Symmetry-restricted phase transitions in two-dimensional solids

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Group-theoretical criteria which determine the possibility of group-subgroup phase transitions have been implemented on a computer. Lower-symmetry groups are determined by the subduction and chain criteria. We list all possible such symmetry-restricted transitions in two dimensions corresponding to \vec{k} points of symmetry. We indicate relative origins and orientations of the prototype group and subgroup sufficient to obtain a wide class of useful experimental information.

I. INTRODUCTION

Phase transitions in three-dimensional solids have been investigated theoretically and experimentally for many years. Mean-field (e.g., Landau theory¹) and renormalization-group (RG) methods yield a well-developed approach to the analysis of space-group changes and the critical phenomena² associated with these transitions. The correspondence between models and physical systems yields similarity (universality) in critical properties for a variety of physical systems. For example, a wide class of ferromagnetic and ferroelectric transitions have the same critical exponents.

More recently, two-dimensional solids have become much more accessible to the experimentalist. Physically and chemically adsorbed atoms and molecules on crystal surfaces, surface reconstruction, domain growth on surfaces, etc., are being actively investigated with new techniques. In some cases, transitions associated with the solid surfaces have been investigated and correspondence made to model systems,^{3,4} e.g., the Ising model, the threeand four-state Potts model, etc., thus providing a physical system to realize the theory. Barber⁵ has written a review of phase transitions in two dimensions, discussing recent developments in theoretical and experimental methods. Based upon group-theoretical criteria. Rottman⁶ has obtained Landau-Ginzburg-Wilson (LGW) Hamiltonians for the irreducible representations of the two-dimensional space groups obeying the Lifshitz criterion. Thus universality classes for these symmetry systems were indicated, and renormalization-group methods could subsequently be used for the description of the associated critical phenomena.

Deonarine and Birman⁷ and independently Maksimov et al.⁸ classified all possible symmetry changes allowed in two dimensions under the restriction that the phase transition correspond to \vec{k} points of symmetry. It would be useful for the experimentalist to know origin and orientation relationships between the prototype space group and its lower symmetry phase, the change in cell size, orderparameter transformation properties, the corresponding representation of the order parameter which can then be used to obtain information about microscopic displacements and orderings, possible rotation and antiphase domains, etc. The tables listed by Maksimov *et al.* and those by Deonarine and Birman do not give sufficient information for the above properties to be obtained. Both papers indicate the irreducible representation (irrep) corresponding to the transition but do not give origin and relative orientations. In addition, both papers contain errors as well as omissions in their tables.

In the present paper, we list all possible group-subgroup transitions in two dimensions corresponding to \vec{k} points of symmetry. The list is of isotropy subgroups and thus include both first- and second-order transitions. This complete list of isotropy groups is helpful in understanding the full phase diagram obtained from terms contributing to arbitrary order in the LGW Hamiltonian. We indicate space-group changes as well as information concerning the relationship of the lower-symmetry space group to the prototype space group sufficient to obtain the experimental information discussed above.

II. LANDAU THEORY AND DIRECT GROUP-THEORETICAL METHODS

Classical Landau theory^{1,9} presents a description of continuous phase transitions in which possible lowersymmetry phases can be predicted from the space group G_0 . Here G_0 and the lower-symmetry group G are each one of the 17 two-dimensional space groups. G is a subgroup of G_0 with possible changes in cell size (lost translational symmetry), as well as possible lost local "point" symmetry.

The classical Landau theory has been reviewed elsewhere^{10,11} and we indicate only the essential steps of that theory. Single irreps drive the transition. Only those irreps which satisfy the Landau and Lifshitz criteria can be active for commensurate transitions. The nonequilibrium (generalized) free energy Φ for the system is to be an invariant function of the order-parameter components C_i^{α} corresponding to irrep D^{α} of G_0 . To lowest order in C_i^{α} (usually fourth order) solutions to extrema are obtained from the equations $\partial \Phi / \partial C_i^{\alpha} = 0$ and subsequently absolute minima are retained. The density function

$$\delta\rho(\vec{\mathbf{r}}) = \sum_{i} C_{i}^{\alpha} \psi_{i}^{\alpha}(\vec{\mathbf{r}})$$

30 5156

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corresponds to the nonzero order-parameter contribution in the lower phase, where $\psi_i^{\alpha}(\vec{r})$ are basis functions of irrep D^{α} . The set of all transformations (of G_0) which leaves $\delta \rho(\vec{r})$ invariant is then the lower-symmetry space group.

Associated with the above formalism, certain direct group-theoretical criteria have been introduced which are necessary conditions for a continuous transition. We only briefly state them here. See Ref. 11 for a more complete discussion.

(1) Subduction criterion. The irrep D^{α} of G_0 must subduce into the identity irrep of G, that is,

$$i(G) = \frac{1}{|G|} \sum_{g} \chi^{\alpha}(g) \neq 0 ,$$

where i(G) is the subduction frequency and $\chi^{\alpha}(g)$ is the character of D^{α} for the element g of G. The summation is taken over all elements g of G.

(2) Chain criterion. If G is a subgroup of another subgroup G' of G_0 [where i(G') is also nonzero for irrep D^{α}], then i(G) must be greater than i(G').

(3) Landau criterion. The symmetrized triple Kronecker product of the irrep D^{α} of G_0 does not contain the identity irrep of G_0 , that is,

$$n_1 = \frac{1}{|G_0|} \sum_{g_0} \left\{ \frac{1}{3} \chi^{\alpha}(g_0^3) + \frac{1}{2} \chi^{\alpha}(g_0) \chi^{\alpha}(g_0^2) + \frac{1}{6} [\chi^{\alpha}(g_0)]^3 \right\} = 0.$$

The summation is taken over all elements g_0 of G_0 .

(4) Lifshitz criterion. The antisymmetrized double Kronecker product of D^{α} does not contain the vector representation of G_0 , that is,

$$n_2 = \frac{1}{|G_0|} \sum_{g_0} \frac{1}{2} \{ [\chi^{\alpha}(g_0)]^2 - \chi^{\alpha}(g_0^2) \} \chi^{\nu}(g_0) = 0 ,$$

where $\chi^{\nu}(g_0)$ is the character of the vector representation of G_0 . Note that in the equations above χ^{α} is the character of a *physically* irreducible representation D^{α} of G_0 . By physical, we mean that if a representation is complex, we consider the direct sum of it and its complex conjugate.

The subduction and chain criteria are valid in a more general transition (first order) if we restrict attention to a group-subgroup transition. These two criteria yield isotropy subgroups of G_0 corresponding to a vector (order parameter) of the representation space. The Landau and Lifshitz criteria in three dimensions are then additional conditions necessary for continuous commensurate transitions. These criteria select from the list of isotropy groups and if one then looks at absolute minima of the free energy a further selection is made. It has been proposed that minimization is equivalent to restricting attention to maximal isotropy groups,¹² i.e., isotropy groups of a given irrep which are not a subgroup of any other for that irrep regardless of subduction frequency. However, a counterexample to this principle has recently been presented.13

Although the Landau criterion appears to be valid in

TABLE I. The basis vectors, \vec{t}_1 and \vec{t}_2 , of the twodimensional Bravais lattices. The vectors are given in terms of (x,y) Cartesian coordinates. We use the convention of Cracknell (Ref. 15).

Lattice	\vec{t}_1	\vec{t}_2
Oblique, p	(<i>a</i> ,0)	$(b\cos\theta, b\sin\theta)$
Rectangular, p	(<i>a</i> ,0)	(0 , <i>b</i>)
Rectangular, c	$(\frac{1}{2}a,\frac{1}{2}b)$	$(-\frac{1}{2}a,\frac{1}{2}b)$
Square, p	(<i>a</i> ,0)	(0 , <i>a</i>)
Hexagonal, p	(0, -a)	$(\frac{1}{2}\sqrt{3}a, \frac{1}{2}a)$

three dimensions, it is not necessary in two dimensions.^{4,5} Thus we will not limit our consideration to only those irreps satisfying the Landau criterion. The Lifshitz criterion restricts our considerations to \vec{k} points of symmetry only, since our interest here is in commensurate transitions.

We have recently implemented on computer an algorithm for obtaining *all* isotropy subgroups of space groups in *two and three dimensions*.¹⁴ The details of the method and the algorithm with the resulting tables for threedimensional space groups are to be published elsewhere. We have also tabulated by computer the Landau and Lifshitz criteria. We do not impose minimization of the lowest-order free-energy expansion which, as mentioned above, would additionally discard possible transitions.

III. PHASE TRANSITIONS IN TWO DIMENSIONS

Irreps of the two-dimensional space groups are obtained by induction from the irreps of the little group of \vec{k} . As stated earlier, we restrict considerations to \vec{k} points of symmetry in the first Brillouin zone since others will not satisfy the Lifshitz criterion and would thus disallow commensurate continuous transitions. Our labeling and choice of irreps will follow that of Cracknell.¹⁵ The short symbol of the space groups is used, and k_i indicates the *i*th irrep of the vector \vec{k} , e.g., Γ_2 is the second irrep of $\vec{k}=0$. If an irrep is complex, we take the physically irreducible representation and, for example, indicate X_1+X_2 as the physical irrep.

So that this paper may be as self-contained as possible and include sufficient detail to obtain the experimental properties listed earlier, we repeat some of the information contained in Cracknell.¹⁵ Tables I and II give the basis vectors of the two-dimensional Bravais and reciprocal lattices. Table III lists the two-dimensional space groups

TABLE II. The basis vectors, \vec{g}_1 and \vec{g}_2 , of the twodimensional reciprocal lattice. The vectors are given in terms of (x,y) Cartesian coordinates.

Lattice	<u>ġ</u> 1	ġ2
Oblique, p	$(2\pi/a)(1, -\cot\theta)$	$(2\pi/b)(0,\csc\theta)$
Rectangular, p	$(2\pi/a)(1,0)$	$(2\pi/b)(0,1)$
Rectangular, c	$2\pi(1/a, 1/b)$	$2\pi(-1/a, 1/b)$
Square, p	$(2\pi/a)(1,0)$	$(2\pi/a)(0,1)$
Hexagonal, p	$(2\pi/a)(1/\sqrt{3},-1)$	$(2\pi/a)(2/\sqrt{3},0)$

System	Number	Symbol	Generating elements
Oblique	1	<i>p</i> 1	{ <i>E</i> 00}
	2	<i>p</i> 2	$\{ C_{2z} \mid 00 \}$
Rectangular	3	pm	$\{\sigma_y \mid 00\}$
	4	pg	$\{\sigma_y \mid \frac{1}{2}0\}$
	5	cm	$\{\sigma_x \mid 00\}$
	6	pmm	$\{C_{2z} \mid 00\}, \{\sigma_y \mid 00\}$
	7	pmg	$\{C_{2z} \mid 00\}, \{\sigma_y \mid \frac{1}{2}0\}$
	8	pgg	$\{C_{2z} \mid 00\}, \{\sigma_x \mid \frac{1}{2}, \frac{1}{2}\}$
	9	cmm	$\{C_{2z} \mid 00\}, \{\sigma_x \mid 00\}$
Square	10	p 4	$\{ C_{4z}^+ 00 \}$
	11	p 4m	$\{C_{4z}^+ \mid 00\}, \{\sigma_x \mid 00\}$
	12	p 4g	$\{C_{4z}^+ \mid 00\}, \{\sigma_x \mid \frac{1}{2} \mid \frac{1}{2}\}$
Hexagonal	13	p 3	$\{C_3^+ \mid 00\}$
-	14	p 3m 1	$\{C_3^+ \mid 00\}, \{\sigma_{v1} \mid 00\}$
	15	p 31m	$\{C_3^+ \mid 00\}, \{\sigma_{d1} \mid 00\}$
	16	<i>p</i> 6	$\{ C_{6}^{+} \mid 00 \}$
	17	p 6m	$\{C_6^+ \mid 00\}, \{\sigma_{d1} \mid 00\}$

TABLE III. The 17 two-dimensional space groups and their generating elements. Vectors are given in terms of components of \vec{t}_1 , \vec{t}_2 . We use the convection of Cracknell (Ref. 15).

and their generating elements. Table IV gives the \bar{k} points of symmetry for each Brillouin zone. Table V gives the irreps of the two-dimensional space groups at the \bar{k} points of symmetry. This table uses notation similar to Table 5.7 in Bradley and Cracknell¹⁶ for the three-dimensional space groups. The irreps and their reality are listed in numerical order. For example, the irreps X_1, X_2, X_3 , and X_4 of space group *pmm* (labeling and numbering follow the convention of Cracknell¹⁵) correspond to the irreps R_1, R_3, R_2 , and R_4 , respectively, of the abstract group G_4^2 listed in Table 5.1 of Bradley and Cracknell.¹⁶ They each have reality of type 1.

In Table VI we list the results of the computer calculation. We give the high-symmetry space group G_0 , its irrep, the Landau criterion n_1 , the Lifshitz criterion n_2 , the number of arms of the star of \vec{k} , the change in primitive cell size (volume), the lower-symmetry space group G, its subduction frequency i(G), the primitive basis vectors of G in terms of the primitive basis vectors of G_0 , and the change of space-group origin (from G_0 to G) in terms of the primitive basis vectors of G_0 . In our tables, we do not indicate which subgroups are maximal since for real irreps the maximal subgroups have subduction frequency i(G) = 1, while for complex irreps, the maximal subgroups have subduction frequency i(G)=2. We have compared our listing of isotropy subgroups with the listing of subgroups given by Sayari et al.¹⁷ We find complete agreement since all of our isotropy subgroups are contained in the appropriate allowed listing as given in their table.

IV. COMPARISON WITH PREVIOUS LISTINGS

Of the many papers written concerning phase transitions in two dimensions, three are notable in that they seek to classify all possible commensurate transitions consistent with mean-field theory (or RG). These are the papers by Rottman,⁶ Maksimov *et al.*,⁸ and Deonarine and Birman.⁷

TABLE IV. The \vec{k} points of symmetry for the twodimensional lattices. The vectors are given in terms of \vec{g}_1 and \vec{g}_2 . We use the convention of Cracknell (Ref. 15).

Lattice		k
Oblique, p	- <u> </u>	Γ(00)
		$X(\frac{1}{2}0)$
	,	$Y(0\frac{1}{2})$
		$A\left(\frac{1}{2}\frac{1}{2}\right)$
Rectangular, p		Γ (00)
		$X(\frac{1}{2}0)$
		$Y(0\frac{1}{2})$
		$S(\frac{1}{2}\frac{1}{2})$
Rectangular, c		Γ(00)
		$S(\frac{1}{2}0)$
		$X(\frac{1}{2}\frac{1}{2})$
Square, p		Γ(00)
		$X(\frac{1}{2}0)$
		$M(\frac{1}{2}\frac{1}{2})$
Hexagonal, p		Γ (00)
		$M(0\frac{1}{2})$
		$K(-\frac{1}{3}\frac{2}{3})$

TABLE V. The irreps of the two-dimensional space groups G_0 at the \vec{k} points of symmetry. The abstract groups are given in Table 5.1 of Bradley and Cracknell (Ref. 16). The generating elements of the abstract groups are P,Q,R (as needed). The irreps are given in numerical order, using the convention of Cracknell (Ref. 15). Each pair of numbers i,j refers to the irrep R_i of the abstract group and reality type equal to j. This table uses notation similar to Table 5.7 in Bradley and Cracknell (Ref. 16) for the three-dimensional space groups.

		Abstract		
G	k	group	P,Q,R	irreps,reality
p 1	Г	G_1^1	{ <i>E</i> 00}	1,1
•	X	$G_{1}^{1} \times T_{2}$	$E \mid 00$	1,1
	Y	$G_1^i \times T_2$	$E 00 \}$	1,1
	A	$G_1^1 \times T_2$	E 00	1,1
p 2	Г	G_2^1	$\{C_{2z} \mid 00\}$	1,1;2,1
	X	$G_2^1 \times T_2$	$\{ C_{2z} \mid 00 \}$	1,1;2,1
	Y ·	$G_2^1 \times T_2$	$\{ C_{2z} \mid 00 \}$	1,1;2,1
	A	$G_2^1 \times T_2$	$\{C_{2z} \mid 00\}$	1,1;2,1
pm	Г	G_2^1	$\{\sigma_y \mid 00\}$	1,1;2,1
	X	$G_2^1 \times T_2$	$\{\sigma_y \mid 00\}$	1,1;2,1
	Y	$G_2^1 \times T_2$	$\{\sigma_y \mid 00\}$	1,1;2,1
	S	$G_2^1 \times T_2$	$\{\sigma_{y} \mid 00\}$	1,1;2,1
pg	Г	G_2^1	$\{\sigma_y \mid \frac{1}{2}0\}$	1,1;2,1
	X	G_4^1	$\{\sigma_y \mid \frac{1}{2}0\}$	2,3;4,3
	Y	$G_2^1 \times T_2$	$\{\sigma_{y}\mid \frac{1}{2}0\}$	1,1;2,1
	S	G_4^1	$\{\sigma_y \mid \frac{1}{2}0\}$	2,3;4,3
cm	Г	G_2^1	$\{\sigma_x \mid 00\}$	1,1;2,1
	- S	$G_1^1 \times T_2$	$\{E \mid 00\}$	1,1
	X	$G_2^1 \times T_2$	$\{\sigma_x \mid 00\}$	1,1;2,1
mm	Γ	G_4^2	$\{C_{2z} 00\}, \{\sigma_{y} 00\}$	1,1;3,1;2,1;4,1
	X	$G_4^2 \times T_2$	$\{C_{2z} \mid 00\}, \{\sigma_y \mid 00\}$	1,1;3,1;2,1;4,1
	Y	$G_4^2 \times T_2$	$\{C_{2z} \mid 00\}, \{\sigma_y \mid 00\}$	1,1;3,1;2,1;4,1
	S	$G_4^2 \times T_2$	$\{C_{2z} \mid 00\}, \{\sigma_y \mid 00\}$	1,1;3,1;2,1;4,1
omg	Γ	G_4^2	$\{C_{2z} \mid 00\}, \{\sigma_x \mid \frac{1}{2}0\}$	1,1;4,1;2,1;3,1
	X	G_8^4	$\{\sigma_{\mathbf{y}} \mid \frac{1}{2}0\}, \{\sigma_{\mathbf{x}} \mid \frac{1}{2}0\}$	5,1
	Y	$G_4^2 \times T_2$	$\{C_{2z} \mid 00\}, \{\sigma_x \mid \frac{1}{2}0\}$	1,1;4,1;2,1;3,1
	S	G_{8}^{4}	$\{\sigma_{\mathbf{y}} \mid \frac{1}{2}0\}, \{\sigma_{\mathbf{x}} \mid \frac{1}{2}0\}$	5,1
pgg	Г	G_4^2	$\{C_{2z} \mid 00\}, \{\sigma_x \mid \frac{1}{2}, \frac{1}{2}\}$	1,1;3,1;2,1;4,1
	X	G_8^4	$\{\sigma_{y} \mid \frac{1}{2} \frac{1}{2}\}, \{C_{2z} \mid 00\}$	5,1
	Y	G_8^4	$\{\sigma_{\mathbf{x}} \mid \frac{1}{2}, \frac{1}{2}\}, \{C_{2\mathbf{z}} \mid 00\}$	5,1
	S	G_{8}^{2}	$\{\sigma_{\mathbf{x}} \mid \frac{1}{2}, \frac{1}{2}, \{C_{2\mathbf{z}} \mid 00\}$	6,3;8,3;4,3;2,3
cmm	Г	G_4^2	$\{C_{2z} \mid 00\}, \{\sigma_y \mid 00\}$	1,1;3,1;2,1;4,1
	S	$G_2^1 \times T_2$	$\{C_{2z} \mid 00\}$	1,1;2,1
	X	$G_4^2 \times T_2$	$\{C_{2z} \mid 00\}, \{\sigma_y \mid 00\}$	1,1;3,1;2,1;4,1
p 4	Γ	G_4^1	$\{C_{4z}^+ 00\}$	1,1;3,1;2,3;4,3
	X	$G_2^1 \times T_2$	$\{C_{2z} \mid 00\}$	1,1;2,1
	М	$G_4^1 \times T_2$	$\{C_{4z}^+ 00\}$	1,1;3,1;2,3;4,3
94m	Γ	G_8^4	$\{C_{4z}^+ 00\}, \{\sigma_y 00\}$	1,1;2,1;3,1;4,1;5,1
	X	$G_4^2 \times T_2$	$\{C_{2z} 00\}, \{\sigma_y 00\}$	1,1;3,1;2,1;4,1
	M	$G_8^4 \times T_2$	$\{C_{4z}^+ 00\}, \{\sigma_y 00\}$	1,1;2,1;3,1;4,1;5,1
94g	Γ	G_8^4	$\{C_{4z}^+ 00\}, \{\sigma_y \frac{1}{2} \frac{1}{2}\}$	1,1;2,1;3,1;4,1;5,1
	X	G_8^4	$\{\sigma_{y} \mid \frac{1}{2} \mid \frac{1}{2} \}, \{\sigma_{x} \mid \frac{1}{2} \mid \frac{1}{2} \}$	5,1
	М	G ¹⁰ ₁₆	$\{C_{4z}^+ \mid 00\}, \{C_{2z} \mid 01\}, \{\sigma_{db} \mid \frac{1}{2}, \frac{1}{2}\}$	8,3;5,3;6,3;7,3;9,1
p 3	Γ	G_3^1	$\{C_3^+ \mid 00\}$	1,1;2,3;3,3
	M	$G_1^1 \times T_2$	$\{E \mid 00\}$	1,1
	K	$G_3^1 \times T_3$	$\{C_3^+ 00\}$	1, x; 2, x; 3, x
3 <i>m</i> 1	Γ	G_{6}^{2}	$\{C_3^+ \mid 00\}, \{\sigma_{v1} \mid 00\}$	1,1;2,1;3,1
	М	$G_2^1 \times T_2$	$\{\sigma_{v1} 00\}$	1,1;2,1
	K	$G_3^1 \times T_3$	$\{C_3^+ 00\}$	1,1;2,1;3,1
31 <i>m</i>	Г	G_6^2	$\{C_3^+ \mid 00\}, \{\sigma_{d1} \mid 00\}$	1,1;2,1;3,1

G	k	Abstract group	P,Q,R	irreps,reality
	М	$G_2^1 \times T_2$	$\{\sigma_{d1} \mid 00\}$	1,1;2,1
,	K	$G_6^2 \times T_3$	$\{C_3^+ 00\}, \{\sigma_{d1} 00\}$	1, x; 2, x; 3, x
p6	Г	G_6^1	$\{C_6^+ \mid 00\}$	1,1;5,3;3,3;4,1;2,3;6,3
•	M	$G_2^1 \times T_2$	$\{C_{2z} \mid 00\}$	1,1;2,1
	K	$G_3^1 \times T_3$	$\{C_3^+ \mid 00\}$	1,1;2,3;3,3
p 6m	Γ	G_{12}^3	$C_6^+ 00\rangle, \{\sigma_{v1} 00\}$	1,1;2,1;4,1;3,1;6,1;5,1
-	M	$G_4^2 \times T_2$	$\{C_{2z} \mid 00\}, \{\sigma_{v1} \mid 00\}$	1,1;3,1;2,1;4,1
	K	$G_6^2 \times T_3$	$\{C_3^+ 00\}, \{\sigma_{d1} 00\}$	1,1;2,1;3,1

TABLE V. (Continued).

TABLE VI. Isotropy subgroups G of the 17 two-dimensional space groups G_0 for the \vec{k} points of symmetry. We give the Landau criterion n_1 , the Lifshitz criterion n_2 , the number of arms of the star of \vec{k} , the change in primitive cell size (volume), the subduction frequency i(G), the primitive basis vectors of G in terms of the primitive basis vectors of G_0 , and the change in space-group origin (from G_0 to G) in terms of the primitive basis vectors of G_0 .

G_0	irrep	<i>n</i> ₁	<i>n</i> ₂	Arms	Size	G	i (G)	Basis vectors		Origin
<i>p</i> 1	Г	1	0	. 1	1	<i>p</i> 1	1	1,0	0,1	0,0
	X_1	0	0	1	2	p 1	1	2,0	0,1	0,0
	\boldsymbol{Y}_1	0	0	1	2	p 1	1	1,0	0,2	0,0
	A_1	0	0	1	2	p 1	1	1,1	1,1	0,0
p 2	Γ_1	1	0	1	1	p 2	1	1,0	0,1	0,0
	Γ_2	0	0	1	1	p 1	1	1,0	0,1	0,0
	· X ₁	0	0	1	2	p 2	1	2,0	0,1	0,0
	X_2	0	0	1	2	<i>p</i> 2	1	2,0	0,1	$\frac{1}{2},0$
	\boldsymbol{Y}_1	0	0	1	2	<i>p</i> 2	1	1,0	0,2	0,0
	Y_2	0	0	1	2	p 2	1	1,0	0,2	$0, \frac{1}{2}$
	A_1	0	0	1	2	p 2	1	1,1	1,1	0,0
	A_2	0	0	1	2	p 2	1	1,1	1,1	$\frac{1}{2},0$
рт	Γ_1	- 1	. 0	1	1	pm	1	1,0	0,1	0,0
1	Γ_2	0	. 0	1	1	<i>p</i> 1	1	1,0	0,1	0,0
	X ₁	0	0	1	2	pm	1	2,0	0,1	0,0
	X_2	0	0	1	2	pg	1	2,0	0,1	0,0
	Y_1	0	0	1	2	pm	1	1,0	0,2	0,0
	Y_2	0	0	1	2	pm	1	1,0	0,2	$0, \frac{1}{2}$
	S_1	0	0	1	2	cm	1	ī,1	Ī,Ī	0,0
	S_2	0	0	1	2	cm	1	Ī,1	<u>1,1</u>	$\frac{1}{2}, \frac{1}{2}$
pg	Γ_1	1	0	1	1	pg	1	1,0	0,1	0,0
10	Γ_2	0	0	1	- 1	p 1	1	1,0	0,1	0,0
	$X_1 + X_2$	0	1	1	2	p 1	2	2,0	0,1	0,0
•	Y ₁	0	0	1	2	PS	- 1	1,0	0,2	0,0
	Y_2	0	0	1	2	pg	1	1,0	0,2	$0, \frac{1}{2}$
	$S_1 + S_2$	0	1	1	2	<i>p</i> 1	2	1,1	1,1	0,0
cm	Γ_1	. 1	0	1	1	cm	1	1,0	0,1	0,0
	Γ_2	0	0	1	1	p 1	1	1,0	0,1	0,0
	\boldsymbol{S}_1	0	0	1	2	<i>p</i> 1	1	1,0	0,2	0,0
						p 1	1	2,0	0,1	0,0
				2	4	ст	1	2,0	0,2	0,0
						p 1	2	2,0	0,2	0,0

G_0	irrep	<i>n</i> ₁	<i>n</i> ₂	Arms	Size	G	i(G)	Basis	vectors	Origin
	X ₁	0	0	1	2	pm	1	ī,ī	1, Ī	0,0
	X_2	0	0	· 1	2	pg	1	<u>1, 1</u>	1,1	$\frac{1}{4}, \frac{1}{2}$
ртт	Γ_1	1	0	1	1	pmm	1	1,0	0,1	0,0
	Γ_2	0	0	1.	1	pm	1	1,0	0,1	0,0
	Γ_3	0	0	1	1	p 2	1	1,0	0,1	0,0
	Γ_4	0	0	1	1	pm	1	0,1	1,0	0,0
	X_1	0	0	1	2	pmm	1	2,0	0,1	0,0
	X_2	0	0	1	2	pmm	1	2,0	0,1	$\frac{1}{2},0$
	X ₃	0	0	1	2	pmg	1	2,0	0,1	0,0
	X4	0	0	1	2	pmg	1	2,0	0,1	$\frac{1}{2},0$
	Y ₁	0	0	1	2	ртт	1	1,0	0,2	0,0
	Y ₂	0	0	1	2	pmg	1	0,2	1,0	$0, \frac{1}{2}$
	Y ₃	0	0	1	2	pmg	1	0,2	1,0	0,0
	Y ₄	0	0	1	2	pmm	1	1,0	0,2	$0, \frac{1}{2}$
	S_1	0	0	1	2	cmm	1	1,1	<u>1</u> ,1	0,0
	S_2	0	• 0	1	2	cmm	1	1,1	<u>1, 1</u>	$\frac{1}{2},0$
	S_3	0	0	1	2	cmm	1	1,1	Ī,1	$\frac{1}{2}, \frac{1}{2}$
	S ₄	0	0	1	2	cmm	1	1,1	ī, 1	$0, \frac{1}{2}$
pmg	Γ_1	1	0	1	1	pmg	1	1,0	0,1	0, ² 0,0
P8	Γ_1	0	0	1	1	pmg Pg	1	1,0	0,1	0,0
•	Γ_3	0	0	1	1	p8 p2	1	1,0	0,1	0,0
	Γ_4	0	0	1	1	pm	1	0, <u>1</u>	1,0	$\frac{1}{4},0$
	X ₁	0	1	1	2	pm	1	0,1	2,0	4, 1 4, (
		Ŭ	•	•	4					
						p 2	1	2,0	0,1	$\frac{1}{2},0$
						p 2	1	2,0	0,1	0,0
	Y ₁	0	0	1		<i>p</i> 1	2	2,0	0,1	0,0
	\boldsymbol{Y}_{1}	0	0	1 1	2	pmg	1 1	1,0	0,2	0,0
	Y ₃	0				Pgg		1,0	0,2	$0, \frac{1}{2}$
	Y ₄	0	0 0	1	2	Pgg	1	1,0	0,2	0,0
				1	2	pmg	1	1,0	0,2	$0, \frac{1}{2}$
	S_1	0	1	1	2	ст	1	1,1	1,1	$\frac{1}{4}, \frac{1}{4}$
						p 2	1	1,1	1,1	$\frac{1}{2},0$
						p 2	1	1,1	1,1	0,0
						<i>p</i> 1	2	1,1	1,1	0,0
Pgg	Γ_1	1	-0	1	1	pgg	- 1	1,0	0,1	0,0
	Γ_2	0	0	1	1	Pg	1	1,0	0,1	$0, \frac{1}{4}$
	Γ_3	0	0	1	. 1	p 2	1	1,0	0,1	0,0
	Γ_4	0	0	1	1	pg	1	0,1	1,0	$\frac{1}{4},0$
	X_1	0	1	1	2	pg	1	0,1	2,0	$\frac{1}{4}, 0$
						p 2	1	2,0	0,1	$\frac{1}{2},0$
						p 2	1	2,0	0,1	0,0
						p 1	2	2,0	0,1	0,0
	\boldsymbol{Y}_1	0	1	1	2	pg	1	1,0	0,2	$0, \frac{1}{4}$
						p 2	1	1,0	0,2	$0, \frac{1}{2}$
				1		- ₽2 ≋	1	1,0	0,2	0,0
						p 1	2	1,0	0,2	0,0

TABLE VI. (Continued).

DORIAN M. HATCH AND HAROLD T. STOKES

G_0	irrep	n_1	<i>n</i> ₂	Arms	Size	G	<i>i</i> (<i>G</i>)	Basis	vectors	Origi
	$S_1 + S_2$	0	0	1	2	p 2	2	1,1	1,1	$\frac{1}{2}$,
	$S_3 + S_4$	0	0	1	2	p 2	2	1, T	1,1	0,0
cmm	Γ_1	1	0	1	1	cmm	1	1,0	0,1	0,0
	Γ_2	0	0	1	1	ст	1	0,1	<u>1</u> ,0	0,0
	Γ3	0	ວ໌	1	1	p 2	1	1,0	0,1	0,0
`. ``	Γ_4	0	0	. 1	1	ст	1	1,0	0,1	0,0
	\boldsymbol{S}_1	0	0	1	2	<i>p</i> 2	1	1,0	0,2	0,0
		,				p 2	1	2,0	0,1	0,0
				2	4	стт	1	2,0	0,2	0,0
						p 2	2	2,0	0,2	0,0
	S_2	0	0	1	2	p 2	1	1,0	0,2	0, -
						p 2	1	2,0	0,1	$\frac{1}{2}$,
				2	4	стт	1	2,0	0,2	$\frac{1}{2}$,
						p 2	2	2,0	0,2	$\frac{1}{2}$,
	X_1	0	0	1	2	pmm	1	1,1	1,1	- 0,0
							1	1,1	<u>1</u> ,1	$0, \frac{1}{2}$
	<i>X</i> ₂	0	0	1	2	pmg				
	X_3	0	0	1	2	Pgg	1	1, <u>1</u>	1,1	0,0
	X ₄	0	0	1	2	pmg	1	1,1	1,1	$\frac{1}{2},($
p 4	Γ_1	1	0	1	1	p 4	1	1,0	0,1	0,0
	Γ_2	0	0	1	1	<i>p</i> 2	1	1,0	0,1	0,0
	$\Gamma_3 + \Gamma_4$	0	0	1	1	<i>p</i> 1	2	1,0	0,1	0,0
	X_1	0	0	1 2	2 4	р2 р4	1	2,0 2,0	0,1 0,2	0,0 0,0
				2	4	р4 p2	2	2,0	0,2	0,0
	X_2	0	0	1	2	p 2 p 2	1	2,0	0,1	$\frac{1}{2},0$
	A ₂	U	U							$\frac{1}{2}, \frac{1}{2}$
				2	4	p 4	1	2,0	0,2	
						p 2	2	2,0	0,2 T	$\frac{1}{2}, \frac{1}{2}$
	\boldsymbol{M}_1	0	0	1	2	<i>p</i> 4	1	1,1	<u>1</u> ,1	0,0
	M_2	0	0	1	2	<i>p</i> 4	1	1,1	1,1	$\frac{1}{2},$
	$M_3 + M_4$	0	0	1	2	p 2	2	1,1	1,1	$\frac{1}{2},$
p 4m	Γ_1	.1	0	1	1	p 4m	1	1,0	0,1	0,0
	Γ_2	0	0	1	1	p 4	1	1,0	0,1	0,0
	Γ_3	0	0	1	1	pmm	1	1,0	0,1	0,0
	Γ_4	0	0	1	1	стт	1	0,1	ī,0	0,0
	Γ_5	0	0	1	1	ст	1	0,1	ī,0	0,0
						pm	1	0,1	1,0	0,0
		.			•	<i>p</i> 1	2	1,0	0,1	0,0
	X_1	0	0	1	2	pmm n Arm	1	2,0 2,0	0,1 0,2	0,0 0,0
				2	4	p 4m pmm	1 2	2,0 2,0	0,2	0,0
	V	0	Δ	1	2	pmm pmm	2	2,0	0,2	$\frac{1}{2}$,
	X ₂	0	0	1						$\frac{1}{2},$
				2	4	p 4m	1	2,0	0,2	
						ртт	2	2,0	0,2	$\frac{1}{2},$
	<i>X</i> ₃	0	0	1 ·	2	pmg	1	2,0	0,1	0,0
				2	4	p 4g	1	2,0	0,2	0,0
						Pgg	2	2,0	0,2	0,0

TABLE VI. (Continued.)

$\overline{G_0}$	irrep	<i>n</i> ₁	<i>n</i> ₂	Arms	Size	G	<i>i</i> (<i>G</i>)	Basis v	vectors	Origin
									an tan dalam ta kara dan menang	
	X ₄	0	0	1	2	pmg	1	2,0	0,1	$\frac{1}{2},0$
				2	4	p 4g	1	2,0	0,2	$\frac{1}{2}, \frac{1}{2}$
	·			· · · ·		Pgg	2	2,0	0,2	$\frac{1}{2}, \frac{1}{2}$
	<i>M</i> ₁	0	0	1	2	p 4m	1	1,1	Ī,1	0,0
	<i>M</i> ₂	0	0	1	2	p 4g	1	1,1	<u>1</u> ,1	0,0
	<i>M</i> ₃	0	0	1	2	p 4g	1	1,1	<u>1,</u> 1	$\frac{1}{2}, \frac{1}{2}$
	M_4	0	0	1	2	p 4m	1	1,1	<u>1</u> ,1	$\frac{1}{2}, \frac{1}{2}$
	M_5	0	0	1	2	стт	1	1,1	<u>1, 1</u>	$\frac{1}{2},0$
						pmg	1	1,1	1,1	$\frac{1}{2},0$
						p 2	2	1,1	1,1	$\frac{1}{2},0$
p 4g	Γ_1	1	0	1	1	p 4g	1	1,0	0,1	0,0
	Γ_2	0	0	1	1	p 4	1	1,0	0,1	0,0
	Γ_3	0	0	1	1	Pgg	1	1,0	0,1	0,0
	Γ_4	0	0	1	1	cmm	1	0,1	<u>1</u> ,0	$0, \frac{1}{2}$
	Γ5	0	0	· 1 · ·	1	ст	1	0,1	1,0	$0, \frac{1}{2}$
						pg	1	0, 1	1,0	$\frac{1}{4},0$
						p 1	2	1,0	0,1	0,0
	X_1	0	1	1	2	Pg	1 -	0, 1	2,0	$\frac{1}{4},0$
						p 2	1	2,0	0,1	$\frac{1}{2},0$
						p 2	1	2,0	0,1	0,0
	2					р 1	2	2,0	0,1	0,0
				2	4	р1 р4	1	2,0	0,1	$\frac{1}{2}, \frac{1}{2}$
				2	-	p4	1	2,0	0,2	2,2 0,0
	к. К					cmm	1	2,0 0,2	0,2 2,0	0,0 $0,\frac{1}{2}$
						cm	2	0,2	2,0	$0, \frac{1}{2}$
						p 2	2	2,0	0,2	$\frac{1}{2}, \frac{1}{2}$
						p 2	2	2,0	0,2	$0, \frac{1}{2}$
						p 2	2	2,0	0,2	0,0
						<i>p</i> 1	4	2,0	0,2	0,0
	$M_1 + M_4$	0	0	1	2	pmm	2	1,1	<u>1, 1</u>	$0, \frac{1}{2}$
	$M_2 + M_3$	0	0	1	2	Pgg	2	1,1	<u>1,1</u>	$0, \frac{1}{2}$
	M_5	0	0	1	2	<i>p</i> 4	1	1,1	1,1	$\frac{1}{2}, \frac{1}{2}$
						p 4	1	1,1	1,1	0,0
						pmg	1	1,1	ī,1	0,0
						p 2	2	1,1	1,1	0,0
<i>p</i> 3	Γ_1	1	0	1	1	<i>p</i> 3	1	1,0	0,1	0,0
	$\Gamma_2 + \Gamma_3$	2	0	1	1	<i>p</i> 1	2	1,0	0,1	0,0
	M_1	1	0	1 3	2 4	<i>p</i> 1	1	1,0	0,2	0,0
				3	4	р3 р1	1 3	2,0 2,0	0,2 0,2	0,0
	$K_1 + K_1^*$	2	0	1	3	р 1 р 3	2	2,0 2,1	0,2 <u>1</u> ,1	0,0 0,0
	$\frac{K_1 + K_1}{K_2 + K_2^*}$	2	0	- 1	· 3	р3 р3	2	2,1	1,1	$\frac{1}{3}, \frac{2}{3}$
	$K_2 + K_2^*$ $K_3 + K_3^*$	2	0	1	. 3	p 3	2	2,1	1,1 1,1	
p 3m 1	Γ_1		0							$\frac{2}{3}, \frac{1}{3}$
p sm 1	Γ_1 Γ_2	1 0	0	1	1	p 3m 1	1	1,0	0,1	0,0
	1 2	U	U	I	1	<i>p</i> 3	1	1,0	0,1	0,0

TABLE VI. (Continued).

DORIAN M. HATCH AND HAROLD T. STOKES

G_0	irrep	<i>n</i> ₁	n	1 2	Arms	Size	G	i(G)	Basis v	ectors	Origin
	Γ_3		1 ·	0	1	1	ст	1	1,1	0,1	0,0
							<i>p</i> 1	2	1,0	0,1	0,0
	M_1		1	0	1	2	pm	1	$\overline{1},\overline{2}$	1,0	0,0
					3	4	p 3m 1	· 1	2,0	0,2	0,0
							cm	2	2,2	0,2	0,0
				· •			<i>p</i> 1	3	2,0	0,2	0,0
	M_2		0	0	1	2	pg	1	1,2	1,0	$\frac{1}{4},0$
					3	4	p 3	1	2,0	0,2	0,0
							ст	1	2,2	0,2	0,0
							<i>p</i> 1	3	2,0	0,2	0,0
	K_1		1	0	2	3	p 31m	. 1	2,1	1,1	0,0
					-		р 3	2	2,1	1,1	0,0
	K ₂		1	0	2	3	p 31m	1	2,1	<u>1, 1</u>	$\frac{1}{3}, \frac{2}{3}$
							<i>p</i> 3	2	2,1	1 , 1	$\frac{1}{3}, \frac{2}{3}$
	K ₃		1	· 0 ·	2	3	p 31m	1	2,1	ī, 1	$\frac{2}{3}, \frac{1}{3}$
	A 3		1	Ū	. 2	5					
				_			<i>p</i> 3	2	2,1	<u>T</u> , 1	$\frac{2}{3}, \frac{1}{3}$
p 31m	Γ_1		1	0	. 1	1	p 31m	1	1,0	0,1	0,0
	Γ_2		0	0	1	1	р3	1	1,0	0,1	0,0
	Γ_3		1	0	1	1	ст	1	0,1	<u>1,1</u>	0,0
							<i>p</i> 1	2	1,0	0,1	0,0
	M_1		1	0	1	2	pm	1	1,0	1,2	0,0
					3	4	p 31m	1	2,0	0,2	0,0
							cm	2	0,2	$\overline{2},\overline{2}$	0,0
			- -				<i>p</i> 1	3	2,0	0,2	0,0
	M_2		0	0	1	2	pg	1	1,0	1,2	$\frac{1}{4}, \frac{1}{2}$
					3	4	<i>p</i> 3	1	2,0	0,2	0,0
							ст	1	0,2	$\overline{2},\overline{2}$	0,0
							<i>p</i> 1	3	2,0	0,2	0,0
	$K_1 + K_1^*$		2	0	1	3	<i>p</i> 3 <i>m</i> 1	2	2,1	1,1	0,0
	$K_2 + K_2^*$		0	0	1	3	<i>p</i> 3	2	2,1	1,1	0,0
	$K_3 + K_3^*$		2	1	1	3	<i>p</i> 3	2	2,1	1,1	$\frac{2}{3}, \frac{1}{3}$
							<i>p</i> 3	2	2,1	1 ,1	$\frac{1}{3}, \frac{2}{3}$
							ст	2	1,1	2,1	0,0
							<i>p</i> 1	4	1,1	2,1	0,0
<i>p</i> 6	Γ_1		1	0	1	1	<i>p</i> 6	1	1,0	0,1	0,0
-	$\Gamma_2 + \Gamma_3$		2	0	1	1	p 2	2	1,0	0,1	0,0
	Γ_4		0	0	1	1	p 3	1 -	1,0	0,1	0,0
	$\Gamma_5 + \Gamma_6$	(0	0	1	1	<i>p</i> 1	2	1,0	0,1	0,0
	M_1		1	0	1	2	p 2	1	1,0	0,2	0,0
					3	4	<i>p</i> 6	1	2,0	0,2	0,0
							p 2	3	2,0	0,2	0,0
	M_2)	0	1	2	<i>p</i> 2	1	1,0	0,2	$0, \frac{1}{2}$
					3	4	<i>p</i> 3	1	2,0	0,2	0,0
			`				p 2	2	2,0	0,2	$0, \frac{1}{2}$
							р1	3	2,0	0,2	0,0
	K_1		1	0	2	3	р 1 р 6	1	2,1	ī,1	0,0
				-			p 3	2	2,1	Ī,1	0,0
	$K_2 + K_3$		2	2	2	3	p 3	2	2,1	Ī,1	$\frac{1}{3}, \frac{2}{3}$

TABLE VI. (Continued).

G_0	irrep	<i>n</i> ₁	<i>n</i> ₂	Arms	Size	G	<i>i</i> (<i>G</i>)	Basis vectors		Origin
						p 2	2	1,⊺	2,1	0,0
						<i>p</i> 1	4	1,1	2,1	0,0
p 6m	Γ_1	1	0	1	1	p 6m	1	1,0	0,1	0,0
	Γ_2	0	0	1	1	<i>p</i> 6	1	1,0	0,1	0,0
	Γ_3	0	0	1	1	p 31m	1	1,0	0,1	0,0
	Γ_4	0	0	1	1	p 3m 1	1	1,0	0,1	0,
	Γ5	0	0	1	1	cm	1	1,1	0,1	0,
						cm	1	0,1	<u>1,1</u>	0,
						<i>p</i> 1	2	1,0	0,1	0,
	Γ_6	1	0	1	1	cmm	1	1,1	0,1	0,
						<i>p</i> 2	2	1,0	0,1	0,
	M_1	1	0	1	2	pmm	1	1,0	1,2	0,
				3	4	p 6m	1	2,0	0,2	0,
						cmm	2	2,2	0,2	0,
				•		p 2.	3	2,0	0,2	0,
	M_2	0	0	1	2	pmg	1	1,0	1,2	$\frac{1}{2}$,
				3	4	p 3m 1	1	2,0	0,2	0,
						cmm	1	2,2	0,2	$\frac{1}{2}$,
						cm	2	2,2	0,2	0,
						p 2	2	2,0	0,2	0,
						р 1	3	2,0	0,2	0,
	M ₃	0	0	1	2	P88	1	2,0 1,0	1,2	0,
	112 3	Ũ	, U	3	4	рвв рб	1	2,0	0,2	0,0
				5		cmm	1	2,0	0,2	0,
						p 2	3	2,0	0,2	0, 0,
	M_4	0	0	1	2	pmg	1	1,2	0,2 1,0	0,
	4	Ŭ	Ū	3	4	p 31m	ı 1	2,0	0,2	0,0
				5	+					
						cmm	1	2,2	0,2	$\frac{1}{2}$,
						cm	2	0,2	$\overline{2},\overline{2}$	0,0
						p 2	2	2,0	0,2	0, -
						p 1	3	2,0	0,2	0,0
	K_1	1	0	2	3	p 6m	1	2,1	<u>1</u> ,1	0,0
						p 3m 1	2	2,1	<u>1</u> ,1	0,0
	K_2	0	0	2	3	<i>p</i> 6	1	2,1	1,1	0,0
						p 31m	1	2,1	<u>1</u> ,1	0,
						p 3	2	2,1	1,1	0,
	K ₃	1	1	2	3	p 31m	1	2,1	ī ,1	$\frac{2}{3}$,
						cmm	1	2,1	1,1	0,
						p 3	2	2,1	1,1	$\frac{1}{3}$,
						cm	2	2,1	ī,1	0,
						cm	2	1,1	2,1	0,
						p 2	2	1,1	2,1	0,
						p 1	4	1,1	2,1	0,

Rottman⁶ lists the irreps which satisfy the Lifshitz criterion $(n_2=0)$ and gives their associated LGW Hamiltonians. (He does not list the low-symmetry space groups.) We compared his list with our results and found

three differences. He lists two irreps for each of the following \vec{k} points: p4gm(j), p3(l), and p3ml(m), which correspond to our \vec{k} points p4g(M), p3(K), and p3m(K). In our Table VI, we list *three* different physical irreps for each of these \vec{k} points.

Maksimov et al.⁸ list the lower-symmetry space groups which arise from irreps which satisfy both the Landau and Lifshitz criteria $(n_1=0 \text{ and } n_2=0)$. Their results correspond to listing only maximal subgroups for a given irrep. In our list these are the isotropy subgroups for which the subduction frequency i(G)=1 if the irrep is real and i(G)=2 if the irrep is complex. We compared their result with ours and found several differences. For example, $p(\sqrt{2} \times \sqrt{2})45^{\circ}$ of space group p4 should give rise to space groups p2,p4, not p1,p4 as they list. As a second example, $p(1\times 1)$ of space group p6 does not give rise to p2 as they list. (Actually, one irrep, $\Gamma_2 + \Gamma_3$ of p6, does give rise to p2, but this irrep fails the Landau criterion.)

Deonarine and Birman⁷ list all the isotropy subgroups

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allowed by the subduction and chain criterion. Again, we find many differences with our results. These differences include omissions of points of symmetry (e.g., Γ , X, and S points of pg), incorrect calculations of the Landau and Lifshitz criteria (e.g., irreps E_1 and E_2 of the Γ point of $p \, 6m$), and incorrect results of the subduction and chain criteria (e.g., incorrect isotropy subgroups arising from the irreps B_1 and B_2 of the $\vec{k}^* = [\frac{1}{2}, 0]$ point of $p \, 2mm$).

The calculations for finding isotropy subgroups are very prone to error as we have seen in the listings of Deonarine and Birman⁷ and also in those of Maksimov *et al.*⁸ Computers are particularly well suited for these kinds of calculations, and up to the present time, we have found our computer-generated tables to be free of any errors.

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