Symmetry Considerations in the Determination of Magnetic Structures

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The connection between magnetic structures and the symmetry of the crystal lattice is investigated in the zero-temperature limit. It is assumed that the magnetic energy is bilinear in the magnetic moments and has the full symmetry of the lattice. A standard group theoretical analysis leads to magnetic configurations belonging to irreducible representation of the space group. The requirement that equivalent magnetic moments have equal magnitude is treated as a set of subsidiary conditions. When these conditions can be fulfilled within one irreducible representation, one gets magnetic structures which are time independent for symmetry reasons.

It is shown how these structures can be found. The possibilities for lattices with a single moment per unit cell are discussed in detail, and the structures on a simple cubic lattice described. For the general case the extension to lattices with several magnetic moments per unit cell is discussed, and some general results are derived.

In general there may also exist additional magnetic structures which have no simple relationship to the crystal symmetry. Both the number and the form of such structures depend on the detailed interaction mechanism. This is demonstrated by comparing two simple examples which can be solved exactly.

I. INTRODUCTION

THE concept of a magnetic structure is essentially classical. An arrangement of magnetic moments on a crystal lattice is considered a structure if each of the moments is pointing in a definite direction parallel to the local field caused by its interactions with all the other moments and with the crystal lattice. These are the time independent states of a classical system of magnetic moments, at zero temperature, and the classical ground state will be one of them. The energy of the system is determined uniquely by the arrangement of the magnetic moments.

For a quantum mechanical system the structure is defined in terms of the expectation values of the individual moments and of the local fields. This is equivalent to the molecular field approximation.

The arrangements of magnetic moments in a crystal lattice have been discussed extensively in recent years. Belov *et al.*[1] and Tavger *et al.*[2] have tabulated the magnetic space and point groups. These describe the symmetry properties of all possible magnetic lattices. As shown in Indenbom,[3] these groups are all isomorphic to the ordinary space and point groups and can be obtained from the alternating representations of the latter.

A different approach was adopted in the work of Villain,[4] Yoshimori,[5] Kaplan,[6] Berthaut,[7] and many others. They have discussed the static arrangements which result when one assumes certain plausible interaction mechanisms. Usually only the translational symmetry of the crystal was taken into account.

The purpose of this work is to see how much information on magnetic structures can be obtained from the symmetry of the crystal lattice. We assume that the magnetic energy of the crystal (i.e., the energy associated with the magnetic structure) is invariant when the symmetry operations of the nonmagnetic space group[8] (NMSG) are applied separately to the crystal lattice or to the magnetic moments. Any magnetic configuration is transformed by the symmetry operations of the NMSG into an equivalent configuration with the same energy (which may or may not coincide with the original configuration). This immediately suggests that one try to describe magnetic structures in terms of the irreducible representations of the NMSG, and apply the group-theoretical techniques developed for investigating lattice vibrations and electronic band structures.[9,10] As in the case of lattice vibrations one has to restrict oneself to interactions which are bilinear in the coordinates (i.e., in the components of the magnetic moments). One can then proceed to find the magnetic configurations which transform like irreducible representations of the NMSG. For bilinear interactions these can always be chosen so that they formally describe time-independent states of the system.

Most of the configurations obtained in this way are, however, not valid solutions of our problem. We have defined a magnetic structure as an arrangement of magnetic dipoles on a lattice, and all equivalent magnetic dipoles must have the same magnitude. This means that a set of nonlinear subsidiary conditions is imposed on the problem. Most of the configurations one finds from symmetry considerations are lattice waves and do not fulfill these conditions. We will refer to magnetic states on which the subsidiary conditions have not been imposed as magnetic configurations. The term magnetic structures will be reserved for states which fulfill these conditions. For special values of the

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[1] N. V. Belov, N. N. Neporova, and T. S. Smirnorna, Trudy Inst. Krist. Akad. Nauk S.S.S.R. **2**, 33 (1955).

[2] B. A. Tavger and V. M. Zaitsev, J. Exptl. Theoret. Phys. (U.S.S.R.) **3**, 430 (1956).

[3] V. L. Indenbom, Kristallografiya **5**, 513 (1960), Transl. p. 493.

[4] T. Villain, J. Phys. Chem. Solids **11**, 303 (1959).

[5] A. Yoshimori, J. Phys. Soc. (Japan) **14**, 807 (1959).

[6] T. A. Kaplan, Phys. Rev. **116**, 888 (1959); T. A. Kaplan and D. H. Lyons, Phys. Rev. **120**, 1580 (1960).

[7] E. F. Berthaut, Compt. rend. **250**, 85 (1960), **252**, 76 (1961).

[8] Throughout this paper the NMSG is the space group determined by x rays when the crystal is in the magnetic state.

[9] M. Lax, Bell Telephone Laboratories, Lecture notes, 1960–61 (unpublished).

[10] G. F. Koster, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957), Vol. 5, p. 174.

wave vector (i.e., for certain discrete increases of the unit cell) and for $\mathbf{k}$'s in some symmetry directions in the crystal it is possible to form magnetic structures which belong to a definite irreducible representation of the NMSG and are time independent. We will show how these structures can be found.

Our approach is closely related to the spherical model of Luttinger and Tisza.[11] We neglect the subsidiary conditions on the magnitude of the moments in the initial symmetry considerations. The configurations obtained in this way would all be legitimate solutions within the spherical model. They have to be rejected when they are not consistent with the full subsidiary conditions on the magnitude of the individual moments.

2. MAGNETIC ENERGY AND STABILITY CONDITIONS

The most general expression for the magnetic energy which is bilinear in the magnetic moments is

$$E=\tfrac{1}{2}\sum_{ij,\nu\mu}(A_{ij}{}^{\nu\mu}\mathbf{S}_i{}^{\nu}\cdot\mathbf{S}_j{}^{\mu}+\mathbf{S}_i{}^{\nu}\cdot\mathbf{B}_{ij}{}^{\nu\mu}\times\mathbf{S}_j{}^{\mu}+\mathbf{S}_i{}^{\nu}\cdot\mathbf{C}_{ij}{}^{\nu\mu}\cdot\mathbf{S}_j{}^{\mu}), \quad (1)$$

where $\mathbf{S}_i{}^{\nu}$ is the magnetic moment at lattice site i and site ν in the unit cell, $A_{ij}{}^{\nu\mu}$ is a scalar, $\mathbf{B}_{ij}{}^{\nu\mu}$ an axial vector and $\mathbf{C}_{ij}{}^{\nu\mu}$ a symmetric tensor, and the summation is over all n sites in the unit cell (ν,μ) and over all unit cells in the crystal (i,j).

We will assume that the magnitude of the moments is absorbed into the interaction constants so that

$$(\mathbf{S}_i{}^{\nu})^2=1. \quad (2)$$

One can now define[7]

$$\mathbf{T}^{\nu}(\mathbf{k})=N^{-\frac{1}{2}}\sum_i \mathbf{S}_i{}^{\nu}e^{i\mathbf{k}\cdot(\mathbf{R}_i+\mathbf{r}_\nu)}, \quad (3)$$

where $\mathbf{k}$ is a wave vector in the first Brillouin zone of the reciprocal lattice, $\mathbf{R}_i$ is a lattice vector, $\mathbf{r}_\nu$ gives the position of ν in the unit cell, and the summation is over all N equivalent sites in the crystal.

From Eq. (2) $\mathbf{T}^{\nu}(-\mathbf{k})$ is the complex conjugate of $\mathbf{T}^{\nu}(\mathbf{k})$:

$$\mathbf{T}^{\nu}(\mathbf{k})^*=\mathbf{T}^{\nu}(-\mathbf{k}). \quad (4)$$

Using the reverse of Eq. (3),

$$\mathbf{S}_i{}^{\nu}=N^{-\frac{1}{2}}\sum_k \mathbf{T}^{\nu}(\mathbf{k})e^{-i\mathbf{k}\cdot(\mathbf{R}_i+\mathbf{r}_\nu)}, \quad (5)$$

one can describe any magnetic structure in terms of the $\mathbf{T}^{\nu}(\mathbf{k})$.

It is convenient to rewrite Eq. (1) as

$$E=\sum_{i,j}\mathbf{S}_i\cdot\mathbf{G}_{ij}\cdot\mathbf{S}_j, \quad (6)$$

where $\mathbf{S}_i$ is the $3n$-dimensional vector whose components are the components of the n $\mathbf{S}_i{}^{\nu}$, and $\mathbf{G}_{ij}$ is a $3n$-dimensional tensor obtained immediately from Eq. (1). One can then use Eq. (5) to obtain[7]

$$E=\sum_k \mathbf{T}(-\mathbf{k})\cdot\mathbf{\Gamma}(\mathbf{k})\cdot\mathbf{T}(\mathbf{k}), \quad (7)$$

where the $\mathbf{T}(\mathbf{k})$ are the $3n$-dimensional vectors derived from the $\mathbf{T}^{\nu}(\mathbf{k})$ and $\mathbf{\Gamma}(\mathbf{k})$ is the Fourier transform of $\mathbf{G}_{ij}$ whose submatrices $\mathbf{\Gamma}^{\mu\nu}(\mathbf{k})$ are defined as

$$\mathbf{\Gamma}^{\mu\nu}(\mathbf{k})=e^{i\mathbf{k}\cdot(\mathbf{r}_\mu-\mathbf{r}_\nu)}\sum_j \mathbf{G}_{ij}{}^{\mu\nu}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}. \quad (8)$$

Equation (7) can be separated further if the $\mathbf{T}(\mathbf{k})$ are written in terms of the eigenvectors of the Hermitian matrices $\mathbf{\Gamma}(\mathbf{k})$. In the absence of the subsidiary conditions these would be the eigenstates of the magnetic system. The eigenvectors of $\mathbf{\Gamma}(\mathbf{k})$ belong to definite irreducible representations of the NMSG, so that group theoretical procedures can be used to find them.

Berthaut[7] has suggested a physically more illuminating approach. Consider the equations of motion for an individual moment which follow from Eq. (1):

$$d\mathbf{S}_i{}^{\nu}/dt=\mathbf{S}_i{}^{\nu}\times\mathbf{h}_i{}^{\nu}, \quad (9)$$

where

$$\mathbf{h}_i{}^{\nu}=\sum_{j\mu}(A_{ij}{}^{\nu\mu}\mathbf{S}_j{}^{\mu}+\mathbf{B}_{ij}{}^{\nu\mu}\times\mathbf{S}_j{}^{\mu}+\mathbf{C}_{ij}{}^{\nu\mu}\cdot\mathbf{S}_j{}^{\mu}) \quad (10)$$

is the local field at the site i.v. A structure is time independent if every $\mathbf{S}_i{}^{\nu}$ is parallel to the local field $\mathbf{h}_i{}^{\nu}$ so that the rhs of Eq. (9) vanishes. This can be written

$$\lambda_i{}^{\nu}\mathbf{S}_i{}^{\nu}=\mathbf{h}_i{}^{\nu}, \quad (11)$$

where $\lambda_i{}^{\nu}$ is defined as the local field constant.

Equation (11) is also the equation one obtains if one uses Lagrange multipliers to minimize the energy (1) with the subsidiary conditions of Eq. (2).[12] This means that the simultaneous solution of Eqs. (11) and (2) are automatically extrema of the energy. All the time-independent magnetic structures possible in a specific case are given by these simultaneous solutions.

Because of the nonlinearity of the normalization conditions [Eq. (2)] it is very hard to make any general statements about the solutions of these equations or even to determine their number. The only structures which are always possible are those whose time independence is due to the symmetry properties of the system. We will discuss in detail the structures which are allowed because of the symmetry of the crystal (i.e., of the NMSG). It should be remembered, however, that the magnetic energy may have higher symmetry (as, e.g., for purely scalar interactions), which may lead to additional structures. For the solutions which are not determined by symmetry the arrangement of the magnetic moments and the number of solutions both depend on the detailed values of the interaction parameters, and no general information can be obtained.

The general solutions of these equations are discussed in Appendix A, where two simple examples in which all solutions can be found are also described.

For further reference it is useful to rewrite our equations in terms of the $\mathbf{T}^{\nu}(\mathbf{k})$. Equations (11) then become

$$\sum_\mu \mathbf{\Gamma}^{\nu\mu}(\mathbf{k})\cdot\mathbf{T}^{\mu}(\mathbf{k})=\sum_\kappa \lambda^{\nu}(\boldsymbol{\kappa})\mathbf{T}^{\nu}(\boldsymbol{\kappa}-\mathbf{k}), \quad (12)$$

[11] T. M. Luttinger and L. Tisza, Phys. Rev. **70**, 954 (1954).

[12] We are grateful to E. I. Blount for pointing this out to us.

where $\Gamma^{\nu\mu}(\mathbf{k})$ is defined in Eq. (8), and the summation on the left is over all n sites (μ) in the unit cell and on the right over all vectors $\boldsymbol{\kappa}$ in the first Brillouin zone, and

$$\lambda^{\nu}(\boldsymbol{\kappa})=\sum_i \lambda_i^{\nu}\exp(i\boldsymbol{\kappa}\cdot\mathbf{R}_i). \tag{13}$$

The subsidiary conditions [Eq. (2)] become

$$\sum_k \mathbf{T}^{\nu}(\mathbf{k})\cdot\mathbf{T}^{\nu}(\boldsymbol{\kappa}-\mathbf{k})=N\delta(\boldsymbol{\kappa}), \tag{14}$$

where $\delta(\boldsymbol{\kappa})$ is the Kronecker delta, the summation is over the first Brillouin zone in $\mathbf{k}$ space, and there is a separate equation for each $\boldsymbol{\kappa}$ in the zone and for each site (ν) in the unit cell.

The strong spherical model (SSM) used, e.g., by Freiser,[13] which requires

$$\sum_i(\mathbf{S}_i^{\nu})^2=N, \tag{15}$$

is equivalent to neglecting all the homogeneous equations in (14). A weaker restriction would be to require one condition:

$$\sum_{\nu}\sum_{i}(\mathbf{S}_i^{\nu})^2=nN; \tag{16a}$$

that is,

$$\sum_{k,\nu}\mathbf{T}^{\nu}(\mathbf{k})\cdot\mathbf{T}^{\nu}(\boldsymbol{\kappa}-\mathbf{k})=\sum_{k}\mathbf{T}(\mathbf{k})\cdot\mathbf{T}(\boldsymbol{\kappa}-\mathbf{k})=nN. \tag{16b}$$

We will refer to Eq. (16) as the weak spherical model (WSM). When there is only one magnetic site in the unit cell the SSM [Eq. (15)] and the WSM [Eq. (16)] are obviously equivalent.

3. CONFIGURATIONS CORRESPONDING TO IRREDUCIBLE REPRESENTATIONS OF THE SPACE GROUP

For a general element of the space group $\langle\alpha|\,\mathbf{v}\rangle$, with with the point operation α and the subsequent translation $\mathbf{v}$, one has

$$\langle\alpha|\,\mathbf{v}\rangle\mathbf{T}^{\nu}(\mathbf{k})=\exp[i(\alpha^{-1}\mathbf{k})\cdot\mathbf{v}]P_{\mu\nu}U(\alpha)\mathbf{T}^{\nu}(\mathbf{k})$$
$$=\{\mathbf{T}^{\mu}(\alpha^{-1}\mathbf{k})\}', \tag{17}$$

where $\alpha^{-1}\mathbf{k}$ is the wave vector into which $\mathbf{k}$ is transformed by the point operation α^{-1}, $P_{\mu\nu}$ permutes site ν into site μ in the unit cell, $U(\alpha)$ is the orthogonal (3-dimensional) matrix representing the point operation α, and $\{\mathbf{T}^{\mu}(\alpha^{-1}\mathbf{k})\}'$ is the wave at site μ *after* the symmetry operation.

It is seen from Eq. (17) that the representation of the space group in terms of the $\mathbf{T}^{\nu}(\mathbf{k})$ is already reduced to a large extent. Under pure translations ($\alpha=e$, the identity of the point group) all $\mathbf{T}^{\nu}(\mathbf{k})$ transform into themselves except for a phase factor ($e^{i\mathbf{k}\cdot\mathbf{v}}$). The other operations of the space group are of two types. Operations for which $\alpha\mathbf{k}=\mathbf{k}$ transform $\mathbf{T}^{\nu}(\mathbf{k})$ into a wave of the same $\mathbf{k}$. Together with the pure translations these operations form the group of the vector $\mathbf{k}$ ($H(\mathbf{k})$). The other operations of the group transform $\mathbf{k}$ into some other wave vectors (e.g., $\mathbf{k}'=\alpha\mathbf{k}$), which can be obtained from $\mathbf{k}$ by the operations of the point group of the crystal. These operations will transform $\mathbf{T}^{\nu}(\mathbf{k})$ into a wave with wave vector $\mathbf{k}'$. However, there is only a small number of vectors $\mathbf{k}'$ which are connected with $\mathbf{k}$ in this way. These vectors are defined as the star of $\mathbf{k}$. Any irreducible representation can be assigned to a definite star in $\mathbf{k}$ space. To obtain the irreducible components we will use the theory of the representations of space groups in the form developed by Lax.[9]

All vectors in a star have isomorphous groups with the same irreducible representations. The operations of the space group which carry $\mathbf{k}$ into some other vector $\mathbf{k}'$ transform the basis vectors of an irreducible representation of $H(\mathbf{k})$ into those of a similar representation of $H(\mathbf{k}')$ in a unique way. [This follows from the completeness of the space group and from the irreducibility of the representations of $H(\mathbf{k})$.] All the vectors obtained in this way from the representations of $H(\mathbf{k})$ form the basis for an irreducible representation of the space group. For a star with r different vectors an s-dimensional representation of $H(\mathbf{k})$ generates an rs-dimensional representation of the space group.

The point operations appearing in $H(\mathbf{k})$ form a point group $G(\mathbf{k})$. For symmorphic space groups, and for $\mathbf{k}$'s in the interior of the Brillouin zone also for nonsymmorphic groups, all relevant representations of $H(\mathbf{k})$ are obtained directly from those of the point group $G(\mathbf{k})$. For the group characters, one has[9]

$$\chi_{H(\mathbf{k})}{}^{\rho}[\langle\alpha|\,\mathbf{v}\rangle]=e^{i\mathbf{k}\cdot\mathbf{v}}\chi_{G(\mathbf{k})}{}^{\rho}[\alpha], \tag{18}$$

where $\chi_{H(\mathbf{k})}{}^{\rho}[\langle\alpha|\,\mathbf{v}\rangle]$ is the character of the element $\langle\alpha|\,\mathbf{v}\rangle$ in the representation ρ of $H(\mathbf{k})$, and $\chi_{G(\mathbf{k})}{}^{\rho}[\alpha]$ is the character of the point operation α in the corresponding representation of the point group $G(\mathbf{k})$. The same factor connects the representative matrices. Equation (18) also holds for most points on the zone boundary in nonsymmorphic groups. The methods for finding the representations where (18) fails were investigated in detail by Lax[9] and can be applied in a straightforward way.[14]

Equation (18) now enables us to find the magnetic configurations which transform like the irreducible representations of the NMSG. These are the $3n$-dimensional basis vectors $\boldsymbol{\tau}_s{}^{\rho}(\mathbf{k})$ of the irreducible representations of $H(\mathbf{k})$, in the $3n$-dimensional space defined by the $3n$ components of the n vectors $\mathbf{T}^{\nu}(\mathbf{k})$, together with the corresponding vectors for the other $\mathbf{k}$'s of the star.

In the definition of $\boldsymbol{\tau}_s{}^{\rho}(\mathbf{k})$, ρ designates the irreducible

[13] M. T. Freiser, Phys. Rev. **123**, 2003 (1961). The SSM leads to nonlinear equations (Sec. 7). An alternative approach which is more general than the WSM, but still linear, has been used by Lyons and Kaplan (second reference 6).

[14] Equation (18) fails only when for some point operations α and β in the point group $G(\mathbf{k})$, $e^{i(\beta\mathbf{k}-\mathbf{k})\cdot\mathbf{u}}\neq e^{i(\alpha\mathbf{k}-\mathbf{k})\cdot\mathbf{v}}$, where $\mathbf{u}$ and $\mathbf{v}$ are translations associated with α and β, respectively, in $H(\mathbf{k})$. In these cases $H(\mathbf{k})$ has no 1-dimensional representations. It's irreducible representations can be found from the multiplier representation of $G(\mathbf{k})$. The procedures are described in detail in reference 9.

representation of $H(\mathbf{k})$ to which it belongs, and s enumerates the different basis vectors for multidimensional representations. The wave vector $\mathbf{k}$ indicates the star to which the irreducible representation belongs and the specific wave vector to which the basis vector belongs. It is convenient to normalize the $\tau_s{}^{\rho}(\mathbf{k})$ so that

$$\begin{aligned}\tau_s{}^{*\rho}(\mathbf{k})\cdot\tau_s{}^{\rho}(\mathbf{k})&=\sum_{\nu=1}^{n}\gamma_s{}^{*\rho\nu}(\mathbf{k})\tau_s{}^{*\rho\nu}(\mathbf{k})\cdot\gamma_s{}^{\rho\nu}(\mathbf{k})\tau_s{}^{\rho\nu}(\mathbf{k}),\\&=\sum_{\nu=1}^{n}\gamma_s{}^{*\rho\nu}(\mathbf{k})\gamma_s{}^{\rho\nu}(\mathbf{k})=n,\end{aligned}\tag{19}$$

where the 3-dimensional vectors $\tau_s{}^{\rho\nu}(\mathbf{k})$ are unit vectors in the direction of the components of $\tau_s{}^{\rho}(\mathbf{k})$ in the subspaces of the respective sites in the unit cell [i.e., of the $\mathbf{T}^{\nu}(\mathbf{k})$], and the $\gamma_s{}^{\rho\nu}(\mathbf{k})$ are (complex) numbers. It should be noted that the $\tau_s{}^{\rho\nu}(\mathbf{k})$ may also be complex. In that case, they always have perpendicular real and imaginary parts of equal magnitude. To find the basis vectors $\tau_s{}^{\rho}(\mathbf{k})$ of the irreducible representations of $H(\mathbf{k})$, one calculates the characters of representative elements of the classes of $H(\mathbf{k})$ in the representation of the $\mathbf{T}^{\nu}(\mathbf{k})$. These characters can then be compared with those of the irreducible representations of $H(\mathbf{k})$ [Eq. (18)] in the usual way.

In doing this it is useful to remember that the group of the vector $\mathbf{k}$ has an invariant subgroup $T_{\mathbf{k}}$ of all translations for which $e^{i\mathbf{k}\cdot\mathbf{R}}=1$. Clearly, all elements of $H(\mathbf{k})$ which differ by such translations have the same effect on the $\mathbf{T}(\mathbf{k})$ and have identical representations. It is therefore sufficient to consider representations of the factor group $H(\mathbf{k})/T_{\mathbf{k}}$, which is much smaller than $H(\mathbf{k})$.

The $\tau_s{}^{\rho}(\mathbf{k})$ span the whole $3n$-dimensional space of $\mathbf{T}(\mathbf{k})$ so that $\mathbf{T}(\mathbf{k})$ can be expressed as

$$\mathbf{T}(\mathbf{k})=\sum_{\rho,s}a_s{}^{\rho}(\mathbf{k})\tau_s{}^{\rho}(\mathbf{k}),\tag{20}$$

and Eq. (13) can then be written in the representation of the irreducible basis vectors. Now, from our initial assumptions it follows that $\mathbf{\Gamma}(\mathbf{k})$ commutes with the symmetry operations in $H(\mathbf{k})$ and therefore only connects vectors $\tau_s{}^{\rho}(\mathbf{k})$ which transform with the same irreducible representation of $H(\mathbf{k})$. When an irreducible representation appears only once, its basis vectors are eigenvectors of $\mathbf{\Gamma}(\mathbf{k})$ so that

$$\mathbf{\Gamma}(\mathbf{k})\tau_s{}^{\rho}(\mathbf{k})=\lambda^{\rho}(\mathbf{k})\tau_s{}^{\rho}(\mathbf{k}),\tag{21}$$

where $\lambda^{\rho}(\mathbf{k})$ is the same for all basis vectors of the representation ρ of $H(\mathbf{k})$ and for the related vectors for the other $\mathbf{k}$'s in the star.

For repeated representations the choice of basis vectors is not determined uniquely by symmetry. To determine the configurations in Eq. (21), one then has to diagonalize the matrix $\mathbf{\Gamma}^{\rho\rho}(\mathbf{k})$ which represents the interactions between the configurations of the irreducible representation ρ chosen in some arbitrary way. The detailed form of the eigenvectors (i.e., the configurations) clearly depends on the interactions. We will restrict our discussion to those properties of the configurations which follow from their symmetry.

When there is only one magnetic moment per unit cell, the solutions of (21) are the only time-independent configurations belonging to the given irreducible representation. They correspond to minimizing the energy within the spherical model. When there are several sites, Eq. (21) is equivalent to minimizing the energy with the sole requirement of the WSM [Eq. (16)]. When the symmetry is sufficient, the SSM [Eq. (15)] may follow automatically. When this does not happen, it may be convenient to allow some additional freedom and introduce the SSM explicitly into the equations. We will discuss this possibility in Sec. 7.

Substituting Eq. (20) into the expression for the energy [Eq. (7)] and using (21), one has

$$E=\sum_{\text{stars}}\sum_{\rho}\lambda^{\rho}(\mathbf{k})\sum_{\mathbf{k},s}a_s{}^{\rho}(\mathbf{k})^{*}a_s{}^{\rho}(\mathbf{k}),\tag{22}$$

where the first summation is over all stars in $\mathbf{k}$ space, the second is over all the irreducible representations ρ belonging to a given star, and the indices $\mathbf{k}$, s designate the distinct basis vectors of the representation.

The matrices $\mathbf{\Gamma}(\mathbf{k})$ are Hermitian and their eigenvalues λ are real and coincide with those of the complex conjugate matrix $\mathbf{\Gamma}(-\mathbf{k})$. There is therefore an inherent degeneracy between $\tau_s{}^{\rho}(\mathbf{k})$ and $\tau_{s'}{}^{\rho'}(-\mathbf{k})=[\tau_s{}^{\rho}(\mathbf{k})]^{*}$, even when $\mathbf{k}$ and $-\mathbf{k}$ do not belong to the same star. They can always be combined to give real configurations so that the $3n$ dimensional moment [in the sense of Eq. (6)] in the unit cell i for the configuration described by $\tau_s{}^{\rho}(\mathbf{k})$ [$S_i(\rho s\mathbf{k})$] is

$$\mathbf{S}_i(\rho,s,\mathbf{k})=2\,\mathrm{Re}[a_s{}^{\rho}(\mathbf{k})\tau_s{}^{\rho}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}_i}],\tag{23}$$

where the rhs is the real part of the bracketed expression. The energy of such a configuration is, from Eq. (22),

$$E=2\lambda^{\rho}(\mathbf{k})\,|\,a_s{}^{\rho}(\mathbf{k})\,|^{2}.\tag{24}$$

The moments at the distinct sites in the unit cell (ν) are given by the components of $\mathbf{S}_i$ in the 3-dimensional subspaces of the $\mathbf{S}_i{}^{\nu}$. In terms of the components $\mathbf{T}_s{}^{\nu}(\mathbf{k})$ one has, in the notation of Eq. (19),

$$\mathbf{S}_i{}^{\nu}(\rho,s,\mathbf{k})=\mathrm{Re}[a_s{}^{\rho}(\mathbf{k})\gamma_s{}^{\rho\nu}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}_i}\tau_s{}^{\rho\nu}(\mathbf{k})].\tag{25}$$

When the $\tau_s{}^{\rho\nu}(\mathbf{k})$ are real, this gives a lattice wave of moments in the direction of $\tau_s{}^{\rho\nu}(\mathbf{k})$:

$$\begin{aligned}\mathbf{S}_i{}^{\nu}(\rho,s,\mathbf{k})=&\,|\,a_s{}^{\rho}(\mathbf{k})\,|\,|\,\gamma_s{}^{\rho\nu}(\mathbf{k})\,|\\&\times\cos[\mathbf{k}\cdot\mathbf{R}_i+\varphi_s{}^{\rho\nu}(\mathbf{k})+\psi_s{}^{\rho}(\mathbf{k})]\tau_s{}^{\rho\nu}(\mathbf{k}),\end{aligned}\tag{26}$$

where $\varphi_s{}^{\rho\nu}(\mathbf{k})$ and $\psi_s{}^{\rho}(\mathbf{k})$ are the phases of $\gamma_s{}^{\rho\nu}(\mathbf{k})$ and

$a_s^\rho(\mathbf{k})$, respectively. When $\tau_s^{\rho\nu}(\mathbf{k})$ is complex, one has

$$[\mathbf{S}_i^\nu(\rho,s,\mathbf{k})]_{\mathrm{Re}}=|a_s^\rho(\mathbf{k})||\gamma_s^{\rho\nu}(\mathbf{k})| \times\cos[\mathbf{k}\cdot\mathbf{R}_i+\varphi_s^{\rho\nu}(\mathbf{k})+\psi_s^\rho(\mathbf{k})], \quad (27)$$

$$[\mathbf{S}_i^\nu(\rho,s,\mathbf{k})]_{\mathrm{Im}}=-|a_s^\rho(\mathbf{k})||\gamma_s^{\rho\nu}(\mathbf{k})| \times\sin[\mathbf{k}\cdot\mathbf{R}_i+\varphi_s^{\rho\nu}(\mathbf{k})+\psi_s^\rho(\mathbf{k})], \quad (28)$$

where the subscripts Re and Im indicate the components of $\mathbf{S}$ in the direction of the real and imaginary parts of τ, respectively. These directions are mutually orthogonal. Equations (27) and (28) describe a spiral structure in which all moments $\mathbf{S}_i^\nu$ with the same ν have equal magnitude. For the magnetic configurations of Eqs. (26), (27), and (28), it follows from Eq. (21) that

$$\begin{aligned}\mathbf{h}_i^\nu(\rho,s,\mathbf{k})&=\mathrm{Re}[\lambda^\rho(\mathbf{k})a_s^\rho(\mathbf{k})\gamma_s^{\rho\nu}(\mathbf{k})e^{i-\mathbf{k}\cdot\mathbf{R}_i}],\\&=\lambda^\rho(\mathbf{k})\mathbf{S}_i^\nu(\rho,s,\mathbf{k}),\end{aligned} \quad (29)$$

and the stability conditions (11) are fulfilled. The configurations obtained in this way have the property

$$\lambda_i^\nu=\lambda^\rho(\mathbf{k}), \quad (30)$$

independent of i and ν. Clearly any superposition of such configurations with the same molecular field constant λ^ρ will obey Eq. (11). When a magnetic structure can be formed from degenerate configurations $\tau_s^\rho(\mathbf{k})$ (with the same λ), it is therefore time independent. This applies, in particular, to combinations of configurations belonging to the same irreducible representation of the NMSG. For purely scalar interactions, it is also true for all configurations obtained from each other by simultaneous rotation of all $\tau_s^{\rho\nu}$ (this was first proved by Kaplan and Lyons[6]).

A second type of combination which is always possible is that of collinear configurations. In the magnetic configurations of Eq. (26) all $\mathbf{S}_i^\nu$ and $\mathbf{h}_i^\nu$ at the same site in the unit cell (ν) have the direction of $\tau_s^{\rho\nu}(\mathbf{k})$ and are therefore parallel to each other. When configurations with the same directions [i.e., with the same $\tau_s^{\rho\nu}(\mathbf{k})$] are combined, the local fields and moments remain parallel to each other so that Eq. (11) still holds. We will discuss the collinear structures which can be formed in this way in Sec. 5 and in Appendix B.

When one tries to go beyond these two cases the situation becomes very complicated, and a description in terms of the irreducible representations may not be useful. For example, one can never combine two noncollinear configurations which are not degenerate. Each configuration contributes a field in the direction of its component of the moment, and because the molecular field constants are different the sum of the local fields cannot have the direction of the resultant moment. For the same reason three configurations cannot be combined unless they are coplanar. Moreover, it is fairly obvious that the λ's for the different directions in space have to be distributed around the same value so as to give the same average in all directions. Since no reasonable structures can be formed by combinations of structures in small regions in $\mathbf{k}$ space (unless they belong to a single $\mathbf{k}$). This seems to indicate that it is hard to gain energy by forming mixed structures with configurations which have a large λ but do not allow the formation of structures.

4. PERIODIC MAGNETIC STRUCTURES

In Eq. (14) the conditions on the magnitude of the individual moments were formulated in terms of the $\mathbf{T}^\nu(\mathbf{k})$.

The simplest case is obviously that of structures belonging to a single $\mathbf{k}$. One then has the two sets of equations:

$$|\mathbf{T}^\nu(-\mathbf{k})|^2+|\mathbf{T}^\nu(\mathbf{k})|^2=N \quad \text{for} \quad \boldsymbol{\kappa}=0, \quad (31)$$

and

$$(\mathbf{T}^\nu(\mathbf{k}))^2+\mathbf{T}^\nu(-\mathbf{k})\cdot\mathbf{T}^\nu(3\mathbf{k})=0 \quad \text{for} \quad \boldsymbol{\kappa}=2k, \quad (32)$$

with its complex conjugate equations for $\boldsymbol{\kappa}=-2\mathbf{k}$. For all other values of $\boldsymbol{\kappa}$ the homogeneous equations in (14) are trivial because we have assumed a single $\mathbf{k}$, i.e.,

$$\mathbf{T}(\mathbf{k}')\equiv 0 \quad \text{for} \quad \mathbf{k}'\neq\pm\mathbf{k}. \quad (33)$$

Now when

$$\mathbf{k}=0, \quad (34a)$$

and when

$$2\mathbf{k}=\mathbf{K}, \quad (34b)$$

where $\mathbf{K}$ is a reciprocal lattice vector, the homogeneous Eqs. (32) do not appear (because $\mathbf{K}=2\mathbf{k}$ is a reciprocal lattice vector), so that only the strong spherical model (SSM) [Eq. (31)] has to be obeyed.

Further, when

$$4\mathbf{k}=\mathbf{K}, \quad (35)$$

Eq. (32) becomes

$$(\mathbf{T}^\nu(\mathbf{k}))^2+(\mathbf{T}^\nu(-\mathbf{k}))^2=0, \quad (36)$$

which can only be obeyed if $\mathbf{T}^\nu(\mathbf{k})^2$ is zero or pure imaginary.

Finally for all other values of $\mathbf{k}$

$$\mathbf{T}(3\mathbf{k})=0, \quad (37)$$

so that Eq. (32) becomes

$$(\mathbf{T}^\nu(\mathbf{k}))^2=0. \quad (38)$$

Thus there are four types of structures. $\mathbf{T}(0)$ describes a structure in which all moments ($\mathbf{S}_i^\nu$) which occupy sites with the same ν are parallel. When there is only one moment per unit cell this is clearly a ferromagnetic structure. When $\mathbf{k}=\frac{1}{2}\mathbf{K}$,

$$e^{i\mathbf{k}\cdot\mathbf{R}}=1 \quad (39)$$

for lattice translations in the plane perpendicular to $\mathbf{K}$, so that all moments at equivalent sites in such a plane point in the same direction. In the direction of $\mathbf{K}$,

$$e^{i\mathbf{k}\cdot\mathbf{R}}=-1 \quad (40)$$

for odd translations, and successive planes have opposite directions of magnetization. Thus the moments at

translationally equivalent sites (ν) constitute a simple antiferromagnetic lattice. For these structures the unit cell is doubled in one or more directions (depending on $\mathbf{K}$).

The general solution of Eq. (36) describes structures which are combinations of a collinear component in one direction with a spiral of pitch $\frac{1}{4}\mathbf{K}$ in the plane perpendicular to it. The interesting point is that collinear structures are possible. This may lead to structures when the the symmetry is not high enough to allow the formation of spirals. In the collinear case one can write

$$\mathbf{T}^\nu(\mathbf{k})=\alpha^\nu(\mathbf{k})e^{i\varphi_\nu(\mathbf{k})}\mathbf{u}^\nu(\mathbf{k}), \tag{41}$$

where $\alpha^\nu(\mathbf{k})$ and $\varphi_\nu(\mathbf{k})$ are real numbers and $\mathbf{u}^\nu(\mathbf{k})$ is a real unit vector. Equation (36) then becomes

$$[\alpha^\nu(\mathbf{k})]^2\cos 2\varphi^\nu(\mathbf{k})=0, \tag{42}$$

and the only solutions for a nonvanishing $\alpha^\nu(\mathbf{k})$ are

$$\varphi^\nu(\mathbf{k})=(n\pm\tfrac{1}{4})\pi, \tag{43}$$

with n an integer. When there is only one moment per unit cell the phase can obviously be chosen so as to satisfy (43). Otherwise (43) requires a relation between the phases at different sites in the unit cell which may or may not be consistent with the structure of the basis vectors.

The collinear structures for $\mathbf{k}=\frac{1}{4}\mathbf{K}$ are somewhat similar to those for $\frac{1}{2}\mathbf{K}$. There are planes of parallel moments perpendicular to $\mathbf{K}$. In the direction of $\mathbf{K}$ one has successively two planes with moments parallel to each other and then two planes pointing in the opposite direction. The choice of phases [Eq. (43)] ensures that the plane wave $\mathbf{T}^\nu(\mathbf{k})$ has equal amplitudes at four successive lattice points.[15]

We now come to the solutions of Eq. (38). These describe spirals. One can always write

$$\mathbf{T}^\nu(\mathbf{k})=\alpha^\nu(\mathbf{k})\exp[i\rho^\nu(\mathbf{k})]\times\{\mathbf{u}_1{}^\nu(\mathbf{k})+\beta^\nu(\mathbf{k})\exp[i\psi^\nu(\mathbf{k})]\mathbf{u}_2{}^\nu(\mathbf{k})\}, \tag{44}$$

where $\mathbf{u}_1{}^\nu(\mathbf{k})$ and $\mathbf{u}_2{}^\nu(\mathbf{k})$ are unit vectors in two orthogonal directions in space, and $\alpha^\nu(\mathbf{k})$, $\beta^\nu(\mathbf{k})$, $\varphi^\nu(\mathbf{k})$, and $\psi^\nu(\mathbf{k})$ are real numbers. To solve Eq. (35) the square of the quantity in brackets has to vanish, i.e.,

$$1+[\beta^\nu(\mathbf{k})]^2\exp[2i\psi^\nu(\mathbf{k})]=0, \tag{45}$$

so that

$$\beta^\nu(\mathbf{k})\exp[i\psi^\nu(\mathbf{k})]=\pm i, \tag{46}$$

and therefore

$$\mathbf{T}^\nu(\mathbf{k})=\alpha^\nu(\mathbf{k})\exp[i\varphi^\nu(\mathbf{k})][\mathbf{u}_1{}^\nu(\mathbf{k})\pm i\mathbf{u}_2{}^\nu(\mathbf{k})], \tag{47}$$

which describes spirals of the type discussed in Eqs. (27) and (28). These are all the structures with a single $\mathbf{k}$.

It is of some interest to discuss the possibilities of combining configurations belonging to the different $\mathbf{k}$'s in a star (which therefore have the same λ) when a single $\mathbf{k}$ does not allow structures. Instead of (38) one then has

$$(\mathbf{T}^\nu(\mathbf{k}))^2+\sum_{\mathbf{k}'=\alpha\mathbf{k}}\mathbf{T}^\nu(\mathbf{k}')\,\mathbf{T}^\nu(2\mathbf{k}-\mathbf{k}')=0, \tag{49}$$

where α is a point operation belonging to the point group of the crystal G. We are looking for solutions for which (38) does not hold {i.e., $(\mathbf{T}^\nu(\mathbf{k}))^2\neq 0$}. It is then necessary that there be a nonvanishing term in the summation, i.e.

$$2\mathbf{k}-\mathbf{k}'=\mathbf{k}''+\mathbf{K}, \tag{50}$$

at least for one $\mathbf{k}'$ of the star with $\mathbf{k}''$ a vector of the star and $\mathbf{K}$ a reciprocal lattice vector. As $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{k}''$ all have the same magnitude and $\mathbf{k}$ and $\mathbf{k}'$ are different by assumption, $\mathbf{K}$ cannot vanish. For points in the interior of the zone it is moreover true that $\mathbf{K}$ cannot have components larger than an elementary reciprocal lattice vector, so that there are very few $\mathbf{K}$'s available.[16] It seems therefore that solutions of Eq. (50) are rather unusual except for the trivial cases $2\mathbf{k}=\mathbf{K}$ and $4\mathbf{k}=\mathbf{K}$. Moreover, Eq. (50) is only a necessary, and by no means sufficient, condition for the existence of structures. In particular, there are always the additional equations with $\mathbf{T}(\mathbf{k})\,\mathbf{T}(\mathbf{k}')$ which may not be consistent with Eq. (49).

Structures with the same λ's (and only such structures) can be combined if the moments are orthogonal to each other at each lattice point. Thus one can always combine a collinear structure with another such structure with orthogonal directions for the $\mathbf{T}^\nu(\mathbf{k})$ even when the $\mathbf{k}$'s are different. The resulting structure is not necessarily collinear. Similarily, a collinear structure can be combined with a spriral in the perpendicular plane to obtain a ferromagnetic spiral with moments lying on a cone. It is however necessary that the two structures have the same λ's (i.e., the same energy) initially, so that for bilinear interactoins nothing can be gained by such combinations.[17]

We will see later that mixed collinear structure with parallel $\mathbf{k}$'s are possible for certain point groups $G(\mathbf{k})$. Structures with two $\mathbf{k}$'s are discussed in Appendix B.

5. IRREDUCIBLE CONFIGURATIONS WITH ONE MOMENT PER UNIT CELL

When there is a single magnetic moment per unit cell, the space group is symmorphic and the configurations are given immediately by the axial vector representations of the point group of $\mathbf{k}$.

[15] For scalar interactions with nearest and *nn* neighbor interaction only, the energy of such structures is the same as that of spiral structures of the same wave vector. Their energy is lower than that of the corresponding $\mathbf{k}=0$ and $\mathbf{k}=\mathbf{K}/2$ structures in the same direction, if the next-nearest-neighbor interaction is antiferromagnetic and larger than half the nearest-neighbor interaction. When there is a single direction of strong anisotropy they might be favored over all spirals.

[16] On the boundary the same argument holds for the component of k which are not half a reciprocal lattice vector. When $2\mathbf{k}\neq\mathbf{K}$ there are always such components.

[17] T. A. Kaplan, Phys. Rev. **124**, 329 (1961).

Of the 32 point groups,[10] 22 can appear only for points on the zone boundary and for $\mathbf{k}=0$. All point groups are possible for $\mathbf{k}=0$. On the boundary the five cubic groups can appear only in the [111] direction, and the other 17 groups which transform $\mathbf{k}$ into $-\mathbf{k}$ are restricted to points for which $2\mathbf{k}=\mathbf{K}$. At all other points only ten point groups are possible. These are the point groups C_1; C_s; C_2; C_{2v}; C_3; C_{3v}; C_4; C_{4v}; C_6; C_{6v}.

C_1

For directions with no symmetry $[G(\mathbf{k})=C_1]$ the magnetic configurations $\tau^\rho(\mathbf{k})$ are determined by the interactions. In general, only the collinear structures ($\mathbf{k}=0$, $\mathbf{K}/2$, $\mathbf{K}/4$) are possible (when they occur in these directions).

C_s; C_2

When the point group is C_s, $\mathbf{k}$ lies in the reflection plane. The component of $\mathbf{T}(\mathbf{k})$ perpendicular to the plane belongs to the identity representation, and the two components in the plane belong to the second representation of the group. The configurations in the plane are therefore not determined by symmetry. The situation is similar for C_2. The wave vector $\mathbf{k}$ is in the direction of the axis, and the longitudinal component belongs to the identity representation. The other two components both belong to the same representation and are therefore not determined.

In both cases only collinear structures can follow from the symmetry. However, the point group is the same for all $\mathbf{k}$'s in a given direction. For C_s one can therefore form mixed collinear structures in the direction perpendicular to the plane, and for C_2 in the direction of the axis. The other basis vectors can have different directions for different $\mathbf{k}$'s so that such mixtures may not be possible.

C_{2v}

For C_{2v} one has three distinct basis vectors belonging to different 1-dimensional representations. The three $\tau^\rho(\mathbf{k})$ are the longitudinal τ in the direction of the axis and the two transverse components along the reflection planes. These directions are the same for all $\mathbf{k}$ along the axis, so that mixed collinear structures can be formed for each component.

All the point groups we have considered so far have only 1-dimensional representations with real characters.

C_3, C_4, C_6

For all three groups, $\mathbf{k}$ points in the direction of the axis. The longitudinal component of $\mathbf{T}(\mathbf{k})$ belongs to the identity representation. For this direction, both single $\mathbf{k}$ and mixed collinear structures are possible. In the transverse plane there are two 1-dimensional vector representations with complex characters. The eigenvectors are also complex and have the form $\mathbf{u}_1 \pm i\mathbf{u}_2$, where $\mathbf{u}_1$ and $\mathbf{u}_2$ are orthogonal unit vectors in the transverse plane. The two vectors describe right- and left-handed spiral structures. When the point group of the crystal has an inversion center or a reflection plane perpendicular to $\mathbf{k}$, the two spirals have the same energy because of the inversion. In most cases these two representations can therefore be regarded as a 2-dimensional representation.

C_{3v} C_{4v} C_{6v}

The structures allowed by these groups are the same as those found when only the rotation axis were present. The only difference is that a 2-dimensional representation replaces the two 1-dimensional representations in the transverse plane.

As pointed out previously, the other point groups can appear only when $\mathbf{k}=0$ or $2\mathbf{k}=\mathbf{K}$. We have shown in section 4 that any basis vector for these values of $\mathbf{k}$ automatically describes a magnetic structure. The point group can help in finding the directions of these structures but otherwise yields no new information.

All $\mathbf{k}$'s in a star have isomorphic point groups and therefore similar structures. As a rule, there will therefore be several structures with the same energy which are transformed into each other by the symmetry operations which carry the $\mathbf{k}$'s into each other. These are, however, different structures, and linear combinations will obey the nonlinear subsidiary conditions only in special cases.

6. MAGNETIC STRUCTURES IN A SIMPLE CUBIC LATTICE

As an example we will apply our results to a simple cubic lattice of magnetic ions.

(a) $\mathbf{k}=0$ *and* $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

In both cases $H(\mathbf{k})$ is the whole space group with the point group O_h. The three components of $\mathbf{T}(\mathbf{k})$ form the basis of a representation derived from the 3-dimensional irreducible representation Γ_{15}' of O_h.[18] For $\mathbf{k}=0$ there are no phase factors, so that this is immediately the representation of the space group. This is clearly a ferromagnetic structure. The fact that the representation is 3-dimensional is to be interpreted as a complete spatial isotropy of the direction of magnetization. This isotropy cannot be removed by bilinear terms in the energy.

For $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ the phase factor is $e^{i\mathbf{k}\cdot\mathbf{R}}=\pm 1$. The minus sign appears whenever $\mathbf{R}$ is an odd lattice translation. The structure has planes of parallel spins, perpendicular to the [111] direction, which alternate in the direction of magnetization. This is the simple antiferromagnetic structure where all nearest neighbors are antiparallel. Again there is complete isotropy of the directions of magnetization.

[18] For notation and character tables of the point groups see reference 10.

(b) $\mathbf{k}=(a,0,0)$ *and* $\mathbf{k}=(a,\frac{1}{2},\frac{1}{2})$

We will first discuss the case $a\neq\frac{1}{2}$. The point group of $\mathbf{k}$ is then C_{4v}. From the operation of the point group elements on $\mathbf{T}(\mathbf{k})$ one obtains the following character table:

E	$2C_x^4$	C_x^2	$2\sigma_v$	$2\sigma_d$
3	1	−1	−1	−1

This breaks up into the 1-dimensional representation Δ_1' and the 2-dimensional representation Δ_5, which describe the longitudinal and the two transverse components of $\mathbf{T}(\mathbf{k})$, respectively.

Because of the sibsidiary conditions, there is only one purely longitudinal structure, namely that for $a=\frac{1}{4}$. The 2-dimensional representation Δ_5 allows us to form transverse spiral structures for all values of a. For $\mathbf{k}=(a,0,0)$ all moments in a yz plane are parallel, and for $\mathbf{k}=(a,\frac{1}{2},\frac{1}{2})$ nearest neighbors in these planes will be antiparallel. Otherwise, we have essentially 1-dimensional spirals with a pitch a in the x direction.

The other members of the stars for $(a,0,0)$ and $(a,\frac{1}{2},\frac{1}{2})$ are $(0,a,0)$, $(0,0,a)$, and $(\frac{1}{2},a,\frac{1}{2})$, $(\frac{1}{2},\frac{1}{2},a)$, respectively. There are corresponding structures for these $\mathbf{k}$'s which have the same energies. It is interesting to point out that the conditions (50) for mixing the different $\mathbf{k}$'s are obeyed for the first time on the zone boundary ($a=\frac{1}{2}$) and therefore give no new structures.

The case of $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ has already been considered. For $\mathbf{k}=(\frac{1}{2},0,0)$ the point group is D_{4h}, and we have the representation M_2 for the longitudinal and the 2-dimensional representation M_5 for the transverse components. The star contains three vectors, and combinations are possible for different $\mathbf{k}$ when the directions of polarization are perpendicular.

(c) $\mathbf{k}=(a,a,0)$ *and* $\mathbf{k}=(a,a,\frac{1}{2})$

For $a\neq\frac{1}{2}$ the point group is C_{2v} which has only 1-dimensional representations. The corresponding configurations are the longitudinal component T_{11} which transforms like Δ_2, the transverse component in the direction of a major crystalline axis (Δ_3) and the transverse component in the xy plane (Δ_4). As the representations are 1-dimensional, only structures for $a=\frac{1}{4}$ and mixed collinear structures are possible. Mixing of different $\mathbf{k}$'s is possible only for $a=\frac{1}{4}$ which gives no new structures.

When $\mathbf{k}=(\frac{1}{2},\frac{1}{2},0)$ the point group is D_{4h} and we have a 1-dimensional representation for T_z and a 2-dimensional representation (M_5) for the components in the xy plane. Because of the special value of $\mathbf{k}$ each component is automatically a structure. These structures can best be visualized as ferromagnetic lines in the z direction with nearest neighbors in the xy plane antiparallel. It is then clear that directions in the plane perpendicular to the z direction should be equivalent.

There are similar structures for the two other vectors of the star, and certain combinations are possible.

(d) $\mathbf{k}=(a,a,a)$ *for* $a\neq\frac{1}{2}$

The point group is C_{3v}. The longitudinal component (in the [111] direction) transforms with the 1-dimensional representation Λ_2. The two transverse components transform with the 2-dimensional representation Λ_3 so that transverse spiral structures are possible.

(e) general $\mathbf{k}$

All other directions in the crystal have point groups of lower symmetry which have only 1-dimensional representations. The only additional pure structures one gets are of the type $\mathbf{k}=(\frac{1}{4},\frac{1}{2},0)$, for which $T_x(\mathbf{k})$, $T_y(\mathbf{k})$ and $T_z(\mathbf{k})$ belong to different representations.

7. STRUCTURES WITH SEVERAL MOMENTS PER UNIT CELL

In Eq. (21) we are essentially looking for minima of the energy with the single explicit restriction of the weak spherical model [Eq. (16a)].[19] When the symmetry of $H(\mathbf{k})$ is sufficient, the SSM [Eq. (15)] may follow automatically, and one can then proceed to check the possibility of forming structures. When this is not the case the ratio of the amplitudes of the $\tau^\rho(\mathbf{k})$ at different sites will depend on the interaction parameters and in general will not be consistent with the SSM. It may then be useful to allow some additional freedom in the choice of the λ's and introduce the SSM explicitly into the equations of motion.[13] In particular, this may be useful when there are different types of sites in the unit cell which are not transformed into each other by the operations of the NMSG. We can then find configurations which belong to a definite irreducible representation of the NMSG and obey the SSM but are not solutions of Eq. (21),[20] because there are different λ's for different sites. In the notation of Eq. (12), we require

$$\sum_\mu \Gamma^{\nu\mu}(\mathbf{k})\cdot\mathbf{T}^\mu(\mathbf{k})=\lambda^\nu\mathbf{T}^\nu(\mathbf{k}), \tag{51}$$

where we are still assuming that $\lambda_i^\nu=\lambda^\nu$ is the same in all unit cells i, and λ^ν is the same for all sites ν for which the magnitude is equal because of $H(\mathbf{k})$. Instead of Eq. (21) one can now write the set of equations

$$\sum_\beta \Gamma^{\alpha\beta}(\mathbf{k})\cdot\tau_s^{\rho\beta}(\mathbf{k})=\lambda^\alpha(\mathbf{k})\tau_s^{\rho\alpha}(\mathbf{k}), \tag{52}$$

where $\tau_s^{\rho\alpha}(\mathbf{k})$ is a basis vector for the irreducible representation ρ of the NMSG in the space defined by the $\mathbf{T}^\nu(\mathbf{k})$ of the set of equivalent sites α, $\lambda^\alpha(\mathbf{k})$ is the λ of the set, and $\Gamma^{\alpha\beta}(\mathbf{k})$ is the interaction matrix between the sets α and β. $\tau_s^{\rho\alpha}(\mathbf{k})$ can interact only with $\tau_s^{\rho\beta}(\mathbf{k})$ which transform with the same irreducible representation of $H(\mathbf{k})$. The solutions of Eq. (52) are the extrema

[19] And therefore with the single Lagrange multiplier $\lambda^\rho(\mathbf{k})$.

[20] The solutions of (21) constitute a complete set so that any structure can be described by them. The structures we are going to consider can be described as combinations of $\tau_s^\rho(\mathbf{k})$ belonging to similar (repeated) irreducible representations. Thus it is really a matter of convenience whether one works with the $\tau_s^\rho(\mathbf{k})$ or the solutions of the modified equations.

of the energy in the presence of the subsidiary conditions, ponents $\mathbf{T}^{\nu}(\mathbf{k})$.

$$\sum_{\nu \subset \alpha} \sum_{i} (\mathbf{S}_i^{\nu})^2 = n_\alpha N, \tag{53}$$

where n_α is the number of different sites in the set α. If the simultaneous solutions of (52) and (53) with minimum energy are sturctures, they will be the ground state structures. It should, however, be noted that the nonlinear conditions (53) are no longer trivial normalization conditions, so that one has to use a procedure of the type suggested in Appendix A to obtain the solutions.

Even for equivalent sites it is probably simplest to investigate the possibilities in each actual case separately. Nevertheless, it seems interesting to see how much can be said about the structure of the basis vectors in general, assuming only the equivalence of the moments under $H(\mathbf{k})$.

The effect of a general operation of the NMSG operating on a vector $\mathbf{T}^{\nu}(\mathbf{k})$ is described by Eq. (17). It is a product of a point operation, a translational phase factor, and a permutation of sites. It can be seen from Eq. (17) that the operation of such a general element of the NMSG on the whole vector $\mathbf{T}(\mathbf{k})$ can be described as the product of a spatial part common to all components and a permutation $P(\alpha)$, i.e.,

$$\langle \alpha | \mathrm{v} \rangle \mathbf{T}(\mathbf{k}) = P(\alpha) e^{i\mathbf{k}' \cdot \mathrm{v}} U(\alpha) \mathbf{T}(\mathbf{k}), \tag{54}$$

where $U(\alpha)$ operates separately on each of the components $\mathbf{T}^{\nu}(\mathbf{k})$.

Distinct elements of the space group with the same α can differ only by lattice translations which can cause no permutations of sites in the unit cell. The permutations $P(\alpha)$ are thus determined by the point operation α and obey the algebra of the point group. The point group of the crystal G is either isomorphic to the group of the permutations $P(\alpha)$ or homomorphic on it. In the latter case the identity of the permutation group is associated with all the elements in an invariant subgroup of the point group, and the permutation group is isomorphic to the factor group of G and the invariant subgroup.

The sites ν in a set α are equivalent only if the permutation group is transitive in the sites. The transitive permutation groups which are consistent with a given point group can be found by well-known procedures.[21] They are isomorphic to the permutations of the cosets found when the group is expanded in cosets of a subgroup. The physical interpretation of such an expansion is that the subgroup contains all operations which leave one site invariant. All the operations in a coset carry that site into one definite other site. A certain care is however required in applying these results, because some of the permutation groups obtained cannot be interpreted as permutations of points in space. For nonsymmorphic groups, for example, the identity permutation group cannot appear. Similarly, for cubic point groups the permutation groups of three objects cannot be interpreted as permutations of sites.[22]

When there is only one site per unit cell we have seen that only the axial vector representations of the point group appear. This no longer applies in the general case. All representations can appear, and there are always repeated representations.

Consider first 1-dimensional representations of $H(\mathbf{k})$ for sites equivalent under $H(\mathbf{k})$. Then, by Eq. (18),

$$\langle \alpha | \mathrm{v} \rangle \tau^{\rho}(\mathbf{k}) = e^{i\mathbf{k} \cdot \mathrm{v}} \chi^{\rho}(\alpha) \tau^{\rho}(\mathbf{k}); \tag{55}$$

and applying (17) and using the notation of Eq. (19), we obtain

$$\chi^{\rho}(\alpha) \gamma^{\rho\mu}(\mathbf{k}) \tau^{\rho\mu}(\mathbf{k}) = \gamma^{\rho\nu}(\mathbf{k}) U(\alpha) \tau^{\rho\nu}(\mathbf{k}); \tag{56}$$

where $\chi^{\rho}(\alpha)$ has magnitude unity, and $\tau^{\rho\mu}(\mathbf{k})$ and $U(\alpha)\tau^{\rho\nu}(\mathbf{k})$ are unit vectors, so that the SSM requirement,

$$|\gamma^{\rho\mu}(\mathbf{k})| = |\gamma^{\rho\nu}(\mathbf{k})|, \tag{57}$$

follows immediately. When the representations at $\mathbf{k}=0$ and $\mathbf{k}=\mathbf{K}/2$ are 1-dimensional, this is sufficient to ensure the existence of structures. The argument can clearly be extended to cases where multidimensional representations of $H(\mathbf{k})$ can be derived from 1-dimensional representations of a subgroup which permutes all sites. For example, this is always possible for the permutations of n sites with point groups C_{nv}.

When the group does not have such a subgroup, the SSM cannot in general be satisfied within one irreducible representation, even when one uses the implicit freedom in choosing the basis vectors for such representations. This may mean that symmetric structures with a single λ are not possible even for $\mathbf{k}=0$ and $2\mathbf{k}=\mathbf{K}$. It should, however, be remembered that the reality of the interaction (i.e., time reversal) may cause additional degeneracies which may allow the formation of structures. This can happen when $\mathbf{k}$ and $-\mathbf{k}$ belong to the same star, but

$$\tau_{s'}{}^{\rho'}(-\mathbf{k}) = \tau_s{}^{\rho}(\mathbf{k})^* \tag{58}$$

does not belong to the same irreducible representation as $\tau_s{}^{\rho}(\mathbf{k})$.

As an example we will discuss the basis vectors of the irreducible representations of the point group C_{3v} in a symmorphic space group with three and six distinct sites in Appendix C.

[21] See e.g., B. L. Van der Waerden, *Modern Algebra #99* (F. Ungar Publishing Company, New York, 1949), p. 150.

[22] These are the permutations of the three crystal axes. Permutations of three objects can only be fitted into a cubic point group if the objects are all invariant under the operations of a subgroup which contains D_2. The subgroup leaves at most one point in the unit cell invariant.

8. CONCLUSIONS

We have found five types of structures:

(a) Structures without increase in the unit cell ($\mathbf{k}=0$).
(b) Structures where the magnetic unit translation is twice the crystalline translation in one or several directions ($\mathbf{k}=\mathbf{K}/2$).
(c) Structures with $\mathbf{k}=\mathbf{K}/4$.
(d) Spiral structures for special symmetry directions in the crystal.
(e) Collinear mixed structures for directions with certain symmetries.

For magnetic lattices with one magnetic ion per unit cell we have shown in detail how these structures can be found and that they are indeed time independent. The extension to the general case is complicated and may not always be possible. In any case it follows from the arguments of Secs. 4 and 7 that no new types of structures appear.

An interesting feature of our analysis is that it applies to quite general bilinear interactions, so that it can be applied to cases where tensorial (dipolar) interactions are important. In particular, it should enable one to find stable structures of a dipolar lattice.

Finally, we would like to stress the limitations of the group-theoretical procedure and the initial assumptions.

The number of structures found is fairly small, and there may exist many other time-independent structures which have no simple relationship to the symmetry of the lattice. At best, one can hope that these mixed solutions are rare.

The assumption of bilinear interactions is probably good in many cases, but there are important exceptions. Sometimes it is possible to regard higher order terms as a perturbation which removes the degeneracy of otherwise degenerate structures or forces special directions on structures which are otherwise isotropic. This happens, for example, for fourth-order anisotropies in cubic ferromagnets. In other cases this is not possible.

Finally, we have assumed a constant magnitude for the moments. This is essentially a zero-temperature approximation. When the magnetic structure of lowest energy is an isolated solution (such as those for $\mathbf{k}=0$ and $\mathbf{k}=\mathbf{K}/2$), it will usually be realistic at all temperatures below the magnetic transition temperature. When there is a practical continuum of structures, as for spirals, the situation becomes much more complicated and the temperature dependence of the average magnitude of the local magnetization may have to be taken into account. Such effects are definitely outside the scope of this work.

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APPENDIX A

Time-Independent Structures in General

The solutions of the stability Eq. (11) do not necessarily have a constant λ. Formally, one can eliminate the $\mathbf{S}_i^{\nu}$ from the stability equation and then determine the λ_i from the conditions on the magnitude of the moments [Eq. (2)]. One can rewrite Eq. (11) as

$$\sum_j \mathbf{D}_{ij}{}^0\cdot\mathbf{S}_j=(\lambda_i-\mathbf{D}_{ii}{}^0)\cdot\mathbf{S}_i, \tag{A1}$$

where the indices i and j designate all magnetic sites on the lattice according to some counting scheme, and thus replace the indices i and ν we used in the text. $\mathbf{D}_{ij}{}^0$ is the interaction tensor between sites i and j. One can now eliminate the moment at site 1 (i.e., $\mathbf{S}_1$) from its equation,

$$\mathbf{S}_1=\sum_{j\neq 1}(\lambda_1-\mathbf{D}_{11}{}^0)^{-1}\mathbf{D}_{1j}{}^0\cdot\mathbf{S}_j, \tag{A2}$$

and substitute in the equations with $i>1$:

$$\sum_{j\neq i;\, i,j>1}\mathbf{D}_{ij}{}^1\cdot\mathbf{S}_j=(\lambda_i-\mathbf{D}_{ii}{}^1)\cdot\mathbf{S}_i, \tag{A3}$$

where we have defined

$$\mathbf{D}_{ij}{}^1=[\mathbf{D}_{ij}{}^0+\mathbf{D}_{i1}{}^0(\lambda_1-\mathbf{D}_{11}{}^0)^{-1}\mathbf{D}_{1j}{}^0]=\mathbf{D}_{ij}{}^1(\lambda_1). \tag{A4}$$

Similarily, after n successive substitutions one obtains

$$\sum_{j\neq i,\, i,j>n}\mathbf{D}_{ij}{}^n\cdot\mathbf{S}_j=(\lambda_i-\mathbf{D}_{ii}{}^n)\cdot\mathbf{S}_i, \tag{A5}$$

with the general definition:

$$\begin{aligned}\mathbf{D}_{ij}{}^n&=\mathbf{D}_{ij}{}^n(\lambda_1,\cdots,\lambda_n)\\&=\mathbf{D}_{ij}{}^{n-1}+\mathbf{D}_{in}{}^{n-1}(\lambda_n-\mathbf{D}_{nn}{}^{n-1})^{-1}\mathbf{D}_{nj}{}^{n-1}.\end{aligned} \tag{A6}$$

Finally, one obtains for the last moment $\mathbf{S}_N$

$$(\mathbf{D}_{NN}{}^{N-1}-\lambda_N)\cdot\mathbf{S}_N=0, \tag{A7}$$

where $\mathbf{D}_{NN}{}^{N-1}$ is a well-defined matrix for any choice of $\lambda_1,\cdots,\lambda_{N-1}$ which does not cause singularities in any $(\lambda_n-\mathbf{D}_{nn}{}^{n-1})^{-1}$. Equation (A7) is an eigenvalue equation and determines λ_N and $\mathbf{S}_N$ in terms of the parameters $\lambda_1,\cdots,\lambda_{N-1}$ which are free so far. One can now proceed backwards to determine the λ_i so as to satisfy the conditions on the magnitude

$$\mathbf{S}_i{}^2=1. \tag{A8}$$

$\mathbf{S}_N$ can clearly be chosen so as to satisfy this. For $\mathbf{S}_{N-1}$ one then has

$$\mathbf{S}_{N-1}=(\lambda_{N-1}-\mathbf{D}_{N-1\,N-1}{}^{N-2})^{-1}\cdot\mathbf{D}_{N-1\,N}{}^{N-2}\cdot\mathbf{S}_N, \quad \text{(A9)}$$

which depends on λ_{N-1} both explicitly and through the dependence of $\mathbf{S}_N$ on λ_{N-1}. Now

$$\mathbf{S}_{N-1}{}^2=\mathbf{S}_N\cdot\mathbf{D}_{N\,N-1}{}^{N-2}(\lambda_{N-1}-\mathbf{D}_{N-1\,N-1}{}^{N-2})^{-2}\times\mathbf{D}_{N-1\,N}{}^{N-2}\cdot\mathbf{S}_N=1, \quad \text{(A10)}$$

where we have used the fact that $\mathbf{D}_{ij}{}^n$ is always the transposed tensor of $\mathbf{D}_{ji}{}^n$ and the quantity in brackets is therefore a symmetric matrix. Equation (A10) can be solved for λ_{N-1} (with $\lambda_1, \cdots, \lambda_{N-2}$ as parameters). It is, however, a very unpleasant equation, mainly because of the complicated dependence of the components of the normalized vector $\mathbf{S}_N$ on λ_{N-1}. It can be expected to have a fairly large number of solutions in terms of the $\lambda_1, \cdots, \lambda_{N-2}$ for each choice of the solution of Eq. (A7). In principle one can proceed in this way to find all the possible choices of λ_i and the corresponding structures. There seems to exist a tremendous number of structures. Many of the solutions probably involve complex λ's and are therefore physically meaningless. The number of real solutions depends on the actual physical situation. To demonstrate that the number of structures can indeed vary, it is illuminating to discuss some simple examples.

The simplest case is that of noninteracting moments, i.e.,

$$\mathbf{D}_{ii}{}^0\neq 0, \quad \text{(A11)}$$

$$\mathbf{D}_{ij}{}^0=0, \quad i\neq j. \quad \text{(A12)}$$

Clearly, a moment can only point in the direction of the principal axes of the tensor $\mathbf{D}_{ii}{}^0$ and therefore has altogether six possible states. The total number of structures for N moments is therfore 6^N.

These are all different structures, and linear combinations of structures are, as a rule, not structures. This is true in spite of the fact that there are obviously only $3N$ linearly independent vectors and the degeneracy in energy is enormous.

A second less trivial case is that of a semi-infinite linear chain with symmetric nearest-neighbor interactions. One has

$$\mathbf{D}\mathbf{S}_2=\lambda_1\mathbf{S}_1 \quad \text{(A13)}$$

and

$$\mathbf{D}\mathbf{S}_{i-1}+\mathbf{D}\mathbf{S}_{i+1}=\lambda_i\mathbf{S}_i, \quad i\neq 1, \quad \text{(A14)}$$

where $\mathbf{D}$ is a symmetric tensor and $\mathbf{S}_1$ is the first moment on the chain. Now assume an arbitrary direction for $\mathbf{S}_1$. Equation (A13) then determines $\mathbf{S}_2$

$$\mathbf{S}_2=\lambda_1\mathbf{D}^{-1}\cdot\mathbf{S}_1, \quad \text{(A15)}$$

and λ_1 is determined, except for sign, by

$$\mathbf{S}_2{}^2=\lambda_1{}^2\mathbf{S}_1\cdot\mathbf{D}^{-2}\cdot\mathbf{S}_1=1, \quad \text{(A16)}$$

where $\mathbf{S}_1\cdot\mathbf{D}^{-2}\cdot\mathbf{S}_1$ is clearly a positive number which can be calculated from the assumed value of $\mathbf{S}_1$ and the known tensor $\mathbf{D}$ (e.g., by expanding $\mathbf{S}_1$ in terms of the eigenvectors of $\mathbf{D}$). One can now proceed to determine $\mathbf{S}_3$ and λ_2 from the stability equation for $\mathbf{S}_2$ and the magnitude of $\mathbf{S}_3$, i.e.,

$$\mathbf{D}\cdot\mathbf{S}_1+\mathbf{D}\cdot\mathbf{S}_3=\lambda_2\mathbf{S}_2; \quad \text{(A17)}$$

and therefore

$$\mathbf{S}_3=\lambda_2\mathbf{D}^{-1}\cdot\mathbf{S}_2-\mathbf{S}_1=[\lambda_1\lambda_2\mathbf{D}^{-2}-1]\cdot\mathbf{S}_1, \quad \text{(A18)}$$

which is linear in λ_2. In general

$$\mathbf{S}_i=\lambda_{i-1}\mathbf{D}^{-1}\cdot\mathbf{S}_{i-1}-\mathbf{S}_{i-2}, \quad \text{(A19)}$$

and therefore

$$\mathbf{S}_i{}^2=\lambda_{i-1}{}^2\mathbf{S}_{i-1}\cdot\mathbf{D}^{-2}\cdot\mathbf{S}_{i-1}-2\lambda_{i-1}\mathbf{S}_{i-2}\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_{i-1}+\mathbf{S}_{i-2}{}^2=1, \quad \text{(A20)}$$

where $\mathbf{S}_{i-1}$ and $\mathbf{S}_{i-2}$ have already been determined previously. Because $\mathbf{S}_{i-2}{}^2=1$, Eq. (A20) becomes

$$\lambda_{i-1}{}^2\mathbf{S}_{i-1}\cdot\mathbf{D}^{-2}\cdot\mathbf{S}_{i-1}-2\lambda_{i-1}\mathbf{S}_{i-2}\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_{i-1}=0, \quad \text{(A21)}$$

with the two solutions

$$\lambda_{i-1}=0 \quad \text{(A22a)}$$

and

$$\lambda_{i-1}=2\frac{\mathbf{S}_{i-2}\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_{i-1}}{\mathbf{S}_{i-1}\cdot\mathbf{D}^{-2}\cdot\mathbf{S}_{i-1}}. \quad \text{(A22b)}$$

Thus there are altogether 2^N structures for each choice of $\mathbf{S}_1$, if one cuts the chain after N moments and assumes boundary conditions which ensure the time independence of the last moment. Altogether there is of course an infinite number of structures because of the freedom in choosing $\mathbf{S}_1$.

An interesting feature of the solutions is that there is really only one structure in which the moments are all pointing in the direction of the field and which therefore can be considered stable. The denominator in (A22b) is obviously positive definite. Substituting from (A19) in the numerator:

$$\mathbf{S}_{i-2}\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_{i-1}=\lambda_{i-2}\mathbf{S}_{i-2}\cdot\mathbf{D}^{-2}\cdot\mathbf{S}_{i-2}-\mathbf{S}_{i-2}\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_{i-3}, \quad \text{(A23)}$$

so that

$$\mathbf{S}_{i-2}\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_{i-1}=\mathbf{S}_{i-3}\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_{i-2}, \quad \text{(A24)}$$

when one assumes $\lambda_{i-2}\neq 0$ and uses Eq. (A21). The first expression of this kind is obviously

$$\mathbf{S}_1\cdot\mathbf{D}^{-1}\cdot\mathbf{S}_2=\lambda_1\mathbf{S}_1\cdot\mathbf{D}^{-2}\cdot\mathbf{S}_1, \quad \text{(A25)}$$

so that the sign of all λ_i is that chosen for λ_1. As one can obviously gain energy at each stage by choosing a negative λ, the lowest energy state for a given $\mathbf{S}_1$ is obtained when one chooses λ_1 negative and all subsequent λ different from zero.

It does not seem feasible to extend these arguments to 3-dimensional lattices or to more than nearest-neighbor interactions. We have demonstrated, however, that the number of solutions is not determined by the general nature of the problem.

APPENDIX B

Collinear Structures with Two Different Wave Vectors

It was pointed out in Sec. 3 that for parallel collinear structures the stability conditions are trivial even for mixtures of nondegenerate configurations. As an example we will discuss structures with two different wave vectors $\mathbf{k}$ and $\mathbf{k}'$. Equation (14) reduces to

$$2|\mathbf{T}(\mathbf{k})|^2+2|\mathbf{T}(\mathbf{k}')|^2=1, \tag{B1}$$

$$\mathbf{T}(\mathbf{k})^2+\mathbf{T}(-\mathbf{k})\mathbf{T}(3\mathbf{k})+\mathbf{T}(\mathbf{k}')\mathbf{T}(2\mathbf{k}-\mathbf{k}')+T(-\mathbf{k}')\mathbf{T}(2\mathbf{k}+\mathbf{k}')=0, \tag{B2a}$$

$$\mathbf{T}(\mathbf{k}')^2+\mathbf{T}(-\mathbf{k}')\mathbf{T}(3\mathbf{k}')+T(\mathbf{k})\mathbf{T}(2\mathbf{k}'-\mathbf{k})+\mathbf{T}(-\mathbf{k})\mathbf{T}(2\mathbf{k}'+\mathbf{k})=0, \tag{B2b}$$

$$2\mathbf{T}(\mathbf{k})\mathbf{T}(\mathbf{k}')+\mathbf{T}(-\mathbf{k})\mathbf{T}(2\mathbf{k}+\mathbf{k}')+\mathbf{T}(-\mathbf{k}')\mathbf{T}(2\mathbf{k}'+\mathbf{k})=0, \tag{B2c}$$

$$2\mathbf{T}(\mathbf{k})\mathbf{T}(-\mathbf{k}')+\mathbf{T}(-\mathbf{k})\mathbf{T}(2\mathbf{k}-\mathbf{k}')+\mathbf{T}(\mathbf{k}')\mathbf{T}(-2\mathbf{k}'+\mathbf{k})=0, \tag{B2d}$$

with their complex conjugate equations. Because of the collinearity the $\mathbf{T}(\mathbf{k})$ can be regarded as numbers. We require solutions for which

$$\mathbf{k}\neq\pm\mathbf{k}', \tag{B3a}$$

$$\mathbf{T}(\mathbf{k})\neq 0, \quad \mathbf{T}(\mathbf{k}')\neq 0, \tag{B3b}$$

$$\mathbf{T}(\mathbf{k}'')=0 \quad \text{for} \quad \mathbf{k}''\neq\mathbf{k},\mathbf{k}'. \tag{B3c}$$

In each of the Eqs. (B2) the first term is, by assumption, nonvanishing. A necessary condition for the existence of a solution is that there should be at least one other nonvanishing term in each equation [consistent with (B3)]. This gives a number of alternative solutions for $\mathbf{k}$ and $\mathbf{k}'$, namely:

$$2\mathbf{k}=\mathbf{K}, \qquad 2\mathbf{k}'=\mathbf{K}', \tag{B4a}$$

$$2\mathbf{k}=\mathbf{K}, \qquad 4\mathbf{k}'=\mathbf{K}', \tag{B4b}$$

$$2\mathbf{k}=\mathbf{K}, \qquad 6\mathbf{k}'=\mathbf{K}+2\mathbf{K}', \tag{B4c}$$

$$4\mathbf{k}=\mathbf{K}, \qquad 4\mathbf{k}'=\mathbf{K}+2\mathbf{K}', \tag{B4d}$$

$$8\mathbf{k}=2\mathbf{K}+\mathbf{K}', \quad 8\mathbf{k}'=2\mathbf{K}+3\mathbf{K}', \tag{B4e}$$

$$10\mathbf{k}=3\mathbf{K}+\mathbf{K}', \quad 10\mathbf{k}'=\mathbf{K}-3\mathbf{K}', \tag{B4f}$$

where $\mathbf{K}$ and $\mathbf{K}'$ are any two reciprocal lattice vectors. In (B4a), (B4b), and (B4d) both $\mathbf{k}$ and $\mathbf{k}'$ allow structures so that nothing is gained by the mixture. For (B4f) the Eqs. (B2) are not consistent. The other two solutions give new structures. One could even construct a model in which these would be the structures of lowest energy. However, these are collinear structures with relatively large periods and could be meaningful only when long-range interactions are very important.

APPENDIX C

Representations of C_{3v} in Symmorphic Space Groups

The group has the character table[10]

	E	$2C_3$	$3\sigma_v$
Λ_1	1	1	1
Λ_2	1	1	−1.
Λ_3	2	−1	0

The representations for a single axial vector are Λ_2 for the component along the axis and Λ_3 for the two other components. Transitive permutation groups of two, three, and six objects are possible. The permutations of two cannot be interpreted as permutatons of sites.[23] For three sites the permutation group is the complete permutation group of three objects. The invariant subgroup C_3 is associated with the cyclic permutations, and the reflection planes each permute two sites and leave the third one invariant.[24] The character table of the representation in terms of the $\mathbf{T}^v(\mathbf{k})$ is therefore

E	$2C_3$	$3\sigma_v$
9	0	−1

so that Λ_1 appears once, Λ_2 twice, and Λ_3 three times.

For six sites we have the regular representaton of the group. The character of E is 18, and all other elements have vanishing characters (because of the permutations). The sites are those obtained from a general point, which is not on the axis or in a reflection plane, by the operations of the group. They divide into two sets of three, each of which is permuted cyclically by C_3. The two sets are permuted into each other by the reflection planes. The two 1-dimensional representations (Λ_1 and Λ_2) each appear three times and the 2-dimensional representation C_3 appears six times.

It is convenient to choose the basis vectors so that they diagonalize the elements of the invariant subgroup C_3. For a single moment there are three such vectors, namely: (a) The component along the axis τ_z which transforms with the identity representation, (b) $\tau_x+i\tau_y$ which is multiplied by $\omega=e^{2\pi i/3}$ by C_3, and (c) $(\tau_x-i\tau_y)$ which is multiplied by ω^2 by the same operation, where τ_x, τ_y, and τ_z are unit vectors in the corresponding directions.

In the larger group C_{3v}, τ_z transforms with the 1-dimensional representation Λ_2, and the two other vectors transform with the 2-dimensional representation Λ_3. With three sites one has for the identity representa-

[23] This follows from the geometric realization and not from the properties of the group. The isomorphic group D_3 can have two sites.

[24] The geometric interpretation is clearly three sites in a plane perpendicular to the axis and lying in the reflection planes.

tion Λ_1 the single vector

$$\mathrm{Re}(\omega(\tau_x+i\tau_y);\ \omega^2(\tau_x+i\tau_y);\ (\tau_x+i\tau_y)), \quad \text{(C1)}$$

where the vectors at the three sites are written successively. This vector is determined uniquely. Equation (C1) describes a 1-dimensional configuration with three real vectors $\tau^{\rho\nu}$ for the directions at the different sites. Structures are therefore possible only for $\mathbf{k}=0$, $\mathbf{k}=\mathbf{K}/2$ and $\mathbf{k}=\mathbf{K}/4$. The SSM is obeyed automatically because the representation is 1-dimensional and the conditions for the solutions at $\mathbf{K}/4$ are obeyed.

For Λ_2 the basis vectors can, e.g., be chosen as

$$(\tau_z;\ \tau_z;\ \tau_z) \quad \text{(C2a)}$$

and

$$\mathrm{Im}(\omega(\tau_x+i\tau_y);\ \omega^2(\tau_x+i\tau_y);\ (\tau_x+i\tau_y)); \quad \text{(C2b)}$$

for $k=0$ one of them describes a ferromagnetic structure and the second a Yafet-Kittel[25] radial structure. The proper choice which diagonalizes the energy is obviously some mixture of these two configurations. All these mixtures obey the SSM because the representation is 1-dimensional. As the two vectors are real, the absolute phase can be chosen so that Eq. (36) is satisfied at all sites for $\mathbf{k}=\frac{1}{4}\mathbf{K}$.

For Λ_3 there are three pairs of solutions, e.g.,

$$(\omega^2\tau_z;\ \omega\tau_z;\ \tau_z), \quad \text{(C3a)}$$

$$((\tau_x+i\tau_y);\ (\tau_x+i\tau_y);\ (\tau_x+i\tau_y)), \quad \text{(C3b)}$$

$$(\omega(\tau_x-i\tau_y);\ \omega^2(\tau_x-i\tau_y);\ (\tau_x-i\tau_y)), \quad \text{(C3c)}$$

for the first vector and, correspondingly,

$$(\omega\tau_z;\ \omega^2\tau_z;\ \tau_z), \quad \text{(C4a)}$$

$$(\tau_x-i\tau_y;\ \tau_x-i\tau_y;\ \tau_x-i\tau_y), \quad \text{(C4b)}$$

$$(\omega^2(\tau_x+i\tau_y;\ \omega(\tau_x+i\tau_y);\ \tau_x+i\tau_y), \quad \text{(C4c)}$$

for the second vectors. We have chosen the vectors so as to diagonalize the rotations. The three vectors (C3) and (C4) transform under C_3 like $\tau_x+i\tau_y$ and $\tau_x-i\tau_y$, respectively. In general the configurations belonging to an irreducible representation will be combinations of these vectors and the right combinations depends on the interactions. The two vectors can, however, always be chosen so as to diagonalize C_3 and in this form they obey the SSM. On the other hand, Eqs. (36) and (38) will only be consistent with this choice in special cases. In general there are, therefore, no structures in the interior of the zone. When there are additional symmetry elements in the NMSG which do not add new sites, time inversion may cause two of the three repeated representations Λ_3 to be degenerate, and this gives enough freedom to allow one to construct spirals for arbitrary magnitudes of $\mathbf{k}$.

We will not write down the vectors for six sites. The sites break up into two sets of three, each of which is permuted cyclically by the subgroup C_3. For the 1-dimensional representations the SSM obviously holds. For Λ_3 one can again choose to diagonalize C_3, and the vectors will then have the form of the τ^ρ of Eq. (C4) for each set separately, with different coefficients and magnitudes in each set. In general it is not possible to combine the two vectors belonging to one representation so as to satisfy the SSM at all sites.

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Phonon-Magnon Interaction in Magnetic Crystals*

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A microscopic theory of phonon-magnon interaction in magnetic crystals is developed from first principles. The crystal field oscillations are treated as perturbations which superpose some excited orbital states on the ground orbital state of the magnetic ions. When use is made of these perturbed states as the starting one-electron functions in the second quantization representation, the formulation of the Heisenberg-type exchange interaction furnishes the relevant phonon-magnon interaction terms. Following the above interactions, the phonon-magnon relaxation times are calculated for the processes involving one-phonon direct and two-phonon Raman processes. Estimates made for iron, where the excited orbitals are taken to be the $4p$ and the ground $3d\gamma$ orbitals, yield values for the relaxation time for the one-phonon processes ($\tau_{sp}\approx 10^{-6}$ sec at 10°K) in agreement with the suggested results. Two-phonon Raman processes do not seem to be important at low temperatures.

INTRODUCTION

THE interaction between spin waves[1] and lattice vibrations is known to play an important role in the relaxation processes occurring in magnetic crystals, particularly at low temperatures.[2] The first theoretical study was made by Akhiezer[3] from a microscopic point of view by expanding the exchange and dipolar terms in power series with normal coordinates of the lattice

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