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General symmetry properties of incommensurately modulated crystals described by projective representations of line groups

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ABSTRACT

After a detailed investigation of some fundamental general orthogonal symmetry properties of incommensurate condensed systems, the line groups are applied for describing the structure of such modulated crystals. It is demonstrated, that use of projective representations of these groups may give a more refined description of such structures and significantly extends applicability of the diffuse scattering formalism.

Introduction

It is well-known, that applications of the exact symmetry theory of discrete crystalline-type quasi-one-dimensional (*Q1D*) systems [1] has been playing, and plays even nowadays a role of crucial importance in both experimental and theoretical investigations of different types of condensed matter systems. Throughout this paper we will call the relevant symmetry groups line groups, as it has been widely accepted in literature e.g. [2], [3]. From the most important applications of them, structural investigation of chain molecules by X-ray diffraction has been known for decades e.g. [4], and played a crucial role in experimental studies at revealing of fundamental structural properties of the DNA-molecule [5-6]. An exact and detailed reformulation of the precise abstract algebraic theory of line groups [2], [7] and their irreducible representations [8-9] came later. A detailed and up-to-date description of this symmetry technique can be found in a recent monograph by Damnjanović and Milošević [3].

A relatively recent important research area, where the application of the line group theory has been demonstrated to be very useful is the investigation of carbon-nanotubes, where after a study of fundamental importance by Damnjanović and co-workers [10] numerous useful applications of the exact representation theory of the symmetry groups of *Q1D* systems has been succesfully demonstrated [11]. Among them, calculation of diffraction intensities on the base of the symmetries of carbon nanotubes e.g. [12] also represents a particularly important and promising technique from the point of view of future applications.

Besides, some very general types of structural phase transitions (including those resulting in incommensurately modulated crystal structures) have also been investigated in detail – but within frame of the mean field

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approximation (MFA) only - by the theory of line groups and their irreducible representations [13-18].

Finally, we would like also to mention here the crucial domain of biopolymers, where beyond the newest modelling results of the elementary excitations (which are in general case of strongly nonlinear character) of the DNA molecules in both quantum-mechanical [19] and classical mechanical sense, (i.e. using tools of the classical elasticity theory [20]), the alpha-helix protein molecule is also one of the best-known examples, whose soliton-type elementary excitations represent active research topic for decades e.g. [21-22], but which have been treated without any detailed application of the theory of line groups and their irreducible representations.

Therefore, it may be stated, that since their discovery, the mathematical formalism of line groups plays a role of continuously increasing importance in various branches of the condensed matter theory, despite of the fact, that there are many intensively studied, but still open research domains where they have not been applied in detail, e.g. in the theory of Peierls' transitions, basic symmetries of liquid crystals and contemporary theories of biopolymers, just to mention a few. In the present work, the author intend to demonstrate, that projective representations of line groups represent a very suitable tool for further refinements of the existing mathematical formalism of scattering processes at *Q1D* systems and propose on this base a novel, more refined description of the diffuse X-ray scattering formalism.

A BRIEF DISCUSSION OF ESSENTIAL FEATURES OF THE EXACT ABSTRACT SYMMETRY AND REPRESENTATION THEORY OF Q1D SYSTEMSAND THEIR APPLICATIONS IN THE EVALUATION OF SCATTERING PROCESSES

Basic elements of the theory of line groups and their irreducible representations

1. The basic algebraic structure

According to the definition, the complete set of symmetry transformations leaving invariant a *Q1D* system belongs to one of the (discrete) infinitely many line groups gathered into 13 families [2]. (We mention here in advance, that the irreducible representation $D^{(\mu)}(L)$ of a full line group L can be obtained from the irreducible representation of symmetry groups (i.e. point groups) of the motifs $D^{(\nu)}(P)$ by use of the induction technique elaborated in the theory of group representations and widely applied in solid state physics e.g. [23-24] and usually denoted by $D^{(\mu)}(L) = D^{(\nu)}(P) \uparrow L$).

2. Application of projective representations

Although some applications of the projective representations of crystallographic point groups in solid state physics are known for decades [25-26] (their relevance in the case of classical description within frame of the Schönfliess-Fedorov Shubnikov theory of crystallographic space groups was also pointed out by Landau and Lifshitz [27]), they are completely absent even from the most complete works about applications of line groups in various types of structural investigations of condensed matter systems [3-4].

In the next section we will demonstrate – following our own earlier basic result [17] (which may be considered as a simple first attempt to introduce the projective representations of line groups into exact

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symmetry theory of incommensurately modulated crystals) – formalism of the projective representations of groups in order to refine the already existing mathematical formalism of the theory of invariants relevant for phase transitions resulting in different types of modulated crystal structures. The same symmetry method will also be applied in formalism of the applied Fourier-analysis necessary for describing the diffuse scattering processes from modulated structures of general type. Finally, we also think, that it must also be pointed out here, that the mathematical terminology emanating from line group theory (which may be considered as the most general algebraic formalism of fractional translations), is not to be confused directly with terminology connected to the most general theory of transport processes, known nowadays under name of anomalous diffusion theory, too (e.g. [28]), despite of the fact, that the latter one has also been topic of very serious and detailed symmetry analyses, too [29].

A novel concept for applying the line group technique in the case of incommensurate systems

In this section we will represent the essential result of the present study on the base of the general symmetry methods explained in [2] and [26]. Accordingly, if a line group L is composed from line groups L_1 and L_2, which have the same translational subgroup T, then its relevant point group P is in relation $P = P_1 \wedge P_2$ with the point groups of its constituent line groups. Then, the following condition (explained by point group elements „R" and fractional translations „v") must be satisfied:

$$v_2 + R_2 v_1 - R' v_2 = v' + t, \quad t = 0, \pm 1, \pm 2, ..., \tag{1}$$

where $\left(R_1 | v_1\right)$ and $\left(R_2 | v_2\right)$ are any coset representatives in L_1 and L_2, respectively (then, the relation $R' = R_2 R_1 R_2^{-1}$ is also valid). Then, if we compare this condition with the one emanating from the general treatment of basic properties of the unimodular group in two dimensions (i.e. characterized by three (continuously varying!) parameters), defined by use of the elementary linear transformation formulae $g_a \equiv x' = a_1 x + a_2, g_b \equiv x'' = b_1 x' + b_2$, it is represented by

$$\xi \mapsto \frac{a_1 \xi + a_2}{b_1 \xi + b_2} \tag{2}$$

(see also the Appendix in this respect). Then, the relevant most general *conjugate* transformation $g_a g_b g_a^{-1}$ from the unimodular group is realized by

$$a_1 x + a_2 b_1 - a_1 b_2 = x' - b_2. \tag{3}$$

Although the simultaneous application of the formulae (1-3) may explain the essential symmetry features of two different translationally invariant (with translational invariance in the same direction, but with generating elements, which can not be interrelated with integer numbers!) *Q1D* systems, this possible connection has not been applied in detail in the case of incommensurately modulated condensed matter systems. Therefore, the essential main new result of the present study is to fill this

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gap in the literature and to lay down mathematical foundation for the relevant Fourier-analysis formalism to be applied in the elastic-, and inelastic scattering experiments playing crucial role in material structure investigation.

Generalization of the concept of structure factors within frame of the theory of projective representations

In the present section we give a refinement of the existing formalism of the diffuse X-Ray scattering formalism on the base of the line group formalism. As it is well-known from the classic literature of the topic e.g. [30] for a non-ideal condensed matter system being able to scatter X-rays coherently, the electron density function can be given in the form of

$$\rho(\vec{r}) = \langle \rho(\vec{r}) \rangle + \Delta\rho(\vec{r}) \tag{4}$$

where $\langle \rho(\vec{r}) \rangle$ denotes the electron density function for the „averaged part" of the lattice being investigated, while $\Delta\rho(\vec{r})$ is related to fluctuational inhomogeneities. Then, the intensity of the diffracted beams can be explained by use of the Patterson autocorrelation function $P(\vec{r})$ defined e.g. [30] by the convolution operation

$$P(\vec{r}) = \{\langle \rho(\vec{r}) \rangle * \langle \rho(-\vec{r}) \rangle\} + \{\Delta\rho(\vec{r}) * \Delta\rho(-\vec{r})\}, \tag{5}$$

and its Fourier-transformed form as

$$I(\vec{\kappa}) = \Im\{P(\vec{r})\} \equiv |\bar{F}|^2 + |\Delta F|^2, \tag{6}$$

where $\vec{\kappa} = \vec{k} - \vec{k}_0$ is the scattering vector (in an elastic scattering process), while $\bar{F}$ and ΔF denote the Fourier transformed forms of the functions $\langle \rho(\vec{r}) \rangle$ and $\Delta\rho(\vec{r})$, respectively. It must also be pointed out here, that from all of the possible variants of diffusively scattered X-rays, electrons or thermal neutrons from condensed matter systems, we base here our modeling work in agreement with the general formalism also described in a suitable manner by Cowley for extended defects, and particularly for the case of stacking faults. Accordingly, the electron-density function is given by the following convolution operation:

$$\rho(\vec{r}) = \rho_0(\vec{r}) * \mathrm{d}(\vec{r}), \tag{7}$$

where $\rho_0(\vec{r})$ denotes the electron density function of a layer consisting of scattering centres, while $\mathrm{d}(\vec{r})$ is a distribution function. The relevant generalized autocorrelation function is given by:

$$P(\vec{r}) = \rho_0(\vec{r}) * \rho_0(-\vec{r}) * D(\vec{r}), \tag{8}$$

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where $D(\vec{r})$ is the generalized autocorrelation function relevant for distribution of layers. It is generally accepted within frame of this formalism, that it can be characterized by Poisson's type probability distribution functions.

Then, in a more specified manner, for the diffuse scattering intensity contribution we may write after [31]:

$$\left|\Delta F\right|^2 \equiv I_{DS}(\vec{\kappa}) = \sum_{\vec{r}} H(\vec{r}) C(\vec{r}) \cdot \mathrm{e}^{-2\pi i \vec{\kappa}\vec{r}}, \tag{9}$$

where $H(\vec{r})$ denotes the supersymmetry function, for which we also postulate here, that it is invariant against symmetry transformations from a group having generalized translations, too (i.e. from a given line group) and which can be therefore represented in a Fourier series form as: $H(\vec{r}) = \sum_{\vec{h}} T_{\vec{h}} \cdot e^{2\pi i \vec{h}\vec{r}}$.

The function $C(\vec{r}) \sim e^{-\lambda r}$ is the so-called spatial correlator realizing randomization of the superstructure being investigated, and whose Fourier-transformed form is of Lorentzian shape (if we accept – following again Naish and Grebennikov – the correlator to be of exponentially decaying character, with characteristic correlation length $\xi \equiv \lambda^{-1}$):

$$\Im\{C(\vec{r})\} \equiv \tilde{C}(\vec{\kappa}) = \frac{\frac{1}{2} sh(\lambda)}{\sin^2(\lambda/2) + \sin^2(\pi\kappa)} \equiv \Lambda(\vec{\kappa}, \lambda). \tag{10}$$

Then, the diffuse scattering intensity contribution is given by:

$$I_{DS}(\vec{\kappa}) = \sum_{\vec{h}} T_{\vec{h}} \cdot \tilde{C}(\vec{\kappa} - \vec{h}) \equiv \sum_{\vec{h}} T_{\vec{h}} \cdot \Lambda(\vec{\kappa} - \vec{h}, \lambda) = \sum_{\vec{h}} T_{\vec{h}} \cdot \frac{\frac{1}{2} sh(\lambda)}{\sin^2(\lambda/2) + \sin^2[\pi(\kappa - h)]}. \tag{11}$$

In an earlier paper of ours [15], we supposed validity of the following simple type invariance properties of the supersymmetry function with respect to symmetry transformations from a given line group $\underline{L}$:

$$(R|\vec{v}_R + \vec{t}) \equiv g \in L \Rightarrow \hat{D}(g) H(\vec{r}) = H(\vec{r}). \tag{12}$$

According to the basic new concept being elaborated in the present paper, the above given simple invariance relation (12) must be generalized in the sense of projective representations. Accordingly (see also the Appendix in this respect), we will have:

$$(R|\vec{v}_R + \vec{t}) \equiv g \in L \Rightarrow \hat{D}(g) H(\vec{r}) = \varepsilon_g H(\vec{r}), \tag{13}$$

i.e., the relevant projective representations of a given line group must be elaborated in detail and applied.

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Appendix

In this Appendix, we summarize briefly some basic features of projective representations of groups after [26]. Accordingly, in the case of projective representation of a group *G*, the basic homomorphism relation relevant for a representation $D(G)$ of its, i.e.

$$\mathrm{D}(g)\mathrm{D}(h)=\mathrm{D}(gh),(\forall g,h\in G),$$

must be replaced by

$$\mathrm{D}(g)\mathrm{D}(h)=\varepsilon_{g,h}\,\mathrm{D}(gh),\left(\forall g,h\in G:\left|\varepsilon_{g,h}\right|=1\right).$$

Then, from relation of the associative law for group elements $(f\cdot g)\cdot h=f\cdot(g\cdot h),(\forall f,g,h\in G)$, we then get directly for the phase factors:

$$\varepsilon_{f,g}\cdot\varepsilon_{fg,h}=\varepsilon_{f,gh}\cdot\varepsilon_{g,h}.$$

It can also be directly seen, that general representations of the Möbius group obey exactly the same system of relations, i.e. they are de facto projective representations.

Namely, if we would like to connect the concept of projective representations to the Bessel's function formalism necessary for description of the X-Ray scattering from ideal *Q1D* systems within frame of kinematic approximation e.g. [4], [30], it is necessary to study bilinear transformations leaving invariant the unit complex circle (whose center is identical with the origin of a complex plane *z*). Therefore, the following type of transformations must be applied:

$$\mathrm{z}\mapsto\mathrm{w}(z)=\frac{az+b}{cz+d},(ad\neq bc),$$

(*a,b,c,d* are in general case all complex numbers), mapping the unit circle $|z|=1$ conformally into $|w|=1$, i.e. into another one unit circle. These types of transformations may be combined and form a group of Möbius' (or: homographic type) transformations [32].

Conclusions

The projective representations of line groups are proposed for detailed analyses of crystals with incommensurately modulated structures. It is shown, that use of projective representations does not lead to contradictions with the already existing formalisms and may significantly extend their domain of applicability. The relevant new mathematical formulae of structure factors are introduced by use of these representations. Finally, the mathematical formalism of the diffuse scattering of X-rays from modulated

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structures is also extended via novel-type formulae of structure factors also generalized by use of projective representations of the exact symmetry groups of quasi-one-dimensional systems.

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