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"Weak Lifshitz condition" and the allowed types of ordering in second-order phase transitions

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It is known that the Lifshitz condition is not a necessary condition for second-order phase transitions in crystals. We show, however, that a certain necessary condition (which we have termed "the weak Lifshitz condition") does exist, though much weaker than the original Lifshitz condition. This necessary condition imposes certain restrictions on the allowed irreducible, or physically irreducible, representations associated with the transition, and accordingly, on the allowed types of ordering below the transition.

I. INTRODUCTION

According to the Landau theory[1] (see also Refs. 2–4), the type of ordering and the change in symmetry characterizing a second-order phase transition in a crystal are associated with a certain irreducible, or physically irreducible, representation $\mathfrak{D}^{(*k_0 n_0)}$ ($\vec{k}_0$ and n_0 are the star and the index of this representation,[3,5] respectively) of the space group G of the higher-symmetry phase. The precise meaning of this is as follows: the density function of the higher-symmetry phase $\rho=\rho_0(\vec{x})$ changes below the transition to a density function $\rho=\rho_0(\vec{x})+\Delta\rho(\vec{x})$, where the change $\Delta\rho(\vec{x})$, describing the type of ordering, is a superposition of basis functions $\phi_i^{(*\vec{k}_0 n_0)}(\vec{x})$ of $\mathfrak{D}^{(*\vec{k}_0 n_0)}$:

$$\Delta\rho(\vec{x})=\sum_i c_i\phi_i^{(*\vec{k}_0 n_0)}(\vec{x}) \ . \tag{1}$$

As was claimed by Lifshitz[6] (see also Refs. 2–4), the antisymmetric square of $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ should not contain any irreducible representation in common with the vector representation of G. This condition can be written (see Ref. 4)

$$([*\vec{k}_0 n_0]_{[2]}|\Gamma^{(v)})=0 \ , \tag{2}$$

where $[*\vec{k}_0 n_0]_{[2]}$ denotes the antisymmetric square of $D^{(*\vec{k}_0 n_0)}$, $\Gamma^{(v)}$ is the vector representation, and the symbol $(\mathfrak{D}|\mathfrak{D}')$ denotes the scalar product of the characters of two representations $\mathfrak{D}$ and $\mathfrak{D}'$. Condition (2), commonly referred to as the Lifshitz condition, drastically limits the types of ordering that are allowed to appear below the transition point. Out of the infinity of irreducible representations of space groups, only a certain finite number of them satisfy this condition. In particular, $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ is forbidden by condition (2) if a wave vector $\vec{k}_0$ in $*\vec{k}_0$ has components differing from 0, $\frac{1}{2}$, $\frac{1}{3}$, $\frac{1}{4}$ (in terms of the fundamental periods of the reciprocal lattice). Lifshitz derived his condition (2) by considering, instead of (1), a more-general change in the density function

$$\Delta\rho(\vec{x})=\sum_i c_i(\vec{x})\phi_i^{(*\vec{k}_0 n_0)}(\vec{x}) \ , \tag{3}$$

where $c_i(\vec{x})$ are slowly varying functions (i.e., varying appreciably only over distances that are large compared with the fundamental lattice periods). The state of the crystal below the transition being described by $\rho=\rho_0(\vec{x})+\Delta\rho(\vec{x})$ with fixed $\phi_i^{(*\vec{k}_0 n_0)}$, the free energy F of the crystal is an integral functional of $c_i(\vec{x})$. In the spirit of Landau's theory, Lifshitz assumed that the integrand of this functional (the density of the free energy) can be expanded in powers of c_i and their gradients $\nabla_\mu c_i$ ($\mu=1,2,3$). Lifshitz proposed that the crystalline, i.e., three-dimensionally periodic, state should be thermodynamically stable below the transition. This means, in particular, that in thermodynamic equilibrium there should be $c_i=\text{const}$ and, therefore, the above expansion of F should not contain antisymmetric terms

$$\int (c_i\nabla_\mu c_j - c_j\nabla_\mu c_i)\, d^3x \ .$$

Since such terms may enter the expansion of F only in the form of invariant combinations

$$\mathcal{I}(c_i)=\sum_{ij\mu} k_{ij\mu}\int (c_i\nabla_\mu c_j - c_j\nabla_\mu c_i)\, d^3x \ , \tag{4}$$

Lifshitz claimed that no such invariants should exist for a representation associated with a second-order phase transition. Condition (2) is the group-theoretical formulation of this claim.

After the discovery of phase transitions accompanied by the formation of spiral magnetic arrangements, in which condition (2) was manifestly violated, Lifshitz's derivation[6] of this condition was disputed by Dimmock.[7] Arguing against Dimmock, Dzyaloshinskii[8] and Haas[9] suggested an alternative deduction of the Lifshitz condition, clarifying its physical meaning. (This deduction was carried out by Goshen *et al.*[10]) The idea of their suggestion is as follows: according to the Landau theory, one should start from a general $\Delta\rho(\vec{x})$ decomposed in terms of all irreducible representations $\mathfrak{D}^{(*\vec{k}n)}$ of G. Designating the basis functions of $\mathfrak{D}^{(*\vec{k}n)}$ as $\phi_i^{(*\vec{k}n)}(\vec{x})$, one can write this decomposition as

$$\Delta\rho(\vec{x}) = \sum_{*\vec{k}} \sum_{n} \sum_{i} c_i^{(*\vec{k}n)} \phi_i^{(*\vec{k}n)}(\vec{x}) . \quad (5)$$

The functions $\phi_i^{(*\vec{k}n)}(\vec{x})$ can be chosen to be real, mutually orthogonal, and normalized. Then the second-order term in the expansion of F in powers of $c_i^{(*\vec{k}n)}$ has the form

$$F_2 = \sum_{*\vec{k}} \sum_{n} A^{(*\vec{k}n)} \sum_{i} (c_i^{(*\vec{k}n)})^2 , \quad (6)$$

where the expansion coefficients $A^{(*\vec{k}n)}$ depend on pressure P and temperature T. A second-order transition to an ordered state occurs when, on varying P and T, the minimal of the coefficients $A^{(*\vec{k}n)}$ changes its sign from positive to negative. The irreducible, or physically irreducible, representation $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ determining the type of ordering below the transition is thus related to the minimal coefficient in (6), $A^{(*\vec{k}_0 n_0)}$. Accordingly, we will name $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ the "minimum representation." The "spectrum" of coefficients $A^{(*\vec{k}n)}$ has a typical band structure in the k space, and $A^{(*\vec{k}_0 n_0)}$ should be the minimum of the lowest band in this structure (if the small representation $\mathfrak{D}^{(\vec{k}_0 n_0)}$ is s dimensional, where $s > 1$, then the minimum $A^{(*\vec{k}_0 n_0)}$ is a sticking point of s bands).[3] Now, one can show[8–10] that if this minimum is an extremum due to symmetry, the "minimum representation" $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ obeys the Lifshitz condition, Eq. (2); if it is not due to symmetry ("accidental" minimum), $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ does not obey this condition and, furthermore, varies as a function of P and T in the lower-symmetry phase.

As claimed by Goshen *et al.*,[10] in the latter case $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ may be *any* irreducible, or physically irreducible, representation of G. This claim does not however take into account the following circumstance: the concept of an ordered phase with a given type of ordering is physically meaningful *only* if this phase occupies a certain *two-dimensional* area on the P-T diagram. Indeed, the point (P,T) at which an experimental determination (say, an x-ray study) of the ordered structure is performed fluctuates within a two-dimensional region determined by the fluctuations of pressure and temperature[2] $\Delta P = (k_B T / V\kappa_S)^{1/2}$ and $\Delta T = (k_B T^2/C_V)^{1/2}$ (here k_B is the Boltzmann constant, κ_S is the adiabatic compressibility, C_V is the specific heat at constant volume, and V is the volume of the crystal). This means that if a given type of ordering exists only at an isolated point, or on an isolated line, on the P-T diagram, it is *unobservable*, however large V may be. Now, if the minimum $A^{(*\vec{k}_0 n_0)}$ at a given point (P,T) is not due to symmetry, an infinitesimal variation of P and T changes the "minimum representation" $\mathfrak{D}^{(*\vec{k}_0 n_0)}$, which determines the type of ordering at this point. Then it may happen, in principle, that this change of $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ gives rise to an abrupt change in the type of ordering associated with $\mathfrak{D}^{(*\vec{k}_0 n_0)}$. In this case, the type of ordering in question will not persist throughout *any* (however small) vicinity of the P-T point in question and will therefore be unobservable.

To clarify this point, consider the following example. Let the space group of the higher-symmetry phase be D_4^1. Suppose that at a certain point (P,T) in the lower-symmetry phase the "minimum representation" of D_4^1 is $\mathfrak{D}^{(*\Gamma 5)}$. ($\Gamma$ denotes the origin of the Brillouin zone, and 5 is the ordinal number of this representation[11]; this representation coincides with the representation E of the point group D_4.[12]) It can be shown[13] that the ordering associated with this representation is of ferroelectric (or ferromagnetic) type, with dipoles being parallel to one of the four rotational axes of second order, so that the space group of the ordered state is C_2^1. [Though the representation in question does not obey the Lifshitz condition (see below), it obeys another necessary condition imposed by the Landau theory (Refs. 1–4): the symmetrical cube of this representation does not contain the identity representation.] However, since $\mathfrak{D}^{(*\Gamma 5)}$ does not[13] obey the Lifshitz condition, an infinitesimal deviation from the point (P,T) will lead to another "minimum representation," with a nonnull star $*\vec{k}_0$ infinitely close to the null star $*\Gamma$. As a result the above dipole ordering will become *sinusoidally modulated*, with a modulation period much larger than, and incommensurable with, the fundamental lattice periods, so that the crystal will become macroscopically inhomogeneous and will not be described by any one of the 230 three-dimensional space groups. This means that the above-mentioned ferroelectric (ferromagnetic) second-order phase transition $D_4^1 \rightarrow C_2^1$, associated with the representation $\mathfrak{D}^{(*\Gamma 5)}$ of $\mathfrak{D}_4^1$, is unobservable.

The irreducible, or physically irreducible, representation associated with an unobservable type of ordering may be regarded as *forbidden*. This means that, though the Lifshitz condition is not in general a necessary condition for a second-order phase transition, there may be a certain weaker necessary condition restricting the allowed representations in the above sense. We shall name it the "weak Lifshitz condition." The purpose of this paper is to give a precise formulation of the "weak Lifshitz condition" and to demonstrate the restrictions it imposes on the space-group representations and the related types of ordering.

One should bear in mind that implicit in our discussion is the applicability of Landau's analytic expansion of F. As is well known,[14] Landau's approach is invalid in the immediate vicinity of phase transition points and leads to incorrect results regarding the critical behavior (critical exponents). However, as regards the determination of the allowed symmetry changes and types of ordering, this approach is believed to yield correct results. It is with this belief in mind that the "weak Lifshitz condition" is proposed.

II. FORMULATION OF THE "WEAK LIFSHITZ CONDITION"

In order to determine the "weak Lifshitz condition," it is convenient to use the original Lifshitz's approach,[6] in which $\Delta\rho(\vec{x})$ is taken in the form (3), and F is presented as a volume integral of a power series in terms of c_i and $\nabla_\mu c_i$. As pointed out by Dzyaloshinskii,[8] this approach is equivalent to his approach, in which one should take $\Delta\rho(\vec{x})$ in the form of a sum (5) over representations $\mathfrak{D}^{(^*kn)}$ that are "close" to $\mathfrak{D}^{(^*\vec{k}_0 n_0)}$ in the sense of compatibility relations [15] and then expand F in both $c_i^{(^*kn)}$ and $\vec{k}-\vec{k}_0$. If $\mathfrak{D}^{(^*\vec{k}_0 n_0)}$ does not satisfy the (original) Lifshitz condition, then the Lifshitz expansion of F should contain a term

$$\sum_\alpha B_\alpha \mathscr{I}_\alpha(c_i) \quad , \tag{7}$$

where $\mathscr{I}_\alpha(c_i)$ $(\alpha=1,2,\dots)$ are independent invariants of the type (4), and B_α are expansion coefficients depending on P and T.

The number and the form of the invariants $I_\alpha(c_i)$ depend on $\mathfrak{D}^{(^*\vec{k}_0 n_0)}$, i.e., on the star $^*\vec{k}_0$ and the index n_0. As is known, for a given space group G, all the stars $^*\vec{k}$ can be classified according to their representative $\vec{k}$ points in the first Brillouin zone; these $\vec{k}$ points are usually designated by certain Latin or Greek symbols.[5,11,15] Every such symbol denotes a certain one-, two-, or three-dimensional domain of $\vec{k}$ points, or an isolated $\vec{k}$ point (which can be regarded as a zero-dimensional domain). A $\vec{k}$ point can move within such a domain without changing its proper symmetry $G(\vec{k})$, which is the subgroup of G that leaves the wave vector $\vec{k}$ invariant (or changes it by a vector of reciprocal lattice). (For physically irreducible representations, the above classification must take into account, besides the space group elements of G, also the inversion of $\vec{k}$ corresponding to the operation of complex conjugation.) Accordingly, all the representations $\mathfrak{D}^{(^*kn)}$ can be classified into the following four types: (i) representations with $\vec{k}$ points in general positions in the $\vec{k}$ space; (ii) representations with $\vec{k}$ points in general positions on certain symmetry planes; (iii) representations with $\vec{k}$ points in general positions on certain symmetry axes; (iv) representations with $\vec{k}$ points in special positions. One can say that in the cases (i), (ii), (iii), and (iv) the $\vec{k}$ point and the representation $\mathfrak{D}^{(^*kn)}$ in question have three, two, one, and zero degrees of freedom, respectively.

When $\vec{k}_0$ varies within the appropriate domain of degrees of freedom [in the cases (i)–(iii)] without crossing its boundary, the representation $\mathfrak{D}^{(^*\vec{k}_0 n_0)}$ varies continuously with $\vec{k}_0$ without the change of the index n_0. The number of independent invariants $\mathscr{I}_\alpha(c_i)$ in the term (7) then remains unchanged, as well as the form of these invariants, i.e., the coefficients $k_{ij\mu}$ in (4). As distinct from this, the coefficients B_α in (7) may vary with $\vec{k}_0$ and are functions of those coordinates of the $\vec{k}_0$ point that are free to vary within the appropriate region. Designating these coordinates as $k_0^{(1)},\dots,k_0^{(m)}$, where $m=m(\vec{k}_0)$ is the number of degrees of freedom of $\vec{k}_0$, one can write $B_\alpha=B_\alpha(P,T;k_0^{(1)},\dots,k_0^{(m)})$.

If the representation $\mathfrak{D}^{(^*\vec{k}_0 n_0)}$ involved in the definition (3) of $\Delta\rho(\vec{x})$ is the "minimum representation" at a certain point (P,T) below a second-order phase transition, then the term (7) automatically vanishes at this point. This means that

$$B_\alpha(P,T;k_0^{(1)},\dots,k_0^{(m)})=0 \tag{8}$$

at this point. The number of independent invariants $\mathscr{I}_\alpha(c_i)$ in (7), which equals $([^*\vec{k}_0 n_0]_{[2]}|\Gamma^{(\nu)})$, may be either equal to $m(\vec{k}_0)$ or larger than $m(\vec{k}_0)$. [One can prove that it can never be smaller than $m(\vec{k}_0)$, but this fact is immaterial for the subsequent results.] If

$$([^*\vec{k}_0 n_0]_{[2]}|\Gamma^{(\nu)})=m(\vec{k}_0) \quad , \tag{9}$$

then the number of equations in (8) equals the number of variables $k_0^{(1)},\dots,k_0^{(m)}$, and one may regard $\vec{k}_0$ as a solution of these equations at the point (P,T) in question. An infinitesimal variation of P and T will lead to an infinitesimal variation of this solution. Then there exists a certain (two-dimensional) vicinity of the point (P,T), in which the index n_0 of the "minimum representation" is the same as at the point (P,T) and the $\vec{k}_0$ point of this representation varies as a function of P,T within a single domain of degrees of freedom. As a result, the ordering below the phase transition described by the function

$$\Delta\rho(\vec{x})=\sum_i c_i\phi_i^{(^*\vec{k}_0 n_0)}(\vec{x}) \quad ,$$

with c_i independent of $\vec{x}$, varies continuously with P,T throughout the above vicinity. However, along with this variation, the symmetry of this ordering and its orientation with respect to the initial crystal structure (of the higher-symmetry phase) remain unchanged, so that in spite of the above variation one can speak of a single *type* of ordering.

For instance, the helicoidal magnetic ordering in Dy is associated with an irreducible representation of the higher-symmetry (paramagnetic) space group D_{6h}^4, which is of the type[11] $\mathfrak{D}^{(*\Delta 5)}$. Throughout the helicoidal phase, the wave vector $\vec{k}_0$ of the above representation varies as a function of P and T within the one-dimensional interval denoted by the symbol $\Delta{:}\vec{k}_0 = k_0\hat{c},\ 0 < k_0 < \pi/c$ ($\hat{c}$ is the unit vector in the direction of the sixfold axis, and c is the lattice period in this direction). This variation exhibits itself in the variation of the pitch of the helix; however, the *type* of ordering— a spiral with the axis parallel to the sixfold axis of the crystal—remains invariable. This type of ordering is determined uniquely by the label ($^*\Delta 5$) of the above representation.

If

$$([^*\vec{k}_0 n_0]_{[2]} | \Gamma^{(\nu)}) > m(\vec{k}_0) \quad ,$$

then the number of independent equations (8) is larger than is the number of variables $k_0^{(1)},\ldots,k_0^{(m)}$. In this case, however small the vicinity of the point (P,T) in question is chosen, Eq. (8) cannot be resolved *throughout* this vicinity. If

$$([^*\vec{k}_0 n_0]_{[2]} | \Gamma^{(\nu)}) = m(\vec{k}_0) + 1 \quad ,$$

these equations can be resolved only on a certain line passing through the point (P,T), and if

$$([^*\vec{k}_0 n_0]_{[2]} | \Gamma^{(\nu)}) = m(\vec{k}_0) + 2 \quad ,$$

they can be resolved only at the point (P,T) itself. It follows immediately that the "weak Lifshitz condition" is expressed by Eq. (9).

To simplify the notations, let us further replace $\vec{k}_0$ with $\vec{k}$ and $\mathfrak{D}^{(*\vec{k}_0 n_0)}$ with $\mathfrak{D}$. If $\mathfrak{D}$ is of the type (iv), it has no degrees of freedom: $m(\vec{k}) = 0$. In this case Eq. (9) reduces to Eq. (2). It follows that *with respect to the representations of type (iv), the "weak Lifshitz condition" is equivalent to the original Lifshitz condition.* The $\vec{k}$ vectors of representations of type (iv) have components 0, $\frac{1}{2}, \frac{1}{3}, \frac{1}{4}$ in terms of the fundamental periods of the reciprocal lattice; therefore the ordering associated with any such representation does not destroy the three-dimensional periodicity of the crystal and leaves the crystal macroscopically homogeneous. The above results means, as should be expected, that the original Lifshitz condition is a necessary condition for those second-order phase transitions in which the crystal remains three-dimensionally periodic in the lower-symmetry phase.

Representations of type (iv) that do not satisfy this condition are thus *forbidden.* An example of such representation has been considered in Sec. I.

Let us now consider the representations of types (i)−(iii). In order to find the number of independent invariants $\mathscr{I}_\alpha(c_i)$ in these cases, let us apply the method developed by Lyubarskii.[3] According to this method, one has to consider two independent bases $\{\phi_i^{(\vec{k})}\}$ and $\{\psi_i^{(\vec{k})}\}(i = 1,\ldots,s)$ of $\mathfrak{D}^{(\vec{k})}$, where $\mathfrak{D}^{(\vec{k})}$ is the small representation of the subgroup $G(\vec{k})$ corresponding to the full-group representation $\mathfrak{D}$. Besides $\{\phi_i^{(\vec{k})}\}$, $\{\psi_i^{(\vec{k})}\}$, one has to consider the complex-conjugate bases[16] $\{\bar{\phi}_i^{(\vec{k})}\}$, $\{\bar{\psi}_i^{(\vec{k})}\}$ of the representation $\bar{\mathfrak{D}}^{(\vec{k})} = \mathfrak{D}^{(-\vec{k})}$. [In the cases (i)−(iii), the vectors $\vec{k}$ and $-\vec{k}$ are nonequivalent, and so are the representations $\mathfrak{D}^{(\vec{k})}$ and $\mathfrak{D}^{(-\vec{k})}$.] The s^2 antisymmetric functions

$$\phi_i^{(\vec{k})}\bar{\psi}_j^{(\vec{k})} - \psi_i^{(\vec{k})}\bar{\phi}_j^{(\vec{k})} \quad (i,j, = 1,\ldots,s) \tag{10}$$

form a basis for a certain representation $\Gamma_{\mathfrak{D}}$ of the subgroup $G(\pm\vec{k})$ consisting of those elements of G which either do not change the vector $\vec{k}$ or transform it into $-\vec{k}$. If G contains an element $\{p|\vec{t}\}$(p is a point group element, and $\vec{t}$ is an appropriate translation vector) which transforms $\vec{k}$ into $-\vec{k}$, then

$$G(\pm\vec{k}) = G(\vec{k}) + \{p|\vec{t}\} \times G(\vec{k}) \quad . \tag{11a}$$

If G does not contain such an element, then

$$G(\pm\vec{k}) = G(\vec{k}) \quad . \tag{11b}$$

The star of the representation $\Gamma_{\mathfrak{D}}$ is obviously the null vector. Therefore, $\Gamma_{\mathfrak{D}}$ can also be regarded as a representation of the point group $\hat{G}(\pm\vec{k})$ corresponding to the space group $G(\pm\vec{k})$. As was shown by Lyubarskii,[3] the number of independent invariants $\mathscr{I}_\alpha(c_i)$ equals the number of times the unit representation of $\hat{G}(\pm\vec{k})$ is contained in the product $\Gamma_{\mathfrak{D}} \times \Gamma_V$, where Γ_V is the vector representation of $\hat{G}(\pm\vec{k})$. The application of the weak Lifshitz condition to the cases (i)−(iii) thus reduces to the determination of $\Gamma_{\mathfrak{D}}$ and the decomposition of $\Gamma_{\mathfrak{D}} \times \Gamma_V$.

III. APPLICATION TO REPRESENTATIONS OF TYPES (i)−(iii)

Let us first consider representations $\mathfrak{D}$ of type (i). In this case $G(\vec{k})$ is simply the subgroup of pure translations, and the small representation $\mathfrak{D}^{(\vec{k})}$ is one dimensional. Therefore, there exists a single antisymmetric combination

$$\phi^{(\vec{k})}\bar{\psi}^{(\vec{k})} - \bar{\phi}^{(\vec{k})}\psi^{(\vec{k})} \quad . \tag{12}$$

The point group $\hat{G}(\pm\vec{k})$ can be either C_1 or C_i. If $G(\pm\vec{k}) = C_1$, then $\Gamma_{\mathfrak{D}} = A$, $\Gamma_V = 3A$; if $\hat{G}(\pm\vec{k}) = C_i$, then $\Gamma_{\mathfrak{D}} = A_u$ (because the inversion element I transforms $\phi^{(\vec{k})}$ into $\bar{\phi}^{(\vec{k})}$ and $\psi^{(\vec{k})}$ into $\bar{\psi}^{(\vec{k})}$) and $\Gamma_V = 3A_u$.[12] In both cases there are *three* independent invariants $\mathscr{I}_\alpha(c_i)$. This means that *any representation $\mathfrak{D}$ of type (i) is allowed by "the weak Lifshitz condition."* Accordingly, sinusoidal arrangements with a general wave vector $\vec{k}$ are always allowed to appear below the transition.

Let us now consider representations of type (ii). Here one encounters the following three possibilities:

$$G(\vec{k}) = C_1^1, \quad \hat{G}(\pm\vec{k}) = C_2; \tag{13a}$$

$$G(\vec{k}) = C_s^m(m=1,\ldots,4), \quad \hat{G}(\pm\vec{k}) = C_s \ ; \tag{13b}$$

$$G(\vec{k}) = C_s^m(m=1,\ldots 4), \quad \hat{G}(\pm\vec{k}) = C_{2h} \ , \tag{13c}$$

where the twofold axis is normal to the plane of the $\vec{k}$ points in question. The small representation $\mathfrak{D}^{(\vec{k})}$ can be either one or two dimensional. If $\mathfrak{D}^{(\vec{k})}$ is one dimensional, then there exists a single antisymmetric function (12). Now, if $G(\vec{k}) = C_s^m$, then the function (12) in question is invariant under C_s^m. If the point group $\hat{G}(\pm\vec{k})$ contains the element C_2 transforming $\vec{k}$ into $-\vec{k}$, then the corresponding space group element $\{C_2|\vec{t}\}$ in $G(\pm\vec{k})$ transforms $\phi^{(\vec{k})}$ into $\bar{\phi}^{(\vec{k})}$ and $\psi^{(\vec{k})}$ into $\bar{\psi}^{(\vec{k})}$. It follows that in all the three cases (13a)–(13c), the representation $\Gamma_{\mathfrak{D}}$ is contained *twice* in the vector representation Γ_v of $\hat{G}(\pm\vec{k})$ [in the cases of (13a)–(13c), $\Gamma_{\mathfrak{D}} = B, A', B_u$, respectively]; therefore there are *two* independent invariants $\mathscr{I}_\alpha(c_i)$. It follows that *if the small representation $\mathfrak{D}^{(\vec{k})}$ is one-dimensional, the full-group representation $\mathfrak{D}$ of type (ii) is allowed by "the weak Lifshitz condition"* and the corresponding type of ordering may appear below the transition.

As distinct from this, if the small representation $\mathfrak{D}^{(\vec{k})}$ is two dimensional, then the representation $\mathfrak{D}$ may be forbidden. For example, let us consider the space group $G = C_{2h}^2$. This group has a physically irreducible representation[11] $\mathfrak{D} = \mathfrak{D}^{(*S\,1)} + \mathfrak{D}^{(*S\,2)}$ corresponding to a general point S on the face of the Brillouin zone normal to the z axis (the twofold axis). The small representation $\mathfrak{D}^{(\vec{k})} = \mathfrak{D}^{(S\,1)} + \mathfrak{D}^{(S\,2)}$ of the space group $G(\vec{k}) = C_s^1$ is two dimensional, the elements E (identity element) and σ^z (reflection in the xy plane) being represented by the matrices

$$\mathfrak{D}^{(\vec{k})}(E) = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \quad \mathfrak{D}^{(\vec{k})}(\sigma^z) = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \ . \tag{14}$$

The element $\{I|\frac{1}{2}c\hat{z}\}$ of the space group $G(\pm\vec{k}) = C_{2h}^2$ (c is the lattice period in the z direction) transforms the basis functions $\phi_1^{(\vec{k})}, \phi_2^{(\vec{k})}$ of the representation $\mathfrak{D}^{(\vec{k})}$ into $\bar{\phi}_2^{(\vec{k})}, \bar{\phi}_1^{(\vec{k})}$, respectively. From here and from (14) it follows that the representation $\Gamma_{\mathfrak{D}}$ of the point group $\hat{G}(\pm\vec{k}) = C_{2h}$ based on four functions (10) with $i,j = 1,2$ has the following table of characters:

E	C_2	σ	I
4	2	0	−2

The decomposition of this representation is

$$\Gamma_{\mathfrak{D}} = A_g + 2A_u + B_u \ .$$

Since the decomposition of the vector representation is

$$\Gamma_V = A_u + 2B_u \ ,$$

it follows that the product $\Gamma_{\mathfrak{D}} \times \Gamma_V$ contains the unit representation four times. Accordingly, there are four independent invariants $\mathscr{I}_\alpha(c_i)$, and the representation $\mathfrak{D} = \mathfrak{D}^{(*S\,1)} + \mathfrak{D}^{(*S\,2)}$ is forbidden by the "weak Lifshitz condition."

Let us now consider representations of type (iii). In this case the point group $\hat{G}(\pm\vec{k})$ can be one of the following groups: C_s, C_2, C_3, C_4, C_6, C_{2v}, C_{3v}, C_{4v}, C_{6v}, S_4, S_6, C_{2h}, C_{3h}, C_{4h}, C_{6h}, D_2, D_3, D_4, D_6, D_{2d}, D_{3d}, D_{2h}, D_{3h}, D_{4h}, D_{6h}, and $G(\pm\vec{k})$ one of the corresponding space groups. If $\hat{G}(\pm\vec{k})$ is one of the groups C_s, C_2, C_{2h}, then the line of $\vec{k}$ points having one and the same symmetry is normal to the reflection plane or parallel to the twofold axis; if $\hat{G}(\pm\vec{k}) = C_{2v}$, this line is either parallel to the twofold axis or normal to one of the reflection planes. The point group $\hat{G}(\vec{k})$ of the $\vec{k}$ point can be one of the following groups: C_1, C_2, C_3, C_4, C_6, C_{2v}, C_{3v}, C_{4v}, C_{6v}, and $G(\vec{k})$ one of the corresponding space groups. The small representation $D^{(\vec{k})}$ can be one dimensional or multidimensional.[11] If $\mathfrak{D}^{(\vec{k})}$ is one dimensional, then a straightforward calculation made for all the above groups $\hat{G}(\pm\vec{k})$ shows that the one-dimensional representation $\Gamma_{\mathfrak{D}}$ is contained in Γ_V *only once;* therefore there is a *single* invariant (4). This means that *if $\mathfrak{D}^{(\vec{k})}$ is one dimensional, the corresponding representation D of type (iii) is allowed by the "weak Lifshitz condition."*

If $\mathfrak{D}^{(\vec{k})}$ is multidimensional, then D may be forbidden. Consider, for example, the space group $G = C_{3v}^1$. This group has a physically irreducible representation $\mathfrak{D} = \mathfrak{D}^{(*\Delta 3)} + \bar{\mathfrak{D}}^{(*\Delta 3)}$ corresponding to a general point Δ on the threefold axis. The small representation $\mathfrak{D}^{(\vec{k})} = \mathfrak{D}^{(\Delta 3)}$ of the group $G(\vec{k}) = C_{3v}^1$ is two dimensional, and its matrices corresponding to the elements of the point group C_{3v} (the space group C_{3v}^1 is symmorphic) coincide with the matrices of the point group representation E. The representation $\Gamma_{\mathfrak{D}}$ of $\hat{G}(\pm\vec{k}) = C_{3v}$ based on four functions (10) has the following table of characters:

E	$2C_3$	3
4	1	0

and its decomposition is

$$\Gamma_{\mathfrak{D}} = A_1 + A_2 + E \ .$$

Since the vector representation of C_{3v} decomposes as $\Gamma_V = A_1 + E$, the product $\Gamma_{\mathfrak{D}} \times \Gamma_V$ contains the unit representation twice. Therefore there are two independent invariants $\mathscr{I}_\alpha(c_i)$, and the representation $\mathfrak{D} = \mathfrak{D}^{(*\Delta 3)} + \bar{\mathfrak{D}}^{(*\Delta 3)}$ is forbidden by the "weak Lifshitz condition."

IV. CONCLUSION

In conclusion, let us summarize the results of this paper. We have found that though the original Lifshitz condition expressed by Eq. (2) is not a necessary condition for second-order phase transitions in crystals, it should not be omitted altogether, but replaced by the "weak Lifshitz condition" expressed by Eq. (9). It turns out that all the irreducible, or physically irreducible, representations of type (i) are allowed by this condition, and so are those representations $\mathfrak{D}$ of types (ii) and (iii) that are induced from one-dimensional small representations $\mathfrak{D}^{(\vec{k})}$. On the other hand, if the dimensionality of $\mathfrak{D}^{(\vec{k})}$ is two or more, then the corresponding representation $\mathfrak{D}$ may be forbidden. One must then calculate the number of independent invariants $\mathscr{I}_\alpha(c_i)$ of the type (4) according to the procedure described in Sec. II, and compare this number with the number of degrees of freedom of $\vec{k}$ [two degrees of freedom in the case (ii), and one in the case (iii)]; if the number of invariants $\mathscr{I}_\alpha(c_i)$ equals the number of degrees of freedom, the representation $\mathfrak{D}$ is allowed by the "weak Lifshitz conditions"; if it is larger, then $\mathfrak{D}$ is forbidden and so is the type of ordering associated with $\mathfrak{D}$. Finally, if the representation $\mathfrak{D}$ is of type (iv), the "weak Lifshitz condition" becomes equivalent to the original Lifshitz condition, and the relevant results of the previous works[3,13] become applicable. In particular, there exist representations of type (iv) forbidden by this condition.

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