Quantum Cryptography

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Time solution of non-linear Schrödinger equation of domain wall for data storage based on polar-active ferroelectric nanofilm with strong optical activity effects

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Spin Hall insulators have connected with respect to dissipationless spin transport via a sample with the spin-orbit interactions (SOI) effects. The extremum rings of the valence band in tensile strained zincblende GaN quantum well as well as the two valley shape of the valence band in GaN nanotube grown along c axis were a collection have attracted our attention both for their fundamental studies and for their device applications. The Quantum Spin Hall effects are shown to be related with intraband transitions of bulk GaN. In the framework of the effective mass theories we have solved the Schrödinger equation if the topological insulator transformation is achieved. The exact solutions of the Schrödinger equations as well as Quantum Spin Hall effect of intraband transitions of bulk GaN are found. For the hexagonal symmetry of GaN the Effective Hamiltonian based on C_{6v} point symmetry group was found. In the article for Quantum Hall effect of intraband phototransitions of bulk GaN the expressions of Berry curvature as well as Hall conductivities have been found when the topological insulator transformation is achieved. Spin Hall insulators have connected with the Topological insulator (TI) as well as Exciton insulators. The dissipationless spin transport via the sample are shown to be related with Spin Hall insulator self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and the local exchange-correlation potential in ZnO quantum well. In ZnO/Zn,MgO quantum well the electron-hole pairing leads to the exciton insulator states. An exciton insulator states with a gap 3.4 eV of ZnO quantum well and at 310 K temperature are predicted. If the electron and hole are separated, their energy is higher on 0.2 meV than if they are paired. The particle-hole pairing leads to the Cooper instability.
Abstract Landau-Ginsburg-Devonshire theory of thin ferroelectric polar-active nanofilms in incommensurate phases and semiconductor heterostructures is presented. The self-consistent time dependence solutions of non-linear Schrödinger equation or Euler-Lagrange equation for the polarization vector with the Maxwell equations for light which propagates along Oz axis in thin ferroelectric polar-active nanofilms have been found. Quantized solutions of one-dimensional Maxwell equations for thin ferroelectric films in Incommensurate phase with space dispersion have been specified as well as soliton time dependence solution of non-linear Schrödinger equation have been found. The analytical solutions of the Maxwell wave equations as well as natural optical gyrotropy effects are found in Rb$_2$ZnBr$_4$ as well as K$_2$SeO$_4$ Incommensurate phases crystals connected with giant light velocity as well as via interaction with coherent phonon oscillations. In the framework of the superspace symmetry group theories the Maxwell wave equations are solved which are shown to be connected with the symmetry group of $D_{16}^{16}$ or isomorphic groups. In the paper the non-zero gyration $g_{33}$ and gyrotropic birefringence $\epsilon_{12}$ tensors of K$_2$SeO$_4$ and Rb$_2$ZnBr$_4$ materials based on $D_{16}^{16}$ space symmetry group were found. The values of natural optical gyrotropy as well as Rashba spin splitting are shown to be specified like $(k^{(0)} \pm k^{(2)})^2$ as displacements of two symmetrically allocated parabolas from Brillouin zone center. In the article the natural optical gyrotropy effects are shown to be found with light velocity like $\epsilon = \hbar c k/eV = 14.0798$ eV but the corresponding wave vector was estimated to be $k = 7.161 \times 10^5$ cm$^{-1}$. The found strong natural optical gyrotropy has been based on available experimental data [Phys. Rev. B 38, 8075, (1988)].

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1 Contents

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2 Introduction

The polar-active properties of ferroelectric films have been calculated in Landau-Ginzburg-Devonshire theory framework [1, 2, 3, 4] with account of polarization vector gradients and surface charges and dipole layers on the interface in the conditions of stability of spontaneous polarization. Under the electric voltage feeds on the electrode or sound of scanning electron microscope the polarization redistributions have been achieved success. Under the increasing the electric voltage the local reversal of polarizations [1, 2, 3, 4] has been achieved which one lied to the creation the intergrown domains in thin films. Under domains recording the velocity of changes of extrinsic electric field \( E \) was negligibly small and without loss of accuracy one can suppose \( \text{rot} E \approx 0 \).

When the propagate waves transport high energy then the medium properties can be transformed. The motion equations were non-linear equations for specified of the creation of domain walls for data storage based on polar-active ferroelectric nanofilm with strong optical activity effects.

Under the spontaneous polarization switching in multiferroic as well as ferroelectric the single domain wall as well as the controlled elements of memory of nanodomain structures with increasing density of nanodomains as well as complicate domain recording of information [1, 2, 3, 4].

It is known [5] vibrations with sine-type modulations can be induced by the impulsive stimulated Raman-scattering process resulting in sine-type oscillations. It explains the coherent oscillations observed in transparent compounds under pumping with a photon energy smaller than an optical gap [5]. In an opaque materials the abrupt modification of pump photons can trigger displaced motions of ions towards new coordinates in the excited state resulting in cosine-type oscillations [5].

The optical activity in \( \text{Rb}_2\text{ZnBr}_4 \), \( \text{Rb}_2\text{ZnCl}_4 \), \( \text{K}_2\text{SeO}_4 \), \( \text{NH}_4\text{I}_2\text{BeF}_6 \), \( \text{N}(\text{CH}_3)_4\text{I}_2\text{MnCl}_4 \) crystals has been measured along three directions in a temperature interval from 400K to 50K [6]. In the incommensurate phase already a nonvanishing element of the gyration tensor has been observed despite the fact that the the average crystal structure has inversion symmetry [6]. In order to explain this phenomenological space dependent dielectric and gyration tensors being invariant with respect to the superspace group of \( \text{Rb}_2\text{ZnBr}_4 \), \( \text{Rb}_2\text{ZnCl}_4 \), \( \text{K}_2\text{SeO}_4 \), \( \text{N}(\text{CH}_3)_4\text{I}_2\text{BeF}_6 \), \( \text{N}(\text{CH}_3)_4\text{I}_2\text{MnCl}_4 \) have been considered [6, 7, 8, 9, 10, 11, 12, 13].

Recently one has seen a growing interest in systems like modulated crystals with charge or spin density waves which can be considered as crystals with a distortion which is periodic in space or in space time [7, 6, 10]. The Euclidean symmetry of these systems was not a three-dimensional space group but a four-dimensional superspace groups [7, 6, 8, 9, 10, 11, 12, 14, 15].

It is known that the spin-orbit coupling originates from gradients of the Coulomb potentials in the atomic cores. The spin-orbit coupling have been presented by \( \Delta = \frac{\hbar}{2m_e} \langle \psi_s | [\nabla V \times \mathbf{p}]_z | \psi_s \rangle \), where \( V \) is the microscopic crystal potential of graphene. In graphene we would have \( \Delta = 0 \) if the basis functions \( | \psi_x \rangle \) and \( | \psi_y \rangle \) were made up on basis of pure \( \pi \) or \( \pi_2 \) orbitals. However spin-orbit coupling induces a mixing of the \( \pi \) or \( \pi_2 \) and \( \sigma \) or \( \pi_2, \pi_2 \) orbitals in graphene that contributes to \( \Delta \) in second order of spin-orbit coupling. In the our case [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26] the strain mediates a coupling between intrinsic-spin and orbital dynamics and the lowest order contribution \( p_{22}^{\text{SS}}(\epsilon_{xy} + \epsilon_{yx})\sigma_x \sigma_y \) constitutes a renormalization of the intrinsic spin-orbit coupling \( p_{22}^{\text{SS}}\sigma_z \). In the article [27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39] a creation of giant spin-orbit splitting (~100 meV) of the graphene Dirac cone up to the Fermi energy are shown to be related with Au intercalation at the graphene-Ni interface. Photoelectron spectroscopy reveals the hybridization with Au 5d states as the source for this giant splitting. A sharp
graphene-Au interface at the equilibrium distance accounts for only $\sim 10$ meV spin-orbit splitting and enhancement is due to the Au atoms in the hollow position that get closer to graphene and do not break the sublattice symmetry.

3 The self-consistent time dependence soliton solutions of non-linear Schrödinger equation or Euler-Lagrange equation for the polarization vector and quantized solutions of one-dimensional Maxwell equations for thin ferroelectric films in Incommensurate phase with space dispersion in framework of Landau-Ginsburg-Devonshire theory

The structure of incommensurate phase is given by the average displacements as well as average dipole momenta and material parameters which may be presented in the form of modulation waves

$$u_n^a = c_n^a(q^l n + \varphi) = \sum_h c_n^a(h) \exp \left( i q^l (n + t_j) + \varphi \right),$$  

$$D_n^a = d_n^a(q^l n + \varphi) = \sum_h d_n^a(h) \exp \left( i q^l (n + t_j) + \varphi \right),$$

where $q^l$ is the wave vector of the incommensurate structure, $c_n^a(\varphi)$ as well as $d_n^a(\varphi)$ are periodic functions of phase $\varphi$ with $2\pi$ period, $h$ is an integer.

From Maxwell equations

$$\text{rot} \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$$

if we have assumed that the magnetic induction $\mathbf{B}$ in Maxwell equation was independent quantity with respect to time then

$$\text{rot} \mathbf{E} \approx 0.$$  

Let us known for the vector of electric field strength following expressions

$$\mathbf{E} = -\nabla \varphi,$$

as well as for the vector of electric-flux density the following Maxwell equations

$$\text{div} \mathbf{D} = \text{div} (\mathbf{E} + 4\pi \mathbf{P}) = \frac{\partial}{\partial z} \rho(\varphi),$$

where $\rho(\varphi)$ is charges density, $\varepsilon_0$ is dielectric constant.

The spontaneous polarization $P_3$ is directed along the polar axis $z$. Further we assume that the dependence of polarization vector acquires the form $[2, 3, 4]$

$$\mathbf{P}(\mathbf{r}) = \left[ \varepsilon_0 (\varepsilon_{11} - 1) E_1, \varepsilon_0 (\varepsilon_{11} - 1) E_2, P_3(\mathbf{E}, \mathbf{r}) + \varepsilon_0 (\varepsilon_{33} - 1) E_3 \right].$$

Let us known the quasi-equilibrium polarization distribution $P_3(x, y, z)$ with taking into account the gyrotropy effects which are shown to be connected with non-linear Schrödinger equation of domain wall found from Euler-Lagrange problem in the framework of Landau-Ginsburg-Devonshire theory (in the articles $[2, 3, 4]$ we have found the space solution of Euler-Lagrange problem in the framework of Landau-Ginsburg-Devonshire theory only) as follows

$$\frac{\partial^2 P_3}{\partial x^2} + \frac{\partial^2 P_3}{\partial y^2} + 2P_3 |P_3|^2 = -\frac{\partial^2 \psi}{\partial z^2}.$$  

with taking into consideration for the vector of electric field strength the following expressions $E_z = -\frac{\partial \psi}{\partial z}$.

Because the equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + 2\psi |\psi|^2 = 0,$$

has the next solution which specified of the next formula by Zakharov and Shabat

$$\psi(\xi, \eta, \delta, t_0) = \frac{2 \exp(\alpha t_0)}{\cosh(2\eta(t_0) - 8\eta(\xi))}.$$  

Hence we have found the time-dependence solution of Eq. (8) in the form

$$P_3 = \psi(\tilde{\xi}, \eta, \delta, t_0) - X,$$

$$\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + 2\psi |\psi|^2 = 0,$$  

$$\psi(\xi, \eta, \delta, t_0) = \frac{2 \exp(\alpha t_0)}{\cosh(2\eta(t_0) - 8\eta(\xi))}.$$  

Hence we have found the time-dependence solution of Eq. (8) in the form

$$P_3 = \psi(\tilde{\xi}, \eta, \delta, t_0) - X.$$
where $\tilde{\xi} = \xi + \frac{q x + q y}{2}$, $\tilde{\varphi} = -\frac{x}{(k^2 + q^2)^2}, X = \frac{\omega^2}{c^2} e^{i\gamma_0(\xi, \varphi) + \frac{1}{2} \gamma_1(\xi, \varphi)}$.

The one-dimensional Maxwell wave equations system of Incommensurate phase crystal thin film for light which propagates along Oz axis with space dispersion is found in the form [1, 14, 15, 40, 41, 42]

$$\nabla_i^2 E + \frac{\omega^2}{c^2} D = 0, \quad (12)$$

where

$$D_i(r, \varphi) = \epsilon_{ij} E_j(r, \varphi) + \epsilon_{ij} q^j r + \varphi) E_j(r, \varphi) + \gamma_{ij}(q^j r + \varphi) \nabla_j E_i(r, \varphi) + \frac{1}{2} \nabla_i \gamma_{ij}(q^j r + \varphi) \cdot E_j(r, \varphi), \quad (13)$$

$$\gamma_{ij} = \epsilon_{ijm} g_{ml}, \quad (14)$$

$$\epsilon_{12}(q^j r + \varphi) = \epsilon_{12} \cos(q^j r + \varphi), \quad (15)$$

$$g_{33}(q^j r + \varphi) = g_{33} \sin(q^j r + \varphi). \quad (16)$$

It is known [5] vibrations with sine-type modulations can be induced by the impulsive stimulated Raman-scattering process resulting in sine-type oscillations. It explains the coherent oscillations observed in transparent compounds under pumping with a photon energy smaller than an optical gap [5]. In an opaque materials the abrupt modification of pump photons can trigger displaced motions of ions towards new coordinates in the excited state resulting in cosine-type oscillations [5].

Hence we have found the one-dimensional Maxwell wave equations system of Incommensurate phase crystal thin film for light which propagates along Oz axis in consideration of both the Gyrotropy effect and dipoles on interface of ferroelectric thin film in incommensurate phase/semiconductor nanoheterostructures as well as free charges for specifying of charge quantization is found in the form

$$((-\frac{c^2}{\omega^2} \Delta) + e) \delta_{ij} + \epsilon_{ij} \delta_{ij} \cos(q_i x_1 + \varphi) + \gamma_{ij} \sin(q_i x_1 + \varphi) \nabla_i + \frac{1}{2} \gamma_{ij} \cos(q_i x_1 + \varphi) q^i E_j = 0, \quad (17)$$

where $x_i \equiv z, e \equiv e + 4\pi \int \frac{\partial \rho}{\partial z} dz - 4\pi \int \frac{\partial \rho}{\partial z} dz + C_i$. We have studied translation symmetry breaking at the normal to interface of ferroelectric thin film in incommensurate phase/semiconductor nanoheterostructures in the direction of light propagation along Oz axis too.

The sought for solution of equation can be presented by following expression according to theorem of Phlocke-Lyapunov

$$E_j = \psi_j(q_j x_1 + \varphi) e^{ik_j x_1}. \quad (18)$$

In according with theorem of Diriklahe the amplitudes of the solutions are presented by the plane waves

$$\psi_j(q_j x_1 + \varphi) = \sum_{n=-\infty}^{\infty} C_j(n) e^{i n(q_j x_1 + \varphi)}. \quad (19)$$

The wave vectors can be extended by series

$$k_i = k_i^{(0)} + k_i^{(1)} + k_i^{(2)} + .... \quad (20)$$

Substituting Eqs. (18), (19), (20) in Eq. (17)

$$\sum_{k, n} e^{i k_i x_1} \frac{(k^{(0)}_i + k^{(1)}_i + k^{(2)}_i + ... + n q_j)}{2} - e) C_j(n) e^{i n(q_j x_1 + \varphi)} = \sum_{k, n} e^{i k_i x_1} \frac{(k^{(0)}_i + k^{(1)}_i + k^{(2)}_i + ... + n q_j)}{2} = (k_i^{(0)} + k_i^{(1)} + k_i^{(2)} + ... + i n q_j) C_j(n) e^{i n(q_j x_1 + \varphi)} e^{i k_i x_1}. \quad (21)$$

The sought for solutions of Eq. (17) one be found as two linear polarization wave in the zero approximation

$$(k_i^{(0)})^2 = \frac{\omega^2}{c^2} \epsilon_{ii}, \quad (22)$$

$$C_{1x} = 1, \quad C_{1y} = 0, \quad (23)$$

$$C_{2x} = 0, \quad C_{2y} = 1. \quad (24)$$
In the first approximation the solutions for wave vectors and field may be now written as

\[ k_i^{(1)} = 0, \]
\[ C_{2x}^{(±1)} = \frac{\omega^2 \epsilon_{ij} \bar{\gamma}_{ij} \sqrt{\epsilon_{ii} + \bar{\gamma}_{ii} q_i^2}}{(k_i^0 ± q)^2 - (k_i^0)^2}, \]
\[ C_{2y}^{(±1)} = 0, \]
\[ C_{1x}^{(±1)} = 0, \]
\[ C_{1y}^{(±1)} = \frac{\omega^2 \epsilon_{ij} \bar{\gamma}_{ij} \sqrt{\epsilon_{ii} + \bar{\gamma}_{ii} q_i^2}}{(k_i^0 ± q)^2 - (k_i^0)^2}. \]

Hence

\[ \psi_1(q_i^2) = \exp(± (q_i^2 x_1, x_2)), \]
\[ \psi_2(q_i^2) = \exp(± (q_i^2 x_1, x_2)). \]

In the second approximation the sought for solutions in series can be found from equation

\[ C_{k_i}^{(2)} : (\epsilon^{(k_i)}_{ij} k_i^{(2)}) C_{k_i}^{(0)} = \epsilon_{ij} C_{i}^{(1)} - \gamma_{ij} k_i^{(0)} C_{i}^{(1)}, \]

in the form

\[ k_i^{(2)} = \frac{\omega^2}{\epsilon} \sqrt{(k_i^{(0)})^2 - 2 \epsilon_{ij} \epsilon_{kl} q_i^2 + 2 \epsilon_{ij} (\epsilon_{kl} q_i^2 - \gamma_{ij} k_i^{(0)}),} \]
\[ k_i^{(2)} = \frac{\omega^2}{\epsilon} \sqrt{(k_i^{(0)})^2 - 2 \epsilon_{ij} \epsilon_{kl} q_i^2 + 2 \epsilon_{ij} (\epsilon_{kl} q_i^2 - \gamma_{ij} k_i^{(0)}).} \]

Hence the values of natural optical gyrotropy as well as Rashba spin splitting [43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57] are shown to be derived like \((k^{(0)} ± k^{(2)})^2\) as displacement of two symmetrically allocated parabolas from Brillouin zone center. We have found the formulas of Gyrotropy splitting of Rb2ZnBr4 as well as K2SeO4 Incommensurate phases crystal from Maxwell wave equations and the magnitude of this Gyrotropy splitting are found to be related with Plank constant as well as electron mass like \(\epsilon = h c k / e V = 14.0798 eV\) but the corresponding wave vector was estimated to be \(k = 7.1614 × 10^5 \text{ cm}^{-1}\). The magnitude of these displacements were estimated correspondingly with formulas Eqs. (31), (32). Hence in the paper we have derived the formulas of Gyrotropy splitting of Rb2ZnBr4 and K2SeO4 Incommensurate phases crystal from Maxwell wave equations and the magnitude of this Gyrotropy splitting are found to be related with light velocity like \(\epsilon = h c k / e V = 14.0798 eV\) but the corresponding wave vector was estimated to be \(k = 7.1614 × 10^5 \text{ cm}^{-1}\).

### Table 2. The material parameters Rb2ZnBr4: refractive index \(n = \frac{\lambda}{\lambda^2}\), gyrotropic birefringence \(\Delta n_{11}\), Gyrotropy \(g\), light wavelength \(\lambda\) in nm, the frequency of light in \(c^{-1}\), lattice constant \(c\) in \(A\), irrational parameter \(\gamma\), wave vector of Incommensurate phase \(q^i\) in \(cm^{-1}\) and temperature \(T\) in K [6], the Gyrotropy splitting \(\epsilon\) in eV, the wave vector of Gyrotropy splitting \(k\) in cm^{-1}.

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<td>5.3 × 10^{-3}</td>
<td>10^{-5}</td>
<td>10^{-4}</td>
<td>632.8</td>
<td>2.9788 × 10^{15}</td>
<td>9.71</td>
<td>0.293</td>
<td>3.0175 × 10^{6}</td>
<td>300</td>
<td>14.0798</td>
</tr>
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</table>

The analytical solutions of the Maxwell wave equations as well as natural optical gyrotropy effects are found in Rb2ZnBr4 as well as K2SeO4 Incommensurate phases crystals connected with giant light velocity as well as via interaction with coherent phonon oscillations [58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 58, 59, 60]. In the framework of the superspace symmetry group theories the Maxwell wave equations are solved which are shown to be connected with the symmetry group of \(D_{2h}^{16}\) or isomorphic groups [62, 63, 65, 66, 67, 68, 69, 70, 71, 72, 73]. In the paper the non-zero gyration \(g_{\lambda}\) and gyrotropic birefringence \(\epsilon_{ij}\) tensors of K2SeO4 and Rb2ZnBr4 materials based on \(D_{2h}^{16}\) space symmetry group were found. The values of natural optical gyrotropy as well as Rashba spin splitting [52, 74, 75, 76, 77, 78, 79] are shown to be found like \((k^{(0)} ± k^{(2)})^2\) as displacement of two symmetrically allocated parabolas from Brillouin zone center. In the article the natural optical gyrotropy effects are shown to be found with light velocity like \(\epsilon = h c k / e V = 14.0798 eV\) but the corresponding wave vector was estimated to be \(k = 7.1614 × 10^5 \text{ cm}^{-1}\) [80, 81, 82, 83, 72, 84]. The found strong natural optical gyrotropy has been based on available experimental data [6].
4 Optical properties of crystals with Incommensurate phases from first principle

Refractive indexes can be determined like the eigenvalues of the dielectric permeability tensor as follows [8]

\[
\det |\epsilon_{\alpha\beta}(\omega, k = 0) - n(\omega)\delta_{\alpha\beta}| = 0.
\]

The tensor \(\epsilon_{\alpha\beta}(\omega, k = 0)\) is expressed by the two-time retarded Green functions [8],

\[
\epsilon_{\alpha\beta}(\omega, k = 0) = \delta_{\alpha\beta} - \frac{8\pi e^2}{v_0^2} \sum_n \langle \hat{P}_n^\alpha \hat{P}_n^\beta \rangle,
\]

where \(P_n^\alpha\) are the operators of the electric dipole momenta of the unit cells of a crystal. Let us know the case of ionic type insulator materials. Their optical properties in the short wave part of the diffraction transparent region were determined by the electronic dipole transitions with the separate ions and ionic groups with accounts coherent phonon oscillations. In the dipole momenta the electronic and ionic components which these that account for phonon oscillations of crystal lattices were separated [8, 13, 85, 86, 87, 88],

\[
\hat{P}_n^\alpha = \sum_k (e\hat{D}_n^\alpha + Z_k u_n^\alpha),
\]

where \(e\) and \(Z_k\) are charges of electron and ion, respectively,

\[
\hat{D}_n^\alpha = \sum_m \mu_{ka}^{\alpha}(\text{R}_{kn}),
\]

is the operator of electron coordinates of the \(k\)-type ion, \(\text{R}_{kn}\) is the sum of the Hubbard operators \(\hat{X}_{nk}^{\alpha'} = |nk\rangle\langle nk|\) acting in the space of electron states \(|\psi_{nk}\rangle\) of the ion, \(\mu_{ka}^{\alpha}\) are the corresponding matrix elements, \(u_n^\alpha\) the components of the ionic displacements from the equilibrium positions account of coherent phonon oscillations of crystal lattices. If we take into consideration the electron excitations only then

\[
\langle \langle \hat{P}_n^\alpha \hat{P}_n^\beta \rangle \rangle_{\omega} = e^2 \sum_{kk'} \langle \langle \hat{D}_n^\alpha \hat{D}_{n'}^\beta \rangle \rangle_{\omega}.
\]

In the article [8] for ionic insulators the Hamiltonian of ionic crystal with account electronic excitation of ionic or ionic complexes as well as phonon lattice vibration oscillations at expansion of interactions in the sets with respect to ionic displacements as well as electric dipole moments has been presented via Hubbard operators \(\hat{X}_{nk}^{\alpha} = |nk\rangle\langle nk|\) from which consist of the basis electronic states of \(|\psi_{nk}\rangle\) ion in the form [8, 26, 89, 90, 91, 92, 93, 72, 20, 94, 95, 96]

\[
H = \sum_{nk} \lambda_{ks} \hat{X}_{nk}^{\alpha} - \sum_{nka,n'k'} \langle j \psi_{nk}(nk,n'k')\hat{D}_n^\alpha \hat{D}_{n'}^\beta + C_{nk}(nk,n'k')\hat{D}_n^\alpha u_{nk}^\beta + D_{nk}(nk,n'k') \hat{D}_n^\alpha u_{nk}^\beta + + \frac{1}{4} \sum_{m'n'a'k''a''k'''} \theta_{\alpha\beta\gamma\delta}(nk,n'k',n''k'',n'''k''') \langle \hat{D}_n^\alpha \hat{D}_{n'}^\beta \hat{D}_{n''}^\gamma \hat{D}_{n'''}^\delta \rangle_{\omega}.
\]

where \(u_{nk}^\alpha\) are ion displacement vectors accordingly equilibrium states, \(\hat{D}_n^\alpha\) is ionic dipole momenta, \(\lambda_{ks}\) is energy of \(s\) state of ion of \(k\) nature.

For the equilibrium positions \(R_{ik}^{(0)} = n + \text{r}_k\) electron wave functions \(\psi_{nk}\) and energies \(\lambda_{ks}\) the ones in the high-temperature commensurate phase of the crystal are chosen.

The structure of the incommensurate phase is given by the average displacements and average dipole momenta which may be presented in the form of modulation waves [8]

\[
u_{nk}^\alpha = \langle u_{nk}^\alpha \rangle + \tilde{u}_{nk}^\alpha,
\]

\[
D_{nk}^\alpha = \langle \hat{D}_{nk}^\alpha \rangle + \tilde{D}_{nk}^\alpha,
\]

where \(\langle u \rangle\) and \(\langle D \rangle\) describe average displacements and average dipole momenta ions (\(\langle u \rangle = 0\) and \(\langle D \rangle = 0\) in high temperature commensurate phases as well as \(\langle u \rangle \neq 0\) and \(\langle D \rangle \neq 0\) in incommensurate phases in low temperature of phase transition) and \(\tilde{u}_{nk}^\alpha\) as well as \(\tilde{D}_{nk}^\alpha\) were deviations from average values.

In order to deposit the electronic subsystem Hamiltonian [8] we have entered main field approximation [97, 98, 99]

\[
\hat{H}_{M_F}^{el} = \sum_{nk} \sum_{\alpha}(\lambda_{ks} \hat{D}_{nk}^\alpha - \sum_{\alpha} F_n^\alpha \mu_{ka}^{\alpha} \hat{X}_{nk}^{\alpha'}),
\]

where

\[
F_{nk}^\alpha = \sum_{n'k'\beta} \langle \psi_{nk}(nk,n'k') \rangle (\hat{D}_{nk}^\beta) + C_{nk}(nk,n'k') \langle u_{nk}^\beta \rangle - \sum_{\alpha\beta\gamma\delta} \langle \hat{D}_{nk}^\alpha \hat{D}_{nk}^\beta \hat{D}_{nk}^\gamma \hat{D}_{nk}^\delta \rangle_{\omega}.
\]

It is known that the Hamiltonian \(\hat{H}_{M_F}^{el}\) describes the influence crystal field of lattice \(F_{nk}^\alpha\) on electronic states of ions [23, 100, 101, 102, 103].

In order to obtain from the Hamiltonian \(\hat{H}_{M_F}^{el}\) the diagonal matrices we have considered the unitary transformation
\[ \hat{X}_{nk}' = \sum_{\mu \nu} u_{\mu n}^* u_{\nu k}^* \hat{\mu}_{\mu \nu}' \]  

where \( u_{\mu n}^* \) were eigenvectors which were found from equations system

\[ \sum_{\nu} (\lambda_{nk} \delta_{\mu \nu} - \sum_{\alpha} D_{nk}^\alpha \bar{k}_{\alpha \nu}^* ) u_{\mu n}^* = \tilde{\lambda}_{nk \mu} u_{\nu k}^* . \]  

Hence

\[ \hat{\mu}_{\mu \nu} = \sum_{\gamma \alpha} f_{\gamma \alpha} u_{\mu \gamma}^* u_{\nu \alpha}^* , \]

where \( \tilde{\lambda}_{nk \mu} \) were new energy levels splitting by Stark effect [104, 84, 101, 105, 106, 107, 108, 109].

We have transformed \( D_{nk}^\alpha \) operators into the form

\[ \hat{D}_{nk}^\alpha = \sum_{\mu \nu} \tilde{\mu}_{\mu \nu}^* X_{nk}^\mu , \]

\[ \tilde{\mu}_{\mu \nu}^* = \sum_{\alpha \gamma \kappa \lambda} f_{\gamma \alpha} u_{\mu \gamma}^* u_{\nu \alpha}^* \]

We have presented dipole-dipole Green function on the basis Eqs. (45), (46) in the form

\[ \langle \langle \hat{D}_{nk}^\alpha | \hat{D}_{n'k'}^\beta \rangle \rangle = \sum_{\mu \nu} u_{\mu n}^* u_{\nu k}^* (\langle \hat{X}_{nk}^\mu | \hat{X}_{n'k'}^\nu \rangle) \omega. \]

The Green function \( \langle \langle \hat{X} \rangle \rangle \) satisfy the motion equation

\[ \hbar \omega - \tilde{\lambda}_{nk \mu} + \tilde{\lambda}_{nk \mu}^* \langle \langle \hat{X}^\mu | \hat{X}^\nu \rangle \rangle = \frac{1}{2} \sum_{\alpha \beta \gamma \delta} \bar{\delta}_{\alpha \beta \gamma \delta} \tilde{\delta}_{\mu \nu}^\alpha \tilde{\delta}_{\mu \nu}^\beta \langle \hat{X}_{nk}^\mu - \hat{X}_{nk}^\nu \rangle - \sum_{\gamma \alpha} \tilde{\mu}_{\mu \nu}^* \langle \hat{X}_{nk}^\mu - \hat{X}_{nk}^\nu \rangle \sum_{m l \delta} \bar{\psi}_{\gamma \delta}(nk, n'k') (\langle \hat{D}_{ml}^\alpha | \hat{X}_{n'k'}^\nu \rangle) \omega, \]

but

\[ \tilde{\psi}_{\alpha \beta}(nk, n'k') = \psi_{\alpha \beta}(nk, n'k') - \frac{1}{2} \sum_{m l \delta} \tilde{\delta}_{m l}^\alpha \bar{\delta}_{\beta \gamma} \tilde{\delta}_{\nu \mu}^\beta \langle \hat{X}_{nk}^\mu - \hat{X}_{nk}^\nu \rangle - \frac{1}{2} \sum_{m l \delta} \bar{\delta}_{\alpha \beta \gamma \delta} \tilde{\delta}_{\nu \mu}^\beta \langle \hat{X}_{nk}^\mu - \hat{X}_{nk}^\nu \rangle \sum_{m l \delta} \bar{\psi}_{\gamma \delta}(nk, ml) (\langle \hat{D}_{ml}^\alpha | \hat{X}_{m k'}^\nu \rangle) \omega, \]

Hence we have derived Tyablickov uncoupling \( \langle \langle \hat{u} \rangle \rangle \) as well as we have cut the expressions with \( \langle \hat{D}_{nk} \hat{X} \rangle \rightarrow \langle \hat{D}_{nk} \hat{X} \rangle \).

We have derived the Bethe-Salpeter equations [110, 111, 112] for Green function in the form

\[ \langle \langle \hat{D}_{nk}^\alpha | \hat{D}_{n'k'}^\beta \rangle \rangle = \frac{1}{2} \sum_{\mu \nu} \bar{\mu}_{\mu \nu}^* \bar{\nu}_{\nu \mu}^* \langle \hat{X}_{nk}^\mu - \hat{X}_{nk}^\nu \rangle , \]

where

\[ \bar{\mu}_{\mu \nu}^* \bar{\nu}_{\nu \mu}^* \langle \hat{X}_{nk}^\mu - \hat{X}_{nk}^\nu \rangle = \sum_{\gamma \alpha} \bar{\psi}_{\gamma \delta}(nk, n'k') (\langle \hat{D}_{ml}^\alpha | \hat{X}_{n'k'}^\nu \rangle) \omega, \]

accounts of electronic polarizability single ion displaced in the field \( F_{nk}^\alpha \) crystal lattice.

### 4.1 Symmetry of Incommensurate phase crystals

It is known from neutron and X-ray scattering that the phase transition from high temperature commensurate phase in incommensurate phase caused by equilibrium breaking in general defined \( q \) point of Brillouin zone [8, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 99]. At these the created structure which displaced low temperature \( T_f \) of phase transition were described for the phase transition of displacement type in \( K_2 SeO_4 \) the modulation wave of ions displacement \( u_{nk} = u_{k}(q' n + \varphi) \) but for the phase transition order-orderless in NaNO\(_2\) by the modulation wave of occupation probability of single ion the one from several equilibrium location \( p_{nk} = p_k(q' n + \varphi) \), where

\[ n = n_1 a_1 + n_2 a_2 + n_3 a_3 \]

was lattice vector of basic high temperature commensurate phase.

The vectors \( u_k(\varphi) \) and \( p_k(\varphi) \) are periodic functions of phase \( \varphi \) with 2\pi period.

Hence like the phase transition of displacement type thus for the phase transition of order-orderless the average displacement of ions [126, 97, 20, 127, 128, 129, 130] in incommensurate phase can be presented in the form

\[ \langle u_{nk} \rangle = C_k(q' n + \varphi), \]

where

\[ C_k(\varphi) = C_k(\varphi + 2\pi). \]

Since the wave vector \( q' \) is incommensurate with inverse lattice vector, (i.e. does not exist of like these integer \( M \) and \( N \) for which
where \( a^* \) is inverse lattice vector.

For study Incommensurate phase symmetry the \( 3 + d \)-dimensional supersymmetry groups have been derived. For experimental observations sufficiently suggest \( d = 1 \) one-dimensional modulation. The supersymmetry group approach was build based on theoretical group analysis or tight-binding method. In which average displacements Eq. (52) were connected with order parameter of phase transition from commensurate phase into incommensurate phase

\[
\langle u_{nk} \rangle = \sum_{q,j} Q(q,j)e_3(q,j) \exp(iq(n+r_i)),
\]

where \( Q(q,j) \) order parameter which transforms like \( j \) irreducible representation for wave vector \( q \), \( e_3(q,j) \) eigenvector this representation; \( \sum_{q,j} \) includes the contributions from main order parameter \( Q(q',j_0) \) corresponding representation \( j_0 \) for the wave vector \( q' \) as well as the contributions from secondary order parameters \( Q(q_i,j_i) \) for which the symmetry allows the existing in Landau expansion for free energy such terms which are proportional to

\[
Q^h(q',j_0)Q(-q_i,j_i)\Delta(n_iq' - q_i),
\]

where \( \Delta(k) = \sum G \delta(k - G) \), but \( G \) is inverse lattice vector. Since

\[
Q(q',j_0) = Q^*(q',j_0) = \eta \exp^{i\varphi},
\]

and take into account the following connections \( \langle u_{nk}^* \rangle \sim Q^*(-q',j_0), q = n,q + m,a^* \) which effluent from Eq. (55) can assure that found expansion for \( \langle u_{nk}^* \rangle \) satisfy the expression Eq. (52).

It is known that the symmetry of average ionic displacements satisfy the condition of invariance of four-dimensional lattice \( (n + r_k + C_q(n + \varphi), \varphi) \) with respect supersymmetry group operations.

The \( g \) elements of supersymmetry group have a form

\[
g = ([\hat{R}t_k], [R_iV_R]),
\]

where \([\hat{R}t_k]\) are elements of the space group of initial high-temperature commensurate phase, but \([R_iV_R]\) corresponding to their transformation of four coordinate of \( \varphi \) phase. The action of operation \( g \) on four-dimensional vector \( (r, \varphi) \) can be entered as

\[
g(r, \varphi) = (r', \varphi'),
\]

where \( r' = \hat{R}r + t_k, \varphi' = R_i\varphi + V_R \) but \( R_i = +1 \) if \( \hat{R}q' = q' \) and \( R_i = -1 \) if \( \hat{R}q' = -q' \).

The translation subgroup contains the following elements \([E|n], [1 - q'|n]]\).

### 4.2 Bethe-Salpeter equation of incommensurate phase

In the initial high temperature commensurate phase \( \langle D_n^{a} \rangle = 0, \langle u_{nk}^a \rangle = 0; \) the matrices of dipole-dipole interactions as well as Fourth constants transform with respect the space group symmetry this phase [23, 131, 21, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142]:

for the element

\[
\psi_{ab}(ml, m'l') = \sum_{n\nu'\nu} R_{\alpha}(R_{\nu'}_{\nu}) \psi_{n\nu'}(nk, n'k'),
\]

where \( m + r_k = \hat{R}(n + r_k) + t_k, m' + r_i = \hat{R}(n' + r_k) + t_k, \)

for translation subgroup

\[
\psi_{ab}(nk, n'k') = \psi_{ab}(n - m, k, n'; m' - m, k').
\]

Correlation functions which were build on a ionic displacements as well as electronic dipole momenta operators [143, 53, 52, 51, 50, 46, 45, 44] satisfy the similar found expressions.

In low-temperature commensurate phase the non-zero averages \( \langle D_n^{a} \rangle = d_n^{a} = d_n^{a+n_{0}c_k} \) and \( \langle u_{nk}^{a} \rangle = C_n^{a} = C_{n+n_{0}c_k}^{a} \) have been created, where \( n_{0} \) is lattice vector of low temperature phase but the renormalized Fourth constants \( \psi_{ab}(nk, n'k') \) Eq. (49) in consideration of lattice anharmonicity transform with respect of the space group of symmetry of this phase.

The structure of the incommensurate phase is given by the average displacements and average dipole momenta [144, 145] which can be presented in the form of modulation waves [8, 146, 147, 148]

\[
\langle u_{nk}^a \rangle = C_n^{a} (q'n + \varphi) = \sum_{h} C_n^{a}(h) \exp(ih + q'n + \varphi),
\]
where $\mathbf{q}'$ is the wave vector of the incommensurate structure, $C'_h(\varphi)$ and $d'_h(\varphi)$ are periodic functions of phase $\varphi$, $h$ is an integer.

The renormalized Fourth constants $\tilde{\psi}_{a\beta}(nk,n'k')$ Eq. (49) and crystal fields of lattice Eq. (41) enclose the following components

$$\tilde{\psi} = \psi + \psi^{(1)} + (\psi^{(2)} + \psi^{(2)}) + \ldots,$$

$$F = F^{(1)} + (F^{(2)} + F^{(2)}) + \ldots,$$

which

$$\psi^{(1)} = -\sigma D^u(u),$$

$$\psi^{(2)} = -\frac{1}{2}\theta(\tilde{u}u),$$

$$F^{(1)} = \psi(D) + C(u),$$

$$F^{(2)} = -\sigma D^u(D\tilde{u}) - \frac{1}{2}\sigma D^u(\tilde{u}u),$$

the contributions from equilibrium displacements,

$$\psi^{(2)} = -\frac{1}{2}\theta(\tilde{u}u),$$

$$F^{(2)} = -\sigma D^u(D\tilde{u}) - \frac{1}{2}\sigma D^u(\tilde{u}u),$$

the contributions which connected from correlation displacements in incommensurate phase.

The crystal field of lattice Eq. (64) as well as the matrix elements Eq. (46) and the energy levels $\tilde{\lambda}_{nk\sigma}$ defined by Eq. (43) in incommensurate phase vary from cell to cell. A distance from the edge of transparent region and for weak internal self-consistent crystal field of lattice the polarizability of ion (ionic group) Eq. (51) can expand in series with respect to power of intrinsic crystal fields of lattice

$$Z_{nk}^\beta(\omega) = Z_{0,k}^\beta(\omega) + \sum_\gamma x_{1,k}^{\beta,\gamma}(\omega)F_{nk}^{(\gamma)} + \frac{1}{2}\sum_\gamma x_{2,k}^{\beta,\gamma}(\omega)F_{nk}^{(1\gamma)}F_{nk}^{(1\gamma)} + \ldots$$

where

$$Z_{0,k}^\beta(\omega) = \sum_{\mu\nu} \mu_{nk}^{\beta}\nu_{nk}^{\beta}(X_{nk}^{\beta} - X_{nk}^{\beta'}).$$

Let us known Eq. (67) in the form of sum of contributions caused different components of field $F_{nk}^{\beta}$ Eq. (64),

$$Z_{nk}^\beta(\omega) = Z_{0,k}^\beta(\omega) + Z_{1,nk}^\beta(\omega) + (Z_{2,nk}^\beta(\omega) + Z_{2,nk}^\beta(\omega)),$$

$$Z_{1,nk}^\beta(\omega) = \sum_\gamma x_{1,k}^{\beta,\gamma}(\omega)F_{nk}^{(1\gamma)},$$

$$Z_{2,nk}^\beta(\omega) = \sum_\gamma x_{2,k}^{\beta,\gamma}(\omega)F_{nk}^{(1\gamma)}F_{nk}^{(1\gamma)},$$

On the basis of Eq. (63) and Eq. (69) the Green function which satisfy of equation Eq. (50) we have presented in the form corresponding series

$$\langle\langle D|D\rangle\rangle_{\omega} = \langle\langle D|D\rangle\rangle_{\omega}^{(0)} + G^{(1)}(\omega) + (G^{(2)}(\omega) + \tilde{G}^{(2)}(\omega)),$$

where Green function of hight temperature commensurate phase $\langle\langle D|D\rangle\rangle_{\omega}^{(0)}$ satisfy the equation

$$\langle\langle D|D\rangle\rangle_{\omega}^{(0)} = \frac{1}{2\pi}Z_{0}\langle\langle D|D\rangle\rangle_{\omega}^{(0)} - Z_{0}(\omega)\psi\langle\langle D|D\rangle\rangle_{\omega}^{(0)},$$

but the remainder contributions in Eq. (73) we have found as

$$G^{(1)}(\omega) = 2\pi\langle\langle D|D\rangle\rangle_{\omega}^{(0)}(Z_{0}^{-1}Z_{0}\psi_{1} - \psi_{1})\langle\langle D|D\rangle\rangle_{\omega}^{(0)},$$

$$G^{(2)}(\omega) = 2\pi\langle\langle D|D\rangle\rangle_{\omega}^{(0)}(Z_{0}^{-1}Z_{0}\psi_{2} - \psi_{2} - Z_{0}^{-1}Z_{1}\psi_{1})\langle\langle D|D\rangle\rangle_{\omega}^{(0)} - 2\pi\langle\langle D|D\rangle\rangle_{\omega}^{(0)}Z_{1}\psi + \psi_{1})G^{(1)}(\omega),$$


\[ G^{(2)}(\omega) = 2\pi \langle (D|D) \rangle^{(0)}_{\omega} (Z_{0}^{-1} Z_{0}^{-1} - \tilde{\psi}_{2}) (\langle D|D \rangle)^{(0)}_{\omega}, \]  

(77)

where Eq. (75), Eq. (76) were corrections linear and quadratic \((\omega)\) and \((D)\), Eq. (77) is correction which was proportional correlation functions \((\tilde{u} \tilde{u})\) and \((\tilde{D} \tilde{u})\).

### 4.3 Symmetry of \(\epsilon_{\alpha\beta}(\omega, k = 0)\) tensor in incommensurate phases

We have presented \(\epsilon_{\alpha\beta}(\omega, k = 0)\) on the basis Eq. (34) and Eq. (37) in the form

\[ \epsilon_{\alpha\beta}(\omega, k = 0) = \delta_{\alpha\beta} - \frac{8\pi^{2}}{V_{c}} \sum_{kk'} \langle \langle \Phi_{kk',\beta}(\omega, k = 0) \rangle \rangle, \]  

(78)

where \(\Phi_{kk',\beta}(\omega, k = 0)\) is Fourier transform of dipole-dipole Green function which includes the contributions corresponding Eq. (73)

\[ \Phi_{kk',\beta}(\omega, k = 0) = \Phi_{kk',\beta}(\omega, k = 0) + \Phi_{kk',\beta}^{(1)}(\omega, k = 0) + \Phi_{kk',\beta}^{(2)}(\omega, k = 0) + \Phi_{kk',\beta}^{(2)}(\omega, k = 0). \]  

(79)

First term enters into the expression for the dielectric permeability tensor for the hight temperature phase

\[ \epsilon_{\alpha\beta}^{0}(\omega, k = 0) = \delta_{\alpha\beta} - \frac{8\pi^{2}}{V_{c}} \sum_{kk'} \langle \langle \Phi_{kk',\beta}^{0}(\omega, k = 0) \rangle \rangle. \]  

(80)

\[ \Phi_{kk',\beta}^{0}(\omega, k = 0) \]  

(81)

The symmetry of contribution \(\Phi^{0}(\omega, k)\) is defined by space group of symmetry of high temperature commensurate phase.

In the Incommensurate phase the average displacements which include coherent phonon oscillations \([43, 57, 56, 55, 64, 2, 3, 4, 1, 14, 15, 40, 41, 42]\) were defined by modulation waves Eqs. (61), (62) as well as an internal self-consistent crystal fields of lattice Eqs. (65), (66) and the polarizabilities of ions Eqs. (70), (71), (72) were modulated with incommensurate period too

\[ F_{nk}^{a} = F_{ka}(q'n + \varphi), \]  

\[ Z_{nk}^{a\beta}(\omega) = Z_{k}^{a\beta}(\omega, q'n + \varphi). \]  

(83)

The renormalized elements of matrix interactions \(\tilde{\psi}\) as well as dependd from \(\varphi\) phase were transformed with respect into superspace group of symmetry:

for the \(((R_{i}k), (R_{j}|V))\) element we have

\[ \tilde{\psi}_{\alpha\beta}(ml, m'l', \varphi') = \sum_{\nu\nu'} R_{\nu\nu'} R_{\beta\nu'} \tilde{\psi}_{\nu\nu'}(nk, n'k', \varphi), \]  

(84)

where

\[ m + \mathbf{r}_{i} = \tilde{R}(\mathbf{n}\mathbf{r}_{i}) + \mathbf{t}_{R}, \]  

\[ m' + \mathbf{r}_{j} = \tilde{R}(\mathbf{n}\mathbf{r}_{j}) + \mathbf{t}_{R}, \]  

(85)

\[ \varphi' = R_{j}\varphi + V_{g}, \]

but for the translation subgroup \(((E) - m), (1|q'|m))\)

\[ \tilde{\psi}_{\alpha\beta}(nk, n'k', \varphi) = \tilde{\psi}_{\alpha\beta}(n - m, k; n' - m, k'; q'|m + \varphi). \]  

(86)

The dipole-dipole Green function Eqs. (74) is depended from \(\varphi\) phase and transforms with respect into superspace group of symmetry:

for \(((R_{i}k), (R_{j}|V))\) element

\[ \langle \langle D_{ml}^{a}|D_{m'l'}^{\beta} \rangle \rangle_{\omega, \varphi'} = \sum_{\nu\nu'} R_{\nu\nu'} R_{\beta\nu'} \langle \langle D_{nk}^{\nu}|D_{n'k'}^{\nu'} \rangle \rangle_{\omega, \varphi}, \]  

(87)

but for translations subgroup

\[ \langle \langle D_{nk}^{a}|D_{n'k'}^{\beta} \rangle \rangle_{\omega, \varphi} = \langle \langle D_{n-m,k}^{a}|D_{n-m,k'}^{\beta} \rangle \rangle_{\omega, \varphi + q'|m}. \]  

(88)

For the defining of non-zero components of gyrotrropy birefringence tensor as well as gyration tensor the Fourier transformations of Green functions Eqs. (88) have been necessary found.
\[
\frac{1}{N} \sum_{m'n'} \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi} \exp^{i(k'n' - k\mathbf{n})},
\]
where sum with respect into \(n\) and \(n'\) calculates \(N\) elements of unit cells. Hence we have found (view of subsection of Appendix)

\[
\frac{1}{N} \sum_{m'n'} \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi} \exp^{i(k'n' - k\mathbf{n})} = \frac{1}{N} \sum_{m'n'} \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi + q\mathbf{n}} \exp^{i(k'n' + (k\mathbf{n})} = \frac{1}{N} \sum_{\Phi} \Phi_{k\alpha,k'\beta}(\omega, k; h) \exp^{i\omega \cdot q} \Delta(k' - k + hq'),
\]
where

\[
\Phi_{k\alpha,k'\beta}(\omega, k; h) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi'} \exp^{i\omega \cdot \mathbf{n}}.
\]
At \(k = k' \neq 0\)

\[
\frac{1}{N} \sum_{m'n'} \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi} \exp^{ik(n-n')} = \Phi_{k\alpha,k'\beta}(\omega, k) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi'} \exp^{i\omega \cdot \mathbf{n}}
\]
but at \(k = k' = 0\)

\[
\frac{1}{N} \sum_{m'n'} \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi} \exp^{ik(n-n')} = \Phi_{k\alpha,k'\beta}(\omega, k = 0) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \langle \langle D_{mk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi'}
\]
The Fourier transforms of the expressions Eqs. (92), (93) are independed from \(\varphi\) phase and can be averaged with respect to \(\varphi\) concerning of period.

We have found Fourier transformations Eq. (90) for Eqs. (75), (76), (77)

\[
\Phi^{(1)}(\omega, k, h) = 2\pi \Phi^{(0)}(\omega, k + hq') (Z_0^{-1}(\omega)Z_1(\omega|h)Z_0^{-1}(\omega) - \psi^{(1)}(k,h)) \Phi^{(0)}(\omega, k),
\]

\[
\Phi^{(2)}(\omega, k, h) = 2\pi \Phi^{(0)}(\omega, k + hq') (Z_0^{-1}(\omega)Z_1(\omega|h)Z_0^{-1}(\omega) - \psi^{(2)}(k,h) - Z_0^{-1}(\omega) \sum_\alpha \psi^{(1)}(k,h_{\alpha}) - 2\pi \Phi^{(0)}(\omega, k + hq') \sum_\alpha \psi^{(1)}(k,h_{\alpha}) + \psi^{(1)}(k+hq',h-h_1)) \Phi^{(0)}(\omega, k),
\]

where

\[
Z_{\alpha j}^{\alpha j}(\omega|h) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi Z_{\alpha j}^{\alpha j}(\omega, \varphi) \exp^{-i\omega \cdot \mathbf{n}},
\]

\[
\psi^{(j)}_{\alpha j}(k, h) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi (\sum_\alpha \psi^{(j)}_{\alpha j}(0k, ml, \varphi) \exp^{i\omega \cdot \mathbf{n}}) \exp^{-i\omega \cdot \mathbf{n}}.
\]
The presence of a modulation wave display itself in the ionic contributions \(Z_1\) conditioned by nonlinear polarizabilities in the crystalline contributions conditioned by anharmonicities and in the mixed contributions which were proportional to \(Z_1 \psi^{(1)}\).

Hence the symmetry of the tensor \(e_{\alpha j}^{(0)}(\omega, k = 0)\) in the incommensurate phase is the same as in the initial hight temperature phase. This result is correct in the presence of external field (electric, magnetic and mechanical strains).

### 4.4 Symmetry of \(K_2SeO_4\) Incommensurate phases crystals

Let us known the symmetry of \(K_2SeO_4\) crystal. Above \(T_1\) temperature the symmetry these crystals was defined by \(D_{16h}\)Pnam space group. The phase transition from high temperature commensurate phase in incommensurate phase conditioned the breaking of crystal equilibrium in \(T_1\) point and Brillouin zone point defined by wave vector \(q' = \frac{1}{N}(1 - \delta)a^*\) (where \(N = 2\) for \((NH_4)_2BeF_4\) and \((N(CH_3)_4)_2MnCl_4\); \(N = 3\) for \(K_2SeO_4\), \(Rb_2ZnCl_4\) [8]) but coherent phonon oscillations amplitude \(Q(q', \Sigma_2)\) with defined symmetry of phonon oscillations \(\Sigma_2\) was main order parameter of phase transition.

Secondary of order parameters which satisfied Eq. (55) are [8]

\[
\begin{align*}
Q(q_1, \Sigma_1) & \rightarrow Q^2(q_1, \Sigma_1), \quad q_1 = 2q', \\
Q(q_2, \Sigma_2) & \rightarrow Q^2(q_2, \Sigma_2), \quad q_2 = 3q', \\
Q(q_3, \Sigma_3) & \rightarrow Q^2(q_3, \Sigma_3), \quad q_3 = 3q' - a^*, \\
Q(q_4, \Sigma_4) & \rightarrow Q^2(q_4, \Sigma_4), \quad q_4 = 2q' - a^*.
\end{align*}
\]

The eigenvectors have next components [8] for translation ionic displacements
\[ e_k^{(r)}(q, \Sigma_1) = (e_{kx}^{(r)}(q, \Sigma_1), e_{ky}^{(r)}(q, \Sigma_1), 0), \]
\[ e_k^{(r)}(q, \Sigma_2) = (0, 0, e_{kz}^{(r)}(q, \Sigma_2)), \]
\[ e_k^{(r)}(q, \Sigma_3) = (0, 0, e_{kz}^{(r)}(q, \Sigma_3)), \]
\[ e_k^{(r)}(q, \Sigma_4) = (e_{kx}^{(r)}(q, \Sigma_4), e_{ky}^{(r)}(q, \Sigma_4), 0), \]
\[ e_k^{(r)}(q, \Sigma_5) = (e_{kx}^{(r)}(q, \Sigma_5), e_{ky}^{(r)}(q, \Sigma_5), 0). \]

as well as for rotation motions of ionic group

\[ e_k^{(r)}(q, \Sigma_1) = (e_{kx}^{(r)}(q, \Sigma_1), e_{ky}^{(r)}(q, \Sigma_1), 0), \]
\[ e_k^{(r)}(q, \Sigma_2) = (0, 0, e_{kz}^{(r)}(q, \Sigma_2)), \]
\[ e_k^{(r)}(q, \Sigma_3) = (0, 0, e_{kz}^{(r)}(q, \Sigma_3)), \]
\[ e_k^{(r)}(q, \Sigma_4) = (e_{kx}^{(r)}(q, \Sigma_4), e_{ky}^{(r)}(q, \Sigma_4), 0). \]

Hence the initial self-consistent crystal field \( F_{nk}^{\prime} \) have in incommensurate phase the same symmetry like symmetry of translation displacement of ions.

Hence for \( K_2SeO_4 \) the non-zero components were \( \epsilon_{12} \) gyrotropy birefringence tensor and \( g_{33} \) gyration tensor specifically from above found results Eqs. (100), (101) but the numerical magnitudes these tensors we have found from experimental data [6].

It is known [8] that temperature law of order parameter \( Q(q^l \Sigma_2) \) in \( K_2SeO_4 \) has good agreement with \( n = 2 \) rank of matrix of Landau-Ginsburg-Vilson Hamiltonian for which

\[ Q(q^l \Sigma_2) \sim (T_f - T^\beta), \]

has been found, where \( T_f \)-Curie temperature, where \( \beta = 0.35 \). But the experimental results of gyrotropy birefringence in incommensurate phase

\[ \Delta n_c \sim (T_f - T)^{2\beta}, \]

have been predicted, where \( 2\beta = 0.75 \) for \( K_2SeO_4 \) as well as \( 2\beta = 0.72 \) for \( Rb_2ZnCl_4 \) defined from \( \Phi^{(2)}_{kx,k'/\rho}(\omega, k = 0, h = 0) \) contribution.

4.5 Appendix

The theoretical justification of transformations Eqs. (90), (91) one can find in the subsection for \( q^l \) incommensurate wave vector and arbitrary integrable concerning the Riemannian periodic function \( f(\varphi) = f(\varphi + 2\pi) \) in the limit \( N \rightarrow \infty \) we have found

\[ \frac{1}{N} \sum_n f(\varphi + q^l n) \exp(i kn) = \sum_{h} \left( \frac{1}{2\pi} \int_0^{2\pi} f(\varphi') \exp(i k\varphi') \Delta(k + hq^l) \right), \]

where

\[ \Delta(k) = i^{1,k=0,G}. \]

\( G \) is inverse lattice vector.

Let us known the \( d = 1 \) one-dimensional modulation. For the incommensurate of \( q^l = \delta a^* \) wave vector the order parameter \( \delta \) can be presented in the form \( \delta = \frac{N_1}{N_0}, \) where \( N_1 \) and \( N_0 \) are integers which have no common divisor and \( \lim_{N_1,N_0 \rightarrow \infty} \frac{N_1}{N_0} = \delta. \) Let us known in crystal the main region which includes \( N_0 \) cells along \( a \) and we have imposed the Born von Karman periodic boundary conditions. Then for wave vector \( k \) we have

\[ k = \frac{m}{N_0} a^* \quad (m = 0, 1, \ldots, N_0 - 1), \]

but for the vector of incommensurate phase

\[ q^l = \frac{N_1}{N_0} a^*. \]

The expression Eq. (104) if based on Eqs. (106), (107) can be rewritten in the form

\[ \frac{1}{N_0} \sum_{n=0}^{N_0-1} f(\varphi + 2\pi \frac{N_1}{N_0} n) \exp(i(2\pi \frac{m}{N_0} n)) = \frac{1}{N_0} \sum_{n=0}^{N_0-1} f(\varphi + 2\pi \frac{N_1}{N_0} n) \exp(i(2\pi \frac{m}{N_0} n)), \]

where at \( \{..\} \) has been accounted fractional part of number.

We have found that for \( 0 \leq n \leq N_0 - 1 \) the sets \( \frac{n}{N_0} \) and \( \{\frac{n}{N_0}\} \) are equivalents. The study sets include \( N_0 \) elements from the interval \([0, 1]\) and the study sets can be like to single-valued correspondence as well as the study sets can not be like to single-valued correspondence. In the second case one can find the such \( n_1 \neq n_2 \) that
\[ \{ \frac{N_1}{N_0} n_1 \} = \{ \frac{N_2}{N_0} n_2 \}. \]  

Then

\[ \frac{N_1}{N_0} n_1 - \frac{N_2}{N_0} n_2 = M, \quad (M \in Z), \]

or \( N_1(n_1 - n_2) = MN_0 \). If \( N_1 \) and \( N_0 \) have no common divisor we have found

\[ n_1 - n_2 = MN_0, \quad (M_1 \in Z). \]

At \( n_1 \geq 0 \), \( N_0 - 1 \geq n_2 \) the latter expression is true only for \( M_1 = 0 \) i.e. \( n_1 = n_2 \) and so we have found contradiction. Hence we have found that the first case is true and the formula Eq. (108) can be rewritten in the form

\begin{align*}
\sum_{-\infty < h < 0} \frac{1}{N_0} \sum_{n=0}^{N_0-1} f \left( \varphi + \frac{2\pi n}{N_0} \right) \exp \left( -i h \left( 2\pi n + \frac{2\pi N_0}{h} \right) \right) \Delta \left( \frac{N_0}{N_0} - 1 \right) = \\
\sum_{-\infty < h < 0} \frac{1}{N_0} \sum_{n=0}^{N_0-1} f \left( \varphi + \frac{2\pi n}{N_0} \right) \exp \left( -i h \left( \varphi + \frac{2\pi N_0}{h} \right) \right) \exp h \Delta (k + hq), 
\end{align*}

(112)

where we impose the identity

\[ \exp \left( i 2\pi \frac{n}{N_0} \right) = \sum_{-N_0/2 < h \leq N_0/2} \exp \left( -i 2\pi \frac{Mh}{N_0} \right) \Delta \left( \frac{M}{N_0} - a \right). \]

(113)

We have entered in Eq. (112) the following key \( \Delta \varphi = \frac{2\pi}{N_0}, \varphi_n = \frac{2\pi}{N_0} n = n\Delta \varphi \) we have found the Riemann integral in Eq. (112) in limit \( N_0 \rightarrow \infty \). Hence Eq. (104) is true.

References


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