

## Physical realizations of $n \geq 4$ -component vector models. I. Derivation of the Landau-Ginzburg-Wilson Hamiltonians\*

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Certain phase transitions which involve an increase of the unit cell in one or more directions, are described by  $n \geq 4$ -component vector models. According to universality, the critical behavior of a system should depend only upon a small number of parameters such as the dimensionality of space, the number of components of the order parameter, and the symmetry of the Hamiltonian. We suggest that it would be of great interest to study these  $n \geq 4$  systems experimentally, and examine the effect of the dimensionality of the order parameter and the anisotropy of the system on the critical behavior. We use the group-theoretical method of Landau and Lifshitz to derive the Landau-Ginzburg-Wilson Hamiltonians corresponding to the following  $n \geq 4$  systems: type-II antiferromagnets TbAs, TbP, TbSb ( $n = 4$ ), and MnO, MnSe, NiO, and ErSb ( $n = 8$ ); type-I antiferromagnet  $\text{UO}_2$  ( $n = 6$ ); type-III antiferromagnet  $\text{K}_2\text{IrCl}_6$  ( $n = 6$ ); sinusoidal magnetic systems  $\text{DyC}_2$  and  $\text{TbAu}_2$  ( $n = 4$ ), and  $\text{TbD}_2$  and Nd ( $n = 6$ ); and an  $n = 4$  system,  $\text{NbO}_2$ , which exhibits a structural transition. In the following paper (II) we use the exact renormalization-group technique in  $d = 4 - \epsilon$  dimensions to study the critical behavior of these Hamiltonians.

### I. INTRODUCTION

In recent years, there has been considerable interest in the study of the critical behavior of  $n$ -component vector models.<sup>1-8</sup> These models have been used to discuss the critical behavior of physical systems which are Ising like<sup>9</sup> ( $n = 1$ ),  $XY$  like<sup>10</sup> ( $n = 2$ ), and Heisenberg like<sup>11</sup> ( $n = 3$ ). Amorphous Ising systems can be described as an  $n \rightarrow 0$  limit of the  $n$ -vector model.<sup>12,13</sup> In the limit  $n \rightarrow \infty$ , the critical behavior of the isotropic  $n$ -vector model becomes exactly that of the spherical model.<sup>14</sup> Recently,<sup>15-17</sup> it has been emphasized that there exist phase transitions in certain physical systems, involving an increase of the unit cell, which are described by  $n \geq 4$ -component models. The critical behavior of these  $n \geq 4$ -component systems is not yet known, and we suggest that it is of great interest to study these systems experimentally. According to the principle of universality, the critical exponents of a system should depend on only a small number of the system's properties, such as spatial dimensionality, the number of components of the order parameter, and the symmetry of the Hamiltonian. Brezin *et al.*<sup>8</sup> have used the  $\epsilon$  expansion to study the effect of anisotropy on the critical behavior of a system. They found that for  $n \leq 3$ -component order parameters, the anisotropy did not affect the critical behavior, while for  $n \geq 4$  anisotropy does affect the critical behavior. In this sense, universality is predicted to be weaker for  $n \geq 4$ -component systems than for  $n \leq 3$  systems. It is important to test this prediction experimentally.

As discussed by Landau,<sup>18</sup> the symmetry-breaking order parameter associated with a second-or-

der phase transition transforms as an irreducible representation of the symmetry group of the disordered phase. The number of independent components of the order-parameter is, therefore, equal to the dimensionality  $n$  of the representation according to which it transforms, and the transition is described by an  $n$ -component model. Transitions which do not involve a change of the unit cell are associated with an irreducible representation of the *point group* of the high-symmetry phase, and the dimensionality of these representations satisfies<sup>19</sup>  $n \leq 3$ . When the unit cell is doubled in one or more directions, the order parameter transforms as an irreducible representation of the *space group* of the high-symmetry phase, and the dimensionality of these representations can satisfy  $n \geq 4$ .

In this paper, we construct Landau-Ginzburg-Wilson (LGW) Hamiltonians for several physical systems which are described by  $n \geq 4$ -component order parameters. The critical behavior of these models is studied in the following paper, using the exact renormalization-group technique in  $d = 4 - \epsilon$  dimensions.<sup>20</sup> A study of the critical behavior of these systems may provide an experimental test for the regions of validity of the  $\epsilon$  expansion.

We construct the LGW Hamiltonian corresponding to a given physical system by using the group-theoretical techniques developed by Landau and Lifshitz.<sup>18</sup> A different method of constructing LGW Hamiltonians has been used by Nelson and Fisher<sup>21</sup> in their recent work on the metamagnet. For the applications we shall consider, the method of Landau and Lifshitz has the advantage of insuring that the Hamiltonian possesses all the fourth-order invariants allowed by symmetry. We have con-

structured LGW Hamiltonians corresponding to the following  $n \geq 4$  physical systems: type-II anti-ferromagnets TbAs, TbP, TbSb ( $n=4$ ), and MnO, MnSe, NiO, and ErSb ( $n=8$ ); type-I antiferromagnet  $\text{UO}_2$  ( $n=6$ ); type-III antiferromagnet  $\text{K}_2\text{IrCl}_6$  ( $n=6$ ); sinusoidal magnetic systems  $\text{DyC}_2$  and  $\text{TbAu}_2$  ( $n=4$ ), and  $\text{TbD}_2$  and Nd ( $n=6$ ). We also consider an  $n=4$  system,  $\text{NbO}_2$ , which exhibits a structural transition.

Our paper is organized as follows: In Sec. II we briefly review the Landau-Lifshitz symmetry arguments which are used in constructing the Hamiltonians. In Sec. III we discuss the dimensionality of the irreducible representations of space groups, and outline the way in which the  $n \geq 4$ -component vector models are derived. In Sec. IV we construct the Hamiltonians for the physical systems. The main results are summarized in Sec. V.

## II. SYMMETRY ARGUMENTS OF LANDAU AND LIFSHITZ

Consider a phase transition in which the symmetry group of the system is reduced from  $G_0$  in the disordered phase to  $G$  in the ordered phase, with  $G$  a subgroup of  $G_0$ . Let the transition be described by an  $n$ -component order-parameter  $\phi_1, \dots, \phi_n$ . Such a transition can be studied by the appropriate Landau-Ginzburg-Wilson Hamiltonian, which is a function of the order-parameter and its derivatives:

$$H = \int d^d x \mathcal{K} \left( \phi_i, \frac{\partial \phi_j}{\partial x_k}, \dots \right), \quad (2.1)$$

where  $\mathcal{K}$  is invariant under the symmetry group  $G_0$ . The partition function is obtained by performing the functional integral

$$Z = \int \prod_{i=1}^n d[\phi_i] e^{-\mathcal{H}}. \quad (2.2)$$

The Hamiltonian density  $\mathcal{K}$  can be written as a sum of two terms:

$$\mathcal{K} \left( \phi_i, \frac{\partial \phi_j}{\partial x_k}, \dots \right) = \mathcal{K}^1(\phi_i) + \mathcal{K}^2 \left( \phi_i, \frac{\partial \phi_j}{\partial x_k}, \dots \right), \quad (2.3)$$

where  $\mathcal{K}^1$  is a function of the order-parameter (and not its derivatives), while  $\mathcal{K}^2$  is a function of the  $\phi$ 's and their derivatives, and it vanishes when all the derivatives vanish. It is assumed that  $\mathcal{K}$  is an analytic function of the order parameter and its derivatives, and that it can be expanded in terms of these variables. We also assume, for reasons which will be discussed later, that the  $n$  components of the order parameter transform into one another according to *one* irreducible representation  $R$  of the group  $G_0$ . Under this assumption, the

expansion of  $\mathcal{K}^1$  will take the form:

$$\mathcal{K}^1 = -\frac{1}{2} \gamma \sum_{i=1}^n \phi_i^2 - \sum_p v_p \sum_{i,j,k=1}^n \alpha_{ijk}^p \phi_i \phi_j \phi_k - \dots, \quad (2.4)$$

where the sum  $\sum_p$  is over the third-order invariants of the group  $G_0$ . The reason that the expansion does not include a linear term is that the representation  $R$  according to which the order parameter transforms is different from the unit representation  $E$  (otherwise, the symmetry group  $G$  of the ordered phase will be the same as the group  $G_0$  of the disordered phase, and no symmetry breaking will occur). The linear term transforms according to the representation  $R$ , and, therefore, it cannot be invariant under  $G_0$ . The expansion includes one second-order term,  $\sum_{i=1}^n \phi_i^2$ , which is the only second-order invariant, but it may include several third- and higher-order terms.

Their number and actual form depend on the specific group  $G_0$  and the representation  $R$ . If the order parameter transforms according to more than one irreducible representation, say two, the second-order term will decompose into a sum of two terms:

$$-\frac{1}{2} \gamma_1 \sum_{i=1}^m \Psi_i^2 - \frac{1}{2} \gamma_2 \sum_{i=m+1}^n \Psi_i^2, \quad (2.5)$$

where  $\Psi_1, \dots, \Psi_n$  are linear combinations of  $\phi_1, \dots, \phi_n$ . Here  $\Psi_1, \dots, \Psi_m$  transform according to an irreducible representation  $R_1$  and  $\Psi_{m+1}, \dots, \Psi_n$  transform according to an irreducible representation  $R_2$ . These two order parameters have, in general, two different transition temperatures  $t_1$  and  $t_2$  determined by  $\gamma_1$  and  $\gamma_2$ . We are interested in the transition from the disordered phase, and, therefore, we consider only the order parameter which has a higher transition temperature, say  $\Psi_1, \dots, \Psi_m$ . This transition can be discussed in terms of an  $m$ -component order parameter. Clearly, it may happen that the two coefficients  $\gamma_1$  and  $\gamma_2$  are accidentally equal, and that one has to consider all the  $n$  components  $\Psi_1, \dots, \Psi_n$ . A point where such an accidental degeneracy occurs is, in fact, a higher-order critical point (bicritical, tetracritical, or higher order). In this work we are interested in ordinary critical points, and therefore, we consider order-parameters which belong to only one irreducible representation. Let us discuss now the Hamiltonian  $\mathcal{K}^2$ . The expansion of  $\mathcal{K}^2(\phi_i, \partial \phi_j / \partial x_k, \dots)$  takes the form:

$$\mathcal{K}^2 = \sum_{i,j=1}^n \sum_{k=1}^d A_{ijk} \phi_i \frac{\partial \phi_j}{\partial x_k} + \sum_{i,j=1}^n \sum_{k,l=1}^d B_{ijkl} \frac{\partial \phi_i}{\partial x_k} \frac{\partial \phi_j}{\partial x_l} + \dots, \quad (2.6)$$

with the restriction that each term is invariant under the group  $G_0$ . The expansion does not include terms linear in the derivatives,

$$\sum_{i=1}^n \sum_{k=1}^d C_k \frac{\partial \phi_i}{\partial x_k},$$

as these are surface terms and they can be neglected in the thermodynamic limit. For the same reason, one should consider only tensors  $A_{ijk}$  which are antisymmetric with respect to the first two indices. The symmetric part of this tensor gives rise to a surface term,

$$\frac{1}{2} \sum_{i,j=1}^n \sum_{k=1}^d (A_{ijk} + A_{jik}) \frac{\partial(\phi_i \phi_j)}{\partial x_k},$$

and it can be neglected.

In the Landau theory, one replaces the functional integral (2.2) by its saddle point value and describes the thermodynamic behavior of the system by the approximate partition function. Using this approximation, Landau and Lifshitz obtained the following results:

(a) For a second-order transition to occur, the third-order term in the expansion (2.4) should vanish at the transition temperature  $T_c$ . One can distinguish between two cases: (i) The third-order term does not appear in the expansion, due to symmetry, so the transition temperature is determined by one equation,  $r=0$ . (ii) The expansion does include a third-order term, but it vanishes at the transition. The transition temperature is now determined by several equations,  $r=0$  and  $v_p=0$ . In order to satisfy these equations one needs, in general, several thermodynamic variables. In this work we are interested in phase transitions which occur when only one thermodynamic variable, the temperature, is changed. We therefore demand that no third-order terms appear in the model Hamiltonians which describe our physical systems. This is equivalent to the restriction that the irreducible representation  $R$  associated with the transition is such that the symmetric part of  $R^3$ , denoted by  $[R^3]$ , does not contain the unit representation  $E$ :

$$[R^3] \not\supset E. \tag{2.7}$$

All the transitions discussed in this work satisfy this condition.

(b) The first term in the expansion (2.6), namely,

$$\sum_{i,j=1}^n \sum_{k=1}^d A_{ijk} \phi_i \frac{\partial \phi_j}{\partial x_k}$$

should vanish at the transition temperature.<sup>22</sup> The physical interpretation of this condition is best seen by rewriting the Hamiltonian (2.1) in terms

of the Fourier components of the order parameter. To second order in the order parameter, the Hamiltonian (2.1) is of the form

$$H = -\frac{1}{2} \sum_{\vec{q}} \sum_i F_i(\vec{q}) \phi_{i,\vec{q}} \bar{\phi}_{i,-\vec{q}} + \dots, \tag{2.8a}$$

where

$$F_i(\vec{q}) = r + \vec{A}^i \cdot \vec{q} + B_{\alpha\beta}^i q_\alpha q_\beta. \tag{2.8b}$$

The linear term in  $\vec{q}$  comes from the first term in (2.6) and the bilinear term in  $q_\alpha$  ( $\alpha, \beta = 1, \dots, d$ ) comes from the second term in (2.6). Since the order parameter which becomes critical at the transition ( $r=0$ ) is  $\phi_{i,0}$  (the  $\vec{q}=0$  Fourier component of  $\phi_i$ ), the coefficients  $F_i(\vec{q})$  should satisfy

$$F_i(\vec{0}) = 0 \tag{2.9a}$$

and

$$F_i(\vec{q}) > 0 \text{ for } \vec{q} \neq \vec{0} \tag{2.9b}$$

at the transition. This may happen only if the linear term in (2.8b) vanishes at  $T_c$ . One can distinguish between two cases: (1) The expansion (2.6) does not include a term

$$\sum_{i,j=1}^n \sum_{k=1}^d A_{ijk} \phi_i \frac{\partial \phi_j}{\partial x_k}$$

due to symmetry. This is the case when the representation  $R$  according to which the transition occurs is such that the direct product of the antisymmetric part of  $R^2$ , denoted by  $\{R^2\}$ , with the vector representation  $V$ , does not include the unit representation

$$\{R^2\} \times V \not\supset E. \tag{2.10}$$

This implies that the minimum of  $F_i(\vec{q})$  is obtained at  $\vec{q}=0$  in a temperature interval which includes  $T_c$ , as shown schematically in Fig. 1(a). (2) The

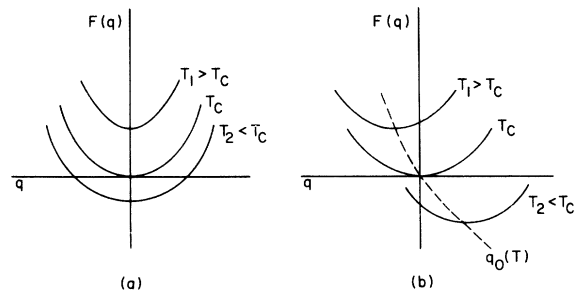


FIG. 1. Schematic form of the function  $F(\vec{q})$  when (a) the condition (2.10) is satisfied, and (b) the condition (2.10) is not satisfied. The vector  $\vec{q}_0$  at which the minimum of  $F(\vec{q})$  is obtained is temperature independent in the first case, but varies with temperature in the second case.

expansion (2.6) does include a term

$$\sum_{i,j=1}^n \sum_{k=1}^d A_{ijk} \phi_i \frac{\partial \phi_j}{\partial x_k},$$

but the coefficients  $A_{ijk}$  vanish at  $T_c$ . For  $T \neq T_c$  the coefficients  $A_{ijk}$  do not vanish, and therefore, the minimum of  $F_i(\vec{q})$  is expected to be at  $\vec{q}_0 \neq 0$ , as shown schematically in Fig. 1(b). The order parameter which appears below the transition is the  $\vec{q}_0$  Fourier component  $\phi_{i,\vec{q}_0}$ , where  $\vec{q}_0(T)$  is expected to vary continuously with temperature, and  $\vec{q}_0(T_c) = 0$ . Some of the physical systems discussed in this work (TbAu<sub>2</sub>, DyC<sub>2</sub>, NbO<sub>2</sub>, and Nd), do not satisfy condition (2.10), and the wave vector  $\vec{q}_0$  of their order parameter is expected to vary with temperature. This prediction of the Landau theory was confirmed experimentally in TbAu<sub>2</sub>, DyC<sub>2</sub>, and Nd. No temperature dependence of  $\vec{q}_0$  was found<sup>23</sup> for NbO<sub>2</sub>. This implies that either the vector  $\vec{q}_0$  varies very slowly with temperature, or that the transition is slightly first order. No evidence for discontinuity of the order parameter was found in this case.

### III. $n \geq 4$ -COMPONENT VECTOR MODELS

We discuss now the dimensionality of the order parameters which may describe transitions (magnetic or nonmagnetic) which occur in crystals. The symmetry groups of the three-dimensional crystals are the 230 space groups, and they are listed in Ref. 24. The irreducible representations of a space group  $G_0$ , are classified in the following way.<sup>25,26</sup> Let  $\vec{k}$  be a vector in the first Brillouin zone. The group of  $\vec{k}$ ,  $G_{\vec{k}}$ , is defined as the group of all the rotational elements (including screw axes and glide planes) of the group  $G_0$  which leave the vector  $\vec{k}$  invariant. The star of  $\vec{k}$  is a set of vectors  $\vec{k}_1 = \vec{k}, \vec{k}_2, \dots, \vec{k}_s$ , which are obtained by applying the symmetry elements of the group  $G_0$  on the vector  $\vec{k}$ . The irreducible representations of the group  $G_0$  are classified according to the parameters  $(\vec{k}, p)$ , where  $\vec{k}$  is a vector in the first Brillouin zone and  $p$  is a discrete parameter which classifies the irreducible representations of the group of  $\vec{k}$ . Let the dimensionality of the representation  $p$  (also called the small representation) be  $l_p$ . The functions which transform into one another as a basis of the representation  $(\vec{k}, p)$  have the form

$$\Psi_{\vec{k}_m, j}(\vec{r}) = U_{\vec{k}_m, j}(\vec{r}) e^{i \vec{k}_m \cdot \vec{r}} \quad (m = 1, \dots, s; j = 1, \dots, l_p), \quad (3.1)$$

where  $U_{\vec{k}_m, j}(\vec{r})$  are invariant under the translation operators of the group  $G_0$ . The functions  $U_{\vec{k}_m, 1}(\vec{r}), \dots, U_{\vec{k}_m, l_p}(\vec{r})$  transform to one another as a basis of the small representation  $p$  of the group

of  $\vec{k}_m$ . The dimensionality  $n$  of the representation  $(\vec{k}, p)$  is, therefore, given by

$$n = s l_p. \quad (3.2)$$

Phase transitions which do not involve a change of the unit cell (i.e., the primitive unit cell above the transition is the same as the one below  $T_c$ ), are associated with a representation which belongs to  $\vec{k} = 0$ . In this case the star of the vector  $\vec{k}$  contains only one vector,  $s = 1$ , and the group  $G_{\vec{k}}$  is isomorphic to the point group of the crystal. The small representation  $p$  is, therefore, a representation of the point group and it satisfies  $l_p \leq 3$ . The order parameter which describes such a transition has  $n \leq 3$ -independent components. If the transition does involve a change of the unit cell, the star of the vector  $\vec{k}$  may include more than one vector and the dimensionality of the representation can be  $n \geq 4$ . Note, however, that not every transition which involves a change of the unit cell is described by an  $n \geq 4$ -component order parameter. As an example, consider a tetragonal crystal whose space group is  $P4/mmm$ , which has one magnetic ion per unit cell. We assume that the crystal undergoes an antiferromagnetic transition which doubles the unit cell in the  $z$  direction, and with the sublattice magnetization along the  $z$  axis (Fig. 2). The order parameter in this case is the sublattice magnetization

$$\phi = S_{A,z} - S_{B,z} \quad (3.3)$$

where  $A$  and  $B$  are the two sublattices.  $\phi$  transforms to  $\pm \phi$  under the operations of the group  $G_0$ , and the order parameter is one dimensional, even though the unit cell is doubled.

The maximal dimensionality of the order parameter which can be achieved in crystals is 48, corresponding to a transition which is associated with a reciprocal-lattice vector  $\vec{k}$  in some general direction, in a crystal whose point group is  $m3m$  ( $O_h$ ). In this case the star of  $\vec{k}$  consists of 48 vectors which are obtained by applying the 48 operators of the group  $O_h$  on the vector  $\vec{k}$ . The group of  $\vec{k}$  is the trivial group, and it has only one one-dimensional representation (the unit representation). For transitions in fluids the dimensionality of the order parameter is not limited. For example, the transitions from liquids to crystals<sup>27,28</sup> or to cholesteric and smectic liquid crystals<sup>29</sup> are described by order parameters of infinite dimensionality. However, the LGW Hamiltonians which describe these transitions contain third-order invariants [they do not satisfy Eq. (2.7)], and the transitions are expected to be first order.

In the present work we construct  $n \geq 4$ -component vector models for several physical systems. We consider model Hamiltonians of the form

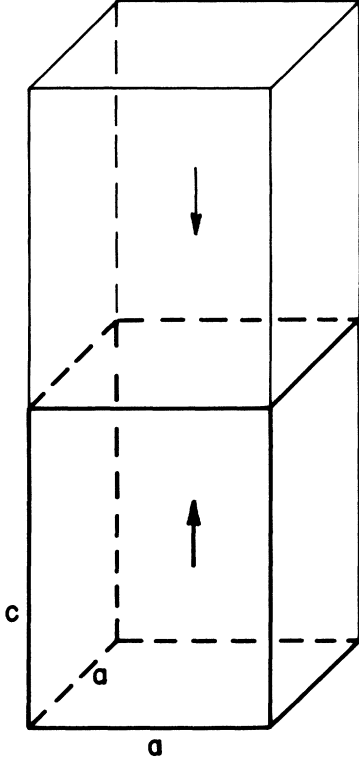


FIG. 2. Magnetic structure and the magnetic unit cell of an antiferromagnetic tetragonal crystal. The chemical unit cell is shown in heavy outline. The transition from the paramagnetic phase to the magnetically ordered phase is described by an  $n = 1$ -component order parameter, even though the unit cell is doubled.

$$\mathcal{H} = -\frac{1}{2} \sum_{i=1}^n [r\phi_i^2 + (\nabla\phi_i)^2] - \sum_{p=1}^m u^p \sum_{ijkl} \beta_{ijkl}^p \phi_i \phi_j \phi_k \phi_l, \quad (3.4)$$

where the sum  $\sum_{p=1}^m$  is over all the possible fourth-order invariants of the group  $G_0$ . All the transitions we shall discuss satisfy Eq. (2.7), and, therefore, the Hamiltonian (3.4) does not include third-order terms. The gradient term in the Hamiltonian (3.4) is assumed to be rotationally invariant in the coordinate space. The anisotropic terms do not affect the critical behavior of the system to first order in  $\epsilon$ , therefore, they are not considered here.<sup>30</sup> By applying a symmetry-breaking field, such as a stress, magnetic field, etc., the paramagnetic space group is lowered and the dimensionality of the order parameter is reduced. Therefore, to experimentally observe the effect of the  $n$  components of the order parameter, care must be taken that no symmetry breaking field is present. Let  $\Gamma$  be the irreducible representation according to which the order parameter  $\phi_1, \dots, \phi_n$  transforms. The fourth-order terms in the Hamil-

tonian (3.4) transform under the operators of  $G_0$  as the symmetric part of the representation  $\Gamma^4$  ( $[\Gamma^4]$ ). The number of fourth-order invariants  $l$  is equal to the number of times the representation  $[\Gamma^4]$  contains the unit representation. The character table  $\chi_4(g)$  of the representation  $[\Gamma^4]$  is given by<sup>31</sup>

$$\chi_4(g) = \frac{1}{4}\chi(g^4) + \frac{1}{3}\chi(g^3)\chi(g) + \frac{1}{4}\chi(g^2)\chi^2(g) + \frac{1}{8}\chi^2(g^2) + \frac{1}{24}\chi^4(g), \quad (3.5)$$

where  $g \in G_0$ , and  $\chi(g)$  is the character table of the representation  $\Gamma$ . One can use this character table and the orthogonality relations to find the number of fourth-order invariants which can be formed by the order-parameter  $\phi_1, \dots, \phi_n$ . Our method for determining the invariants was not systematic. We made educated guesses and then explicitly checked that our forms were invariant under the operations of the group. Since we knew the number of independent invariants from the character table, we knew when we had constructed a complete set.

#### IV. CONSTRUCTING THE HAMILTONIANS

##### A. Type-II antiferromagnets

We consider the transition from the paramagnetic to the magnetically ordered phase in type-II antiferromagnets.<sup>32</sup> The paramagnetic space group of these fcc crystals is  $Fm\bar{3}m$ . The magnetic structure below the transition consists of ferromagnetic (111) planes which are coupled antiferromagnetically. This structure belongs to a reciprocal-lattice vector  $\vec{k}_1 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})(2\pi/a)$ , where  $a$  is the lattice constant of the nonprimitive unit cell. The star of  $\vec{k}_1$  consists of four vectors:  $\vec{k}_1 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})(2\pi/a)$ ,  $\vec{k}_2 = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})(2\pi/a)$ ,  $\vec{k}_3 = (-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})(2\pi/a)$ , and  $\vec{k}_4 = (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})(2\pi/a)$ . The four magnetic lattices which correspond to these four vectors are given in Fig. 3. The group of  $\vec{k}_1$  is  $D_{3d}$ , and, therefore, any order parameter which belongs to  $\vec{k}_1$ , should transform as a basis of an irreducible representation of  $D_{3d}$ . This restricts the direction of the magnetic moments to be either parallel to  $\vec{k}_1$ , where it belongs to a one-dimensional representation of  $D_{3d}$ , or to lie in a plane perpendicular to  $\vec{k}_1$ , where it has two independent components. In the first case (which occurs in<sup>33</sup> TbAs, TbP, and TbSb), the system is described by an  $n = 4$ -component order parameter, while in the second case (which occurs in<sup>34</sup> MnO,<sup>35</sup> MnSe, NiO,<sup>36</sup> and<sup>37,38</sup> ErSb) the system is described by an  $n = 8$ -component order parameter. We note, however, that there exist some type-II antiferromagnets (as<sup>33</sup> DySb and HoSb) where the magnetic moment lies along the [001] direction with nonvanishing components both parallel and

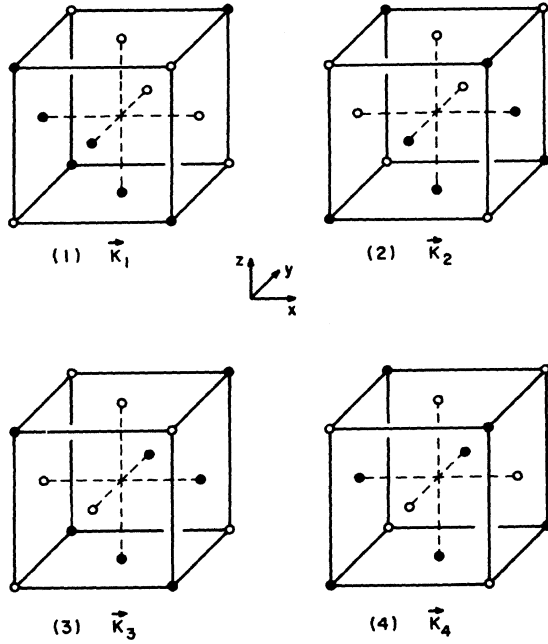


FIG. 3. Four magnetic lattices of type-II antiferromagnets. Black dots indicate "up" spins and white dots indicate "down" spins. The lattices 1, . . . , 4 belong to the wave vectors  $\vec{k}_1 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})(2\pi/a)$ ,  $\vec{k}_2 = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})(2\pi/a)$ ,  $\vec{k}_3 = (-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})(2\pi/a)$ , and  $\vec{k}_4 = (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})(2\pi/a)$ , respectively.

perpendicular to  $\vec{k}_i$ . The order parameter which describes these systems belongs to two irreducible representations, and it has 12 independent components. According to Landau theory the transition in these systems is either first order, or second order with the critical point being a bicritical or tetracritical point (where two different representations become critical simultaneously). In the present work we consider only ordinary critical points. Let us discuss now the transitions described by the  $n=4$  and  $n=8$  models.

#### 1. $\vec{m} \parallel \vec{k}$

When the magnetic moment  $\vec{m}$  is parallel to the reciprocal-lattice vector  $\vec{k}$ , the order parameter has four independent components  $\phi_i$  ( $i=1, \dots, 4$ ). These components are defined in the following way:

$$\phi_i = \sum_{\alpha \in \{B\}_i} \vec{S}_\alpha \cdot \hat{k}_i - \sum_{\alpha \in \{W\}_i} \vec{S}_\alpha \cdot \hat{k}_i, \quad i=1, \dots, 4 \quad (4.1)$$

where the sums  $\sum_{\alpha \in \{B\}_i}$  and  $\sum_{\alpha \in \{W\}_i}$  are over sites  $\alpha$  of the black and white sublattices, respectively, of the structure which belongs to  $\vec{k}_i$  (see Fig. 3). The vectors  $\hat{k}_i$  are unit vectors in the  $\vec{k}_i$  directions. The order parameter (4.1)

transforms under the generators of the group  $Fm3m$  as follows:

$$\begin{aligned} C_4([111]): \quad & \phi_1 \rightarrow \phi_2, \phi_2 \rightarrow \phi_3, \phi_3 \rightarrow \phi_4, \phi_4 \rightarrow \phi_1, \\ i: \quad & \phi_i \rightarrow -\phi_i, \quad i=1, \dots, 4 \\ C_3([111]): \quad & \phi_1 \rightarrow \phi_1, \phi_2 \rightarrow -\phi_3, \phi_3 \rightarrow -\phi_4, \phi_4 \rightarrow \phi_2, \\ C_2([110]): \quad & \phi_1 \rightarrow \phi_3, \phi_3 \rightarrow \phi_1, \phi_2 \rightarrow \phi_2, \phi_4 \rightarrow \phi_4, \\ t([\frac{1}{2}\frac{1}{2}0]): \quad & \phi_1 \rightarrow -\phi_1, \phi_2 \rightarrow \phi_2, \phi_3 \rightarrow -\phi_3, \phi_4 \rightarrow \phi_4, \end{aligned} \quad (4.2)$$

where  $C_l([\dots])$  is an  $l$ -fold rotation axis along the direction  $[\dots]$ ,  $i$  is the inversion, and  $t([\frac{1}{2}\frac{1}{2}0])$  is a translation of  $(\frac{1}{2}, \frac{1}{2}, 0)a$ . Using these transformations we found that the order parameter has three fourth-order invariants. The LGW Hamiltonian which describes the system is

$$\begin{aligned} \mathcal{H}_3 = & -\frac{1}{2} \sum_{i=1}^4 [r\phi_i^2 + (\nabla\phi_i)^2] - u \left( \sum_{i=1}^4 \phi_i^2 \right)^2 \\ & - v \sum_{i=1}^4 \phi_i^4 - w \phi_1 \phi_2 \phi_3 \phi_4. \end{aligned} \quad (4.3)$$

#### 2. $\vec{m} \perp \vec{k}$

In this case there are two components  $\phi_i$  and  $\bar{\phi}_i$  associated with each vector  $\vec{k}_i$ ,  $i=1, \dots, 4$ , and the representation according to which the transition occurs is eight dimensional. For each vector  $\vec{k}_i$  we define two unit vectors  $\vec{\nu}_i$  and  $\vec{\mu}_i$  perpendicular to it:

$$\begin{aligned} \vec{\nu}_1 &= (1/\sqrt{2})(1, -1, 0), \quad \vec{\mu}_1 = (1/\sqrt{6})(1, 1, -2), \\ \vec{\nu}_2 &= (1/\sqrt{2})(1, 1, 0), \quad \vec{\mu}_2 = (1/\sqrt{6})(-1, 1, -2), \\ \vec{\nu}_3 &= (1/\sqrt{2})(-1, 1, 0), \quad \vec{\mu}_3 = (1/\sqrt{6})(-1, -1, -2), \\ \vec{\nu}_4 &= (1/\sqrt{2})(-1, -1, 0), \quad \vec{\mu}_4 = (1/\sqrt{6})(1, -1, -2). \end{aligned} \quad (4.4)$$

Using these unit vectors, the eight components of the order parameter are defined by

$$\begin{aligned} \phi_i &= \sum_{\alpha \in \{B\}_i} \vec{S}_\alpha \cdot \vec{\nu}_i - \sum_{\alpha \in \{W\}_i} \vec{S}_\alpha \cdot \vec{\nu}_i, \quad i=1, \dots, 4 \\ \bar{\phi}_i &= \sum_{\alpha \in \{B\}_i} \vec{S}_\alpha \cdot \vec{\mu}_i - \sum_{\alpha \in \{W\}_i} \vec{S}_\alpha \cdot \vec{\mu}_i, \quad i=1, \dots, 4 \end{aligned} \quad (4.5)$$

where the sums  $\sum_{\alpha \in \{B\}_i}$  and  $\sum_{\alpha \in \{W\}_i}$  are defined as before. The order parameter (4.5) transforms under the generators of the group  $Fm3m$  in the following way:

$$\begin{aligned}
C_4([001]): & \phi_1 - \phi_2, \phi_2 - \phi_3, \phi_3 - \phi_4, \phi_4 - \phi_1, \bar{\phi}_1 - \bar{\phi}_2, \bar{\phi}_2 - \bar{\phi}_3, \bar{\phi}_3 - \bar{\phi}_4, \bar{\phi}_4 - \bar{\phi}_1, \\
i: & \phi_i - -\phi_i, \bar{\phi}_i - -\bar{\phi}_i, \quad i=1, \dots, 4 \\
C_2([110]): & \phi_1 - -\phi_3, \phi_2 - -\phi_2, \phi_3 - -\phi_1, \phi_4 - -\phi_4, \bar{\phi}_1 - \bar{\phi}_3, \bar{\phi}_2 - \bar{\phi}_2, \bar{\phi}_3 - \bar{\phi}_1, \bar{\phi}_4 - \bar{\phi}_4, \\
C_3([111]): & \phi_1 - -\frac{1}{2}\phi_1 - \frac{1}{2}\sqrt{3}\bar{\phi}_1, \phi_2 - \frac{1}{2}\phi_3 + \frac{1}{2}\sqrt{3}\bar{\phi}_3, \phi_3 - \frac{1}{2}\phi_4 - \frac{1}{2}\sqrt{3}\bar{\phi}_4, \phi_4 - -\frac{1}{2}\phi_2 + \frac{1}{2}\sqrt{3}\bar{\phi}_2, \bar{\phi}_1 - \frac{1}{2}\sqrt{3}\phi_1 - \frac{1}{2}\bar{\phi}_1, \\
& \bar{\phi}_2 - \frac{1}{2}\sqrt{3}\phi_3 - \frac{1}{2}\bar{\phi}_3, \bar{\phi}_3 - -\frac{1}{2}\sqrt{3}\phi_4 - \frac{1}{2}\bar{\phi}_4, \bar{\phi}_4 - -\frac{1}{2}\sqrt{3}\phi_2 - \frac{1}{2}\bar{\phi}_2, \\
t([\frac{1}{2}\frac{1}{2}0]): & \phi_1 - -\phi_1, \phi_2 - \phi_2, \phi_3 - -\phi_3, \phi_4 - \phi_4, \bar{\phi}_1 - -\bar{\phi}_1, \bar{\phi}_2 - \bar{\phi}_2, \bar{\phi}_3 - -\bar{\phi}_3, \bar{\phi}_4 - \bar{\phi}_4.
\end{aligned} \tag{4.6}$$

This order parameter has six fourth-order invariants, and the LGW Hamiltonian is given by

$$\mathcal{H}_2 = -\frac{1}{2} \sum_{i=1}^4 [\gamma(\phi_i^2 + \bar{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\bar{\phi}_i)^2] - \sum_{i=1}^6 u_i O_i(\phi_i, \bar{\phi}_i), \tag{4.7}$$

where

$$\begin{aligned}
O_1 &= \sum_{i=1}^4 (\phi_i^2 + \bar{\phi}_i^2)^2, \\
O_2 &= \sum_{i < j} (\phi_i^2 \phi_j^2 + \bar{\phi}_i^2 \bar{\phi}_j^2 + \phi_i^2 \bar{\phi}_j^2 + \bar{\phi}_i^2 \phi_j^2), \\
O_3 &= \phi_1 \phi_2 \bar{\phi}_3 \bar{\phi}_4 + \bar{\phi}_1 \bar{\phi}_2 \phi_3 \phi_4 + \phi_1 \bar{\phi}_2 \bar{\phi}_3 \phi_4 + \bar{\phi}_1 \phi_2 \phi_3 \bar{\phi}_4 - \phi_1 \bar{\phi}_2 \phi_3 \bar{\phi}_4 - \bar{\phi}_1 \phi_2 \bar{\phi}_3 \phi_4 - 3\phi_1 \phi_2 \phi_3 \phi_4 - 3\bar{\phi}_1 \bar{\phi}_2 \bar{\phi}_3 \bar{\phi}_4, \\
O_4 &= \sum_{i < j} (\phi_i^2 \phi_j^2 + \bar{\phi}_i^2 \bar{\phi}_j^2) - 2(\phi_1 \bar{\phi}_1 \phi_2 \bar{\phi}_2 + \phi_2 \bar{\phi}_2 \phi_3 \bar{\phi}_3 + \phi_1 \bar{\phi}_1 \phi_4 \bar{\phi}_4 + \phi_3 \bar{\phi}_3 \phi_4 \bar{\phi}_4 - \phi_1 \bar{\phi}_1 \phi_3 \bar{\phi}_3 - \phi_2 \bar{\phi}_2 \phi_4 \bar{\phi}_4), \\
O_5 &= 2(\phi_1^2 \phi_3^2 - \bar{\phi}_1^2 \bar{\phi}_3^2) + 2(\phi_2^2 \phi_4^2 - \bar{\phi}_2^2 \bar{\phi}_4^2) - (\phi_1^2 \phi_2^2 - \bar{\phi}_1^2 \bar{\phi}_2^2) - (\phi_1^2 \phi_4^2 - \bar{\phi}_1^2 \bar{\phi}_4^2) - (\phi_2^2 \phi_3^2 - \bar{\phi}_2^2 \bar{\phi}_3^2) \\
& \quad - (\phi_3^2 \phi_4^2 - \bar{\phi}_3^2 \bar{\phi}_4^2) + \sqrt{3}(\phi_1 \bar{\phi}_1 - \phi_3 \bar{\phi}_3)(\phi_4^2 + \bar{\phi}_4^2 - \phi_2^2 - \bar{\phi}_2^2) + \sqrt{3}(\phi_2 \bar{\phi}_2 - \phi_4 \bar{\phi}_4)(\phi_1^2 + \bar{\phi}_1^2 - \phi_3^2 - \bar{\phi}_3^2),
\end{aligned} \tag{4.8}$$

and

$$\begin{aligned}
O_6 &= 4(\phi_1^2 \phi_2^2 + \phi_2^2 \phi_3^2 + \phi_3^2 \phi_4^2 + \phi_4^2 \phi_1^2 + \bar{\phi}_1^2 \bar{\phi}_2^2 + \bar{\phi}_2^2 \bar{\phi}_3^2 + \bar{\phi}_3^2 \bar{\phi}_4^2 + \bar{\phi}_4^2 \bar{\phi}_1^2) \\
& \quad + 12(\phi_1 \bar{\phi}_1 \phi_3 \bar{\phi}_3 + \phi_2 \bar{\phi}_2 \phi_4 \bar{\phi}_4) + (\phi_1^2 \phi_3^2 + \phi_2^2 \phi_4^2 + \bar{\phi}_1^2 \bar{\phi}_3^2 + \bar{\phi}_2^2 \bar{\phi}_4^2) + 3(\phi_1^2 \bar{\phi}_3^2 + \bar{\phi}_1^2 \phi_3^2 + \phi_2^2 \bar{\phi}_4^2 + \bar{\phi}_2^2 \phi_4^2) \\
& \quad + 2\sqrt{3}(\phi_1 \bar{\phi}_1 - \phi_3 \bar{\phi}_3)(\phi_4^2 - \bar{\phi}_4^2 - \phi_2^2 + \bar{\phi}_2^2) + 2\sqrt{3}(\phi_2 \bar{\phi}_2 - \phi_4 \bar{\phi}_4)(\phi_1^2 - \bar{\phi}_1^2 - \phi_3^2 + \bar{\phi}_3^2).
\end{aligned}$$

#### B. Type-I antiferromagnets, $\bar{m} \perp \bar{k}$

Consider the transition from the paramagnetic to the magnetically ordered phase in type-I antiferromagnets. These are fcc crystals whose paramagnetic space group is  $Fm\bar{3}m$ . The magnetic structure consists of ferromagnetic (100) planes coupled antiferromagnetically. This structure belongs to a reciprocal-lattice vector  $\bar{k}_1 = (1, 0, 0)(2\pi/a)$ , where  $a$  is the lattice constant of the non-primitive unit cell. The star of  $\bar{k}_1$  consists of three vectors:  $\bar{k}_1 = (1, 0, 0)(2\pi/a)$ ,  $\bar{k}_2 = (0, 1, 0)(2\pi/a)$ , and  $\bar{k}_3 = (0, 0, 1)(2\pi/a)$ . The three magnetic lattices which correspond to these three vectors are given in Fig. 4. The fact that the order parameter which belongs to  $\bar{k}_1$  should transform according to one irreducible representation of the group of  $\bar{k}_1$  ( $D_{4h}$ ), imposes restrictions on the possible direction of the sublattice magnetization: it can be either parallel or perpendicular to  $\bar{k}_1$ . In the first case, the representation of the group of  $\bar{k}_1$  is one dimensional, and the order parameter has only three components. We shall not consider this case. In the sec-

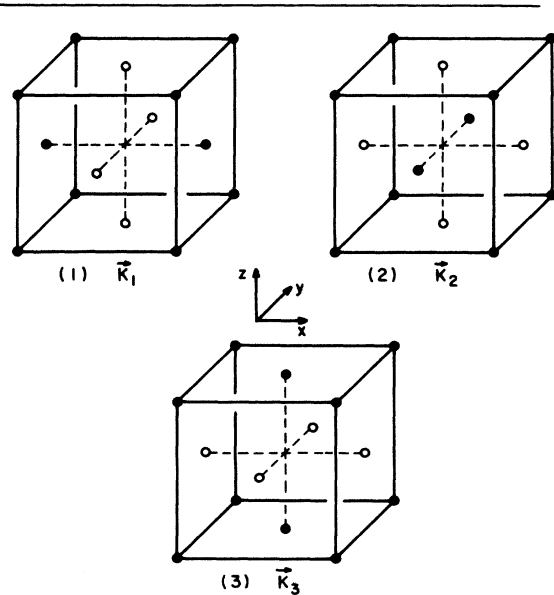


FIG. 4. Three magnetic lattices of type-I antiferromagnets. The lattices 1, 2, 3 belong to the wave vectors  $\bar{k}_1 = (1, 0, 0)(2\pi/a)$ ,  $\bar{k}_2 = (0, 1, 0)(2\pi/a)$ , and  $\bar{k}_3 = (0, 0, 1)(2\pi/a)$ , respectively.

ond case (which occurs<sup>39</sup> in  $\text{UO}_2$ ), the representation of the group of  $\vec{k}_1$  is two dimensional, and the order parameter has six independent components,  $\phi_i, \bar{\phi}_i, i=1, 2, 3$ . The order parameter is defined by:

$$\begin{aligned}
\phi_1 &= \sum_{\alpha \in \{B\}_1} S_{\alpha,x} - \sum_{\alpha \in \{W\}_1} S_{\alpha,x}, \\
\bar{\phi}_1 &= \sum_{\alpha \in \{B\}_1} S_{\alpha,y} - \sum_{\alpha \in \{W\}_1} S_{\alpha,y}, \\
\phi_2 &= \sum_{\alpha \in \{B\}_2} S_{\alpha,x} - \sum_{\alpha \in \{W\}_2} S_{\alpha,x}, \\
\bar{\phi}_2 &= \sum_{\alpha \in \{B\}_2} S_{\alpha,z} - \sum_{\alpha \in \{W\}_2} S_{\alpha,z}, \\
\phi_3 &= \sum_{\alpha \in \{B\}_3} S_{\alpha,y} - \sum_{\alpha \in \{W\}_3} S_{\alpha,y}, \\
\bar{\phi}_3 &= \sum_{\alpha \in \{B\}_3} S_{\alpha,x} - \sum_{\alpha \in \{W\}_3} S_{\alpha,x},
\end{aligned} \tag{4.9}$$

where  $S_{\alpha,\mu}$ ,  $\mu=x, y, z$ , is the  $\mu$  component of the spin on site  $\alpha$ . This order parameter transforms under the generators of the group  $Fm\bar{3}m$  as follows:

$$\begin{aligned}
C_4([001]): \quad & \phi_1 \rightarrow \bar{\phi}_2, \phi_2 \rightarrow \bar{\phi}_1, \phi_3 \rightarrow -\bar{\phi}_3, \\
& \bar{\phi}_1 \rightarrow -\phi_2, \bar{\phi}_2 \rightarrow \phi_1, \bar{\phi}_3 \rightarrow \phi_3, \\
i: \quad & \phi_i \rightarrow \phi_i, \bar{\phi}_i \rightarrow \bar{\phi}_i, \quad i=1, 2, 3 \\
C_3([111]): \quad & \phi_1 \rightarrow \phi_3, \phi_2 \rightarrow \phi_1, \phi_3 \rightarrow \phi_2, \\
& \bar{\phi}_1 \rightarrow \bar{\phi}_3, \bar{\phi}_2 \rightarrow \bar{\phi}_1, \bar{\phi}_3 \rightarrow \bar{\phi}_2, \\
C_2([110]): \quad & \phi_1 \rightarrow -\bar{\phi}_2, \phi_2 \rightarrow \bar{\phi}_1, \phi_3 \rightarrow \bar{\phi}_3, \\
& \bar{\phi}_1 \rightarrow \phi_2, \bar{\phi}_2 \rightarrow -\phi_1, \bar{\phi}_3 \rightarrow \phi_3, \\
t([\frac{1}{2}\frac{1}{2}0]): \quad & \phi_1 \rightarrow -\phi_1, \phi_2 \rightarrow -\phi_2, \phi_3 \rightarrow \phi_3, \\
& \bar{\phi}_1 \rightarrow -\bar{\phi}_1, \bar{\phi}_2 \rightarrow -\bar{\phi}_2, \bar{\phi}_3 \rightarrow \bar{\phi}_3.
\end{aligned} \tag{4.10}$$

The order-parameter has five fourth-order invariants, and the LGW Hamiltonian which describes the system is:

$$\begin{aligned}
\mathcal{H}_4 = & -\frac{1}{2} \sum_{i=1}^3 [\gamma(\phi_i^2 + \bar{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\bar{\phi}_i)^2] \\
& - u_1 \sum_{i=1}^3 (\phi_i^4 + \bar{\phi}_i^4) - u_2 \sum_{i=1}^3 \phi_i^2 \bar{\phi}_i^2 \\
& - u_3 \sum_{i<j} (\phi_i^2 \phi_j^2 + \bar{\phi}_i^2 \bar{\phi}_j^2) - u_4 (\bar{\phi}_1^2 \phi_2^2 + \bar{\phi}_2^2 \phi_3^2 + \bar{\phi}_3^2 \phi_1^2) \\
& - u_5 (\phi_1^2 \bar{\phi}_2^2 + \phi_2^2 \bar{\phi}_3^2 + \phi_3^2 \bar{\phi}_1^2).
\end{aligned} \tag{4.11}$$

### C. Type-III antiferromagnets

These are fcc crystals whose paramagnetic space group is  $Fm\bar{3}m$ . The magnetic structure

below the transition belongs to a reciprocal-lattice vector  $\vec{k}_1 = (\frac{1}{2}, 0, 1)(2\pi/a)$  with the nonprimitive unit cell doubled in one direction ( $x$  in this case). The star of the vector  $\vec{k}_1$  consists of six vectors:  $\pm\vec{k}_1 = (\pm\frac{1}{2}, 0, 1)(2\pi/a)$ ,  $\pm\vec{k}_2 = (1, \pm\frac{1}{2}, 0)(2\pi/a)$ , and  $\pm\vec{k}_3 = (0, 1, \pm\frac{1}{2})(2\pi/a)$ , and the group of  $\vec{k}_1$  is  $C_{4v}$ . As in the previous cases, for the order parameter to belong to one irreducible representation of the group of  $\vec{k}_1$ , the sublattice magnetization should be either parallel to the  $x$  direction (with one independent component) or be in the  $y-z$  plane (with two linearly independent components). Here we consider only the first case (occurs<sup>40</sup> in  $\text{K}_2\text{IrCl}_6$ ), which is described by a six-dimensional order parameter. Let  $\Psi_{\pm\vec{k}_j}$  be the components of the order parameter which belong to the reciprocal-lattice vectors  $\pm\vec{k}_j, j=1, 2, 3$ . We define these components in terms of six functions  $\phi_j$  and  $\bar{\phi}_j$  ( $j=1, 2, 3$ ):

$$\Psi_{\pm\vec{k}_j} \equiv (\phi_j + \bar{\phi}_j) \pm i(\phi_j - \bar{\phi}_j), \tag{4.12}$$

where  $\phi_j$  and  $\bar{\phi}_j$  are defined by

$$\begin{aligned}
\phi_1 &= \sum_{\alpha \in \{B\}_1} S_{\alpha,x} - \sum_{\alpha \in \{W\}_1} S_{\alpha,x}, \\
\bar{\phi}_1 &= \sum_{\alpha \in \{B\}_{\bar{1}}} S_{\alpha,x} - \sum_{\alpha \in \{W\}_{\bar{1}}} S_{\alpha,x}, \\
\phi_2 &= \sum_{\alpha \in \{B\}_2} S_{\alpha,y} - \sum_{\alpha \in \{W\}_2} S_{\alpha,y}, \\
\bar{\phi}_2 &= \sum_{\alpha \in \{B\}_{\bar{2}}} S_{\alpha,y} - \sum_{\alpha \in \{W\}_{\bar{2}}} S_{\alpha,y}, \\
\phi_3 &= \sum_{\alpha \in \{B\}_3} S_{\alpha,z} - \sum_{\alpha \in \{W\}_3} S_{\alpha,z}, \\
\bar{\phi}_3 &= \sum_{\alpha \in \{B\}_{\bar{3}}} S_{\alpha,z} - \sum_{\alpha \in \{W\}_{\bar{3}}} S_{\alpha,z},
\end{aligned} \tag{4.13}$$

where the magnetic lattices  $j, \bar{j}, j=1, 2, 3$  are defined in Fig. 5. The order parameters  $\phi_j, \bar{\phi}_j$  transform, under the generators of the group  $Fm\bar{3}m$ , in the following way:

$$\begin{aligned}
C_4([001]): \quad & \phi_1 \rightarrow \bar{\phi}_2, \phi_2 \rightarrow \bar{\phi}_1, \phi_3 \rightarrow \bar{\phi}_3, \\
& \bar{\phi}_1 \rightarrow \phi_2, \bar{\phi}_2 \rightarrow \bar{\phi}_1, \bar{\phi}_3 \rightarrow \phi_3, \\
i: \quad & \phi_j \rightarrow -\bar{\phi}_j, \bar{\phi}_j \rightarrow -\phi_j, \quad j=1, 2, 3 \\
C_3([111]): \quad & \phi_1 \rightarrow \phi_3, \phi_2 \rightarrow \phi_1, \phi_3 \rightarrow \phi_2, \\
& \bar{\phi}_1 \rightarrow \bar{\phi}_3, \bar{\phi}_2 \rightarrow \bar{\phi}_1, \bar{\phi}_3 \rightarrow \bar{\phi}_2, \\
C_2([110]): \quad & \phi_1 \rightarrow \bar{\phi}_2, \phi_2 \rightarrow \bar{\phi}_1, \phi_3 \rightarrow \phi_3, \\
& \bar{\phi}_1 \rightarrow \phi_2, \bar{\phi}_2 \rightarrow \phi_1, \bar{\phi}_3 \rightarrow \bar{\phi}_3, \\
t([\frac{1}{2}\frac{1}{2}0]): \quad & \phi_1 \rightarrow -\bar{\phi}_1, \phi_2 \rightarrow \bar{\phi}_2, \phi_3 \rightarrow -\phi_3, \\
& \bar{\phi}_1 \rightarrow \phi_1, \bar{\phi}_2 \rightarrow -\phi_2, \bar{\phi}_3 \rightarrow -\bar{\phi}_3.
\end{aligned} \tag{4.14}$$



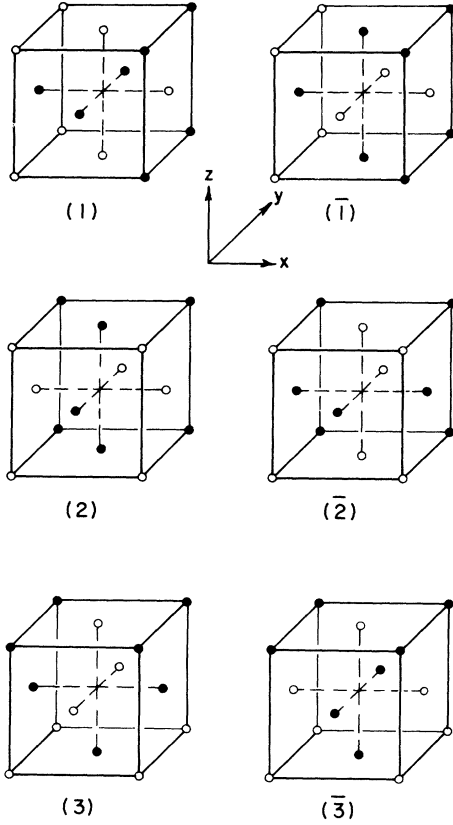


FIG. 5. Six magnetic lattices of type-III antiferromagnets.

We found that this order parameter has three fourth-order invariants. The LGW Hamiltonian which describes the system is

$$\begin{aligned} \mathcal{H} = & -\frac{1}{2} \sum_{i=1}^3 [\mathcal{r}(\phi_i^2 + \bar{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\bar{\phi}_i)^2] \\ & - u \left( \sum_{i=1}^3 \phi_i^2 + \bar{\phi}_i^2 \right)^2 - v \sum_{i=1}^3 (\phi_i^2 + \bar{\phi}_i^2)^2 \\ & - w \sum_{i=1}^3 \phi_i^2 \bar{\phi}_i^2. \end{aligned} \quad (4.15)$$

#### D. DyC<sub>2</sub> and TbAu<sub>2</sub>

These are tetragonal crystals<sup>41</sup> whose paramagnetic space group is  $I4/mmm$  ( $D_{4h}^{17}$ ). Below the Néel temperature, they exhibit a transverse sinusoidal magnetic structure with the sublattice magnetization being parallel to the  $z$  axis (Fig. 6). We consider first the DyC<sub>2</sub>. The magnetic structure of this compound belongs to a reciprocal-lattice vector  $\vec{k}_1 = (k, 0, 0)(2\pi/a)$ , where  $k \sim 0.77$  and  $a$  is the lattice constant of the  $x$ - $y$  plane. The

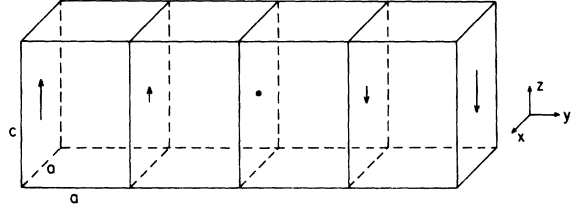


FIG. 6. Transverse sinusoidal magnetic structure, such as the one which exists in DyC<sub>2</sub>. The  $\vec{k}$  vector is along the  $y$  axis and the magnetization is along the  $z$  axis. The  $x$ - $z$  planes are ferromagnetic.

star of  $\vec{k}_1$  consists of four vectors:  $\pm\vec{k}_1 = (\pm k, 0, 0) \times (2\pi/a)$  and  $\pm\vec{k}_2 = (0, \pm k, 0)(2\pi/a)$  (Fig. 7). The sublattice magnetization is along the  $z$  axis and, therefore, the order parameter belongs to a one-dimensional representation of the group of  $\vec{k}_1$  ( $C_{2v}$ ). The order parameter has four linearly independent components:

$$\Psi_{\pm\vec{k}_j} \equiv \phi_j \pm i\bar{\phi}_j = \sum_{\vec{r}} e^{i\vec{k}_j \cdot \vec{r}} S_{\vec{r},z}, \quad (4.16)$$

where the sum  $\sum_{\vec{r}}$  is over the sites of the magnetic ions, and  $S_{\vec{r},z}$  is the  $z$  component of the spin located at  $\vec{r}$ . The fourth-order invariants of this order parameter are constructed by noting that the only fourth-order terms which are translationally invariant are those which can be written as products of two terms of the form  $\Psi_{\vec{k}_i} \Psi_{-\vec{k}_i}$ . The two functions of  $\Psi_{\vec{k}_1} \Psi_{-\vec{k}_1}$  and  $\Psi_{\vec{k}_2} \Psi_{-\vec{k}_2}$  are invariants under the translation operators of the group  $D_{4h}^{17}$ , and they transform to one another as a basis of a two-dimensional representation of the point group  $D_{4h}$ . By finding the second-order invariants of this representation, one obtains all the possible invariants fourth order in  $\Psi_{\vec{k}_i}$ . The functions  $\Psi_{\vec{k}_1} \Psi_{-\vec{k}_1}$  and  $\Psi_{\vec{k}_2} \Psi_{-\vec{k}_2}$  transform under the generators of  $D_{4h}$  in the following way:

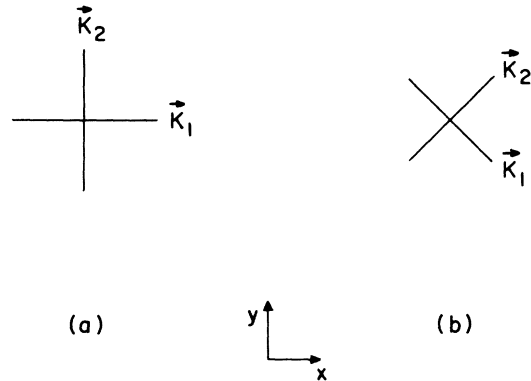


FIG. 7. Star of the wave vector  $\vec{k}$  of the magnetic structure of (a) DyC<sub>2</sub>, and (b) TbAu<sub>2</sub>.

$$C_4: \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1} \leftrightarrow \Psi_{\vec{k}_2} \Psi_{-\vec{k}_2}$$

$$i: \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j} - \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j}, \quad j=1, 2 \quad (4.17)$$

and

$$C_2([100]): \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j} \leftrightarrow \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j}, \quad j=1, 2.$$

Using these transformations we found that there are two invariants, fourth order in the order parameter. The LGW Hamiltonian which describes the system is

$$\begin{aligned} \mathcal{H} = & -\frac{1}{2} \sum_{i=1}^2 [\gamma(\phi_i^2 + \bar{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\bar{\phi}_i)^2] \\ & - u \left( \sum_{i=1}^2 \phi_i^2 + \bar{\phi}_i^2 \right)^2 - v \sum_{i=1}^2 (\phi_i^2 + \bar{\phi}_i^2)^2. \end{aligned} \quad (4.18)$$

The magnetic structure of TbAu<sub>2</sub> is similar to that of DyC<sub>2</sub>, except that the propagation vector  $\vec{k}_1$  is  $\vec{k}_1 = (k, k, 0)(2\pi/a)$  with  $k \sim 0.83$ . The star of  $\vec{k}_1$  consists of the four vectors:  $\pm\vec{k}_1 = (\pm k, \pm k, 0)(2\pi/a)$  and  $\pm\vec{k}_2 = (\pm k, \mp k, 0)(2\pi/a)$ , so the order parameter is four dimensional. One can define the order parameter as in Eq. (4.16) and find the LGW Hamiltonian in the way discussed above. The result is that the Hamiltonian (4.18) is also relevant for DyAu<sub>2</sub>.

#### E. TbD<sub>2</sub>

TbD<sub>2</sub> is an fcc crystal<sup>42</sup> whose paramagnetic space group is  $Fm\bar{3}m$ . Below the Néel temperature, it exhibits a longitudinal sinusoidal magnetic structure, associated with a reciprocal-lattice vector  $\vec{k}_1 = (k, 0, 0)(2\pi/a)$ , where  $k \sim 0.21$  and  $a$  is the lattice constant. The star of the vector  $\vec{k}_1$  consists of six vectors:  $\pm\vec{k}_1 = (\pm k, 0, 0)(2\pi/a)$ ,  $\pm\vec{k}_2 = (0, \pm k, 0)$ , and  $\pm\vec{k}_3 = (0, 0, \pm k)(2\pi/a)$  (Fig. 8), and

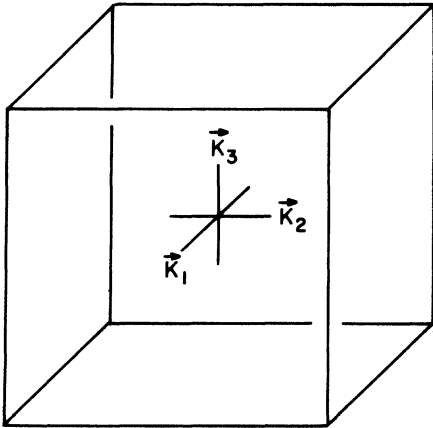


FIG. 8. Star of the wave vector  $\vec{k}$  of the magnetic structure of TbD<sub>2</sub>.

the group of  $\vec{k}_1$  is  $D_{4v}$ . The sublattice magnetization is parallel to  $\vec{k}_1$ , and, therefore, the order parameter which belongs to  $\vec{k}_1$  transforms as a one-dimensional representation of the little group. The order parameter has six independent components, defined by

$$\begin{aligned} \Psi_{\pm\vec{k}_j} & \equiv \phi_j \pm i\bar{\phi}_j \\ & = \sum_{\vec{r}} e^{\pm i\vec{k}_j \cdot \vec{r}} \vec{S}_{\vec{r}} \cdot \hat{k}_j, \quad j=1, 2, 3 \end{aligned} \quad (4.19)$$

where the sum  $\sum_{\vec{r}}$  is over the sites of the magnetic ions and  $\hat{k}_j$  is a unit vector parallel to  $\vec{k}_j$ . We use the method described in Sec. IV D to find the fourth-order invariants of this order parameter. The functions  $\Psi_{\vec{k}_j} \Psi_{-\vec{k}_j}$  ( $j=1, 2, 3$ ) transform under the generators of the point group  $m\bar{3}m$  ( $O_h$ ) as

$$\begin{aligned} C_4([001]): \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1} & \leftrightarrow \Psi_{\vec{k}_2} \Psi_{-\vec{k}_2}, \\ & \Psi_{\vec{k}_3} \Psi_{-\vec{k}_3} \leftrightarrow \Psi_{\vec{k}_3} \Psi_{-\vec{k}_3}, \\ i: \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j} & \leftrightarrow \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j}, \quad j=1, 2, 3 \\ C_3([111]): \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1} & \leftrightarrow \Psi_{\vec{k}_2} \Psi_{-\vec{k}_2} \\ & \leftrightarrow \Psi_{\vec{k}_3} \Psi_{-\vec{k}_3} \leftrightarrow \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1}, \\ C_2([110]): \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1} & \leftrightarrow \Psi_{\vec{k}_2} \Psi_{-\vec{k}_2}, \\ & \Psi_{\vec{k}_3} \Psi_{-\vec{k}_3} \leftrightarrow \Psi_{\vec{k}_3} \Psi_{-\vec{k}_3}. \end{aligned} \quad (4.20)$$

The order parameter has two fourth-order invariants, and the LGW Hamiltonian which describes the system is

$$\begin{aligned} \mathcal{H} = & -\frac{1}{2} \sum_{i=1}^3 [\gamma(\phi_i^2 + \bar{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\bar{\phi}_i)^2] \\ & - u \left( \sum_{i=1}^3 \phi_i^2 + \bar{\phi}_i^2 \right)^2 - v \sum_{i=1}^3 (\phi_i^2 + \bar{\phi}_i^2)^2. \end{aligned} \quad (4.21)$$

#### F. Nd

The crystallographic structure of Nd is double hexagonal close packed,<sup>43</sup> with four-layer stacking sequence of type  $ABAC$ , and whose space group is  $P6_3/mmc$ . Each unit cell contains four ions located on sites  $(2a)$  and  $(2d)$ . The ions on site  $(2d)$  (layers  $B, C$ ) order magnetically at 19 °K, with an antiferromagnetic arrangement between alternate hexagonal layers, and with sinusoidal modulation within each layer. The magnetic structure is associated with a reciprocal-lattice vector  $\vec{k}_1 = (k, 0, 0)(2\pi/a)$ , where  $k \approx 0.31$ ,  $a$  is the lat-

tice constant in the basal plane, and the three axes  $\vec{b}_1 = (1, 0, 0)$ ,  $\vec{b}_2 = (0, 1, 0)$ , and  $\vec{b}_3 = (0, 0, 1)$  are defined in Fig. 9. The sublattice magnetization is parallel to the vector  $\vec{k}_1$ . The star of  $\vec{k}_1$  consists of six vectors:  $\pm\vec{k}_1 = (\pm k, 0, 0)$  ( $2\pi/a$ ),  $\pm\vec{k}_2 = (0, \pm k, 0)$  ( $2\pi/a$ ), and  $\pm\vec{k}_3 = (0, 0, \pm k)$  ( $2\pi/a$ ), and the group of  $\vec{k}_1$  is  $C_{2v}$ . The order parameter which belongs to  $\vec{k}_1$  transforms as a one-dimensional representation of the group of  $\vec{k}_1$  and, therefore, it has six independent components:

$$\begin{aligned} \Psi_{\pm\vec{k}_j} &\equiv \phi_j \pm i\bar{\phi}_j \\ &= \sum_{\vec{r} \in B} e^{\pm i\vec{k}_j \cdot \vec{r}} \vec{S}_{\vec{r}} \cdot \hat{k}_j - \sum_{\vec{r} \in C} e^{\pm i\vec{k}_j \cdot \vec{r}} \vec{S}_{\vec{r}} \cdot \hat{k}_j, \\ & \quad j=1, 2, 3 \end{aligned} \quad (4.22)$$

where the sums  $\sum_{\vec{r} \in B}$  and  $\sum_{\vec{r} \in C}$  are over the sites of layers  $B$  and  $C$ , respectively, and  $\hat{k}_j$  is a unit vector parallel to  $\vec{k}_j$ . The functions  $\Psi_{\vec{k}_j} \Psi_{-\vec{k}_j}$ ,  $j=1, 2, 3$ , transform under the generators of the rotational part of the group  $P6_3/mmc$  according to

$$\begin{aligned} C_{6_3}: \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1} &\rightarrow \Psi_{\vec{k}_2} \Psi_{-\vec{k}_2} \rightarrow \Psi_{\vec{k}_3} \Psi_{-\vec{k}_3} \rightarrow \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1}, \\ i: \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j} &\rightarrow \Psi_{\vec{k}_j} \Psi_{-\vec{k}_j}, \quad j=1, 2, 3 \\ C_2([100]): \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1} &\rightarrow \Psi_{\vec{k}_1} \Psi_{-\vec{k}_1}, \\ \Psi_{\vec{k}_2} \Psi_{-\vec{k}_2} &\rightarrow \Psi_{\vec{k}_3} \Psi_{-\vec{k}_3}. \end{aligned} \quad (4.23)$$

The order parameter has two fourth-order invariants. The LGW Hamiltonian which describes the Nd was found to be the same as the Hamiltonian which describes  $TbD_2$ , and it is given by Eq. (4.21).

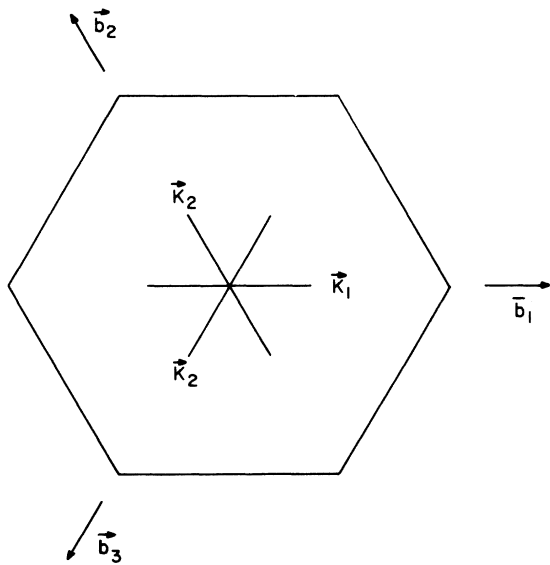


Fig. 9. Star of the wave vector  $\vec{k}$  of the magnetic structure of Nd.

### G. $NbO_2$

$NbO_2$  is a tetragonal crystal<sup>44-46</sup> whose space group is  $P4_2/mnm (D_{4h}^{14})$ . At  $\sim 800^\circ C$  it undergoes a structural transition, in which its symmetry is reduced to  $I4_1/a (C_{4h}^2)$ . The structure below the transition is associated with a reciprocal-lattice vector  $\vec{k}_1 = (\frac{1}{4}, \frac{1}{4}, \frac{1}{2}) (2\pi/a)$ , where  $a$  is the lattice constant in the basal plane. The star of  $\vec{k}_1$  consists of four vectors:  $\pm\vec{k}_1 = (\pm\frac{1}{4}, \pm\frac{1}{4}, \frac{1}{2}) (2\pi/a)$ , and  $\pm\vec{k}_2 = (\mp\frac{1}{4}, \pm\frac{1}{4}, \frac{1}{2}) (2\pi/a)$  and the group of  $\vec{k}_1$  is  $C_{2v}$ . The order parameter which is associated with  $\vec{k}_1$  transforms according to one irreducible representation of the group of  $\vec{k}_1$ , and neutron-diffraction studies show that this representation is either  $A_1$  or  $A_2$ .<sup>46</sup> Both cases give rise to the same LGW Hamiltonian, and, therefore we assume that the order parameter belongs to the representation  $A_1$ . The structure below the transition is discussed in detail by Pynn, Axe, and Thomas.<sup>46</sup> The order parameter has four components:

$$\Psi_{\pm\vec{k}_j} \equiv \phi_j \pm i\bar{\phi}_j, \quad j=1, 2 \quad (4.24)$$

where  $\phi_j, \bar{\phi}_j$ ,  $j=1, 2$ , are real parameters. Under the generators of the group  $D_{4h}^{14}$  they transform as:

$$\begin{aligned} C_{4_2}: \phi_1 &\rightarrow \phi_2, \phi_2 \rightarrow \bar{\phi}_1, \\ \bar{\phi}_1 &\rightarrow \bar{\phi}_2, \bar{\phi}_2 \rightarrow \phi_1, \\ i: \phi_1 &\rightarrow -\phi_1, \phi_2 \rightarrow \phi_2, \\ \bar{\phi}_1 &\rightarrow \bar{\phi}_1, \bar{\phi}_2 \rightarrow -\bar{\phi}_2, \\ C_2([100]): \phi_1 &\rightarrow \phi_2, \phi_2 \rightarrow \bar{\phi}_1, \\ \bar{\phi}_1 &\rightarrow \bar{\phi}_2, \bar{\phi}_2 \rightarrow -\phi_1, \\ t([010]): \phi_1 &\rightarrow \bar{\phi}_1, \phi_2 \rightarrow \bar{\phi}_2, \\ \bar{\phi}_1 &\rightarrow -\phi_1, \bar{\phi}_2 \rightarrow -\phi_2. \end{aligned} \quad (4.25)$$

The order parameter has three fourth-order invariants, and the LGW Hamiltonian which describes the system is<sup>47</sup>

$$\begin{aligned} \mathcal{H} &= -\frac{1}{2} \sum_{i=1}^2 [\nu(\phi_i^2 + \bar{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\bar{\phi}_i)^2] \\ &\quad - u \left( \sum_{i=1}^2 \phi_i^2 + \bar{\phi}_i^2 \right)^2 - v \sum_{i=1}^2 (\phi_i^2 + \bar{\phi}_i^2)^2 \\ &\quad - w \sum_{i=1}^2 \phi_i^2 \bar{\phi}_i^2. \end{aligned} \quad (4.26)$$

Let us define a  $2m$ -component vector model

TABLE I. Physical systems which correspond to the model Hamiltonians  $\mathcal{H}_1 - \mathcal{H}_4$ . The notation of the space groups is defined in Ref. 24.  $\vec{m}$  and  $\vec{k}$  are the magnetization and propagation vectors, respectively.

Substance	Dimensionality of the order parameter	Model Hamiltonian	Space group $T > T_c$	Structure $T < T_c$	References
TbAu <sub>2</sub> , DyC <sub>2</sub>	$2m=4$	$\mathcal{H}_1, w=0$	$I4/mmm$	Sinusoidal, $\vec{k} \parallel [110]$ (TbAu <sub>2</sub> ) $\vec{k} \parallel [100]$ (DyC <sub>2</sub> ), $\vec{m} \parallel [001]$	41
NbO <sub>2</sub>	$2m=4$	$\mathcal{H}_1$	$P4_2/mnm$	$\vec{k} = (\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	44, 45
TbD <sub>2</sub>	$2m=6$	$\mathcal{H}_1, w=0$	$Fm3m$	Sinusoidal $\vec{m} \parallel \vec{k} \parallel [100]$	42
Nd	$2m=6$	$\mathcal{H}_1, w=0$	$P6_3/mmc$	Sinusoidal $\vec{m} \parallel \vec{k} \parallel [1000]$	43
K <sub>2</sub> IrCl <sub>6</sub>	$2m=6$	$\mathcal{H}_1$	$Fm3m$	Type-III antiferromagnet $\vec{k} = (\frac{1}{2}, 0, 1)$ $\vec{m} \parallel [100]$	40
MnO, MnSe, NiO, ErSb	8	$\mathcal{H}_2$	$Fm3m$	Type-II antiferromagnet $\vec{m} \perp \vec{k}$	34-38
TbAs, TbP, TbSb	4	$\mathcal{H}_3$	$Fm3m$	Type-II antiferromagnet $\vec{m} \parallel \vec{k}$	33
UO <sub>2</sub>	6	$\mathcal{H}_4$	$Fm3m$	Type-I antiferromagnet $\vec{m} \perp \vec{k}$	39

$$\begin{aligned}
\mathcal{H}_1 = & -\frac{1}{2} \sum_{i=1}^m [\gamma(\phi_i^2 + \bar{\phi}_i^2) + (\nabla\phi_i)^2 + (\nabla\bar{\phi}_i)^2] \\
& -u \left( \sum_{i=1}^m \phi_i^2 + \bar{\phi}_i^2 \right)^2 - v \sum_{i=1}^m (\phi_i^2 + \bar{\phi}_i^2)^2 \\
& -w \sum_{i=1}^m \phi_i^2 \bar{\phi}_i^2. \quad (4.27)
\end{aligned}$$

As shown in Secs. II C-II G, this model is the appropriate LGW Hamiltonian for the systems K<sub>2</sub>IrCl<sub>6</sub> ( $2m=6$ ), Nd and TbD<sub>2</sub> ( $2m=6, w=0$ ), NbO<sub>2</sub> ( $2m=4$ ), and TbAu<sub>2</sub> and DyC<sub>2</sub> ( $2m=4, w=0$ ).

## V. SUMMARY

We constructed four different  $n \geq 4$ -component vector models,  $\mathcal{H}_1 - \mathcal{H}_4$ , which describe the crit-

ical behavior of several physical systems. The physical systems which correspond to these Hamiltonians are listed in Table I. All the substances in this table, except NbO<sub>2</sub>, exhibit antiferromagnetic transitions, while NbO<sub>2</sub> exhibits a structural transition. In the following paper we study the critical behavior of the Hamiltonians  $\mathcal{H}_1 - \mathcal{H}_4$  using the exact renormalization group in  $d=4-\epsilon$  dimensions. It would be interesting to test the predictions of the  $\epsilon$ -expansion calculations by studying these systems experimentally.

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