LINE GROUP TECHNIQUES IN DESCRIPTION OF THE STRUCTURAL PHASE TRANSITIONS IN SOME SUPERCONDUCTORS

Cs. Mészáros[1], Á. Bálint[2] and J. Bánkuti[1]

(1) Department for Low Temperature Physics, Roland Eötvös University, Budapest, Hungary

(2) Department of Chemistry and Biochemistry, University of Agricultural Sciences, Gödöllő, Hungary

ABSTRACT

The main features of the theory of line groups, and their irreducible representations are briefly discussed, as well as the most important applications of them. A new approach in the general symmetry analysis of the modulated systems is presented. It is shown, that the line group formalism could be a very effective tool in the examination of the structural phase transitions in High Temperature Superconductors. As an example, the material $YBa_2Cu_3O_{7-x}$ is discussed briefly.

INTRODUCTION

The geometrical symmetries of a system possessing periodicity in one dimension form a line group by definition. The line groups were first derived by Hermann [1], and 75 line groups were found with "crystallographic character". Omitting the detailed discussion of the intermediate steps in the development of the line group theory is mentioned the X-ray structure analysis of polymers [2] based on this theory. The line group theory is the base for the Fourier-Bessel synthesis of structural investigations of polymers, as well as the Schönfliess' theory in the structural investigations of *3D* crystals. This paper presents and adopts completely the formalism and notation of the line groups, described and later repeatedly exploited by Vujičić et al [3-6]. It has been proved, that all of the innumerable line groups can be gathered into thirteen families containing "non-crystallographical" symmetry transformations among the group elements, too. There is a crucial difference between the derivation of the line groups and the space groups of the ordinary, *3D* crystals. In the case of the line groups, the possible symmetries of the motif (monomer - in the case of polymers), is examined leaving invariant the main axis of the system, too. While in the construction of the space groups of *3D* crystals the symmetry relations between the possible translations in the crystal and the point group-symmetries of the unit cell (and not of the molecule!) are studied. Thus the usefulness and the advantage of the line group formalism is obvious: starting from the *quantum-mechanical description of the motif*, there is a valuable tool to examine the electron (or spin-) density functions in the condensed matter. Such a Q1D subsystems have been examined in detail in some well-known superconductors [7]. Besides, there are some interesting results, which also show that the modulation of the crystal structure could be very interesting in the examination of the High Temperature Superconductivity Phenomena [8]. In this paper we show, that the line group formalism is very appropriate for the description of the modulation. The new thermodynamical methods [9] would also give valuable contributions in these investigations.

1. SUBGROUP STRUCTURE AND IRREDUCIBLE REPRESENTATIONS OF LINE GROUPS

1.1. Subgroup structure

Recognizing the line groups being the subgroups of the Euclidean group, the use of the usual Koster symbol for the general line group element [3] is convenient:

$$\underline{L} \ni (R \mid v+t); \quad v \in [0,1), \quad t \in Z \tag{1}$$

The line group elements in their orthogonal part possess the elements R_i, which constitute the *isogonal point group* $\underline{P}$, $|\underline{P}| = N_p$. $\underline{P}$ is always an axial point group when one deals with line groups. There are two types of point and line groups. Namely, if the point group $\underline{P}$ contains an element R^-, which reverses the direction of the main axis, then it will be denoted as $\underline{P}^-$, which has the following subgroup structure:

$$\underline{P}^- = \underline{P}^+ + R^-\underline{P}^+ \tag{2}$$

i.e. $\underline{P}^+$ is an index-two invariant subgroup in $\underline{P}^-$. Similarly, all the line groups are $\underline{L}^+$ or $\underline{L}^-$ type, depending on the type of isogonal point group. The list of all line groups is completed by use of the concept of the generalized semi-direct product of the line groups [3].

1.2. Irreducible representations

In the short description of the irreducible representations we use the technique and notation presented in [4-5]. The general formula for the irreducible representation of the $\underline{L}^+$ type line group element can be written as:

$$_kD_m(R \mid v+t) = D_m(R)\exp[ik(v+t)a] \tag{3}$$

i.e. it is built up from the irreducible representations of $\underline{P}$ and $\underline{T}$. The irreducible representations of $\underline{P}$ and $\underline{T}$ are labelled by indices m and k, respectively ($k \in (-\pi/a, \pi/a]$). With the matrices $_kD_m(\underline{L}^+)$, the irreducible representations of $\underline{L}^-$ can be obtained by *induction* technique [4],[12].

2. SOME APPLICATIONS OF LINE GROUP FORMALISM IN CONDENSED MATTER PHYSICS

There are some remarkable results, which show the power and the usefulness of the line group formalism. It is well-known in the mathematical crystallography, that the non-symmorphic space groups of 3D crystals are not factorized yet in the

sense of the product of its subgroups [10]. The algorithms developed in the elaboration of the abstract line group theory would be also useful in the solving of this important crystallographic problem [11].

With the addition of the time-reversal symmetry to geometrical symmetry transformations of the line group, the *magnetic line groups* tabulated in [6] can be obtained. This result is completely analogous to the derivation of Heesch-Shubnikov point-, and space-groups (see for example in [12]). The irreducible representations of the magnetic line groups have also been derived and tabulated already and completely can be found in [13-14].

A general discussion of the normal modes of QID systems as well as the complete classification of the orbits of the line groups is given in [15]. There is another important result in the same paper: the classical Jahn-Teller theorem is generalized to the case of systems, whose symmetry groups are line groups.

The line group formalism was introduced in the structural investigation of modulated crystals in our earlier paper [16]. It was shown, in the Landau power expansion of thermodynamic potential (for description of the phase transitions, in which modulated structures could appear), that the terms concerning translational invariance are exactly line group invariants.

This thermodynamical analysis gave us the following geometrical result: let the function $\rho(\vec{r})$ be the electron (or spin-) density function with the ordinary space-group symmetry, and let $f(\vec{r})$ be the modulation function in one particular direction only. The function $f(\vec{r})$ must be invariant under the symmetry transformations of the supersymmetry - which is a particular line group. Thus, to describe the scattering experiments and to obtain the adequate structure factors of the modulated structures we have the formula:

$$F_{mod}(S) = \mathscr{F}\{f(\vec{r}) * \rho(\vec{r})\} = \mathscr{F}\{f(\vec{r})\} \cdot F(S) , \qquad (4)$$

where the sign * denotes the convolution operation, instead of the usual expression $F(S) = \mathscr{F}\{\rho(\vec{r})\}$ applied for ordinary structures. It is convenient and customary [2] to use cylindrical coordinates in this calculation of the modulated structure factor. In the fully developed form, formula (4) can be written as:

$$F_l(R,\Psi,lc^*) = \sum_j \sum_n f_j J_n(2\pi r_j R) \exp [i(n(\Psi + \frac{\pi}{2}) - n\psi_j + 2\pi l \frac{z_j}{c})] \qquad (5)$$

This description de facto implies the following factorization of the symmetry group $\underline{G}_S$ of the modulated crystals:

$$\underline{G}_S = \underline{G} \circ \underline{G}_M (\text{ or } \underline{G}_S = \underline{G}_M \circ \underline{G}) \qquad (6)$$

In this formula $\underline{G}$ means the space group according to Schönfliess, while $\underline{G}_M$ denotes symmetry group, which describes the modulation of the structure. $\underline{G}_M$ could be a line group, but the nature of the product $\circ$ is not clear yet (i.e. when it is a weak-direct, a semi-direct or a direct product [6] of the subgroups, which constitute the full group)

and it requires further group-theoretical investigations concerning the general problem of the orthogonal invariance in the modulated systems. This investigation in progress gives the result will be applied in the examination of structural phase transitions in liquid crystals, as well as in the complete classification of them. Moreover, this approach would be very useful in the investigation of the crucial properties of the heavy-fermion superconductor UPt_3, because some interesting results [17] show clearly the possibility of influence of incommensurate modulation of the crystal structure on the superconductivity in such a systems.

The suitability of the presented formalism can be accepted for the structural investigation of High Temperature Superconductors (HTSC), too. There are many experimental results, which show, that some of the HTSC materials also have modulated structures [18-20]. The technique proposed in [16] would provide crucial results in the symmetry analysis of the structures of these superconductors. Moreover, the advantage of the line group technique is obvious in the investigation of the structural phase transitions in HTSC-s. For such investigations we also have fully elaborated techniques based on the line group theory. The polar-vector and axial-vector representations of line groups are also well-known and presented in [21]. Connecting the line group formalism with Ascher's epikernel technique [22], Damnjanović showed, [23-24], that the reduction of symmetry during the continuous phase transition of some 3D crystals can be studied equally well using line groups. Recently, this method has been developed for the phase transitions without translation lost, i.e. for the equitranslational phase transitions only. The extension to the general case is also possible [11]. As it is well-known [22], the phase transitions with $k=0$ can be described as equitranslational phase transitions i.e. one should deal with the irreducible representations of point groups only:

$$D_m(R) \equiv {}_k D_m(R \mid v+t) \qquad (7)$$

The procedure is the following: let $\underline{L}_0$ be one line group and let $\underline{L}_l$ be one of its equitranslational epikernels concerning irreducible representation ${}_k D_m(\underline{L}_0)$. Then, if $\underline{P}_l$ is the isogonal point group of $\underline{L}_l$, then it is also an epikernel of $\underline{P}_0$, corresponding to the representation $D_m(\underline{P}_0)$. In this case an epikernel $\underline{P}_l$ of $\underline{P}_0$ belongs to each equitranslational epikernel $\underline{L}_l$ of $\underline{L}_0$, and $\underline{P}_l$ is the isogonal point group of $\underline{L}_l$. Obviously, the described line group-epikernel formalism (LEF) is a very suited technique for description of the tetragonal-orthorhombic structural phase transition in $YBa_2Cu_3O_{7-x}$. Using some results of the phenomenological description of this phase transition based on Landau's theory [25] and on group-subgroup technique [26], we have enough information for application of the LEF. Namely, it is shown in [25], that the primary order parameter for this transition is the quantity $\eta = n_b - n_a$, i.e. the difference between oxygen atom rate along b and a axes, respectively. It is pointed out in both [25] and [26], that the above mentioned phase transition is exactly equitranslational. Thus, the order parameter η also could be treated by LEF and this method would provide a valuable new method to describe the oxygen atom ordering, which is believed to be crucial in the examination of the High Temperature Superconductivity mechanism. Namely, the irreducible representation relevant for

this phase transition denoted by B_{1g} in [25] can be identified as B_1^+ in the tables given in [24]. At first, we give in Table 1. the adequate space- ($\underline{G}_i$) and point groups ($\underline{P}_i$) (i=0 and 1 for the high- and low-symmetry phase, respectively).

Table 1.*   Space and point groups of high (tetragonal) and low temperature (orthorombic) phase

	Space Group	Point Group
High Temperature Phase ($\underline{G}_o,\underline{P}_o$)	P4/mmm (D_{4h}^1)	4/mmm (D_{4h})
Low Temperature Phase ($\underline{G}_1,\underline{P}_1$)	Pmmm (D_{2h}^1)	mmm (D_{2h})

*The Schönfliess symbols are given in brackets.

The symmetry analysis based on the above mentioned epikernel-technique gives the results, presented in Table 2. Thus, we have two line groups as the possible equi-translational epikernels and also two strictly determined *supersymmetries* for description of the ordering *of oxygen atoms*. Then, formula (5) gives also possibility to calculate the intensity spectra in the diffuse X-ray scattering and for the direct comparison of such a results with the already existing profiles (see for example the adequate references in [20]). The new results concerning the general problem of the scattering processes from a *real* superlattices [27], as well as the suited available experimental data [28-30] provide possibilities for doing such a calculations.

Table 2. The maximal $Q1D$ subsystems in $YBa_2Cu_3O_{7-x}$ and the adequate equitranslational epikernels in the low temperature phase according to B_I^+:

	Line Groups		
High Temperature Phase Line groups as maximal subgroups	$\underline{L}(4)/mmm$	$\underline{L}(4)/mcc$	$\underline{L}(4)_2/mcc$
Low Temperature Phase The equitranslational epikernels	$\underline{L}(\bar{4})/2m$	$\underline{L}(\bar{4})/2c$	$\underline{L}(\bar{4})/2c$

CONCLUSIONS

The line group formalism provides a very effective tool in the symmetry analysis of different $Q1D$ (sub-)systems in the condensed matter. Due to their obvious suitness, the line group techniques could penetrate into many recently developing areas, which are exactly in the front of the condensed matter physics and it could provide some valuable new results. The superconductivity is expected to be an especially fruitful topic.

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