## Landau, Lifshitz, and weak Lifshitz conditions in the Landau theory of phase transitions in solids

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Landau theory provides a group-theoretical method for determining which symmetry changes can occur in second-order phase transitions in solids. The irreducible representations of the space group of the higher-symmetry phase must satisfy certain conditions. For transitions to commensurate crystalline structures, the Landau and Lifshitz conditions must be satisfied. For transitions to incommensurate structures, the Landau and "weak Lifshitz" conditions must be satisfied. The irreducible representations of each of the 230 crystallographic space groups that violate these conditions are listed.

Landau theory<sup>1,2</sup> uses group-theoretical methods to describe second-order phase transitions in crystalline solids. In this theory, a transition is driven by an order parameter  $\eta$ . The components of  $\eta$  transform like basis functions of an irreducible representation (IR) of the space group of the higher-symmetry phase.

Near the transition, the free energy of the crystal is expanded about  $\eta = 0$ . The space-group symmetry of the crystal requires that only invariant polynomials in this expansion can contribute. The invariant terms in the expansion determine the nature of the phase transition. If the transition is to be second order, then certain kinds of terms must *not* appear in the free-energy expansion. These terms are forced not to appear by symmetry. These considerations have resulted in two conditions which must be satisfied if the transition is to be second order: the Landau and Lifshitz conditions.

The Landau condition states that no third-degree terms of the form  $\eta_i \eta_j \eta_k$  can be allowed to appear in the free-energy expansion. This condition is satisfied if the symmetrized triple Kronecker product of the IR does not contain the identity representation.

The Lifshitz condition states that no terms of the form  $\eta_i(\partial \eta_j/\partial x_k)$  can be allowed to appear in the free-energy expansion. Invariant polynomials in the expansion which contain terms of this form are called "Lifshitz invariants." The Lifshitz condition is satisfied if the antisymmetrized double Kronecker product of the IR does not contain the vector representation.

If we consider second-order transitions to incommensurate phases, the Lifshitz condition need not be satisfied. Instead, the so-called "weak Lifshitz condition," introduced by Michelson<sup>3,2</sup> must be satisfied. This condition states that the number of Lifshitz invariants in the freeenergy expansion must equal the number of degrees of freedom of the **k** vector associated with the IR. Bradley and Cracknell<sup>4</sup> classify **k** vectors as belonging to either points of symmetry, lines of symmetry, planes of symmetry, or general points. Points of symmetry have zero degrees of freedom; lines of symmetry have one degree of freedom; planes of symmetry have two degrees of freedom; and general points have three degrees of freedom.

TABLE I. IR's and PIR's which violate the Landau condition. The trivial case of the identity IR's  $(\Gamma_1, \Gamma_1^+)$  has been omitted from the table. All of the identity IR's violate the Landau condition.

Space groups	IR's, PIR's
Hexagonal R	
146	$\Gamma, \Sigma, F$
148	$\Gamma_2^+\Gamma_3^+, \Sigma, F_1^+$
155	$\Gamma_3, \Sigma_1 \Sigma_1, F_1$
160,161	$\Gamma_3, \Sigma, F_1$
166,167	$\Gamma_3^+, \Sigma_1, F_1^+$
Hexagonal P	- 3, -1, -1
143–145	$\Gamma, \Lambda, \Sigma, K, M, B$
147	$\Gamma_2^+\Gamma_3^+, \Lambda, \Sigma, K, M_1^+, B$
149,151,153,156,158	$\Gamma_3,\Lambda,\Sigma_1\Sigma_1,K,M_1,B$
150,152,154,157,159	$\Gamma_3, \Lambda_1 \Lambda_1, \Sigma, K_1 K_1, K_3 K_3, M_1, B$
162-165	$\Gamma_3^+, \Lambda_1, \Sigma_1, K_1, K_3, M_1^+, B$
168–173	$\Gamma_3, \Lambda_1, \Sigma_1, \Lambda_1, \Lambda_3, M_1, D$ $\Gamma_3\Gamma_5, \Lambda, \Sigma, K, M_1, B$
174	$\Gamma_3\Gamma_5, \Lambda_1\Lambda_1, \Sigma_1\Sigma_1, K_1K_1, K_3K_3,$
	$K_5K_5, M_1, B_1B_1$
175,176	$\Gamma^{+}\Gamma^{+} \Lambda_{1} \Sigma_{1} K_{1} K_{2} K_{2} M^{+} B_{2}$
177–186	$\Gamma_3^+\Gamma_5^+, \Lambda_1, \Sigma_1, K_1, K_3K_5, M_1^+, B_1$ $\Gamma_5, \Lambda_1, \Sigma_1, K_1, K_3, M_1, B$
187,188	$\Gamma_5, \Lambda_1, \Sigma_1, \Sigma_1, K_1, K_3, K_5, M_1, B_1B_1$
189,190	$\Gamma_5, \Lambda_1 \Lambda_1, \Sigma_1, K_1 K_1, K_5 K_5, M_1, B_1 B_1$
191–194	$\Gamma_5^+, \Lambda_1, \Sigma_1, K_1, K_5, M_1^+, B_1$
Cubic P	15,11,21,11,15,111,21
195,198	$\Gamma, \Sigma, M$
200	$\Gamma_2^+\Gamma_3^+, \Gamma_4^+, \Sigma, M_1^+, M_2^+, M_3^+, M_4^+$
201,205	$\Gamma_2^+\Gamma_3^+, \Gamma_4^+, \Sigma, M$
207	$\Gamma_3,\Gamma_5,\Sigma_1,M_1,M_4,M_5$
208	$\Gamma_3, \Gamma_5, \Sigma_1, M_2, M_3, M_5$
212,213	$\Gamma_3, \Gamma_5, \Sigma_1, M_1M_4, M_5$
215,218	$\Gamma_3, \Gamma_4, \Sigma, M_1, M_3, M_5$ $\Gamma_3^+, \Gamma_5^+, \Sigma_1, \Sigma_4, M_1^+, M_4^+, M_5^+$
221,223	
222,224	$\Gamma_3^+,\Gamma_5^+,\Sigma_1,\Sigma_4,M_1,M_3$
Cubic F	0 0
196	$\Gamma, \Sigma, X$
202	$\Gamma_2^+\Gamma_3^+, \Gamma_4^+, \Sigma, X_1^+, X_2^+, X_3^+, X_4^+$
203	$\Gamma_2^+\Gamma_3^+, \Gamma_4^+, \Sigma, X$
203	$\Gamma_{2}^{\Gamma_{2}}\Gamma_{3}^{\Gamma_{4}}, \Gamma_{4}^{L}, X_{1}, X_{4}, X_{5}$
210	$\Gamma_3, \Gamma_5, \Sigma_1, X_1, X_4, X_5$ $\Gamma_3, \Gamma_5, \Sigma_1, X_2, X_3, X_5$
216,219	$\Gamma_3, \Gamma_4, \Sigma, X_1, X_2, X_3, X_5$ $\Gamma_3, \Gamma_4, \Sigma, X_1, X_3, X_5$
225,226	$\Gamma_3^+, \Gamma_5^+, \Sigma_1, \Sigma_4, X_1^+, X_4^+, X_5^+$
227,228	$\Gamma^+_3,\Gamma^+_5,\Sigma_1,\Sigma_4,X_1,X_3$
Cubic I	
197,199	$\Gamma, \Sigma, N$
204	$\Gamma_2^+\Gamma_3^+, \Gamma_4^+, \Sigma, N_1^+, N_2^+$
206	$\Gamma_2^+\Gamma_3^+, \Gamma_4^+, \Sigma, N$
211,214	$\Gamma_3, \Gamma_5, \Sigma_1, N_1, N_3$
217	$\Gamma_3, \Gamma_4, \Sigma, N_1, N_4$
220	$\Gamma_3, \Gamma_4, \Sigma, N$
229	$\Gamma_{3}^{+}, \Gamma_{5}^{+}, \Sigma_{1}, \Sigma_{4}, N_{1}^{+}, N_{3}^{+}$
230	$\Gamma_3^+,\Gamma_5^+,\Sigma_1,\Sigma_4,N_2$

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## BRIEF REPORTS

TABLE II. IR's and PIR's which violate the weak Lifshitz condition.

Space groups	IR's, PIR's	Space groups	IR's, PIR's
Monoclinic P		82	$\Sigma, \Delta, Q, Y, A, B$
4,11	C, D, E, Z, G	87	$\Sigma, \Delta, P_3 P_4, Q, Y, A, B$
7,13	A, B, D, E, U, V	88 97	$\Sigma, \Delta, X, M_1, P, Q, W, Y, A, B$
14 Aonoclinic A	A, B, C, Z, U, V, G	97 98	$\Gamma_5, M_5, P_3P_4$ $\Gamma_5, M_5, P$
9,15	A, M, U	107	$P_3P_4$
Orthorhombic	P	108, 120, 140	N, P, Q
17,26	Z, T, U, R, A, B, P, E, W	109	$X, M_1 M_2, M_3 M_4, P, W, Y$
18,55,59	X, Y, T, U, C, D, P, E, G, H, L, N	110	$X, M_1 M_2, M_3 M_4, N, P, Q, W, Y$
19	X, Y, Z, R, A, B, C, D, G, H, L, N, W	121 122	$P_5 P_5 X, M_5, P, W, Y$
27,49 28	Z, T, U, R, A, B, P, E X, S, U, R, D, P, Q, G	139	$P_5$
29	X, Z, S, T, U, R, A, B, D, P, Q, E, G, W	141	$X, M_1, M_2, P, W, Y$
30	Y, Z, S, T, U, R, A, B, C, P, Q, H	142	$X, M_1, M_2, N, P, Q, W, Y$
31,53	X, Z, S, T, A, B, D, P, Q, E, G, W	Hexagonal $R$	
32,50	X, Y, S, T, U, R, C, D, P, E, G, H	146	$\Gamma_2\Gamma_3, \Sigma, T_2T_3, Y, C$
33 34,48	X, Y, Z, S, U, R, A, B, C, D, P, E, G, H, W X, Y, Z, S, T, U, A, B, C, D, G, H	$\frac{148}{155}$	$\Lambda_2 \Lambda_3, \Sigma, Y, C$ $\Gamma_3, T_3$
51	X, Y, Z, S, T, O, A, B, C, D, G, H X, S, U, R, D, P, Q, G, L	160	$\Lambda_3 \Lambda_3$
52	X, Y, Z, S, U, R, A, B, C, D, Q, E, G, H, N	161	$\Lambda_3 \Lambda_3, L, T, Y$
54	X, Z, S, T, U, R, A, B, D, P, Q, E, G, L	166	$\Lambda_3$
56	X,Y,Z,T,U,A,B,C,D,P,E,G,H,L,N	167	$\Lambda_3, L, T, Y$
57	Y, Z, S, T, U, R, A, B, C, P, Q, E, H, N, W	Hexagonal $P$	
58	X, Y, Z, A, B, C, D, P, E, G, H, L, N	143,145	$\Gamma_2\Gamma_3, \Lambda, \Sigma, A_2A_3, H, K, Q, R, U, B, C, D, E$
60 61	X, Y, Z, T, U, R, A, B, C, D, P, Q, E, G, H, L, W	$\frac{144}{147}$	$\Gamma_2\Gamma_3,\Lambda,\Sigma,A_1A_3,H,K,Q,R,U,B,C,D,E \ \Delta_2\Delta_3,\Lambda,\Sigma,H,K,P_2P_3,Q,R,U,B,C,D,E$
62	X, Y, Z, S, T, U, A, B, C, D, P, Q, E, G, H, L, N, W X, Y, Z, S, R, A, B, C, D, Q, G, H, L, N, W	149,151,153	$\Gamma_3, \Lambda, A_3, H, K, Q, U, B, D, E$
rthorhombic		150, 152, 154	$\Gamma_3, \Sigma, A_3, H_3H_3, K_3K_3, R, U, B, C, E$
20,36,63	Z, R, T, A, B, Q	156	$\Delta_3\Delta_3, \Sigma, R, U, B, C, E$
37,40,66	Z, T, A, B	157	$\Delta_3\Delta_3, \Lambda, H, K, P_3P_3, Q, U, B, D, E$
39,67	R, S, D	158	$\Delta_3 \Delta_3, \Sigma, A, H, L, Q, R, U, B, C, E$
41,68	Z, R, S, T, A, B, D	$\begin{array}{c} 159 \\ 162 \end{array}$	$\Delta_3\Delta_3, \Lambda, A, H, K, L, P_3P_3, Q, R, U, B, D, E$
64 orthorhombic	Z, S, T, A, B, D, Q	162	$\Delta_3, \Lambda, H, K, P_3, Q, U, B, D, E  \Delta_3, \Lambda, A, H, K, L, P_3, Q, R, U, B, D, E$
24	W	164	$\Delta_3, \Sigma, H_3, K_3, P_2P_3, R, U, B, C, E$
45,72	S, R, Q, D, W	165	$\Delta_3, \Sigma, A, H, K_3, L, P_2P_3, Q, R, U, B, C, E$
46	R,Q,W	168,171	$\Gamma_{3}\Gamma_{5}, \Gamma_{4}\Gamma_{6}, \Lambda, \Sigma, A_{3}A_{5}, A_{4}A_{6}, H_{2}H_{3}, K_{2}K_{3}, Q, R, C$
73	S, R, T, Q, P, D, W	169, 170, 173	$\Gamma_3\Gamma_5, \Gamma_4\Gamma_6, \Lambda, \Sigma, A, H, K_2K_3, L, Q, R, C, D, E$
74	T, P, W	172	$\Gamma_{3}\Gamma_{5}, \Gamma_{4}\Gamma_{6}, \Lambda, \Sigma, A_{1}A_{5}, A_{2}A_{6}, H_{1}H_{3}, K_{2}K_{3}, Q, R, C$
Orthorhombic 43,70		$\frac{174}{175}$	$\Lambda, \Sigma, Q, R, C, D$ $\Lambda, \Sigma, H_3H_5, H_4H_6, K_3K_5, K_4K_6, P_2P_3, Q, R, C, D$
23,70 Tetragonal P	Z,T,Y,A,B,H	176	$\Lambda, \Sigma, A, H_1H_2, K_3K_5, K_4K_6, L, P_2P_3, Q, R, C, D, E$
75	$\Gamma_3\Gamma_4, \Sigma, \Delta, M_3M_4, A_3A_4, Z_3Z_4, Y, S, T, U, B, C, F$	177,180,181	$\Gamma_5, \Gamma_6, A_5, A_6, H_3, K_3$
76,78	$\Gamma_3\Gamma_4, \Sigma, \Delta, M_3M_4, A, R, Z, Y, S, T, U, B, C, E, F$	178,179,182	$\Gamma_5, \Gamma_6, A, H, K_3, L, Q, R, E$
77	$\Gamma_3\Gamma_4, \Sigma, \Delta, M_3M_4, A_1A_2, Z_1Z_2, Y, S, T, U, B, C, F$	183	$H_3, K_3, P_3P_3$
81,83	$\Sigma, \Delta, Y, S, T, U, B, C, F$	184	$A, H, K_3, L, P_3P_3, Q, R$
84	$\Sigma, \Delta, A_1, Z_1, Y, S, T, U, B, C, F$ $\Sigma, \Delta, M, Y, \Delta, B, Y, W, S, T, U, B, C, F$	$\frac{185}{186}$	$A, H, K_3, L, P_3P_3, Q, R, E \\ A, H_1H_2, K_3, L, P_3P_3, Q, R, E$
85 86	$\Sigma,\Delta,M_1,X,A_1,R,Y,W,S,T,U,B,C,F$ $\Sigma,\Delta,M_1,X,R,Z_1,Y,W,S,T,U,B,C,F$	188	A, H, L, Q, R
89,93	$\Gamma_5, M_5, A_5, Z_5$	189	$H_5H_5, H_6H_6, K_5K_5, K_6K_6, P_3P_3$
90,94	$\Gamma_5, X, R, Z_5, Y, W, T, F$	190	$A, H_3H_3, K_5K_5, K_6K_6, L, P_3P_3, Q, R$
91,95	$\Gamma_5, M_5, A, R, Z, S, T, U, E$	191	$H_5, H_6, K_5, K_6, P_3$
92,96	$\Gamma_5, X, A, Z, Y, W, S, U, E, F$	192	$A, H, K_5, K_6, L, P_3, Q, R$
100	$M_1 M_3, M_2 M_4, X, A_1 A_3, A_2 A_4, R, Y, W, T$	193	$A, H, K_5, K_6, L, P_3, Q, R, E$
101 102	$A_1A_3, A_2A_4, R, Z_1Z_3, Z_2Z_4, T, U$ $M_2M_2, M_2M_4, X, R, Z_1Z_2, Z_2Z_4, Y, W, U$	194 Cubic P	$A, H_3, K_5, K_6, L, P_3, Q, R, E$
102	$M_1M_3, M_2M_4, X, R, Z_1Z_3, Z_2Z_4, Y, W, U$ A, R, Z, S, T, U	195	$\Gamma_4, \Sigma, R_4, S, C$
104	$M_1M_3, M_2M_4, X, A_1A_2, A_3A_4, R, Z, Y, W, S, U$	198	$\Gamma_4, \Sigma, R, X, S, Z, C, B$
105	$A_1A_2, A_3A_4, Z_1Z_2, Z_3Z_4, S$	200	$\Lambda_2\Lambda_3, \Sigma, S, C$
106	$M_1M_3, M_2M_4, X, A, R, Z_1Z_2, Z_3Z_4, Y, W, S, T$	201	$\Lambda_2\Lambda_3, \Sigma, X, M, S, Z, C$
112	$A_5, Z_5, S$	205	$\Lambda_2\Lambda_3, \Sigma, X, M, S, T, Z, C, B$
113,127,129	X, R, Y, W, T, F	207,208 212,213	$\Gamma_4, \Gamma_5, R_4, R_5, X_5, M_5 \ \Gamma_4, \Gamma_5, R, X, S, Z, B$
114 116	$X, A_5A_5, R, Z_5, Y, W, S, T, F$ $A_5, R, Z_5, T, U$	212,213	$\Lambda_3 \Lambda_3$
117	$M_5, X, A_5, R, Y, W, T$	218	$\Lambda_3 \Lambda_3, R_4 R_5, X_5, S$
118	$M_5, X, R, Z_5, Y, W, U$	221	$\Lambda_3$
125	$M_3, M_4, X, A_3, A_4, R, Y, W, T$	222	$\Lambda_3, R_4, X, M_3, M_4, S, Z$
126	$M_3, M_4, X, A_3, A_4, R, Z, Y, W, S, U$	223	$\Lambda_3, R_4, X_1, X_2, S$
128	$X, A_3A_4, Z, Y, W, S, T, U, F$	224 Cubic F	$\Lambda_3, X_1, X_2, M_1, M_2, Z$
130 131	X, A, R, Z, Y, W, S, T, U, F $A_1, A_2, Z_1, Z_2, S$	196	$\Gamma_4, \Sigma, L_2L_3, W, Q, C$
131	$A_1, A_2, Z_1, Z_2, S$ $A_1, A_2, R, Z_1, Z_2, T, U$	202	$\Lambda_2 \Lambda_3, \Sigma, W, Q, C$
133	$M_1, M_2, X, A, R, Z_1, Z_2, Y, W, S, T$	203	$\Lambda_2 \Lambda_3, \Sigma, X, W, Q, V, C$
134	$M_1, M_2, X, R, Z_1, Z_2, Y, W, U$	209	$\Gamma_4,\Gamma_5,L_3,X_5,W_3W_4$
135	$X, A, R, Z_1, Z_2, Y, W, S, T, F$	210	$\Gamma_4, \Gamma_5, L_3, X_5, W$
136	$X, Z_1, Z_2, Y, W, T, U, F$	216	$\Lambda_3 \Lambda_3$
137	$X, A_3A_4, R, Z_1, Z_2, Y, W, S, T, F$	219 225	$\Lambda_3 \Lambda_3, L, W, Q$
138 Tetragonal I	$X, R, Z_1, Z_2, Y, W, T, U, F$	225	$\Lambda_3, W_5$ $\Lambda_3, L, W, Q$
contragonal 1	D.D. S.A.M.M. D.D. O.V.A.P.	227	$\Lambda_{3}, X_{1}, X_{2}, W, V$
79	$\Gamma_3\Gamma_4, \Sigma, \Delta, M_3M_4, P_2P_2, Q, Y, A, B$	221	

TABLE II. (Continued).

pace groups	IR's, PIR's	Space groups	IR's, PIR's
Cubic I			
197	$\Gamma_4, \Sigma, H_4, P_4P_4, G, C$	214	$\Gamma_4, \Gamma_5, H_4, H_5, P$
199	$\Gamma_4, \Sigma, H_4, P, G, C$	217	$\Lambda_3\Lambda_3, P_4P_4, P_5P_5$
204	$\Lambda_2\Lambda_3, \Sigma, P_4, G, C$	220	$\Lambda_3\Lambda_3, H_4H_5, N, P_3P_3, D, G$
206	$\Lambda_2\Lambda_3, \Sigma, N, P, D, G, C$	229	$\Lambda_3, P_4, P_5$
211	$\Gamma_4, \Gamma_5, H_4, H_5, P_4$	230	$\Lambda_3, H_4, N, P, D, G$

Second-order transitions to commensurate phases must be driven by an order parameter belonging to an IR associated with a  $\mathbf{k}$  point of symmetry. Hence we have the Lifshitz condition as a special case of the weak Lifshitz condition: The number of Lifshitz invariants must be zero.

The Landau and weak Lifshitz conditions are entirely determined by the IR. Among the 230 crystallographic space groups, there are 10285 IR's which need to be considered. These IR's include all those associated with each **k** point of symmetry and also those associated with an arbitrary  $\mathbf{k}$  vector on each inequivalent  $\mathbf{k}$  line of symmetry and on each inequivalent  $\mathbf{k}$  plane of symmetry, and those associated with an arbitrary general  ${\bf k}$  vector. We list in Table I the IR's which violate the Landau condition and in Table II the IR's which violate the weak Lifshitz condition. In Table I we omit the trivial case of the identity IR's which always violate the Landau condition. Note the surprising result that none of the IR's (except the identity IR's) of the space groups in the triclinic, monoclinic, orthorhombic, or tetragonal systems violate the Landau condition. The IR's in Table II which are associated with  $\mathbf{k}$  points of symmetry are also those which violate the Lifshitz condition. The data in both of these tables were generated by computer calculations using the database from Ref. 5. The mathematical equations used in these calculations are given in Ref. 6.

We use the IR labeling from Miller and Love.<sup>7,5</sup> (Note that Ref. 5 is an updated version of Ref. 7 and contains some additional **k** vectors. Reference 8 contains a useful table giving the corresponding labeling of IR's by Kovalev,<sup>9</sup> Bradley and Cracknell,<sup>4</sup> and Zak<sup>10</sup> for **k** points of symmetry. Also, a forthcoming English edition of Kovalev<sup>11</sup> gives the mapping of all **k** vectors from Miller and Love to Kovalev.) The IR symbols in Tables I and II are represented by a letter  $(\Sigma, \Lambda, A, B, \ldots)$ , which denotes the **k** vector, and a subscript number, which de-

TABLE III. Equivalent  ${\bf k}$  values in the Miller and Love labeling of IR's. Groups of symbols separated by semicolons are labels for equivalent  ${\bf k}$  values.

Lattice	k values
Orthorhombic $C$	$\Delta, F; \Sigma, C; A, E; B, G; K, L; M, N$
Orthorhombic I	$\Delta, U; \Lambda, G; \Sigma, F; A, K; B, L; C, M$
Orthorhombic $F$	$\Delta, R; \Lambda, Q; \Sigma, U; A, C; B, D; H, G;$
	$E,F;\ J,K;\ M,N$
Tetragonal I	$\Sigma, F; \Lambda, V; Y, U; A, E; C, D$
Hexagonal $R$	$\Lambda, P; \Sigma, Q; Y, B; C, D, E$
Hexagonal P	$\Lambda, T; Q, S; C, F$
Cubic P	C, J
Cubic F	$\Sigma, S; C, J; A, B$
Cubic I	$\Lambda, F; C, J, B$

notes the IR associated with that **k** vector. If the subscript is absent, then all of the IR's associated with that **k** vector are implied. For example, we see in Table I that all of the  $\Sigma$  IR's of space group 146 violate the Landau condition, whereas only the one IR  $\Sigma_1$  of space group 166 violates the Landau condition.

In Landau theory, only physically irreducible representations (PIR's) are considered. If an IR is not real, the PIR is formed from the direct sum of the IR with its complex conjugate. This is indicated in the tables by combining two IR symbols to form a single symbol. For example, in Table I, we see that PIR  $\Sigma_1 \Sigma_1$  of space group 155 violates the Landau condition. This PIR is formed from the direct sum of the IR  $\Sigma_1$  with its complex conjugate. In Table II, we see that PIR  $P_2P_3$  of space group 147 violates the weak Lifshitz condition. This PIR is formed from the direct sum of  $P_2$  with its complex conjugate. In this case, the complex conjugate of  $P_2$  happens to be equivalent to the IR  $P_3$ . Hence we use the label  $P_2P_3$ .

Some of the **k** vectors listed in Refs. 7 and 5 are equivalent to each other. These are listed in Table III. We do not list IR's with equivalent **k** vectors in Tables I and II. For example, from Table I we see that IR  $\Sigma_1$  of space group 166 violates the Landau condition. In Table III we find that **k** vectors  $\Sigma$  and Q are equivalent for the hexagonal R lattice. Therefore, IR  $Q_1$  of space group 166 also violates the Landau condition, even though it is not listed in Table I.

In Ref. 8, the Landau and Lifshitz conditions have been previously determined for all IR's associated with **k** points of symmetry. In Ref. 12, the Landau condition for all real IR's can be easily obtained from the tables of symmetrized triple Kronecker products. Other papers<sup>13–16</sup> have listed IR's which satisfy the Landau and/or Lifshitz conditions for various space groups, but these lists contain errors.<sup>17</sup> The tables in Refs. 8 and 5 were typeset by computer directly from data files and therefore almost certainly do not contain any errors. Also, Tables I and II in this Brief Report were composed directly by the computer and therefore also should not contain any errors.

Using our data, we can comment on some assertions made by Michelson<sup>3</sup> regarding the weak Lifshitz condition. First of all, he asserts that all IR's associated with general  $\mathbf{k}$  points satisfy the weak Lifshitz condition. There are no general  $\mathbf{k}$  points listed in Table II, in agreement with his assertion.

Second, he asserts that IR's associated with  $\mathbf{k}$  planes and  $\mathbf{k}$  lines of symmetry satisfy the weak Lifshitz condition if the small representation is one dimensional. We have found two ways in which this rule can be violated. If the IR is not real, the PIR may not satisfy the weak Lifshitz condition. For example, the PIR  $A_1A_2$  of space group 17 is associated with a **k** line of symmetry. The small representations  $A_1$  and  $A_2$  are both one dimensional. However, there are three Lifshitz invariants in the free-energy expansion for the PIR  $A_1A_2$ . Since the **k** vector has only one degree of freedom, this PIR violates the weak Lifshitz condition.

The other way in which Michelson's rule can be violated is illustrated by the following example. The IR  $\Delta_1$ of space group 75 is associated with a **k** line of symmetry (one degree of freedom). The small representation  $\Delta_1$  is one dimensional. However, there are two Lifshitz invariants in the free-energy expansion, and the weak Lifshitz condition is violated. There is a special circumstance here that allows Michelson's rule to be violated. If we consider the full symmetry of the tetragonal P lattice,

- <sup>1</sup>L. D. Landau and E. M. Lifshitz, *Statistical Physics*, 3rd ed. (Pergamon, Oxford, 1980), Pt. 1, Chap. XIV.
- <sup>2</sup>J.-C. Tolédano and P. Tolédano, The Landau Theory of Phase Transitions (World Scientific, Singapore, 1987).
- <sup>3</sup>A. Michelson, Phys. Rev. B **18**, 459 (1978).
- <sup>4</sup>C. J. Bradley and A. P. Cracknell, *The Mathematical Theory of Symmetry in Solids* (Clarendon, Oxford, 1972).
- <sup>5</sup>A. P. Cracknell et al., General Introduction and Tables of Irreducible Representations of Space Groups, Kronecker Product Tables, Vol. 1 (IFI/Plenum, New York, 1979).
- <sup>6</sup>G. Ya. Lybarskii, *Applications of Group Theory in Physics* (Pergamon, New York, 1963).
- <sup>7</sup>S. C. Miller and W. F. Love, Tables of Irreducible Representations of Space Groups and Co-Representations of Magnetic Space Groups (Pruett, Boulder, 1967).
- <sup>8</sup>H. T. Stokes and D. M. Hatch, *Isotropy Subgroups of the 230 Crystallographic Space Groups* (World Scientific, Singapore, 1988).
- <sup>9</sup>O. V. Kovalev, Irreducible Representations of the Space Groups (Gordon and Breach, New York, 1965); Irreducible and Induced Representations and Corepresentations of the

the point group of every  $\mathbf{k}$  vector on  $\Delta$  is mm2. If we consider only the symmetry of the space group, then the point group of  $\mathbf{k}$  vectors on  $\Delta$  is 1, the same as the point group of a general  $\mathbf{k}$  point. One might argue that  $\mathbf{k}$  vectors on that line do not really belong to a  $\mathbf{k}$  line of symmetry in space group 75, but are actually general  $\mathbf{k}$  points and have three degrees of freedom. However, by mathematical definition, the  $\mathbf{k}$  vectors that lie on  $\Delta$  have only one degree of freedom, and therefore, if there is more than one Lifshitz invariant in the free energy, the weak Lifshitz condition is violated. The minimum of the free energy cannot fall on that line. In general, Michelson's rule may be violated in cases where  $\mathbf{k}$  vectors on a  $\mathbf{k}$  line or plane of symmetry do not have more symmetry than surrounding  $\mathbf{k}$  vectors.

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Fedorov Groups (Nauka, Moskow, 1986), in Russian.

- <sup>10</sup> The Irreducible Representations of the Space Groups, edited by J. Zak (Benjamin, New York, 1969).
- <sup>11</sup>O. V. Kovalev, Irreducible and Induced Representations and Corepresentations of the Crystallographic Space Groups, edited by H. T. Stokes and D. M. Hatch (Gordon and Breach, London, in press).
- <sup>12</sup>B. L. Davies and A. P. Cracknell, Symmetrized Powers of Irreducible Representations of Space Groups, Kronecker Product Tables, Vol. 4 (IFI/Plenum, New York, 1980).
- <sup>13</sup>P. Tolédano and J.-C. Tolédano, Phys. Rev. B 14, 3097 (1976).
- <sup>14</sup>P. Tolédano and J.-C. Tolédano, Phys. Rev. B 16, 386 (1977).
- <sup>15</sup>P. Tolédano and G. Pascoli, Ferroelectrics 25, 427 (1980).
- <sup>16</sup>H. W. Kunert, in *Group Theoretical Methods in Physics*, edited by M. Serdaroglu and E. Inönü, Lecture Notes in Physics Vol. 180 (Springer, Berlin, 1983), p. 329.
- <sup>17</sup>H. T. Stokes and D. M. Hatch, Phys. Rev. B **30**, 4962 (1984). Also see erratum in *ibid.* **31**, 4700 (1985).