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Line group theory of commensurate and incommensurate modulations

I. Kirschner[1,a], Cs. Mészáros[2], and R. Laiho[3]

[1] Department for Low Temperature Physics, Eötvös University, 1088 Budapest, Hungary
[2] Department of Physics and Process Control, Gödöllö University of Agricultural Sciences, 2103 Gödöllö, Hungary
[3] Wihuri Physical Laboratory, University of Turku, 20500 Turku, Finland

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Abstract. It is shown that the line group formalism proposed is suitable to describe both commensurate and incommensurate modulations. Symmetry groups of modulated crystal lattices can completely be characterized by symmetry transformations existing in real space, without any application of the formalism based on reciprocal space. As typical examples of the method elaborated, the fundamental invariance and symmetry properties of spin density functions and the soliton lattice are determined.

PACS. 02.20.-a Group theory – 64.70.Rh Commensurate-incommensurate transitions – 75.40.Cx Static properties (order parameter, static susceptibility, heat capacities, critical exponents, etc.)

Introduction

As numerous former studies show [1–3], different kinds of geometrical groups, namely point groups, line groups and space groups can play a distinguished role in the description of symmetry properties of the solid states. In the general case of magnetic structures the geometrical groups have to be generalized [4] to involve the requirement of time reversal symmetry, too [5]. The exact symmetry theory of quasi-one-dimensional (Q1D) systems [6,7] provides powerful methods for the analysis of condensed matter by using irreducible representations (irreps) of the symmetry groups [8–10], which are generally line groups.

These methods can be employed in the research of Q1D subsystems of real crystals [11,12], polymers [13], modulated systems [14,15] especially non-collinear magnetic superstructures [16] and special materials, *e.g.* high-T_c superconductors [17–19] having ordered or other superstructural units in their structures.

One of our earlier papers was dealing with the problem of the translational symmetry of modulated crystals [12]. When finding the line groups to characterize the actual symmetry groups of given materials, the relation for structure factors of polymers can be extended to describe the modulation. In the case of $K_2SeO_4^-$ and $MnAu_2$ type materials the characteristic line group invariants were shown to be just the translational invariants.

Another research [20] was devoted to the modelling of the oxygen ordering in $Y_1Ba_2Cu_3O_{7-\delta}$ high temperature superconductors by the line group method. The result of this symmetry analysis reflects all the possible types of oxygen ordering which can appear in the solid state system under investigation. The line group-epikernel technique led to the possible supersymmetries of the oxygen ordering as L($\overline{4}$)/2c, L($\overline{4}$)/2m, L2/mmm and L2/mcc. In this symmetry analysis the *c*-axis of the orthorhombic $Y_1Ba_2Cu_3O_{7-\delta}$ was chosen as the main one of the system described by line group formalism. It makes possible to calculate directly the (0,0,1) type superlattice diffuse scattering curves. The method of the determination of Fourier coefficients was similar to the structure analysis of polymers, giving algorithms to approach the experimental curves of whatever kind of supersymmetry. The results obtained provided the possibility for comparison of theoretical and experimental intensity profiles, leading to a good agreement between them.

In a later paper [15] line groups were proposed to describe the symmetry properties of systems with non-collinear magnetic structure. A general method was elaborated to obtain the irreducible representation of the symmetry groups of modulated crystals by using that of the line groups. As a demonstrative example, the structural phase transition leading to the modulated magnetic superstructure in $MnAu_2$ type compounds was analyzed by the employment of the line group technique. It was shown that the Dzyaloshinskii invariant is the most general one according to symmetry properties of the order parameter space investigated.

Although the Dzyaloshinskii's theory [16,21,22] gives a possibility for describing each important physical property of modulated magnetic crystals, there is no symmetry theory, which can completely describe these types of structures. It means, that no symmetry groups exist, the symmetry transformations of which act in the real space

[a] Fax: (36-1) 266-0206

only and are able to reflect exactly the structure of modulated crystals.

The present paper intends to prove that the application of line groups gives a possibility to construct such a kind of symmetry theory. It will be shown, that symmetries of ideal as well as modulated crystals can be given generally in the form

$$\mathrm{G} = \mathrm{S} \otimes \mathrm{L} \tag{1}$$

where G is a space group, S is a plane group and L is a line group, which may have both crystallographic (for ideal crystals) or non-crystallographic character (for modulated crystals). The formalism based on the fundamental formula (1) is consistent with Dzyaloshinskii's theory, but its scope is more general.

Calculation technique

According to the general interpretation, the line group L represents a regular arrangement of identical motifs in a given direction. In such a way it contains all the symmetry elements, which are responsible to preserve the Q1D system to be invariant along the direction indicated. Corresponding to this, the line group is generally the symmetry group of the systems of Q1D geometrical character, thus it can characterize 3D systems of translational invariance in at least one direction. The line group theory is able to provide information on both symmetry transformations of crystallographic and non-crystallographic character, too. Each line group L is built up from two different subgroups, namely Z, which characterizes the generalized translations and P, which describes the rotations (and/or the reflections), respectively. Therefore, each line group is given as a product of

$$\mathrm{L} = \mathrm{Z} \star \mathrm{P}; \star \in \{\cdot, \wedge, \otimes\}, \tag{2}$$

where the symbols $\cdot$, $\wedge$, $\otimes$ denote the weak-direct, semidirect and direct product of the constitutive groups, respectively [3]. Having all the possible factorizations, the irreps can be built for every line group family. Knowing irreps $\mathrm{D}^{(\nu)} = \mathrm{D}^{(\nu)}(\mathrm{P})$ of the isogonal point group P of a line group the irreps of the line group can be constructed by an induction technique [23] used in the case of ideal 3D crystals, too, *i.e.*

$$\mathrm{D}^{(\mu)}(\mathrm{L}) = \mathrm{D}^{(\nu)}(\mathrm{P}) \uparrow \mathrm{L}. \tag{3}$$

As is known [22,24] modulated crystal structures are described by the so-called non-Lifshitz type stars in the form of

$$\mathbf{k} = \mathbf{k}_0 + \delta\mathbf{k} \tag{4}$$

in which the vectors $\mathbf{k}_0$ refer to highly symmetric points in the first Brillouin zone and the vectors $\delta\mathbf{k}$ realize the modulation.

The concept of translation can be generalized in the line group theory by the following way. Instead of usual translations composed from the integer linear combinations of some three non-coplanar elementary translational vectors (*i.e.* which originate from the Bravais-lattice) we have the following extension of these pure translational symmetry transformations:

$$(E|\mathbf{t}) \Rightarrow (R_{\boldsymbol{\nu}}|\boldsymbol{\nu} + \mathbf{T}); \quad \boldsymbol{\nu} = \nu\mathbf{e},\ \mathbf{e} = \frac{\mathbf{T}}{|\mathbf{T}|},\ \nu \in [0,1) \tag{5}$$

i.e. the elementary non-symmorphic symmetry transformations are the most general translation operations. Although we can deal with these generalized translations in the usual 3D crystal space too, we would restrict the number of linearly independent vectors of the Bravais-lattice from three to one, simply because we need only the integer ("pure") translations along the main direction of the Q1D system. The choice of the translational subgroup determines the algebraic structure of the full line group [2]. The integer translations $\mathbf{T} \equiv T\mathbf{a}$ appearing in the group of generalized translations should not be confused with the elements $\mathbf{t}$ of Bravais lattice of the 3D crystal. They are identical only in the trivial case when the modulation is absent or is reduced to the appearance of orthogonal symmetry transformations with "non-crystallographic" character. The groups of generalized translations are infinite cyclic groups, generated by the elementary non-symmorphic symmetry elements of an arbitrary order corresponding to Seitz-operators [4]. In particular, the irreps for group $\mathrm{n_r}$ can be determined by a simple method [8]. As usual, for the cyclic group C_n we have

$$\mathrm{g} \equiv \mathrm{C}_n^s \Rightarrow \mathrm{A}_m(\mathrm{C}_n^s) = \mathrm{e}^{ims\alpha};\ 0 \le s \le n-1;\ \alpha = \frac{2\pi}{n} \tag{6}$$

and so the irreps for the full line group $\mathrm{Ln_p}$ are

$${}_k\mathrm{A}_m(\mathrm{C}_n^s|\mathrm{Fr}(sp/n) + T) \equiv \mathrm{e}^{ims\alpha}\mathrm{e}^{i\mathbf{k}[\mathrm{Fr}(sp/n)+T]\mathbf{a}}, \tag{7}$$

where $\mathrm{Fr}(y)$ denotes the fractional part of y, and thus it represents the fractional translations $\nu \equiv \mathrm{Fr}(sp/n)$. Therefore, the irreps of the elements $(\mathrm{E}|\boldsymbol{\nu} + \mathbf{T})$ can always be separated from the orthogonal part, independently of the algebraic nature of the factorization we used.

In order to describe briefly the general algorithm for constructing irreducible representation of product groups, the Hamermesh's idea [1] will be followed. Let a group G be the direct product of its subgroups H and K, the irreducible representations of which are known as

$$\begin{aligned} &\mathrm{G} = \mathrm{H} \otimes \mathrm{K};\ \mathrm{D}^{(\mu)} = \mathrm{D}^{(\mu)}(\mathrm{H}), \\ &\mathrm{D}^{(\nu)} = \mathrm{D}^{(\nu)}(K);\ \dim\{\mathrm{D}^{(\mu)}\} = n_\mu,\ \dim\{\mathrm{D}^{(\nu)}\} = n_\nu. \end{aligned} \tag{8}$$

The irreducible representations are realized over irreducible vector spaces $\mathrm{V}^{(\mu)}$ and $\mathrm{V}^{(\nu)}$ with the bases given by the following sets of functions

$$\begin{aligned} \mathrm{B}(\mathrm{V}^{(\mu)}) &= \{\psi_1^{(\mu)}, \psi_2^{(\mu)}, ..., \psi_{n_\mu}^{(\mu)}\}, \\ \mathrm{B}(\mathrm{V}^{(\nu)}) &= \{\psi_1^{(\nu)}, \psi_2^{(\nu)}, ..., \psi_{n_\nu}^{(\nu)}\}. \end{aligned} \tag{9}$$

The symmetry operator of the constitutive subgroups acting on the relevant irreducible subspaces is

$$h \in \mathrm{H} \Rightarrow \hat{\mathrm{D}}(h)\psi_i^{(\mu)} = \sum_k \psi_k^{(\mu)} D_{ki}^{(\mu)}(h);$$
$$k \in \mathrm{K} \Rightarrow \hat{\mathrm{D}}(k)\psi_j^{(\nu)} = \sum_l \psi_l^{(\nu)} D_{lj}^{(\nu)}(k), \qquad (10)$$

which implies that in the vector space obtained by direct product of subspaces $\mathrm{V}^{(\mu)}$ and $\mathrm{V}^{(\mu)}$ the symmetry operator corresponding to a general group element of G acts as follows:

$$\hat{\mathrm{D}}(g = hk)\{\psi_i^{(\mu)}\psi_j^{(\nu)}\} = \{\hat{\mathrm{D}}(h)\psi_i^{(\mu)}\{\hat{\mathrm{D}}(k)\psi_j^{(\nu)}\}$$
$$= \sum_{k,l} \psi_k^{(\mu)}\psi_l^{(\nu)} D_{ki}^{(\mu)}(h) D_{lj}^{(\nu)}(k). \qquad (11)$$

It means, that each group element of G is obtained by the direct product representation $\mathrm{D}^{(\mu)\otimes(\nu)}(\mathrm{G}) = \mathrm{D}^{(\mu)}(\mathrm{K}) \otimes \mathrm{D}^{(\nu)}(\mathrm{H})$ with matrix elements

$$D_{kl,ij}^{[(\mu)\otimes(\nu)]}(hk) = D_{ki}^{(\mu)}(h) D_{ij}^{(\nu)}(k). \qquad (12)$$

Description of commensurate and incommensurate modulations

Taking into account the general type of simple spiral (SS) structures, the line group method used in this paper is shown to be able to describe both commensurate and incommensurate modulations. This statement is demonstrated by the analysis of the invariance properties of spin density functions and soliton lattices.

Invariance properties of the spin density functions

Under the commensurate modulation we mean that the elementary period of the ordinary Bravais lattice divided by the elementary period of the superlattice is a rational number, while in the case of the incommensurate modulation the elementary translations of the two mentioned subsystems are related to each other by an irrational number. Let us specify a translation $\mathbf{t}_m \equiv m\mathbf{a}_1$ of the Bravais-lattice of the ordinary 3D crystal, which is parallel to a translation $\mathbf{T}_l + \boldsymbol{\nu} \equiv l\mathbf{a}_2 + \frac{z}{n}\mathbf{a}_2$ of the line group related to the superstructure and calculate their difference. The result obtained is

$$\mathbf{t}_m - \mathbf{T}_l - \boldsymbol{\nu} \equiv m\mathbf{a}_1 - l\mathbf{a}_2 - \frac{z}{n}a_2$$
$$= p\mathbf{a}_2 + \frac{w}{s}\frac{\mathbf{a}}{n} - \frac{z}{n}\mathbf{a}_2 = p\mathbf{a}_2 + \frac{w - zs}{ns}\mathbf{a}_2 \equiv \mathbf{T}_p + \boldsymbol{\nu}' \quad (13)$$

where p is an integer and $w/s < n$. It is obvious that the number w can possess both rational and irrational values. This simple formula presents a useful tool for examining the transformation properties of the spin density functions in the case of modulated structure.

If $S(\mathbf{r})$ denotes the conventional spin density function and $f(\mathbf{r})$ the modulation function, the structure factor of one-dimensionally modulated system can be written [15] in the form

$$F_{\mathrm{mod}}(\boldsymbol{\kappa}) = \mathcal{F}\{f(\mathbf{r}) * S(\mathbf{r})\} = \mathcal{F}\{f(\mathbf{r})\}F(\boldsymbol{\kappa}), \qquad (14)$$

where * marks the convolution operation, $\boldsymbol{\kappa}$ is the scattering vector and the scattering amplitude

$$F(\boldsymbol{\kappa}) = \mathcal{F}\{S(\mathbf{r})\} \qquad (15)$$

corresponds to the ordinary structures. The function $f(\mathbf{r})$ has to be invariant against the symmetry transformation of the given supersymmetry to which a characteristic line group belongs. Applying this consideration to some kind of magnetic interactions, it is seen that the scattering amplitude depends directly on the line group invariant spin density function

$$\hat{\mathrm{D}}(g_1)\mathrm{S}(\mathbf{r}) = S(\mathbf{r});\ g_1 \in \mathrm{L}. \qquad (16)$$

The functionals (14-16) can immediately be introduced into the relevant expression for the magnetic elastic scattering cross-section [22]:

$$\frac{\mathrm{d}\sigma^{\mathrm{M}}}{\mathrm{d}\Omega} = (r_0\gamma)^2\{|\mathbf{F}(\boldsymbol{\kappa})|^2 - |\mathbf{e}\mathbf{F}(\boldsymbol{\kappa})|^2\}, \qquad (17)$$

where $\mathbf{e}$ is the scattering unit vector. The atomic spin for the SS structures in the zeroth unit cell has the position

$$\mathbf{S}_0^{\mathbf{k}} = \frac{1}{2}S_0(\mathbf{m}_1 + i\mathbf{m}_2), \qquad (18)$$

where $\mathbf{k}$, $\mathbf{m}_1$ and $\mathbf{m}_2$ are mutually orthogonal vectors.

In order to prove our statement in this case, we start from the most simple spin density function (with only one atom carrying nonzero spin in the motif)

$$\mathbf{S}_n^{\mathbf{k}} = \mathbf{S}_0^{\mathbf{k}}\mathrm{e}^{i\mathbf{k}\mathbf{t}_n} + \mathbf{S}_0^{\mathbf{k}*}\mathrm{e}^{-i\mathbf{k}\mathbf{t}_n}, \qquad (19)$$

which can be written with $\delta\mathbf{k}$ in the following form:

$$\mathbf{S}_n^{\mathbf{k}} = S_0\{\mathbf{m}_1\cos[(\delta\mathbf{k})\mathbf{t}_n] - \mathbf{m}_2\sin[(\delta\mathbf{k})\mathbf{t}_n]\} \qquad (20)$$

separating the function by using the bases of

$$\mathrm{B}_1 = \{\mathbf{m}_1, \mathbf{m}_2\};\ \mathrm{B}_2 = \{\cos[(\delta\mathbf{k})\mathbf{t}_n], \sin[(\delta\mathbf{k})\mathbf{t}_n]\}. \qquad (21)$$

Since the adequate line group $\mathrm{Ln_p}$ has the subgroup structure of $\mathrm{Ln_p} = \mathrm{q_r} \otimes \mathrm{C_n}$, it can be represented by matrices built up in the form of a Kronecker-product

$$g_l \in \mathrm{Ln_p} \Rightarrow \mathrm{D}^{(\mu)}(\mathrm{g}_l) \equiv \mathrm{D}^{(\mu)}(\mathrm{Q}|\boldsymbol{\nu}_{\mathrm{R}} + \mathbf{T})$$
$$= \mathrm{D}^{(\nu)}(\mathrm{C_n^s}|\mathbf{0}) \otimes \mathrm{D}^{(\lambda)}(\mathrm{R}|\boldsymbol{\nu}_{\mathrm{R}} + \mathbf{T}). \qquad (22)$$

Considering that the constitutive subgroups of $\mathrm{Ln_p}$ are commutative groups whose irreps are one dimensional, and an algebraically convenient subgroup structure of this group, we may perform the following transcription of the irrep (22) as

$$\mathrm{D}^{(\mu)}(\mathrm{Q}|\boldsymbol{\nu}_{\mathrm{R}} + \mathbf{T}) = \mathrm{D}^{(\nu)\otimes(\kappa)}(\mathrm{C}_n^s\mathrm{R})\mathrm{e}^{i\mathbf{k}(\nu_{\mathrm{R}}+T)\mathbf{a}}, \qquad (23)$$

where $\mathrm{D}^{(\kappa)}$ denotes the irrep of the orthogonal part of the Seitz-generator of the subgroup of generalized translations. The elements (being axial vectors) of the basis B_1 transform according to the pseudovectorial representation [1,22] and the elementary rotational transformations with respect to $\mathrm{D}^{(\nu)\otimes(\kappa)}(\mathrm{C}_n^s\mathrm{R})$ can be left. Let us consider the action of the symmetry operator from the group of generalized translations on the basis functions:

$$\hat{\mathrm{D}}(\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})\cos[(\delta\mathbf{k})\mathbf{t}_n] = \cos[(\delta\mathbf{k})(\mathbf{T}_\mathrm{p}-\boldsymbol{\nu}')] = \hat{\mathrm{D}}(\boldsymbol{\nu}')\cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] \quad (24)$$

$$\hat{\mathrm{D}}(\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})\sin[(\delta\mathbf{k})\mathbf{t}_n] = \sin[(\delta\mathbf{k})(\mathbf{T}_\mathrm{p}-\boldsymbol{\nu}')] = \hat{\mathrm{D}}(\boldsymbol{\nu}')\sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}]. \quad (25)$$

In these equations we used the given line group property (21) and separated the fractional translations from the integer ones and reduced the problem to the examination of the action of the operators of fractional translations on the basis functions. Then, from (24,25) the relations

$$\hat{\mathrm{D}}(\boldsymbol{\nu}')\cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] = \cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}]\cos[(\delta\mathbf{k})\nu'\mathbf{a})] + \sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}]\sin[(\delta\mathbf{k})\nu'\mathbf{a}] \quad (26)$$

$$\hat{\mathrm{D}}(\boldsymbol{\nu}')\sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] = \sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}]\cos[(\delta\mathbf{k})\nu'\mathbf{a}_2)] - \cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}]\sin[(\delta\mathbf{k})\nu'\mathbf{a}_2] \quad (27)$$

can be got. If two strictly fractional translations are taken from the relevant line group (*e.g.* $(\mathrm{E}|\boldsymbol{\nu}_1)$,$(\mathrm{E}|\boldsymbol{\nu}_2)$; $\nu_1,\nu_2\in[0,1)$) which also generate two strictly fractional translations ν' and ν'' and supposing that their sum does not exceed the elementary integer translation of the line group of the examined superstructure, these lead to the results

$$\hat{\mathrm{D}}(\boldsymbol{\nu}')\hat{\mathrm{D}}(\boldsymbol{\nu}'')\cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] = \cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] \times\cos[(\delta\mathbf{k})(\nu'+\nu'')\mathbf{a}]+\sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}]\sin[(\delta\mathbf{k})(\nu'+\nu'')\mathbf{a}] \quad (28)$$

$$\hat{\mathrm{D}}(\boldsymbol{\nu}')\hat{\mathrm{D}}(\boldsymbol{\nu}'')\sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] = \sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] \times\cos[(\delta\mathbf{k})(\nu'+\nu'')\mathbf{a}_2]-\cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}]\sin[(\delta\mathbf{k})(\nu'+\nu'')\mathbf{a}_2]. \quad (29)$$

These equations show immediately that the requirement of the homomorphism is really satisfied, *i.e.*

$$\mathrm{D}(\boldsymbol{\nu}'+\boldsymbol{\nu}'') = \hat{\mathrm{D}}(\boldsymbol{\nu}')\hat{\mathrm{D}}(\boldsymbol{\nu}'') \quad (30)$$

implying directly that

$$\mathrm{D}(\boldsymbol{\nu}_1)\hat{\mathrm{D}}(\boldsymbol{\nu}_2) = \hat{\mathrm{D}}(\boldsymbol{\nu}_1+\boldsymbol{\nu}_2). \quad (31)$$

In the case, when the sum of the fractional translations generated by (13) exceeds the elementary integer translation of the line group, we have

$$\boldsymbol{\nu}'+\boldsymbol{\nu}'' = \mathbf{a}_2+\boldsymbol{\nu}''' \quad (32)$$

and so from (28,29) the relations

$$\hat{\mathrm{D}}(\boldsymbol{\nu}'+\boldsymbol{\nu}'')\cos[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] = \cos[(\delta\mathbf{k})\nu'''\mathbf{a}]\cos[(\delta\mathbf{k})(\mathbf{T}_\mathrm{p}-\mathbf{a})] + \sin[(\delta\mathbf{k})\nu'''\mathbf{a}]\sin[(\delta\mathbf{k})(\mathbf{T}_\mathrm{p}-\mathbf{a})] \quad (33)$$

$$\hat{\mathrm{D}}(\boldsymbol{\nu}'+\boldsymbol{\nu}'')\sin[(\delta\mathbf{k})\mathbf{T}_\mathrm{p}] = \cos[(\delta\mathbf{k})\nu'''\mathbf{a}]\sin[(\delta\mathbf{k})(\mathbf{T}_\mathrm{p}-\mathbf{a})] - \sin[(\delta\mathbf{k})\nu'''\mathbf{a}]\cos[(\delta\mathbf{k})(\mathbf{T}_\mathrm{p}-\mathbf{a})] \quad (34)$$

follow and one can perform again the complete procedure to prove the homomorphism for the case (32), too.

Therefore each non-colinear SS-type magnetic structure can be connected exactly with line groups of the simplest family $\mathrm{Ln_p}$, independently of the commensurate or incommensurate character of the modulation.

Invariance properties of the soliton lattice

As some earlier results show [20], the static soliton lattice characterizes the structures consisting of commensurate domains separated by thin incommensurate domain boundaries. Let the unmodulated electron density function be invariant with respect to symmetry transformations from the space group of the crystal

$$\rho(\mathbf{r}) = \rho(\mathbf{r}-\mathbf{R}_{n\gamma}) \quad (35)$$

where the index n counts the elementary cells and the index γ counts the scattering centres inside the unit cell.

In the case of a modulation the scattering centres are displaced from their ideal places by $\mathbf{u}_{n\gamma}$ and the modulated electron density function has a form of

$$\rho(\mathbf{r}-\mathbf{R}_{n\gamma}) \Rightarrow \varrho(\mathbf{r}-\mathbf{R}_{n\gamma}-\mathbf{u}_{n\gamma}) \equiv \rho_1(\mathbf{r}-\mathbf{u}_{n\gamma}) \quad (36)$$

and so, we can employ the Fourier expansion of series

$$\rho_1(\mathbf{r}) = \sum_\mathbf{k}\rho_{1\mathbf{k}}\mathrm{e}^{2\pi i\mathbf{kr}}\mathrm{e}^{-2\pi i\mathbf{ku}_{n\gamma}} \approx \sum_\mathbf{k}\rho_{1\mathbf{k}}\mathrm{e}^{2\pi i\mathbf{kr}} - 2\pi i\sum_\mathbf{k}\mathbf{ku}_{n\gamma}\rho_{1\mathbf{k}}\mathrm{e}^{2\pi i\mathbf{kr}}. \quad (37)$$

Using the Fourier expansion of the function $\mathbf{ku}_{n\gamma}$, we have the following simplified form of the new, "modulated" electron density function in the given approximation as

$$\rho_1(\mathbf{r}) = \sum_\mathbf{k}\rho_{1\mathbf{k}}\mathrm{e}^{2\pi i\mathbf{kr}} - 2\pi i\sum_\mathbf{k}\sum_\mathbf{h}\rho_{1\mathbf{k}}\mathrm{T}_{\mathbf{h},\mathbf{k}}\mathrm{e}^{2\pi i(\mathbf{k}+\mathbf{h})\mathbf{r}}. \quad (38)$$

Therefore, the amplitude of the X-rays scattered in the direction $\mathbf{k}$ can be obtained by the following Fourier transform

$$\mathrm{A}(\boldsymbol{\kappa}) = \mathcal{F}\{\rho(\mathbf{r}-\mathbf{u}_{n\gamma})\} = \sum_\mathbf{k}\rho_{1\mathbf{k}}\delta(\boldsymbol{\kappa}-\mathbf{k}) - 2\pi i\sum_\mathbf{k}\sum_\mathbf{h}\rho_{1\mathbf{k}}\mathrm{T}_{\mathbf{h},\mathbf{k}}\delta(\boldsymbol{\kappa}-\mathbf{k}-\mathbf{h}), \quad (39)$$

i.e. the main Bragg reflections are determined by the equation $\boldsymbol{\kappa}=\mathbf{k}$ while the satellite reflections are centered around $\mathbf{k}$ and situated at $\boldsymbol{\kappa}=\mathbf{k}+\mathbf{h}$.

Properties of the modulated electron density function can also be examined by line group symmetry transformations, *i.e.* we examine the effect of the symmetry operator $\hat{\mathrm{D}}(g_l)$ on $\rho_1(r)$, $g_l\in\mathrm{Ln_p}$ by applying the line group technique for the description of this incommensurate modulation. If the displacement function can be written as

$$\mathbf{u}_{n\gamma} = \mathbf{u}_\gamma\mathrm{e}^{i\Phi(z)} = \mathbf{u}_\gamma\mathrm{e}^{i(\Phi_0+2\pi\frac{m}{p})}, \quad (40)$$

then it is assumed to be corresponding to a line group invariant function

$$g_l \in \mathrm{L} \Rightarrow \hat{\mathrm{D}}(g_l)\mathbf{u}_{n\gamma} = \mathbf{u}_{n\gamma}, \tag{41}$$

which can be decomposed by using again the direct product of the given line groups and the rules for the irreducible representations of the product groups. The product of the symmetry operators is

$$\{\hat{\mathrm{D}}[(\mathrm{C}_n^s|\mathbf{0})\mathbf{u}_\gamma]\}\{\hat{\mathrm{D}}[(R|\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})]\mathrm{e}^{i\Phi(z)}\}, \tag{42}$$

i.e. the amplitude vector $\mathbf{u}_\gamma$ is invariant with respect to the transformations of the cyclic group C_n, and the phase function $\mathrm{e}^{i\Phi(z)}$ according to the transformations of the subgroup of generalized translations q_r. Due to the properties of the polar-vectorial and axial-vectorial (or: pseudovectorial) representations, we do not perform here the calculations concerning the first part of the product (40), but limit ourselves to the second factor only. Specifying $\boldsymbol{\nu}_\mathrm{R} = \frac{m}{p}\mathbf{a}$, the calculation can be realized in the form

$$\begin{aligned}
&\hat{\mathrm{D}}[(R|\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})]\mathrm{e}^{i(\Phi_0+2\pi\frac{m}{p})} = \mathrm{e}^{i\Phi_0}\hat{\mathrm{D}}[(R|\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})]\mathrm{e}^{i2\pi\frac{m}{p}}\\
&\equiv \mathrm{e}^{i\Phi_0}\hat{\mathrm{D}}[(R|\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})]\mathrm{e}^{2\pi i(\mathbf{e}_\mathrm{d},\frac{m}{p}\mathbf{a})}\\
&= \mathrm{e}^{i\Phi_0}\mathrm{e}^{2\pi i(\mathbf{e}_\mathrm{d},(R^{-1}|-R^{-1}\boldsymbol{\nu}_\mathrm{R})\frac{m}{p}\mathbf{a})}\mathrm{e}^{-2\pi i(\mathbf{e}_\mathrm{d},R^{-1}\mathbf{T})},
\end{aligned} \tag{43}$$

where the last exponential factor is equal to unity, because the rotational operation on a line group does not change the vectors of its integer translations, but may reverse their directions. The consideration leads to

$$\begin{aligned}
&\hat{\mathrm{D}}[(R|\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})]\mathrm{e}^{i(\Phi_0+2\pi\frac{m}{p})} = \mathrm{e}^{i\Phi_0}\mathrm{e}^{2\pi i(\mathbf{e}_\mathrm{d},R^{-1}\frac{m-k}{p}\mathbf{a})}\\
&= \mathrm{e}^{i\Phi_0}\mathrm{e}^{2\pi(R\mathbf{e}_\mathrm{d},\frac{m}{p}\mathbf{a})}\mathrm{e}^{-2\pi i(R\mathbf{e}_\mathrm{d},\frac{k}{p}\mathbf{a})}\\
&= \mathrm{e}^{i\Phi_0}\mathrm{e}^{2\pi i(\mathbf{e}_\mathrm{d},\frac{m}{p}\mathbf{a})}\mathrm{e}^{-2\pi i(\mathbf{e}_\mathrm{d},\frac{k}{p}\mathbf{a})} \equiv \mathrm{e}^{i(\Phi+2\pi\frac{m}{p})}\mathrm{e}^{-2\pi i\frac{k}{p}},
\end{aligned} \tag{44}$$

i.e. the displacement function is a genuine line group invariant function at least in the sense of projective representations, where the unit vector of the direct space is denoted by $\mathbf{e}_\mathrm{d}$. The last equation before the identity is valid because the point group relationships are identical in the real space of the crystal and its dual space, *i.e.* the symmetry operation R may at most reverse the direction of $\mathbf{e}_\mathrm{d}$ but not change its direction.

Finally, we prove the homomorphism for the case of soliton lattices, too. The result of the symmetry operation of a line group on the modulated electron density function is

$$\hat{\mathrm{D}}(Q|\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})\rho_1(\mathbf{r}-\mathbf{u}_{n\gamma}) = \sum_\mathbf{k}\rho_{1Q\mathbf{k}}(\mathbf{T})\mathrm{e}^{2\pi i(Q\mathbf{k},\mathbf{r}-\mathbf{u}_{n\gamma})} \tag{45}$$

where we defined the modified Fourier-coefficients (*i.e.* structure factors corresponding to the modulation) by the formula

$$\rho_{1Q\mathbf{k}}(\mathbf{T}) = \rho_{1\mathbf{k}}\mathrm{e}^{-2\pi i(Q\mathbf{k},\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})}. \tag{46}$$

Since in general the isogonal point group of the line group differs from the point group of the crystal being modulated, the action of Q on the vector $\mathbf{k}$ results in a new reciprocal-space vector, which can be expressed as

$$Q\mathbf{k} = \mathbf{k} + \delta\mathbf{k}. \tag{47}$$

This is a relation of crucial importance, because it connects to an *orthogonal* symmetry operation of the isogonal point group of a line group with the modulation. Using this formula, it is possible to prescribe the exponential factor as

$$\begin{aligned}
\mathrm{e}^{-2\pi i(Q\mathbf{k},\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})} &= \mathrm{e}^{-2\pi i(\mathbf{k}+\delta\mathbf{k},\boldsymbol{\nu}_\mathrm{R}+\mathbf{T})}\\
&= \mathrm{e}^{-2\pi i(\mathbf{k}+\delta\mathbf{k}',m\mathbf{d})},
\end{aligned} \tag{48}$$

i.e. we used the vector $\mathbf{d}$ from the direct lattice in order to explain the modulation $\delta\mathbf{k}'$ which can be registrated in the scattering experiments. The homomorphism can be proven by the application of two line group symmetry operators on the same electron density function

$$\begin{aligned}
&\hat{\mathrm{D}}[(P|\boldsymbol{\nu}_1+\mathbf{T}_1)]\hat{\mathrm{D}}[Q|\boldsymbol{\nu}_2+\mathbf{T}_2)]\rho_1(\mathbf{r}-\mathbf{u}_{n\gamma})\\
&= \hat{\mathrm{D}}[(PQ|\boldsymbol{\nu}_1+\mathbf{T}_1+P\boldsymbol{\nu}_2+P\mathbf{T}_2)]\rho_1(\mathbf{r}-\mathbf{u}_{n\gamma})\\
&= \sum_\mathbf{k}\rho_{1PQ\mathbf{k}}(\mathbf{T}_1+\mathbf{T}_2)\mathrm{e}^{2\pi i(PQ\mathbf{k},\mathbf{r}-\mathbf{u}_{n\gamma})}
\end{aligned} \tag{49}$$

with transformed structure factors in the following form of

$$\rho_{1PQ\mathbf{k}}(\mathbf{T_1}+\mathbf{T_2}) = \rho_{1\mathbf{k}}\mathrm{e}^{-2\pi i(PQ\mathbf{k},\boldsymbol{\nu}_1+\mathbf{T}_1+P\boldsymbol{\nu}_2+P\mathbf{T}_2)}. \tag{50}$$

The same result must be obtained by succesive application of the symmetry operators:

$$\begin{aligned}
&\hat{\mathrm{D}}[(P|\boldsymbol{\nu}_1+\mathbf{T}_1)]\hat{\mathrm{D}}[(Q|\boldsymbol{\nu}_2+\mathbf{T}_2)]\rho_1(\mathbf{r}-\mathbf{u}_{n\gamma})\\
&= \hat{\mathrm{D}}[(P|\boldsymbol{\nu}_1+\mathbf{T}_1)]\sum_\mathbf{k}\rho_{1Q\mathbf{k}}(\mathbf{T}_2)\mathrm{e}^{2\pi i(Q\mathbf{k},\mathbf{r}-\mathbf{u}_{n\gamma})}\\
&= \sum_\mathbf{k}\rho_{1Q\mathbf{k}}(\mathbf{T}_2)\hat{\mathrm{D}}[(P|\boldsymbol{\nu}_1+\mathbf{T}_1)]\mathrm{e}^{2\pi i(Q\mathbf{k},\mathbf{r}-\mathbf{u}_{n\gamma})}\\
&= \sum_\mathbf{k}\rho_{1Q\mathbf{k}}(\mathbf{T}_2)\mathrm{e}^{2\pi i(Q\mathbf{k},(P|\boldsymbol{\nu}_1+\mathbf{T}_1)^{-1}(\mathbf{r}-\mathbf{u}_{n\gamma}))}\\
&= \sum_\mathbf{k}\rho_{1Q\mathbf{k}}(\mathbf{T}_2)\mathrm{e}^{2\pi i(Q\mathbf{k},P^{-1}(\mathbf{r}-\mathbf{u}_{n\gamma}-\boldsymbol{\nu}_1-\mathbf{T}_1))}\\
&= \sum_\mathbf{k}\rho_{1Q\mathbf{k}}(\mathbf{T}_2)\mathrm{e}^{2\pi i(PQ\mathbf{k},\mathbf{r}-\mathbf{u}_{n\gamma})}\mathrm{e}^{-2\pi i(PQ\mathbf{k},\boldsymbol{\nu}_1+\mathbf{T}_2)}.
\end{aligned} \tag{51}$$

The Fourier coefficients are also the same as in the case of equation (45), which are demonstrated in the next relations

$$\begin{aligned}
&\rho_{1Q\mathbf{k}}(\mathbf{T}_2)\mathrm{e}^{-2\pi i(PQ\mathbf{k},\boldsymbol{\nu}_1+\mathbf{T}_1)} \equiv \rho_{1\mathbf{k}}\mathrm{e}^{-2\pi i(Q\mathbf{k},\boldsymbol{\nu}_1+\mathbf{T}_2)}\\
&\times \mathrm{e}^{-2\pi i(PQ\mathbf{k},\boldsymbol{\nu}_1+\mathbf{T}_1)} = \rho_{1\mathbf{k}}\mathrm{e}^{-2\pi i(P^{-1}PQ\mathbf{k},\boldsymbol{\nu}_2+\mathbf{T}_2)}\\
&\times \mathrm{e}^{-2\pi i(PQ\mathbf{k},\boldsymbol{\nu}_1+\mathbf{T}_1)} = \rho_{1\mathbf{k}}\mathrm{e}^{-2\pi i(PQ\mathbf{k},P(\boldsymbol{\nu}_2+\mathbf{T}_2))}\\
&\times \mathrm{e}^{-2\pi i(PQ\mathbf{k},\boldsymbol{\nu}_1+\mathbf{T}_1)} = \rho_{1\mathbf{k}}\mathrm{e}^{-2\pi i(PQ\mathbf{k},P\boldsymbol{\nu}_2+P\mathbf{T}_2+\boldsymbol{\nu}_1+\mathbf{T}_1)}
\end{aligned} \tag{52}$$

showing obviously their identity.

Conclusions

1. As is shown, the formalism developed is suitable to characterize both commensurate and incommensurate modulations. On the basis of this experience, the main advantage of the method discussed above is its validity when describing phase transitions independently of their commensurate or incommensurate character.
2. The new formula (46) obtained for the structure amplitude of X-ray scattering may be used for further development of the general formalism needed for the structural analysis of modulated crystals.
3. The results obtained concerning the symmetry properties of the Q1D subsystems of 3D systems may be applied in the examination of different properties of charge density waves (CDW) and spin density waves (SDW) [25] too. The selection rules based on the employment of the irreps of line groups would be especially useful in the investigation of the dynamics of CDW-s and SDW-s. Therefore, the research of these problems represents prospective directions of the application of line group technique, elaborated above.

References

1. M. Hamermesh, *Group Theory and its Application to Physical Problems* (New York: Dover Publications, Inc., 1979); G.Ya. Lyubarskii, *The Application of Group Theory in Physics* (Oxford: Pergamon Press, 1960).
2. B.K. Vainshtein, *Diffraction of X-Rays by Chain Molecules* (Amsterdam: Elsevier Publ. Co., 1966).
3. O.V. Kovalev, *Irreducible Representations of The Space Groups* (New York: Gordon and Breach, 1965).
4. L.D. Landau, E.M. Lifshitz, *Electrodynamics of Continuous Media* (Oxford: Pergamon Press, 1960).
5. E.P. Wigner, *Group Theory and its Application to The Quantum Mechanics of Atomic Spectra* (New York: Academic Press, 1959).
6. M. Vujičić, I.B. Božović, F. Herbut, J. Phys. **A10**, 1271 (1977).
7. M. Damnjanović, M. Vujičić, Phys. Rev. **B25**, 6987 (1982).
8. I.B. Božović, M. Vujičić, F. Herbut, J. Phys. **A10**, 2133 (1978); I.B. Božović, M. Vujičić, J. Phys. **A14** 777 (1981).
9. M. Damnjanović I. Milošević, M. Vujičić, Phys. Rev. **B39**, 4610 (1989); M. Damnjanović, I. Milošević, Phys. Rev. **B43**, 13482 (1991).
10. M. Damnjanović, Phys. Lett. **A94**, 337 (1983); I. Milošević, Phys. Lett. **A204**, 63 (1995).
11. M. Damnjanović, J. Phys. C: Solid State Phys. **15**, 2321 (1982).
12. Cs. Mészáros, J. Bánkuti, Phys. Status Solidi **B183**, 73 (1994).
13. I. Milošević, M. Damnjanović, Phys. Rev **B47**, 7805 (1993).
14. T. Vuković, I. Milošević, M. Damnjanović, Phys. Lett. **A216**, 307 (1996).
15. I. Kirschner, Cs. Mészáros, R. Laiho, Z. Phys. B **104**, 289 (1997).
16. I.E. Dzyaloshinskii, Sov. Phys.-JETP **19**, 960 (1964); **20**, 223 (1965); **20**, 665 (1965).
17. I. Kirschner, S. Leppävuori, A.C. Bódi, A. Uusimäki, I. Dódony, Appl. Supercond. **1**, 1721 (1993).
18. T. Kármán, E. Lähderanta, S. Leppävuori, R. Laiho, I. Halász, I. Dódony, I. Kirschner, A. Uusimäki, T. Porjesz, Gy. Kovács, Z. Phys. **B78**, 169 (1990).
19. I.B. Božović, J.N. Eckstein, in *Physical Properties of High Temperature Superconductors*, vol. 5, pp. 101-206, edited by D.M. Ginsberg (Singapore, New-Jersey, London: World Scinetific, 1996).
20. Cs. Mészáros, Á Bálint, I. Kirschner, R. Laiho, R. Lähderanta, J. Bánkuti, Superlattices Microstruct. **21**, 381 (1997).
21. Yu.A. Izyumov, V.M. Laptev, Fiz. Met. Metalloved. **56**, 877 (1983).
22. Yu. A. Izyumov, V.N. Syromyatnikov, *Phase Transitions and Crystal Symmetry* (Dordrecht: Kluwer Academic Publishers, 1990).
23. S.L. Altmann, *Induced Representations in Crystals and Molecules* (London, New York, San Francisco: Academic Press, 1977).
24. Yu. A. Izyumov, V.E. Naish, R.P. Ozerov, *Neutronography of Magnetic Materials* (in Russian) (Moscow: Atomizdat, 1981).
25. G. Grüner, Rev. Mod. Phys. **66**, 1 (1994).