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

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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 & 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 we 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 \( G_0 \) to another 2-D space group \( G \) of lower symmetry, \( G \supset G_0 \). In a previous paper 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 (Liu & Birman[2]) we use group theory criteria (Birman[3]). We summarize them below:

(i) \( G \subset G_0 \)

(ii) The order parameters form the basis of an irrep of \( G_0 \): \( D^{1k}_{G_0} \)

(iii) The irrep must be Landau-active: \( \Gamma^{1+}_{G_0} \not\in \{ D^{1k}_{G_0} \} \)

(iv) The irrep must be Lifshitz-active: \( \Gamma^{v}_{G_0} \not\in \{ D^{1k}_{G_0} \} \)

(v) For a three-chain of maximal subgroups \( G_0 \supset G' \supset G'' \)

if \( p \Gamma^{1+}_{G'} \in \{ D^{1k}_{G_0} \} \)
and \( q \Gamma^{1+}_{G''} \in \{ D^{1k}_{G_0} \} \)

then for \( p > 0 \) \( G_0 \rightarrow G' \) is permitted.

for \( q = p \) \( G_0 \rightarrow G' \) is allowed; \( G_0 \rightarrow G'' \) is not allowed.

for \( q > p \) both \( G_0 \rightarrow G' \) and \( G_0 \rightarrow G'' \) are allowed.

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

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§ 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:

\[ P_4 = \{(E, 0, 0), (E, 0, 1), (C_4z + 10, 0)\} \]  \hspace{1cm} (1)

Go = P4 is generated by the two translations \([E, 1, 0], [E, 1, 1]\) and the 4-fold rotation \([C_4z + 10, 0]\). In a table of Coexter 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

\[ P_4 = \{(E, 1, 1), (E, 1, -1), (C_4z + 10, 0)\} \]  \hspace{1cm} (2)

is such a subgroup of index 2.

However, it is erroneous to 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

\[ P_4 = \{(E, 1, 1), (E, 1, -1), (C_4z + 10, 1)\} \]  \hspace{1cm} (3)

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

\[ (C_4z + 10, 1) \]

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

\[ n \Gamma_{G}^{1+} \in (\mathcal{D}_{Go}^{kk} \cdot G) \]

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 symmetry points \(k = 0\). 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 \(*k = \{1/2, 0, 1/2\}\). In Table 1, 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 wavevector 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 \((E \cdot 0, 1)\) \((E \cdot 1, 0)\) \((C4z+0, 0)\) that are allowed in a continuous phase transition

<table>
<thead>
<tr>
<th>irrep</th>
<th>n</th>
<th>G</th>
<th>(k = {1/2, 1/2}) index</th>
<th>generators</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1</td>
<td>P4</td>
<td>2 ((E \cdot 1, 1)) ((E \cdot 1, -1)) ((C4z+10, 0))</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>1</td>
<td>P4</td>
<td>2 ((E \cdot 1, 1)) ((E \cdot 1, -1)) ((C4z+10, 0))</td>
<td></td>
</tr>
<tr>
<td>E1</td>
<td>1</td>
<td>P2</td>
<td>4 ((E \cdot 1, 1)) ((E \cdot 1, -1)) ((C2z+10, 0))</td>
<td></td>
</tr>
<tr>
<td>E2</td>
<td>1</td>
<td>P2</td>
<td>4 ((E \cdot 1, 1)) ((E \cdot 1, -1)) ((C2z+10, 0))</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>irrep</th>
<th>n</th>
<th>G</th>
<th>(k = {(1/2, 0); (0, 1/2)}) index</th>
<th>generators</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1</td>
<td>P4</td>
<td>4 ((E \cdot 1, 2)) ((E \cdot 10, 0)) ((C4z+11, 0))</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>1</td>
<td>P4</td>
<td>4 ((E \cdot 1, 2)) ((E \cdot 10, 0)) ((C4z+11, 0))</td>
<td></td>
</tr>
<tr>
<td>B</td>
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<td>P2</td>
<td>4 ((E \cdot 1, 0)) ((E \cdot 10, 2)) ((C2z+10, 0))</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>1</td>
<td>P2</td>
<td>4 ((E \cdot 1, 0)) ((E \cdot 10, 0)) ((C2z+10, 0))</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>2</td>
<td>P2</td>
<td>8 ((E \cdot 1, 0)) ((E \cdot 10, 0)) ((C2z+11, 0))</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>2</td>
<td>P2</td>
<td>8 ((E \cdot 1, 0)) ((E \cdot 10, 0)) ((C2z+11, 0))</td>
<td></td>
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REFERENCES

*additional references may be found in the works cited*

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