The calculation of parameters for Stevens Hamiltonian in a crystalline field generated by the electric charge uniformly extended in one direction

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Exact expressions for the parameters of Stevens Hamiltonian are derived within the framework of a specific model that assumes uniform character of charge density distribution in a certain direction over crystalline lattice.

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1. FORMULATION OF THE MODEL

The well-known point charge model is widely used both for description of crystal electric field (CEF) effects and for analysis of the related experimental results. A standard form of its application is based on the so-called equivalent Stevens Hamiltonian (ESH) [1,2,3,4]. The respective coefficients for the Hamiltonian have been tabulated already for many crystal structures. It should be noted that this Hamiltonian is not directly relevant to the point character of the electric charges forming CEF. Therefore, methods to calculate the Hamiltonian coefficients can be generalized for a more complicated case. For instance, in [3] they are determined with taking into account of screening effects by using of ligand electrostatic potential in the form of Yukawa. The numerical methods for calculation of the ESH parameters are also in use. In particular, it is possible to advance point charge model for more realistic assuming about electron density distribution by introducing a net of negatively charged points in interion space [6]. (This approach will be described in details in item 6 of the present paper.)

The perovskite-related compounds comprising CuO₂-planes in the structure were a subject of intensive studies during the last decade. It is of a general believement that the charge state of these planes is responsible for the unusual properties of the layered copper perovskites as, for instance, the high-temperature superconductivity is. The inelastic neutron scattering has proved to be a powerful tool for studying the charge states in the high-temperature superconductors containing rare-earth elements with f-shells [7,8,9]. A numerical analysis of the data collected in the scattering experiments enabled us to obtain earlier some evidences in proof of extended, stripe-like charge structures in the CuO₂-planes [10]. When analyzing these data we have found rather general method to obtain exact solutions for ESH parameters of a crystal field generated by the charge system with density being uniform in one direction.

The specific goal of this paper is the systematic description of the mathematical apparatus developed for analytical calculation of ESH parameters for this geometry of charge distribution and also the analysis of the consequences resulted from the model.

Since the charge systems described by our theory are assumed to have sufficiently high symmetry (at least orthorhombic) it is convenient to use the local coordinate system (x̂, ŷ, ẑ) shown at Fig. 1 with the origin at the rare earth ion and the electric charges situated within two parallel planes ẑ = ±H. The density of the uniformly extended in x̂ direction charge can be described by the function f(L) where L is the distance in ŷ-direction between ẑ-axis and the partial charge filament [11].

At first let us consider the electrostatic potential generated by the infinite uniformly charged filament oriented along x̂-axis. If the rare-earth ion has f-electron at x̂̂, ŷ̂, ẑ̂ then the perturbing crystalline potential generated by the filament will be:

\[ U(x̂, ŷ, ẑ) = U(ŷ, ẑ) = ξ \ln \frac{H^2 + L^2}{(L - ŷ)^2 + (H - ẑ)^2}; \quad (1.1) \]

where ξ is the linear charge density.

Taking into account that due to the small radii of the f-shell the inequalities |ŷ|; |ẑ| ≪ \sqrt{L^2 + H^2} are satisfied and introducing the notations:

\[ \alpha = \frac{ŷ}{\sqrt{L^2 + H^2}}; \quad β = \frac{ẑ}{\sqrt{L^2 + H^2}}; \]
\[ M = -\frac{2L}{\sqrt{L^2 + H^2}}; \quad N = -\frac{2H}{\sqrt{L^2 + H^2}}; \quad (1.2) \]

one can present the expression (1.1) as a polynomial expansion:

\[ U(ŷ, ẑ) = ξ \sum_{p,q} F_{p,q} α^p β^q. \quad (1.3) \]

As a consequence of the selection rules for the ESH matrix elements [12] the non-zero contribution into ESH is produced only by the members of expansion (1.3) with \( p + q = 2, \ p + q = 4 \) and \( p + q = 6 \), for which after

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To obtain the potential generated by the whole system of the equally oriented filaments it is necessary to sum partial contributions (1.3) with their corresponding coordinates. In particular, it includes such important cases as the crystals with orthorhombic and tetragonal symmetry. In the local coordinate system presented at Fig. 1 our pair has the coordinates as \((L, H)\) and \((-L, H)\). It is obvious that the summation of the contributions (1.3) for this pair results in vanishing of the terms in which \(M\) occurs to an odd power. As a result, the relevant part of the electric potential generated by the pair of the uniformly charged parallel filaments will be:

\[
U(\tilde{y}, \tilde{z}) = U_2(\tilde{y}, \tilde{z}) + U_4(\tilde{y}, \tilde{z}) + U_6(\tilde{y}, \tilde{z}),
\]

(1.5)

where

\[
U_2(\tilde{y}, \tilde{z}) = 2\xi g_2(L, H) (\tilde{z}^2 - \tilde{y}^2),
\]

(1.6)

\[
U_4(\tilde{y}, \tilde{z}) = 2\xi g_4(L, H) (\tilde{y}^4 - 6\tilde{y}^2\tilde{z}^2 + \tilde{z}^4),
\]

(1.7)

\[
U_6(\tilde{y}, \tilde{z}) = 2\xi g_6(L, H) \{(\tilde{z}^6 - \tilde{y}^6)
-15\tilde{y}^2\tilde{z}^2(\tilde{z}^2 - \tilde{y}^2)\},
\]

(1.8)

\[
g_2(L, H) = \frac{H^2 - L^2}{(H^2 + L^2)^2},
\]

(1.9)

\[
g_4(L, H) = \frac{1}{2} \frac{H^4 - 6H^2L^2 + L^4}{(H^2 + L^2)^4},
\]

(1.10)

\[
g_6(L, H) = \frac{1}{3} \frac{(H^6 - L^6) - 15H^2L^2(H^2 - L^2)}{(H^2 + L^2)^6}.
\]

(1.11)

The coefficient 2 is introduced into expressions (1.6)-(1.8) to emphasize that the field in question is assumed to be generated by the pair of the charged filaments. Thus, the factors \(g_2, g_4, g_6\) describe the contribution from the one charged filament in given symmetric configuration. For the system of the charged filaments with the coordinates \((L, H), (-L, H), (L, -H), (-L, -H)\) the coefficient 2 in (1.6)-(1.8) is replaced by the factor of 4.

The results (1.3)-(1.11) can be generalized for the charged distributed in the plane \(\tilde{z} = H\) with the surface density \(f(L)\) which is a constant in \(\tilde{x}\)-direction and \(f(L) = f(-L)\). Then in the formula (1.6)-(1.7) the linear charge density \(\xi\) will be replaced by \(f(L) dL\). As a result, the final expressions for the summary contribution from this charged plane in the crystalline field potential in the point \((\tilde{x}, \tilde{y}, \tilde{z})\) look as:

\[
U_2(\tilde{y}, \tilde{z}) = 2G_2 \cdot (\tilde{z}^2 - \tilde{y}^2),
\]

(1.12)

\[
U_4(\tilde{y}, \tilde{z}) = 2G_4 \cdot (\tilde{y}^4 - 6\tilde{y}^2\tilde{z}^2 + \tilde{z}^4),
\]

(1.13)

\[
U_6(\tilde{y}, \tilde{z}) = 2G_6 \cdot \{(\tilde{z}^6 - \tilde{y}^6) - 15\tilde{y}^2\tilde{z}^2(\tilde{z}^2 - \tilde{y}^2)\},
\]

(1.14)

where

\[
G_n = G_n(H) = \int_0^\infty dL f(L) \cdot g_n(L, H).
\]

(1.15)

In the case of two parallel identically charged planes situated at \(\tilde{z} = H\) and \(\tilde{z} = -H\), the coefficient 2 in (1.12)-(1.14) is replaced by 4. The expressions (1.12)-(1.14) stay formally valid not only for two dimension charge but for the volume one too if its distribution described by the density \(f(L, H)\), i.e. if it does not depend of the \(\tilde{x}\)-coordinate and \(f(L, H) = f(-L, H)\). For instance, it takes place when the electric field is generated by two cords of arbitrary cross section form. For such a case:

\[
G_n = \int_0^\infty dL \int dH f(L, H) \cdot g_n(L, H)
\]

(1.16)

and again if the charge distribution is symmetric relatively not only \(\tilde{y} = 0\) plane but also \(\tilde{z} = 0\) plane, the
coefficient 2 in \([1.12]-[1.14]\) should be substituted by 4 and
\[
G_n = \int_0^\infty dL \int_0^\infty dH f(L, H) g_n(L, H).
\]
(1.17)
As in the case of the point-charge model the determination of the perturbing Hamiltonian is the evaluation of the appropriate electrostatic potential. One-particle Hamiltonian for the f-electron in a crystalline electric field:
\[
\hat{h} = eU(\tilde{y}, \tilde{z}).
\]
(1.18)
The calculation of the ESH parameters becomes much more convenient when using the spherical coordinates \(r, \tilde{\vartheta}, \tilde{\varphi}\) in expression for \(U(\tilde{y}, \tilde{z})\) instead of the rectangular coordinates \(x, y, z\):
\[
\tilde{x} = r \sin \tilde{\vartheta} \cos \tilde{\varphi}, \quad \tilde{y} = r \sin \tilde{\vartheta} \sin \tilde{\varphi}, \quad \tilde{z} = r \cos \tilde{\vartheta}.
\]
(1.19)
On proceeding of this substitution in \([1.3]-[1.14]\) one can obtain after algebraic transformations the following expression for the electrostatic potential:
\[
U(\tilde{y}, \tilde{z}) = \sum_{n,m} \hat{A}_{nm} r^n Y_n^m (\tilde{\vartheta}, \tilde{\varphi}),
\]
(1.20)
where \(n = 2, 4, 6; m = 0, \pm 2, \pm 4, \ldots \pm n\) and the coefficients \(\hat{A}_{nm}^m\) are equal:
\[
\begin{align*}
\hat{A}_{2}^0 &= 2G_2 \cdot 2 \left(\frac{\pi}{5}\right)^{1/2}, \\
\hat{A}_{4}^2 &= 2G_4 \cdot 2 \left(\frac{2\pi}{15}\right)^{1/2}, \\
\hat{A}_{4}^0 &= 2G_4 \cdot 2 \left(\frac{3\pi}{5}\right)^{1/2}, \\
\hat{A}_{4}^{12} &= 2G_4 \cdot 2 \left(\frac{2\pi}{3}\right) \left(\frac{2\pi}{5}\right)^{1/2}, \\
\hat{A}_{4}^{14} &= 2G_4 \cdot 2 \left(\frac{2\pi}{3}\right) \left(\frac{2\pi}{35}\right)^{1/2}, \\
\hat{A}_{4}^0 &= 2G_6 \cdot 2 \left(\frac{\pi}{13}\right)^{1/2}, \\
\hat{A}_{6}^{12} &= 2G_6 \cdot 2 \left(\frac{2\pi}{2730}\right)^{1/2}, \\
\hat{A}_{6}^{14} &= 2G_6 \cdot 2 \left(\frac{14\pi}{13}\right) \left(\frac{14\pi}{13}\right)^{1/2}, \\
\hat{A}_{6}^{14} &= 2G_6 \cdot 2 \left(\frac{231\pi}{13}\right)^{1/2},
\end{align*}
\]
(1.21)
It should be noted that during these manipulations we used the notations for the spherical harmonics from \([1]\).

In real crystalline structures the potential of electric field are formed simultaneously by the ligand charges (described, for instance, in framework of the point-charge model) and by the extended charge structures described by the expressions \([1.21]-[1.22]\). The calculation of a such superposition potential and analysis of summary system properties can be carried out with the most convenience using the coordinate system associated with the crystallographic symmetry axes. Let us consider the case when the local coordinate system \(\tilde{x}, \tilde{y}, \tilde{z}\) is oriented relatively the crystallographic system \(x, y, z\) as at the Fig. 1. It is the orientation that is of the most importance for description of orthorhombic and tetragonal systems. In the spherical coordinate system connected with the crystallographic axes:
\[
x = r \sin \vartheta \cos \varphi, \quad y = r \sin \vartheta \sin \varphi, \quad z = r \cos \vartheta.
\]
(1.22)
Correspondingly in the local coordinate system (see \([1.19]\)) we have:
\[
\tilde{\vartheta} = \vartheta, \quad \tilde{\varphi} = \varphi - \Delta.
\]
(1.23)
As a result, in \([1.20]\) the replacement arises:
\[
\hat{A}_{nm}^m \rightarrow A_{nm}^m = \hat{A}_{nm}^m e^{-i\Delta
\]

Then
\[
U(r, \vartheta, \varphi) = \sum_{n,m} A_{nm}^m r^n Y_n^m (\vartheta, \varphi)
\]
(1.24)
where the potential \(U(r, \vartheta, \varphi)\) is assumed to be notated in the crystallographic coordinates whereas the coefficients \(A_{nm}^m\) are calculated in the local one. Three charge configurations with different symmetry are shown at the Fig. 2. Corresponding set of the \(A_{nm}^m\)-coefficients are presented in the Table 1. It should be noted that at \(\Delta \neq 0, \pm \frac{\pi}{2}\) the coefficients \(A_{nm}^m\) have imaginary parts.

2. CALCULATION OF THE ESH PARAMETERS

Following the procedure proposed in \([3]\) for determination of the ESH parameters we shall turn to tesseral
harmonics from spherical ones in \([1,24]\). Accordingly for even \(m\) the tesseral harmonics can be expressed via spherical harmonics as:

\[
Z_{n0}^0 = Y_{n0}^0, \quad Z_{nm}^c = \frac{1}{\sqrt{2}} \{ Y_{nm}^c + Y_{-m}^c \}, \quad Z_{nm}^s = \frac{1}{\sqrt{2}} \{ Y_{nm}^s - Y_{-m}^s \},
\]

where \(m=2,4,6\) \(m\leq n\). Accordingly:

\[
Y_{n0}^m = \frac{1}{\sqrt{2}} \{ Z_{nm}^c + iZ_{nm}^s \}, \quad Y_{n0}^{-m} = \frac{1}{\sqrt{2}} \{ Z_{nm}^c - iZ_{nm}^s \}.
\]

Taking into account \([2.1]-[2.2]\), one can obtain from \([1.24]\):

\[
U(r, \theta, \varphi) = \sum_n r^n \sum_{m \geq 0} \sum_\alpha \gamma_{nm}^\alpha Z_{nm}^\alpha, \quad (2.3)
\]

where \(\alpha = 0, c, s\).

Then for the charge system formed on the basis of the \(\gamma_{nm}^\alpha\) the tesseral harmonics as a functions of the rectangular coordinates is completed below with the \(s\)-harmonics from \([1,24]\) by the corresponding choice of the coordinate system where \(\gamma_{nm}^s = 0\). However, aiming to derive formulas suitable for calculation of superposition potentials we shall not restrict extension of our expressions. The collection of formulas expressing the tesseral harmonics as functions of the rectangular coordinates is completed below with the \(s\)-harmonics. Using the notations:

\[
Z_{nm}^c = K_{nm} f_{nm}^c, \quad Z_{nm}^s = K_{nm} f_{nm}^s, \quad Z_{nm}^0 = K_{nm} f_{nm}^0,
\]

and the expressions \([2.1],[2.2]\) and also the spherical harmonics from \([1,24]\), we have obtained the formulas for the \(f_{nm}^c, f_{nm}^s, f_{nm}^0\) listed in the Table \([1]\).

The Hamiltonian of the f-shell in the CEF is as follows:

\[
\hat{H}_{cf} = -|e| \sum_i U(x_i; y_i; z_i), \quad (2.6)
\]

where we are normally concerned with the summation over the f-electrons. Thus:

\[
\hat{H}_{cf} = -|e| \sum_n \sum_{m \geq 0} \sum_\alpha \gamma_{nm}^\alpha K_{nm} \cdot \sum_i f_{nm}^\alpha(x_i; y_i; z_i),
\]

\[
(2.7)
\]

Using Wigner-Eckart theorem \([1,2]\) one can replace:

\[
\sum_i f_{nm}^\alpha (x_i; y_i; z_i) = \Theta_n(r^n) \hat{O}_{nm}^\alpha, \quad (2.8)
\]

Then:

\[
\hat{H}_{cf} = \sum_n \sum_{m \geq 0} \sum_\alpha B_{nm}^\alpha \hat{O}_{nm}^\alpha, \quad (2.9)
\]

where \(\hat{O}_{nm}^\alpha\) - operator equivalents introduced by Stevens \([2]\) and

\[
B_{nm}^\alpha = -|e| \gamma_{nm}^\alpha K_{nm} \Theta_n(r^n), \quad (2.10)
\]

The so-called irreducible matrix elements \(\Theta_n\) are listed in \([1]\). They are often denoted as \(\Theta_n = \alpha_f, \beta_f, \gamma_f\) for \(n=2, 4, 6\), respectively. The averaged value for the \(n\)-th power of the f-shell radii is denoted as \(\langle r^n \rangle\) \([1]\). Taking into account \([2.1], [2.4]\) let us write down now the expressions for the \(B_{nm}^\alpha\) for the charge system characterized by the angle of rotation \(\Delta\) relatively crystallographic coordinate system as at Fig. 1:

\[
B_{20} = \frac{1}{2} b_2, \quad B_{22}^c = \frac{1}{2} \cos(2\Delta) b_2, \quad B_{22}^a = \frac{1}{2} \sin(2\Delta) b_2, \quad B_{40} = \frac{1}{8} b_4, \quad B_{42}^c = \frac{1}{2} \cos(2\Delta) b_4, \quad B_{42}^a = \frac{1}{2} \sin(2\Delta) b_4, \quad B_{44}^c = \frac{1}{8} \cos(4\Delta) b_4, \quad B_{44}^a = \frac{1}{8} \sin(4\Delta) b_4, \quad B_{60} = \frac{1}{16} b_6, \quad B_{62}^c = \frac{15}{32} \cos(2\Delta) b_6, \quad B_{62}^a = \frac{15}{32} \sin(2\Delta) b_6, \quad B_{64}^c = \frac{3}{16} \cos(4\Delta) b_6, \quad B_{64}^a = \frac{3}{16} \sin(4\Delta) b_6, \quad B_{66}^c = \frac{1}{32} \cos(6\Delta) b_6, \quad B_{66}^a = \frac{1}{32} \sin(6\Delta) b_6, \quad (2.11)
\]
TABLE II: Components of the tesseral harmonics expressed in Cartesian coordinates.

| n,m | $K_{nm}$ | $f_{nm}^s$ | $f_{nm}^s$ |
|-----|---------|----------|----------|
| 2,0 | $\frac{1}{4} \left( \frac{3}{2} \right)^{1/2}$ | $x^2 - y^2$ | $3z^2 - r^2$ |
| 2,2 | $\frac{1}{4} \left( \frac{1}{2} \right)^{1/2}$ | $r \sqrt{2}$ | $2xy$ |
| 4,0 | $\frac{1}{4} \left( \frac{3}{2} \right)^{1/2}$ | $(7z^2 - r^2)(x^2 - y^2)$ | $(7z^2 - r^2)2xy$ |
| 4,4 | $\frac{1}{4} \left( \frac{1}{2} \right)^{1/2}$ | $x^4 - 6x^2y^2 + y^4$ | $4xy(x^2 - y^2)$ |
| 6,0 | $\frac{1}{4} \left( \frac{1}{2} \right)^{1/2}$ | $231z^6 - 315z^4r^2 + 105z^2r^4 - 5r^6$ | $(16z^4 - 16(x^2 + y^2)^2)z^2 + (x^2 + y^2)^2z^2 + (x^2 + y^2)^22xy$ |
| 6,2 | $\frac{1}{4} \left( \frac{1}{2} \right)^{1/2}$ | $(11z^2 - r^2)(x^4 - 6x^2y^2 + y^4)$ | $(11z^2 - r^2)4xy(x^2 - y^2)$ |
| 6,6 | $\frac{1}{4} \left( \frac{1}{2} \right)^{1/2}$ | $x^6 - 15x^4y^2 + 15x^2y^4 - y^6$ | $2xy(4(x^2 - y^2)^2 - (x^2 + y^2)^2)$ |

where:

$$b_n = -\hat{C}\langle e|G_\alpha\Theta_n(r^n)\rangle,$$  \hspace{1cm} (2.12)

and the coordination number $\hat{C}$ is equal 2 for the charge distributed within the $z = H$ plane with the density $f(L) = f(-L)$, and $\hat{C} = 4$ when the charge is placed within the $z = \pm H$ planes with the density $f(L, H) = f(-L, H) = f(-L, -H)$. Naturally, the coefficient $\hat{C}$ takes the same values for the cases described by the formulas \eqref{1.12}, \eqref{1.16} respectively.

The Stevens operator equivalents are listed for $\alpha = 0; c$ in \cite{1}. The expressions for the operators with $\alpha = s$ can be derived by means of well-known procedure consisting of the replacement of the coordinates $x, y, z$ in the expressions for $f_{nm}^s$ by the corresponding components $J_x; J_y; J_z$ of the angular momentum operator $J$. It is the reason why the formulas for the tesseral harmonics in CEF-formalism are transformed back to Cartesian coordinates. It should be noted that it is conventional in Stevens formality to use the operators $\hat{J}_n$ without $\hbar$ in the commutation rules, i.e.:

$$[\hat{J}_x; \hat{J}_y] = i\hat{J}_z,$$
$$[\hat{J}_y; \hat{J}_z] = i\hat{J}_x,$$
$$[\hat{J}_z; \hat{J}_x] = i\hat{J}_y,$$  \hspace{1cm} (2.13)

For the operators $\hat{J}_\pm$ defined as:

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y,$$  \hspace{1cm} (2.14)

we have:

$$\hat{J}_\pm |J, M\rangle = \sqrt{J(J+1) - M(M \pm 1)} |J, M \pm 1\rangle.$$  \hspace{1cm} (2.15)

However, as long as the commutation rules for the operators $\hat{x}; \hat{y}; \hat{z}$ and $\hat{J}_x; \hat{J}_y; \hat{J}_z$ are different, the replacement procedure demands preliminary symmetrization of $f_{nm}^s$ over all possible permutations of the coordinates $x, y, z$. For $f_{22}^s, f_{44}^s, f_{66}^s$ this manipulation is trivial. For example:

$$f_{22}^s = 2xy = \frac{1}{2i} \{(x + iy)^2 - (x - iy)^2\},$$  \hspace{1cm} (2.16)

Correspondingly:

$$\hat{O}_{22} = \frac{1}{2i} \{ \hat{j}_+^2 - \hat{j}_-^2 \},$$  \hspace{1cm} (2.17)

And:

$$f_{44}^s = \frac{1}{2i} \{ (x + iy)^4 - (x - iy)^4 \},$$  \hspace{1cm} (2.18)

$$\hat{O}_{44} = \frac{1}{2i} \{ \hat{j}_+^4 - \hat{j}_-^4 \},$$  \hspace{1cm} (2.19)

$$f_{66}^s = \frac{1}{2i} \{ (x + iy)^6 - (x - iy)^6 \},$$  \hspace{1cm} (2.20)

$$\hat{O}_{66} = \frac{1}{2i} \{ \hat{j}_+^6 - \hat{j}_-^6 \},$$  \hspace{1cm} (2.21)

However, the method that requires less tedious algebraic manipulations than the universally adopted one, may be applied to obtain the expressions for arbitrary operators $O_{nm}^s$. Let us take into account that:

$$f_{nm}^s = \frac{1}{K_{nm}} \frac{1}{\sqrt{2i}} \left( r^nY^m_n - r^{-n}Y^{-m}_n \right),$$  \hspace{1cm} (2.22)

The functions $Y^m_n; Y^{-m}_n$ themselves form the full set of the irreducible tensor operators. Thus, accordingly Wigner-Eckart theorem the combinations $\sum_i r_iY^m_n$ may be directly (i.e. without using of rectangular coordinates) substituted by the set of the equivalent tensor operators of the same rank:

$$\sum_i r_i^nY^m_n(\vartheta_i, \phi_i) = \Theta_n(r^n)\tilde{W}^m_n,$$  \hspace{1cm} (2.23)

Accordingly the algorithm proposed in \cite{12}, one can choose the operator proportional to $\hat{J}_n$ as the equivalent tensor operator $\tilde{W}^m_n$. Other operators of the full set can be obtained with using the recurrent formula:

$$[\hat{J}_-; \tilde{W}^m_n] = \sqrt{n(n+1) - m(m-1)}\tilde{W}^{m-1}_n,$$  \hspace{1cm} (2.24)
It is easy to see that by accepting the definition $\hat{W}_n^m = \frac{1}{\sqrt{2}} K_{nm} j_v^n$, we completely match this procedure with the formulas $\hat{W}_n^m$, $\hat{W}_n^{-m}$, $\hat{W}_n^m$ so that:

$$\hat{O}_{nm} = \frac{1}{\sqrt{2}K_{nm}} \left( \hat{W}_n^m + \hat{W}_n^{-m} \right),$$

$$\hat{O}_{nm} = \frac{1}{i\sqrt{2}K_{nm}} \left( \hat{W}_n^m - \hat{W}_n^{-m} \right), \quad (2.25)$$

The calculations for the $\hat{O}_{nm}$ yields:

$$\hat{O}_{42} = \frac{1}{2i} \left\{ \hat{j}_z^2 \left[ 7\hat{j}_z^2 + 14\hat{j}_z - J(J+1) + 9 \right] - \hat{j}_z^2 \left[ 7\hat{j}_z^2 - 14\hat{j}_z - J(J+1) + 9 \right] \right\}, \quad (2.26)$$

$$\hat{O}_{62} = \frac{1}{2i} \left\{ \hat{j}_z^2 \left[ 33\hat{j}_z^4 + 132\hat{j}_z^3 - 18J(J+1)\hat{j}_z^2 + 273\hat{j}_z^2 - 36J(J+1)\hat{j}_z + 282\hat{j}_z + J(J+1)^2 - 26J(J+1) + 120 \right] - \hat{j}_z^2 \left[ 33\hat{j}_z^4 - 132\hat{j}_z^3 - 18J(J+1)\hat{j}_z^2 + 273\hat{j}_z^2 - 36J(J+1)\hat{j}_z - 282\hat{j}_z + J(J+1)^2 - 26J(J+1) + 120 \right] \right\}, \quad (2.27)$$

$$\hat{O}_{64} = \frac{1}{2i} \left\{ \hat{j}_z^4 \left[ 11\hat{j}_z^2 + 44\hat{j}_z - J(J+1) + 50 \right] - \hat{j}_z^4 \left[ 11\hat{j}_z^2 - 44\hat{j}_z - J(J+1) + 50 \right] \right\}, \quad (2.28)$$

Jointly with the formulas listed in [4], the expressions $\hat{W}_n^m$, $\hat{W}_n^{-m}$, $\hat{W}_n^m$ and $\hat{W}_n^{-m}$ in (2.25) respectively. Replacing this difference by sum and the factor $1/2i$ by $1/2$, one can obtain, as it is clear from the algorithm used, the expressions for the corresponding $\hat{O}_{nm}$. It is easy to make sure after simple transformations that these coincide with the formulas from [4].

3. THE DETAILS OF THE CHARGE DISTRIBUTION

Main distinctive feature of the charge systems studied in this paper is their extended (“filament-like”) character, i.e. the absence of dependence for charge density distribution in the $\hat{z}$ direction. As it can be seen from (2.11), this fact has already estated the strong interrelations between the coefficients $B_{nm}^n$ at given $n$. For instance, $B_{22}^n = \cos(2\Delta) B_{20}^n$.

It should be stressed that these relations are independent of the other details of the charge distribution. The similar relations between the coefficients for more complex superposition systems are demonstrated in the [4].

Let us consider more closely the case when the electric charge is distributed along the $\hat{z} = H$ plane with the surface density $f(L) = f(-L)$, i.e. when the coefficients $G_n$ are determined by (1.13). Introducing the parameter $\lambda = L/H$, one can obtain from (1.9), (1.11), (1.17):

$$G_n = C_n \int_0^\infty d\lambda f(H\lambda) \chi_n(\lambda), \quad (3.1)$$

where:

$$C_2 = \frac{1}{H}, \quad C_4 = \frac{1}{2H^3}, \quad C_6 = \frac{1}{3H^5}, \quad (3.2)$$

$$\chi_2(\lambda) = \frac{1 - \lambda^2}{(1 + \lambda^2)^2}, \quad \chi_4(\lambda) = \frac{1 - 6\lambda^2 + \lambda^4}{(1 + \lambda^2)^4}, \quad \chi_6(\lambda) = \frac{1 - \lambda^6 - 15\lambda^2(1 - \lambda^2)}{(1 + \lambda^2)^6}, \quad (3.3)$$

The formulas (3.1)-(3.3) describe the contributions of the “partial filaments” with the coordinates $L = H\lambda$ into the potentials of the 2-nd, 4-th and 6-th orders respectively. The functions $\chi_n(\lambda)$ play the role of the weighting factors. It is clear from Fig. [4] that these contributions oscillate with $\lambda$ not synchronously. Moreover, the rates of their damping are also sufficiently different.

At last for a certain practical calculations it is rather convenient to define the parameter $t$ as follows:

$$L = H \tan\left(\frac{t}{2}\right), \quad (3.4)$$

Then:

$$G_n = C_n \int_0^\pi dt f(H\tan\left(\frac{t}{2}\right)) \cdot \Omega_n(t), \quad (3.5)$$

$$\Omega_2(t) = \cos(t), \quad (3.6)$$

$$\Omega_4(t) = \frac{1}{4} \left\{ \cos(3t) + 2\cos(2t) + \cos(t) \right\}, \quad (3.7)$$

$$\Omega_6(t) = \frac{1}{16} \left\{ \cos(5t) + 4\cos(4t) + 6\cos(3t) + 4\cos(2t) + \cos(t) \right\}, \quad (3.8)$$

The plots for the functions $\Omega_n(t)$ are shown at Fig. [4].

4. THE MODEL OF THE CHARGED STRIPES

Let us consider the case when the electric charge is distributed along the plane $\hat{z} = H$ within the system of the parallel stripes uniformly charged with the surface density $F_0$. As usual, it is assumed that $f(L) = f(-L)$. 
The contribution into $G_n$ from the stripe situated in the range $L_N \leq L \leq (L_N + W_N)$ can be calculated using (3.1) or (3.3). As a result one obtains:

$$G_n^{(N)} = F_0 C_n \{ \nu_n(\beta_N) - \nu_n(\alpha_N) \},$$

(4.1)

$$\nu_2(\lambda) = \frac{\lambda}{1 + \lambda^2},$$

$$\nu_4(\lambda) = \frac{\lambda(3 - \lambda^2)}{3(1 + \lambda^2)^3},$$

$$\nu_6(\lambda) = \frac{\lambda(5 - 10\lambda^2 + \lambda^4)}{5(1 + \lambda^2)^5},$$

(4.2)

where the variables

$$\alpha_N = \frac{L_N}{H}, \quad \beta_N = \frac{L_N + W_N}{H},$$

(4.3)

are the values of the parameter $\lambda$ corresponding to the stripe left and right edges. The summation contribution from the total system of the charged stripes can be calculated accordingly:

$$G_n = \sum_N G_n^{(N)},$$

(4.4)

At last it is useful to write down the final formula for the coefficients $b_n$ taking into account the contribution from the N-th stripe. From (2.12) and (1.3) it follows:

$$b_n^{(N)} = -\tilde{C}e^2 \sigma(r^n) \Theta_n C_n \{ \nu_n(\beta_N) - \nu_n(\alpha_N) \},$$

(4.5)

The symbol $\sigma$ here means the surface concentration of the carriers generating the stripe charge, so that:

$$F_0 = \sigma |e|,$$

(4.6)

where $e$ is the elementary charge and the variable $\sigma$ is positive for the holes and negative for the electrons. It is convenient during the practical calculations to replace positive for the holes and negative for the electrons. It simultaneously expressing all the lengths in Angstroms. The coefficient $\tilde{C}$ in (1.5) is of the same sense as in (2.12). Carrying out summation of the expression (1.3) over N with corresponding values of the angle $\Delta$ in (2.11), one can obtain the formulas for the ESH parameters in the cases of rather complex superposition systems.

5. PERIODICAL TWO DIMENSIONAL LATTICES OF THE CHARGED STRIPES

Now we consider the case when the surface charge density $f(L)$ in (1.15) is a periodic function with the period $T$.

$$f(L + T) = f(L).$$

(5.1)

Introducing the surface density $\sigma(L)$ of the number of the carriers:

$$f(L) = |e|\sigma(L).$$

(5.2)

Expanding $\sigma(L)$ to Fourier series results in:

$$\sigma(L) = \sigma_0 + \sum_{k=1}^{\infty} \sigma_k \cos\left(\frac{2\pi k}{T}L\right).$$

(5.3)

The term $\sigma_0$ in (5.3) corresponds to the uniformly charged plane. This part of the charge density generates only the uniform electric field with the constant gradient and naturally with the zero contributions of the 2-nd, 4-th and 6-th orders into the potential. It is easy to see from (3.1) - (3.7) that our results satisfy to this condition. Then combining (3.1) and (5.3):

$$G_n = |e|C_n \sum_{k=1}^{\infty} E_{nk} \sigma_k,$$

(5.4)

where the coefficients

$$E_{nk} = \int_{0}^{\infty} d\lambda \chi_n(\lambda) \cos\left(\frac{2\pi k H}{T}\lambda\right)$$

(5.5)

depend only on the relation $H/T$ and are not connected with the other details of the charge distribution described by the coefficients $\sigma_k$. The formulas (1.5) stay to be valid for the system in question but now they look as:

$$b_n = -\tilde{C}e^2 C_n \Theta_n \sum_{k=1}^{\infty} E_{nk} \sigma_k,$$

(5.6)

As it is clear from (4.5), the full set of the coefficients $B_{nm}^{(2)}$ within the framework of the model developed is completely defined by the values of the three parameters $b_2, b_3, b_6$, which can be obtained, for example, by fitting of the experimental and calculated neutron spectra. Thus, the experimental information can be a tool for verification both of the microscopic and of the phenomenological models of the charge distribution with three arbitrary parameters. It should be noted that the expressions (2.4) - (2.6) describe the contributions from one or two charged planes dependingly of the coefficient $\tilde{C}$ ($\tilde{C} = 2$ or 4, respectively). But they can be easily generalized for more complicate configurations. For instance, in the case of a stack of identically charged planes, in (2.6) one should estate $\tilde{C} = 4$ and substitute the coefficients $E_{nk}$ by the $\tilde{E}_{nk}$:

$$\tilde{E}_{nk} = \sum_{H} E_{nk},$$

(5.7)

where the summation of (5.5) is carried out over the plane coordinates $H > 0$.

Now a few words about the periodicity of the charge distribution. Well-defined character of the experimental neutron spectra gives us the evidence of the fact that
the crystal lattice and charge distribution periods are commensurate. In other case the spectrum would be smoothed. Moreover, the coefficient interrelating these periods should be not large due to the same reasons. There are three examples shown at the Fig. 5.

- The period of the charge distribution is equal to the lattice one. In such a case we have identical positions for every Rare-Earth ion and only one set of the crystalline electric field parameters.

- If \( T = 2a \), the situation is different. We have two types of the REI positions with their own crystal field. If the condition \( f(L) = f(-L) \) is satisfied then both positions are symmetric.

- If \( T = 3a \) there exist three types of positions. But if we deal with the systems with at least orthorhombic symmetry then the charge distribution in the elementary cell should be rather symmetric too. In other case the distortions seem to be inevitable. The condition \( f(L) = f(-L) \) guarantees, at least, the symmetry of distribution for one type of positions. Then immediately we get rather interesting thing: there are two different positions ("1" and "2") for the REI in such a system. But the "1" position is asymmetric. As a consequence there must be the \( B_{nm} \) coefficients with both even and odd \( m \).

As a rather general example, let us consider the model of two parabolas (Fig. 4) when the period \( T = a \) and the function \( \sigma(L) \) in the range of \( (0, \frac{a}{2}) \) is assumed to be equal to:

\[
\sigma(L) = \sigma_0 + \kappa L^2 + \Theta(L - L_0) \frac{\mu}{\delta} \left( \delta^2 - \left( L - \frac{a}{2} \right)^2 \right),
\]

(5.8)

where \( L_0 = \frac{a}{2} - \delta; \sigma_0 \) is the constant that does not affect \( b_2, b_4, b_6 \) and should be obtained by means of a certain additional speculations

\[
\Theta(L - L_0) = \begin{cases} 1, & L \geq L_0, \\ 0, & L < L_0. \end{cases}
\]

Thus, accordingly this model the function \( \sigma(L) \) in the range of \( (0, \frac{a}{2}) \) is a superposition of the two parabolas with the extremums in the points \( L = 0 \) and \( L = a/2 \) respectively. The coefficients \( \kappa \) and \( \mu \) can be of arbitrary signs. Also taking into account the possibility of adding of an arbitrary constant to \( \sigma_0 \), one can see that this formula describes rather wide set of the charge distributions. After calculation of the Fourier coefficients for the function \( \sigma(L) \) we obtain:

\[
\sigma_k = (-1)^k \frac{a}{\pi^2 k^2} \left\{ a \kappa + 2 \mu \left[ \frac{a}{2 \pi k \delta} \sin \left( \frac{2 \pi k \delta}{a} \right) - \cos \left( \frac{2 \pi k \delta}{a} \right) \right] \right\},
\]

(5.9)

As a result, the system of the three equations (at \( n = 2, 4, 6 \)) interrelating the variables \( \kappa, \mu, \delta \) may be derived from (5.6), (5.9):

\[
P_n = \kappa Q_n + \mu S_n(\delta),
\]

(5.10)

where:

\[
P_n = -\frac{b_n \pi^2}{C e^2 \Theta_n \langle r \rangle^2 a},
\]

(5.11)

\[
Q_n = a \sum_{k=1}^\infty E_{nk} \frac{( -1 )^k}{k^2},
\]

(5.12)

\[
S_n(\delta) = 2 \sum_{k=1}^\infty E_{nk} \frac{(-1)^k}{k^2} \left[ \frac{a}{2 \pi k \delta} \sin \left( \frac{2 \pi k \delta}{a} \right) - \cos \left( \frac{2 \pi k \delta}{a} \right) \right]
\]

(5.13)

The equations (5.10) are linear relatively the variables \( \kappa, \mu \). The solution of this system easily can be reduced to determination of \( \delta \) from the following transcendent equation:

\[
(Q_2 P_4 - Q_4 P_2) S_6(\delta) + (Q_6 P_2 - Q_2 P_6) S_4(\delta) + (Q_4 P_6 - Q_6 P_4) S_2(\delta) = 0.
\]

(5.14)

After solving of (5.14), other parameters will be determined immediately:

\[
\mu = \frac{Q_2 P_4 - Q_4 P_2}{Q_2 S_4(\delta) - Q_4 S_2(\delta)},
\]

\[
\kappa = \frac{P_2 S_4(\delta) - P_4 S_2(\delta)}{Q_2 S_4(\delta) - Q_4 S_2(\delta)}.
\]

(5.15)

Sometimes from certain additional speculations (for example, concerning the concentration of dopants in the crystalline lattice) one can independently indicate the concentration of the carriers injected into the plane \( z = H \). Let us denote the total number of these carriers per the element \( a \times d \) of the charged plane shown at the Fig. 4 as \( N_0 \). In such a case the expressions (5.14) - (5.15) can be completed by the formulas for determination of the \( \sigma_0 \) term from (5.8). Really:

\[
N_0 = 2d \int_0^H dL \sigma(L),
\]

(5.16)

Substituting (5.8) into (5.16) yields:

\[
\sigma_0 = \frac{N_0}{a d} - \frac{1}{12} \frac{a^2 k}{\delta} \frac{8}{3a} \mu \delta^2,
\]

(5.17)

Sometimes the calculation of \( b_n \) is convenient not making use of Fourier expansions. For example, direct summation of the expressions (4.5) over \( \Lambda \) is possible for the model of the charged stripes. Accordingly (2.12):

\[
b_n = -\tilde{C} \cdot |e| \cdot \Theta_n \cdot \langle r \rangle \sum_{N=1}^\infty G_n^{(N)},
\]

(5.18)
For the periodic lattice of the stripes charged with the surface density \( F_0 = \sigma |e| \) we have: \( f(H\lambda) = F_0 \) at \( \lambda \in (\alpha_N; \beta_N) \) and \( f(H\lambda) = 0 \) at \( \lambda \not\in (\alpha_N; \beta_N) \), where

\[
\alpha_N = (Na - a + W/2)/H, \\
\beta_N = (Na - a - W/2)/H, \tag{5.19}
\]

\( W \) is the width of a stripe.

It is possible to accelerate the convergence of the series in (5.18) using the fact that one can add an arbitrary constant to the charge density in the expression (5.1).

For example:

\[
G_n = C_n \int_{0}^{\infty} d\lambda \cdot \left[ f(H\lambda) - \frac{F_0 W}{a} \right] \cdot \chi_n(\lambda), \tag{5.20}
\]

where we have extracted from the charge density its average value. In practice, the summation in (5.18) is carried out up to a certain maximal stripe number \( N = M \). Representing (5.20) as:

\[
G_n = C_n \cdot \int_{0}^{\beta_M} d\lambda \cdot \left[ f(H\lambda) - \frac{F_0 W}{a} \right] \cdot \chi_n(\lambda) + \\
C_n \cdot \int_{\beta_M}^{\infty} d\lambda \cdot \left[ f(H\lambda) - \frac{F_0 W}{a} \right] \cdot \chi_n(\lambda), \tag{5.21}
\]

we then take into account that at large \( \beta_M \), as it can be seen from the Fig. 3, the second integral contains the product of a slow varying function and the function oscillating around the zero average value. It gives us the possibility to neglect the second integral (from the physical point of view it corresponds to the mutual compensation of the two neighboring stripes carrying the charges of the equal value but of the opposite signs). Then calculating the first integral we obtain:

\[
G_n \approx C_n F_0 \sum_{N=1}^{M} \left\{ \nu_n(\beta_N) - \nu_n(\alpha_N) \right\} - \frac{W}{a} \nu_n(\beta_M). \tag{5.22}
\]

Correspondingly:

\[
b_n = -\tilde{C}e^2 \sigma \Theta_n (\nu^n) C_n \sum_{N=1}^{M} \left\{ \nu_n(\beta_N) - \frac{W}{a} \nu_n(\beta_M) \right\}. \tag{5.23}
\]

6. POINT CHARGE MODEL CALCULATION OF THE ESH PARAMETERS FOR THE COMPLEX CHARGE CONFIGURATIONS

Below we list the formulas adopted for numerical calculation of the coefficients \( B_{nm}^\alpha \) generated by the clouds of charged points. Then we use the results obtained for evaluation of an applicability of the charged filaments model to description of real systems. In the point-charge model the coefficients \( \gamma_{\alpha}^{nm} \) are expressed via the spherical coordinates \( R_j, \vartheta_j, \varphi_j \) of the charges generating the crystalline electric field as [1]:

\[
\gamma_{\alpha}^{nm} = \sum_{j} \frac{4\pi q_j}{2n+1} \frac{Z_{\alpha}^{nm}(\vartheta_j; \varphi_j)}{R_j^{n+1}}. \tag{6.1}
\]

The necessary expressions for the tesseral harmonics are listed in Table I. In this section we use for the Cartesian coordinates of the charges the traditional capital letters \( X_j, Y_j, Z_j \) instead of \( D_j, L_j, H_j \) that are reserved only for filaments. As a result, one can obtain from (5.10) and Table I the following list of the formulas:

\[
B_{20} = -|e| \frac{1}{4} \Theta_2 (r^2) \sum_j q_j \frac{3Z_j^2 - R_j^2}{R_j^5},
\]

\[
B_{22} = -|e| \frac{3}{4} \Theta_2 (r^2) \sum_j q_j \frac{Z_j^2 - Y_j^2}{R_j^3},
\]

\[
B_{22} = -|e| \frac{3}{4} \Theta_2 (r^2) \sum_j q_j \frac{2X_j Y_j}{R_j^3},
\]

\[
B_{40} = -|e| \frac{1}{64} \Theta_4 (r^4) \sum_j q_j \frac{35Z_j^4 - 30Z_j^2 R_j^2 + 3R_j^4}{R_j^9}.
\]
The expressions (6.2) are convenient for numerical calculations in the models representing the electric charge distributed in the lattice as a net of the charged points. Let us use this formulas for evaluation of the inaccuracy induced by the replacement of a finite filament by an infinite one. As it can be seen from (6.2), the coefficients $B_{nm}^a$ decrease with a distance as:

$$B_{2m}^a \sim R_j^{-3}, \quad B_{4m}^a \sim R_j^{-5}, \quad B_{6m}^a \sim R_j^{-7}. \quad (6.3)$$

Thus, it is obvious that the replacement in question contributes the maximal error at $n = 2$. So, it is reasonable for our evaluation to calculate the coefficients $B_{20}^a$ and $B_{30}^a$ for the finite charged filament (exactly speaking, belonging to the configuration of the filaments in
the sense of the formulas (6.4)-(6.5) oriented along the x-axis in the range \((-D; +D)\) and characterized by the coordi-
ates \(Y = L, Z = H\). Such a configuration automatically
applies \(B_{nm}(x, y, z) = 0\). Replacing \(q_1 \rightarrow \xi dx\) and transforming
\[ (6.2) \] from the sum to the integral yield:

\[
B_{20} = -|e| \cdot \xi \cdot \Theta_2 \cdot (\xi^2) \cdot \frac{1}{2} \cdot \sin(\phi_0) \cdot \left( \frac{H^2 - L^2}{(H^2 + L^2)^2} \right) \cdot \left( \frac{H^2 - L^2}{(H^2 + L^2)^2} \right) \cdot \left( \sin^2(\phi_0) \right), \tag{6.4}
\]

\[
B_{22} = -|e| \cdot \xi \cdot \Theta_2 \cdot (\xi^2) \cdot \left( \frac{2}{4} \cdot \frac{3}{2} \cdot \sin(\phi_0) \cdot \sin^2(\phi_0) \right) \cdot \left( \frac{H^2 - L^2}{(H^2 + L^2)^2} \right) \cdot \left( \frac{H^2 - L^2}{(H^2 + L^2)^2} \right) \cdot \left( \sin^2(\phi_0) \right), \tag{6.5}
\]

\[
\phi_0 = \arctan(\frac{D}{\sqrt{H^2 + L^2}}). \tag{6.6}
\]

For the infinite filament \(\phi_0 = \frac{\pi}{2}\). Assuming
\(\sqrt{H^2 + L^2} \ll D\), let us expand the expressions (6.4)-(6.5)
over this parameter. As a result, the following convenient
formulas for evaluation of relative inaccuracy appear:

\[
B_{20} = B_{20}(\infty) \cdot \left( 1 - \frac{1}{2} \cdot \frac{H^2 + L^2}{L^2 - H^2} \cdot \frac{H^2 + L^2}{D^2} \right), \tag{6.7}
\]

\[
B_{22} = B_{22}(\infty) \cdot \left( 1 + \frac{3}{2} \cdot \frac{H^2 + L^2}{L^2 - H^2} \cdot \frac{H^2 + L^2}{D^2} \right). \tag{6.8}
\]

where \(B_{20}(\infty), B_{22}(\infty)\) - are the corresponding expres-
sions for the infinite filament. Naturally the formulas
(6.7)-(6.8) are not applicable for the case \(L = H\) when
\(B_{20}(\infty), B_{22}(\infty)\) are equal to zero. In the latest case
only absolute evaluations on the basis of the expressions
(6.4)-(6.5) are possible. At \(L = 0\) the value of the ratio
\(D/H = 10\) is follows from (6.7)-(6.8) to be enough to
provide the accuracy of 1% for the model of the infinite
filament. To achieve the same accuracy at \(L \sim 5H\) one
needs of the ratio \(D/H \sim 50\). However, when the lat-
tice of the stripes is described, such an increase concerns
only the relative error of the far stripes input whereas
the main contribution to the potential is generated by the
nearby ones.

7. CONCLUSION

The new model is developed to strengthen the possi-
bilities for analysis of experimental data obtained by
inelastic neutron scattering. It is particularly valu-
able for studying the charge distribution in the layered
perovskite-like compounds doped with the rare-earth ions
being used as a local probe. In contrast to the widely
adopted point-charge model, the new approach directly
takes into account the extended character of the charge
distribution in one direction. The model provides clear
analytical expressions for the crystalline electric field pa-
rameters, which may be used efficiently in further eval-
uations. As a result, the strong interrelations between
these parameters were found to originate from the spe-
cific charge distribution topology. The similar relations
may easily be established for more complicated, super-
positional systems. The model enabled us to develop
methods of the charge profile reconstruction from the ex-
perimental data.

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of the ligands but we would like to reserve \(Y\) and \(Z\)
for spherical and tesseral harmonics. To avoid a mish-
mash we’ll use for coordinates of the crystal electric field
sources in \((\tilde{x}, \tilde{y}, \tilde{z})\)-system the capital letters \(D, L, H\)
respectively.
[14] Naturally, the same result takes place for the pair \((L, H)\),
\((L, -H)\).
FIG. 1: The local $\tilde{x}; \tilde{y}; \tilde{z}$ and crystallographic $x; y; z$ coordinate systems for description of the field generated in the point $r$ by the charged filaments $AB$ and $A'B'$.

FIG. 2: Superpositional charged systems characterized by three parameters: (a) - symmetry $mmm(D_{2h})$; (b) - symmetry $\bar{4}2m(D_{2d})$; (c) - symmetry $4/mmm(D_{4h})$.

FIG. 3: Weighting functions $\chi_n(\lambda)$ for the contributions to the crystalline field potential of the 2, 4 and 6 orders, respectively.

FIG. 4: Weighting functions $\Omega_n(t)$ for the contributions to the crystalline field potential of the 2, 4 and 6 orders, respectively.

FIG. 5: Schematic charge distribution profiles with different periodicity.

FIG. 6: The model of two parabolas. The summary carrier concentration $\sigma(L)$ consists of the two prabolic contributions $\sigma_1(L)$ and $\sigma_2(L)$ and may be added by the constant $\sigma_0$. 
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