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THE FIELD-INDUCED PHASE TRANSITIONS IN FeBr₂ CRYSTAL

J. Kociński

Warsaw Technical University, Institute of Physics, Koszykowa 75, 00-662 Warszawa, Poland

Abstract. – The field-induced phase transitions in FeBr₂-type crystal under hydrostatic pressure have been determined in terms of Landau's theory, with the paramagnetic phase described by a unitary or a non-unitary group. The sets of low-temperature symmetry groups implied by these two descriptions partly overlap.

Introduction

The field-induced phase transition in FeBr₂ crystal from the paramagnetic phase (P) to the antiferromagnetic phase (AF) was experimentally detected by Vetier et al. [1]. Transitions to AF and ferrimagnetic (Fi) phases were discussed [2] and the corresponding phase diagrams were analysed [3]. A review of metamagnetic transitions was presented by Stryjewski and Giordano [4]. Applying Landau’s theory, we will give a group-theoretical discussion of the low-temperature phases which can emerge after field-induced phase transitions, accounting for the influence of external pressure.

Symmetry group of the paramagnetic phase and order parameters

The paramagnetic phase of a FeBr₂ crystal in an external magnetic field parallel to the threefold axis is characterized by the symmetry group G_{OM}=P3m' determined by the elements:

\[ a_1, a_2, a_3, 1, R_3, R_6, R_{13}, R_{17} \]

\[ \Theta R_7, \Theta R_9, \Theta R_{11}, \Theta R_{19}, \Theta R_{21}, \Theta R_{23} \] (1)

numbered according to Kovalev [5, 6], where \( \Theta \) is the time-reversal operation, and \( a_1, a_2, a_3 \) are the basis vectors of the Bravais lattice. According to the Curie principle, this is the maximal common subgroup of the symmetry group of the unmagnetized crystal and the magnetic field, for a fixed mutual orientation of their symmetry elements. To distinguish between the AF and Fi phases, each consisting of two sublattices, two axial-vector order parameters are required. For the AF phase we define the order parameter by

\[ \delta S_B (x_p) = e_z \left[ + \sqrt{ (S_A^z (x_p))^2 - S_B^z (x_p) } \right] \] (2)

where \( e_z \) is the unit vector along the threefold axis and \( S_B^z (x_p) < 0 \) is the mean spin \( z \)-component of the point \( x_p \) of the B-sublattice. The mean spin \( z \)-component in the A-sublattice is assumed to be positive and antiparallel to the external magnetic field. For the Fi phase we define the order parameter by

\[ \Delta S (x_p) = S_A^z (x_p) - S_B^z (x_p+a) \] (3)

where \( S_A^z (x_p) \) and \( S_B^z (x_p+a) \) are the mean spins in A and B sublattices at the points \( x_p \) and \( x_p+a \), respectively. Notice that parameter equation (3) can also describe the AF phase, however, parameter equation (2) cannot describe the Fi phase (cf. [4]). By definition, the symmetry of the AF and Fi phases is determined by the symmetry of parameters equations (2) and (3), respectively.

Active representations and corepresentations

The paramagnetic phase can be described in terms of a unitary or a non-unitary group and consequently, phase transitions can be induced by active representations (reps) or corepresentations (coreps), respectively. These two methods are based on the isomorphism of the two groups: \( G_{OM} \) in (1) and \( G_{OM} = P3m1 \), the latter obtained from the former by omitting the time-reversal operation. To obtain a representation of the magnetic group (1) of the P phase, the matrices of a rep of the group P3m1 connected with these rotational elements which in (1) appear together with the time-reversal operation, have to be multiplied by \(-1\). For those groups, six real irreps, and two real and two physically irreducible type (a) coreps are connected with the vector \( k = b_3/2 \) which must be chosen to obtain the observed AF phase (see Bradley and Cracknell [6], Kovalev and Gorbanyuk [7]). We have one-arm star and therefore all the irreps and coreps are Landau-active, and it can be verified that they are Lifshitz-active. We assume that different low-temperature phases are induced by different reps or coreps. The two-dimensional irreps can be transformed to a real form with help of the matrix

\[ D = \begin{pmatrix} -1 & -1 \\ i & 1 \end{pmatrix} \] (4)

which implies that the complex basis functions fulfill the equality \( \varphi_2 = \varphi_1^* \). The order parameters equations (2) and (3) are expanded in terms of the basis functions of an active irrep or corep,

\[ \delta S (x_p) = \sum_i \eta_i \varphi_i (x_p) \] (5)

\[ \Delta S (x_p) = \sum_j \xi_j \psi_j (x_p) \] (6)
with $i, j = 1, 2$, depending on the rep or corep dimension. The symmetry groups of the low-temperature phases are determined on the basis of these two expansions.

**Low-temperature symmetry groups**

An analysis of the spin structures connected with the order parameters equations (2) and (3) shows that the irreps $73$ and $76$ can induce the AF and Fi phases. The same holds for the coreps $d_1$ and $d_4 \oplus d_5$. The remaining reps and coreps cannot induce those phases. The low-temperature symmetry groups connected with $73$ and $d_1$ are $G_{OM}$ in (1), with the unit cell doubled compared to that of the P phase. The low-temperature groups connected with $75$ add $d_3 \oplus d_5$. The lowest-degree mixed invariants connected with the interaction of the order parameters with $M$, can be incorporated into the second-degree invariants appearing in $\Phi_1$ and $\Phi_2$, respectively. By applying the condition $\partial \Phi / \partial e_v = 0$, we eliminate the strain tensor components and obtain an effective potential density $\Phi'$. The second-degree invariants in $\Phi'$ have the effective coefficients

$$A'_i = A_i + \frac{\beta_i}{2\alpha} \sigma_v, \quad i = 1, 2.$$  (8)

The form of $A'_i$ explains the experimentally determined linear dependence of the critical end-point temperature on the hydrostatic pressure [1]. According to equation (8), the bicritical end-point is expected to behave in the same way.

**Thermodynamic potential density**

It has the same form for reps and coreps, since for the two-dimensional reps we have the equality: $\varphi_2 = \varphi_2^*$. The influence of hydrostatic pressure is accounted for by the invariants connected with the rep $\Gamma_1^+$ at $k = 0$. Expressed with accuracy to the sixth-degree the potential density is

$$\Phi = \Phi_1 + \Phi_2 + \Phi_3 + \Phi_{12} + \Phi_{13} + \Phi_{23} - e_v \sigma_v$$  (7)

where

$$\Phi_1 = A_1 \eta^2 + C_1 \xi^4 + D_1 \eta^6$$

$$\Phi_2 = A_2 |\xi|^2 + C_2 |\xi|^4 + D_2 |\xi|^6 + E_2 \xi^6 + E_2^* \xi^{*6}$$

$$\Phi_3 = \alpha \xi^2,$$  $\quad \Phi_{12} = \gamma \xi^2 |\xi|^2 + \delta \eta (\xi^3 + \xi^{*3})$  

$$\Phi_{13} = \beta_1 \eta^2 \xi v,$$  $\quad \Phi_{23} = \beta_2 |\xi|^2 \eta v$

where $A_i \sim (T - T_{c,i}), \quad i = 1, 2$ with $T_{c,i}$ denoting the transition temperature at zero external stress, $C_i, D_i, E_2, \alpha, \beta_i, \gamma$ and $\delta_i$ are temperature-independent, and where $e_v = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$ and $\sigma_v = \sigma_{xx} + \sigma_{yy} + \sigma_{zz}$ are the basis function of $\Gamma_1^+$ and the respective external stress. The term in the potential connected with the magnetization $M$ in the external field does not influence symmetry change, and has been omitted. The lowest-degree mixed invariants connected with the interaction of the order parameters with $M$, can be incorporated into the second-degree invariants appearing in $\Phi_1$ and $\Phi_2$, respectively. By applying the condition $\partial \Phi / \partial e_v = 0$, we eliminate the strain tensor components and obtain an effective potential density $\Phi'$. The second-degree invariants in $\Phi'$ have the effective coefficients

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