d}{dE} \sum_n G^0_{nl} G^0_{mn} = -\frac{d}{dE} G^0_{ml}, \qquad (3.11)$$

$$D = \sum_p (1 - G^0 V)_{mp} C_{mp}. \qquad (3.12)$$

Thus, differentiating (3.12) with respect to E, we get

$$\frac{d}{dE} D = -\sum_{mlp} V_{lp} C_{mp} \frac{d}{dE} G^0_{ml}, \qquad (3.13)$$

precisely the expression appearing in (3.10) after substitution from (3.11). Thus we have

$$\frac{1}{N} \operatorname{Sp} G(E) = G_0{}^0 + \frac{1}{N} \frac{d}{dE} \ln D. \qquad (3.14)$$

Now, according to (3.8) and (3.14), we can write

$$g(E) = g_0(E) + \frac{1}{\pi N} \operatorname{Im} \frac{D_E'(E - i\mathscr{E})}{D(E - i\mathscr{E})}, \qquad (3.15)$$

where $g_0(E) = \pi^{-1} \operatorname{Im} G_0^0$ is the density of states for the ideal crystal. The second term gives the change in the density of states caused by the impurity.

From (3.4), we have

$$\frac{D_E'}{D} = \frac{D_E'(s)}{D(s)} + 3\frac{D_E'(p)}{D(p)} + 2\frac{D_E'(d)}{D(d)}. \qquad (3.16)$$

This means that the different branches (s, p, d) of local vibrations contribute additively to the density of states, with weights corresponding to the degree of degeneracy of the local levels.

4. TRANSITION TO THE FOURIER REPRESENTATION

For a complete solution of the problem, we must find not only the poles of the Green's function and the density of states, but must calculate the Green's function. The expression (3.1) simplifies considerably if we note that for p > (z + 1),

$$\left(\frac{1}{1 - G^0 V}\right)_{np} = \delta_{np}. \qquad (4.1)$$

It can be written in the form

$$G_{nm} = \sum_{p=1}^{z+1} \left(\frac{1}{1 - G^0 V}\right)_{np} G^0_{pm} + \sum_{p=z+2}^{N} \delta_{np} G^0_{pm}, \qquad (4.2)$$

so that G_{nm} will be calculated from the G^0_{pm}, if we know the matrix elements $(1 - G^0 V)^{-1}_{np}$. In particular one can in this way get the expression for the important function G_{11}:

$$G_{11} = D^{-1}(s) \left\{ \left[1 + (2JS) \left(z\gamma G_{12}{}^0 - \rho \sum_{i=2}^{z+1} G^0_{i2} \right) \right] G_{11}{}^0 - z(2JS)(\gamma G_{11}{}^0 - \rho G_{12}{}^0) G_{12}{}^0 \right\}. \qquad (4.3)$$

(We have used the relation $G^0_{1i} = G^0_{12}$; i = 2, ..., z + 1, which follows from the cubic symmetry of the crystal.)

For calculations regarding the crystal as a whole, one may need the functions G_{nm} with large index n, for which computations using formula (4.2) are ineffective. For this purpose it is convenient to go over to the Fourier representation. But we must immediately point out that since the system "crystal plus impurity" no longer has translational symmetry, the function G_{nm} no longer depends only on the difference n − m, but involves the arguments individually; thus G_{nm} cannot be expanded into a single Fourier series. It is still useful to use a mixed representation, in which G_{nm} is expanded in a Fourier series in the difference n − m, while we retain the dependence of the Fourier coefficients on one of the indices, say n.

Thus we set

$$G_{nm} = \frac{1}{N} \sum_{\mathbf{k}} G^{(n)}(\mathbf{k}) e^{i\mathbf{k}(\mathbf{n}-\mathbf{m})}. \qquad (4.4)$$

Using the equation for the function G in the form (2.15), (2.16) or (3.9), we get equations for $G^{(n)}(\mathbf{k})$. We first consider Eq. (2.16) in matrix form:

$$G_{nm} = G^0_{nm} + \sum_{l,\,p=1}^{z+1} G^0_{nl} V_{lp} G_{pm}. \qquad (4.5)$$

Here the indices n and m run from 1 to N, whereas l and p actually go from 1 to z + 1, since the matrix V is truncated.

Substituting (4.4) in (4.5), we get the relation

$$G^{(n)}(\mathbf{k}) = G^0(\mathbf{k}) + \sum_{p=1}^{z+1} (G^0 V)_{np} e^{i\mathbf{k}(\mathbf{p}-\mathbf{n})} G^{(p)}(\mathbf{k}). \qquad (4.6)$$

This relation, for n = 1, ..., z + 1, gives a closed system of equations for the first z + 1 values $G^{(n)}(\mathbf{k})$. Having solved them, we substitute the results for $G^{(p)}(\mathbf{k})$ on the right of (4.6), which will then determine the other values for n = z + 2, ... Thus the problem of finding all the $G^{(n)}(\mathbf{k})$ has been reduced to the solution of a system of z + 1 equations.

For applications it may be more convenient to use (3.9), which has the following matrix form:

$$G_{nm} = G_{nm}{}^{0} + \sum_{l,\,p,\,j=1}^{z+1} G_{nl}{}^{0} V_{lp} \left(\frac{1}{1 - G^{0}V} \right)_{pj} G_{jm}{}^{0}. \tag{4.7}$$

Substituting the expansion (4.4) and (2.5), we find

$$G^{(n)}(\mathbf{k}) = G^{0}(\mathbf{k}) + \sum_{l,\,p,\,j=1}^{z+1} G^{0}_{nl} V_{lp} \left(\frac{1}{1 - G^{0}V} \right)_{pj} e^{i\mathbf{k}(\mathbf{j}-\mathbf{n})} G^{0}(\mathbf{k}). \tag{4.8}$$

Although this formula gives an explicit expression for $G^{(n)}(k)$, one should not be misled, since the triple summation has not yet been carried out. Nevertheless, it is useful for many applications, in particular for calculating the important expression $\sum_{n=1}^{N} G^{(n)}(k)$, which occurs in scattering theory.

To do this, we sum the left and right sides of (4.8) over n from 1 to N. Using relation (3.2), we find

$$\sum_{n=1}^{N} G^{(n)}(\mathbf{k}) = NG^{0}(\mathbf{k}) + W(\mathbf{k})/D, \tag{4.9}$$

$$W(\mathbf{k}) = [G^{0}(\mathbf{k})]^{2} \sum_{l,\,p,\,j=1}^{z+1} V_{lp} C_{jp} e^{i\mathbf{k}(\mathbf{j}-\mathbf{l})}. \tag{4.10}$$

The quantity W(k) can be immediately computed, although the calculation is very lengthy. We find that

$$\begin{aligned} W(\mathbf{k}) = {} & Y(\mathbf{k}, s) D^{3}(p) D^{2}(d) + 3Y(\mathbf{k}, p) D(s) D^{2}(p) D^{2}(d) \\ & + 2Y(\mathbf{k}, d) D(s) D^{3}(p) D(d), \end{aligned} \tag{4.11}$$

$$\begin{aligned} Y(\mathbf{k}, s) = {} & (2JS)\,[G^{0}(\mathbf{k})]^{2} \Big\{ (\varepsilon z - \gamma z e^{i\mathbf{k}(\mathbf{1}-\mathbf{2})}) \\ & \times \Big[1 + (2JS) \Big(z\gamma G_{12}{}^{0} - \rho \sum_{i=2}^{z+1} G_{i2}{}^{0} \Big) \Big] \\ & + \Big(\rho \sum_{i=2}^{z+1} e^{i\mathbf{k}(\mathbf{i}-\mathbf{2})} - \gamma z e^{i\mathbf{k}(\mathbf{1}-\mathbf{2})} \Big) [1 - (2JS)(\varepsilon z G_{11}{}^{0} - \gamma z G_{12}{}^{0})] \\ & + z\,(2JS)\,(\varepsilon z e^{i\mathbf{k}(\mathbf{1}-\mathbf{2})} - \gamma \sum_{i=2}^{z+1} e^{i\mathbf{k}(\mathbf{i}-\mathbf{2})})\,(\rho G_{12}{}^{0} - \gamma G_{11}{}^{0}) \\ & + z\,(2JS) \Big(\varepsilon z G_{12}{}^{0} - \gamma \sum_{i=2}^{z+1} G_{i2}{}^{0} \Big) (\rho e^{i\mathbf{k}(\mathbf{1}-\mathbf{2})} - \gamma) \Big\} \end{aligned} \tag{4.12}$$

$$Y(\mathbf{k}, p) = (2JS)\,[G^{0}(\mathbf{k})]^{2} \rho\,(1 - e^{i\mathbf{k}(\mathbf{2}-\mathbf{3})}), \tag{4.13}$$

$$Y(\mathbf{k}, d) = (2JS)\,[G^{0}(\mathbf{k})]^{2} \rho\,(1 + e^{i\mathbf{k}(\mathbf{2}-\mathbf{3})} - 2e^{i\mathbf{k}(\mathbf{2}-\mathbf{4})}). \tag{4.14}$$

Using (4.11) and (3.4), one can write the relation

$$\frac{W(\mathbf{k})}{D} = \frac{Y(\mathbf{k}, s)}{D(s)} + 3\frac{Y(\mathbf{k}, p)}{D(p)} + 2\frac{Y(\mathbf{k}, d)}{D(d)}, \tag{4.15}$$

which is very similar to (3.16). One can show that

$$\frac{1}{N} \sum_{\mathbf{k}} Y(\mathbf{k}, s) = D_{E}'(s),$$

$$\frac{1}{N} \sum_{\mathbf{k}} Y(\mathbf{k}, p) = D_{E}'(p), \quad \frac{1}{N} \sum_{\mathbf{k}} Y(\mathbf{k}, d) = D_{E}'(d). \tag{4.16}$$

Using these equalities, one can show from (4.11) that

$$\frac{1}{N} \sum_{\mathbf{k}} W(\mathbf{k}) = D_{E}'. \tag{4.17}$$

Summing (4.15) over k and using the relations (4.16) and (4.17), we again arrive at formula (3.16), which is a check of relations (4.12)–(4.14).

5. APPLICATION OF THE THEORY TO INELASTIC MAGNETIC SCATTERING OF NEUTRONS

Local oscillations of the spins in a ferromagnetic crystal can be detected by means of inelastic magnetic scattering of neutrons, similarly to the way considered earlier[4] for studying local lattice vibrations by means of inelastic nuclear scattering. We shall therefore calculate the cross section for one-magnon scattering of neutrons in a ferromagnet containing an impurity.

The second derivative of the cross section for magnetic scattering of neutrons by a crystal can be written in the familiar form (cf., for example,[11]):

$$\begin{aligned} \frac{d^{2}\sigma}{d\Omega\,dE'} = {} & (r_{0}\eta)^{2} \frac{p'}{p} \sum_{nm} F_{n}(\mathbf{q}) F_{m}(\mathbf{q}) e^{-i\mathbf{q}(\mathbf{n}-\mathbf{m})} \sum_{\alpha\beta} (\delta_{\alpha\beta} - e_{\alpha}e_{\beta}) \\ & \times \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{i(E'-E)t} \langle S_{n}{}^{\alpha}(0) S_{m}{}^{\beta}(t) \rangle, \end{aligned} \tag{5.1}$$

where E, **p** and E′, **p**′ are the energy and momentum of the incident and scattered neutron; **q** = **p** − **p**′ is the scattering vector; **e** is the unit scattering vector; $F_n(q)$ is the magnetic form factor of the atom at site n; r_0 is the electromagnetic radius of the electron, and $\eta = 1.93$ is the magnetic moment of the neutron in nuclear magnetons.

The inelastic scattering is related to the correlations of the "transverse" components of the spin vectors $\langle S_n^{+}(0) S_m^{-}(t) \rangle$ and $\langle S_n^{-}(0) S_m^{+}(t) \rangle$. Selecting the appropriate term from the general expression (2.2), we get the cross section for one-magnon scattering in the form

$$\begin{aligned} \frac{d^{2}\sigma_{\mathrm{in}}}{d\Omega\,dE'} = {} & \frac{1}{2} (r_{0}\eta)^{2} \frac{p'}{p} [1 + (\mathbf{em})^{2}] \sum_{nm} F_{n}(\mathbf{q}) F_{n}(\mathbf{q}) (S_{n}S_{m})^{1/2} \\ & \times e^{-i\mathbf{q}(\mathbf{n}-\mathbf{m})} \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{i(E'-E)t} \{ \langle a_{n}{}^{+}(0) a_{m}(t) \rangle \\ & + \langle a_{n}(0) a_{m}{}^{+}(t) \rangle \} \end{aligned} \tag{5.2}$$

(**m** is a unit vector along the direction of the spontaneous magnetic moment of the crystal). Here S_n (like S_m) is equal to S if a host atom is at site n, and S′ if an impurity atom is at site n. Similarly, the form factors of host atoms and impurity atoms will be denoted by F(q) and F′(q). We shall continue to assume that the impurity atom is at the site labelled 1.

Part of the expression (5.2) coming from the first term in the curly bracket corresponds to scattering of the neutron with absorption of a spin wave, and another part—with emission of a spin wave. Using (2.4), which relates the correlation function to the Green's function, we write the cross section (5.2) in the form

$$\frac{d^2\sigma_{\text{in}}}{d\Omega\, dE'} = \frac{d^2\sigma^-}{d\Omega\, dE'} + \frac{d^2\sigma^+}{d\Omega\, dE'} \tag{5.3}$$

$$\frac{d^2\sigma^\pm}{d\Omega\, dE'} = \frac{1}{2}(r_0\eta)^2\,\frac{p'}{p}\,[1+(\mathbf{em})^2]\sum_{nm} F_n(\mathbf{q})\,F_m(\mathbf{q})\,(S_nS_m)^{1/2}$$
$$\times\, e^{\mp i\mathbf{q}(\mathbf{n}-\mathbf{m})}\,\frac{1}{\pi}\,\operatorname{Im} G_{nm}(\Delta E - i\mathscr{E})\left[n(\Delta E)+\frac{1}{2}\pm\frac{1}{2}\right]. \tag{5.4}$$

Here the plus sign corresponds to emission and the minus to absorption of a magnon; ΔE = |E′ − E| is the transition energy; n(ΔE) is the Bose distribution function. The expression for the one-magnon scattering in this form is convenient for the further discussion.

Assuming that the impurity atom is at site 1, it is convenient to separate in the sum over n and m in (5.4) the terms in which a) n = 1, m = 1; b) n = 1, m ≠ 1; c) n ≠ 1, m = 1.

If we then add to the sums $\Sigma_{n\neq 1}$ and $\Sigma_{m\neq 1}$, and to the double sum $\Sigma_{n\neq 1}\Sigma_{m\neq 1}$ the terms with n = 1 and m = 1, which correspond to the case where there would be a host atom at site 1 (and, of course, subtract these same terms), (5.4) splits into the sum of the following three terms:

$$\frac{d^2\sigma_1^\pm}{d\Omega\, dE'} = \frac{1}{2}(r_0\eta)^2\frac{p'}{p}[1+(\mathbf{em})^2][F'(\mathbf{q})\,(S')^{1/2} - F(\mathbf{q})S^{1/2}]^2$$
$$\times\,\frac{1}{\pi}\operatorname{Im} G_{11}(\Delta E - i\mathscr{E})\left[n(\Delta E)+\frac{1}{2}\pm\frac{1}{2}\right], \tag{5.5}$$

$$\frac{d^2\sigma_2^\pm}{d\Omega\, dE'} = \frac{1}{2}(r_0\eta)^2\frac{p'}{p}[1+(\mathbf{em})^2]F^2(\mathbf{q})S$$
$$\times\,\frac{1}{\pi}\operatorname{Im}\sum_{n=1}^{N} G^{(n)}(\Delta E - i\mathscr{E}, \boldsymbol{\tau}\pm\mathbf{q})\left[n(\Delta E)+\frac{1}{2}\pm\frac{1}{2}\right], \tag{5.6}$$

$$\frac{d^2\sigma_3^\pm}{d\Omega\, dE'} = \frac{1}{2}(r_0\eta)^2\frac{p'}{p}[1+(\mathbf{em})^2]$$
$$\times\, F(\mathbf{q})S^{1/2}[F'(\mathbf{q})\,(S')^{1/2} - F(\mathbf{q})S^{1/2}]$$
$$\times\,\frac{1}{\pi}\Pi(\Delta E - i\mathscr{E}, \boldsymbol{\tau}\pm\mathbf{q})\left[n(\Delta E)+\frac{1}{2}\pm\frac{1}{2}\right], \tag{5.7}$$

where τ is a reciprocal lattice vector, multiplied by 2π, and

$$\Pi(\Delta E - i\mathscr{E}, \boldsymbol{\tau}\pm\mathbf{q}) = \sum_{n=1}^{N}\{e^{\mp i\mathbf{q}(\mathbf{1}-\mathbf{n})}\operatorname{Im} G_{1n}(\Delta E - i\mathscr{E})$$
$$+\, e^{\mp i\mathbf{q}(\mathbf{n}-\mathbf{1})}\operatorname{Im} G_{n1}(\Delta E - i\mathscr{E})\}. \tag{5.8}$$

In carrying out the summation over n and m in formula (5.4), leading to (5.6), we have used the expansion of the Green's function G_{nm} in Fourier series in accordance with (4.4). For example,

$$\sum_{n,m=1}^{N} e^{i\mathbf{q}(\mathbf{n}-\mathbf{m})}G_{nm} = \sum_{n}\sum_{\mathbf{k}} G^{(n)}(\mathbf{k})\,\delta_{\mathbf{k},\boldsymbol{\tau}-\mathbf{q}} = \sum_{n} G^{(n)}(\boldsymbol{\tau}-\mathbf{q}).$$

In formula (5.8) one can similarly complete the summation over n for the first term, which then gives the expression

$$\sum_{n=1}^{N} e^{\mp i\mathbf{q}(\mathbf{1}-\mathbf{n})}\operatorname{Im} G_{1n}(\Delta E - i\mathscr{E}) = \operatorname{Im} G^{(1)}(\Delta E - i\mathscr{E}, \boldsymbol{\tau}\pm\mathbf{q}),$$

which is quite complicated when written out explicitly, and will not be given here.

We note that when S′ = S and F′(q) = F(q), expressions (5.5) and (5.7) vanish, and the remaining expression (5.6), under the condition J′ = J, will describe the coherent scattering of the ideal crystal. Formula (5.5) describes purely incoherent one-magnon scattering, whereas (5.7) and (5.6) together determine the coherent part of the scattering of the crystal containing the impurity.

The expression for G_{11} was given in Sec. 4 [formula (4.3)]. The sum over n in (5.6) can be written, using the relation (4.9), as

$$\sum_{n} G^{(n)}(\Delta E - i\mathscr{E}, \boldsymbol{\tau}\pm\mathbf{q}) = NG^0(\Delta E - i\mathscr{E}, \boldsymbol{\tau}\pm\mathbf{q})$$
$$+\, W(\Delta E - i\mathscr{E}, \boldsymbol{\tau}\pm\mathbf{q})/D, \tag{5.9}$$

where W/D is given by (4.15). It follows that all the singularities of the scattering cross section determined by (5.6) are related to the conditions for existence of local vibrations of the s, p and d types, which, as we see from (4.15), contribute additively to the cross section. At the same time it follows from expression (4.3) for G_{11} that the singularities of the cross section for the incoherent part of the scattering (5.5) are determined by the condition for existence of local vibrations of the s type only.

Let us consider in more detail the incoherent part of the cross section. The energy dependence of this cross section is determined by the imaginary part of the Green's function G_{11}. Using the relation between the different Green's functions for the ideal crystal,[8] we can transform (4.3) to the simple form:

$$G_{11}(E) = \left\{\left[1+\frac{\rho}{z}\,\frac{2JSz-E}{2JS}\right]G_{11}{}^{0} + \frac{\rho}{2JSz}\right\}\Big/\, D(s). \tag{5.10}$$

We separate out the imaginary part of $G_{11}(E - i\mathscr{E})$, for which we note that

$$D(s, E - i\mathscr{E}) = \operatorname{Re} D(s) + i \operatorname{Im} D(s), \qquad (5.11)$$

where, as is easily shown from (3.5),

$$\operatorname{Re} D(s) = 1 + 2\gamma + \gamma^2 - \varepsilon\rho - \rho(2JSz - E)\,/\,2JSz + M \operatorname{Re} G_{11}{}^0, \qquad (5.12)$$

$$\operatorname{Im} D(s) = M \operatorname{Im} G_{11}{}^0 = \pi M g_0(E), \qquad (5.13)$$

$$M = -2JSz\varepsilon + (2JSz - E)(2\gamma + \gamma^2 - \varepsilon\rho) - \rho(2JSz - E)^2\,/\,2JSz, \qquad (5.14)$$

where $g_0(E)$ is the density of spin wave states for the ideal crystal.

Starting from expressions (5.10) and (5.11), one can show that

$$\frac{1}{\pi} \operatorname{Im} G_{11}(E - i\mathscr{E}) = \Big\{\Big[1 + \frac{\rho}{z}\frac{2JSz - E}{2JS}\Big] \operatorname{Re} D(s) \Big/ \{[\operatorname{Re} D(s)]^2 + [\pi M g_0(E)]^2\} - M\Big[\Big(1 + \frac{\rho}{z}\frac{2JSz - E}{2JS}\Big)\operatorname{Re} G_{11}{}^0 + \frac{\rho}{2JSz}\Big] \Big/ \{[\operatorname{Re} D(s)]^2 + [\pi M g_0(E)]^2\}\Big\} g_0(E). \qquad (5.15)$$

We see that the analytic properties of the cross section as a function of the argument $E = \Delta E$, depend essentially on whether the local level $E = E_S$, which is a root of the equation

$$\operatorname{Re} D(s) = 0, \qquad (5.16)$$

lies in the region of the continuous spin wave spectrum of the ideal crystal (case a), or above it (case b). Formula (5.15) describes both cases, but can be transformed differently in the two cases.

Case a. At the point $E = E_S$, $\operatorname{Im} D(s) \neq 0$, because $g_0(E_S) \neq 0$. The denominator of (5.16) does not vanish, but reaches its minimum value at the point $E = E_S$. Thus, near this point the function (5.15) has a definite maximum, whose sharpness is determined by the value of $\pi M g_0(E_S)$.

Near the point $E = E_S$, the quantity $\operatorname{Re} D(s)$ can be expanded in series:

$$\operatorname{Re} D(s) = (E - E_s) \operatorname{Re} D'_{E=E_s}(s) + \ldots, \qquad (5.17)$$

Substituting this expansion in (5.15), we find that

$$\pi^{-1} \operatorname{Im} G_{11}(E - i\mathscr{E}) \sim \Gamma_s\,/\,\pi[(E - E_s)^2 + \Gamma_s{}^2], \qquad (5.18)$$

$$\Gamma_s = -\pi M g_0(E_s) / \operatorname{Re} D'_{E=E_s}(s). \qquad (5.19)$$

Thus, near the virtual level of the local vibration, formula (5.18), and consequently the cross section (5.5), has a resonance bump described by a Lorentzian line with width Γ_S, corresponding to the damping of the local level because of interaction with the levels of the continuous spectrum of the crystal. If Γ_S is comparable to E_S, (5.18) will not give a definite maximum.

Case b. If the level $E = E_S$ is above the band, then for values of the argument E lying within the band the cross section is given by the function (5.15) which contains no singularities. Outside the band the expression (5.15) is zero, because the function $g_0(E)$ is equal to zero everywhere except at the point $E = E_S$ at which the denominator vanishes. Going to the limit $E \to E_S$, we find that outside the limits of the band the expression (5.15) is proportional to $\delta(E - E_S)$. A similar treatment can be given for the coherent part of the scattering.

The treatment given in this section permits us to draw the following conclusions:

1. Slow neutrons when scattered by a ferromagnetic crystal containing an impurity can excite local magnetic vibrations of types s, p, and d. One can therefore observe in the energy distribution of the inelastically scattered neutrons sharp peaks corresponding to those local vibrations for which the local levels lie above the spin wave band. But if the local levels fall within the band, the cross section may show maxima whose widths are determined by the damping of the local levels.

2. Only local levels of s type can participate in incoherent magnetic scattering, whereas vibrations of all three types participate in coherent scattering.

3. The peaks corresponding to local magnetic oscillations can be distinguished from those corresponding to local phonon vibrations, studied by Kagan and Iosilevskiĭ, because of the special angular dependence of the inelastic magnetic scattering associated with the factor $1 + (\mathbf{e} \cdot \mathbf{m})^2$.

In this paper we have given a general treatment of the problem. A detailed specific analysis of the conditions under which one gets local magnetic vibrations is more difficult than for the case of local lattice vibrations because of the large number of parameters describing the local magnetic vibrations. In a later paper we shall give such an analysis based on numerical computations. We also intend to discuss in detail the multi-impurity problem for a ferromagnet.

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