Computer Generation of Subduction Frequencies for 2nd Order Phase Transitions in 2-D †

S. Deonarine(a), D.B Litvin(b) & Joseph L. Birman(a)
(a) Physics Dept., City College (CUNY), NY 10031
(b) Physics Dept., Penn. State University Berks Campus, Reading, PA 19608

ABSTRACT

We have written a RATFOR/FORTRAN program for the VAX11-780 which will generate the subduction frequencies for allowed 2nd order phase transitions in 2-D systems describable by the 17 plane space groups. The Landau theory of 2nd order phase transitions and group theory criteria are used to determine which subgroups can occur in such transitions. Previous work by Deonarine & Birman on these subgroups of the 2-D space groups was based on the ITXRC§ and the tables of Coxeter & Moser. These tables do not list all the possible subgroups of a space group.Using the tables of Sayari,Billiet & Zarrouk & the ITC§§ our program gives a complete tabulation of the allowed 2nd order phase transitions in 2-dimensions.

INTRODUCTION

Two dimensional systems are being widely studied at the present time. Improvements in technology have made it possible to create and analyze quasi-2D systems/models (see review by Barber[1]).One aspect of phase changes in 2-D deals with the symmetry change from an initial 2-D crystal space group Go to another 2-D space group G of lower symmetry, Go $\supseteq$ G.In a previous paper[2] we calculated by hand the various changes for each irrep (irreducible representation) of the 17 groups for points of high symmetry in their respective Brillouin Zones. Instead of the usual algebraic extremization of a free energy polynomial(Liubarskii [3]) we use group theory criteria (Birman [4]). We summarize them below:

(i) $G \subseteq Go$

(ii) The order parameters form the basis of an irrep of Go : $D^{j,k}_{Go}$

(iii) The irrep must be Landau-active : $\Gamma^{1+}_{Go} \notin [D^{j,k}_{Go}]^3$

(iv) The irrep must be Lifshitz-active : $\Gamma^{v}_{Go} \notin \{D^{j,k}_{Go}\}^2$

(v) For a three-chain of maximal subgroups $Go \supseteq G' \supseteq G''$

if $p\,\Gamma^{1+}_{G'} \in (D^{j,k}_{Go} \downarrow G')$
and
if $q\,\Gamma^{1+}_{G''} \in (D^{j,k}_{Go} \downarrow G'')$

then for $p > 0$ Go —> G′ is permitted.
for $q = p$ Go —> G′ is allowed ; Go —> G″ is not allowed.
for $q > p$ both Go —> G′ and Go —> G″ are allowed.

Since fluctuations play an important role in 2D we have applied the criteria to all the irreps , irespective of their activity.

† This work was supported in part by PSC-BHE ,FRAP and NSF

§ ITXRC-International tables of X-Ray Crystallography(1965)
Vol I: Symmetry Groups

§§ ITC-International Tables for Crystallography(1983)
Vol A: SPACE-GROUP SYMMETRY

GROUPS and SUBGROUPS

One needs to take special care in determining all subgroups of a given space group . For example consider the 2D space group P4 :

$$P4 = \{(E \mid 1, 0), (E \mid 0, 1), (C4z+ \mid 0, 0)\} \qquad (1)$$

Go = P4 is generated by the two translations {E | 1,0},{E | 0,1 } and the 4-fold rotation {C4z+ | 0,0 }. In a table of Coxeter and Moser [5] on group-subgroup relations this group is listed as containing a subgroup (or subgroups - the table is not clear) of index 2 which is also denoted as P4 . The group generated by

$$P4 = \{(E \mid 1, 1), (E \mid 1, -1), (C4z+ \mid 0, 0)\} \qquad (2)$$

is such a subgroup of index 2 .

However, it is erroneous take this as the only subgroup of index 2 belonging to the family of 2-D space groups denoted by the symbol **P4** . A second such subgroup exists . The subgroup generated by

$$P4 = \{(E \mid 1, 1), (E \mid 1, -1), (C4z+ \mid 0, 1)\} \qquad (3)$$

is a subgroup of index 2 which is also denoted by the symbol P4. Because of the non-primitive translation in the generator

$$(C4z+ \mid 0, 1)$$

the group given by equation 3 is not in the ' standard form ' of a space group denoted by **P4**.

This group can be cast in the ' standard form ' by translating to a new origin at (1/2,1/2) . It is necessary to consider both subgroups, equations 2 ,3 in determining all possible transitions from a parent space group Go . Considering only the subgroup given in equation 2 leads to an incomplete list of subgroups , a type of error warned against by Billiet [6] and an incomplete list of phase transitions.

We have written a program for the VAX11-780 to calculate the subduction frequencies ' n ' in

$$n\ \Gamma_{G}^{1+} \in (D_{Go}^{j,k} \downarrow G)$$

where Go is one of the 17 2D space groups and G is a subgroup of Go. We have obtained results for the irreps at high symmtery points $k \neq 0$. The input consists of G as subroutines and character tables of the multiplier reps of Gk, the group of the k-vector of Go (Vol. 1 : Cracknell , Davies , Miller & Love [7]).The various shifts in origin and new translation lattices were programmed according to the tables of Sayari, Billiet & Zarrouk [8].

As an example of the use of these tables we have applied the chain subduction criteria to Go = P4 for *k = { 1/2,1/2 } and *k = { 1/2,0 ; 0,1/2 }. In Table I , all allowed 2-D phase transitions between the group and its subgroups are given. In column 1 we list the irreps via the irreps of the point group Pk of Gk-the wave-vector group.The bracket ' } ' denotes a physically irreducible representation . The subduction frequency ,class symbol of the subgroup G and the subgroup index are given in columns 2,3,4. Complete tables will be published elsewhere [9].

TABLE I

Subgroups of the 2-D space group P4 generated by {(E | 0 ,1) , (E | 1, 0) ,(C4z+ | 0 ,0)} that are allowed in a continuous phase transition

*k = {1/2 , 1/2}

irrep	n	G	index	generators		
A	1	P4	2	(E | 1 , 1)	(E | 1 , -1)	(C4z+ | 0 , 0)
B	1	P4	2	(E | 1 , 1)	(E | 1 , -1)	(C4z+ | 0 , 1)
E1	1	P2	4	(E | 1 , 1)	(E | 1 , -1)	(C2z+ | 0 , 1)
E2	1	P2	4	(E | 1 , 1)	(E | 1 , -1)	(C2z+ | 0 , 1)

*k = {(1/2 , 0) ; (0 , 1/2)}

irrep	n	G	index	generators		
A	1	P4	4	(E | 2 , 0)	(E | 0 , 2)	(C4z+ | 0 , 0)
A	1	P4	4	(E | 2 , 0)	(E | 0 , 2)	(C4z+ | 1 , 1)
B	1	P4	4	(E | 2 , 0)	(E | 0 , 2)	(C4z+ | 1 , 0)
B	1	P4	4	(E | 2 , 0)	(E | 0 , 2)	(C4z+ | 0 , 1)
A	1	P2	4	(E | 1 , 0)	(E | 0 , 2)	(C2z+ | 0 , 0)
B	1	P2	4	(E | 1 , 0)	(E | 0 , 2)	(C2z+ | 0 , 1)
A	1	P2	4	(E | 2 , 0)	(E | 0 , 1)	(C2z+ | 0 , 0)
B	1	P2	4	(E | 2 , 0)	(E | 0 , 1)	(C2z+ | 1 , 0)
A	2	P2	8	(E | 2 , 0)	(E | 0 , 2)	(C2z+ | 0 , 0)
B	2	P2	8	(E | 2 , 0)	(E | 0 , 2)	(C2z+ | 1 , 1)

REFERENCES

{additional references may be found in the works cited}

[1] M. N. Barber : Phys . Rep . 59, 375 (1980)

[2] S. Deonarine & J. L. Birman : Phys. Rev. B27, 2855 (1983)

[3] G. Ya. Liubarskii : The Application of Group Theory in Physics (Pergamon, New York,1960)

[4] J. L. Birman : Group theoretical Methods in Physics Vol 79,LECTURE NOTES IN PHYSICS ,edited by P. Kramer & A. Riekers (Springer, New York 1978)

[5] H. S. M. Coxeter & W. O. Moser : Generators and relations for Discrete Groups (Springer ,New York,1965)

[6] Y. Billiet : Acta. Cryst. A37 p649 (1981)

[7] Kronecker Product tables - Volume I: A. P. Cracknell, B. L. Davies , S. C. Miller & W. F. Love (Plenum Press, 1979)

[8] A. Sayari ,Y. Billiet & H. Zarrouk : Acta Cryst.,A34, 553-555 (1978); Y. Billiet : MATCH 9 , p177 (1980)

[9] S. Deonarine , D. B. Litvin & J. L. Birman (to be published)

XIIIth International Colloquium on

GROUP THEORETICAL METHODS IN PHYSICS

College Park, Maryland, USA
21-25 May 1984

Edited by W W Zachary

World Scientific