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## Spin-wave theory of impurity states in a Heisenberg ferromagnet with planar anisotropy

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**Abstract.** The linear spin-wave theory of a single magnetic impurity in a Heisenberg ferromagnet with planar single-ion anisotropy is presented. The impurity–host exchange is assumed to be ferromagnetic or antiferromagnetic and the ground state of the host taken to be the classical aligned state. The calculation consists of deriving the double-time thermodynamic Green function from the corresponding equation of motion. From the poles of the Green functions the criteria for the impurity modes are obtained and calculations of their energies as functions of various perturbation parameters and for various values of the anisotropy given.

### 1. Introduction

There has been much interest in the effect of impurities on the continuous energy spectrum of the elementary excitations in solids. The perturbation produced by the impurity is characterised by its spatial extent, and for sufficiently small perturbations the energy levels of the impurity–host system may be solved exactly. The impurity and perturbed region of the host form a complex with discrete energy levels that may lie within or outside the energy band of the host, virtual and localised states, respectively. The virtual levels decay into the band with a finite lifetime and may have a significant effect on the thermodynamic properties of the system. Localised levels have a long lifetime and in general are of less importance to the thermodynamic properties but may have an important role in magneto-optical transitions.

The literature on the effects of impurities in simple metals, crystals and ferromagnets is very extensive. There have been several reviews and we refer the reader to those by Izyumov (1965) and Maradudin (1966).

The energy states in an isotropic Heisenberg ferromagnet containing a ferromagnetically coupled impurity have been examined by Wolfram and Callaway (1963), Takeno (1963) and Izyumov and Medvedev (1965). They find that the energy levels may be classified according to the symmetry elements of the crystal lattice. The corresponding problem for an antiferromagnetically coupled impurity has been discussed by Ishii *et al* (1965) and Parkinson (1967). In addition to the energy modes found with the ferromagnetically coupled impurity there always exists a localised mode below the energy band of the host. This mode may be understood as one in which the impurity precesses in a natural sense and the host spins driven through the exchange coupling precesses in the same sense.

The problem of the inelastic one-magnon–neutron cross section in the isotropic Heisenberg ferromagnet with a ferromagnetically or antiferromagnetically coupled impurity has been considered by Izyumov and Medvedev (1965) and Lovesey (1967).

Lovesey (1968a, b) considered the linear spin-wave theory of a single magnetic impurity in a body-centred Heisenberg antiferromagnet and calculated the inelastic neutron cross section in the case of positive and negative impurity–host exchange coupling.

Parkinson (1969a, b) has applied the theory of defects in antiferromagnetic insulators to discuss optical properties of perovskite and layer antiferromagnets with  $K_2NiF_4$  structure.

On the other hand, ferromagnetic systems with planar anisotropy have received much theoretical and experimental attention too. As in antiferromagnets the ground state of the Heisenberg ferromagnet with planar (or general non-axial) single-ion anisotropy is unknown and obtaining a systematic treatment of the anisotropy is difficult. In a series of papers (see Lindgard and Kowalska (1976), Rastelli and Lindgard (1979) and Rastelli and Tassi (1984) and references therein), Lindgard and coworkers have analysed the pure Heisenberg ferromagnet with planar anisotropy and derived low temperature spin-wave renormalisation for that system by means of a perturbation expansion in  $n_q/S$ ,  $d/S$  and  $n_q d/S$  (where  $n_q$  is the spin-wave population factor,  $S$  is the spin of the system and  $d$  is the renormalised anisotropy).

We consider in this paper the spin-wave theory of the Heisenberg ferromagnet with planar anisotropy containing a single magnetic impurity ferromagnetically or antiferromagnetically coupled to the host.

The model Hamiltonian may be written

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \quad (1.1)$$

where  $\mathcal{H}_0$  is the Hamiltonian of the pure host and  $\mathcal{H}_1$  accounts for a single impurity ion of spin  $S'$  coupled to the host by an exchange integral of magnitude  $J'$ . With only nearest-neighbour coupling ( $J > 0$ ),  $\mathcal{H}_0$  is

$$\mathcal{H}_0 = -J \sum_{\langle n, \delta \rangle} \hat{S}_n \cdot \hat{S}_{n+\delta} + D \sum_n (\hat{S}_n^x)^2 \quad (1.2)$$

$D > 0$  is the single-ion planar anisotropy strength and  $\hat{S}_n$  is the spin operator of the site  $n$ .  $\delta$  is the vector connecting nearest neighbours. The impurity Hamiltonian  $\mathcal{H}_1$  is given by

$$\mathcal{H}_1 = 2J \sum_{n(0)} \hat{S}_n \cdot \hat{S}_0 + 2J' \sum_{n(0)} \hat{S}_n \cdot \hat{S}'_0 - D(\hat{S}'_0)^2 + D'(\hat{S}'_0^x)^2 \quad (1.3)$$

where  $0$  denotes the impurity site and the anisotropy strength  $D'$  is in general different from  $D$ . In the case of large spin  $S$  and low temperatures, Rastelli and Lindgard (1979) proved that the linear spin-wave theory is a good working approximation. It is introduced through the following transformation. For the host,

$$\hat{S}_n^- = \sqrt{2S} \hat{a}_n^+ \quad \hat{S}_n^+ = \sqrt{2S} \hat{a}_n \quad \hat{S}_{nz} = S - \hat{a}_n^+ \hat{a}_n. \quad (1.4a)$$

For a ferromagnetic impurity,

$$\hat{S}'_0^- = \sqrt{2S'} \hat{a}'_0^+ \quad \hat{S}'_0^+ = \sqrt{2S'} \hat{a}'_0 \quad \hat{S}'_{0z} = S' - \hat{a}'_0^+ \hat{a}'_0. \quad (1.4b)$$

For antiferromagnetic impurity,

$$\hat{S}'_0^- = \sqrt{2S'} \hat{a}'_0 \quad \hat{S}'_0^+ = \sqrt{2S'} \hat{a}'_0^+ \quad \hat{S}'_{0z} = -S' + \hat{a}'_0^+ \hat{a}'_0. \quad (1.4c)$$

$\mathcal{H}$  reduced to terms quadratic in the spin deviation operators  $\hat{a}_n$  and  $\hat{a}_n^+$ .  $\hat{a}_n$  and  $\hat{a}_n^+$  satisfy Bose commutation rules.

In section 2, we give the formalism of Green functions applied to our system and derive their equations of motion. In section 3, numerical calculations of the energies of the various ferromagnetic impurity modes are presented and their dependence on the anisotropy of the host analysed. In section 4, the case of the antiferromagnetic impurity is presented. The conclusions are given in section 5.

## 2. The Green functions and their equations of motion

The Green function that we use is the thermodynamic two-time retarded Green function for Bose operators  $\hat{a}_n$ :

$$G_{mn}(t) = -i\vartheta(t)\langle[\hat{a}_m(t), \hat{a}_n^+(0)]_-\rangle \equiv \langle\langle \hat{a}_m(t); \hat{a}_n^+(0) \rangle\rangle \quad (2.1)$$

which satisfies the following equation of motion:

$$E\langle\langle \hat{a}_m; \hat{a}_n^+ \rangle\rangle_E = \delta_{mn} + \langle\langle [\hat{a}_m, \mathcal{H}]_-; \hat{a}_n^+ \rangle\rangle_E. \quad (2.2)$$

$\vartheta(t)$  is the unit step function,  $\delta_{mn}$  is the Kronecker symbol,  $[\hat{a}_m, \hat{a}_n]_-$  is the commutator of  $\hat{a}_m$  and  $\hat{a}_n$ , and  $\langle \dots \rangle$  represents the average over the grand canonical ensemble at a temperature  $\beta = 1/k_B T$ .

The necessary theory of the Green functions is given in the review by Zubarev (1960).

In order to obtain an explicit expression for the Green functions it is necessary to approximate the higher-order Green functions that occur in the equation of motion. This decoupling is for the low temperatures into the approximate ground state (linear in  $D/J$ ) in which all the spins are aligned, and is automatically obtained when the linearised Holstein–Primakoff (HP) transformation in the Hamiltonian was used.

On the right-hand side of equation (2.2) another Green function is generated

$$K_{mn}(E) = \langle\langle \hat{a}_m^+; \hat{a}_n^+ \rangle\rangle_E. \quad (2.3)$$

The equation of motion for  $K_{mn}$  is

$$E\langle\langle \hat{a}_m^+; \hat{a}_n^+ \rangle\rangle_E = \langle\langle [\hat{a}_m^+, \mathcal{H}]_-; \hat{a}_n^+ \rangle\rangle_E. \quad (2.4)$$

If we calculate explicitly the commutators in (2.2) and (2.4) and introduce some appropriate abbreviations we obtain the following system of equations:

$$\begin{aligned} (E - A)G_{mn} - DSK_{mn} + 2JS \sum_{i(m)} G_{in} &= \delta_{mn} + \Lambda_{mn} \\ (E + A)K_{mn} + DSG_{mn} - 2JS \sum_{i(m)} K_{in} &= -\Theta_{mn} \end{aligned} \quad (2.5)$$

with

$$A = 2ZJS + DS \quad (2.6)$$

where  $Z$  is the number of nearest neighbours. In the following we consider the case of simple cubic lattice where  $Z = 6$ :

$$\begin{aligned} \Lambda_{mn} &= (12JS\varepsilon\delta_{0m} + 2JS\rho\Delta_{0m} + DS\theta\delta_{0m})G_{mn} \\ &+ DS\theta\delta_{0m}K_{mn} - 2JS\gamma\Delta_{0m}G_{0n} - 2JS\gamma\delta_{0m} \sum_{i(m)} G_{in} \end{aligned} \quad (2.7a)$$

$$\begin{aligned} \Theta_{mn} &= (12JS\varepsilon\delta_{0m} + 2JS\rho\Delta_{0m} + DS\theta\delta_{0m})K_{mn} \\ &+ DS\theta\delta_{0m}G_{mn} - 2JS\gamma\Delta_{0m}K_{0n} - 2JS\gamma\delta_{0m} \sum_{i(m)} K_{in} \end{aligned} \quad (2.7b)$$

where  $\Delta_{mn}$  is equal to unity if indices  $n, m$  connect nearest neighbours and otherwise is

zero. The perturbation parameters are

$$\begin{aligned}\varepsilon &= J'/J - 1 & \rho &= J'S'/JS - 1 \\ \theta &= D'S'/DS - 1 & \gamma &= J'/J\sqrt{S'/S} - 1.\end{aligned}\quad (2.8)$$

Symbolically we can write the system (2.5) as

$$\hat{\mathbf{G}} = \hat{\mathbf{G}}^0 + \hat{\mathbf{K}}^0 \hat{\Theta} + \hat{\mathbf{G}}^0 \hat{\Lambda} \quad \hat{\mathbf{K}} = \hat{\mathbf{K}}^0 + \hat{\mathbf{G}}^0(-E)\hat{\Theta} + \hat{\mathbf{K}}^0 \hat{\Lambda} \quad (2.9)$$

with

$$\hat{\Lambda} = \hat{\mathbf{V}}_1 \hat{\mathbf{G}} + \hat{\mathbf{V}}_2 \hat{\mathbf{K}} \quad \hat{\Theta} = \hat{\mathbf{V}}_1 \hat{\mathbf{K}} + \hat{\mathbf{V}}_2 \hat{\mathbf{G}} \quad (2.10)$$

$\mathbf{G}^0$  and  $\mathbf{K}^0$  are the pure system Green functions:

$$G_{mn}^0(E) = \frac{1}{N} \sum_{\mathbf{k}} \frac{E + 12JS + DS - 2JS\gamma_{\mathbf{k}}}{E^2 - E^2(\mathbf{k})} \exp[i\mathbf{k} \cdot (\mathbf{m} - \mathbf{n})] \quad (2.11a)$$

$$K_{mn}^0(E) = \frac{1}{N} \sum_{\mathbf{k}} \frac{-DS}{E^2 - E^2(\mathbf{k})} \exp[i\mathbf{k} \cdot (\mathbf{m} - \mathbf{n})]. \quad (2.11b)$$

$N$  is the number of atoms in the lattice and  $\mathbf{k}$  is the wavevector of the first Brillouin zone.  $V_1$  and  $V_2$  are the impurity perturbation matrices:

$$\begin{aligned}(V_1)_{mm'} &= (12JS\varepsilon\delta_{0m} + 2JS\rho\Delta_{0m} + DS\theta\delta_{0m})\delta_{mm'} \\ &\quad - 2JS\gamma\Delta_{0m}\delta_{mm'} - 2JS\gamma\delta_{0m}\Delta_{mm'}\end{aligned}\quad (2.12a)$$

$$(V_2)_{mm'} = DS\theta\delta_{0m}\delta_{mm'} \quad (2.12b)$$

for the ferromagnetic impurity case.

In the case of the antiferromagnetic impurity,  $V_1$  and  $V_2$  are

$$\begin{aligned}(V_1)_{mm'} &= (12JS\varepsilon\delta_{0m} + 2JS\rho\Delta_{0m} + DS\theta\delta_{0m})\delta_{mm'} \\ &\quad + 2JS\Delta_{0m}\delta_{0m'} + 2JS\delta_{0m}\Delta_{mm'}\end{aligned}\quad (2.12c)$$

$$(V_2)_{mm'} = DS\theta\delta_{0m}\delta_{mm'} + 2JS(\gamma + 1)(\Delta_{0m}\delta_{0m'} + \delta_{0m}\Delta_{mm'}). \quad (2.12d)$$

$E(\mathbf{k})$  is the dispersion relation for linear spin waves in the pure host:

$$E^2(\mathbf{k}) = 4JS(6 - \gamma_{\mathbf{k}})[JS(6 - \gamma_{\mathbf{k}}) + DS] \quad (2.13)$$

with  $\gamma_{\mathbf{k}} \equiv \sum_{\delta} \exp(i\mathbf{k} \cdot \delta)$ , obtained from the system (2.5) by excluding the impurity site Green function matrix elements.

Equation (2.13) differs from the corresponding equation (17) of Rastelli and Lindgard (1979) by the factor  $1 - 1/2S$  multiplying  $DS$  in (2.13). They obtained that factor by renormalising spin waves beyond the linear HP transformation. If we restrict our attention to large spins ( $S > 1$ ), our equation (2.13) is a good approximation of the result of Rastelli and Lindgard.

Having this in mind, we can solve the impurity–host system (2.5) for the Green functions  $\mathbf{G}$  and  $\mathbf{K}$ :

$$\begin{aligned}\hat{\mathcal{D}}(E)\hat{\mathbf{G}} &= \hat{\mathbf{G}}^0 + \hat{\mathbf{K}}^0\hat{\mathbf{V}}_1[1 - \hat{\mathbf{G}}^0(-E)\hat{\mathbf{V}}_1 - \hat{\mathbf{K}}^0\hat{\mathbf{V}}_2]^{-1}\hat{\mathbf{K}}^0 \\ &\quad + \hat{\mathbf{G}}^0\hat{\mathbf{V}}_2[1 - \hat{\mathbf{G}}^0(-E)\hat{\mathbf{V}}_1 - \hat{\mathbf{K}}^0\hat{\mathbf{V}}_2]^{-1}\hat{\mathbf{K}}^0\end{aligned}\quad (2.14)$$

$$\begin{aligned}\hat{\mathcal{D}}(-E)\hat{\mathbf{K}} &= \hat{\mathbf{K}}^0 + \hat{\mathbf{K}}^0\hat{\mathbf{V}}_1(1 - \hat{\mathbf{G}}^0\hat{\mathbf{V}}_1 - \hat{\mathbf{K}}^0\hat{\mathbf{V}}_2)^{-1}\hat{\mathbf{G}}^0 \\ &\quad + \hat{\mathbf{G}}^0(-E)\hat{\mathbf{V}}_2(1 - \hat{\mathbf{G}}^0\hat{\mathbf{V}}_1 - \hat{\mathbf{K}}^0\hat{\mathbf{V}}_2)^{-1}\hat{\mathbf{G}}^0\end{aligned}$$

with

$$\begin{aligned}\hat{\mathcal{D}}(E) &= 1 - \hat{\mathbf{K}}^0\hat{\mathbf{V}}_2 - \hat{\mathbf{G}}^0\hat{\mathbf{V}}_1 - (\hat{\mathbf{K}}^0\hat{\mathbf{V}}_1 + \hat{\mathbf{G}}^0\hat{\mathbf{V}}_2) \\ &\quad \times [1 - \hat{\mathbf{G}}^0(-E)\hat{\mathbf{V}}_1 - \hat{\mathbf{K}}^0\hat{\mathbf{V}}_2]^{-1}[\hat{\mathbf{G}}^0(-E)\hat{\mathbf{V}}_2 + \hat{\mathbf{K}}^0\hat{\mathbf{V}}_1].\end{aligned}\quad (2.15)$$

$\hat{\mathcal{D}}(-E)$  is obtained from (2.15) by permuting energy signs in  $\hat{\mathbf{G}}^0(E \rightarrow -E)$ .

Since we are interested in the positions of impurity levels only, we shall concentrate our attention on the condition

$$\text{Re } D(E) \equiv \text{Re}[\det|\hat{\mathcal{D}}(E)|] = 0 \tag{2.16}$$

which determines the poles of  $\mathbf{G}$ , corresponding to impurity levels in the system.  $\text{Re } D(E)$  is the real part of the complex function  $D(E)$ .

In the limit of zero anisotropy ( $D \rightarrow 0$ ), the energy spectrum  $E(\mathbf{k})$  and Green function  $\hat{\mathbf{G}}^0(E)$  reduce to the well known expressions for the isotropic Heisenberg system, and  $\hat{\mathbf{K}}^0(E)$  vanishes. Equation (2.16) reduces to Izyumov's (1965) and Lovesey's (1967) results for the magnetic impurity in the isotropic Heisenberg ferromagnet, which can be seen by writing down the impurity matrices  $\hat{\mathbf{V}}_1$  and  $\hat{\mathbf{V}}_2$  for the simple-cubic nearest-neighbour case explicitly.

Equation (2.16) is in the nearest-neighbour case of the order  $Z + 1$  and can be factorised by transforming to the representation determined by the basis functions for the irreducible representations of the cubic point group. Thus (2.16) is split into three equations of the lower order:

$$\text{Re } D_p(E) = 0 \quad \text{Re } D_d(E) = 0 \quad \text{Re } D_s(E) = 0 \tag{2.17}$$

with

$$D_p(E) = 1 - 2JS\rho[G_{00}^0(E) - G_{12}^0(E)] - \frac{4J^2S^2\rho^2[K_{00}^0(E) - K_{12}^0(E)]^2}{\{1 - 2JS\rho[G_{00}^0(-E) - G_{12}^0(-E)]\}} \tag{2.18}$$

$$D_d(E) = 1 - 2JS\rho[G_{00}^0(E) + G_{12}^0(E) - 2G_{13}^0(E)] - \frac{4J^2S^2\rho^2[K_{00}^0(E) + K_{12}^0(E) - 2K_{13}^0(E)]^2}{\{1 - 2JS\rho[G_{00}^0(-E) + G_{12}^0(-E) - 2G_{13}^0(-E)]\}}. \tag{2.19}$$

The expressions for  $D_s(E)$  are too complicated to be explicitly written here. Owing to the symmetry properties in the final expression, only a few Green functions appear:  $G_{00}^0$  and  $K_{00}^0$ ,  $G_{12}^0$  and  $K_{12}^0$ , and  $G_{13}^0$  and  $K_{13}^0$ .  $G_{12}^0$  and  $K_{12}^0$  connect any pair of atoms placed symmetrically around the impurity;  $G_{13}^0$  and  $K_{13}^0$  connect any pair of nearest atoms in the first coordination sphere.

Solving (2.17), we obtain local spin states of the s, p and d type. p states are doubly degenerate, and d states triply degenerate. We note that they depend only on the single perturbation parameter  $\rho$ . In the limit of zero anisotropy, (2.18) and (2.19) reduce to Izyumov's results.

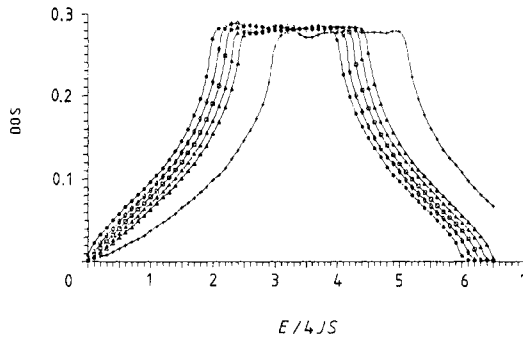
### 3. Numerical results: ferromagnetic impurity

Equations (2.17) are solved numerically. Green functions are obtained using the Simpson integration rule and the summation was done over 42 000 points in the reduced Brillouin zone in order to obtain the following sums:

$$\begin{aligned} S_1 &= \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{E^2 - E^2(\mathbf{k})} & S_3 &= \frac{1}{N} \sum_{\mathbf{k}} \frac{\gamma_{2k}}{E^2 - E^2(\mathbf{k})} \\ S_2 &= \frac{1}{N} \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}}{E^2 - E^2(\mathbf{k})} & S_4 &= \frac{1}{N} \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}\gamma_{2\mathbf{k}}}{E^2 - E^2(\mathbf{k})}. \end{aligned} \tag{3.1}$$

The small imaginary part of the complex energy was  $-0.02$ .

In the isotropic case, integrals over the Brillouin zone may be reduced to the complete elliptic integrals of the first kind, which saves computing time and increases the accuracy.



**Figure 1.** The influence of the anisotropy on the DOS in the pure host: ●,  $D/J = 0$ ; ◇,  $D/J = 0.5$ ; □,  $D/J = 1.0$ ; ▲,  $D/J = 1.5$ ; △,  $D/J = 2.0$ ; +,  $D/J = 5.0$ .

Energies of s, p and d modes are obtained as functions of the perturbation parameters  $S'/S$ ,  $J'/J$  and  $D/J$ . In order to reduce the number of independent parameters and to save the computing time, we have set  $D'/D = 1$  for most values of  $S'/S$ . A representative value of  $S'/S$  was chosen to examine the influence of different anisotropy constant  $D'$ .

We show the influence of the anisotropy on the density of states (DOS) in the pure system in figure 1. As the anisotropy increases the DOS near the top of the band is shifted towards higher energies, while the shape near the bottom of the band is deformed. The Goldstone symmetry is preserved.

In figure 2 the energies of the p and d modes are given as a function of the perturbation parameter  $J'S'/JS$  for different values of the anisotropy constant  $D/J$ . In the limit  $D \rightarrow 0$  we reproduce Izyumov's result. As the anisotropy increases, p and d states are shifted toward higher energies.

In figure 3 the energies of the virtual s modes that occur at the bottom of the band are shown as a function of  $J'/J$ , for different values of  $S'/S$ . As the parameter  $S'/S$  increases, the influence of the anisotropy becomes more pronounced. If  $S'/S > 1$ , resonant levels are moved deeper in the band with increase in the anisotropy and the interval  $J'/J$  in which they exist is reduced. However, for  $S'/S < 1$ , resonant levels are slightly shifted towards the bottom of the band with increase in the anisotropy, and this occurs only for larger values of the parameter  $J'/J$ .

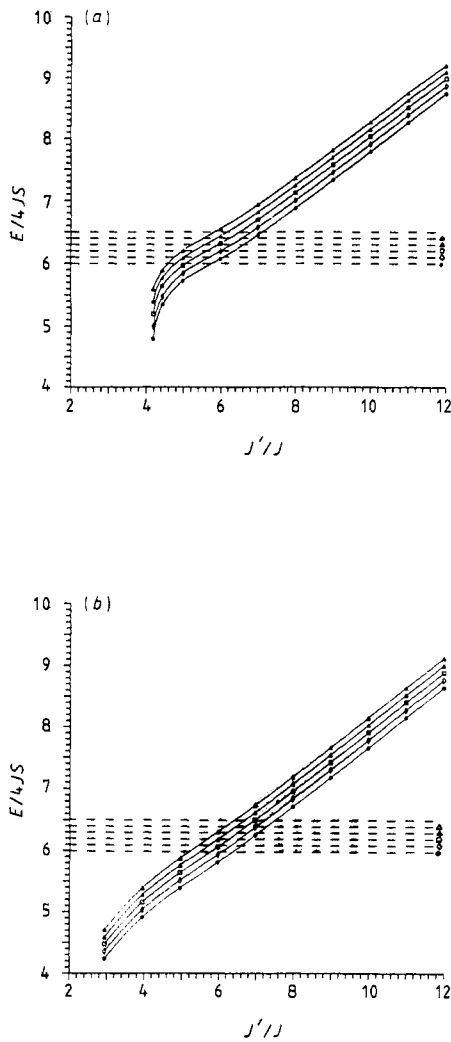
In figure 3(c) the impurity anisotropy constant  $D'$  is varied and the results compared with the appropriate curve for  $D' = D$  and  $D/J = 0.5$ , for three different values of  $D' \neq D$ . The influence of different impurity anisotropy constant  $D' \neq D$  on the resonant states near the bottom of the band is very pronounced. If  $D'/D < 1$  the change  $D' \neq D$  introduces a decrease in the energies of virtual states for the given  $J'/J$  and  $D/J$  compared with the case when  $D' = D$ . That decrease is more pronounced if  $D'/D$  is smaller.

In figure 4 the influence of the anisotropy on the energies of localised and resonant modes near the top of the band is shown. Again, the influence of the anisotropy becomes more pronounced with increase in the parameter  $S'/S$ . For  $S'/S > 1$  the influence of the anisotropy is almost independent of  $S'/S$ . There are no resonant modes near the top of the band for  $S'/S > 1$ .

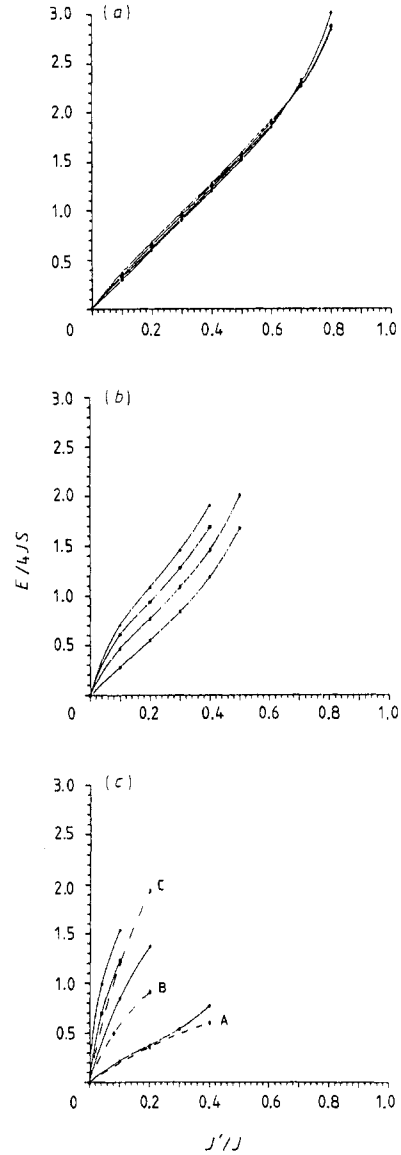
The impurity anisotropy constant  $D'$  is varied for parameter  $S'/S = 2$  and  $D/J = 0.5$ , and the results compared with the appropriate curve where  $D' = D$ , for three different values of  $D' \neq D$ . The influence of different impurity anisotropy constants  $D' \neq D$  on the localised states near the top of the band is not as pronounced as in the case of resonant states near the bottom of the band.

#### 4. Numerical results: antiferromagnetic impurity

As we have already mentioned, the solutions for s, p and d states are obtained numerically. In the case of the antiferromagnetic impurity the p- and d-type modes remain the

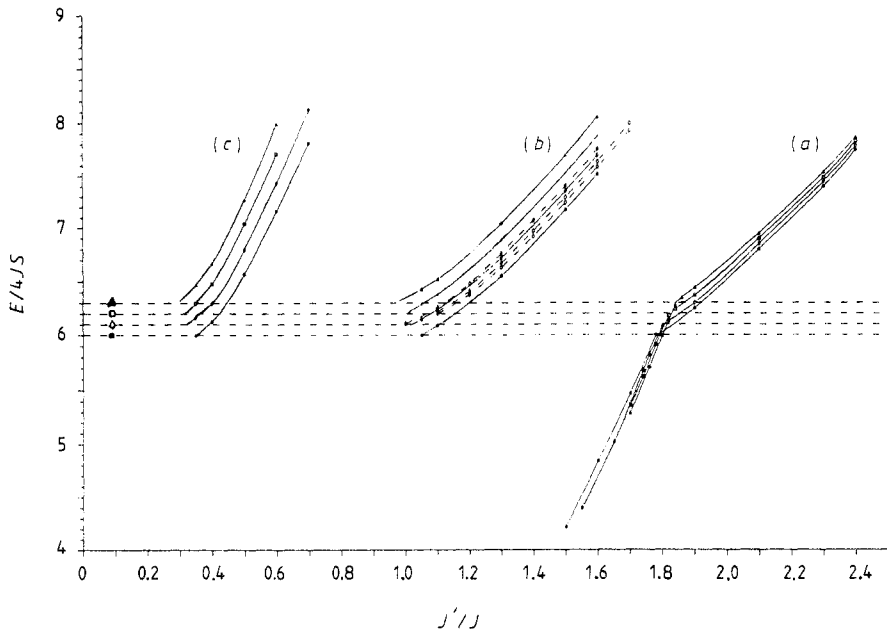


**Figure 2.** The influence of the anisotropy on (a) the p and (b) d states: ●,  $D/J = 0$ ; ◇,  $D/J = 0.5$ ; □,  $D/J = 1.0$ ; ▲,  $D/J = 1.5$ ; the broken horizontal lines represent the top of the band for the above values of  $D/J$  parameter.



**Figure 3.** For a ferromagnetic impurity; the influence of the anisotropy on the virtual s states near the bottom of the band for (a)  $S'/S = 0.25$ ; (b)  $S'/S = 2$  and (c)  $S'/S = 10.0$  and for different values of  $D'/D$ : —●—,  $D/J = 0$ ,  $D'/D = 1.0$ ; —◇—,  $D/J = 0.5$ ,  $D'/D = 1.0$ ; —□—,  $D/J = 1.0$ ,  $D'/D = 1.0$ ; —▲—,  $D/J = 1.5$ ,  $D'/D = 1.0$ ; curve A, ---,  $D/J = 0.5$ ,  $D'/D = 0$ ; curve B, -.-,  $D/J = 0.5$ ,  $D'/D = 0.5$ ; curve C, ---,  $D/J = 0.5$ ,  $D'/D = 1.5$ .





**Figure 4.** For a ferromagnetic impurity, the influence of the anisotropy on the top of the band for (a)  $S'/S = 0.25$ , (b)  $S'/S = 2.0$  and (c)  $S'/S = 10.0$ ; the symbols are as in figure 3.

same (because the state vector describing the p- and d-type impurity states have zero amplitude at the impurity site), but the s-type mode changes.

In this case there are antiresonant states which are located around the middle of the band, with a large negative width. They are more difficult to position but nevertheless the influence of the anisotropy is not significant and therefore they are not represented by the figure.

In the case of the antiferromagnetic impurity there are no resonant states near the bottom of the band, but there exist solutions for negative energies. As discussed by Izyumov and Medvedev (1973) these solutions are related to the inhomogeneity of the ground state around the impurity.

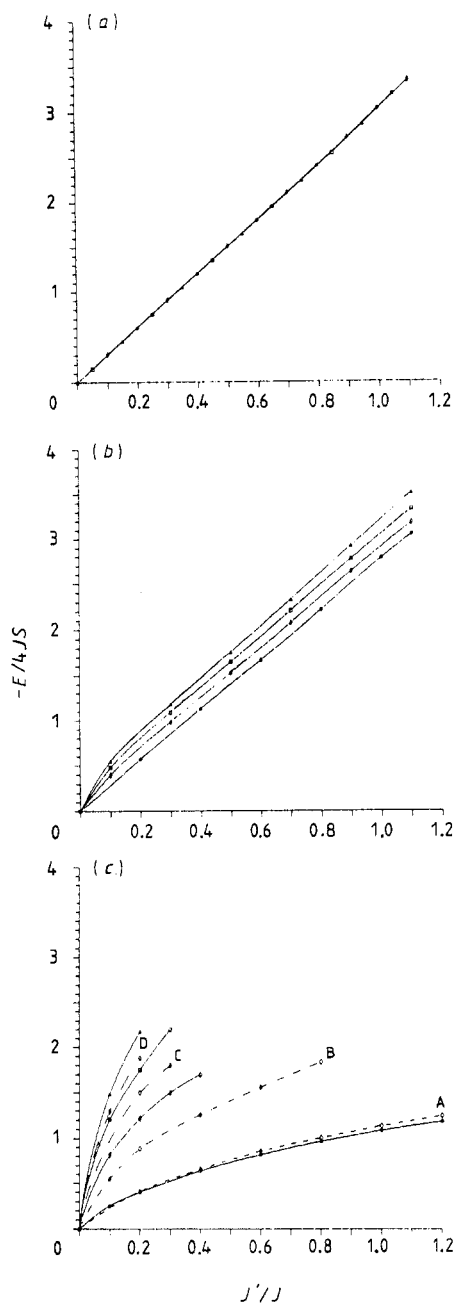
In figure 5 we show the influence of the anisotropy on negative solutions for different values of  $S'/S$ . For  $S'/S < 1$  the anisotropy has almost no influence on the inhomogeneity of the ground state. For  $S'/S \geq 1$  the range of that inhomogeneity is reduced with increase in the anisotropy. This influence is more pronounced for larger values of  $S'/S$ .

The influence of  $D' \neq D$  is demonstrated in figure 5(c) for  $D/J = 0.5$  and  $S'/S = 10.5$ . If  $D'/D < 1$  the range of the inhomogeneity of the ground state is extended compared with the case  $D' = D$ , in accordance with the decrease in  $D'/D$ .

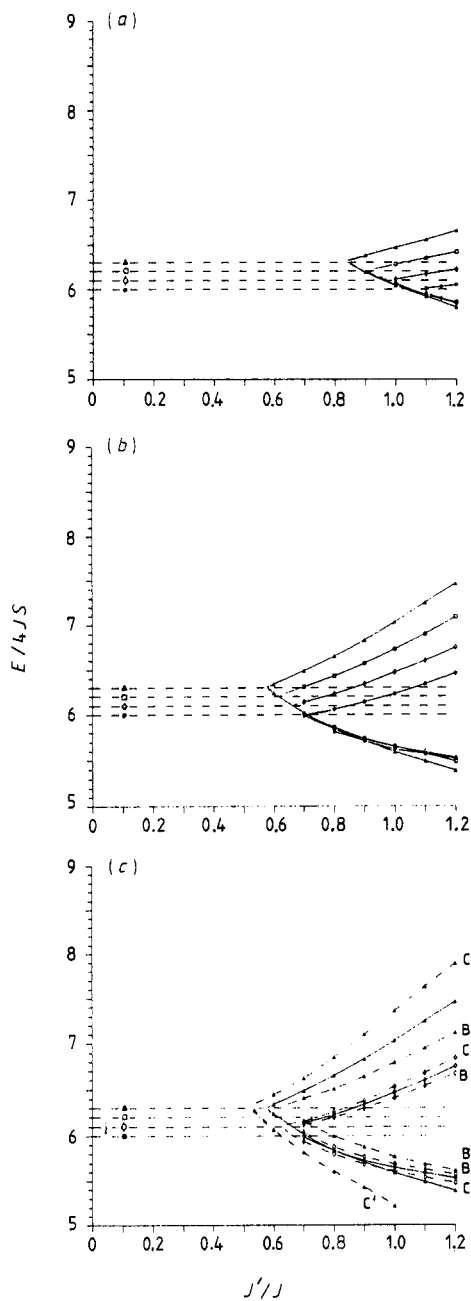
In figure 6 we show the influence of the anisotropy on the virtual and localised states near the top of the band for two different values of  $S'/S$ . Localised s states are shifted towards higher energies as the anisotropy increases. This shift is more pronounced for large values of  $J'/J$ .

The resonant s states near the top of the band are only slightly shifted towards higher energies with increase in the anisotropy, but the introduction of the anisotropy enlarges the range of  $J'/J$  in which both resonant and localised states near the top of the band exist.

The influence of the impurity anisotropy constant  $D' \neq D$  on the localised and resonant states near the top of the band is shown in figure 6(c) for  $S'/S = 8$  and two values



**Figure 5.** For an antiferromagnetic impurity, the influence of the anisotropy on the negative  $s$  solutions for (a)  $S'/S = 0.1$ , (b)  $S'/S = 1.0$  and (c)  $S'/S = 10.5$  and for different values of  $D'/D$ : the symbols and curves are as in figure 3; curve A:  $D/J = 0.5$ ,  $D'/D = 0$ ; curve B:  $D/J = 0.5$ ,  $D'/D = 0.5$ ; curve C:  $D/J = 0.5$ ,  $D'/D = 1.5$ ; curve D:  $D/J = 0.5$ ,  $D'/D = 2.0$ .



**Figure 6.** For an antiferromagnetic impurity, the influence of the anisotropy on the virtual and localised  $s$  states near the top of the band for (a)  $S'/S = 6.0$  and (b), (c)  $S'/S = 8.0$ . The symbols and curves are as in figure 3. Virtual and localised curves: B:  $D'/D = 0.5$ ,  $D/J = 0.5$ ; B':  $D'/D = 0.5$ ,  $D/J = 1.5$ ; C:  $D'/D = 1.5$ ,  $D/J = 0.5$ ; C':  $D'/D = 1.5$ ,  $D/J = 1.5$ . The broken horizontal lines are as in figure 2.

of  $D/J$ . As before, if  $D'/D < 1$ , the change  $D' \neq D$  introduces a decrease in the energies of localised states near the top of the band while, if  $D'/D > 1$ , the change introduces an increase in energies with respect to the case  $D' = D$ . For the resonant states near the top of the band, the opposite happens. If  $D/J$  is larger, this influence is more pronounced.

One can conclude that the impurity anisotropy constant  $D' \neq D$  significantly changes the total influence of anisotropy on the impurity states, i.e. the range of  $J'/J$  and energy range change with the introduction of a new parameter  $D' \neq D$ .

## 5. Conclusions

We have calculated the impurity energy states for a Heisenberg ferromagnet with planar anisotropy containing a single magnetic impurity ferromagnetically or anti-ferromagnetically coupled to the host, using the linear spin-wave approximation. p, d and most s modes are shifted towards higher energies as the anisotropy increases. In some cases, the interval of  $J'/J$  in which localised or resonant states exist is reduced when the anisotropy is included.

The antiresonant states are not much influenced by the anisotropy.

In the case of an antiferromagnetic impurity the negative solution near the bottom of the band is also influenced by the anisotropy in the case  $S'/S \geq 1$ . It is related to the inhomogeneity of the ground state around the impurity and the anisotropy reduces the range of that inhomogeneity.

The introduction of a different impurity anisotropy constant  $D' \neq D$  shows the interdependence of two parameters  $D/J$  and  $D'/J$  generally increases the total influence of the anisotropy if  $D'/D > 1$ . If  $D'/D < 1$  the total influence of the anisotropy is diminished.

All the experimental examples of systems with competing interactions known to us have more complex symmetry than simple cubic. Nevertheless, the above conclusions about the influence of the anisotropy on the localised and resonant states (in particular that the range of  $J'/J$  changes in which localised and resonant states exist and that this change in energy position for fixed  $S'/S$  and  $J'/J$  is introduced by the anisotropy) should hold for more realistic systems too. The work on an experimental example is in progress.

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## References

- Ishii H, Kanamori J and Nakamura T 1965 *Prog. Theor. Phys.* **33** 795
- Izyumov Yu A 1965 *Adv. Phys.* **14** 569
- Izyumov Yu A and Medvedev M V 1965 *Zh. Eksp. Teor. Fiz.* **49** 1887
- 1973 *Magnetically Ordered Crystals Containing Impurities* (New York: Consultants Bureau) pp 61–7
- Lindgard P A and Kowalska A 1976 *J. Phys. C: Solid State Phys.* **9** 2081
- Lovesey S W 1967 *Proc. Phys. Soc.* **91** 658
- Lovesey S W 1968a *J. Phys. C: Solid State Phys.* **1** 102
- 1968b *J. Phys. C: Solid State Phys.* **1** 118

- Maradudin A A 1966 *Solid State Phys.* **19** 1  
Parkinson J B 1967 *Solid State Commun.* **5** 419  
—— 1969a *J. Phys. C: Solid State Phys.* **2** 2003  
—— 1969b *J. Phys. C: Solid State Phys.* **2** 2012  
Rastelli E and Lindgard P A 1979 *J. Phys. C: Solid State Phys.* **12** 1989  
Rastelli E and Tassi A 1984 *J. Phys. C: Solid State Phys.* **17** 727  
Takeno S 1963 *Prog. Theor. Phys.* **30** 731  
Wolfram T and Callaway J 1963 *Phys. Rev.* **130** 2207  
Zubarev D N 1960 *Sov. Phys.-Usp.* **3** 320