TABLE III. $H_0+\Delta$ matrix.

$H_0+\Delta$	$[\psi(\frac{1}{2})]$	$[\psi(-\frac{1}{2})]$
$[\psi(\frac{1}{2})]$	$[H_0]+(1+\alpha_3)[\delta]$	$-(\alpha_1+i\ \alpha_2)[\delta]$
$[\psi(-\frac{1}{2})]$	$-(\alpha_1-i\ \alpha_2)[\delta]$	$[H_0]+(1-\alpha_3)[\delta]$

talline Stark effect) on the orbit, and then indirectly on the spin through the $\vec{L}\cdot\vec{S}$ coupling. (A recent work of Lowther[20] studies the effects of cubic and axial crystal fields on the spin-orbit splittings of the energy levels in rare-earth ions, but does not compute the anisotropy.) These mechanisms are much different from the ones in transition metals. We will thus not draw any conclusion for materials other than the transition metals.

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Distortion in an Impure Spiral Magnet

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A classical first-order calculation of the static distortion in a magnetic spiral with a magnetic impurity is performed. The distortion for any spin in the spiral is defined as its change of orientation in the ground state due to the impurity. The impurity is assumed to introduce a different spin on a particular site, and to change the exchange coupling of this spin with all others by a constant ratio. With these assumptions, a general expression for the distortion in any crystal with the spins arrayed on a Bravais lattice is derived. The expression is analytically evaluated for a special one-dimensional spiral. The distortion is found to be localized about the impurity for the one-dimensional case so one would expect good localization in higher dimensions due to the additional couplings. Nevertheless, the distortion has to be viewed as an extended rather than a point defect in the magnetic crystal.

I. INTRODUCTION

Magnetic spiral structures are well known to occur in nature.[1] In rare earths where the spins are large, ground-magnetic-state structures are often calculated by classical methods.[2] The interactions between spins in magnetic spirals are known to be of a range greater than nearest neighbor[3] and the presence of a magnetic impurity will cause torques to be exerted on spins in the locale of the impurity, and hence the spiral will be distorted in the whole neighborhood of the impurity. This distortion does not appear to have been explicitly considered in the literature before. However, the problems arising from long-range interactions between impurities and certain rare-earth-host crystals have been discussed.[4] A small concentration of magnetic impurities should have observable effects on elastic neutron scattering from spiral magnets. A more regular distortion, the "bunching" of spins due to hexagonal anisotropy, has had observable effects.[5]

Allowing long-range interactions, but assuming that the distortion produced by the impurity is small, this paper uses classical methods to derive a first-order expression for the distortion at any lattice site for any Bravais lattice of spins. It is assumed that the effect of the impurity is to introduce a different spin on a particular site and to modify the exchange coupling of this site with other sites by a constant ratio. The ground-state configuration of the impure crystal is obtained by minimizing the magnetic energy of the crystal in the same way that the ground-state configuration has been calculated by many authors[2,6] for perfect crystals. The resulting expression for the distortion would, in general, require numerical methods for its evaluation. In order to obtain some analytical results, a model of one-dimensional exchange coupling for a spiral, similar to one suggested by Nagamiya,[3] has been considered. For this model it is possible, in first order, to derive simple expressions for the distortion produced by a magnetic impurity in a crystal which has a spiral of arbitrary turn angle.

II. MODEL

Long-range Heisenberg coupling between the spins is assumed. The spins are further assumed to all reside in planes perpendicular to the z axis (which is thus the axis of the spiral) and so the Hamiltonian of the perfect crystal can be written[6]

$$H_0 = -S^2 \sum_{i,j} J_{ij} \cos(\phi_i - \phi_j), \tag{1}$$

where ϕ_i is the angle spin i (of magnitude S) makes with the x axis and J_{ij} characterizes the exchange coupling between spins i and j. It is further assumed that $J_{ii}=0$ and $J_{ij}=J_{ji}$. Spin i is assumed to be located at the lattice site $\vec{R}_i$. The impurity spin with magnitude S' is assumed to be placed at $\vec{R}_0$. If the exchange coupling J_{0j} is changed to μJ_{0j} by the impurity[4] and if we define

$$\rho = \mu(S'/S) - 1, \tag{2}$$

then the perturbation of the crystal by the impurity can be represented by the Hamiltonian

$$H_1 = -2S^2 \rho \sum_i J_{i0} \cos\phi_i, \tag{3}$$

where no twisting of the spins out of their planes is considered (from effective local field torque considerations, this is physically reasonable) and ϕ_0 is chosen to be zero to fix the one arbitrary angle. We define the distortion Δ_j at lattice site j by

$$\Delta_j = \phi_j - \vec{q}\cdot\vec{R}_j \equiv \phi_j - \alpha_j, \tag{4}$$

where $\alpha_j = \vec{q}\cdot\vec{R}_j$ is the equilibrium turn angle of the perfect crystal, i.e., $\vec{q}$ is along the z axis and the Fourier component of J_{ij} is a maximum when evaluated at the point in reciprocal space where $\vec{k}=\vec{q}$.

We assume ρ to be small so Δ_j will be small. With appropriate numbering of the crystal lattice, we choose $\phi_j = -\phi_{-j}$. The equilibrium configuration of spins is then determined by requiring

$$\frac{\partial}{\partial\phi_p}(H_0 + H_1) = 0. \tag{5}$$

Within the context of our model, this gives the exact condition

$$\sum_j J_{pj} \sin(\phi_j - \phi_p) = \rho J_{p0} \sin\phi_p. \tag{6}$$

To first order in ρ and Δ, Eq. (6) becomes, with $\Delta_{jp} = \Delta_j - \Delta_p$ and $\alpha_{jp} = \alpha_j - \alpha_p$,

$$\sum_j J_{pj} (\cos\alpha_{jp}) \Delta_{jp} = \rho J_{p0} \sin\alpha_p. \tag{7}$$

Equation (7) can be solved by Fourier analysis in reciprocal space. We assume periodic boundary conditions and write

$$J_{pj} = \frac{1}{N} \sum_{\vec{k}} e^{-i\vec{k}\cdot(\vec{R}_p - \vec{R}_j)} J(\vec{k}) \tag{8}$$

and

$$\Delta_j = \frac{1}{N} \sum_{\vec{k}'} e^{i\vec{k}'\cdot\vec{R}_j} \Delta(\vec{k}'), \tag{9}$$

where the sums over $\vec{k}$ and $\vec{k}'$ are over the first Brillouin zone. We substitute Eqs. (8) and (9) into (7), do a little manipulation, and find the following relatively simple expression for $\Delta(\vec{k})$;

$$\Delta(\vec{k}) = i\rho \frac{J(\vec{k}+\vec{q}) - J(\vec{k}-\vec{q})}{J(\vec{k}+\vec{q}) + J(\vec{k}-\vec{q}) - 2J(\vec{q})} \equiv -i\rho f(\vec{k}). \tag{10}$$

Using Eqs. (8) and (9) we can write

$$\Delta_j = \frac{\rho}{N} \sum_{\vec{k}} f(\vec{k}) \sin\vec{k}\cdot\vec{R}_j, \tag{11}$$

where $f(\vec{k})$ is defined by Eq. (10). This explicitly displays the expected property $\Delta_j = -\Delta_{-j}$.

III. ONE-DIMENSIONAL CASE

Following Nagamiya[3] we limit ourselves to nearest-neighbor and next-nearest-neighbor interactions. If a represents the distance between adjacent spins in our one-dimensional crystal, we thus write

$$J(k) = 2J_1 \cos(ka) + 2J_2 \cos(2ka). \tag{12}$$

Requiring $J(q)$ to be the absolute maximum for the range $-\pi < ka \leqslant \pi$, we find that Eq. (12) can be written

$$J(k) = 4J[\cos qa \cos ka - \tfrac{1}{4}\cos(2ka)], \tag{12'}$$

where J is an arbitrary positive constant measuring the over-all strength of the exchange coupling.

For our one-dimensional case, we use Eq. (12′) to evaluate $f(k)$ and substitute in Eq. (11). The sum over the Brillouin zone can be converted to an integral in the usual way. Making the substitution $y = ka$ for the dummy integration variable we find that Eq. (11) becomes

$$\Delta_n = -\frac{\rho}{2\pi}\sin(2qa)\int_0^{2\pi}\frac{\sin y\,\sin(ny)\,dy}{1-\cos(2qa)\cos y}\,. \qquad (13)$$

If we let $z = e^{iy}$ and integrate over the unit circle, Eq. (13) can readily be evaluated from the residues at the poles interior to the unit circle. The result is the following simple equation:

$$\Delta_n = -\rho\tan 2\theta\left(\frac{1-|\sin 2\theta|}{\cos 2\theta}\right)^n, \quad n>0; \qquad (14)$$

$$\Delta_0 = 0, \qquad (14')$$

$$\Delta_n = -\Delta_{-n}, \qquad (14'')$$

where $\theta = qa$ is the equilibrium turn angle of the perfect crystal between adjacent spins.

IV. DISCUSSION OF RESULTS

Equation (14) shows that the distortion is dependent on turn angle. This makes sense when one considers that the torque exerted on spins adjacent to the impurity is dependent on the angle they make with the impurity. From such considerations, one would expect no distortion for the ferromagnetic ($\theta = 0$) and antiferromagnetic ($\theta = \pi$) cases and this is what Eq. (14) predicts. For $\theta = 45°$, Eq. (14) predicts $\Delta_1 = -\Delta_{-1} = -\frac{1}{2}\rho$ and $\Delta_n = 0$ otherwise. For this case the distortion is of minimal range. Other angles show somewhat longer-range distortion but for all θ, $\Delta_n \to 0$ *as* $n \to \infty$. When $\theta = 30°$ one has for $n > 0$, $\Delta_n = -\rho\sqrt{3}\,(2-\sqrt{3}\,)^n$ and $\theta = 60°$ gives for the same case $\Delta_n = (-)^n\rho\sqrt{3}(2-\sqrt{3}\,)^n$. Equation (14) shows a type of compensation. For very small θ (in radians), $\Delta_n = -2\rho\theta(1-2\theta)^n$ with $n > 0$, so that although the distortion is very small it is also very long range. When the distortion becomes comparable to ρ (e.g., the $\theta = 45°$ case), then it also becomes rather short range. Actually the localization about the impurity would be expected from the structure of Eq. (11) which applies to one, two, or three dimensions. The fact that we do get localization in one dimension only confirms the belief that the additional couplings in higher dimensions will produce well-localized distortions about the impurity. The main point of this paper is to emphasize that a magnetic impurity in a magnetic spiral introduces a localized but not point defect as far as the change in the ground-state structure is concerned.

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