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Normal Spin-Wave Modes of Complex Exchange-Coupled Crystals

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Recently, the author constructed a spin-wave theory of the Holstein-Primakoff type applicable to exchange-coupled crystals with an arbitrary number of magnetic ions per primitive magnetic unit cell. In the present report, a simple, explicit, and general procedure is given for finding a complete set of normal spin-wave modes within the context of the above theory. A comparison of our procedure with the corresponding one of Wallace reveals that the present method is considerably easier to apply than his in practical computations involving an extensive class of complex exchange-coupled spin structures.

INTRODUCTION

In a recent paper (1), we developed a spin-wave theory of the Holstein-Primakoff variety for exchange-coupled solids with an arbitrary number of magnetic ions per primitive magnetic unit cell. The only condition on the spin ordering in that theory was that the spins should point parallel or antiparallel to a given direction, except for the effect of spin-wave fluctuations. A procedure for determining the spin-wave energies and the corresponding normal modes was given in I,* where the problem of determining these energies was treated in detail for various cases of interest and where the solution to the problem of determining the normal modes in question was presented schematically.

The main purpose of the present report is to show that the formulation of the normal-mode problem given in I and a line of attack inspired by a classical procedure (2) of the theory of small oscillations lead in an elegant and simple way to an explicit general solution of this problem which is quite convenient for practical computational work involving typical complex exchange-coupled solids.

Recently, Wallace (3) has published a method for determining the normal spin-wave modes of exchange-coupled solids of the type considered in I. We shall compare our solution of this normal mode problem with his in the two final paragraphs of the main body of this report.†

DETERMINATION OF SPIN-WAVE NORMAL MODES

It was established in I that the spin-wave Hamiltonian (2.9I) could be reduced to the diagonal form (2.19I), provided that for each magnon wavenumber $\boldsymbol{\kappa}$ one could find $n \times n$ transformation matrices T_κ satisfying the equations

$$\sigma L_\kappa T_\kappa = T_\kappa \mu_\kappa, \tag{1}$$

$$T_\kappa^\dagger \sigma T_\kappa = \omega, \tag{2}$$

$$T_{-\kappa} = T_\kappa^*, \tag{3}$$

where the dagger and asterisk refer to the Hermitian conjugate and complex conjugate, respectively, of the matrices of interest. The $n \times n$ matrices σ, ω, μ_κ, and L_κ in Eqs. (1) and (2) have the following significance. We define $\sigma \equiv [\sigma_\alpha \delta_{\alpha\beta}]$, σ_α being 1 (-1) if the αth spin in a primitive unit cell points "up" ("down") along the direction of spin alignment. The matrix L_κ, given by Eq. (2.6I), is Hermitian and can be made positive definite (det $[L_\kappa] > 0$) for all $\boldsymbol{\kappa}$ by an appropriate choice of the anisotropy constants A_α in Eq. (2.4I). This global positive definiteness property of L_κ should be understood to hold henceforth. We define $\mu_\kappa \equiv [\mu_{\kappa,\alpha}\delta_{\alpha\beta}]$, where the $\mu_{\kappa,\alpha}$ are the eigenvalues of σL_κ, these eigenvalues being real and nonzero by a standard theorem of linear algebra (as given, for example, by Ref. 4). We shall always suppose

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*Reference 1 is herein denoted by I, and, for example, Eq. (2.9) thereof is quoted as (2.9I).

†Those primarily interested in the practical aspects of this report, may find it advisable to omit Appendixes A and B, as well as the discussion in the paragraph containing Eq. (12), at least in an initial reading of this report.

that the $\mu_{\kappa,\alpha}$ have been numbered in such a way as to possess the continuity properties mentioned in I and in Appendix A. Under this proviso, it is shown in this appendix that the sign of $\mu_{\kappa,\alpha}$, denoted by ω_α, is independent of $\boldsymbol{\kappa}$ and of the A_β when the latter constants are chosen as indicated above. We set $\omega \equiv [\omega_\alpha\, \delta_{\alpha\beta}]$.

Let t_κ be a nonsingular matrix satisfying the eigenvalue equation

$$\sigma L_\kappa t_\kappa = t_\kappa \mu_\kappa. \qquad (1')$$

Such matrices t_κ exist for each $\boldsymbol{\kappa}$ by virtue of the hermiticity and positive definiteness of L_κ for all $\boldsymbol{\kappa}$. The last assertion follows from Theorem B of Appendix B when one sets $P = \sigma$ and $Q = L_\kappa$. An equivalent theorem was established in a different way in Sec. 4.082 of Ref. 2.

The hermiticity of L_κ, the reality of $\mu_{\kappa,\alpha}$, and Eq. (1′) imply

$$(t_\kappa{}^\dagger \sigma t_\kappa)\mu_\kappa = \mu_\kappa (t_\kappa{}^\dagger \sigma t_\kappa) = t_\kappa{}^\dagger L_\kappa t_\kappa. \qquad (4)$$

Let $\epsilon_\kappa \equiv [|\mu_{\kappa,\alpha}|\delta_{\alpha\beta}]$ be the positive definite diagonal matrix of spin-wave energies which was introduced in I. The commutativity of μ_κ and $t_\kappa{}^\dagger L_\kappa t_\kappa$ asserted by Eq. (4) is easily seen to imply that $t_\kappa{}^\dagger L_\kappa t_\kappa$ commutes with ϵ_κ and therefore also with $\epsilon_\kappa{}^{-1}$. Combining this remark with Eq. (4) and with the obvious equation

$$\epsilon_\kappa = \omega \mu_\kappa, \qquad (5)$$

we conclude that $t_\kappa{}^\dagger \sigma t_\kappa$ has the form

$$t_\kappa{}^\dagger \sigma t_\kappa = \omega D_\kappa, \qquad (6)$$

where

$$D_\kappa \equiv \epsilon_\kappa{}^{-1}(t_\kappa{}^\dagger L_\kappa t_\kappa) = (t_\kappa{}^\dagger L_\kappa t_\kappa)\epsilon_\kappa{}^{-1}. \qquad (7)$$

It is clear from Eq. (7) and the hermiticity of L_κ that D_κ is Hermitian. D_κ is also positive definite, since Eq. (7) entails that $\det[D_\kappa] = |\det[t_\kappa]|^2 \times \det[L_\kappa]/\det[\epsilon_\kappa] > 0$, because t_κ is nonsingular and because L_κ and ϵ_κ are positive definite.

From Eqs. (4) and (6), one finds

$$D_\kappa \mu_\kappa = \mu_\kappa D_\kappa. \qquad (8)$$

The commutativity of D_κ with μ_κ and the hermiticity and positive definiteness of D_κ imply that there exists a unitary matrix Z_κ having the properties

$$Z_\kappa{}^\dagger D_\kappa Z_\kappa = d_\kappa, \qquad (9)$$

$$Z_\kappa \mu_\kappa = \mu_\kappa Z_\kappa, \qquad (10)$$

where d_κ stands for the positive definite diagonal matrix $[d_{\kappa,\alpha}\delta_{\alpha\beta}]$.

Define

$$T_\kappa \equiv t_\kappa Z_\kappa d_\kappa{}^{-1/2}, \qquad (11)$$

where $d_\kappa{}^{-1/2} \equiv [d_{\kappa,\alpha}{}^{-1/2}\delta_{\alpha\beta}]$. Then T_κ satisfies Eq. (1) by virtue of Eqs. (1′), (10), and (11), and T_κ obeys Eq. (2) because of Eqs. (5) and (8) and the commutativity of Z_κ with ω which follows readily from (10).

Using the procedures just given, there is no practical difficulty in finding matrices T_κ which, outside of obeying Eqs. (1) and (2) for each $\boldsymbol{\kappa}$, also fulfill Eq. (3) for every $\boldsymbol{\kappa}$. However, for the sake of mathematical completeness, we shall give an explicit procedure for solving Eqs. (1) to (3) once the solution of Eqs. (1) and (2) is known in "one half" of $\boldsymbol{\kappa}$ space. We divide $\boldsymbol{\kappa}$ space into two parts, R_+ and R_-, such that if $\boldsymbol{\kappa} \in R_+$ then $-\boldsymbol{\kappa} \in R_-$ for each $\boldsymbol{\kappa}$. For example, choose R_+ (R_-) to be the set of all $\boldsymbol{\kappa}$ such that $\kappa_x \geqslant 0$ (< 0), where x designates some fixed direction in the crystal. Let T_κ be given by Eq. (11) whenever $\boldsymbol{\kappa} \in R_+$, so that T_κ obeys (1) and (2) throughout R_+. Define the matrices T_κ in R_- as follows in terms of the corresponding matrices in R_+:

$$T_\kappa \equiv T_{-\kappa}{}^*, \ \boldsymbol{\kappa} \in R_-. \qquad (12)$$

By virtue of this definition, Eq. (3) holds automatically for all $\boldsymbol{\kappa}$. It remains solely to show that Eqs. (1) and (2) are obeyed by the present T_κ for every $\boldsymbol{\kappa} \in R_-$. That Eq. (1) is fulfilled in this sense results from the defining Eq. (12) coupled with the facts that $L_{-\kappa} = L_\kappa{}^*$ [Eq. (2.81)] and that $\mu_{-\kappa} = \mu_\kappa$ [this equation is implied by Eq. (2.121) and the reality of μ_κ]. The T_κ of interest satisfy Eq. (2) for $\boldsymbol{\kappa} \in R_-$ because of Eq. (12) and the reality of σ and ω.

For purposes of comparison with Ref. 3, we shall recapitulate succinctly the present method for finding solutions T_κ of Eqs. (1) to (3), *i.e.*, for finding a complete set of normal spin-wave modes.

In this recapitulation and in all other subsequent remarks of this section, we shall only be concerned with the nontrivial case $\sigma \neq I$, *i.e.*, with spin structures in which some spins point "up" and some "down." As is well known, no refined methods are required to determine these normal modes in the ferromagnetic case $\sigma = I$, even when $n > 1$. Omitting the simple matter of satisfying Eq. (3), the present method involves two steps: (a) one obtains the eigenvalues $\mu_{\kappa,\alpha}$ and determines a particular nonsingular solution of Eq. (1); (b) one constructs the corresponding matrix D_κ using Eq. (6), finds its eigenvalues $d_{\kappa,\alpha}$, and determines a diagonalizing unitary matrix Z_κ fulfilling Eqs. (9) and (10). Notice that, by suitably permuting the rows and columns of D_κ, this matrix acquires a block structure in which the size of the blocks is equal to the degeneracy of the $\mu_{\kappa,\alpha}$. Hence D_κ is diagonal for any $\boldsymbol{\kappa}$ such that all the $\mu_{\kappa,\alpha}$ are distinct. In the latter case, the problem of finding d_κ and Z_κ is trivial once step (a) has been effected. In cases of small degeneracy of the $\mu_{\kappa,\alpha}$, say double or triple degeneracy, it should be clear from our remark on the block structure of D_κ, that step (b) involves only a modest amount of labor. Most of the actual exchange-coupled spin structures probably obey this low-degeneracy condition. For example, the condition in question is satisfied by the exchange-coupled models of magnetite (A-B interactions) (see, for instance, footnote 26, page 1948, of I) and YIG (a-a, d-d, and a-d interactions), excluding possible accidental degeneracy effects in the case of this last substance.*

In Wallace's approach (3), one has to (a′) find the eigenvalues of a matrix which he terms L_k (his $\mathbf{k}$ is our $\boldsymbol{\kappa}$ and his L_k is unitarily equivalent to our L_κ); (b′) determine the corresponding eigenvalues and a corresponding diagonalizing unitary matrix of a matrix which he denotes by R_k [see Eq. (25), Ref. 3]. Even when all the $\mu_{\kappa,\alpha}$ are distinct for a given $\boldsymbol{\kappa}$, L_k and R_k cannot in general be reduced to matrices having a simple block structure by permutations of rows and columns. Hence, the main advantage of our method over that in Ref. 3 in the above low-degeneracy case is the fact that the latter involves two lengthy diagonalization procedures, while only one lengthy step, namely (a), is required in our approach.

For either of the normal-mode methods under discussion, cases of high degeneracy of the $\mu_{\kappa,\alpha}$ would in general necessitate the aid of an electronic computer to obtain detailed numerical results. In a complex situation of this type, it is probable that the method advocated in this report would be simpler for coding purposes than that of Ref. 3.

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*The spin-wave excitations of this model of YIG have been studied by Douglass (5). Although Douglass' paper deals only with restricted regions of $\boldsymbol{\kappa}$ space, one can deduce from it, by simple additional reasoning, that the low-degeneracy condition mentioned in the text of this report holds for all $\boldsymbol{\kappa}$, exception made of the above accidental degeneracy phenomena.

APPENDIX A

In I, reasons of brevity precluded giving a complete proof of the important fact that the sign of $\mu_{\kappa,\alpha}$, for fixed α, is independent of $\boldsymbol{\kappa}$ and of the anisotropy constants A_β when L_κ is positive definite for all $\boldsymbol{\kappa}$. We shall devote this appendix to a detailed proof of this fact.*

Consider the Euclidean space $R^{(n)}$ composed of the n-ples $(A_1, \ldots, A_n)$; *i.e.,* consider the set of all such n-ples provided with a Euclidean distance function

$$d(P', P'') = \left[\sum_{\alpha=1}^{n} [A_\alpha' - A_\alpha'']^2 \right]^{1/2}$$

corresponding to the points $P' = (A_1', \ldots, A_n')$ and $P'' = (A_1'', \ldots, A_n'')$. Let S be the subset of points of $R^{(n)}$ such that L_κ is positive definite for all $\boldsymbol{\kappa}$.

Lemma. S is a connected set.

Proof. From Eq. (2.61), one sees that

$$L_\kappa = L_\kappa^{(0)} + [A_\alpha \delta_{\alpha\beta}], \qquad \text{(A1)}$$

where $L_\kappa^{(0)}$ is independent of the A_β.

Let $(A_1', \ldots, A_n')$ and $(A_1'', \ldots, A_n'')$ be two elements of $R^{(n)}$ and let L_κ' and L_κ'' be the corresponding matrices L_κ. Then Eq. (A1) implies

$$L_\kappa'' = L_\kappa' + [(A_\alpha'' - A_\alpha')\delta_{\alpha\beta}]. \qquad \text{(A2)}$$

We now restrict $(A_1', \ldots, A_n')$ to lie in S and suppose that $A_\alpha'' \geqslant A_\alpha'$ for $\alpha = 1, \ldots, n$. Then the matrix L_κ' is positive definite for all $\boldsymbol{\kappa}$, and the $\boldsymbol{\kappa}$-independent matrix $[(A_\alpha'' - A_\alpha')\delta_{\alpha\beta}]$ is positive semidefinite. Since Eq. (A2) asserts that L_κ is the sum of the last two matrices, L_κ'' is positive definite for all $\boldsymbol{\kappa}$; *i.e.* $(A_1'', \ldots, A_n'') \in S$. Hence, we have shown that if $(A_1', \ldots, A_n') \in S$, then $(A_1'', \ldots, A_n'') \in S$ if $A_\alpha'' \geqslant A_\alpha'$ for all α. This is easily seen to imply that S is connected.*

Theorem A. For fixed α, sgn $\mu_{\kappa,\alpha}$ is independent of $\boldsymbol{\kappa}$ and of the A_β, provided that $(A_1, \ldots, A_n) \in S$.

Proof. As usual, we regard $\boldsymbol{\kappa}$ space as a three-dimensional Euclidean space, which will be called K. Since K is (trivially) connected and since the connectivity of S follows from the lemma just proved, we see that the product space $K \times S$ is connected (see, for example, Ref. 6).

Now $\mu_{\kappa,\alpha}$ is a real-valued, nonvanishing, and jointly continuous function of $\boldsymbol{\kappa}$ and of all the A_β on $K \times S$.† Hence, by a well-known theorem [see Theorem (3.19.8), page 66, Ref. 6] of real-variable theory, the sign of $\mu_{\kappa,\alpha}$, for fixed α, is the same throughout K × S, which completes our proof.

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*From the mere equality of the signatures of μ_κ and σ when L_κ is positive definite for all $\boldsymbol{\kappa}$, it is, of course, not obvious that sgn $\mu_{\kappa,\alpha}$, for given α, is independent of $\boldsymbol{\kappa}$ and of the A_β when L_κ is of this type. This signature property is entirely algebraic, while the said property of sgn $\mu_{\kappa,\alpha}$ is of an analytical character. We regret the confusing passage on p. 1943 of I, from which one would gather the erroneous impression that we established the equality of the signatures of μ_κ and σ by continuity arguments. It may be of interest to present our original proof of this equality. If L_κ has the above global positive definiteness property, Sylvester's theorem of inertia tells us that the signatures of $L_\kappa^{1/2}\sigma L_\kappa^{1/2}$ and σ are the same, because then the "positive square root" $L_\kappa^{1/2}$ of L_κ is nonsingular. But since the matrices AB and BA have the same eigenvalues (see the second paragraph of the proof of Theorem A in this appendix), we conclude that the eigenvalues $\mu_{\kappa,\alpha}$ of σL_κ are the same as the eigenvalues of $L_\kappa^{1/2}\sigma L_\kappa^{1/2}$. Hence, the signature of $\mu_{\kappa,\alpha}$ is the same as that of σ. This fact is also proved in Ref. 3. Notice that in that reference, it is implicitly assumed, not proved, that sgn $\mu_{\kappa,\alpha}$ is independent of $\boldsymbol{\kappa}$ and of the A_β under the present hypotheses.

*For $n = 2$, this connectedness property is readily verified graphically.

†More precisely, for given α, $\mu_{\kappa,\alpha}$ is a jointly continuous function of the $3 + n$ variables κ_x, κ_y, κ_z, $A_1, \ldots, A_n$, where κ_x, κ_y, κ_z are the components of $\boldsymbol{\kappa}$ with respect to an arbitrary Cartesian system. It is hardly necessary to state the continuity is understood here in the familiar sense of classical analysis.

APPENDIX B

In this appendix, we prove a theorem equivalent to the "theorem of the separation of the roots," established by analytical procedures in Ref. 3. Our proof is both simple and purely algebraic.

Theorem B. Let P and Q be $n \times n$ Hermitian matrices and let Q be positive definite. Let λ_α be the αth eigenvalue of PQ. Then there exists a nonsingular matrix X satisfying

$$(PQ)X = X\lambda, \tag{B1}$$

where $\lambda \equiv [\lambda_\alpha \delta_{\alpha\beta}]$.

Proof. Define the matrix

$$B_\alpha \equiv PQ - \lambda_\alpha I, \tag{B2}$$

where I is the $n \times n$ unit matrix. It is well known from elementary linear algebra that a necessary and sufficient condition for the existence of a nonsingular matrix X obeying Eq. (B1) is that B_α have rank $n - m_\alpha$ for each α, where m_α is the multiplicity of the eigenvalue λ_α. We proceed to prove that B_α has this rank.

Set

$$H_\alpha \equiv Q^{1/2} B_\alpha Q^{-1/2} = Q^{1/2} P Q^{-1/2} - \lambda_\alpha I, \tag{B3}$$

where $Q^{1/2}$ is the Hermitian nonsingular matrix which is the "positive square root" of Q, and where $Q^{-1/2}$ is the inverse of $Q^{1/2}$. The matrix $Q^{1/2}PQ^{1/2}$ is obviously Hermitian and its eigenvalues are the same as the eigenvalues λ_α of PQ. To prove this last statement, one writes $Q^{1/2}PQ^{1/2} = Q^{1/2} \cdot (PQ^{1/2})$ and $PQ = (PQ^{1/2}) \cdot Q^{1/2}$ and invokes the theorem that AB and BA have the same eigenvalues for arbitrary $n \times n$ matrices A and B (see, for example, Ref. 7). But, if H is any $n \times n$ Hermitian matrix and ρ_α is its αth eigenvalue, the rank of $H - \rho_\alpha I$ is equal to n minus the multiplicity of ρ_α, since the hermiticity of H entails that the maximum number of linearly independent eigenvectors belonging to ρ_α is equal to this multiplicity. Hence, the hermiticity of $Q^{1/2}PQ^{1/2}$ and the fact that its eigenvalues are the λ_α implies that H_α in Eq. (B3) has rank $n - m_\alpha$ for each α.

Since H_α is obtained from B_α by pre- and post-multiplication with the nonsingular matrices $Q^{1/2}$ and $Q^{-1/2}$, respectively, the ranks of H_α and B_α are identical, which completes our proof.

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