Giant nature optical activity coupled with incommensurate phase transition and integer quantum Hall effect in Weil 2D half layered materials: Group-VI Dichalcogenides and Rb$_2$ZnBr$_4$, Ca$_2$RuO$_4$, Cr$_2$O$_3$, MnTiO$_3$, La-doped BiFeO$_3$, PtCl$_3$, PdBr$_3$, RuCl$_3$, PtI$_3$

Available online 13 March 2020: https://communities.acs.org/people/LiubovLokot/content

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Abstract In the article we have found that the Weyl Hall semiconductor (WHS) states allow the topological phase transition happened between two quantum anomalous Hall (QAH) insulator phase with opposite Chern numbers and we have based on phonon dispersion of Weil 2D half semiconductor monolayers group like PtCl$_3$. Landau-Ginzburg-Devonshire theory of thin ferroelectric polar-active nanofilms in incommensurate phases and semiconductor heterostructures is presented. The self-consistent solutions of the Euler-Lagrange equation for the polarization vector and 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. 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 $D_{16}^{2h}$ or isomorphic groups. In the paper the non-zero gyration $g_{33}$ and gyrotropic birefringence $\varepsilon_{12}$ tensors of K$_2$SeO$_4$ and Rb$_2$ZnBr$_4$ materials based on $D_{16}^{2h}$ space symmetry group were found. The values of natural optical gyrotropy as well as Rashba spin splitting are shown to be specified like $(\kappa(0) \pm \tilde{\kappa}(2))^2$ as displacements of two symmetrically allocated parabolas from Brillouin zone center. Hence if sine-type edges of Group-VI Dichalcogenides and Rb$_2$ZnBr$_4$, Ca$_2$RuO$_4$, Cr$_2$O$_3$, MnTiO$_3$, La-doped BiFeO$_3$, PtCl$_3$, PdBr$_3$, RuCl$_3$, PtI$_3$, and carbon nanoribbons may be approximated armchair or zigzag edges then in the sections 5 are found that structure phase transitions to be related with giant spin-orbit interaction (SOI). In the article a creation of giant spin-orbit splitting (\sim 2.5 eV) coupled with the carbon Dirac cones (K and K') are shown to be related with structure phase transition in carbon nanoribbon with armchair or zigzag edges of honeycomb lattice of Group-VI Dichalcogenides and Rb$_2$ZnBr$_4$, Ca$_2$RuO$_4$, Cr$_2$O$_3$, MnTiO$_3$, La-doped BiFeO$_3$, PtCl$_3$, PdBr$_3$, RuCl$_3$, PtI$_3$, and carbon nanoribbons. In the article the natural optical gyrotropy effects are shown to be found with light velocity like $e = \hbar c k/eV = 14.0798$ eV, $e = \hbar c k/eV = 27.6009$ eV, $e = \hbar c k/eV = 7.5726$ eV, with the corresponding considered in Tables 4,5,6 of gyrotropic birefringences $\Delta n_{11}$ and gyrotropies g.

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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.
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## 2 Introduction

It is known [1] 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 [1]. 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 [1].

The optical activity in Rb₂ZnBr₄, Rb₂ZnCl₄, K₂SeO₄, (NH₄)₂BeF₄, (N(CH₃)₄)₂MnCl₄ crystals has been measured along three directions in a temperature interval from 400K to 50K [2]. 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 [2]. In order to explain this phenomenological space dependent dielectric and gyration tensors being invariant with respect to the superspace group of Rb₂ZnBr₄, Rb₂ZnCl₄, K₂SeO₄, (NH₄)₂BeF₄, (N(CH₃)₄)₂MnCl₄ have been considered [2, 3, 4, 5, 6, 7, 8, 9]. 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 [3, 2, 6]. The Euclidean symmetry of these systems was not a three-dimensional space group but a four-dimensional superspace groups [3, 2, 4, 5, 6].

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 Δ = \( \frac{\hbar}{2m_0c^2} \langle \psi_x | (V \times p_x) \rangle \psi_y \), where V is the microscopic crystal potential of graphene. In graphene we would have Δ = 0 if the basis functions |ψₓ⟩ and |ψᵧ⟩ were made up on basis of pure π or (pₓ) orbitals. However spin-orbit coupling induces a mixing of the π or (pₓ) and σ or (pₓ, pᵧ) orbitals in graphene that contributes to Δ in second order of spin-orbit coupling. In the our case [10, 11, 12, 13, 14, 15, 16, 17, 18, 19] the strain mediates a coupling between intrinsic-spin and orbital dynamics and the lowest order contribution \( p_{xy}^{(2)}(c_{xx} + c_{yy}) \delta_{xy} \sigma_z \) constitutes a renormalization of the intrinsic spin-orbit coupling \( p_{xy}^{(2)} \delta_{xy} \). In the article [20] 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 ~ 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 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 [4]

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

(1)

The tensor \( \epsilon_{\alpha\beta}(\omega, k = 0) \) is expressed by the two-time retarded Green functions [4],

\[
\epsilon_{\alpha\beta}(\omega, k = 0) = \delta_{\alpha\beta} - \frac{8\pi^2}{\nu} \sum_{\text{ion}} \langle \hat{p}_{\alpha} \hat{p}_{\beta} \rangle, 
\]

(2)
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 shirt 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 [4, 9, 21, 22, 23, 24],

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

(3)

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

\[
\hat{D}_n^{\alpha k} = \sum_{\mu} \hat{\mu}_{\alpha k}^\mu \hat{x}_{n\mu}^\nu
\]

(4)
is the operator of electron coordinates of the \( \kappa \)-type ion, written in the representation of the Hubbard operators \( \hat{x}_{n\mu}^\nu = \{nk\} \langle \nu | s' \rangle \) acting in the space of electron states \( \{\psi_{nks}\} \) of the ion, \( \hat{\mu}_{\alpha k}^\mu \) are the corresponding matrix elements, \( \hat{n}_n^\alpha \) 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

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

(5)

In the article [4] for ionic insulator crystals the Hamiltonian of ionic crystal with account electronic excitation of ions 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 \( \hat{x}_{n\mu}^\nu = \{nk\} \langle \nu | s' \rangle \) from which consist of the basis electronic states of \( \psi_{nks} \) ion in the form [4, 19, 25, 26, 27, 28, 29, 30, 14, 31, 32, 33]

\[
H = \sum_{nks} \lambda_{ks} \hat{x}_{n\mu}^\nu \hat{\mu}_{\alpha k}^\mu - \sum_{nks,nk's} \frac{1}{2} \sum_{\alpha\beta} (\psi_{nk,k'}^{\alpha\beta} (n, k, n', k') \hat{D}_{n\kappa}^{\alpha k} \hat{D}_{m\kappa'}^{\beta k'} + C_{\alpha\beta} (n, k, n', k') \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \theta_{\alpha\beta\gamma\delta} \hat{\mu}_{\alpha k}^{\mu} (n, k, n', k') \hat{\mu}_{\beta k'}^{\nu} + \hat{\mu}_{\gamma k'}^{\nu} \hat{\mu}_{\delta k}^{\mu} \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} + \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} - \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \theta_{\alpha\beta\gamma\delta} \hat{\mu}_{\alpha k}^{\mu} (n, k, n', k') \hat{\mu}_{\beta k'}^{\nu} \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} + \hat{\mu}_{\gamma k'}^{\nu} \hat{\mu}_{\delta k}^{\mu} \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'}) + \sum_{\alpha\beta\gamma\delta} \theta_{\alpha\beta\gamma\delta} \hat{\mu}_{\alpha k}^{\mu} (n, k, n', k') \hat{\mu}_{\beta k'}^{\nu} \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} + \hat{\mu}_{\gamma k'}^{\nu} \hat{\mu}_{\delta k}^{\mu} \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'})
\]

(6)

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

For the equilibrium positions \( R_{nk}^{(0)} = n + r_k \) electron wave functions \( \psi_{nks} \) 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 [4]

\[
\begin{align*}
    u_{nk}^\alpha &= \langle u_{nk}^\alpha \rangle + \tilde{u}_{nk}^\alpha, \\
    D_{nk}^\alpha &= \langle D_{nk}^\alpha \rangle + \tilde{D}_{nk}^\alpha,
\end{align*}
\]

(7)

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 [4] we have entered main field approximation [34, 35, 36]

\[
\hat{H}_{MF}^{el} = \sum_{nks} \sum_{\alpha\beta} (\lambda_{ks} \delta_{\alpha\beta} - \sum_{\mu} F_{nk}^\alpha \hat{\mu}_{\alpha k}^{\mu} \hat{x}_{n\mu}^{\nu}),
\]

(8)

where

\[
F_{nk}^\alpha = \sum_{n'k'} \frac{1}{2} (\psi_{nk,k'}^{\alpha\beta} (n, k, n', k') \hat{D}_{n\kappa}^{\alpha k} \hat{D}_{n'\kappa'}^{\beta k'} + C_{\alpha\beta} (n, k, n', k') \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \theta_{\alpha\beta\gamma\delta} \hat{\mu}_{\alpha k}^{\mu} (n, k, n', k') \hat{\mu}_{\beta k'}^{\nu} + \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} - \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \theta_{\alpha\beta\gamma\delta} \hat{\mu}_{\alpha k}^{\mu} (n, k, n', k') \hat{\mu}_{\beta k'}^{\nu} \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} + \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} - \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \theta_{\alpha\beta\gamma\delta} \hat{\mu}_{\alpha k}^{\mu} (n, k, n', k') \hat{\mu}_{\beta k'}^{\nu} \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'} + \hat{n}_n^{\alpha k} \hat{n}_{n'}^{\beta k'})
\]

(9)

It is known that the Hamiltonian \( \hat{H}_{MF}^{el} \) describes the influence crystal field of lattice \( F_{nk}^\alpha \) on electronic states of ions [16, 37, 38, 39, 40].

In order to obtain from the Hamiltonian \( \hat{H}_{MF}^{el} \) the diagonal matrices we have considered the unitary transformation

\[
\hat{x}_{n\mu}^{\nu} = \sum_{\mu'\nu'} u_{nk}^{\mu'\nu'} \hat{x}_{n\mu'\nu'}
\]

(10)

where \( u_{nk}^{\mu'\nu'} \) were eigenvectors which were found from equations system

\[
\sum_{\mu} (\lambda_{ks} \delta_{\mu\nu} - \sum_{\alpha} F_{nk}^\alpha \hat{\mu}_{\alpha k}^{\mu}) u_{nk}^{\mu} = \tilde{\lambda}_{nk} u_{nk}^{\mu},
\]

(11)

Hence
H_{\text{MF}}^{\alpha} = \sum_{\nu \mu} \alpha_{\nu \mu} \hat{X}_{\nu \mu}^{\mu}, \quad (12)

where \( \lambda_{\nu \mu} \) were new energy levels splitting by Stark effect [41, 42, 38, 43, 44, 45, 46, 47]. We have transformed \( D_{nk}^{\alpha} \) operators into the form

\[ D_{nk}^{\alpha} = \sum_{\mu \nu} \tilde{\mu}_{nka}^{\mu \nu} X_{\mu \nu}^{\nu}, \quad (13) \]

\[ \tilde{\mu}_{nka}^{\mu \nu} = \sum_{\alpha \beta \gamma \delta \epsilon \zeta} \delta_{\mu \alpha} \delta_{\nu \beta} \delta_{\delta \gamma} \delta_{\epsilon \zeta} u_{\alpha \beta \gamma \delta \epsilon \zeta}^{\nu \mu}, \quad (14) \]

We have presented dipole-dipole Green function on the based Eqs. (13), (14) in the form

\[ \langle \langle D_{nk}^{\alpha} | D_{nk'}^{\beta} \rangle \rangle_\omega = \sum_{\mu \nu \mu' \nu'} \mu_{nka}^{\mu \nu} \delta_{\mu \mu'} \delta_{\nu \nu'} \langle \langle \hat{X}_{\nu \mu}^{\mu} | \tilde{X}_{\nu' \mu'}^{\nu'} \rangle \rangle_\omega. \quad (15) \]

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

\[ (\hbar \omega - \tilde{\lambda}_{\nu \mu} + \tilde{\lambda}_{\mu \nu}) \langle \langle \hat{X}_{\nu \mu}^{\mu} | \hat{X}_{\nu' \mu'}^{\nu'} \rangle \rangle_\omega = \frac{1}{2\pi} \delta_{\eta \eta'} \delta_{\nu \nu'} \delta_{\mu \mu' \nu \mu} \delta_{\nu \nu'} \delta_{\alpha \alpha'} (\hat{X}_{\nu \mu}^{\mu} - \hat{X}_{\nu' \mu'}^{\nu'}) - \sum_{\gamma \delta \epsilon \zeta} \mu_{nka}^{\mu \nu} \delta_{\mu \mu'} \delta_{\nu \nu'} \delta_{\alpha \alpha'} \langle \langle \hat{X}_{\nu \mu}^{\mu} \rangle \rangle_\omega, \quad (16) \]

\[ \tilde{\psi}_{\alpha \beta}(\nu, \eta') = \psi_{\alpha \beta}(\nu, \eta') - \sum_{\gamma \delta \epsilon \zeta} \mu_{nka}^{\mu \nu} \delta_{\mu \mu'} \delta_{\nu \nu'} \delta_{\alpha \alpha'} \langle \langle \hat{X}_{\nu \mu}^{\mu} \rangle \rangle_\omega - \frac{1}{2\pi} \delta_{\eta \eta'} \delta_{\nu \nu'} \delta_{\mu \mu'} \delta_{\alpha \alpha'} (\hat{X}_{\nu \mu}^{\mu} - \hat{X}_{\nu' \mu'}^{\nu'}). \quad (17) \]

Hence we have derived Tyablickov uncoupling \( \langle \langle u | \hat{X} \rangle \rangle \) as well as we have used the expressions with \( \langle \langle \hat{u} \hat{X} \rangle \rangle \) Green function as well as we have uncoupled \( \langle \langle \hat{u} \hat{u} \rangle \rangle \) and \( \langle \langle \hat{u} \rangle \rangle \) in additions.

Hence we have derived the Bethe-Salpeter equations \([48, 49, 50]\) for Green function in the form

\[ \langle \langle D_{nk}^{\alpha} | D_{nk'}^{\beta} \rangle \rangle_\omega = \frac{1}{2\pi} \delta_{\mu \mu'} \delta_{\nu \nu'} \langle \langle \hat{X}_{\nu \mu}^{\mu} | \hat{X}_{\nu' \mu'}^{\nu'} \rangle \rangle_\omega = - \sum_{\gamma \delta \epsilon \zeta} \psi_{\gamma \delta \epsilon \zeta}(\nu, \eta') \langle \langle \hat{X}_{\nu \mu}^{\mu} \rangle \rangle_\omega, \quad (18) \]

\[ \tilde{Z}_{nk}^{\nu \mu}(\omega) = \sum_{\mu \nu \mu' \nu'} \tilde{\mu}_{nka}^{\mu \nu} \delta_{\mu \mu'} \delta_{\nu \nu'} \langle \langle \hat{X}_{\nu \mu}^{\mu} \rangle \rangle_\omega - \langle \langle \hat{X}_{\nu \mu}^{\mu} \rangle \rangle_\omega, \quad (19) \]

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

### 3.1 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 \( q^i \) point of Brillouin zone \([4, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 36]\). At these the created structure which displaced low temperature \( T_i \) of phase transition were described for the phase transition of displacement type in \( K_2SeO_3 \) the modulation wave of ions displacement \( u_{nk} = U_i(q^i n + \varphi) \) but for the phase transition order-orderless in \( NaNbO_4 \) by the modulation wave of occupation probability of single ion the one from several equilibrium location \( p_{nk} = p_k(q^i n + \varphi) \), 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 \( U_i(q^i) \) and \( p_k(q^i) \) are periodic functions of phase \( \varphi \) with \( 2\pi \) period.

Hence like for phase transition of displacement type thus for the phase transition of order-orderless the average displacement of ions \([64, 34, 14, 65, 66, 67, 68]\) in incommensurate phase can be presented in the form

\[ \langle u_{nk} \rangle = C_k(q^i n + \varphi), \quad (20) \]

where \( \varphi \) = \( \varphi + 2\pi \). Since the wave vector \( q^i \) is incommensurate with inverse lattice vector, (i.e. does not exist of like these integer \( M \) and \( N \)) for which

\[ Nq^i + M a^* = 0, \quad (21) \]

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. \( 20 \) were connected with order parameter of phase transition from commensurate phase into incommensurate phase
\[ \langle u_{nk} \rangle = \sum q_{ij} Q(q, j) e_i(q, j) \exp(iq(n + r_i)), \] (22)

where \( Q(q, j) \) order parameter which transforms like \( j \) irreducible representation for wave vector \( q, e_i(q, j) \) eigenvector this representation; \( \sum q_{ij} \) 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 \( Q(q, j) \) for which the symmetry allows the existing in Landau expansion for free energy such terms which are proportional to

\[ Q^n(q', j_0)Q(-q, j)\Delta(n_i q' - q_i), \] (23)

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

Since

\[ Q(q', j_0) = \eta \exp^{i\varphi}, \] (24)

and take into account the following connections \( Q(q, j) \sim Q^n(-q', j_0), q_i = n_i q' + m_i a^* \) which effluent from Eq. (23)

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

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

\[ g = ([\hat{R}(t_k)], [R|V_R]), \] (25)

where \([\hat{R}(t_k)]\) are elements of the space group of initial high-temperature commensurate phase, but \([R|V_R]\) 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

\[ g(r, \varphi) = (r', \varphi'), \] (26)

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]).\]

### 3.2 Bethe-Salpeter equation of incommensurate phase

In the initial high temperature commensurate phase \( \langle D_{nk}^a \rangle = 0, \langle u_{nk}^a \rangle = 0 \); the matrices of dipole-dipole interactions as well as Fourth constants transform with respect the space group symmetry this phase \([16, 69, 15, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80]:\)

for the element

\[ \psi_{ab}(m l, m'l') = \sum_{\nu \nu'} R_{\alpha \nu} R_{\nu' \beta} \psi_{\nu \nu'}(nk, n' k'), \] (27)

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

for translation subgroup

\[ \psi_{ab}(nk, n' k') = \psi_{ab}(n - m, k; n' - m, k'). \] (28)

Correlation functions which were build on a ionic displacements as well as electronic dipole momenta operators \([81, 82, 83, 84, 85, 86, 87, 88]\) satisfy the similar found expressions.

In low-temperature commensurate phase the non-zero averages \( \langle D_{nk}^a \rangle = d_{nk}^a = d_{nk}^a, \) and \( \langle u_{nk}^a \rangle = C_{nk}^a = C_{nk}^a \) have been created, where \( n_0 \) is lattice vector of low temperature phase but the renormalized Fourth constants \( \tilde{\psi}_{ab}(nk, n' k') \)

Eq. (17) 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 which can be presented in the form of modulation waves \([4]\)

\[ \langle u_{nk}^a \rangle = C_k^a(q' n + \varphi) = \sum_h C_k^a(h) \exp(i h + q'(n + r_i)), \] (29)

\[ \langle D_{nk}^a \rangle = d_k^a(q' n + \varphi) = \sum_h d_k^a(h) \exp(i h + q'(n + r_i)), \] (30)

where \( q' \) is the wave vector of the incommensurate structure, \( C_k^a(\varphi) \) and \( d_k^a(\varphi) \) are periodic functions of phase \( \varphi, h \) is an integer.

The renormalized Fourth constants \( \tilde{\psi}_{ab}(nk, n' k') \) Eq. (17) and crystal fields of lattice Eq. (9) enclose the following components

\[ \tilde{\psi} = \psi + \psi^{(1)}(1 + \psi^{(2)}(2) + \ldots, \] (31)
\[ F = F^{(1)} + (F^{(2)} + F^{(2)}) + ..., \]  

which

\[ \psi^{(1)} = -\sigma^{D} X(u), \]
\[ \psi^{(2)} = -\frac{1}{2} \theta(u) \langle u \rangle, \]
\[ F^{(1)} = \psi(D) + C(u), \]
\[ F^{(2)} = -\sigma^{D} X(D) \langle u \rangle - \frac{1}{2} \sigma^{D} \langle u \rangle, \]

the contributions from equilibrium displacements,

\[ \psi^{(2)} = -\frac{1}{2} \theta \langle u \tilde{u} \rangle, \]
\[ F^{(2)} = -\sigma^{D} \langle D \tilde{u} \rangle - \frac{1}{2} \sigma^{D} \langle u \tilde{u} \rangle, \]

the contributions which connected from correlation displacements in incommensurate phase.

The crystal field of lattice Eq. (32) as well as the matrix elements Eq. (14) and the energy levels \( \lambda_{\text{hkl}} \) defined by Eq. (11) in incommensurate phase vary from cell to cell. A distant from the edge of transparent region and for weak internal self-consistent crystal field of lattice the polarizability of ion (ionic group) Eq. (19) can expand in series with respect to power of intrinsic crystal fields of lattice

\[ \tilde{Z}^{a\beta}_{nk}(\omega) = Z^{a\beta}_{0,k}(\omega) + \sum_{\gamma} \sum_{l,k} \alpha^{a\beta}_{\gamma l} F^{(1)\gamma}_{nk} + \frac{1}{2} \sum_{l,k} \sum_{\gamma} \sum_{l,k} \alpha^{a\beta}_{\gamma l} F^{(1)\gamma}_{nk} F^{(2)\gamma}_{nk} + ... \]  

where

\[ Z^{a\beta}_{0,k}(\omega) = \sum_{\gamma} \mu^{a\beta}_{\gamma l}(\omega) X^{ss}_{nk}(\omega) X^{s\prime s\prime}_{nk}(\omega). \]

Let us known Eq. (35) in the form of sum of contributions caused different components of field \( F^{a}_{nk} \) Eq. (32),

\[ \tilde{Z}^{a\beta}_{nk}(\omega) = Z^{a\beta}_{0,k}(\omega) + Z^{a\beta}_{1,nk}(\omega) + (Z^{a\beta}_{2,nk}(\omega) + \tilde{Z}^{a\beta}_{nk}(\omega)), \]

\[ Z^{a\beta}_{1,nk}(\omega) = \sum_{\gamma} \sum_{l,k} \alpha^{a\beta}_{\gamma l} F^{(1)\gamma}_{nk} F^{(1)\gamma}_{nk} , \]

\[ Z^{a\beta}_{2,nk}(\omega) = \sum_{\gamma} \sum_{l,k} \sum_{\gamma} \sum_{l,k} \alpha^{a\beta}_{\gamma l} F^{(1)\gamma}_{nk} F^{(1)\gamma}_{nk} \]

On the basis of Eq. (31) and Eq. (37) the Green function which satisfy of equation Eq. (18) 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

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

but the remainder contributions in Eq. (41) we have found as

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

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

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

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

where Eq. (43), Eq. (44) were corrections linear and quadratic \( \langle u \rangle \) and \( \langle D \rangle \), Eq. (45) is correction which was proportional correlation functions \( \langle \tilde{u} \tilde{u} \rangle \) and \( \langle \tilde{D} \tilde{u} \rangle \).
3.3 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. (2) and Eq. (5) in the form

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

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

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

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

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

\( \Phi_{k\alpha,k'\beta}^{0}(\omega, k = 0) \) can be found from Eq. (42)

\[
\Phi_{k\alpha,k'\beta}^{0}(\omega, k) = \frac{1}{2\pi} \delta_{kk'} z_{\alpha\beta}^{q}(\omega) - \sum_{q} z_{\alpha\beta}^{q}(\omega) \sum_{l,\delta} \psi_{k\gamma,l,\delta}(k) \Phi_{l,\delta,k'\beta}^{0}(\omega, k),
\]

\[
\psi_{k\gamma,l,\delta}(k) = \sum_{n-n'} \psi_{\gamma}(nk, n'k') \exp^{-ik(n-n')}. \tag{50}
\]

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 [89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102] were defined by modulation waves Eqs. (29), (30) as well as an internal self-consistent crystal fields of lattice Eqs. (33), (34) and the polarizabilities of ions Eqs. (38), (39), (40) were modulated with incommensurate period too

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

\[
Z_{nk}^{a\beta}(\omega) = Z_{k}^{\alpha}(\omega, q'n + \varphi). \tag{51}
\]

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

for the \( ((\hat{R}|t_{R}), (R|V)) \) element we have

\[
\hat{\psi}_{ab}(ml, m'l', \varphi') = \sum_{vv'} R_{a\nu} R_{\beta
u'} \psi_{vv'}(nk, n'k', \varphi),
\]

where

\[
\begin{align*}
m + r_{i} &= \hat{R}(nr_{i}) + t_{R}, \\
m' + r_{i'} &= \hat{R}(nr_{i'}) + t_{R}, \\
\varphi' &= R_{i}\varphi + V_{R}.
\end{align*} \tag{53}
\]

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

\[
\hat{\psi}_{ab}(nk, n'k', \varphi) = \hat{\psi}_{ab}(n - m, k; n' - m, k'; q'm + \varphi). \tag{54}
\]

The dipole-dipole Green function Eq. (42) is depended from \( \varphi \) phase and transforms with respect into superspace group of symmetry:

for \( ((\hat{R}|t_{R}), (R|V_{R})) \) element

\[
\langle D_{ml}^{a} | D_{m'l'}^{\beta} \rangle_{\omega, \varphi'} = \sum_{vv'} R_{a\nu} R_{\beta
u'} \langle D_{ml}^{v} | D_{m'l'}^{\nu'} \rangle_{\omega, \varphi}, \tag{55}
\]

but for translations subgroup

\[
\langle D_{nk}^{a} | D_{n'k'}^{\beta} \rangle_{\omega, \varphi} = \langle D_{n-m,k}^{a} | D_{n'-m,k'}^{\beta} \rangle_{\omega, \varphi + q'm}. \tag{56}
\]

For the defining of non-zero components of gyrotrypt birefringence tensor as well as gyration tensor the Fourier transformations of Green functions Eq. (56) have been necessary found.

\[
\frac{1}{N} \sum_{n'n'} \langle D_{nk}^{a} | D_{n'k'}^{\beta} \rangle_{\omega, \varphi} \exp^{i(k'n' - kn)}, \tag{57}
\]

where sum with respect into \( n \) and \( n' \) calculates \( N \) elements of unit cells. Hence we have found (view of subsection of Appendix)
\[
\frac{1}{N} \sum_{\text{nnr}} \langle \langle D_{nk}^a | D_{n'k'}^\beta \rangle \rangle_{\omega',\varphi} \exp^{i(k' - k)n} = \frac{1}{N} \sum_{\text{nnr}} \langle \langle D_{nk}^a | D_{n'k'}^\beta \rangle \rangle_{\omega',\varphi} \exp^{i(k' - k)n} = 0
\]
where
\[
\Phi_{k',k'}(\omega, k; h) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \left( \sum_{\omega'} \langle \langle D_{n'k'}^a | D_{n'k'}^\beta \rangle \rangle_{\omega',\varphi'} \exp^{i\omega n} \right). \tag{59}
\]
At \(k = k' \neq 0\)
\[
\frac{1}{N} \sum_{\text{nnr}} \langle \langle D_{n}^a | D_{n'}^\beta \rangle \rangle_{\omega,\varphi} \exp^{i\omega(n-n')} = \Phi_{k',k}(\omega, k) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \left( \sum_{\omega'} \langle \langle D_{n}^a | D_{n'}^\beta \rangle \rangle_{\omega',\varphi'} \exp^{i\omega n} \right), \tag{60}
\]
but at \(k = k' = 0\)
\[
\frac{1}{N} \sum_{\text{nnr}} \langle \langle D_{n}^a | D_{n'}^\beta \rangle \rangle_{\omega,\varphi} \exp^{i\omega(n-n')} = \Phi_{k,0}(\omega, k = 0) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \left( \sum_{\omega'} \langle \langle D_{n}^a | D_{n'}^\beta \rangle \rangle_{\omega',\varphi'} \right). \tag{61}
\]
The Fourier transforms of the expressions Eqs. (60), (61) are independent from \(\varphi\) phase and can be averaged with respect to \(\varphi\) concerning of period.

We have found Fourier transformations Eq. (58) for Eqs. (43), (44), (45)
\[
\Phi^{(1)}(\omega, k, h) = 2\pi \Phi^{(0)}(\omega, k + hq') (Z_{1}^{-1}(\omega) Z_{2}(\omega) h) Z_{1}^{-1}(\omega) - \psi^{(1)}(k, h) \Phi^{(0)}(\omega, k), \tag{62}
\]
\[
\Phi^{(2)}(\omega, k, h) = 2\pi \Phi^{(0)}(\omega, k + hq') (Z_{1}^{-1}(\omega) Z_{2}(\omega) h) Z_{1}^{-1}(\omega) - \psi^{(1)}(k, h) - Z_{1}^{-1}(\omega) \psi^{(1)}(k + h, h') \Phi^{(0)}(\omega, k) - 2\pi \Phi^{(0)}(\omega, k + hq') \sum_{\text{nnr}} \psi^{(1)}(\omega, k + h, h') \Phi^{(1)}(\omega, k, h'), \tag{63}
\]
where
\[
Z^{ab}_{i,j}(\omega) h = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \left( Z^{ab}_{i,j}(\omega, \varphi) \exp^{i(h\varphi)} \right), \tag{65}
\]
\[
\psi^{(j)}(k, h, l) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \left( \sum_{ml} \psi^{(j)}(0k, ml, 0) \exp^{i(km\varphi)} \exp^{i(h\varphi)} \right). \tag{66}
\]
The presence of a modulation wave display itself in the ionic contributions \(Z_{i}\) conditioned by nonlinear polarizabilities in the crystalline contributions conditioned by anharmonicities and in the mixed contributions which were proportional to \(Z_{1}\).

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

### 3.4 Symmetry of \(K_{2}SeO_{4}\) Incommensurate phases crystals

Let us known the symmetry of \(K_{2}SeO_{4}\) crystal. Above \(T_{c}\) temperature the symmetry these crystals was defined by \(D_{2h}^{16}\) Pnma space group. The phase transition from high temperature commensurate phase in incommensurate phase conditioned the breaking of crystal equilibrium in \(T_{c}\) point and Brillouin zone point defined by wave vector \(q' = \frac{1}{N}(1 - \delta)\alpha\) ( where \(N = 2\) for \((NH_{4})_{2}BeF_{4}\) and \((NH_{4})_{2}MnCl_{4}\); \(N = 3\) for \(K_{2}SeO_{4}, Rb_{2}ZnCl_{4}\) [4]) 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. (23) are [4]
\[
Q(q_{1}, \Sigma_{1}) \longrightarrow Q^{2}(q_{1}, \Sigma_{2}), \quad q_{1} = 2q',
\]
\[
Q(q_{2}, \Sigma_{2}) \longrightarrow Q^{2}(q_{2}, \Sigma_{2}), \quad q_{2} = 3q',
\]
\[
Q(q_{3}, \Sigma_{3}) \longrightarrow Q^{2}(q_{2}, \Sigma_{2}), \quad q_{3} = 3q' - \alpha',
\]
\[
Q(q_{4}, \Sigma_{4}) \longrightarrow Q^{2}(q_{4}, \Sigma_{2}), \quad q_{4} = 2q' - \alpha'.
\]

The eigenvectors have next components [4]
for translation ionic displacements
\[
e^{(i)}(q, \Sigma_{1}) = (e^{(i)}_{\alpha}(q, \Sigma_{1}), e^{(i)}_{\beta}(q, \Sigma_{1}), 0),
\]
\[
e^{(i)}(q, \Sigma_{2}) = (0, 0, e^{(i)}_{\alpha}(q, \Sigma_{2})),
\]
\[
e^{(i)}(q, \Sigma_{3}) = (0, 0, e^{(i)}_{\beta}(q, \Sigma_{3})),
\]
\[
e^{(i)}(q, \Sigma_{4}) = (e^{(i)}_{\alpha}(q, \Sigma_{4}), e^{(i)}_{\beta}(q, \Sigma_{4}), 0),
\]
\[
(67)
\]
\[
(68)
\]
as well as for rotation motions of ionic group

\[
e_{k}^{(r)}(q, \Sigma) = (e_{kx}^{(r)}(q, \Sigma_{x}), e_{ky}^{(r)}(q, \Sigma_{y}), 0),
\]

\[
e_{k}^{(r)}(q, \Sigma_{z}) = (0, 0, e_{kz}^{(r)}(q, \Sigma_{z})),
\]

\[
e_{k}^{(r)}(q, \Sigma_{x}) = (e_{kx}^{(r)}(q, \Sigma_{x}), e_{ky}^{(r)}(q, \Sigma_{y}), 0).
\]

(69)

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

Hence for \( K_{2}SeO_{4} \) the non-zero components were \( e_{12} \) gyrotry birefringence tensor and \( g_{33} \) gyration tensor specifically from above found results Eqs. (68), (69) but the numerical magnitudes these tensors we have found from experimental data [2].

It is known [4] that temperature law of order parameter \( Q(q^{4}e_{0}) \) in \( K_{2}SeO_{4} \) has good agreement with \( n = 2 \) rank of matrix of Landau-Ginsburg-Vilson Hamiltonian for which

\[
Q(q^{4}e_{0}) \sim (T_{c} - T)^{\beta},
\]

(70)

has been found, where \( T_{c} \)-Curie temperature, where \( \beta = 0.35 \). But the experimental results of gyrotry birefringence in incommensurate phase

\[
\Delta n_{g} \sim (T_{c} - T)^{2\beta},
\]

(71)

have been predicted, where \( 2\beta = 0.75 \) for \( K_{2}SeO_{4} \) as well as \( 2\beta = 0.72 \) for \( Rb_{2}ZnCl_{4} \) defined from \( \Phi_{\kappa\alpha\kappa\rho}(\omega, k = 0, h = 0) \) contribution.

### 3.5 Appendix

The theoretical justification of transformations Eqs. (58), (59) one can find in the subsection for \( q^{l} \) incommensurate wave vector and arbitrary integrable concerning the Riemannian periodic function \( f(\phi) = f(\phi + 2\pi) \) in the limit \( N \rightarrow \infty \) we have found

\[
\frac{1}{N} \sum_{n=1}^{N} f(\phi + q^{l}(n)) \exp^{(in \kappa)} = \sum_{n=1}^{N} \left( \frac{1}{2\pi} \int_{0}^{2\pi} f(\phi') \exp^{(i\phi')} d\phi' \right) \exp^{(i\kappa \phi)} \Delta(k + hq^{l}),
\]

(72)

where

\[
\Delta(k) = \left\{ 1, k \equiv G \right\}_{\kappa=G}.
\]

(73)

\( G \) 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

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

(74)

but for the vector of incommensurate phase

\[
q^{l} = \frac{N_{1}}{N_{0}} a^{*}.
\]

(75)

The expression Eq. (72) if based on Eqs. (74), (75) can be rewritten in the form

\[
\frac{1}{N} \sum_{n=0}^{N_{0} - 1} f(\phi + 2\pi \frac{N_{0}}{N_{1}} n) \exp^{(i2\pi \frac{m}{N_{0}} n)} = \frac{1}{N_{0}} \sum_{n=0}^{N_{0} - 1} \left( \frac{1}{2\pi} \int_{0}^{2\pi} f(\phi + 2\pi \frac{N_{0}}{N_{1}} n) \right) \exp^{(i2\pi \frac{m}{N_{0}} n)},
\]

(76)

where at \( \{ \ldots \} \) 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

\[
\{ \frac{N_{1}}{N_{0}} n_{1} \} = \{ \frac{N_{1}}{N_{0}} n_{2} \}.
\]

(77)

Then

\[
\frac{N_{1}}{N_{0}} n_{1} - \frac{N_{1}}{N_{0}} n_{2} = M, \quad (M \in Z),
\]

(78)
or $N_1(n_1 - n_2) = MN_0$. If $N_1$ and $N_0$ have no common divisor we have found

$$n_1 - n_2 = MN_0, \quad (M_1 \in \mathbb{Z}).$$

(79)

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. (76) can be rewritten in the form

$$\sum_{-N_0 \leq h < l \leq N_0} \left( \frac{1}{g} \sum_{n=0}^{N_0-1} f(\varphi + 2\pi \frac{N_0}{N_0} n) \exp -i h(2\pi \frac{N_0}{N_0} n) \Delta(\frac{m + hN_0}{N_0} - a^*) \right) =$$

(80)

where we impose the identity

$$\exp^{2\pi \frac{N_0}{N_0} n} = \sum_{-N_0 \leq h \leq N_0} \exp^{-2\pi \frac{N_0}{N_0} n} \Delta(\frac{m + hN_0}{N_0} - a^*).$$

(81)

We have entered in Eq. (80) 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. (80) in limit $N_0 \rightarrow \infty$. Hence Eq. (72) is true.

4 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

$$u_{nx}^b = e_0^b(q' n + \varphi) = \sum_{h} e_0^b(h) \exp hq'(n + r_i) + \varphi,$$

(82)

$$D_{nx}^a = d_0^a(q' n + \varphi) = \sum_{h} d_0^a(h) \exp hq'(n + r_i) + \varphi,$$

(83)

where $q'$ is the wave vector of the incommensurate structure, $e_0^b(\varphi)$ as well as $d_0^a(\varphi)$ are periodic functions of phase $\varphi$ with $2\pi$ period, $h$ is an integer.

From Maxwell equations

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

(84)

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

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

(85)

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

$$E = -\nabla \varphi,$$

(86)

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

$$\text{div} D = \text{div}(E + 4\pi P) = \frac{\Delta \varphi}{\epsilon_0} \rho(\varphi),$$

(87)

where $\rho(\varphi)$ is charges density, $\epsilon_0$ is dielectric constant.

The spontaneous polarization $P_0$ is directed along the polar axis $z$. Further we assume that the dependence of polarization vector acquires the form [94, 95, 96]

$$P(r) = [\epsilon_0(\epsilon_{11} - 1)E_1, \epsilon_0(\epsilon_{11} - 1)E_2, P_3(E, r) + \epsilon_0(\epsilon_{33} - 1)E_3].$$

(88)

Let us known the quasi-equilibrium polarization distribution $P_2(x, y, z)$ with taking into account the gyrotropy effects which are shown to be found from Euler-Lagrange boundary problem in the framework of Landau-Ginsburg-Devonshire theory [94, 95, 96] as follows

$$\alpha P_3 + \beta |P_3|^2 P_3 - g(\Delta_0 + \frac{\partial^2}{\partial z^2}) P_3 = -\frac{\partial \varphi}{\partial z},$$

(89)

with the next boundary conditions
\begin{align}
(P_3 + \lambda_1 \frac{\partial P_3}{\partial z})|_{z=0} &= -P_b, \quad (90) \\
(P_3 - \lambda_2 \frac{\partial P_3}{\partial z})|_{z=-L} &= 0, \quad (91)
\end{align}

with taking into consideration for the vector of electric field strength the following expressions 
\(E_z = \frac{\partial \varphi}{\partial z}\).

We seek the solution the Euler-Lagrange equation Eq. (113) in the form
\[
P_3(x, y, z) = P_3 \exp(i kr) \exp(i k_z z), \quad (92)
\]

Substituting the solution Eq. (114) in Eq. (113) we have found non-linear equation with respect to \(P_3\)
\[
\alpha P_3 + \beta P_3^3 + g k_2^2 P_3 - g \frac{\partial^2}{\partial z^2} P_3 = -\frac{\partial \varphi}{\partial z}. \quad (93)
\]

Hence we have found the non-linear cubic equation with respect to polarization vector component \(P_3\)
\[
f = \alpha P_3 + \beta P_3^3 + g k_2^2 P_3 + g k_2^2 P_3 - E_z = 0, \quad (94)
\]

the solutions of which meet the next expressions
\[
P_3^{(1)} = \frac{1}{6} \left( \frac{\left(12 \sqrt{3} R + 108 \epsilon_3^2 \right)^{1/3}}{\beta} - \frac{2g \left( k_2^2 + k_3^2 + a \right)}{\left(12 \sqrt{3} R + 108 \epsilon_3^2 \right)^{1/3}} \right), \quad (95)
\]

as well as
\[
P_3^{(2)} = P_3^{(3)} = -\frac{1}{12} \left( \frac{\left(12 \sqrt{3} R + 108 \epsilon_3^2 \right)^{1/3}}{\beta} + \frac{\left( g \left( k_2^2 + k_3^2 + a \right) \right)}{\left(12 \sqrt{3} R + 108 \epsilon_3^2 \right)^{1/3}} \right), \quad (96)
\]

where
\[
R = \sqrt{\frac{1}{\beta} \left( 4g^3 (k_2^2 + k_3^2) + 12g^3 k_2^2 k_3^2 (k_2^2 + k_3^2) + 12 \alpha g^2 (k_2^2 + k_3^2)^2 + 12 \alpha^2 g (k_2^2 + k_3^2) + 27 \epsilon_3^2 \beta + 4 \alpha^3 \right)}. \quad (97)
\]

The Maxwell equations we have specified for three regions: for contact clearance \((-H - L < z < -L)\), for ferroelectric thin polar-active nanofilm \(-L < z < 0\) and for semiconductor \(z > 0\) [94, 95, 96]
\[
\epsilon_0 \frac{\partial^2 \varphi}{\partial z^2} + \Delta \varphi = 0, \quad -H - L < z < -L, \\
\epsilon^{\perp} \frac{\partial^2 \varphi}{\partial z^2} + \epsilon_{11} \Delta \varphi = \frac{1}{\epsilon_0} \left( \frac{\partial P_3}{\partial z} - \rho f (\varphi) \right), \quad -L < z < 0, \\
\epsilon_0 \epsilon_{11} \frac{\partial^2 \varphi}{\partial z^2} + \Delta \varphi = -\rho_j (\varphi), \quad z > 0, \quad (98)
\]

where \(\epsilon^{\perp}, \epsilon_{11} = \epsilon_{22}\) are permittivities of gyrotropic medium with taking to account the optical activity effects, \(\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\).

For the light which propagates along Oz axis for first contact clearance \((-H - L < z < -L)\) the solution of Maxwell equation for the vector of electric field strength we have found by using Green function method
\[
\text{div} \mathbf{E} = \frac{4 \pi \rho}{\epsilon_0}, \quad (99)
\]

where \(\rho\) is charge density,
\[
\frac{\partial \varphi}{\partial z} \mathbf{E} = \frac{4 \pi \rho(z)}{\epsilon_0}, \quad (100)
\]

where \(e_z\) is unit vector in Oz axis
\[
\frac{\partial \varphi}{\partial z} G_z = \frac{4 \pi \delta(z)}{\epsilon_0}, \quad (101)
\]

where \(G_z\) is Green step Hevithaide function, \(\delta(z)\) is Dirac delta function,
\[
G_z \equiv e_z G = \frac{4 \pi e_z}{\epsilon_0} \frac{4 \pi e_z}{|z|}. \quad (102)
\]

The solution the equation Eq. (100) we have found in the form
\[
E(z_0) = \int G(z_0 - z) \rho(z) dz + C_1. \quad (103)
\]

Since for scalar potential we have found the following equations
\[
E = -\text{grad} \varphi = -e_i \frac{\partial \varphi}{\partial x_i}, \quad (104)
\]
The self-consistent stationarity quantized solutions of non-linear Schrödinger or Euler-Lagrange boundary problem for the polarization vector with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire theory

The polar-active properties of ferroelectric films have been calculated in Landau-Ginsburg-Devonshire theory framework \cite{97, 94, 95, 96} 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 we assume that the dependence of plane polarization components on external fields. The spontaneous polarization $P_0 \approx 1,2$ zero electric field. We assume that the dependence of polarization vector acquires the form

\begin{equation}
\varphi = -\int E_z \, dz + C_2.
\end{equation}

Substituting Eq. (103) in Eq. (106) the solution the Maxwell equation for the first contact clearance ($-H - L < z < -L$) we have presented like follows

\begin{equation}
\varphi = -\int dz_0(\int G(z_0 - z)\rho(z) \, dz + C_1) + C_2.
\end{equation}

4.1 The self-consistent stationarity quantized solutions of non-linear Schrödinger or Euler-Lagrange boundary problem for the polarization vector with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire theory

The polar-active properties of ferroelectric films have been calculated in Landau-Ginsburg-Devonshire theory framework \cite{97, 94, 95, 96} 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 interface in the conditions of stability of spontaneous polarization. Under the electric voltage feeds on the electrode the spontaneous polarization $P_0 \approx 1,2$ zero electric field. We assume that the dependence of plane polarization components on external fields. The spontaneous polarization $P_0$ is connected with the stationary non-linear Schrödinger equation of domain wall found from Euler-Lagrange problem in the framework of Landau-Ginsburg-Devonshire theory \cite{97, 94, 95, 96} 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 $\text{rot} E \approx 0$. From Maxwell equations

\begin{equation}
\text{rot} E = -\frac{\partial \mathbf{B}}{\partial t},
\end{equation}

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

\begin{equation}
\text{rot} E \approx 0.
\end{equation}

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

\begin{equation}
\mathbf{E} = -\nabla \varphi,
\end{equation}

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

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

where $\rho(\varphi)$ is charges density, $\epsilon_0$ is dielectric constant.

The ferroelectric film that occupies the region $-L < z < 0$ is transversally isotropic i.e. permittivity $\epsilon_{11} = \epsilon_{22}$ at zero electric field. We assume that the dependence of plane polarization components on $E_{1,2}$ can be linearized as $P_{1,2} \approx \epsilon_0(\epsilon_{11} - 1)E_{1,2}$ ($\epsilon_0$ is the universal dielectric constant) while the polarization component $P_3$ nonlinear depends on external fields. The spontaneous polarization $P_3$ is directed along the polar axis $z$. Further we assume that the dependence of polarization vector acquires the form \cite{94, 95, 96}

\begin{equation}
\mathbf{P}(\mathbf{r}) = [\epsilon_0(\epsilon_{11} - 1)E_1, \epsilon_0(\epsilon_{11} - 1)E_2, P_3(\mathbf{E}, \mathbf{r}) + \epsilon_0(\epsilon_{33} - 1)E_3].
\end{equation}

Let us known the quasiequilibrium polarization distribution $P_0(x, y, z)$ with taking into account the gyrotropy effects which are shown to be connected with the stationary non-linear Schrödinger equation of domain wall found from Euler-Lagrange problem in the framework of Landau-Ginsburg-Devonshire theory \cite{94, 95, 96} we have found the space solution of Euler-Lagrange problem in the framework of Landau-Ginsburg-Devonshire theory only as follows

\begin{equation}
\imath \alpha \frac{\partial P_3}{\partial t} - g(\Delta_z + \frac{\partial^2}{\partial z^2})P_3 + \beta P_3|P_3|^2 = -\frac{\partial \varphi}{\partial z}.
\end{equation}

with taking into consideration for the vector of electric field strength the following expressions $E_z = -\frac{\partial \varphi}{\partial z}$, with the following boundary conditions

\begin{equation}
(P_3 + \lambda_1 \frac{\partial P_3}{\partial z})|_{z=0} = -P_b,
\end{equation}

\begin{equation}
(P_3 - \lambda_2 \frac{\partial P_3}{\partial z})|_{z=-L} = 0.
\end{equation}
where we introduce $\Delta_i = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ Laplace operator. Inhomogeneity $P_b$ describes the effects of interface polarization stemming from the interface bonding effect and associated interface dipole. Hence the translation symmetry breaking inevitably in the vicinity of any interface will give rise to inhomogeneity in the boundary conditions in Eqs. (113), (114), (115). The equations Eqs. (111), (113), (114), (115) yield the coupled system

\[
\left(\frac{\partial^2 \phi}{\partial z^2} + \Delta_i \phi\right) = 0, \quad -H - L < z < -L, \quad \text{(116)}
\]

\[
e_{b} e_{33}^{b} \frac{\partial^2 \phi}{\partial z^2} + \epsilon_{11} \Delta_i \phi = \frac{1}{e_{0}} \left(\frac{\partial \rho}{\partial z} + \rho_{f}(\phi)\right), \quad -L < z < 0, \quad \text{(117)}
\]

\[
\epsilon_{0} \epsilon_{i} \left(\frac{\partial^2 \phi}{\partial z^2} + \Delta_i \phi\right) = -\rho_{f}(\phi), \quad z > 0, \quad \text{(118)}
\]

where the $e_{33}^{b}$ is background insulator permittivity of incipient ferroelectric, $\epsilon_{i}$ is the semiconductor bare lattice permittivity. The equations Eqs. (116), (117), (118) were supplemented with the boundary conditions $\phi(x, y, -L - H) = U_{b}(x, y)$, $\phi(x, y, L + 0) = \phi(x, y, L - 0)$, $\phi(x, y, z \rightarrow \infty) = 0$, $\phi(x, y, +0) - \phi(x, y, -0) = U_{b}$, $\epsilon_{0} e_{33}^{b} \frac{\partial \phi(x, y, -0)}{\partial z} - P_{b}(x, y, -0) = \sigma_{s}(x, y)$, $-\epsilon_{0} e_{33}^{b} \frac{\partial \phi(x, y, +0)}{\partial z} + P_{3}(x, y, -0) = \epsilon_{0} e_{33}^{b} \frac{\partial \phi(x, y, -0)}{\partial z} = \sigma_{f}(x, y)$, where $U_{b}$ is the contact potential difference at the insulator-semiconductor interface, $\epsilon_{33}^{b}$ is the dielectric constant of the dielectric gap between the tip and ferroelectric surface.

We have assumed that polarization vector $P_{3}$ is directed along z axis that corresponds to the plane electrodes.

The space charge density inside the doped p-type (or n-type) semi-infinite semiconductor has the form $\rho_{i}(\phi) = q \left[ p(\phi) + N_{d}^{0}(\phi) - n(\phi) - N_{a}^{-}(\phi) \right]$, $p(\phi) = N_{d}^{0} F \left( \frac{\phi - E_{d}}{k_{B}T} \right)$, $N_{d}^{+}(\phi) = N_{d} F \left( \frac{E_{d} - \phi}{k_{B}T} \right)$, $n(\phi) = N_{d}^{0} F \left( \frac{E_{d} - \phi}{k_{B}T} \right)$, $N_{a}^{-}(\phi) = N_{a} F \left( \frac{E_{a} - \phi}{k_{B}T} \right)$, where $F(\theta) = \left( \exp^{\theta} - 1 \right)^{-1}$, is the Fermi-Dirac distributional function, $q$ is carriers charge, $E_{d}$, $E_{a}$, $E_{F}$, $E_{v}$, $E_{c}$, $E_{s}$, $E_{d}$, $E_{a}$ are the energies of Fermi level, valence band conductivity, and donor and acceptor levels in the quasineutral region of the semiconductor correspondingly. We have assumed $p(0) + N_{d}^{+}(0) - n(0) - N_{a}^{-}(0) = 0$, $N_{d}^{+} \approx \text{const}$, $N_{a}^{-} \approx \text{const}$, and Boltzman approximation for electrons $E_{c} - E_{F} - q\varphi >> k_{B}T$ or holes $E_{F} - E_{v} + q\varphi >> k_{B}T$ lead to expressions $\rho_{i} \approx q p_{d}^{0} \left[ \exp^{\frac{-E_{d}}{k_{B}T}} - 1 \right]$, $\rho_{s} \approx q n_{i}^{0} \left[ \exp^{\frac{-E_{a}}{k_{B}T}} - 1 \right]$ correspondingly where $p_{d}^{0}$ and $n_{i}^{0}$ are equilibrium concentrations of holes and electrons in the quasineutral region of the semiconductor.

Hence in abrupt junction approximation the space charge density near the interface of the strongly doped p-type (or n-type) semi-infinite semiconductor has the form $\rho_{i}(\phi) = q p_{d}^{0} \left[ \exp^{\frac{-E_{d}}{k_{B}T}} - 1 \right]$, where we assume the charge density $p_{d}^{0}$ with depth $W_{i} = W_{sp}$ (or $p_{s}^{0} = -q n_{i}^{0}$ with depth $W_{i} = W_{sp}$).

We have supposed that the ferroelectric film is wide-gap semiconductor or insulator. Hence $\rho_{f}(\phi) \approx 0$ at region $-L < z < 0$. Keeping in mind the above found boundary conditions the one-dimension solutions of Eqs. (116), (117), (118) have the form

\[
\phi(z) = -\frac{P_{3}(z)}{\epsilon_{33}^{b}} (W_{i} - z)^{2} \theta(W_{i} - z), \quad z > 0, \quad \text{(119)}
\]

\[
\phi(z) = \int_{-L}^{z} P_{3}(z) d\tilde{z} - (L + z) \left( \frac{W_{i} - \sigma_{f}}{\epsilon_{33}^{b}} \right) + U_{b} + \frac{H}{\epsilon_{33}^{b}} (\sigma_{s} + \sigma_{f} - \rho_{f}^{0} W_{i}), \quad -L \leq z < 0, \quad \text{(120)}
\]
Hence we have found the electric field \( E \) after the following elementary algebraic transformations we have found \( \theta \) where \( \epsilon \) and as well as with the Maxwell equation in thin polar active ferroelectric film

Under variate Eq. (127) we have found \( -\sigma_f = D_3(-L) \) has been created at second interface \( z = -L \), and the electroneutral condition has the form \( -\sigma_f + \rho_0^3W_s + \sigma_f = 0 \). Hence we have found the self-consistent stationarity soliton solution of non-linear Schrödinger or Euler-Lagrange boundary problem for the polarization vector distributions with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire theory as following

Hence the compensated free charge \( -\sigma_f = D_3(-L) \) has been created at second interface \( z = -L \), and the electroneutral condition has the form \( -\sigma_f + \rho_0^3W_s + \sigma_f = 0 \). Hence we have found the self-consistent stationarity soliton solution of non-linear Schrödinger or Euler-Lagrange boundary problem for the polarization vector distributions with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire theory as following

\[
\varphi(z) = U_\epsilon + \frac{\mu + L}{\epsilon_0^3}(\sigma_z + \rho_0^3W_s), \quad -L - H \leq z < -L, \quad (121)
\]

where \( \theta(z) \) is the Hevithaide step function.

Hence we have found the electric field \( E_3 \) with \( E_3(z) = -\frac{\partial \varphi}{\partial z} \) and electrical displacement \( D_3 \) distributions based on Eqs. (119), (120), (121) in the form

\[
E_3(z) = -\frac{P_3(z)}{\epsilon_0^3} + \frac{\rho_0^3W_s - \sigma_z}{\epsilon_0^3}, \quad (122)
\]

\[
D_3(z) = \rho_0^3W_s - \sigma_z, \quad -L < z < 0, \quad (123)
\]

\[
E_3(z) = \frac{\rho_0^3}{2\epsilon_0^3}(z - W_s)\theta(W_s - z), \quad z > 0, \quad (124)
\]

\[
D_3(z) = \rho_0^3(z - W_s)\theta(W_s - z), \quad z > 0, \quad (125)
\]

\[
P_3(z) = \rho_0^3\frac{s}{\epsilon_0^3}(z - W_s)\theta(W_s - z), \quad z \geq 0. \quad (126)
\]

Hence the compensated free charge \( -\sigma_f = D_3(-L) \) has been created at second interface \( z = -L \), and the electroneutral condition has the form \( -\sigma_f + \rho_0^3W_s + \sigma_f = 0 \). Hence we have found the self-consistent stationarity soliton solution of non-linear Schrödinger or Euler-Lagrange boundary problem for the polarization vector distributions with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire theory as following

\[
a P_3 + \beta P_3^3 - g(\Delta_1 + \frac{\partial^2}{\partial z^2})P_3 = -\frac{\partial \varphi}{\partial z}, \quad (127)
\]

Under variate Eq. (127) we have found

\[
a \frac{\partial P_3}{\partial z} + 3\beta P_3 \frac{\partial P_3}{\partial z} - g \Delta_1 \frac{\partial P_3}{\partial z} - g \frac{\partial^2}{\partial z^2} P_3 = -\frac{\partial^2 \varphi}{\partial z^2}, \quad (128)
\]

with the Maxwell equation in thin polar active ferroelectric film

\[
\frac{\epsilon_b^3}{2} \frac{\partial^2}{\partial z^2} + \epsilon_{11}^3 \Delta_1 \varphi = \frac{1}{\epsilon_0^3} \left( \frac{\partial P_3}{\partial z} - \rho_f(\varphi) \right), \quad -L < z < 0, \quad (129)
\]

after the following elementary algebraic transformations we have found

\[
-\frac{\partial^2 \varphi}{\partial z^2} + \frac{\epsilon_0^3}{\epsilon_{33}^3} \Delta_1 \varphi - \frac{1}{\epsilon_0^3} \left( \frac{\partial P_3}{\partial z} - \rho_f(\varphi) \right), \quad -L < z < 0, \quad (130)
\]

as well as

\[
\frac{\partial^2 P_3}{\partial z^2}(\alpha + 3\beta P_3)^2 + \frac{1}{\epsilon_0^3} \left( \frac{\partial P_3}{\partial z} - \rho_f(\varphi) \right) = 0. \quad (131)
\]
Hence under integrate transformations of Eq. (131) we have found
\[
\int dz \frac{\partial P_3}{\partial z} (\alpha + 3\beta (P_3) + 2 + \frac{1}{\epsilon_3^{e33}}) - g \frac{1}{L} \int_0^L dz \int \frac{\partial \xi}{\partial z} P_3 (P_3) - \int_0^L dz \frac{\partial \xi}{\partial z} P_3 (P_3) + C_1 = 0, 
\]
under the second integrate transformation of Eq. (132) we have written
\[
P_3 (\alpha + 3\beta (P_3) + 2 + \frac{1}{\epsilon_3^{e33}}) - g \frac{1}{L} \int_0^L dz \int \frac{\partial \xi}{\partial z} P_3 (P_3) - \frac{\partial \xi}{\partial z} P_3 (P_3) + C_1 = 0, 
\]
under the third integrate transformation of Eq. (133) we have derived
\[
P_3 (\alpha + 3\beta (P_3) + 2 + \frac{1}{\epsilon_3^{e33}}) - g \frac{1}{L} \int_0^L dz P_3 (P_3) - \frac{\partial \xi}{\partial z} P_3 (P_3) + C_1 = 0, 
\]
the equation from which one can find polarization \( P_3 \) via average polarization \( \langle P \rangle \) in the form
\[
P_3 (\alpha + 3\beta (P_3) + 2 + \frac{1}{\epsilon_3^{e33}}) - g (P_3)^3 - \frac{\partial \xi}{\partial z} P_3 (P_3) + C_1 = 0.
\]
Keeping in mind the found boundary condition we have found
\[
P_3 = \frac{g (P_3)^2}{(\alpha + 3\beta (P_3) + 2 + \frac{1}{\epsilon_3^{e33}})} + C_1,
\]
as well as
\[
P_3 = \frac{g (P_3)^2}{(\alpha + 3\beta (P_3) + 2 + \frac{1}{\epsilon_3^{e33}})} + C_1,
\]
for the coupled states of particles from the conditions that the first quantized wave function or first quantized polarization \( P_3 \) has not the node on quantum well width and keeping in mind the next boundary conditions we have found \( \psi = A\xi \sinh (\xi), \psi_1 = A\lambda_1 \cosh (\frac{\xi}{\lambda_1}), \phi = A\xi \cos (\xi), \phi_1 = -A\lambda_2 \sinh (\frac{\xi}{\lambda_2}) \), where \( \xi = \sqrt{\epsilon_0 \epsilon_3^{e33}} g \) [38, 42, 41, 40, 39, 38, 37, 34, 14, 103, 104], the following trial wave functions and the following normalization condition for wave function with boundary conditions in the form \( \frac{\partial \psi}{\partial z} = \frac{-1}{2} \xi \psi \) and \( \lambda_1 \cosh (\frac{\xi}{\lambda_1}) \), the following two constants of integrations \( \psi (z, L) = 1 - A^2 \xi (\sin (\xi z) - \lambda_1 \cosh (\frac{\xi}{\lambda_1}) = xi \sinh (\frac{\xi}{\lambda_1}) z) + A^2 \xi (\sin (\frac{\xi}{\lambda_1}) z + \lambda_2 \cosh (\frac{\xi}{\lambda_1}) = xi \cos (\frac{\xi}{\lambda_1}) z) \), and \( \phi (z, L) = A^2 \xi (\sin (\frac{\xi}{\lambda_1}) z + \lambda_2 \cosh (\frac{\xi}{\lambda_1}) = xi \cos (\frac{\xi}{\lambda_1}) z) \) for the first quantized polarization \( P_3 \)
\[
P_3^{first \ quantized \ polarization} = \frac{g (P_3)^2}{(\alpha + 3\beta (P_3) + 2 + \frac{1}{\epsilon_3^{e33}})} \psi (z, L) - P_b \phi (z, L).
\]
The first energy level of an electron in the quantum well of width \( w \) is equal to \( E_1 = \frac{2 e^2 \hbar^2}{m w^2} \), where \( m \) is an electron effective mass and \( \xi \) is determined from equation \( \cosh (\frac{\xi}{\lambda_1}) = \pm \xi \), where \( \gamma = \frac{\hbar^2}{2 m w^2} \tan (\xi) > 0 \), and \( \xi = \frac{\hbar w}{2} \). For \( k_h \) the following equality holds arcsinh \( \frac{k_h}{\sqrt{w^2 n^2}} = \frac{\pi (n - \frac{k_h}{w})}{w} \), where \( n = 1, 2, 3, \ldots \) i.e is an integer number. Hence we have derived the quantized polarization vector \( P_3 \) as well as the quantized energies. For the average polarization \( P_3 \) we have written the following expression
\[
\langle P_3 \rangle = \rho_0^b W_s - \sigma_j + \frac{\epsilon_0 \epsilon_3^{e33}}{2 \epsilon_3^{e33}} W_s^2 - \frac{\epsilon_0 \epsilon_3^{e33}}{L} (U_b + U_c) + \frac{\hbar \sigma_j}{\epsilon_3^{e33}} (\sigma_j + \sigma_j - P_0^b W_s)),
\]
where \( z = \frac{\epsilon_0 \epsilon_3^{e33}}{2 \epsilon_3^{e33}} W_s \), and for the average polarization \( P_3 \) we can derive the cubic equation like
\[
(\alpha + \frac{1}{\epsilon_3^{e33}}) \langle P_3 \rangle + (P_3)^3 (3\beta - g \langle \psi \rangle) + 3\beta P_b \langle \phi \rangle \langle P_3 \rangle^2 = \frac{\rho_0^b W_s - \sigma_j}{\epsilon_3^{e33}} \langle \psi \rangle - P_b \langle \phi \rangle (\alpha + \frac{1}{\epsilon_3^{e33}}),
\]
where for average magnitudes one can find the next expressions \( \langle \psi \rangle = 1 - \frac{\epsilon_0 \epsilon_3^{e33}}{\epsilon_3^{e33} (L + \frac{\xi}{\lambda_1} + \frac{\xi}{\lambda_2} + \frac{\xi}{\lambda_1} \lambda_2)}, \langle \phi \rangle = \frac{\epsilon_0 \epsilon_3^{e33}}{\epsilon_3^{e33} (L + \frac{\xi}{\lambda_1} + \frac{\xi}{\lambda_2} + \frac{\xi}{\lambda_1} \lambda_2)} \),
\]
then the cubic equation for average polarization \( P_3 \) we can derive as follows
\[
(\alpha + \frac{1}{\epsilon_3^{e33}} (1 - \frac{\epsilon_0 \epsilon_3^{e33}}{\epsilon_3^{e33} (L + \frac{\xi}{\lambda_1} + \frac{\xi}{\lambda_2} + \frac{\xi}{\lambda_1} \lambda_2)})) \langle P_3 \rangle + (P_3)^3 (3\beta - g \langle \psi \rangle) + 3\beta P_b \langle \phi \rangle \langle P_3 \rangle^2 = E_b (L, H) + E_c (L, H),
\]
where \( E_b'(L, H) = \frac{c_{13}^{L}(\varphi)}{c_{33}^{L}+c_{33}^{H}}(U_b + \frac{H\sigma_r}{c_{33}^{T}}) - \frac{P_b}{c_{33}^{T}}(\varphi) \), \( E_c'(L, H) = \frac{c_{13}^{c}(\varphi)}{c_{33}^{L}+c_{33}^{H}} \), are built-in electrostatic field and the external field correspondingly. From the equation \( a + \frac{1}{c_{13}^{c}}(1 - \frac{c_{13}^{c}}{c_{33}^{L}+c_{33}^{H}}) = 0 \)

For the proper ferroelectrics the coefficient \( a(T) = a_f(T - T_c) \), where \( T \) is an absolute temperature, \( T_c \) is the Curie temperature renormalized by the epitaxial misfit strain \( u_m \). The strain originates from the thin film (a) and the semiconductor (c) lattice constants mismatch [76, 78, 16, 68, 36, 44, 43].

we have found Curie temperature for phase transition from ferroelectric phase into high symmetric paraelectric phase like

\[
T_{\text{phase transition}} = T_{\text{Curie}} + \frac{2\mu_0 q_0 c_{22} - c_{11} q_1}{c_{11}} [105].
\]

For the cube-on-cube epitaxy of perovskites and considered out-of-plane polarization geometry \( T_c = T_c + \frac{q_{44}}{4c_{12}^2} \) where \( u_m \) is the effective misfit strain, \( s_{ijkl} \) is compliances tensor, \( Q_{ijkl} \) is the electrostriction strain tensor [94, 95].

In Fig. 1 we have presented the quantized out-of-plane polarizations \( P_3 \) dispersion for LSMO/BFO interface of polar-active ferroelectric nanofilm with semiconductor with boundary parameters: \( \lambda_1 = 5 \text{ nm}, \lambda_2 = 50 \text{ nm}, \sigma_z = 0.1 \text{ C/cm}^2, P_b = 0.2 \text{ C/m}^2. \)

In Fig. 2 we have presented the quantized out-of-plane polarizations \( P_3 \) dispersion for LSMO/BFO interface of polar-active ferroelectric nanofilm with semiconductor with boundary parameters: \( \lambda_1 = 0, \lambda_2 = 0, \sigma_z = 0 \text{ C/cm}^2, P_b = 0.1 \text{ C/m}^2. \)

The quantized out-of-plane \( P_3 \) polarizations were clearly visible like the festive fires of candles.

### 4.2 The self-consistent 5-polynomial quantized solutions of stationary Schrödinger or Euler-Lagrange boundary problem for the polarization vector with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire theory

Let us know the quasi-equilibrium polarization distribution \( P_3(x, y, z) \) with taking into account the gyrotropy effects which are shown to be connected with the stationary non-linear Schrödinger equation of domain wall found from Euler-Lagrange problem in the framework of Landau-Ginsburg-Devonshire theory (in the articles [94, 95, 96] we have found the space solution of Euler-Lagrange problem in the framework of Landau-Ginsburg-Devonshire theory only) as follows

\[
\begin{align*}
\iota a \frac{\partial P_3}{\partial z} + \beta P_3 |P_3|^2 + \gamma P_3 (|P_3|^2)^2 - g(\Delta_1 + \frac{\partial^2 \varphi}{\partial z^2}) P_3 &= -\frac{\partial \varphi}{\partial z}, \\
(P_3 + \lambda_1 \frac{\partial P_3}{\partial z})|_{z=0} &= -P_b, \\
(P_3 - \lambda_2 \frac{\partial P_3}{\partial z})|_{z=-L} &= 0,
\end{align*}
\]

with taking into consideration for the vector of electric field strength the following expressions \( E_z = -\frac{\partial \varphi}{\partial z} \), with the following boundary conditions

\[
\begin{align*}
(P_3 + \lambda_1 \frac{\partial P_3}{\partial z})|_{z=0} &= -P_b, \quad (P_3 - \lambda_2 \frac{\partial P_3}{\partial z})|_{z=-L} = 0,
\end{align*}
\]

where we introduce \( \Delta_1 = \frac{\partial^2 \varphi}{\partial z^2} + \frac{\partial^2 \varphi}{\partial z^2} \) Laplace operator. Inhomogeneity \( P_b \) describes the effects of interface polarization stemming from the interface bonding effect and associated interface dipole. Hence the translation symmetry breaking inevitably in the vicinity of the any interface will give rise to inhomogeneity in the boundary conditions in Eqs. (143), (144), (145). The equations Eqs. (111), (143), (144), (145) yield the coupled system

\[
\begin{align*}
\left( \frac{\partial^2 \varphi}{\partial z^2} + \Delta_1 \varphi \right) &= 0, \quad -H < z < -L, \\
\epsilon_{33} \frac{\partial^2 \varphi}{\partial z^2} + \epsilon_{11} \Delta_1 \varphi &= \frac{1}{\epsilon_0} \left( \frac{\partial \varphi}{\partial z} - \rho_f(\varphi) \right), \quad -L < z < 0, \\
\epsilon_0 \epsilon_{33} \frac{\partial^2 \varphi}{\partial z^2} + \Delta_1 \varphi &= -\rho_i(\varphi), \quad z > 0,
\end{align*}
\]

where the \( \epsilon_{33} \) is background insulator permittivity of incipient ferroelectric, \( \epsilon_0 \) is the semiconductor bare lattice permittivity. The equations Eqs. (146), (147), (148) were supplemented with the boundary conditions \( \varphi(x, y, -L - H) = U_0(x, y), \varphi(x, y, -L + 0) = \varphi(x, y, -L - 0), \varphi(x, y, z) \to \infty \to 0, \varphi(x, y, +0) - \varphi(x, y, -0) = U_b \), \( \epsilon_0 \epsilon_{33} \frac{\partial \varphi(x, y, -0)}{\partial z} - P_3(x, y, 0) - \epsilon_0 \epsilon_{33} \frac{\partial \varphi(x, y, +0)}{\partial z} = \sigma_r(x, y), -\epsilon_0 \epsilon_{33} \frac{\partial \varphi(x, y, -L + 0)}{\partial z} + P_3(x, y, -L + 0) + \epsilon_{33} \epsilon_0 \frac{\partial \varphi(x, y, -L)}{\partial z} = \sigma_f(x, y), \)}}
Table 2. The material parameters: Band gap, (eV), Carriers concentrations cm$^{-3}$, Background permittivity, LGD-expansion coefficient for ferroelectrics, electrostriction, and elastic constants [94, 95, 96, 105].

<table>
<thead>
<tr>
<th>Material</th>
<th>Band gap, (eV)</th>
<th>Concentrations cm$^{-3}$</th>
<th>LGD-expansion coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>LaSrMnO$_3$ (LSMO) half-metal</td>
<td>1 p type</td>
<td>1.83 x 10$^{22}$</td>
<td>Permittivity</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\varepsilon_s = 30$ (effective lattice constant $a = 3.876$ Å)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Nonferroelectric</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\varepsilon_3^b = 9.0$  (effective lattice constant $a_{hex} = 5.58$ Å)</td>
</tr>
<tr>
<td>BiFeO$_3$ (BFO) ferroelectric</td>
<td>3</td>
<td>Wide band-gap semiconductor</td>
<td></td>
</tr>
<tr>
<td>SrTiO$_3$ (STO)</td>
<td>3</td>
<td>Dielectric</td>
<td>(without impurities)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\varepsilon_{33}^g = 43$, $\varepsilon_{33}^b = 5.7$, $a = 0.3905$ Å, $\alpha_T = 1.26 \times 10^6$ m/(FK), $T_c = 38$ K, $T_q = 84$ K, $\beta_b = 8.1 - 6.8 \times 10^9$ m$^5/(C^2F)$, $\gamma = 4 \times 10^{12}$ m$^9/(C^4F)$, $g = 10^{-8} - 10^{-9}$ (m$^3$/F), $g = 0.99 \times 10^{-9}$ (m$^3$/F), $Q_{11} = 0.051$ (m$^4$/C$^2$), $Q_{12} = -0.016$, (m$^4$/C$^2$), $Q_{44} = 0.020$, (m$^4$/C$^2$), $s_{11} = 3.89 \times 10^{-12}$, (m$^2$/N), $s_{12} = -1.06 \times 10^{-12}$, (m$^2$/N), $s_{44} = 8.20 \times 10^{-12}$, (m$^2$/N),</td>
</tr>
</tbody>
</table>

where $U_b$ is the contact potential difference at the insulator-semiconductor interface, $\varepsilon_{33}^g$ is the dielectric constant of the dielectric gap between the tip and ferroelectric surface.

We have assumed that polarization vector $P_3$ is directed along $z$ axis that corresponds to the plane electrodes.

Hence we have found the self-consistent stationarity quantized solution of 5-polynomial Schrödinger or Euler-Lagrange boundary problem for the polarization vector distributions with one-dimensional Maxwell equations system at interface of thin ferroelectric films and semiconductor in framework of Landau-Ginsburg-Devonshire theory as following

$$\alpha P_3 + \beta P_3^3 + \gamma P_3^5 - g(\Delta_T + \frac{\partial^2}{\partial x^2})P_3 = -\frac{2\gamma}{\alpha^2} \frac{\partial^2}{\partial x^2},$$ (149)
The renormalization of $T_{Curie}^c$ by misfit strain and dislocations originated at critical film thickness $h_d$: $T_{Curie}^c$ at $L \leq h_d$, $T_{Curie}^c + \frac{\mu_a}{\sigma_3} \frac{4Q_{12}}{33}$; $T_{Curie}^c$ at $L > h_d$, $T_{Curie}^c + \frac{\mu_a}{\sigma_3} \frac{4Q_{12}}{33}$ $[94, 95, 96, 105]$. 

<table>
<thead>
<tr>
<th>Interface orientation</th>
<th>$u_m$</th>
<th>$h_d$, nm</th>
<th>$T_{Curie}^c$ at $L \leq h_d$</th>
<th>$T_{Curie}^c$ at $L &gt; h_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LSMO/STO [100]</td>
<td>-0.0074</td>
<td>10.8</td>
<td>-12 $T_{Curie}$</td>
<td>$T_{Curie}^c(1 - \frac{3h_d}{L})$</td>
</tr>
<tr>
<td>LSMO/BFO [100]</td>
<td>-0.0230</td>
<td>2.4</td>
<td>0.6 $T_{Curie}$</td>
<td>$T_{Curie}^c(1 - \frac{0.4h_d}{L})$</td>
</tr>
</tbody>
</table>

Under variate Eq. (149) we have found

$$
\frac{\partial P_1}{\partial x} + 3\beta P_3^4 \frac{\partial P_3}{\partial x} + 5\gamma P_3^4 \frac{\partial P_3}{\partial x} - g \Delta t \frac{\partial P_3}{\partial x} - g \frac{\partial}{\partial x} \frac{\partial f}{\partial x} P_3 = - \frac{\partial^2 \varphi}{\partial x^2},
$$

(150)

with the Maxwell equation in thin polar active ferroelectric film

$$
\varepsilon_b \frac{\partial^2 \varphi}{\partial x^2} + \varepsilon_{11} \Delta \varphi = \frac{1}{\varepsilon_0} \left( \frac{\partial f}{\partial x} - \rho_f(\varphi) \right), -L < z < 0,
$$

(151)

after the following elementary algebraic transformations we have found

$$
- \frac{\partial^2 \varphi}{\partial x^2} = \frac{\partial^2}{\partial x^2} \Delta \varphi - \frac{\partial}{\partial x} \left( \frac{\partial f}{\partial x} - \rho_f(\varphi) \right), -L < z < 0,
$$

(152)

as well as

$$
\frac{\partial P_3}{\partial x} (\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0}) - g \frac{\partial^2}{\partial x^2} P_3 - \frac{\rho_f(\varphi)}{\varepsilon_0} = 0.
$$

(153)

Hence under integrate transformations of Eq. (153) we have found

$$
\int dz \frac{\partial P_3}{\partial x} (\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0}) - g \frac{1}{L} \int_0^L dz \frac{\partial^2}{\partial x^2} P_3 - \int_0^L \frac{dW_s}{\varepsilon_0} + C_1 = 0,
$$

(154)

under the second integrate transformation of Eq. (154) we have written

$$
P_3 (\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0}) - g \frac{1}{L} \int_0^L dz \frac{\partial^2}{\partial x^2} P_3 + \frac{\rho_f W_{s_3}}{\varepsilon_0} + C_1 = 0,
$$

(155)

under the third integrate transformation of Eq. (155) we have derived

$$
P_3 (\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0}) - g \frac{1}{L} \int_0^L dz P_3 (\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0}) - \frac{\rho_f W_{s_3}}{\varepsilon_0} + C_1 = 0,
$$

(156)

the equation from which one can find polarization $P_3$ via average polarization $(P_3)$ in the form

$$
P_3 (\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0}) - g (P_3)^3 - \frac{\rho_f W_{s_3}}{\varepsilon_0} + C_1 = 0.
$$

(157)

Keeping in mind the found boundary condition we have found

$$
P_3 = \frac{g (P_3)^3 + \frac{\rho_f W_{s_3}}{\varepsilon_0}}{(\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0})} + C_1,
$$

(158)

as well as

$$
P_3 = \frac{g \rho_f W_{s_3}}{(\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0})} + C_1,
$$

(159)

for the coupled states of particles from the conditions that the first quantized wave function or first quantized polarization $P_3$ has not the node on quantum well width and keeping in mind the next boundary conditions we have found $\psi = A \xi \sinh(\frac{\xi}{\lambda})$, $\psi_1 = A \lambda \cosh(\frac{\xi}{\lambda})$, $\phi = A \xi \cosh(\frac{\xi}{\lambda})$, $\phi_1 = -A \lambda \sinh(\frac{\xi}{\lambda})$, where $\xi = \sqrt{\varepsilon_0 \varepsilon_b \varepsilon_3} Z [38, 42, 41, 40, 39, 38, 37, 34, 14, 103, 104]$, the following trial wave functions and the following normalization condition for wave function with boundary conditions in the form $\frac{\partial}{\partial x} 0 \int L d \xi \xi \sinh(\xi \frac{\xi}{\lambda}) + \lambda \cosh(\xi \frac{\xi}{\lambda})$, $\xi \cosh(\xi \frac{\xi}{\lambda}) + \xi \sinh(\xi \frac{\xi}{\lambda}) = 1$ hence from the normalization condition for wave function with wavevector $A \xi \cosh(\xi \frac{\xi}{\lambda}) + \xi \cosh(\xi \frac{\xi}{\lambda}) = 1$ we have found the two constants of integrations $\psi(z, L) = 1 - A \xi \psi(\xi \frac{\xi}{\lambda}) - \lambda \cosh(\xi \frac{\xi}{\lambda}) + \xi \cosh(\xi \frac{\xi}{\lambda}) + \lambda \cosh(\xi \frac{\xi}{\lambda})$ and $\psi(z, L) = A \xi \psi(\xi \frac{\xi}{\lambda}) + \lambda \cosh(\xi \frac{\xi}{\lambda})$ for the first quantized polarization $P_3$

$$
P_3^{first \ quantized \ polarization} = \frac{g \rho_f W_{s_3}}{(\alpha + 3\beta P_3^4 + 5\gamma P_3^4 + \frac{1}{\varepsilon_0})} \psi(z, L) - P_0 \phi(z, L),
$$

(160)
\[ P^3 = \frac{g_{15}^{13}(P^1 + \rho W - \sigma)}{(c_0 c_{13}^2 + 3P^1 + 5P^1)} \psi(z, L) = P_3 \phi(z, L), \]

where \( \psi(z, L) = 1 - A^2 \xi (\xi -\xi \sinh(\frac{2\xi}{\xi}) - \lambda_1 \cosh(\frac{2\xi}{\xi}) + \xi \cosh(\xi + \lambda_2 \sinh(\frac{2\xi}{\xi}) + \lambda_2 \cosh(\xi + \lambda_2 \sinh(\frac{2\xi}{\xi})) \xi (\lambda_1 + \lambda_2) \cosh(\frac{2\xi}{\xi})) = 1. \)

For the average polarization \( P_3 \) we have written the following expression

\[ (P_3) = \rho W - \sigma + \frac{\langle \rho W \rangle}{e_{c_{13}^2}} \left( U_0 + U + \frac{\rho}{e_{c_{13}^2}} (\sigma_s + \sigma_f - \rho W) \right), \]

where \( z = \frac{I_W}{2e_s} \), and for the average polarization \( P_3 \) we can derive the 5-polynomial equation like

\[ (\alpha + \frac{1}{e_{c_{13}^2}})(P_3) + (P_3)^3(3\beta - \langle \psi \rangle) + 3\beta P_3(\langle \psi \rangle + P_3)^2 + 5\gamma P_3(\langle \psi \rangle + P_3)^4 + 5\gamma(\langle \psi \rangle + P_3)^5 = \frac{\rho^2 W - \sigma}{e_{c_{13}^2}} \langle \psi \rangle - P_3(\alpha + \frac{1}{e_{c_{13}^2}}), \]

where for average magnitudes one can find the next expressions \( \langle \psi \rangle = 1 - \frac{\xi^2(2\xi + \lambda_1 + \lambda_2)}{(\xi + \lambda_1 + \lambda_2) + 2\xi + \lambda_2}, \phi = \frac{\xi^2}{\xi(\xi + \lambda_2)}. \)

4.3 Conclusion

The computation solutions of order parameters for ferroelectric phase transition and applicable that Fractional Quantum Hall Effect (FQHE) in the form of nanosize quantized as well as Landau quantized hysteresis loops that were clearly visible like Fairy-tale Phoenix [106, 107, 108]. The computer solution of quantized energies or wave vectors of stationary inhomogeneous Schrödinger boundary problem for \( Q_f, Q_p, Q_s \) with sinusoidal depolarization waves for the thin PmBaMn\(_6\)O\(_8\) as well as SmBaMn\(_6\)O\(_8\) in magnetic field applied in symmetric gauge ferroic nanofilms are specified. We have presented the computation solutions of quantized normalized charges densities of the stationary Schrödinger boundary problem for different thickness of PmBaMn\(_6\)O\(_8\) as well as SmBaMn\(_6\)O\(_8\) in magnetic field applied in symmetric gauge ferroelectric (FE) nanofilms [108]. The thin Os\(_3\)Ra\(_{1-x}\)Fe\(_3\)O\(_9\) nanofilms have quasiparticle excitations that can be described by (2+1)-dimensional Dirac theory from developed a four-sublattice model (FSM) for the analytical description of A-cation displacements in (anti)ferroelectric-antiferrodistortive perovskites of ABO\(_3\) type. We have found that FSM explains the coexistence of rhombohedral (R), orthorhombic (O) and spatially modulated phases observed by atomic-resolution scanning transmission electron microscopy (STEM) in Os-doped RaFe\(_3\). Using this approach we atomically resolve the theoretical model of the sublatice symmetry inherent to the case of the A-site Os/Ra cation sublattice in Os\(_3\)Ra\(_{1-x}\)Fe\(_3\)O\(_9\) polymorphs. We have shown that this produces an unconventional form of the quantized Hall conductivity \( \sigma_{xy} = -(2e^2/h)(2n + 1) \) with \( n = 0, 1, 2, .. \) [106, 107, 108, 109].

4.4 Summary

In the article we have found the chiral solutions of Schrödinger boundary problem for domain wall for data storage of nanosize PmBaMn\(_6\)O\(_8\) ferroics with incommensurately modulated sinusoidal polarization waves \( Q_f, Q_p, Q_s \). The computer solution of quantized energies or wave vectors of stationary inhomogeneous Schrödinger boundary problem for \( Q_f, Q_p, Q_s \) with sinusoidal depolarization waves for the thin PmBaMn\(_6\)O\(_8\) nanofilm are specified. We have specified the analytical quantized solutions for the band energy dispersion in nanosize ferroics in framework of Landau-Ginsburg-Devonshire (LGD) theory as well as the numerical computer calculation results for the thin PmBaMn\(_6\)O\(_8\) nanofilm have been presented. We have presented the computation solutions of quantized normalized charges densities of the stationary Schrödinger boundary problem for different thickness \( h \) of PmBaMn\(_6\)O\(_8\) ferroelectric (FE) nanofilms [108]. We have found the computation solutions of order parameters of ferroelectric phase transition in the form of quantized hysteresis loops. We have found the quantized out-of-plane polarizations \( P_3 \) dispersion for LSMO/BFO interface of polar-active ferroelectric nanofilm with semiconductor with different boundary parameters. The quantized out-of-plane \( P_3 \) polarizations were clearly visible like the festive fires of candles. I think in the article [95] the derived of Finite size and intrinsic field effect on the polar-active properties of ferroelectric-semiconductor heterostructures by A.N. Morozovska et.al. were not allowed and consequently quantized energies or wave vectors were not found by means of the uncertain inference of just these similar symmetrical expressions into (160), (161).

5 Theory of Gyrotropic Birefringence: Quantum-Mechanical treatment at 0\(^0\)K

In this section we formally calculate the elements of the gyrotropic birefringence tensor at 0\(^0\)K [110]. Consider a perfect crystal acted upon by a monochromatic plane wave of frequency \( \omega \) and wave vector \( k \). The electric field vector is taken as \( e = \frac{1}{2} [E_\theta e^{i\omega t} e^{-i\omega t} + E_\phi e^{-i\omega t} e^{i\omega t}] \) and may be derived from the vector potential \( \mathbf{A} = -\frac{\mathbf{E}}{c} e^{i\omega t} \) according to the relation \( \mathbf{e} = -\frac{i}{c} \frac{\partial \mathbf{A}}{\partial t} \). The magnetic field associated with the plane wave is then given by \( \mathbf{h} = rot\mathbf{A} \). We take the field strengths to be such that only terms linear in \( A \) need be included in our Hamiltonian. Then in the
presence of the plane wave we have $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1(t)$, where $\mathcal{H}_0$ is the Hamiltonian of the unperturbed system and $\mathcal{H}_1(t)$ is given by

$$\mathcal{H}_1(t) = \sum_{r_i}[\sum \frac{\epsilon_{r_i}}{2m}[A_{r_i} \pi_{r_i} + \pi_{r_i}A_{r_i}] - \frac{ie}{m} \sum_{r_i} S_{r_i} \gamma_i \kappa_i - \frac{\xi}{\gamma_i} \sum_{r_i} (\gamma_i(r_i) e_{r_i} A_{r_i} S_{r_i} \gamma_i \kappa_i)].$$  \hspace{1cm} (164)

The quantities in (164) are as follows; $e$ and $m$ are the electron charge and mass, respectively; $r_{\gamma_i}$, $\pi_{r_i}$ and $S_{r_i}$ are respectively the $i$th Cartesian components of the position, mechanical momentum and spin operators of the $\gamma$ electron; $\xi(r_i)$ expresses the radial dependence of the spin-orbit term of the $\gamma$ electron, $e_{r_i}$ is the antisymmetric unit tensor, and summation over repeated indices is understood. The $\gamma$ summation indicates that the contributions of all electrons in the crystal must be included. It is straightforward to show that the spin-orbit term in Eq. (164) contributes only to the magnetoelectric type term and not to the electric quadrupole effect. We shall also, at this point discard the Zeeman term in Eq. (164). The effect of this term will be reintroduced in Eq. (??) by the simple expedient of replacing the orbital angular momentum operator $l$ by $l + 2s$.

We will thus work with the perturbation

$$\mathcal{H}_1(t) = \sum_{r_i}[\sum \frac{\epsilon_{r_i}}{2m}[A_{r_i} \pi_{r_i} + \pi_{r_i}A_{r_i}]].$$  \hspace{1cm} (165)

Using time-dependent perturbation theory to second order, the expectation value of any operator $F(r)$ is found to be

$$(F) = \langle 0|F|0 \rangle - \Re\{\sum_{q \neq 0} \langle 0|F|q \rangle \langle q, n|\mathcal{H}_0^{-1}|0 \rangle \frac{e^{-i\omega t}}{\hbar} + \sum_{q \neq 0} \langle 0|F|q \rangle \langle q, n|\mathcal{H}_1^s|0 \rangle \frac{e^{i\omega t}}{\hbar}\},$$  \hspace{1cm} (166)

where we write $\mathcal{H}_1(t) = \frac{1}{\hbar} \int \exp(i\omega t) \mathcal{H}_1(t) \exp(-i\omega t) dt$, where $\hbar$ is the energy of the state $|q, n \rangle$ and we have fixed the zero of energy by taking $\langle 0|\mathcal{H}_0^{-1}|0 \rangle = 0$.

Consider now the matrix element $\langle n, q|\mathcal{H}_0^{-1}|0 \rangle$; we wish to known for which values of $q$ this matrix element will be nonzero. These values may be found as follows: let $T_n$ be the operator that translates the lattice a distance $\eta$ and let $\eta$ be such a translation that $[T_n, \mathcal{H}_0] = 0$. Then $T_n|n, q \rangle = e^{i\eta n}|n, q \rangle$. We also have from the form of $\mathcal{H}_0^{-1}$, $T_n \mathcal{H}_0^{-1} (T_n)^{-1} = e^{i\eta n} \mathcal{H}_0^{-1}$. It then follows that $\langle n, q|\mathcal{H}_0^{-1}|0 \rangle = 0$ if and only if $\eta = 2\pi l$, where $l$ is an integer. This requires that $q = 2\pi l b$, where $b$ is any whole-number multiple of a reciprocal lattice vector. Thus in conclusion of the matrix elements $\langle n, q|\mathcal{H}_0^{-1}|0 \rangle$, only the elements $\langle n, k|\mathcal{H}_0^{-1}|0 \rangle$ need be considered. Similarly it may be shown that of the matrix elements $\langle n, q|\mathcal{H}_0^{-1}|0 \rangle$ only the elements $\langle n, -k|\mathcal{H}_0^{-1}|0 \rangle$ need be considered. We now take as $F$ the current operator $J(r)$. To the same approximation as in Eq. (176) this operator may be written as $J(r) = \sum_{r_i} \frac{\epsilon_{r_i}}{2m} [\pi_{r_i} (r_{r_i} - \gamma_i) + \delta (r_{r_i} - \gamma_i) \pi_{r_i}]$, where $\delta (u)$ is the Dirac delta function. However it will be more convenient to calculate $\langle J(k, \omega) \rangle$ as $\langle J(r, \omega) \rangle$. We therefore Fourier transform Eq. for $J(r)$ using $\delta (r_{r_i} - \gamma_i) = \frac{1}{(2\pi l)} \int \epsilon^{ik(r_{r_i} - \gamma_i)} d\gamma_i$ to obtain

$$J(k) = \sum_{r_i} \frac{\epsilon_{r_i}}{2m} [\pi_{r_i} \epsilon^{ikr_i} + \epsilon^{ikr_i} \pi_{r_i}],$$

Now using (166) and the Eq. for $J(k)$ and the relation $\langle J_i(k_0, \omega) \rangle - \langle J_i(0) \rangle = \sigma_{ij}(E_0)$, where $\langle J_i(0) \rangle$ is the current present in the absence of the plane wave (due to permanent electric and/or magnetic moments), we obtain for the complex conductivity tensor

$$\sigma_{ij}(k, \omega) = \frac{ieN}{m_0} \delta_{ij} + \frac{ie^2}{4\pi m_0} \sum_{\delta, s, \eta=0} \left[ \frac{1}{\omega - \omega_{\eta s}} \right] \langle 0|\pi_{r_i} \epsilon^{ikr_i} + e^{-ikr_i} \pi_{r_i}, k |n, k|\pi_{\eta s} \epsilon^{ikr_i}; e^{ikr_i} + e^{ikr_i} \pi_{\eta s} |0 \rangle = \text{Re}\left\{ \frac{ieN}{m_0} \delta_{ij} \right\},$$  \hspace{1cm} (167)

where $N$ is the total number of electrons in the system and $\delta_{ij}$ is the Kronecker delta.

5.1 Armchair nanoribbon: Electron wavefunctions

The energy dispersion relation for armchair nanoribbons is written as [112]

$$E^i(k, \theta) = s\gamma_0 \sqrt{1 + 4cos(\theta)^2 - 4cos(\theta)cos(kl)},$$  \hspace{1cm} (168)

where $\gamma_0$ is the hopping integral ($\gamma_0 = 3$ eV) and $l \equiv \sqrt{3}a/2$ (a is a lattice constant $[a = 2.46\ \text{Å}]$). The energy is characterized by the band index $s$ and two parameters $k$ and $\theta$. The superscript $s$ represents the conduction (valence) energy band and takes values $s = \pm 1$, $k$ is the wave vector parallel to the edge, and $\theta$ stands for the phase in the direction perpendicular to the edge.

The wave functions are given by [112]

$$\phi^s_{j}(k, \theta) = \frac{1}{\sqrt{N}} e^{-ikl(1-j)} \sin(J\theta) \parallel e^{-i\theta / s},$$  \hspace{1cm} (169)

where $J = 1, \ldots, N$ is the coordinate perpendicular to the edge. The upper (lower) component of Eq. (169) represents the amplitude at A-atom (B-atom).

The wave function vanishes at $J = 0$ and $J = N + 1$ (i.e. at fictitious edge sites). The boundary condition for $J = 0$ is given by $\phi^s_{J=0}(k, \theta) = 0$ which is satisfied with arbitrary values of $\theta$. The phase $\theta$ is quantized by the boundary condition for $J = N + 1$, $\phi^s_{J=N+1}(k, \theta) = 0$ as [112]
Figure 3. (Color online) (Figures from Ref. [111]) Carbon nanoribbon with armchair and zigzag edges.

Figure 4. (Color online) Single-particle spectrum $\epsilon = v_F f(k)$ of carbon armchair nanoribbon (the width of the ribbon is $N=202$ unit cells) [112] for wave vectors in a ranges $k = -2.318..2.318$ in a units of $1/A$. 
\[ \theta_n = \frac{m\pi}{N}, \quad (n = 1, \ldots, N), \]  
\text{(170)}

where \( n \) represents the subband index. Meanwhile we assume that the wave vector \( k \) parallel to the edge is a continuous variables. Since \( k \) is not changed by the perturbations which preserve translational symmetry along the edge.

### 5.2 Optical transitions in carbon armchair nanoribbon

The electron-light interaction is written as \( H_{\text{em}} = -e\mathbf{v}A \), where \(-e\) is the electron charge, \( \mathbf{v} = (v_x, v_y) \) is the velocity operator and \( A \propto e^{-i\omega t}e \) is a spatially uniform vector potential. Here \( \hbar \omega \) corresponds to the energy of the incident light and \( \epsilon \) denotes the polarization. The matrix elements of \( \mathbf{v} \) are classified into inter-band \( \langle \phi^k_n | \mathbf{v} | \phi^\ell_m \rangle \) and intra-band \( \langle \phi^\ell_m | \mathbf{v} | \phi^k_n \rangle \) transitions, hereafter we abbreviate \( \phi^k_j(k, \theta_j), \Theta(k, \theta_j) \) and \( \epsilon'(k, \theta_j) \) by omitting \( k \) and \( \theta \) as \( \phi_n^k, \Theta_n \) and \( \epsilon^i \) respectively.

First we consider the intra-band transition. The matrix elements of \( \mathbf{v} \) are found to be [112]

\[ \langle \phi^k_n | \mathbf{v}_x | \phi^\ell_m \rangle = \begin{cases} 0, m - n \in \text{even} \\ -i \frac{2v_y}{m-n} \langle \sigma_y \rangle_{mn}, m - n \in \text{odd}, \end{cases} \]  
\text{(171)}

\[ \langle \phi^k_n | \mathbf{v}_x | \phi^\ell_m \rangle = \delta_{mn}v_y \langle \sigma_y \rangle_{mn}, \]  
\text{(172)}

where \( \delta_{mn} \) is the Kronecker delta, \( v_y = \gamma_0 / \hbar \) is the Fermi velocity and \( \sigma_i \), where \( i = x, y \) denotes the Pauli matrices. The matrix elements of \( \sigma_i \) are written as [112]

\[ \langle \sigma_x \rangle_{mn} = \frac{1}{2}(e^{i\Theta_n} + e^{-i\Theta_n}), \]  
\text{(173)}

\[ \langle \sigma_y \rangle_{mn} = -i\hbar \langle v_y \rangle_{mn} \]  
\text{(174)}

where \( \Theta_n \) is given by (170). The summation takes a non-zero value only when \( m - n \equiv \Delta n \) is an odd number. The momentum conservation for \( \langle \phi^k_n | \mathbf{v}_x | \phi^\ell_m \rangle \) leads to the following summation with respect to the out-of-phase trigonometric functions [112]

\[ \frac{1}{N} \sum_{J=1}^{N} \sin(J\theta_m) \cos(J\theta_n) = \begin{cases} 0, m - n \in \text{even} \\ 2 \frac{1}{m-n}, m - n \in \text{odd}, \end{cases} \]  
\text{(175)}

where \( \theta_n \) is given by (170). The summation takes a non-zero value only when \( m - n \equiv \Delta n \) is an odd number. The momentum conservation for \( \langle \phi^k_n | \mathbf{v}_x | \phi^\ell_m \rangle \) leads to the summation of the in-phase trigonometric functions, so that the summation takes a non-zero value only for \( m = n \). Hereafter we call the process satisfying \( m - n \in \text{odd} \) an indirect transition for which the wavenumber of the initial state changes \( \Delta n \), and the process satisfying \( m = n \) is called a direct transition \( \Delta n = 0 \).

We have seen that the velocity matrix element is determined by two factors: pseudospin and momentum conservation. Next we consider the inter-band transition based on this understanding. The calculated matrix elements are given by [112]

\[ \langle \phi^\ell_m | \mathbf{v}_x | \phi^k_n \rangle = \begin{cases} 0, m - n \in \text{even} \\ -\frac{2v_y}{m-n} \langle \sigma_y \rangle_{mn}, m - n \in \text{odd}, \end{cases} \]  
\text{(176)}

In Eq. (176), \( \delta_{mn} \) shows that the \( y \)-polarized light \( (A_y) \) results in a direct inter-band transition. Thus, the transition amplitude depends on the diagonal matrix element of the pseudospin \( \langle \sigma_y \rangle_{mn} \). From Eq. (173) we see that \( \langle \sigma_y \rangle_{mn} \) takes a maximum value of \( \langle \sigma_y \rangle_{mn} = \cos(\Theta_n) = \pm 1 \) for \( \Theta_n = 0 \) or \( \pi \). On the other hand, \( \langle \sigma_y \rangle_{mn} \) vanishes for \( \Theta_n = \pm \pi/2 \). Therefore, the electrons on the \( \theta \)-axis \( (\Theta_n = 0 \text{ or } \pi) \) are selectively excited by \( A_y \), while the electrons near the \( k \)-axis \( (\Theta_n = \pm \pi/2) \) are excited very little.

As we can see in Eq. (175), the \( x \)-polarized light \( (A_x) \) results in an indirect transition. An interband transition amplitude \( \langle \phi^\ell_m | A_x | \phi^0 \rangle \) is enhanced because the strength of the pseudospin takes a maximum value of \( \langle |\sigma_y|\rangle_{mn} = 1 \). This indirect inter-band transition is a forward scattering, namely, the electron crosses the Dirac point. An inter-band transition that is not across the Dirac point, such as a (backward) transition from \( \Theta_n = 0 \) to \( \Theta_n = 0 \), is allowed by momentum conservation if \( m - n \) is an odd number. However, it is strongly suppressed by the pseudospin because \( \langle \sigma_y \rangle_{mn} = 0 \) for the emitted process.
The energy dispersion relation for zigzag nanoribbons is given by [112]

$$\epsilon^2(k, \theta) = s_0^2 \sqrt{1 + 4 \cos^2 \left(\frac{k \pi}{2}\right) + 4 \cos \left(\frac{k \pi}{2}\right) \cos \theta},$$

(177)

where $k$ is the wave vector along the zigzag edge and $\theta$ denotes the phase in the direction perpendicular to the edge. The two Dirac points are non-equivalent, i.e., the Brillouin zone (BZ) of zigzag nanoribbons contains the two independent Dirac points (K and K'). This contrasts with the fact that the BZ of armchair nanoribbons has a single Dirac point. The difference in the number of Dirac points is because the reflection of an electronic wave at the zigzag edge constitutes intravalley scattering, while the reflection at the armchair edge is intervalley scattering [112].

The wave functions are expressed by [112]

$$\phi_j^s(k, \theta) = \begin{bmatrix} e^{i\Theta(k, \theta)} \\ e^{-i\Theta(k, \theta)} \end{bmatrix} s \begin{bmatrix} e^{i\Theta(k, \theta)} \\ e^{-i\Theta(k, \theta)} \end{bmatrix} s,$$

(178)

where $J = 1, \ldots, N$ is a coordinate perpendicular to the zigzag edge.

The wave function has two components [112]

$$\phi_j^s(k, \theta) = \begin{bmatrix} \phi_{A J}^s(k, \theta) \\ \phi_{B J}^s(k, \theta) \end{bmatrix} = \begin{bmatrix} \frac{i}{\sqrt{N}} \sin (J \theta - \Theta(k, \theta)) \\ \frac{\sin (n \pi)}{\sqrt{N}} \sin (n \pi) \end{bmatrix},$$

(179)

where the first (second) component represents the amplitude at A-atom (B-atom). Note that the minus sign in front of the second term on the right-hand side of Eq. (178) ensures that the wave function satisfies the boundary condition at $J = 0$ given by $\phi_{B J=0}^s = 0$. The phase $\theta$ is quantized as $\theta_n$ by the boundary condition at $J = N + 1$, $\phi_{A J=N+1}^s = 0$.

This boundary condition gives the constraint condition between $k$ and $\theta_n$, $\Theta(k, \theta_n) - (N + 1) \theta_n = -n \pi$, which is rewritten as [112]

$$\theta_n = \frac{n \pi + \Theta(k, \theta_n)}{N + 1}.$$  

(180)

It can be shown that $\theta_0(k)$ acquires an imaginary part after crossing the $k$-axis as $\theta_0(k) = i/\xi(k)$. In Eq. (178) $\xi(k)$ corresponds to the localization length. By putting $\theta_n(k) = i/\xi(k)$ into (180), we see that $\Theta(k, \theta_0(k))$ also acquires an imaginary part as $\Theta(k, \theta_0(k)) = i(N + 1)/\xi(k)$. The localized states near the zigzag edge are known as the edge states. The curved line is essential to the existence of the edge localized states in the zigzag nanoribbons.

### 5.4 Optical transitions in carbon zigzag nanoribbon

Let us known that

$$\langle \phi_m^e | v_x | \phi_n^e \rangle = i v_F \langle \phi_m^e | \sigma_y | \phi_n^e \rangle,$$

$$\langle \phi_m^e | v_y | \phi_n^e \rangle = i v_F \langle \phi_m^e | \sigma_x | \phi_n^e \rangle.$$ 

(181)
The calculations for the pseudospin of the standing wave on the right-hand side of Eq. (181) is straightforward with the studies of Eqs. (180) and (178) are presented to be [112]

\[
\langle \phi^c_n | \sigma_x | \phi^c_n \rangle = -\sin (\Theta_n) \left\{ \frac{\sin \left( \frac{2\pi (n+m)}{n} \right)}{\pi} \frac{\sin \left( \frac{2\pi (n-m)}{m} \right)}{\sin \left( \frac{2\pi (n-m)}{m} \right)} \right\} + \frac{2}{\pi} \cdot \frac{\sin \left( \frac{2\pi (n-m)}{m} \right)}{\sin \left( \frac{2\pi (n-m)}{m} \right)} + \frac{2}{\pi} \cdot \frac{\sin \left( \frac{2\pi (n-m)}{m} \right)}{\sin \left( \frac{2\pi (n-m)}{m} \right)} \right\}
\]

(182)

\[
i\langle \phi^c_n | \sigma_y | \phi^c_n \rangle = -\sin (\Theta_n) \left\{ \frac{\sin \left( \frac{2\pi (n+m)}{n} \right)}{\pi} \frac{\sin \left( \frac{2\pi (n-m)}{m} \right)}{\sin \left( \frac{2\pi (n-m)}{m} \right)} \right\} + \frac{2}{\pi} \cdot \frac{\sin \left( \frac{2\pi (n-m)}{m} \right)}{\sin \left( \frac{2\pi (n-m)}{m} \right)} + \frac{2}{\pi} \cdot \frac{\sin \left( \frac{2\pi (n-m)}{m} \right)}{\sin \left( \frac{2\pi (n-m)}{m} \right)} \right\}
\]

(183)

We have considered a case where the polarization of the incident light is parallel to the zigzag nanoribbon. By setting \( m = n \) in (183) we have \( \langle \phi^c_n | \sigma_y | \phi^c_n \rangle = 0 \). Since \( \langle \phi^c_n | \sigma_y | \phi^c_n \rangle = 0 \) leads \( \langle \phi^c_n | v_x | \phi^c_n \rangle = 0 \) in (181) we conclude that the x-polarized light does not cause a direct inter-band transition. Therefore, the possible inter-band transition is an indirect one. To further explore the inter-band transitions produced by the x-polarized light, let us examine the electrons with \( \Theta = \pi/2 \) (or \( k = 4\pi/3a \)). By putting \( \Theta_n = \pi/2 \) and \( \Theta_m = \pi/2 \) into Eq. (183), we obtain [112]

\[
\langle \phi^c_n | v_x | \phi^c_n \rangle = v_F \frac{2}{\pi} \left\{ \frac{\sin \left( \frac{2\pi (n-m)}{m} \right)}{\sin \left( \frac{2\pi (n-m)}{m} \right)} \right\}
\]

(184)

Eq. (184) suggests that the x-polarized light induces indirect transitions when \( m - n = \Delta n \) is an odd number. The inter-band transitions with \( \Delta n = \pm 1 \) have advantage over the transitions with \( \Delta n = \pm 3, \ldots \) in producing prominent peaks in the dynamical conductivity since the suppression due to the momentum conservation is minimum when \( \Delta n = \pm 1 \).

Next we consider a case where the polarization of the incident light is perpendicular to the zigzag nanoribbon. When \( m = n \), Eq. (182) leads to [112]

\[
\langle \phi^c_n | v_x | \phi^c_n \rangle = \cos (\Theta_n) - \frac{\sin (\Theta_n)}{\pi/2 - \Theta_n}
\]

(185)

The second term on the right-hand side is suppressed by the factor of \( (\pi/2 - \Theta_n)^{-1} \) when \( n \geq 1 \). For \( n = 0 \), \( \langle \phi^c_n | v_x | \phi^c_n \rangle \) is zero when \( \Theta_n = 0 \) and -1 when \( \Theta_n = \pi \). Thus the y-polarized light gives rise to direct inter-band transitions, by which the electrons near the k-axis (\( \Theta = 0 \) or \( \pi \)) are selectively excited. Since there is not a large density of states for the states near the k-axis, the direct inter-band transition does not result in a prominent absorption peak.

By putting \( \Theta_n = \pi/2 \) and \( \Theta_m = \pi/2 \) into Eq. (182), we obtain [112]

\[
\langle \phi^c_n | v_y | \phi^c_n \rangle = -iv_F \frac{2}{\pi} \left\{ \frac{\sin \left( \frac{2\pi (n+m+1)}{m+1} \right)}{\sin \left( \frac{2\pi (n+m+1)}{m+1} \right)} \right\}
\]

(186)

Eq. (186) suggests that the y-polarized light gives rise to an indirect inter-band transition when \( n+m+1 \) is an even number. For example the transition \( \phi^c_0 \rightarrow \phi^c_1 \) satisfies this condition. However the amplitude of this emitted or absorption process is small due to the suppression by momentum conservation. The indirect inter-band transitions caused by y-polarized light can be neglected.

We have shown that the x-polarized light (parallel to zigzag edge) results in inter-band inter-band transitions (\( \Delta n = \pm 1 \)) for the states near the band edges. The y-polarized light induces direct inter-band transitions (\( \Delta n = 0 \)) selectively for the states near the k-axis. The polarization dependence of the inter-band optical transition in zigzag nanoribbon exhibits a \( \pi/2 \) phase shift with respect to that derived for armchair nanoribbons.

The velocity matrix elements for the intra-band transition are written as [112]

\[
\langle \phi^c_m | v_x | \phi^c_n \rangle = -v_F \langle \phi^c_n | \sigma_x | \phi^c_m \rangle,
\]

\[
\langle \phi^c_m | v_y | \phi^c_n \rangle = v_F \langle \phi^c_m | \sigma_y | \phi^c_n \rangle.
\]

(187)

From Eqs. (187) and (181) we see that

\[
|\langle \phi^c_m | v_x | \phi^c_n \rangle| = |\langle \phi^c_n | v_x | \phi^c_m \rangle|,
\]

\[
|\langle \phi^c_m | v_y | \phi^c_n \rangle| = |\langle \phi^c_n | v_y | \phi^c_m \rangle|.
\]

(188)

The equations mean that the selection rule for intra-band transitions can be obtained from that for inter-band transitions by changing the polarization direction. For the intra-band transitions the x-polarized light results in a direct transition (\( \Delta n = 0 \)), while the y-polarized light results in an indirect transition (\( \Delta n = \pm 1 \)).
5.5 Dynamical conductivity

With the optical selection rule established by Eqs. (171), (172), (175), (176) let us known the absorption of light. The dynamical conductivity is given by \( \sigma_{xx}(\omega) = \frac{\hbar}{i S} \sum_{l} \sum_{nmk} \left[ f(\epsilon_{l}^* - f(\epsilon_{l}^*)) |(\phi_{l}^* - e_{n} | \phi_{m}^* |)^{2} \right] \left( \epsilon_{l}^* - \epsilon_{n} \right) \left( \epsilon_{m}^* - \epsilon_{l} \right) \),\(^{(189)}\)

where \( f(\epsilon) \) is the Fermi distribution function, \( S \) is the nanoribbon area, and \( \delta \) is inversely proportional to the relaxation time of the excited electron. The real part of the dynamical conductivity \( \Re(\sigma_{xx}) \), \( \Re(\sigma_{xy}) \) represents the absorption spectrum of x-polarized (y-polarized) light.

5.6 Giant natural optical activity in \( \text{Rb}_{2}\text{ZnBr}_{4} \)

The constitutive equation which takes account of the natural optical activity effects of homogeneous medium was found as

\[ D_{i} = \epsilon_{ij}E_{j} + \gamma_{ijk} \partial_{k}E_{j}. \]

(190)

The constitutive equation which takes account of the natural optical activity effects of inhomogeneous medium was presented of single possible equation \[ \int \mathbf{E}' d\mathbf{v} = \int \mathbf{E}'' d\mathbf{v}, \]

(192)

where \( \mathbf{E}' \) and \( \mathbf{E}'' \) are two different choice set of value \( \mathbf{E} \) electric field strength, and \( \mathbf{D}' \) and \( \mathbf{D}'' \) corresponding it choice set of value \( \mathbf{D} \) magnetic induction. Substituting (191) into (192) under partial integration with takes account of whole space and tensor symmetry as well as the absence of an electric fields in infinity we have found \[ \int (\alpha_{ikj}E_{i}'\partial_{k}E_{j}' - \beta_{ikj}E_{i}'\partial_{k}E_{j}')d\mathbf{v} = \int (\alpha_{ikj}E_{i}''\partial_{k}E_{j}' + \beta_{ikj}E_{i}''\partial_{k}E_{j}')d\mathbf{v}, \]

(193)

which can be rewritten as follows

\[ \int (\alpha_{ikj}E_{i}'\partial_{k}E_{j}' - \beta_{ikj}E_{i}'\partial_{k}E_{j}')d\mathbf{v} = 0, \]

(194)

with arbitrary of choice set of values \( \mathbf{E}' \) and \( \mathbf{E}'' \) electric field strength we have \[ \alpha_{ikj} = -\beta_{ikj}. \]

(195)

Hence the constitutive equation which takes account of the natural optical activity effects of inhomogeneous medium was presented of single possible equation like \[ D_{i} = \epsilon_{ij}E_{j} + \alpha_{ikj} \partial_{k}E_{j} + \partial_{i}(\alpha_{jk}E_{j}). \]

(196)

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 [97, 98, 99, 100, 101, 102]

\[ \nabla_{i}^{2}E + \frac{\omega^{2}}{c^{2}}D = 0, \]

(197)

with the constitutive equation which takes account of the natural optical activity effects of inhomogeneous medium was presented of single possible equation in which \( \gamma_{ij} \equiv \alpha_{ij} \) like \[ \mathbf{D}_{i}(\mathbf{r}, \varphi) = \epsilon_{ij}E_{j}(\mathbf{r}, \varphi) + \epsilon_{ij}(\mathbf{q}' \mathbf{r} + \varphi)E_{j}(\mathbf{r}, \varphi) + \gamma_{ij}(\mathbf{q}' \mathbf{r} + \varphi)\nabla_{i}E_{j}(\mathbf{r}, \varphi) + \frac{1}{2} \nabla_{i}\gamma_{ij}(\mathbf{q}' \mathbf{r} + \varphi) \cdot E_{j}(\mathbf{r}, \varphi), \]

(198)

in which

\[ \gamma_{ij} = \epsilon_{ijm} \delta_{ml}, \]

(199)

where \( \epsilon_{ijm} \) is unit Levi-Chevita tensor and with consideration of inhomogeneous medium

\[ \epsilon_{12} = \epsilon_{12} \cos(\mathbf{q}' \mathbf{r} + \varphi), \]

(200)

as well as
\[ g_{33}(q' r + \varphi) = g_{33} \sin(q' r + \varphi). \] (201)

It is known [1] 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 [1]. In an opaque materials the abrupt modulation of pump photons can trigger displaced motions of ions towards new coordinates in the excited state resulting in cosine-type oscillations [1].

If sine-type edges of Group-VI Dichalcogenides and Rb₂ZnBr₄, Ca₂RuO₄, Cr₂O₃, MnTiO₃, La-doped BiFeO₃, PtCl₃, PdBr₃, RuCl₃, PtI₃, and carbon nanoribbons may be approximated armchair or zigzag edges then in the sections 5 are found that structure phase transitions to be related with giant spin-orbit interaction (SOI). In the article a creation of giant spin-orbit splitting (∼ 2.5 eV) coupled with the carbon Dirac cones (K and K') are shown to be related with structure phase transition in carbon nanoribbon with armchair or zigzag edges of honeycomb lattice of Group-VI Dichalcogenides and Rb₂ZnBr₄, Ca₂RuO₄, Cr₂O₃, MnTiO₃, La-doped BiFeO₃, PtCl₃, PdBr₃, RuCl₃, PtI₃, and carbon nanoribbons.

Hence we have replaced the Eqs. (98) in the space region \(-L < z < 0\) by of the one-dimensional Maxwell wave equations system of Incommensurate phase crystal thin film of the space region \(-L < z < 0\) 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

\[
\left[\left(\frac{c^2}{\omega^2} \Delta_l + e_i \delta_{ij} \cos(q_i' x_i + \varphi) + \gamma_{ijl} \sin(q_i' x_i + \varphi)\right) \nabla_i + \frac{1}{2} \gamma_{ijl} \cos(q_i' x_i + \varphi) q_l^j\right] E_j = 0, \] (202)

where \(x_i \equiv z, e \equiv e + 4\pi P_j - 4\pi \int \frac{x_i}{z} \rho_i(z) dz + C_1\). 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

\[ E_j = \psi_j(q_i' x_i + \varphi)e^{i k_n x_n}. \] (203)

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

\[ \psi_j(q_i' x_i + \varphi) = \sum_{n=-\infty}^{\infty} C_j^{(n)} e^{i n(q_i' x_i + \varphi)}. \] (204)

The wave vectors can be extended by series

\[ k_i = k_i^{(0)} + k_i^{(1)} + k_i^{(2)} + \ldots. \] (205)

Substituting Eqs. (203), (204), (205) in Eq. (202)

\[
= \sum_{n=-\infty}^{\infty} \left( (e_{ij} + \frac{1}{2} \gamma_{ijl} q_l^j) e^{i q_i' x_i + \varphi} e^{i k_n x_n} - e \right) C_j^{(n)} e^{i n(q_i' x_i + \varphi)} e^{i k_n x_n} = \sum_{n=-\infty}^{\infty} \left( (q_i' q_i^{(0)} + k_i^{(1)} + \ldots + n q_l^j) - e \right) C_j^{(n)} e^{i n(q_i' x_i + \varphi)} e^{i k_n x_n}. \] (206)

The sought for solutions of Eq. (202) one be found as two linear polarization wave in the zero approximation

\[ (k_i^{(0)})^2 = \frac{\omega^2}{c^2} e_{ii}, \] (207)

\[ C_{1x}^{(0)} = 1, \quad C_{1y}^{(0)} = 0, \] (208)

\[ C_{2x}^{(0)} = 0, \quad C_{2y}^{(0)} = 1. \] (209)

In the first approximation the solutions for wave vectors and field may be now written as

\[ k_i^{(1)} = 0, \] (210)

\[ C_{2x}^{(\pm 1)} = \frac{\omega^2 c_{1x} (\sqrt{2} \pm \sqrt{1 + \frac{1}{\gamma_{1x} q_i^j}})}{((k_i^{(0)})^2 - (k_i^{(1)})^2)}, \quad C_{2y}^{(\pm 1)} = 0, \] (211)
Hence

\[
\psi_1(q_i^j) = \frac{1}{c^2} \left( \psi_{1i} + \psi_{2j} \right) \exp(\pm i k_i x) \exp(\pm i k_j y),
\]

(213)

\[
\psi_2(q_i^j) = \frac{1}{c^2} \left( \psi_{1i} - \psi_{2j} \right) \exp(\pm i k_i x) \exp(\pm i k_j y),
\]

(214)

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

\[
\varepsilon \frac{d^2}{d\tilde{q}_i^j}(k_{i}^{(1)})^2 + 2k_{i}^{(0)}k_{i}^{(2)}C_{i}^{(0)} = \varepsilon_{ij} \left( C_{i}^{(0)} - \frac{\varepsilon_{ij}}{c^2} \frac{\varepsilon}{\varepsilon} \right) - \gamma_{ij} \left( C_{i}^{(1)} + \frac{\varepsilon_{ij}}{2} \frac{\varepsilon}{\varepsilon} \right),
\]

(215)

in the form

\[
\tilde{E}_{ij}^{(2)} = -k_{i}^{(0)} - \frac{\omega^2}{c^2} \sqrt{(k_{i}^{(0)})^2 \frac{\varepsilon}{\varepsilon} + 2 \frac{\varepsilon^2}{c^2} \left( \frac{\varepsilon_{ij}}{2} \frac{\varepsilon}{\varepsilon} \right) \left( C_{i}^{(1)} + \frac{\varepsilon_{ij}}{2} \frac{\varepsilon}{\varepsilon} \right) - \gamma_{ij} \left( C_{i}^{(1)} + \frac{\varepsilon_{ij}}{2} \frac{\varepsilon}{\varepsilon} \right)},
\]

(216)

\[
\tilde{E}_{ij}^{(2)} = -k_{i}^{(0)} - \frac{\omega^2}{c^2} \sqrt{(k_{i}^{(0)})^2 \frac{\varepsilon}{\varepsilon} + 2 \frac{\varepsilon^2}{c^2} \left( \frac{\varepsilon_{ij}}{2} \frac{\varepsilon}{\varepsilon} \right) \left( C_{i}^{(1)} + \frac{\varepsilon_{ij}}{2} \frac{\varepsilon}{\varepsilon} \right) - \gamma_{ij} \left( C_{i}^{(1)} + \frac{\varepsilon_{ij}}{2} \frac{\varepsilon}{\varepsilon} \right)},
\]

(217)

Hence the data of natural optical gyrotropy as well as Rashba spin splitting are shown to be derived like \( (k^{(0)} \pm k^{(2)})^2 \) as displacement of two symmetrically allocated parabolas from Brillouin zone center. We have found the formulas of Gyrotropy splitting of Rb_2ZnBr_4 as well as K_2SeO_4 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 \( e = \hbar c k / eV = 138.7202 \text{ eV cm}^{-1} \) but the corresponding wave vector was estimated to be \( k = 7.1614 \times 10^5 \text{ cm}^{-1} \). The magnitude of these displacements were estimated correspondingly with formulas Eqs. (216), (217). Hence in the paper we have derived the formulas of Gyrotropy splitting of Rb_2ZnBr_4 and K_2SeO_4 Incommensurate phases crystal from Maxwell wave equations and the magnitude of this Gyrotropy splitting are found to be related with light velocity like \( e = \hbar c k / eV = 14.0798 \text{ eV} \) but the corresponding wave vector was estimated to be \( k = 7.1614 \times 10^5 \text{ cm}^{-1} \).

Table 4. The material parameters Rb_2ZnBr_4: refractive index \( n = \frac{\lambda}{\varepsilon} k \), gyrotropic birefringence \( \Delta n_{11} \), Gyrotropy \( g \), light wavelength \( \lambda \) in nm, the frequency of light in \( c^{-1} \), lattice constant \( a \) in A, irrational parameter \( \gamma \), wave vector of Incommensurate phase \( q^l \) in \( c^{-1} \) and temperature \( T \) in K [2], the Gyrotropy splitting \( e \) in eV, the wave vector of Gyrotropy splitting \( k \) in cm^{-1}.

<table>
<thead>
<tr>
<th>( n = \frac{\lambda}{\varepsilon} k )</th>
<th>( \Delta n_{11} )</th>
<th>( g )</th>
<th>( \lambda )</th>
<th>( \Omega )</th>
<th>( c^* )</th>
<th>( \gamma )</th>
<th>( q^l )</th>
<th>( T )</th>
<th>( \epsilon )</th>
<th>( k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.65</td>
<td>5.3 \times 10^{-3}</td>
<td>10^{-5}..10^{-4}</td>
<td>632.8</td>
<td>2.9788 \times 10^{-15}</td>
<td>9.71</td>
<td>0.293</td>
<td>3.0175 \times 10^6</td>
<td>300</td>
<td>14.0798</td>
<td>7.1614 \times 10^5</td>
</tr>
</tbody>
</table>

The analytical solutions of the Maxwell wave equations as well as natural optical gyrotropy effects are found in Rb_2ZnBr_4 as well as K_2SeO_4 Incommensurate phases crystals connected with giant light velocity as well as via interaction with coherent phonon oscillations [114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 30, 127, 114, 115, 116]. 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_{16h} or isomorphic groups [118, 119, 120, 121, 122, 123, 124, 125, 126, 30, 127]. In the paper the non-zero gyration \( g_{33} \) and gyrotropic birefringence \( e_{12} \) tensors of K_2SeO_4 and Rb_2ZnBr_4 materials based on D_{16h} space symmetry group were found. The values of natural optical gyrotropy as well as Rashba spin splitting are shown to be found like \( (k^{(0)} \pm k^{(2)})^2 \) 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 \( e = \hbar c k / eV = 14.0798 \text{ eV} \) but the corresponding wave vector was estimated to be \( k = 7.1614 \times 10^5 \text{ cm}^{-1} \). The found strong natural optical gyrotropy has been based on available experimental data [2].

Hence if sine-type edges of Group-VI Dichalcogenides and Rb_2ZnBr_4, Ca_2RuO_4, Cr_2O_3, MnTiO_3, La-doped BiFeO_3, PtCl_3, PdBr_3, RuCl_3, PtI_3, and carbon nanoribbons may be approximated armchair or zigzag edges then in the sections 5 are found that structure phase transitions to be related with giant spin-orbit interaction (SOI). In the article a creation of giant spin-orbit splitting (~ 2.5 eV) coupled with the carbon Dirac cones (K and K') are shown to be related with structure phase transition in carbon nanoribbon with armchair or zigzag edges of honeycomb lattice of Group-VI Dichalcogenides and Rb_2ZnBr_4, Ca_2RuO_4, Cr_2O_3, MnTiO_3, La-doped BiFeO_3, PtCl_3, PdBr_3, RuCl_3, PtI_3, and carbon
The material parameters $\gamma, T, q, \lambda, c, \Delta$.

<table>
<thead>
<tr>
<th>$n = \frac{5}{2} k$</th>
<th>$\Delta n_{11}$</th>
<th>$g$</th>
<th>$\lambda$</th>
<th>$\Omega$</th>
<th>$c^g$</th>
<th>$\gamma$</th>
<th>$q^I$</th>
<th>$T$</th>
<th>$e$</th>
<th>$k$</th>
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</thead>
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<tr>
<td>1.65</td>
<td>$5.5 \times 10^{-3}$</td>
<td>$2 \times 10^{-3}$</td>
<td>632.8</td>
<td>$2.9788 \times 10^{15}$</td>
<td>9.71</td>
<td>0.293</td>
<td>$3.0175 \times 10^6$</td>
<td>300</td>
<td>27.6009</td>
<td>$1.4038717 \times 10^6$</td>
</tr>
</tbody>
</table>

Table 5: The material parameters $A_2BX_4$: refractive index $n = \frac{5}{2} k$, gyrotropic birefringence $\Delta n_{11}$, Gyrotropy $g$, light wavelength $\lambda$ in nm, the frequency of light in $c^{-1}$, lattice constant $c^g$ in $\AA$, irrational parameter $\gamma$, wave vector of Incommensurate phase $q^I$ in $cm^{-1}$ and temperature $T$ in K [2], the Gyrotropy splitting $e$ in eV the wave vector of Gyrotropy splitting $k$ in $cm^{-1}$.

<table>
<thead>
<tr>
<th>$n = \frac{5}{2} k$</th>
<th>$\Delta n_{11}$</th>
<th>$g$</th>
<th>$\lambda$</th>
<th>$\Omega$</th>
<th>$c^g$</th>
<th>$\gamma$</th>
<th>$q^I$</th>
<th>$T$</th>
<th>$e$</th>
<th>$k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.65</td>
<td>$4.5 \times 10^{-3}$</td>
<td>$5 \times 10^{-5}$</td>
<td>632.8</td>
<td>$2.9788 \times 10^{15}$</td>
<td>9.71</td>
<td>0.293</td>
<td>$3.0175 \times 10^6$</td>
<td>300</td>
<td>7.5726</td>
<td>$3.851647380 \times 10^5$</td>
</tr>
</tbody>
</table>

Table 6: The material parameters $A_2BX_4$: refractive index $n = \frac{5}{2} k$, gyrotropic birefringence $\Delta n_{11}$, Gyrotropy $g$, light wavelength $\lambda$ in nm, the frequency of light in $c^{-1}$, lattice constant $c^g$ in $\AA$, irrational parameter $\gamma$, wave vector of Incommensurate phase $q^I$ in $cm^{-1}$ and temperature $T$ in K [2], the Gyrotropy splitting $e$ in eV the wave vector of Gyrotropy splitting $k$ in $cm^{-1}$.

nanoribbons. In the article the natural optical gyrotyropy effects are shown to be found with light velocity like $e = \hbar ck/eV = 14.0798 eV, e = \hbar ck/eV = 27.6009 eV, e = \hbar ck/eV = 7.5726 eV$ with the corresponding considered in Tables 4,5,6 of gyrotyropy birefringences $\Delta n_{11}$, Gyrotropies $g$ [132, 129, 129, 130, 131, 30, 42, 133].

6 Tight-binding method of phonon modes dispersion in Weil 2-Dimensional half semiconductors: Group-VI Dichalcogenides and PtCl$_3$, PdBr$_3$, RuCl$_3$, PtI$_3$, Cr$_2$Ge$_2$Te$_6$, VCl$_3$, OsCl$_3$

The two-dimensional Group-VI Dichalcogenides include layered materials: MoX$_2$, WX$_2$, (X=S, Se, Te) [134]. The two-dimensional Weil half semiconductors include the next layered materials with the honeycomb lattice with two atoms per unit cell: PtCl$_3$, graphene, PtBr$_3$, PtI$_3$, PdCl$_3$, PdBr$_3$, PdI$_3$, RuCl$_3$, Cr$_2$Ge$_2$Te$_6$, VCl$_3$, OsCl$_3$, CrI$_3$, VSe$_2$ [135, 136, 137]. For explanation of strong spin-orbit splitting and enhancement due to the Au atoms in the hollow position that get closer to graphene and do not break the sublattice symmetry we have calculated phonon dispersion of graphene as well as their wave vectors with accounts oscillation interactions [34, 117, 118, 139, 139, 140, 85, 134, 104, 103] between the first and second nearest neighbors in the basis of the Born-von Karman model [20, 141, 137, 1, 9, 10, 142, 143, 34, 11, 138, 134, 12, 16, 17]. Analytical expressions were derived for the out-of-plane modes as well as for the in-plane modes [137].

The topological invariant or Chern number defined for the integer quantum Hall system the TKNN [144, 145] invariant is closely related to the Berry phase. We have derived the TKNN invariant by calculating the Hall conductivity of a two-dimensional (2D) electron system in perpendicular magnetic field where the electric field $E$ and the magnetic field $B$ were applied along the $y$ and $z$ axes respectively.

The Heisenberg equation of motion $\frac{d}{dt} y = v_y = \frac{i}{\hbar} [y, H]$ leads to [145]

$$\langle m|v_y|n\rangle = \frac{i}{\hbar}(E_n - E_m)\langle m|y|n\rangle,$$

which allows one to calculate the Hall conductivity [145]

$$\sigma_{xy} = \frac{\langle j_x \rangle}{e} = -\frac{\hbar e^2}{2}\sum_{m \neq m} f(E_n)\frac{\langle n|v_x|m\rangle\langle m|y|n\rangle - \langle n|y|m\rangle\langle m|v_x|n\rangle}{(E_n - E_m)^2},$$

(219)

where $v_x$ is the electron velocity along the $x$ direction and $f(E_n)$ is the Fermi distribution function. If we study a system in the periodic potential and its Bloch states $|u_{nk}\rangle$ as the eigenstates the identity [145]

$$\langle u_{nk}|v_y|u_{nk}\rangle = \frac{1}{\hbar}(E_{nk} - E_{mk})\langle u_{nk}|\frac{\partial}{\partial k_y}|u_{nk}\rangle,$$

(220)

allows one to rewrite [145]

$$\sigma_{xy} = \frac{\langle j_x \rangle}{e} = -\frac{\hbar e^2}{2}\sum_{k} \sum_{m \neq m} f(E_n)(\frac{\partial}{\partial k_y} \langle u_{nk}|\frac{\partial}{\partial k_y} u_{nk}\rangle - \frac{\partial}{\partial k_y} \langle u_{nk}|\frac{\partial}{\partial k_y} u_{nk}\rangle),$$

(221)

the Berry connection can be written as Bloch states [145]

$$a_n(k) = -\epsilon (u_{nk}|\nabla_k|u_{nk}) = -\epsilon (u_{nk}|\frac{\partial}{\partial k}|u_{nk}),$$

(222)
the Hall conductivity reduces to \( \sigma_{xy} = \frac{\nu}{h} \), with

\[
\nu = \gamma = \sum_n \int_{BZ} d^2 k \left( \frac{\partial n_{x y}}{\partial k_x} - \frac{\partial n_{x x}}{\partial k_y} \right),
\]  

(223)

where \( \nu = \gamma = \sum_n \nu_n \), which was connected with the Berry phase [145]

\[

v_n = \int_{BZ} d^2 k \left( \frac{\partial n_{x y}}{\partial k_x} - \frac{\partial n_{x x}}{\partial k_y} \right) = \frac{1}{2\pi} \oint_{BZ} d\mathbf{k} a_n(\mathbf{k}) = \frac{1}{2\pi} \gamma_n[\partial BZ],
\]

(224)

hence \( \gamma_n[\partial BZ] = 2\pi m, (m \in Z) \) [145].

Hence \( v_n \) can only take an integer value and hence \( \sigma_{xy} \) is quantized to integer multiples of \( \frac{e^2}{h} \). The integers \( v = \gamma \) were called TKNN invariant or Chern number and it plays the role of the topological invariant of the quantum spin Hall effect is represented by adding a mass term \( H_A = \pm \sigma_z \) [135].

In the basis of the two-dimensional (2D) irreducible representation \( E \) for \( C_{3v} \) point symmetry the effective model takes the form of the 2D Weyl model for PtCl\(_3\) [135]

\[
\hat{H}_0(\mathbf{q}) = v_F(\tau q_x \hat{\sigma}_x + q_y \hat{\sigma}_y),
\]

(225)

where \( v_F \) is the Fermi velocity, \( \tau = \pm \) for the K and K' point, \( \hat{\sigma} \) are the Pauli matrices acting in the space of the two basis states, and for the MoS\(_2\) [134]

\[
\hat{H}_0(\mathbf{q}) = at(\tau q_x \hat{\sigma}_x + q_y \hat{\sigma}_y) + \hat{\sigma}_z - \lambda \tau \frac{\sigma_z - 1}{2} \hat{\gamma}_z,
\]

(226)

where \( \hat{\gamma}_z = \pm \frac{\hat{\gamma}_z}{2}, \hat{\lambda} \) is spin-valley splitting of valence band in the basis of the two-dimensional (2D) irreducible representation two valued \( \Gamma_7 \) for \( C_{3h} \) point symmetry.

Hence we can conclude [135] that the ground state of monolayer PtCl\(_3\) indeed realizes a 2D WHS with a pairs of fully polarized fermions at Weyl points robust under SOC.

A prominent property of Dirac fermions is that they carry the Berry phase of \( \pm \pi \) Hence the Chern number \( \gamma = \pm 1 \).

Let us known 2D massless Weyl fermions with the Fermi velocity \( v_F \) for which the \( 4 \times 4 \) Dirac equation reduces to \( 2 \times 2 \) Weyl equation [145]

\[
E\psi(\mathbf{r}) = \hbar v_F \hat{\sigma} \mathbf{k} \psi(\mathbf{r}) = -i\hbar v_F \hat{\sigma} \nabla \psi(\mathbf{r}),
\]

(227)

the eigenvectors of this equation are

\[
\psi_{\pm}(\mathbf{r}) = \begin{cases} 
\exp^{-i\theta(\mathbf{k})/2} & \text{for } \pm \exp^{i\theta(\mathbf{k})/2}, \text{ } u_{\pm}(\mathbf{k}) \exp^{ikr},
\end{cases}
\]

(228)

where \( \theta(\mathbf{k}) = \arctan \frac{k_x}{k_y} \) and the energy eigenvalue are

\[
E_{\pm} = \pm \hbar v_F k.
\]

(229)

Keeping in mind the Stocks theorem one can find [145]

\[
\gamma = \oint_{C} d\mathbf{k} \langle u_{\pm}(\mathbf{k})|\nabla \psi|u_{\pm}(\mathbf{k})\rangle = \pm \pi.
\]

(230)

We have found that Landau quantization occurs in the manner [145]

\[
E_{\pm}(N) = \pm \sqrt{2e\hbar v_F B/c} N,
\]

(231)

where \( N = 0, 1, 2, 3, \ldots \)

If the Landau quantization of the form Eq. (231) is true the associated QHE becomes unusual \( \sigma_{xy} = -\frac{\pi}{e} (N + \frac{1}{2}) \) which is called half-integer quantization. Hence the half-integer quantization can also be understood to be a result of the \( \pm \pi \) Berry phases or \( \pm 1 \) Chern numbers [145].

The two QAH phases with \( \gamma = \pm 1 \) have edge channels propagating in opposite directions. Because the chirality of the edge channel is determined by the sign of Chern number.

Each atom has three first neighbors in the other sublattice i.e. \( B \) with the relative vectors and six second neighbors in the same sublattice \( A \) with the relative vectors too

\[
\begin{align*}
B_1 &= a(1, 0), & B_2 &= a(-\frac{1}{2}, \frac{\sqrt{3}}{2}), & B_3 &= a(-\frac{1}{2}, -\frac{\sqrt{3}}{2}), \\
A_1 &= a(0, \sqrt{3}), & A_2 &= a(-\frac{3}{2}, -\frac{\sqrt{3}}{2}), & A_3 &= a(-\frac{3}{2}, \frac{\sqrt{3}}{2}), \\
A_4 &= a(0, -\sqrt{3}), & A_5 &= a(-\frac{3}{2}, \frac{\sqrt{3}}{2}), & A_6 &= a(-\frac{3}{2}, -\frac{\sqrt{3}}{2}).
\end{align*}
\]

(232)

The motion equations system in harmonic approximation we seek as follows [137]
where the vectors $a_n$ numerate the lattice cells the $\kappa$ and $\kappa'$ note two sublattices $A$ and $B$ and the $i, j = x, y, z$ accounts three values corresponding space coordinates. Since the potential energy is the quadratic function of the atomic displacements $u_i^a(a_n)$ and $u_i^b(a_n)$, the forth constant matrix can be taken in the symmetrical form

$$\Phi_{ij}^{AB}(a_n) = \Phi_{ji}^{AB}(a_n),$$  \hspace{1cm} (234)

and its Fourier transform i.e. the dynamical matrix is a Hermitian matrix. For the nearest neighbors (in the $B$ sublattice) the dynamical matrix has the form

$$\Phi_{ij}^{AB}(q) = \sum_{\kappa=1}^{3} \Phi_{ij}^{AB}(B_\kappa) \exp(\imath q B_\kappa),$$  \hspace{1cm} (235)

and for the next neighbors (in the $A$ sublattice)

$$\Phi_{ij}^{AB}(q) = \Phi_{ij}^{AB}(A_0) + \sum_{\kappa'=1}^{6} \Phi_{ij}^{AB}(A_{\kappa'}) \exp(\imath q A_{\kappa'}),$$  \hspace{1cm} (236)

where $A_0$ indices the atom chosen at the center of the coordinate system in the $A$ sublattice and $q$ is the wave vector.

The constants

$$\alpha_z \equiv \Phi_{zz}^{AB}(B_1),$$  \hspace{1cm} (237)

$$\gamma_z \equiv \Phi_{zz}^{AB}(A_1).$$  \hspace{1cm} (238)

We have found the stability condition

$$\Phi_{zz}^{AB}(A_0) + 6\Phi_{zz}^{AB}(A_1) + 3\Phi_{zz}^{AB}(B_1) = 0,$$  \hspace{1cm} (239)

and the similar form for the $\xi \eta$ components, where off-diagonal elements are given by

$$\begin{align*}
\Phi_{\xi}(q) &= \Phi_{\xi}(B_1) \exp(\imath q B_1) + \Phi_{\xi}(B_2) \exp(\imath q B_2) + \Phi_{\xi}(B_3) \exp(\imath q B_3) = \\
&= \Phi_{\xi}(B_1) \exp(\imath \frac{\pi}{3}) + \exp(-2\imath \frac{\pi}{3}) \exp(-\imath \frac{\pi}{3}) \exp(-\imath \frac{\pi}{3}) = \\
&= \beta(\exp^\imath \frac{\pi}{3} + 2 \exp(-\imath \frac{\pi}{3}) \cos(\frac{\sqrt{3} \pi}{2} q_y + \frac{2}{3} \pi)),
\end{align*}$$  \hspace{1cm} (240)
Figure 7. (Color online) Frequency dispersions or Phonon dispersion spectrums in MoS$_2$ from point K $(0,1)$ $\frac{4\pi}{3\sqrt{3}a}$ to $\Gamma$ $(0,0)$.

Figure 8. (Color online) Frequency dispersions or Phonon dispersion spectrums in MoS$_2$ from point $\Gamma$ $(0,0)$ to M $(1, \sqrt{3}) \frac{2\pi}{3a}$ and from point M $(1, \sqrt{3}) \frac{2\pi}{3a}$ to K $(0,1)$ $\frac{2\pi}{3\sqrt{3}a}$.

Figure 9. (Color online) Frequency dispersions or Phonon dispersion spectrums in MoS$_2$ from point K $(0,1)$ $\frac{4\pi}{3\sqrt{3}a}$ to $\Gamma$ $(0,0)$. 
Figure 10. (Color online) Frequency dispersions or Phonon dispersion spectrums in $\text{PlCl}_3$ from point $\Gamma (0,0)$ to $M (1, \sqrt{3} \frac{a}{3a})$ and from point $M (1, \sqrt{3} \frac{a}{3a})$ to $K (0,1) \frac{4\pi}{3\sqrt{3}a}$.

Figure 11. (Color online) Frequency dispersions or Phonon dispersion spectrums in $\text{PlCl}_3$ from point $K (0,1) \frac{4\pi}{3\sqrt{3}a}$ to $\Gamma (0,0)$.

Figure 12. (Color online) Frequency dispersions or Phonon dispersion spectrums in $\text{PlCl}_3$ from point $\Gamma (0,0)$ to $M (1, \sqrt{3} \frac{a}{3a})$ and from point $M (1, \sqrt{3} \frac{a}{3a})$ to $K (0,1) \frac{4\pi}{3\sqrt{3}a}$. 
Figure 13. (Color online) Frequency dispersions or Phonon dispersion spectrums in PlCl$_3$ from point K (0,1) to Γ (0,0).

Figure 14. (Color online) Figures from Phys. Rev. B 100 (064408) 2019.
\[ \Phi_{\xi \zeta}^A(B_1) = \Phi_{\xi \zeta}^A(B_2) \exp^{2\pi i/3} = \Phi_{\xi \zeta}^A(B_3) \exp^{-2\pi i/3}, \]

\[ \Phi_{\xi \zeta}^B(A_1) = \Phi_{\xi \zeta}^B(A_3) \exp^{-2\pi i/3} = \Phi_{\xi \zeta}^B(A_5) \exp^{-2\pi i/3}, \]

\[ \Phi_{\xi \zeta}^B(A_2) = \Phi_{\xi \zeta}^B(A_6) \exp^{2\pi i/3}. \]

(242)

The dynamical matrix for the in-plane oscillations for the honeycomb lattice with two atoms per unit cell for \( N \times N \) unit cells has the form

\[ \Phi_{\xi \zeta}^A(A_0) + 6 \Phi_{\xi \zeta}^A(A_1) + 3 \Phi_{\xi \zeta}^B(B_1) = 0. \]

(243)

The point group \( D_{6h} \) of the honeycomb lattice is generated by \( \{C_6, \sigma_x, \sigma_z\} \) where \( \sigma_z \) is a reflection \( z \rightarrow -z \) by the plane that contains the graphene layer, \( C_6 \) is a rotation by \( \pi/3 \) around the \( z \)-axis and \( \sigma_x \) is a reflection by the \( xz \) plane. To find the dynamic matrix we introduce variables \( \xi, \eta = x \pm iy \) transforming under the rotation \( C_6 \) around the \( z \)-axis (taken at the \( A_0 \) atom) as follows (\( \xi, \eta \) \( \rightarrow \) (\( \xi, \eta \)) \( \exp^{\pm 2\pi i/3} \)). At the rotation the atoms change their positions \( B_1 \rightarrow B_2 \rightarrow B_3, A_1 \rightarrow A_3 \rightarrow A_5 \) and \( A_2 \rightarrow A_4 \rightarrow A_6 \). Hence all forth constant \( \Phi_{\xi \eta}^B(B_a) \) with the different \( \kappa \) (as well as \( \Phi_{\xi \eta}^A(B_a) \)) are equal to one another but the force constants with the coincident subscripts \( \xi \) or \( \eta \) transform as covariant variables.

\[ \Phi_{\xi \eta}^B(B_a) = \Phi_{\xi \zeta}^A(B_a) \exp^{2\pi i/3} = \Phi_{\xi \zeta}^A(B_a) \exp^{-2\pi i/3}, \]

\[ \Phi_{\xi \eta}^B(B_a) = \Phi_{\xi \zeta}^A(B_a) \exp^{2\pi i/3} = \Phi_{\xi \zeta}^A(B_a) \exp^{2\pi i/3}. \]

(244)
The equations allow us to express the phonon frequencies of the out-of-plane branches and in-plane modes at the critical points $\Gamma$, $K$ and $M$ in the term of force constants

\[
\delta(\exp^{\sqrt{3}q_y} + 2\exp^{-\sqrt{3}q_y}\cos\left(\frac{2\sqrt{3}}{3}q_y + \frac{2\pi}{3}\right)) = \\
= \delta(\cos(\sqrt{3}q_y) + \sqrt{3}\sin(\sqrt{3}q_y) + 2(2\cos(\sqrt{3}q_y) - \sqrt{3}\sin(\sqrt{3}q_y))\cos(\frac{3}{2}q_y + \frac{3\pi}{2})) + \\
+ \delta^* (\cos(\sqrt{3}q_y) - \sqrt{3}\sin(\sqrt{3}q_y) + 2(2\cos(\sqrt{3}q_y) + \sqrt{3}\sin(\sqrt{3}q_y))\cos(\frac{3}{2}q_y - \frac{3\pi}{2})) = \tag{247}
\]

We have found the matrix factor for the equation of motion in the form

\[
\Phi^{AB}_{\xi\xi}(q) - \omega^2 \\
\Phi^{AB}_{\xi\eta}(q) - \omega^2 \\
\Phi^{AB}_{\eta\eta}(q) - \omega^2 \\
\Phi^{AB}_{\eta\xi}(q) - \omega^2 \\
\Phi^{AB}_{\eta\xi}(q) - \omega^2 \\
\Phi^{AB}_{\eta\eta}(q) - \omega^2
\]

where

\[
\Phi^{AB}_{\xi\xi}(q) = \beta(\exp^{q_x} + 2\exp^{-q_x}\cos(\frac{\sqrt{3}}{2}q_y - \frac{3\pi}{2})), \tag{249}
\]

\[
\Phi^{AB}_{\eta\eta}(q) = \alpha_1(\exp^{q_x} + \exp^{-q_x}\cos(\frac{\sqrt{3}}{2}q_y)), \tag{250}
\]

\[
\Phi^{AB}_{\eta\xi}(q) = \Phi^{AB}_{\xi\eta}(q) = \alpha_2(\exp^{q_x} + 2\exp^{-q_x}\cos(\frac{\sqrt{3}}{2}q_y)). \tag{251}
\]

The phonon dispersion for the out-of-plane modes is found the equations of motion

\[
\det \begin{bmatrix} 
\Phi^{AB}_{\xi\xi}(q) - \omega^2 \\
\Phi^{AB}_{\xi\eta}(q) \\
\Phi^{AB}_{\eta\eta}(q) - \omega^2 \\
\end{bmatrix} = 0, \tag{255}
\]

\[
(\Phi^{AB}_{\xi\xi}(q) - \omega^2)^2 - |\Phi^{AB}_{\xi\eta}(q)|^2 = 0, \tag{256}
\]

\[
\Phi^{AB}_{\xi\xi}(q) - \omega^2 = \pm|\Phi^{AB}_{\xi\eta}(q)|, \tag{257}
\]

\[
\Phi^{AB}_{\xi\xi}(q) \mp |\Phi^{AB}_{\xi\eta}(q)| = \omega^2, \tag{258}
\]

\[
\omega(q) = \sqrt{\Phi^{AB}_{\xi\xi}(q) + |\Phi^{AB}_{\xi\eta}(q)|}. \tag{259}
\]
The Force parameters of phonon oscillating matrices of graphene

\[ \Gamma(0, 0), \]
\[ M(1, \sqrt{3}) \frac{q_x}{\sqrt{2}}, \]
\[ K(0, 1) \frac{q_x}{3\sqrt{2}}, \]
\[ \Gamma - M, \]
\[ \frac{q_y}{q_x} = \sqrt{3}, \]
\[ q_y = q, \]
\[ q_x = \frac{q}{\sqrt{3}}, \]
\[ \omega(q_y = q, q_x = \frac{q}{\sqrt{3}}) = \sqrt{\Phi_{zz}^{\Delta}(q_y = q, q_x = \frac{q}{\sqrt{3}}) + |\Phi_{zz}^{\Delta}(q_y = q, q_x = \frac{q}{\sqrt{3}})|}, \]
\[ k_y = 0.. \frac{\sqrt{3} \pi}{3a}, \]
\[ M - K, \]
\[ \frac{q_y}{q_x} = \tan \left( \frac{\pi}{6} \right) = \frac{1}{\sqrt{3}}, \]
\[ q_y = q, \]
\[ q_x = \sqrt{3}q, \]
\[ \omega(q_y = q, q_x = \sqrt{3}q) = \sqrt{\Phi_{zz}^{\Delta}(q_y = q, q_x = \sqrt{3}q) + |\Phi_{zz}^{\Delta}(q_y = q, q_x = \sqrt{3}q)|}, \]
\[ k_y = \frac{\sqrt{2} \pi}{3a} \ldots \frac{4\pi}{3\sqrt{3}a}, \]
\[ K - \Gamma, \]
\[ q_y = q, \]
\[ q_x = 0, \]
\[ \omega(q_y = q, q_x = 0) = \sqrt{\Phi_{zz}^{\Delta}(q_y = q, q_x = 0) + |\Phi_{zz}^{\Delta}(q_y = q, q_x = 0)|}, \]
\[ k_y = \frac{4\pi}{3\sqrt{3}a}..0, \]

Table 8. The Force parameters of phonon oscillating matrices of graphene [137].

<table>
<thead>
<tr>
<th>( a_x )</th>
<th>( \gamma_x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.27</td>
<td>0.204</td>
</tr>
</tbody>
</table>

\[ a_x (\exp^{q_x} + 2 \exp^{-i \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2}} q_y) = a_x (\cos q_x + i \sin q_x + 2(\cos \frac{q_x}{2} - i \sin \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2})) = \]
\[ = a_x (\cos q_x + 2 \cos \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2} q_y + i(\sin q_x - 2 \sin \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2})), \]
\[ |a_x (\cos q_x + 2 \cos \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2} q_y + i(\sin q_x - 2 \sin \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2})))| = \]
\[ = a_x \sqrt{(\cos q_x + 2 \cos \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2} q_y)^2 + (\sin q_x - 2 \sin \frac{q_x}{2} \cos \frac{\sqrt{3}q_y}{2})^2}, \]

So we found the three acoustic branches and optical branches which are in close agreement with Ref. [137, 135, 146, 147, 148, 149, 150, 129, 130, 131, 151, 152, 153]. In the framework our calculations one can conclude that in the K point the acoustic and optical branches have Dirac point similarly to the Dirac cone in graphene and light cone in relativistic physics, where the light velocity is substituted by the phonon velocity and describes by the Dirac equation. In Fig. 9 we have presented (a) schematic depiction of the orbital splitting in monolayer PtCl\(_3\). In (b) Spin-resolved partial density of states (PDOS) for monolayer PtCl\(_3\) projected on different orbitals. In (c) band structure without spin-orbit coupling (SOC). The red and blue bands are for spin-majority (spin-up) and spin-minority (spin-down) channels respectively. In (d) enlarged view of the band structure around the Weyl point. The red solid (blue dashed) lines are
located at K/K’ points without SOC (blue points), and they are shifted along the x direction on the mirror-invariant line after considering SOC (red points) [135]. In (a) top and side views of monolayer PtCl₃, with the edge-sharing PtCl₃ octahedron forming a honeycomb lattice. In (b) first Brillouin zone for monolayer PtCl₃ with high-symmetry D₃d point group symmetry. We also mark the three vertical mirror planes for the lattice structure (red lines) [135]. Let us known the phonon dispersions and their wave vectors from the equations of motion

\[
\begin{align*}
\begin{bmatrix} \Phi^{AB}_{zz}(\mathbf{q}) - \omega^2 & \Phi^{AB}_{xx}(\mathbf{q}) \\ \Phi^{AB}_{xx}(\mathbf{q}) & \Phi^{AB}_{zz}(\mathbf{q}) - \omega^2 \end{bmatrix} \begin{bmatrix} u_A(\mathbf{q}) \\ u_B(\mathbf{q}) \end{bmatrix} = 0,
\end{align*}
\]

(276)

\[
(\Phi^{AB}_{zz}(\mathbf{q}) - \omega^2)u_A(\mathbf{q}) + \Phi^{AB}_{xx}(\mathbf{q})u_B(\mathbf{q}) = 0,
\]

(277)

\[
\omega_+ : u_A(\mathbf{q}) = -\frac{\Phi^{AB}_{zz}(\mathbf{q})}{\Phi^{AB}_{xx}(\mathbf{q}) - \omega^2} u_B(\mathbf{q}),
\]

(278)

\[
\Phi^{AB}_{xx}(\mathbf{q})u_A(\mathbf{q}) + (\Phi^{AB}_{zz}(\mathbf{q}) - \omega^2)u_B(\mathbf{q}) = 0,
\]

(279)

with orthonormalized condition of wave vectors of out-of plane modes of coherent phonon oscillation of lattice

\[
|u_A(\mathbf{q})|^2 + |u_B(\mathbf{q})|^2 = 1,
\]

(280)

\[
|\frac{\Phi^{AB}_{zz}(\mathbf{q})}{\Phi^{AB}_{xx}(\mathbf{q}) - \omega^2}|^2 |u_B(\mathbf{q})|^2 + |u_B(\mathbf{q})|^2 = 1,
\]

(281)

\[
u_B(\mathbf{q}) = \frac{1}{\sqrt{1 + |\frac{\Phi^{AB}_{zz}(\mathbf{q})}{\Phi^{AB}_{xx}(\mathbf{q}) - \omega^2}|^2}} = \frac{1}{\delta},
\]

(282)

\[
\begin{bmatrix} \Phi^{AA}_{zz}(\mathbf{q})u_A(\mathbf{q}) + (\Phi^{AA}_{zz}(\mathbf{q}) - \omega^2)u_A(\mathbf{q}) = 0,
\end{bmatrix}
\]

(284)

\[
u_B(\mathbf{q}) = -\frac{\Phi^{AB}_{zz}(\mathbf{q})}{\Phi^{AB}_{xx}(\mathbf{q}) - \omega^2} u_A(\mathbf{q}),
\]

(285)

\[
|u_A(\mathbf{q})|^2 + |u_B(\mathbf{q})|^2 = 1,
\]

(286)

\[
|u_A(\mathbf{q})|^2 + |\frac{\Phi^{AB}_{zz}(\mathbf{q})}{\Phi^{AB}_{xx}(\mathbf{q}) - \omega^2}|^2 |u_A(\mathbf{q})|^2 = 1,
\]

(287)

\[
u_A(\mathbf{q}) = \frac{1}{\sqrt{1 + |\frac{\Phi^{AB}_{zz}(\mathbf{q})}{\Phi^{AB}_{xx}(\mathbf{q}) - \omega^2}|^2}} = \frac{1}{\delta},
\]

(288)

\[
\begin{bmatrix} \Phi^{AA}_{zz}(\mathbf{q}) - \omega^2 & \Phi^{AA}_{xx}(\mathbf{q}) \\ \Phi^{AA}_{xx}(\mathbf{q}) & \Phi^{AA}_{zz}(\mathbf{q}) - \omega^2 \end{bmatrix} \begin{bmatrix} u_A(\mathbf{q}) \\ u_A(\mathbf{q}) \end{bmatrix} = 0,
\]

(290)

The phonon dispersions and their wave vectors for in-plane coherent phonon branches of oscillation of lattice

\[
(\Phi^{AA}_{zz}(\mathbf{q}) - \omega^2)u_A(\mathbf{q}) + \Phi^{AA}_{xx}(\mathbf{q})u_A(\mathbf{q}) + (\Phi^{AA}_{xx}(\mathbf{q}) - \omega^2)u_A(\mathbf{q}) + (\Phi^{AA}_{zz}(\mathbf{q}) - \omega^2)u_B(\mathbf{q}) = 0,
\]

(291)
\[
\begin{align*}
\mathbf{u}_A(q) &= -\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q), \\
\mathbf{u}_A'(q) &= -\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q), \\
\mathbf{u}_B(q) &= -\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q), \\
\mathbf{u}_B'(q) &= -\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q).
\end{align*}
\]
\[
\begin{align*}
\mathbf{u}_A(q)(1 - \frac{\Phi^{AA}(q)^2}{\Phi^{AA}(q) - \omega^2}) &= \left(\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q)\right), \\
\mathbf{u}_A'(q) &= -\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q), \\
\mathbf{u}_B(q) &= -\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q), \\
\mathbf{u}_B'(q) &= -\frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_A(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q).
\end{align*}
\]
\[
\begin{align*}
\mathbf{u}_A(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_A'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_B'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) = 0, \\
\mathbf{u}_A(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_A'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_B'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) = 0, \\
\mathbf{u}_A(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_A'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_B'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) = 0, \\
\mathbf{u}_A(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_A'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) + \left(\frac{\Phi^{AA}(q) - \omega}{\Phi^{AA}(q) - \omega^2}\right)^{-1}\mathbf{u}_B'(q) - \frac{\Phi^{AA}(q)}{\Phi^{AA}(q) - \omega} u_B(q) = 0.
\end{align*}
\]
\[
\frac{1}{\delta} = -\left(\left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)^{-1}(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}) - \Phi_{\text{C}}(q) - \Phi_{\text{L}}(q)\right)^{-1}\left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)^{-1}\left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)^{-1}\times

\frac{u_B(q)}{u_B(q)} = \frac{1}{\delta} u_B(q),
\]

with orthonormalized condition of wave vectors for in-plane modes of coherent phonon branches of oscillations of lattice

\[u_A(q)u_A(q)^\dagger + u_B(q)u_B(q) = 1, \quad (308)\]

\[u_A(q) = \frac{1}{\delta} u_B(q), \quad (311)\]

\[u_A(q)(1 - \frac{|\Phi_{\text{C}}(q)|^2}{|\Phi_{\text{C}}(q)|^2}) = \left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)u_B(q) + \left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)u_B(q)^\dagger, \quad (312)\]

\[u_A(q) = \left(\left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right) - \Phi_{\text{C}}(q) - \Phi_{\text{L}}(q)\right)\left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)^{-1}\left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)^{-1}\left(\frac{\Phi_{\text{C}}(q)}{\psi_{\text{C}}(q)} - \frac{\Phi_{\text{L}}(q)}{\psi_{\text{L}}(q)}\right)^{-1}, \quad (313)\]

\[u_A(q) = \frac{1}{\delta} u_B(q), \quad (315)\]

\[u_A(q) = \frac{1}{\delta} u_B(q), \quad (316)\]

\[\psi_1(q) = \frac{1}{\alpha} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad (317)\]

\[\psi_2(q) = \frac{1}{\alpha} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad (318)\]

\[\psi_3(q) = \frac{1}{\alpha} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad (319)\]

\[\psi_4(q) = \frac{1}{\alpha} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad (320)\]

We seek linearly independent solutions of wave vectors of coherent phonon oscillations [154, 155, 156, 150, 157, 158, 132] Eqs. (320), (319), (318) from (317) like \(A \rightarrow B, B \rightarrow A, \ast \rightarrow \circ, \circ \rightarrow \ast\).
Hence we have found that the Weyl Hall semiconductor (WHS) states allow the topological phase transition happened between two quantum anomalous Hall (QAH) insulator phase with opposite Chern numbers and we have based on phonon dispersion of Weil 2D half semiconductor monolayers group like PtCl$_3$. The ground state of monolayer PtCl$_3$ allows the creation of the 2D WHS states with the pairs of fully polarized fermions at Weyl points which robust under spin-orbit coupling (SOC). We have proposed the switching of the quantum anomalous Hall states by rotating the magnetization vector on the basis of PtCl$_3$ monolayer. So we have proposed the switchable QAH phases will enable new designs of topological nano electronic devices in basis on group materials like 2D PtCl$_3$ type [114, 115, 116, 117, 159, 118, 119, 120, 121, 122, 123, 124, 125].

In the article we have found that the Weyl Hall semiconductor (WHS) states allow the topological phase transition happened between two quantum anomalous Hall (QAH) insulator phase with opposite Chern numbers and we have based on phonon dispersion of Weil 2D half semiconductor monolayers group like PtCl$_3$. The ground state of monolayer PtCl$_3$ allows the creation of the 2D WHS states with the pairs of fully polarized fermions at Weyl points which robust under spin-orbit coupling (SOC). The two QAH phases with $\epsilon' = \pm 1$ have edge channels propagating in opposite directions. Because the chirality of the edge channel is determined by the sign of Chern number. We have predicted the switching of the Quantum Anomalous Spin Hall states by rotating the magnetization vector on the basis of PtCl$_3$ monolayer and we have based on phonon dispersion of Weil 2D half semiconductor monolayers group like PtCl$_3$. Landau-Ginsburg-Devonshire theory of thin ferroelectric polar-active nanofilms in incommensurate phases and semiconductor heterostructures is presented. The self-consistent solutions of the Euler-Lagrange equation for the polarization vector and 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. 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 $D_{16}$ or isomorphic groups. In the paper the non-zero gyration $g_{32}$ and gyrotropic birefringence $e_{12}$ tensors of K$_2$SeO$_4$ and Rb$_2$ZnBr$_4$ materials based on $D_{16}$ space symmetry group were found. The values of natural optical gyrotropy as well as Rashba spin splitting are shown to be specified like $\nu (k_{0}^{(0)} \pm k_{2}^{(2)})$ 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 $\epsilon = hck/eV = 14.0798$ eV but the corresponding wave vector was estimated to be $k = 7.161 \times 10^6$ cm$^{-1}$. The found strong natural optical gyrotropy has been based on available experimental data [Phys. Rev. B 38, 8075, (1988)].

References


