Quantum Cryptography

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Landau-Ginsburg-Devonshire theory of thin ferroelectric polar-active nanofilms in Incommensurate Phases and semiconductor heterostructures

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

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1 Contents

2 Optical properties of crystals with Incommensurate phases from first principle

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 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. In an opaque material the abrupt modification of pump photons can trigger displaced motions of ions towards new coordinates in the excited state resulting in cosine-type oscillations. It explains the coherent oscillations observed in transparent compounds under pumping with a photon energy smaller than an optical gap [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 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].

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

\[ \Delta = \frac{\hbar}{2m} \left( \right| \nabla \mathbf{V} \times \mathbf{p} \left| \right| \psi, \right) \]

where \( \mathbf{V} \) is the microscopic crystal potential of graphene. In graphene we would have \( \Delta = 0 \) if the basis functions \( |\psi_\sigma \rangle \) and \( |\psi_p \rangle \) were made up on basis of pure \( \pi \) or \( \sigma \) orbitals. However spin-orbit coupling induces a mixing of the \( \pi \) or \( \sigma \) or \( (\sigma_x, \sigma_y) \) orbitals in graphene that contributes to \( \Delta \) in second order of spin-orbit coupling. In the our case [7, 8, 9, 10, 11, 12, 13, 14, 15, 16] the strain mediates a coupling between intrinsic-spin and orbital dynamics and the lowest order contribution \( p_{22}^{\alpha\beta}(\epsilon_{xx} + \epsilon_{xy})s_{z} \sigma_{z} \) constitutes a renormalization of the intrinsic spin-orbit coupling \( p_{22}^{\alpha\beta} s_{z} \sigma_{z} \). In the article [17] 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.

Refractive indexes can be determined like the eigenvalues of the dielectric permeability tensor as follows [4]

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

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

\[ \epsilon_{\alpha\beta}(\omega, \mathbf{k} = 0) = \delta_{\alpha\beta} - \frac{s_{\alpha\beta}^{2}}{\omega} \sum_{\mathbf{n} \mathbf{n} \mathbf{n} \mathbf{n}} \langle \left\{ \mathbf{p}_{\mathbf{n}}^{\alpha} \mathbf{p}_{\mathbf{n}}^{\beta} \right\} \rangle, \]

where \( \mathbf{p}_{\mathbf{n}}^{\alpha} \) 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].

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Table 1. Chapters.

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It is known that the Hamiltonian 

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

where $e$ and $Z_k$ are charges of electron and ion, respectively,

\[ \hat{D}_n^\alpha = \sum_{k\beta} \mu_{k\alpha}^\beta \hat{X}_{nk}^\beta, \]

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

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

In the article [4] for ionic insulator crystals the Hamiltonian of ionic crystal with account electronic excitation of ionics or ionic complexes as well as phonon lattice vibration oscillations at expansion of interactions in the sets with phonon to ionic displacements as well as electric dipole moments has been presented via Hubbard operators $\hat{X}_{nk}^\beta = |nk\rangle \langle k^\beta|$ from which consist of the basis electronic states of $|\psi_{nk}\rangle$ ion in the form [4]

\[ H = \sum_{nks} \lambda_{ks} \hat{X}_{nk}^s - \sum_{nks, n'k} \left( \frac{1}{2} \psi_{nk}(nk') \hat{D}_{nk}^\alpha \hat{D}_{nk'}^\beta \right) + C_{nk'}(nk, n'k') \hat{D}_{nk}^\alpha u_{nk'}^\beta + \sum_{n'n''k} \left( \sigma_{nk}^{D_{nk}}(nk, n''k') \hat{D}_{nk}^\alpha u_{nk''}^\beta + \sigma_{nk''}^{D_{nk}}(nk, n''k') \hat{D}_{nk}^\alpha u_{nk'}^\beta \right) + \frac{1}{4} \sum_{n'n''k} \left( \sum_{nk'} \theta_{nk} \hat{D}_{nk}^\alpha u_{nk'}^\beta \right) \]

where $u_n^\alpha$ are ion displacement vectors accordingly equilibrium states, $\hat{D}_{nk}^\alpha$ 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 $\psi_{nk}$ and energies $\lambda_{ks}$ the ones in the high-temperature commensurate phase of the crystal are chosen.

The structure of the incommensurate phase is given by the average displacements and average dipole momenta which may be presented in the form of modulation waves [4]

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

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

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

In order to deposit the electronic subsystem Hamiltonian [4] we have entered main field approximation

\[ H_{MF}^{el} = \sum_{nk} \sum_{n'k'} (\lambda_{ks} \delta_{n'n'} - \sum_{\alpha} F_{nk}^{\alpha} \bar{X}_{nk}^{\alpha} \bar{X}_{nk'}^{\alpha}), \]

where

\[ F_{nk}^{\alpha} = \sum_{n'k'} \left( \psi_{nk}(nk') \left( \hat{D}_{nk'}^\alpha \right) + C_{nk'}(nk, n'k') \left( u_{nk'}^\beta \right) \right) - \sum_{n''k} \left( \sigma_{nk}^{D_{nk}}(nk, n''k') \left( \hat{D}_{nk'}^\alpha \right) \left( u_{nk''}^\beta \right) + \sigma_{nk''}^{D_{nk}}(nk, n''k') \left( \hat{D}_{nk'}^\alpha \right) \left( u_{nk'}^\beta \right) \right) \]

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.

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

\[ \bar{X}_{nk}^{\alpha} = \sum_{\nu} \mu_{nk}^{\nu} \bar{X}_{nk}^{\alpha}, \]

where $\mu_{nk}^{\nu}$ were eigenvectors which were found from equations system

\[ \sum_{\nu} (\lambda_{ks} \delta_{n'n'} - \sum_{\alpha} F_{nk}^{\alpha} \bar{X}_{nk}^{\nu}) u_{nk}^{\nu} = \tilde{\lambda}_{nk} u_{nk}^{\nu}. \]

Hence

\[ \bar{H}_{MF}^{el} = \sum_{nk\mu} \tilde{\lambda}_{nk} \bar{X}_{nk}^{\mu}, \]

where $\tilde{\lambda}_{nk\mu}$ were new energy levels splitting by Stark effect. We have transformed $\bar{D}_{nk}$ operators into the form

\[ \bar{D}_{nk}^{\alpha} = \sum_{\mu\nu} \tilde{\mu}_{nk\alpha}^{\mu\nu} \bar{X}_{nk}^{\nu}, \]
Hence we have derived the Bethe-Salpeter equations for Green function in the form

\[ \langle \hat{D}^{\mu}_{nk} | \hat{D}^{\nu}_{n'k'} \rangle_\omega = \sum_{\mu'\nu'} \hat{\mu}^{\nu'}_{nk} \hat{\nu}^{\mu'}_{nk'} \langle \hat{X}^{\mu'\nu'}_{nk} | \hat{X}^{\nu'\mu'}_{n'k'} \rangle_\omega. \]  

(14)

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

\[ \langle \hat{D}^{\mu}_{nk} | \hat{D}^{\nu}_{n'k'} \rangle_\omega = \sum_{\mu'\nu'} \hat{\mu}^{\nu'}_{nk} \hat{\nu}^{\mu'}_{nk'} \langle \hat{X}^{\mu'\nu'}_{nk} | \hat{X}^{\nu'\mu'}_{n'k'} \rangle_\omega. \]  

(15)

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

\[ (\hbar \omega - \tilde{\sigma}_{nk} + \tilde{\sigma}_{nk}^\dagger) \langle \hat{X}^{\mu\nu}_{nk} | \hat{X}^{\nu\mu}_{n'k'} \rangle = \frac{1}{2\pi} \delta_{n'n} \delta_{kk'} \delta_{\mu'\mu} \delta_{\nu'\nu} \langle \hat{X}^{\mu\nu}_{nk} - X^{\mu\nu}_{nk} \rangle - \sum_{\mu'\nu'} \hat{\mu}^{\nu'}_{nk} \langle \hat{X}^{\mu\nu}_{nk} - X^{\mu\nu}_{nk} \rangle \sum_{m\ell \delta} \tilde{\psi}_{\gamma\delta}(nk, n'k') \langle \hat{D}^\delta_{m\ell} | \hat{X}^{\nu'\mu'}_{n'k'} \rangle_\omega, \]  

(16)

but

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

(17)

Hence we have derived Tyablikov uncoupling \( \langle \langle u | \tilde{X} \rangle \rangle \) as well as we have cut the expressions \( \langle \hat{D} \tilde{u} | \hat{X} \rangle \) Green function as well as we have uncoupled \( \langle \tilde{u} \tilde{u} | \hat{X} \rangle \) and \( \langle D | D | \rangle \) in additions.

Hence we have derived the Bethe-Salpeter equations for Green function in the form

\[ \langle \langle \hat{D}^{\mu}_{nk} | \hat{D}^{\nu}_{n'k'} \rangle \rangle_\omega = \frac{1}{2\pi} \delta_{n'n} \delta_{kk'} \langle \tilde{X}^{\mu\nu}_{nk} \rangle_\omega - \sum_{\mu'\nu'} \langle \tilde{X}^\delta_{nk} \rangle_\omega \sum_{m\ell \delta} \tilde{\psi}_{\gamma\delta}(nk, n'k') \langle \hat{D}^\delta_{m\ell} | \hat{D}^{\mu}_{n'k'} \rangle_\omega, \]  

where

\[ \langle \tilde{X}^\mu_{nk} \rangle_\omega = \sum_{\mu'\nu'} \frac{\mu^{\nu'}_{nk} \nu^{\mu'}_{nk} \langle \hat{X}^{\mu'\nu'}_{nk} - X^{\mu'\nu'}_{nk} \rangle \langle \hat{D}^\delta_{m\ell} | \hat{X}^{\nu'\mu'}_{n'k'} \rangle_\omega}{\hbar \omega - \tilde{\sigma}_{nk} + \tilde{\sigma}_{nk}^\dagger}. \]  

(18)

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

## 2.1 Symmetry of Incommensurate phase crystals

It is known from neutron and X-ray scattering that the phase transition from high temperature commensurate phase in incommensurate phase caused by equilibrium breaking in general defined \( q \) point of Brillouin zone [4]. At these the created structure which displaced low temperature \( T_1 \) of phase transition were described for the phase transition of displacement type in \( K_2SeO_4 \) the modulation wave of ions displacement \( u_{nk} = u(q|n + \varphi) \) but for the phase transition order-orderless in \( NaN_2O_2 \) by the modulation wave of occupation probability of single ion the one from several equilibrium location \( p_{nk} = p_{k}(q|n + \varphi) \), where \( n = n_1 a_1 + n_2 a_2 + n_3 a_3 \) was lattice vector of basic hight temperature commensurate phase.

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

Hence like for the phase transition of displacement type thus for the phase transition of order-orderless the average displacement of ions in incommensurate phase can be presented in the form

\[ \langle u_{nk} \rangle = \mathbf{C}_k(q|n + \varphi), \]  

(20)

where \( \mathbf{C}_k(q) = \mathbf{C}_k(q + 2\pi). \)

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

\[ Nq^I + Ma^I = 0, \]  

(21)

where \( a^I \) 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

\[ \langle u_{nk} \rangle = \sum_{q,j} Q(q, j) \mathbf{e}_j(q, j) \exp(iq|n + r_j)), \]  

(22)

where \( Q(q, j) \) order parameter which transforms like \( j \) irreducible representation for wave vector \( q \), \( \mathbf{e}_j(q, j) \) eigenvector this representation; \( \sum_{q,j} \) includes the contributions from main order parameter \( Q(q^I, j_I) \) corresponding representation \( j_I \) for the wave vector \( q^I \) as well as the contributions from secondary order parameters \( Q(q_{II}, j_{II}) \) for which the symmetry allows the existing in Landau expansion for free energy such terms which are proportional to

\[ Q^5(q^I, j_I)Q(-q^I, j_I)\Delta(n, q^I - q^I), \]  

(23)
where $\Delta(k) = \sum_\alpha \delta(k - G)$, but $G$ is inverse lattice vector. 

Since 

$$Q(q', j_0) = Q(-q', j_0) = \eta \exp^{i\varphi},$$  \hspace{1cm} (24)$$

and take into account the following connections $Q(q, j_0) \sim Q^0(-q', j_0)$, $q_0 = n_q q' + m_a a^*$ which effluent from Eq. (23) can assure that found expansion for $\langle u_{nk}^a \rangle$ satisfy the expression Eq. (20). 

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 $\hat{g}$ elements of supersymmetry group have a form 

$$\hat{g} = ([\hat{R}t_k], [R|V_R]),$$ \hspace{1cm} (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 $\hat{g}$ on four-dimensional vector $(r, \varphi)$ can be entered as 

$$\hat{g}(r, \varphi) = (r', \varphi'),$$ \hspace{1cm} (26)$$

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

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

### 2.2 Bethe-Salpeter equation of incommensurate phase

In the initial hight 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: for the element 

$$\psi_{ab}(ml, m'l') = \sum_{\nu\nu'} R_{ab\nu} R_{b\nu'} \psi_{\nu\nu'}(nk, n'k'),$$ \hspace{1cm} (27)$$

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

$$\psi_{ab}(nk, n'k') = \psi_{ab}(n - m, k; n' - m, k'),$$ \hspace{1cm} (28)$$

Correlation functions which were build on anionic displacements as well as electronic dipole momenta operators satisfy the similar found expressions. 

In low-temperature commensurate phase the non-zero averages $\langle D_{nk}^a \rangle = d_{nk}^a = d_{nk}^a = \delta_{nk}^a = \delta_{nk}^a n_{n_k}$ have been created, where $n_k$ is lattice vector of low temperature phase but the renormalized Fourth constants $\bar{\psi}_{ab}(nk, n'k')$ 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 effluent from Eq. (23)

$$\langle u_{nk}^a \rangle = C_k^a(q' n + \varphi) = \sum_h C_k^a(h) \exp^{ihq(n + r_i)},$$ \hspace{1cm} (29)$$

$$\langle D_{nk}^a \rangle = d_k^a(q' n + \varphi) = \sum_h d_k^a(h) \exp^{ihq(n + r_i)},$$ \hspace{1cm} (30)$$

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

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

$$\tilde{\psi} = \psi + \psi^{(1)} + (\psi^{(2)} + \bar{\psi}^{(2)}) + ..., \hspace{1cm} (31)$$

$$F = F^{(1)} + (F^{(2)} + \bar{F}^{(2)}) + ..., \hspace{1cm} (32)$$

which 

$$\psi^{(1)} = -\sigma^{Dnk}(u), \hspace{1cm} \psi^{(2)} = -\frac{1}{2} \theta(u) \langle u \rangle,$$

$$F^{(1)} = \psi(D) + C \langle u \rangle, \hspace{1cm} (33)$$

$$F^{(2)} = -\sigma^{Dnk}(D) \langle u \rangle - \frac{1}{2} \sigma^{Duk}(u) \langle u \rangle,$$
the contributions from equilibrium displacements,
\[
\psi^{(2)} = -\frac{i}{2} \delta (\hat{u} \hat{u}),
\]
\[
F^{(2)} = -\sigma^{\delta \mu \nu} (\hat{D} \hat{u}) - \frac{i}{2} \sigma^{\delta \mu \nu} (\hat{u} \hat{u}),
\]
(34)
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 \( \tilde{\epsilon}_{\nu k } \) 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 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
\[
\tilde{Z}_{nk}^{\alpha\beta} (\omega) = Z_{0,k}^{\alpha\beta} (\omega) + \sum_{y} z_{1,k}^{\alpha\beta,\gamma} (\omega) F_{nk}^{y} + \sum_{y} z_{2,k}^{\alpha\beta,\gamma} (\omega) F_{nk}^{y} F_{nk}^{y} + \ldots,
\]
(35)
where
\[
Z_{nk}^{\alpha\beta} (\omega) = \sum_{\omega} \frac{\nu_{\alpha\beta,\gamma}^{nk}}{\hbar \omega - E_{\alpha\beta,\gamma}^{nk} + \lambda_{\alpha\beta}} (X_{\gamma}^{nk} - X_{\gamma}^{nk}).
\]
(36)
Let us known Eq. (35) in the form of sum of contributions caused different components of field \( F_{nk}^{\alpha} \) Eq. (32),
\[
\begin{align*}
\tilde{Z}_{nk}^{\alpha\beta} (\omega) &= Z_{0,k}^{\alpha\beta} (\omega) + \sum_{\gamma} z_{1,k}^{\alpha\beta,\gamma} (\omega) (F_{nk}^{1}\gamma) + \sum_{\gamma} z_{2,k}^{\alpha\beta,\gamma} (\omega) (F_{nk}^{1}\gamma) F_{nk}^{1}\gamma ,
\end{align*}
\]
(37)
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
\[
\langle \langle D|D \rangle \rangle_{\omega} = \langle \langle D|D \rangle \rangle_{\omega}^{(0)} + G^{(1)}(\omega) + (G^{(2)}(\omega) + \tilde{G}^{(2)}(\omega)),
\]
(41)
where Green function of hight temperature commensurate phase \( \langle \langle D|D \rangle \rangle_{\omega}^{(0)} \) satisfy the equation
\[
\langle \langle D|D \rangle \rangle_{\omega}^{(0)} = \frac{1}{2\pi} Z_{0}(\omega) - Z_{0}(\omega) \psi \langle \langle D|D \rangle \rangle_{\omega}^{(0)},
\]
(42)
but the remainder contributions in Eq. (41) we have found as
\[
G^{(1)}(\omega) = 2\pi \langle \langle D|D \rangle \rangle_{\omega}^{(0)} (Z_{0}^{-1} Z_{1} Z_{0}^{-1} - \psi_{1}) \langle \langle D|D \rangle \rangle_{\omega}^{(0)},
\]
(43)
\[
G^{(2)}(\omega) = 2\pi \langle \langle D|D \rangle \rangle_{\omega}^{(0)} (Z_{0}^{-1} Z_{2} Z_{0}^{-1} - \psi_{2} - Z_{0}^{-1} Z_{1} \psi_{1}) \langle \langle D|D \rangle \rangle_{\omega}^{(0)} - 2\pi \langle \langle D|D \rangle \rangle_{\omega}^{(0)} (Z_{0}^{-1} Z_{1} \psi + \psi_{1}) G^{(1)}(\omega),
\]
(44)
\[
\tilde{G}^{(2)}(\omega) = 2\pi \langle \langle D|D \rangle \rangle_{\omega}^{(0)} (Z_{0}^{-1} Z_{2} Z_{0}^{-1} - \psi_{2}) \langle \langle D|D \rangle \rangle_{\omega}^{(0)},
\]
(45)
where Eq. (43), Eq. (44) were corrections linear and quadratic \( \langle \hat{u} \rangle \) and \( \langle D \rangle \), Eq. (45) is correction which was proportional correlation functions \( \langle \hat{u} \hat{u} \rangle \) and \( \langle \hat{D} \hat{u} \rangle \).

### 2.3 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
\[
\epsilon_{\alpha\beta}(\omega, k = 0) = \delta_{\alpha\beta} - \frac{8\pi^{2}}{\nu_{\alpha\beta}} e^{2} \sum_{kk'} \langle \langle \Phi_{k\alpha,k'\beta}(\omega, k = 0) \rangle \rangle,
\]
(46)
where \( \Phi_{k\alpha,k'\beta}(\omega, k = 0) \) is Fourier transform of dipole-dipole Green function which includes the contributions corresponding Eq. (77)
\[
\Phi_{k\alpha,k'\beta}(\omega, k = 0) = \Phi_{k\alpha,k'\beta}(\omega, k = 0) + \Phi_{k\alpha,k'\beta}^{(1)}(\omega, k = 0) + (\Phi_{k\alpha,k'\beta}^{(2)}(\omega, k = 0) + \tilde{\Phi}_{k\alpha,k'\beta}^{(2)}(\omega, k = 0)).
\]
(47)
First term enters into the expression for the dielectric permeability tensor for the hight temperature phase
\[
\epsilon_{0\alpha\beta}(\omega, k = 0) = \delta_{\alpha\beta} - \frac{8\pi^{2}}{\nu_{\alpha\beta}} e^{2} \sum_{kk'} \langle \langle \Phi_{k\alpha,k'\beta}(\omega, k = 0) \rangle \rangle.
\]
(48)
\[ \Phi_{k,a,k',p}(\omega, k = 0) \] can be found from Eq. (42)

\[ \Phi_{k,a,k',p}(\omega, k) = \frac{1}{2\pi} \delta_{kk'} \tilde{Z}_{a,b}^{\alpha}(\omega) - \sum_{\alpha} \tilde{Z}_{a,b}^{\alpha}(\omega) \sum_{i,\delta} \psi_{k,i,\delta}(k) \Phi_{\delta,\delta,k',p}(\omega, k), \] (49)

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

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 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

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

\[ Z^{a,b}_{nk}(\omega) = Z^{a,b}_{k}(\omega, q'n + \varphi). \] (51)

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

for the \((|R|_k), (R, |V|)\) element we have

\[ \tilde{\psi}_{ab}(m_l, m_l', \varphi') = \sum_{v,v'} R_{a,v} R_{b,v'} \psi_{v,v'}(nk, n'k', \varphi), \] (52)

where

\[ m + r_l = \tilde{R}(nr_l) + t_{g}, \]

\[ m' + r_l = \tilde{R}(nr'_l) + t_{g}, \]

\[ \varphi' = R_l \varphi + V_g, \] (53)

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

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

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

for \((|R|_k), (R, |V|)\) element

\[ \langle \langle D_{m,l}^\alpha | D_{m',l'}^\beta \rangle \rangle_{\omega, \varphi'} = \sum_{v,v'} R_{a,v} R_{b,v'} \langle \langle D_{nk}^\alpha | D_{n'k'}^\beta \rangle \rangle_{\omega, \varphi}, \] (55)

but for translations subgroup

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

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

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

where sum with respect into \( n \) and \( n' \) calculates \( N \) elements of unit cells. Hence we have found (view of subsection of Appendix)

\[ \frac{1}{N} \sum_{mn} \langle \langle D_{nk}^m | D_{n'k'}^m \rangle \rangle_{\omega, \varphi} \exp^{i(m'n' - mn)} = \frac{1}{N} \sum_{mn} \langle \langle D_{nk}^m | D_{n'k'}^m \rangle \rangle_{\omega, \varphi + q' \exp^{i(m'n' - (k'n' - kn)}} = \]

\[ \frac{1}{N} \sum_{k'} \Phi_{k,a,k',p}(\omega, k; h) \exp^{i\delta h_\varphi} \Delta(k' - k + hq'), \]

where

\[ \Phi_{k,a,k',p}(\omega, k; h) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \langle \langle D_{nk}^a | D_{n'k'}^b \rangle \rangle_{\omega, \varphi'} \exp^{im'\varphi'}. \] (59)

At \( k = k' \neq 0 \)

\[ \frac{1}{N} \sum_{mn} \langle \langle D_{nk}^m | D_{n'k'}^m \rangle \rangle_{\omega, \varphi} \exp^{i(m'n' - mn)} = \Phi_{k,a,k',p}(\omega, k) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \langle \langle D_{nk}^a | D_{n'k'}^b \rangle \rangle_{\omega, \varphi'} \exp^{im'\varphi'}. \] (60)

but at \( k = k' = 0 \)

\[ \frac{1}{N} \sum_{mn} \langle \langle D_{nk}^a | D_{n'k'}^b \rangle \rangle_{\omega, \varphi} \exp^{i(m'n' - mn)} = \Phi_{k,a,k',p}(\omega, k = 0) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \langle \langle D_{nk}^a | D_{n'k'}^b \rangle \rangle_{\omega, \varphi'}. \] (61)
The Fourier transforms of the expressions Eqs. (60), (61) are independent of \( \varphi \) phase and can be averaged with respect to \( \varphi \) concerning of period.

We have found Fourier transformations Eq. (58) for Eqs. (43), (44), (45)

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

\[
\Phi^{(2)}(\omega, k, h) = 2\pi \Phi^{(0)}(\omega, k + h q^0) (Z_0^{-1}(\omega)Z_2(\omega | h)Z_0^{-1}(\omega) - \psi^{(2)}(k, h), h - h_1)) \Phi^{(0)}(\omega, k) - 2\pi \Phi^{(0)}(\omega, k + h q^0) (Z_0^{-1}(\omega)Z_1(\omega | h_1)\psi^{(1)}(k + h_1 q^0) + \psi^{(1)}(k + h_1 q^0, h - h_1)) \Phi^{(1)}(\omega, k, h_1),
\]

where

\[
Z_{j,k}^{n}\psi^{(j)}(\omega, k, h) = \int_0^{2\pi} d\varphi \Phi_{j,k}^{n}(\omega, \varphi) \exp^{-i(h \varphi)},
\]

\[
\psi_{k}^{(j)}(\omega, k, h) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi (\sum_{m} \psi_{\pi}^{(j)}(0k, ml, \varphi) \exp^{ikm}) \exp^{-i(h \varphi)}. \tag{66}
\]

The presence of a modulation wave display itself in the ionic contributions \( Z_j \), conditioned by nonlinear polarizabilities in the crystalline contributions conditioned by anharmonicities and in the mixed contributions which were proportional to \( Z_j \psi^{(j)} \).

Hence the symmetry of the tensor \( e_{ab}(\omega, k = 0) \) 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).

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

Let us known the symmetry of \( K_2SeO_4 \) 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 \( q^0 = \frac{1}{N} (1 - \delta) a^* \) (where \( N = 2 \) for \( \text{(NH}_4)\text{BeF}_4 \) and \( \text{(N(CH}_3)\text{)}_2\text{MnCl}_4 \); \( N = 3 \) for \( K_2SeO_4, Rb_2ZnCl_4 \) [4]) but coherent phonon oscillations amplitude \( Q(q^0, \Sigma_2) \) 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]

\[
Q(q_1, \Sigma_1) \rightarrow Q^2(q_1, \Sigma_2), \quad q_1 = 2q^0,
\]

\[
Q(q_2, \Sigma_2) \rightarrow Q^2(q_2, \Sigma_2), \quad q_2 = 3q^0,
\]

\[
Q(q_3, \Sigma_3) \rightarrow Q^2(q_3, \Sigma_2), \quad q_3 = 3q^0 - a^*,
\]

\[
Q(q_4, \Sigma_4) \rightarrow Q^2(q_4, \Sigma_2), \quad q_4 = 2q^0 - a^*.
\]

The eigenvectors have next components [4] for translation ionic displacements

\[
e^{(1)}_k(q, \Sigma_1) = (e^{(1)}_k(q, \Sigma_1), (e^{(1)}_k(q, \Sigma_2)), 0),
\]

\[
e^{(2)}_k(q, \Sigma_2) = (0, 0, (e^{(2)}_k(q, \Sigma_3)),
\]

\[
e^{(3)}_k(q, \Sigma_3) = (0, 0, (e^{(3)}_k(q, \Sigma_4)),
\]

\[
e^{(4)}_k(q, \Sigma_4) = (e^{(4)}_k(q, \Sigma_1), (e^{(4)}_k(q, \Sigma_2)), 0),
\]

as well as for rotation motions of ionic group

\[
e^{(1)}_k(q, \Sigma_1) = (e^{(1)}_k(q, \Sigma_1), (e^{(1)}_k(q, \Sigma_2)), 0),
\]

\[
e^{(2)}_k(q, \Sigma_2) = (0, 0, (e^{(2)}_k(q, \Sigma_3)),
\]

\[
e^{(3)}_k(q, \Sigma_3) = (0, 0, (e^{(3)}_k(q, \Sigma_4)),
\]

\[
e^{(4)}_k(q, \Sigma_4) = (e^{(4)}_k(q, \Sigma_1), (e^{(4)}_k(q, \Sigma_2)), 0).
\]

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 \( K_2SeO_4 \) the non-zero components were \( e_{12} \) gyrotropy 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 \(Q(q'\Sigma_2)\) in \(K_2\text{SeO}_4\) has good agreement with \(n = 2\) rank of matrix of Landau-Ginsburg-Vilson Hamiltonian for which

\[
Q(q'\Sigma_2) \sim (T - T_c)^\beta , 
\]

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

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

have been predicted, where \(2\beta = 0.75\) for \(K_2\text{SeO}_4\) as well as \(2\beta = 0.72\) for \(Rb_2\text{ZnCl}_4\) defined from \(\Phi^{(2)}_{\omega,k/\rho}(\omega, k = 0, h = 0)\) contribution.

### 2.5 Appendix

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

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

where

\[
\Delta(k) = \frac{1}{-1, k = G}.
\]

\(G\) is inverse lattice vector.

Let us known the \(d = 1\) one-dimensional modulation. For the incommensurate of \(q' = \delta a^*\) 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 \(\lim_{N_1, N_0 \to \infty} \frac{N_1}{N_0} = \delta\). Let us known in crystal the main region which includes \(N_0\) cells along \(a\) and we have imposed the Born von Karman periodic boundary conditions. Then for wave vector \(k\) we have

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

but for the vector of incommensurate phase

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

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

\[
\frac{1}{N_0} \sum_{n=0}^{N_0-1} f(\varphi + 2\pi \frac{N_1}{N_0} n) \exp^{i2\pi \frac{N_1}{N_0} n} \delta(2\pi \frac{N_1}{N_0} n) = \frac{1}{N_0} \sum_{n=0}^{N_0-1} f(\varphi + 2\pi \frac{N_1}{N_0} n) \exp^{i2\pi \frac{N_1}{N_0} n} ,
\]

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 equivalent. 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

\[
\{\frac{N_1}{N_0} n_1\} = \{\frac{N_1}{N_0} n_2\}.
\]

Then

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

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

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

At \(n_1 \geq 0, N_0 - 1 \geq n_2\) the latter expression is true only for \(M_1 = 0\) i.e. \(n_1 = n_2\) and so we have found contradiction. Hence we have found that the first case is true and the formula Eq. (76) can be rewritten in the form

\[
\sum_{-\frac{N_0}{2} < h < \frac{N_0}{2}} \left( \frac{1}{N_0} \sum_{n=0}^{N_0-1} f(\varphi + 2\pi \frac{N_1}{N_0} n) \exp^{-i(h(2\pi \frac{N_1}{N_0} n))} \Delta(\frac{m + hN_1}{N_0} a^*) \right) =
\]

\[
\sum_{-\frac{N_0}{2} < h < \frac{N_0}{2}} \left( \sum_{n=0}^{N_0-1} f(\varphi + 2\pi \frac{N_1}{N_0} n) \exp^{-i(h(\varphi + 2\pi \frac{N_1}{N_0} n))} \exp^{i\varphi n} \Delta(k + hq') \right),
\]

where we impose the identity
\[ \exp \left( \frac{2\pi n N_0}{N_0} \right) = \sum_{h=-N_0}^{N_0} \exp \left( \frac{-2\pi h n N_0}{N_0} \Delta \left( \frac{m + h N_0}{N_0} \right) \right). \]  

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 \( N_0 \to \infty \). Hence Eq. (72) is true.

### 3 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

\[ (u^{\alpha}_n) = c^{\alpha} e^{i(q' \cdot n + \varphi)} = \sum_{h} c^{\alpha}_e(h) \exp^h(q'(n + h) + \varphi), \]  

\[ (D^{\alpha}_n) = d^{\alpha}_e n + \varphi = \sum_{h} d^{\alpha}_e(h) \exp^h(q'(n + h) + \varphi), \]  

where \( q' \) is the wave vector of the incommensurate structure, \( c^{\alpha} e(\varphi) \) as well as \( d^{\alpha}_e(\varphi) \) are periodic functions of phase \( \varphi \) with \( 2\pi \) period, \( h \) is an integer.

From Maxwell equations

\[ \nabla \times E = -\frac{\varrho}{\varepsilon}, \]  

(84)

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

\[ \nabla \times E \approx 0. \]  

(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

\[ \nabla \cdot D = \nabla \cdot (E + 4\pi P) = \frac{2\pi}{\varepsilon_0} \rho(\varphi), \]  

(87)

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

The spontaneous polarization \( P_3 \) is directed along the polar axis \( z \). Further we assume that the dependence of polarization vector acquires the form \( [18, 19, 20] \)

\[ P(r) = [\varepsilon_0 (\epsilon_{11} - 1) E_1, \varepsilon_0 (\epsilon_{11} - 1) E_2, P_3(E, r) + \varepsilon_0 (\epsilon_{33} - 1) E_3]. \]  

(88)

Let us known the quasiequilibrium polarization distribution \( P_3(x, y, z) \) 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 \( [18, 19, 20] \) as follows

\[ \alpha P_3 + \beta |P_3|^2 P_3 - g(\Delta_{\perp} + \frac{\partial^2}{\partial x^2}) P_3 = -\frac{\partial \varphi}{\partial x}, \]  

(89)

with the next boundary conditions

\[ (P_3 + \lambda_1 \frac{\partial P_3}{\partial x})|_{x=0} = -P_b, \]  

(90)

\[ (P_3 - \lambda_2 \frac{\partial P_3}{\partial x})|_{x=-L} = 0, \]  

(91)

with taking into consideration for the vector of electric field strength the following expressions \( E_z = -\frac{\partial \varphi}{\partial x} \). We seek the solution the Euler-Lagrange equation Eq. (89) in the form

\[ P_3(x, y, z) = P_3 \exp(i kr) \exp(i k z). \]  

(92)

Substituting the solution Eq. (92) in Eq. (89) we have found non-linear equation with respect to \( P_3 \)
\[ \alpha P_3 + \beta P_3 + gk^2P_3 - g \frac{e^2}{\varepsilon} P_3 = -\frac{\varepsilon}{\varepsilon}, \]  

(93)

Hence we have found the next non-linear cubic equation with respect to polarization vector component \( P_3 \)

\[ f = \alpha P_3 + \beta P_3 + gk^2P_3 + gk^2P_3 - E_z = 0, \]

(94)

the solutions of which meet the next expressions

\[ p_1^{(1)} = \frac{1}{6} \left( \frac{12(\sqrt{3} \varepsilon + 108E_0) \varepsilon^2}{\beta} \right)^{1/3} - \frac{2(12(\sqrt{3} \frac{k_1^2}{\varepsilon} + \varepsilon))^2}{(12(\sqrt{3} \frac{k_1^2}{\varepsilon} + \varepsilon))^2}, \]

(95)

as well as

\[ p_1^{(2)} = p_1^{(3)} = -\frac{1}{12} \left( \frac{12(\sqrt{3} \varepsilon + 108E_0) \varepsilon^2}{\beta} \right)^{1/3} + \frac{(12(\sqrt{3} \frac{k_1^2}{\varepsilon} + \varepsilon))^2}{(12(\sqrt{3} \frac{k_1^2}{\varepsilon} + \varepsilon))^2}, \]

(96)

where

\[ R = \sqrt{\frac{1}{\beta}} \left( 4g^3(k_1^6 + k_0^6) + 12g^3k_1^2k_2^2(k_1^2 + k_2^2) + 12\alpha g^2(k_1^2 + k_2^2)^2 + 12\alpha^2 g(k_1^2 + k_2^2) + 27E_0^2 \frac{\beta}{\varepsilon} + 4\alpha^3 \right). \]

(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 \(z > 0\) [18, 19, 20]

\[ \left( \frac{\partial^2 \varphi}{\partial z^2} + \Delta_\perp \varphi \right) = 0, \quad -H - L < z < -L, \]

(98)

\[ \left( \frac{\partial^2 \varphi}{\partial z^2} + \varepsilon_{11} \Delta_\perp \varphi \right) = \frac{1}{\varepsilon_0} \left( \frac{\partial P_3}{\partial z} - \rho_f(\varphi) \right), \quad -L < z < 0, \]

\[ \varepsilon_0 \varepsilon \left( \frac{\partial^2 \varphi}{\partial z^2} + \Delta_\perp \varphi \right) = -\rho_f(\varphi), \quad z > 0, \]

where \( \varepsilon_{33}^b, \varepsilon_{11} = \varepsilon_{22} \) are permittivities of gyrotropic medium with taking to account the optical activity effects, \( \Delta_\perp = \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial x^2} \).

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

\[ \text{div} \mathbf{E} = \frac{4\pi \rho}{\varepsilon_0}, \]

(99)

where \( \rho \) is charge density,

\[ \frac{\partial E_\parallel}{\partial z} = \frac{4\pi \rho(z)}{\varepsilon_0}, \]

(100)

where \( e_z \) is unit vector in \( Oz \) axis

\[ \frac{\partial E_\parallel}{\partial z} = \frac{4\pi \delta(z)}{\varepsilon_0}, \]

(101)

where \( G_z \) is Green step Hevithaide function, \( \delta(z) \) is Dirac delta function,

\[ G_z \equiv e_z G = \frac{4\pi e_z}{\varepsilon_0} = \frac{4\pi z}{\varepsilon_0} [\zeta]. \]

(102)

The solution the equation Eq. (100) we have found in the form

\[ E(z_0) = \int G(z_0 - z) \rho(z) dz + C_1. \]

(103)

Since for scalar potential we have found the following equations

\[ E = -\text{grad} \varphi = -e_z \frac{\partial \varphi}{\partial z}, \]

(104)

then

\[ e_z E_z = -e_z \frac{\partial \varphi}{\partial z}, \]

(105)

hence for the solution the Eq. (105) we have derived a formula in the form

\[ \varphi = -\int E_z dz + C_2. \]

(106)

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

\[ \varphi = -\int dz_0 \int G(z_0 - z) \rho(z) dz + C_1 + C_2. \]

(107)
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 [21, 22, 23, 24, 25, 26]

$$\nabla_i^2 E + \frac{\omega^2}{c^2} D = 0, \quad (108)$$

where

$$D_i(r, \varphi) = \epsilon_{ij}E_j(r, \varphi) + \epsilon_{ij}E_j(r, \varphi) E_i(r, \varphi) + \gamma_{ij}(q'r + \varphi) \nabla_j E_i(r, \varphi) + \frac{1}{2} \nabla_i \gamma_{ij}(q'r + \varphi) \cdot E_j(r, \varphi), \quad (109)$$

$$\gamma_{ij} = \epsilon_{ijm}g_{ijm}, \quad (110)$$

$$\epsilon_{ij}(q'r + \varphi) = \epsilon_{ij} \cos(q'r + \varphi), \quad (111)$$

$$g_{ij}(q'r + \varphi) = g_{ij} \sin(q'r + \varphi). \quad (112)$$

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].

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

$$((-\frac{\epsilon^2}{\omega^2} \Delta + \epsilon)\delta_{ij} + \epsilon_{ij} \delta_{ij} \cos(q'_i x_i + \varphi) + \gamma_{ij} \sin(q'_i x_i + \varphi) \nabla_i + \frac{1}{2} \gamma_{ij} \cos(q'_i x_i + \varphi) q_i') E_j = 0, \quad (113)$$

where $x_i \equiv z, \epsilon \equiv \epsilon + 4\pi P_3 - 4\pi \int \frac{\epsilon}{|z|} \rho_f(z) dz + C_1$. 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

$$E_j = \psi_j(q'_i x_i + \varphi) e^{i k_i x_i}. \quad (114)$$

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

$$\psi_j(q'_i x_i + \varphi) = \sum_{n=-\infty}^{\infty} C_{ij} e^{i n(q'_i x_i + \varphi)}. \quad (115)$$

The wave vectors can be extended by series

$$k_i = k_i^{(0)} + k_i^{(1)} + k_i^{(2)} + .... \quad (116)$$

Substituting Eqs. (114), (115), (116) in Eq. (113)

$$= \sum_{n=-\infty}^{\infty}((\epsilon_{ij} + \frac{1}{2} \gamma_{ij} q'_i)^2 + \gamma_{ij} \frac{1}{2} (4nq_i^2 - 2) + \gamma_{ij} (4nq_i^2 - 2)) C_{ij} e^{i n(q'_i x_i + \varphi)} e^{i k_i x_i} \quad (117)$$

The sought for solutions of Eq. (113) one be found as two linear polarization wave in the zero approximation

$$\left(\frac{k_i^{(0)}}{2}\right)^2 = \frac{\omega^2}{c^2} \epsilon_{ij}, \quad (118)$$

$$C_{1x} = 1, \quad C_{1y} = 0, \quad (119)$$

$$C_{2x} = 0, \quad C_{2y} = 1. \quad (120)$$
In the first approximation the solutions for wave vectors and field may be now written as

\[ k_1^{(1)} = 0, \]

\[ C_{2x}^{(±1)} = \frac{\epsilon c^2}{\gamma} \sqrt{\frac{\gamma}{(k_x^2 - q_x^2)^2 - (k_y^2)^2}}, \quad C_{2y}^{(±1)} = 0, \]

\[ C_{1x}^{(±1)} = 0, \quad C_{1y}^{(±1)} = \frac{\epsilon c^2}{\gamma} \sqrt{\frac{\gamma}{(k_x^2 - q_x^2)^2 - (k_y^2)^2}}. \]

Hence

\[ \psi_1(q_y^i) = \frac{1}{\sqrt{c^2}} \exp^{±2i(q_x^iy_i + \phi_1)} \varepsilon_{ij} \frac{C_{1y}^{−1}C_{1x}^{−1} + C_{1x}^{−1}C_{1y}^{−1}}{2}, \]

\[ \psi_2(q_y^i) = \frac{1}{\sqrt{c^2}} \exp^{±2i(q_x^iy_i + \phi_1)} \varepsilon_{ij} \frac{C_{1y}^{−1}C_{1x}^{−1} + C_{1x}^{−1}C_{1y}^{−1}}{2}. \]

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

\[ \frac{c^2}{\omega^2} \left((k_x^2)^2 - 2k_x^{(1)}k_x^{(2)}C_{1y}^{(0)} = \frac{1}{\omega^2} \frac{C_{1y}^{−1}C_{1x}^{−1} + C_{1x}^{−1}C_{1y}^{−1}}{2} \right), \]

in the form

\[ \tilde{k}_1^{(2)} = -\frac{c^2}{\omega^2} \left((k_x^{(1)})^2 - 2k_x^{(1)}k_x^{(2)}C_{1y}^{(0)} = \frac{1}{\omega^2} \frac{C_{1y}^{−1}C_{1x}^{−1} + C_{1x}^{−1}C_{1y}^{−1}}{2} \right), \]

\[ \tilde{k}_2^{(2)} = -\frac{c^2}{\omega^2} \left((k_x^{(1)})^2 - 2k_x^{(1)}k_x^{(2)}C_{1y}^{(0)} = \frac{1}{\omega^2} \frac{C_{1y}^{−1}C_{1x}^{−1} + C_{1x}^{−1}C_{1y}^{−1}}{2} \right). \]

Hence the values of natural optical gyrotyropy as well as Rashba spin splitting can be derived like \((k_x^{(0)} ± \tilde{k}_x^{(2)})^2\) as displacement of two symmetrically allocated parabolas from Brillouin zone center. We have found the formulas of Gyrotropy splitting of Rb₂ZnBr₄ as well as K₂SeO₄ Incommensurate phases crystal from Maxwell wave equations and the magnitude of this Gyrotropy splitting are found to be related with Plank constant as well as electron mass like \(\epsilon = h/\omega \equiv 138.7202 \text{ eV} \times \text{cm}^{-1}\) 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. (127), (128). Hence in the paper we have derived the formulas of Gyrotropy splitting of Rb₂ZnBr₄ and K₂SeO₄ Incommensurate phases crystal from Maxwell wave equations and the magnitude of this Gyrotropy splitting are found to be related with light velocity like \(\epsilon = h/\omega \equiv 14.0798 \text{ eV} \times \text{cm}^{-1}\) but the corresponding wave vector was estimated to be \(k = 7.1614 \times 10^5 \text{ cm}^{-1}\).

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

<table>
<thead>
<tr>
<th>(\frac{\omega}{k} )</th>
<th>(\Delta n_{11} )</th>
<th>(g )</th>
<th>(\lambda )</th>
<th>(\Omega )</th>
<th>(c )</th>
<th>(\gamma )</th>
<th>(\mathbf{q} )</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 gyrotyropy effects are found in Rb₂ZnBr₄ as well as K₂SeO₄ Incommensurate phases crystals connected with giant light velocity as well as via interaction with coherent phonon oscillations [27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 27, 28, 29]. 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 [31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41]. In the paper the non-zero gyration \(S_{23} \) and gyrotropic birefringence \(e_{12} \) tensors of K₂SeO₄ and Rb₂ZnBr₄ materials based on \(D_{16h} \) space symmetry group were found. The values of natural optical gyrotyropy as well as Rashba spin splitting are shown to be found like \((k_x^{(0)} ± \tilde{k}_x^{(2)})^2\) as displacement of two symmetrically allocated parabolas from Brillouin zone center. In the article the natural optical gyrotyropy effects are shown to be found with light velocity like \(\epsilon = h/\omega \equiv 14.0798 \text{ eV} \times \text{cm}^{-1}\) but the corresponding wave vector was estimated to be \(k = 7.1614 \times 10^5 \text{ cm}^{-1}\) [42, 43, 44, 45, 40, 46]. The found strong natural optical gyrotyropy has been based on available experimental data [2].
4 Spin Hall Effects in semiconductor nanoheterostructures: ZnO and GaN Quantum Wells and GaN nanotubes without Landau levels

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 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,Mg)O 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.

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 coinciding with the geometric axis of cylinder are a collection have attracted our attention both for their fundamental studies and for their device applications.

Although the extremum loop or ring effects in wurtzite crystals were studied [12, 47, 48, 49, 50, 51, 52, 53, 54, 55], the both the suppressing of laser effect and Spin Hall effects in bulk GaN as well as in GaN/AlGaN Quantum wells were not found in publications 1996, 1997 New Years Eve [56, 57, 58, 59, 60]. It should be noted that in 1998 the Science discovery of Quantum Fractional Hall Effects in Quantum Matter was Nobel Prize winner by Kingdom Academy of Sciences of Sweden.

The strong strain induces warping considerable Rashba spin-orbit (SO) interactions (SOI) on Fermi surfaces that may transform the valence band system into a topological insulator (TI). The latter testify about the significant increased value of Quantum Spin Hall (QSH) effects. The basic idea is as follows. A set of hole bands that in absence SO coupling belongs to orbital momentum $L$, in presence of SO coupling have been described by the total angular momentum $J = L + S$. The TI state can be achieved in semiconductors with inverted bands and in usually driven by the intrinsic SOI arising from heavy host atoms [45, 44, 43, 8, 52, 61, 62, 63, 64, 65, 66, 67, 68, 69].

Hence Spin Hall insulators have connected with the Topological insulator (TI) as well as Exciton insulators. Since the dissipationless spin transport via the sample are shown to be related with Spin Hall insulator solutions of theoretical studies of the space separation of electron and hole wave vectors by 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.

The zinc oxides present a new state of matter where the electron-hole pairing leads to the exciton insulator states [70]. The Coulomb interaction leads to the electron-hole bound states scrutiny study of which acquire significant attention in the explanations of high-temperature superconductivity.

There has been widely studied in the blue, ultraviolet spectral ranges lasers based on direct wide-bandgap hexagonal wurtzite crystal material systems such as ZnO [71, 72, 73, 74, 75, 76]. Significant success has been obtained in growth ZnO quantum wells with (ZnMg)O barriers by scrutinized methods of growth [77, 78]. The carrier relaxation from (ZnMg)O barrier layers into a ZnO quantum well through time-resolved photoluminescence spectroscopy is studied in the paper [79]. The time of filling of particles for the single ZnO quantum well is found to be 3 ps [79].

In the paper we present a theoretical investigation of the intricate interaction of the electron-hole plasma with a polarization-induced electric fields. The confinement of wave functions has a strong influence on the optical properties which is observed with a dependence from the intrinsic electric field which is calculated to be 0.37 MV/cm [80], causing to the quantum-confined Stark effect (QCSE). In this paper we present the results of theoretical studies of the space separation of electron and hole wave functions by 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 addition large electron and hole effective masses, large carrier densities in quantum well ZnO are of cause for population inversions. These features are comparable to GaN based systems [81, 40].

A variational simulation in effective-mass approximation is used for the conduction band dispersion and for quantization of holes a Schrödinger equation is solved with wurtzite hexagonal effective Hamiltonian [11] including defor-
mation potentials [82]. Keeping in mind the above mentioned equations and the potential energies which have been included in this problem from Poisson’s equations we have obtained completely self-consistent band structures and wave functions.

We consider the pairing between oppositely charged particles with complex dispersion. If the exciton Bohr radius is grater than the localization range particle-hole pair, the excitons may be spontaneously created. If the Hartree-Fock band gap energy is greater than the exciton energy in ZnO/(Zn,Mg)O quantum wells then excitons may be spontaneously created. It is known that under the compressive biaxial strain, the matrix elements of optical transitions from the heavy hole band have the strict x (or y) light polarization. The origin of the large negative mass concerned of geometry of the valence band spectra and the strong modification of the momentum matrix elements are shown to be related to the tensile biaxial strain effects. The casual twofold degeneration of the heavy hole and the light hole states at the Brillouin zone center additional to double spin-degeneration is derived. The strong momentum matrix element for the z polarization is found. Both Rashba spin splitting in zinc-blende GaN quantum wells as well as the concerned geometry of the valence band spectra are shown to be related with the found optical transitions of z light polarization. In the article RSOI (Rashba spin-orbit interaction) effect is found. The biaxial strain causes quite significant changes to the gain spectra in spatially confined structures. It is shown, that laser effect is suppressed with arising of the circular loop of valence band maxima in the heterostructure under the tensile strain, while under the compressive strain, the stimulated optical transitions give rise to the large optical gain. Our results show the internal strain effects are important in optical properties of GaN and associated quantum well structures. Comparison with available experimental data shows good agreement [Phys. Rev. B 79, 121308(R), (2009)].

In section a theoretical studies of the space separation of electron and hole wave functions in the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O are presented. For this aim the 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 local exchange-correlation potential is found. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions. In ZnO/(Zn,Mg)O quantum well the electron-hole pairing leads to the exciton insulator states. An exciton insulator states with a gap 3.4 eV are predicted. The particle-hole pairing leads to the Cooper instability. The paper is organized as follows.

4.1 Derivation of effective Hamiltonian of wurtzite band dispersion

<table>
<thead>
<tr>
<th>$C_{6v}$</th>
<th>e</th>
<th>C$_3$</th>
<th>2C$_3$</th>
<th>2C$_6$</th>
<th>3σ</th>
<th>3σ'</th>
</tr>
</thead>
<tbody>
<tr>
<td>τ$_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>τ$_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>τ$_3$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>τ$_4$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>τ$_5$</td>
<td>2</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>τ$_6$</td>
<td>2</td>
<td>-2</td>
<td>-1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>τ$_7$</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>$\sqrt{3}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>τ$_8$</td>
<td>2</td>
<td>0</td>
<td>-1</td>
<td>$-\sqrt{3}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>τ$_9$</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>τ$_7$ + τ$_9$</td>
<td>4</td>
<td>0</td>
<td>-1</td>
<td>$\sqrt{3}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\chi_v$</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>
Table 4. The irreducible representation of $C_{6v}$ [9, 11, 13].

<table>
<thead>
<tr>
<th>$C_{6v}$</th>
<th>$\Gamma_1 + \Gamma_5$</th>
<th>$E$</th>
<th>$C_2$</th>
<th>$2C_3$</th>
<th>$2C_6$</th>
<th>$3\sigma_v$</th>
<th>$3\sigma'_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi^6_0(g)$</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$\frac{g^2}{v}$</td>
<td>9</td>
<td>1</td>
<td>0</td>
<td>4</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$\chi^6_H(g^2)$</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$\frac{1}{2}[+]$</td>
<td>6</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>$2\Gamma_1 + \Gamma_5 + \Gamma_6$</td>
</tr>
<tr>
<td>$\frac{1}{2}[-]$</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
<td>$\Gamma_2 + \Gamma_5$</td>
</tr>
</tbody>
</table>

Table 5. The vector irreducible representation of $C_{6v}$ [9, 11, 13].

<table>
<thead>
<tr>
<th>$C_{6v}$</th>
<th>$E$</th>
<th>$C_2$</th>
<th>$2C_3$</th>
<th>$2C_6$</th>
<th>$3\sigma_v$</th>
<th>$3\sigma'_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_v$</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$\frac{1}{2}[+]$</td>
<td>6</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>$\frac{1}{2}[-]$</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>-1</td>
<td>-1</td>
</tr>
</tbody>
</table>

An irreducible representation for the orbital angular momentum $j$ can be built from the formulas

$$\chi_j(\varphi) = \sum_n D_{j,m} \exp im \varphi = \frac{\sin((j+\frac{1}{2})\varphi)}{\sin \frac{\varphi}{2}} = 1 + 2 \cos \varphi,$$

(129)

$$\chi(C_0) = \chi(\frac{2\pi}{\beta}) = 2,$$

$$\chi(C_2) = \chi(\frac{2\pi}{\beta}) = 0,$$

$$\chi(C_2) = \chi(\frac{2\pi}{\beta}) = -1,$$

(130)

$$\sigma = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ -y \\ z \end{bmatrix},$$

$$\sigma = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$  

(131)

The direct production of two irreducible representations of both wave vector and wave function of difference $\kappa - \Gamma$ expansion with taken into account time inversion can be expanded on

$$p^\alpha : (\Gamma_1 + \Gamma_5) \times (\Gamma_2 + \Gamma_5) = (2\Gamma_1 + \Gamma_5 + \Gamma_6),$$

$$p^\beta : (2\Gamma_1 + \Gamma_5 + \Gamma_6) \times (2\Gamma_1 + \Gamma_5 + \Gamma_6) = 4\Gamma_1 + \Gamma_5 + \Gamma_6 \times \Gamma_5 + \Gamma_5 + \Gamma_6,$$

(132)

$$\sigma_\mu, H_\mu : (\Gamma_2 + \Gamma_5) \times (\Gamma_2 + \Gamma_5) = \Gamma_2 \times \Gamma_2 + \Gamma_5 \times \Gamma_5.$$  

Table 6. The bases functions and operators of irreducible representation of $C_{6v}$ [9, 11, 13].

<table>
<thead>
<tr>
<th>$C_{6v}$</th>
<th>$\Gamma_1$</th>
<th>$\Gamma_2$</th>
<th>$\Gamma_3$</th>
<th>$\Gamma_4$</th>
<th>$\Gamma_5$</th>
<th>$\Gamma_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_x^2$</td>
<td>$k_y^2$</td>
<td>$\epsilon_{+z}$, $\epsilon_{-z}$</td>
<td>$\sigma_{\pm,\pm}$, $\sigma_{\pm,-}$</td>
<td>$J_z$</td>
<td>$J_z$</td>
<td>$J_z$</td>
</tr>
<tr>
<td>$\frac{1}{2}[+]$</td>
<td>$\frac{1}{2}(-\sigma_{\pm} \mp \sigma_{\pm})$</td>
<td>$\frac{1}{2}(\pm \sigma_x \mp \sigma_y)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\frac{1}{2}[-]$</td>
<td>$\frac{1}{2}(\pm \sigma_x \mp \sigma_y)$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$k_{\pm} = k_x \pm i k_y, k_z = k_x^2 + k_y^2, j_z = \frac{1}{\sqrt{2}(J_x \pm i J_y)}, 2[J_x, J_z] = J_x J_z + J_z J_x,$

$$\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm \sigma_y), e_{\pm \pm} = \pm \epsilon_{\pm \pm} = \epsilon_{\pm \pm} = e_{\pm \pm} \pm 2 \epsilon_{\pm \pm} = e_{\pm \pm} \pm 2 \epsilon_{\pm \pm} = e_{\pm \pm} \pm 2 \epsilon_{\pm \pm},$$

(133)
In the low-energy the Hamiltonian with wurtzite symmetry one can find in the form

\[
H_0^{\text{wur}} = (\Delta_1 + \Delta_2) + \Delta_1 J_z^2 + \Delta_2 J_x \sigma_+ + \sqrt{2} \Delta_3 (J_+ \sigma_- + J_- \sigma_+),
\]

\[
H_k^{\text{wur}} = A_1 k_x^2 + A_2 k_y^2 + (A_3 k_x^2 + A_4 k_y^2) J_z^2 + A_5 k_z (2[J_{x+}] k_x + 2[J_{y-}] k_y + A_6 (J_z^2 k_x^2 + J_z k_y^2) + \Delta_5 (J_z k_x - J_- k_y) + \Delta_6 (J_z k_y - J_+ k_x) + \delta (J_z^2 k_x^2 + J_z k_y^2) + D_1 e_{xx} + D_2 e_{yt} + (D_3 e_{zz} + D_4 e_{yt}) J_z^2 + D_5 (2[J_{x+}] e_{xy} + 2[J_{y-}] e_{yx}) + D_6 (J_z^2 e_{xx} + J_z^2 e_{yy}),
\]

where

\[
\begin{align*}
J_x &= \frac{\lambda}{2} (J_+ + J_-), \\
\sigma &= \frac{\lambda}{2} (\sigma_+ + \sigma_-), \\
2[J_{x+}] &= J_x J_+ + J_x J_-,
\end{align*}
\]

so we have specified the bases \{\[Y_1, Y_{10}, Y_{1-1}\] with the operator matrices \{J_x, J_y, J_z\}. Hence the Effective Hamiltonian can be rewritten in the invariant method like in the article \[13\]

\[
H = (\Delta_1 + \Delta_2) J_z^2 + \Delta_1 J_x \sigma_+ + \Delta_2 J_y \sigma_- + \lambda (J_+ \sigma_- + J_- \sigma_+) - (K J_z^2 + K J_y^2) - (H^2 J_z \sigma_+ + H^2 J_z \sigma_-),
\]

where

\[
\begin{align*}
F &= \Delta_1 + \Delta_2 + \lambda + \theta, \\
G &= \Delta_1 - \Delta_2 + \lambda + \theta, \\
\lambda &= \frac{\delta}{2} \left[ A_1 k_x^2 + A_4 k_y^2 \right] + \lambda_z, \\
\delta_x &= D_1 e_{xx} + D_2 (e_{zx} + e_{zy}), \\
\theta &= \frac{\delta}{2} \left[ A_3 k_x^2 - A_4 k_y^2 \right] + \theta_z, \\
\theta_x &= D_3 e_{xx} + D_4 (e_{zx} + e_{zy}), \\
K &= \frac{\delta}{2} \left[ A_5 k_x + \theta k_y \right]^2 + D_5 e_{zz}, \\
H &= \frac{\delta}{2} \left[ A_6 k_z + \theta k_y \right]^2 + D_6 e_{zz}, \\
\Delta &= \sqrt{2} \Delta_3, \\
\epsilon_{\pm} &= \epsilon_{xx} \pm 2 \epsilon_{xy} - \epsilon_{zy}, \\
\epsilon_{\pm x} &= \epsilon_{xx} \pm \epsilon_{xy}.
\end{align*}
\]

In the article \[13\] the following expressions are shown to be related with the cubic approximation for effective mass parameters and deformation parameters

\[
\begin{align*}
A_1 - A_2 &= -A_3 = 2A_4, \\
A_3 + 4A_5 &= \sqrt{2} A_6, \\
\Delta_3 &= \Delta_3, \\
D_1 - D_2 &= D_3 = 2D_4, \\
D_3 + 4D_5 &= \sqrt{2} D_6.
\end{align*}
\]

In the article \[13\] in the following basis

\[
\{[Y_{11} \uparrow], [Y_{10} \uparrow], [Y_{1-1} \uparrow], [Y_{11} \downarrow], [Y_{10} \downarrow], [Y_{1-1} \downarrow]\},
\]

are shown to be found the Effective Hamiltonian in the form

\[
H = \begin{pmatrix}
F & -H^* & -K^* \\
-H & \lambda & H^* \\
-K & H & G \\
0 & \Delta & 0 \\
0 & \Delta & -H & \lambda & H^* \\
0 & 0 & -K & H & F
\end{pmatrix}
\begin{pmatrix}
Y_{11} \uparrow \\
Y_{10} \uparrow \\
Y_{1-1} \uparrow \\
Y_{11} \downarrow \\
Y_{10} \downarrow \\
Y_{1-1} \downarrow
\end{pmatrix},
\]

\[
(142)
\]
where

\[ K = K_t \exp 2\phi, \]
\[ K_t = \frac{\hbar}{2m} A_0 k_z^2, \]
\[ H = H_t \exp i\phi, \]
\[ H_t = \frac{\hbar}{2m} A_0 k_z, \]
\[ (k_x + i k_y) = k_t \exp i\phi, \]
\[ (k_x^2 + k_y^2) = k_t^2. \]  

By introducing the bases \([\exp (-i3\phi/2)|Y_{11} \uparrow], \exp (i\phi/2)|Y_{-1,1} \uparrow], \exp (-i\phi/2)|Y_{10} \uparrow], \exp (3\phi/2)|Y_{1,1} \uparrow], \exp (-i\phi/2)|Y_{11} \downarrow \]

and by using the basis transformation

\[ T = \begin{bmatrix} a^* & 0 & 0 & a & 0 & 0 \\ 0 & \beta & 0 & 0 & \beta^* & 0 \\ 0 & 0 & \beta & 0 & 0 & \beta^* \\ a^* & 0 & 0 & -a & 0 & 0 \\ 0 & \beta^* & 0 & 0 & \beta & 0 \\ 0 & 0 & -\beta^* & 0 & 0 & \beta \end{bmatrix}, \]

where

\[ a = \frac{1}{\sqrt{2}} \exp(i(\frac{5\phi}{4} + \frac{3\phi}{2})), \]

the block diagonal 3 \( \times \) 3 Effective Hamiltonian have been found [13]

\[ H' = UHU^\dagger = T^\dagger HT', \]

in the following form

\[ H = \begin{bmatrix} F & K_t & -i H_t & 0 & 0 & 0 \\ K_t & G & \Delta - i H_t & 0 & 0 & 0 \\ i H_t & \Delta + i H_t & \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & F & K_t & i H_t \\ 0 & 0 & 0 & -i H_t & \Delta - i H_t & \lambda \end{bmatrix}. \]  

The valence subband energy surfaces \( E^\nu_v(k_x, k_y) \) of \( \nu \)-type hole with spin \( \zeta = \pm 1/2 \) and momentum \( k_x, k_y \) can be determined by solving Schrödinger equations system \( \hat{H}\psi = E\psi \). It is known that the cubic equation with respect to \( E \):

\[ \det(\hat{H} - E\hat{I}) = 0 \]

was the necessary and sufficient conditions of existing of solutions of Schrödinger equations system. The solutions of Schrödinger equations we have found in the form of energy surfaces \( E^\nu_v(k_x, k_y) \) as we have shown in Fig.1.

We take the following wave functions written as vectors in the three-dimensional Bloch space:

\[ |\nu, \zeta, k_t \rangle = \sum_{i=1}^{m} |\Psi^{(1)}_{k_t} [i, \nu] \psi_i(Z) \rangle |1, \zeta \rangle \]
\[ \sum_{i=1}^{m} |\Psi^{(2)}_{k_t} [i, \nu] \psi_i(Z) \rangle |2, \zeta \rangle. \]
\[ \sum_{i=1}^{m} |\Psi^{(3)}_{k_t} [i, \nu] \psi_i(Z) \rangle |3, \zeta \rangle. \]

The Bloch vector of \( \nu \)-type hole with spin \( \zeta = \pm 1/2 \) and momentum \( k_t \) is specified by its three coordinates \( [\Psi^{(1)}_{k_t} [m, \nu], \Psi^{(2)}_{k_t} [m, \nu], \Psi^{(3)}_{k_t} [m, \nu]] \) in the basis \([1, \zeta], [2, \zeta], [3, \zeta] \) [13], known as spherical harmonics with the orbital angular momentum \( l = 1 \) and the eigenvalue \( m \) its \( z \) component. The envelope \( Z \)-dependent part of the quantum well eigenfunctions can be specified from the boundary conditions \( \psi_m(Z = 0) = \psi_m(Z = 1) = 0 \) of the infinite quantum well as

\[ \psi_m(Z) = \sqrt{\frac{2}{\pi}} \sin(\pi m Z), \]

where \( Z = (\zeta + \frac{1}{2}) \), \( m \) is a natural number. Thus the hole wave function can be written as

\[ \Psi_{\nu, \zeta, k_t}(r) = \frac{e^{ik_t r}}{\sqrt{\lambda}} |\nu, \zeta, k_t \rangle. \]

The valence subband structure \( E^\nu_v(k_t) \) can be determined by solving equations system:

\[ \sum_{j=1}^{2} (H^{\nu_v}_{jj}(k_t) - i \frac{\phi}{2}) + V(z) + \delta_{ij}E^\nu_v(k_t) \times \phi^{(3)}_{i}(z, k_t) = 0, \]
Figure 1. (Color online) Upper band and Light band as well as Spin Splitting band energies in the axes of reference $k_x = 1.38 \times 10^4$, $k_z = 1.38 \times 10^4$ in the units $cm^{-1}$ for bulk ZnO materials.
where \( \phi^{\langle i \rangle} \xi_i(z, k_i) = \sum_{n=1}^{m} \psi^{\langle i \rangle} [n, v] \psi_i(z) \), \( i = 1, 2, 3 \). The solutions of Schrödinger equations can be found in the form Eq. (148) by premultiply the equations system on Eq. (151) functions and by integrating the later equations system on quantum well boundaries.

Let us known the following integral relations for the found solutions algebra equation systems

\[
\int_0^1 w \psi(n, Z) \psi(n, Z) dZ = 1, \tag{152}
\]

\[
\int_0^1 w \psi(n, Z) \psi(k, Z) dZ = 0, \tag{153}
\]

if \( n \neq k \),

\[
\int_0^1 \psi(n, Z) \frac{d}{dZ} \psi(n, Z) dZ = 0, \tag{154}
\]

if \( n \neq k \),

\[
\int_0^1 \psi(n, Z) \frac{d}{dZ} \psi(n, Z) dZ = 0, \tag{155}
\]

\[
\int_0^1 \psi(n, Z) \frac{d}{dZ} \psi(n, Z) dZ = -\frac{n^2}{w}, \tag{156}
\]

if \( n \neq k \),

\[
\int_0^1 \psi(n, Z) (Z - \frac{1}{2}) \psi(n, Z) dZ = \frac{1}{2} \pi n w (n + k)^2 (n + k)^2
\]

\[
= -\frac{1}{2} \pi n w (n + k)^2 (n + k)^2 (-4nk(-1)^{-n+k} + 8nk(1)^{n+k} + 2(-1)^{-n+k} + (-1)^{n+k})(n^2 + k^2), \tag{157}
\]

if \( n \neq k \),

\[
\int_0^1 \psi(n, Z) (Z - \frac{1}{2}) \psi(n, Z) dZ = 0. \tag{158}
\]

### 4.2 Momentum matrix elements of interband phototransitions of GaN/AlGaN Quantum well

Consider a perfect crystal acted upon by a monochromatic plane wave of wave vector \( k \) and frequency \( \omega \). The vector potential of electrical field can be written as follows

\[
A(r, t) = eA_0 \exp (ikr - i\omega t). \tag{159}
\]

Hence the electric field vector is taken as

\[
E = \frac{\epsilon \omega}{c} A. \tag{160}
\]

The magnetic field associated with a plane wave is then given by the following Maxwell equation

\[
\nabla A = 0. \tag{161}
\]

The light and matter interaction Hamiltonian as usually we have written as follows

\[
\tilde{\mathcal{H}}_{\text{int}} = \frac{\epsilon}{mc^2} (A\tilde{p} + \frac{\epsilon}{2c^2} \tilde{A}^2), \tag{162}
\]

where momentum operator is written a like

\[
\tilde{p} = -i\hbar \nabla. \tag{163}
\]

Hence the matrix elements of the light and matter interaction Hamiltonian with the considered a perfect crystal acted upon by a monochromatic plane wave of selected vector potential we have described as

\[
\langle \psi_{j'_{\sigma'}} | \tilde{\mathcal{H}}_{\text{int}} | \psi_{j_{\sigma}} \rangle = \delta_{j_{\sigma}, j'_{\sigma'}} \frac{eA_0}{mc} \int d^3r U_{j_{\sigma}j_{\sigma}} k \hat{e}[\tilde{p} + \hbar k \hat{e}] U_{j'_{\sigma'}j'_{\sigma'}}, \tag{164}
\]

where we have written momentum matrix elements for interbands phototransitions as

\[
M_{j_{\sigma} \rightarrow j'_{\sigma'}}(k) = \int d^3r U_{j_{\sigma}j_{\sigma}} k \tilde{e} \tilde{p} U_{j'_{\sigma'}j'_{\sigma'}}, \tag{165}
\]

as well as

\[
M_{j_{\sigma} \rightarrow j'_{\sigma}}(k) = \langle S | (\sigma \tilde{e} \tilde{p}) \sigma_{\nu} | j_{\sigma} \rangle, \tag{166}
\]
For the momentum matrix elements of interband phototransitions of bulk GaN.

\[ H_{\text{initial}} = \sum_{\sigma'} \left| \langle \sigma | \psi \rangle \right|^2 \delta_{\sigma\sigma'} \]

\[ M_{\sigma\sigma',-c\sigma_c}(k) = \langle S|\sigma_c|\sigma\rangle \]

(167)

The allowed matrix elements of momentum operator can express by using Klebs-Gordon coefficients as

\[ \langle n'j'm'|f_{km}|njm\rangle = \frac{e^{i(kx-my)}}{(2\pi)^{3/4}} \left| \begin{array}{ccc} j' & k & j \end{array} \right| \left| \begin{array}{ccc} n' & j' & m' \end{array} \right| \left| \begin{array}{ccc} n & j & m \end{array} \right| (n'j'm|f_{km}|njm) \]

(168)

The matrix elements \( f_{km} \) components of irreducible tensor of \( k \) rank have nonzero values for the transitions \( jm \rightarrow j'm' \) which allow by the momentum composition rules \( j' = j + k, m' = m + q \).

For irreducible representation of \( C_{6v} \) point group one can insert the basis

\[ \Gamma_1 + \Gamma_5 : Y_{1,\pm 1} = |1, \pm 1\rangle, \ Y_{10} = |10\rangle. \]

(169)

The allowed matrix elements of momentum operator can express by using Klebs-Gordon coefficients as

\[ \hat{\mathbf{p}} \cdot \langle L', m'|\mathbf{p}|L,m\rangle, \quad L = 1, \ L' = 0, \]

(170)

via \( \langle L'|\mathbf{p}|L\rangle \).

Hence one can find

\[ \langle S|\hat{P}_y|10\rangle = P_x, \quad \langle S|\hat{P}_x|1, -1\rangle = -\langle S|\hat{P}_x|11\rangle = \sqrt{2}P_z. \]

(171)

In spherical coordinate axis the electric field vector has the form \( \mathbf{e} = (\sin(\theta)\cos(\varphi), \sin(\theta)\sin(\varphi), \cos(\theta)) \). The total momentum matrix elements can write as follows

\[ M_{\sigma\sigma',-c\sigma_c}(k) = \sum_{l=1}^{2} \langle S|\sigma_c|\sigma_l\rangle \]

(172)

In the basis

\[ |1, \varsigma_1\rangle = \frac{1}{\sqrt{2}}(Y_1^1(1/2)e^{3\varpi/2}e^{3\varpi/4} \pm Y_1^{-1}(1/2)e^{3\varpi/2}e^{3\varpi/4}) \]

(173)

the Hamiltonian may be transformed to the diagonal form indicating two spin degeneracy [13]:

\[ H_{\pm} = \begin{pmatrix} F & K_t & \mp iH_t \\ K_t & G \mp \Delta & iH_t \\ \pm iH_t & \Delta & \mp iH_t \end{pmatrix} \]

(174)

By using matrix algebra calculations one can find

\[ \langle S|\sigma_c|\sigma_l\rangle \]

(175)

\[ \frac{1}{\sqrt{2}}(Y_1^1(1/2)e^{-3\varpi/2}e^{-3\varpi/4} \pm Y_1^{-1}(1/2)e^{-3\varpi/2}e^{-3\varpi/4}) = -\frac{1}{2}P_z \exp(-i\frac{\varpi}{4}) \sin(\theta), \]

(176)

\[ \frac{1}{\sqrt{2}}(Y_1^1(1/2)e^{-3\varpi/2}e^{-3\varpi/4} \pm Y_1^{-1}(1/2)e^{-3\varpi/2}e^{-3\varpi/4}) = \frac{1}{2}P_z \exp(-i\varpi) \exp(i\frac{\varpi}{4}) \sin(\theta), \]

(177)

\[ \frac{1}{\sqrt{2}}(Y_1^1(1/2)e^{-3\varpi/2}e^{-3\varpi/4} \pm Y_1^{-1}(1/2)e^{-3\varpi/2}e^{-3\varpi/4}) = \frac{1}{2}P_z \exp(i\varpi) \exp(-i\frac{\varpi}{4}) \sin(\theta), \]

(178)
\[ \langle S\rangle = \langle \frac{1}{\sqrt{2}} (Y_1(1/2)e^{-i\pi/2}e^3 + Y_1^{-1}(1/2)e^{i\pi/2}e^{3\pi/4}) = \pm \frac{1}{2} P_e (\cos(\theta)) \sin^2(\theta) \] (179)

\[ \langle S\rangle = \langle \frac{1}{\sqrt{2}} (Y_1(1/2)e^{-i\pi/2}e^{-3\pi/4} + Y_1^{-1}(1/2)e^{i\pi/2}e^{3\pi/4}) = \pm \frac{1}{2} P_e (\cos(\theta)) \sin(\theta) \] (180)

\[ \langle S\rangle = \langle \frac{1}{\sqrt{2}} (Y_1(1/2)e^{-i\pi/2}e^{-3\pi/4} + Y_1^{-1}(1/2)e^{i\pi/2}e^{3\pi/4}) = \frac{1}{\sqrt{2}} P_e (\cos(\theta)) \sin(\theta) \] (181)

### Table 8.
The momentum matrix elements of interband phototransitions of bulk GaN.

| \( |v_{1,\pm}\rangle \) | \( |v_{2,\pm}\rangle \) | \( |v_{\mp,\pm}\rangle \) |
|---|---|---|
| \( \langle S\rangle \) | \( -\frac{1}{2} P_e \exp(\theta) \cos(\frac{\pi}{2}) \sin^2(\theta) \) | \( \frac{1}{2} P_e \exp(-\theta) \cos(\theta) \) | \( \pm \frac{1}{2} P_e \exp(-\theta) \sin(\theta) \) |
| \( \langle S\rangle \) | \( \frac{1}{2} P_e \exp(\theta) \cos(\theta) \) | \( \frac{1}{2} P_e \exp(-\theta) \cos(\theta) \) | \( \pm \frac{1}{2} P_e \exp(\theta) \sin(\theta) \) |

### 4.3 Quantum Hall Plateaus of Gain coefficients of GaN/AlGaN Quantum well including Lorenz broadening

It is known [30], that the optical material gain can be calculated from Fermi golden rule:

\[ a_0 = \frac{\sigma^2}{c\sqrt{m_0} \omega} \sum_{\sigma_{\alpha} = \pm} \sum_{\sigma_{\alpha'} = \pm} \sum_{m,a} \int k_i d k_i \int \frac{d\theta}{2\pi} \left| \mathbf{M}^{\sigma_{\alpha} \sigma_{\alpha'}}_{m,a} (k) \right|^2 (f_{m_i}^\sigma (k_i) - f_{m_{\alpha}}^\sigma (k)) \delta(E^{\sigma_{\alpha}}_{m,a} (k_i) - \hbar\omega), \] (182)

where \( e \) is the magnitude of the electron charge, \( m_0 \) is the electron rest mass in free space, \( c \) is the velocity of light in free space, \( \varepsilon \) is the permittivity of the host material, \( f_{m_i}^\sigma \), \( f_{m_{\alpha}}^\sigma \) are the Fermi-Dirac distributions for electrons in the conduction and valence bands, \( e \) is a unit vector of vector potential of electromagnetic field, \( E^{\sigma_{\alpha}}_{m,a} (k_i) \) is the interband energy of the conduction and valence bands, and \( \hbar \omega \) is an optical energy. We consider the electromagnetic wave, which propagates in plane of quantum well.

Although the carriers within each band are in a strongly nonequilibrium states, however interband relaxation times are much larger than intraband relaxation times. Therefore the Fermi-Dirac statistics may be used in the calculations. \( M^{\sigma_{\alpha} \sigma_{\alpha'}}_{m,a} (k) = \langle \Psi^{\sigma_{\alpha}}_{m,k} \mid \mathbf{p} \Psi^{\sigma_{\alpha'}}_{m,k} \rangle \) is the momentum matrix elements for transitions between the conduction band state \( \Psi^{\sigma_{\alpha}}_{m,k} (z) \) and the valence band state \( \Psi^{\sigma_{\alpha'}}_{m,k} (z) \) and \( \mathbf{p} \) is momentum operator.

The optical material gain [30, 13, 85] can be calculated from Fermi golden rule:

\[ a_0 = \frac{\sigma^2}{c\sqrt{m_0} \omega} \sum_{\sigma_{\alpha} = \pm} \sum_{\sigma_{\alpha'} = \pm} \sum_{m,a} \int k_i d k_i \int \frac{d\theta}{2\pi} \left| \mathbf{M}^{\sigma_{\alpha} \sigma_{\alpha'}}_{m,a} (k) \right|^2 \frac{(f_{m_i}^\sigma (k_i) - f_{m_{\alpha}}^\sigma (k)) (\frac{1}{2} \sum_{m,a} \int k_i d k_i)}{(E^{\sigma_{\alpha}}_{m,a} (k_i) - \hbar\omega)^3 + (\hbar\gamma)^3}, \] (183)

where \( e \) is the magnitude of the electron charge, \( m_0 \) is the electron rest mass in free space, \( c \) is the velocity of light in free space, \( \kappa = 8.27 \) is the permittivity of the host material, \( f_{m_i}^\sigma \), \( f_{m_{\alpha}}^\sigma \) are the Fermi-Dirac distributions for electrons in the conduction and valence bands, \( e \) is a unit vector of vector potential of electromagnetic field, \( E^{\sigma_{\alpha}}_{m,a} (k_i) \) is the interband energy of the conduction and valence bands, and \( \hbar \omega \) is an optical energy, \( \hbar \gamma \) is a half linewidth of the Lorentzian functions, which is equal 6.56 meV.

In the article in Figs.2.3 the considerable plateaus in the Gain coefficients calculations at interband phototransitions without including Lorenz broadening are shown to be related with Quantum Spin Hall effects in intraband phototransitions of GaN/AlGaN Quantum well.

### 4.4 Quantum Spin Hall effect in intersubband transitions of GaN/AlGaN Quantum well without Landau levels

We take the following plain wave functions written as vectors in the three-dimensional Bloch space:

\[ \Psi_{j\sigma k}(r) = \exp(ikr)\Psi_{j\sigma k}(r), \] (184)

where \( j = HH, LH, SH \),

\[ \Psi_{j\sigma k}(r) = (r|j\sigma k) + O(k), \] (185)

\[ |j\sigma k\rangle = \phi^{(1)}_{j\sigma k}\phi_{1,\sigma} + \phi^{(2)}_{j\sigma k}\phi_{2,\sigma} + \phi^{(3)}_{j\sigma k}\phi_{3,\sigma}, \] (186)
Figure 2. (Color online) Gain coefficient for the quantum well GaN/Al$_{0.3}$Ga$_{0.7}$N with a width 26Å, at a carriers concentration $10^{13}$ cm$^{-2}$, at a temperature 4.4 K.

Figure 3. (Color online) Gain coefficient for the quantum well GaN/Al$_{0.3}$Ga$_{0.7}$N with a width 26Å, at a carriers concentration $10^{13}$ cm$^{-2}$, at a temperature 4.4 K, 77 K and 300 K including Lorentz broadening.
Hall effect. The intrinsic Hall conductivity can be written as follows:

\[ \sigma_{ijk} = \frac{e^2}{\pi h} \int d^3 k \mathbf{f}(k) \Omega(k), \]

(179)

Quantum Hall effect is connected with intersubband transitions of bulk GaN. Quantum Hall effect is specified as spin

\[ \sigma = \sigma_{ijk} \]

(180)

where \( \sigma_{ijk} \) is the conductivity tensor.

From the conditions of orthonormal basis of wave plane vectors if \( k_x = 0 \) then \( \phi_{jk}^+ = \phi_{jk}^- = \phi_{jk} \). Hence

\[ \phi_{jk} = \begin{pmatrix} \phi_{jk}^{(1)} \\ \phi_{jk}^{(2)} \\ \phi_{jk}^{(3)} \end{pmatrix} = \begin{pmatrix} \cos \theta_{jk} \\
\cos \phi_{jk} \sin \theta_{jk} \\
\sin \phi_{jk} \sin \theta_{jk} \end{pmatrix}, \]

(181)

The solutions of Schrödinger equation can be sought in the form Eq. (190) by premultiplying the integral Eq. (191) on Eq. (149) functions and integrating Eq. (191) on quantum well boundaries

\[ \sum_{i=1}^{m} \cos \theta_{i,j,k} \psi_i(Z) = \begin{pmatrix} 1, \zeta_v \\
2, \zeta_v \\
3, \zeta_v \end{pmatrix}, \]

(192)

where from conditions of inverted bands

\[ \theta_{hh} = 0, \]

(193)

\[ \theta_{hh} = \frac{\pi}{2}, \]

\[ \phi_{lh} = \phi_{hl} \frac{\pi}{2}. \]

(194)

In the basis

\[ \begin{pmatrix} 1, \zeta_v \\
2, \zeta_v \\
3, \zeta_v \end{pmatrix} = \begin{pmatrix} Y_1^1(1/2) e^{-i \phi/2} e^{-i \phi/4} + Y_1^{-1}(1/2) e^{i \phi/2} e^{i \phi/4} \\
Y_1^1(1/2) e^{-i \phi/2} e^{-i \phi/4} + Y_1^{-1}(1/2) e^{i \phi/2} e^{i \phi/4} \\
Y_1^1(1/2) e^{-i \phi/2} e^{-i \phi/4} + Y_1^{-1}(1/2) e^{i \phi/2} e^{i \phi/4} \end{pmatrix}, \]

(195)

the Hamiltonian may be transformed to the diagonal form indicating two spin degeneracy [13]:

\[ H_{hh} = \begin{pmatrix} F & K_t & \mp iH_t \\
K_t & G & \Delta \mp iH_t \\
\pm iH_t & \Delta \pm iH_t & \lambda \end{pmatrix}, \]

(196)

We have considered intersubband phototransitions because the influence of time inversion operator has been importantly inserted [10]:

\[ K^{(r,t)} = \frac{m_e}{\hbar c k_x}, \]

(197)

\[ K^{(p)} = \frac{m_e}{\hbar c k_x} \{ H_{xx}, \frac{dU}{d\varphi} \}, \]

(198)

Quantum Hall effect is connected with intersubband transitions of bulk GaN. Quantum Hall effect is specified as spin Hall effect. The intrinsic Hall conductivity can write as follows [86]

\[ \sigma_{int} = \frac{e^2}{\pi} \int d^3 k \mathbf{f}(k) \Omega(k), \]

(199)

where three dimensional space can be specified as follows

\[ \frac{1}{V} \sum_k \rightarrow \frac{1}{V} \int \frac{d^3 k}{(2\pi)^3} \frac{1}{2\pi} \int k_i d k_i d k_i, \]

(200)
\[ \frac{1}{\delta} \sum_{\mathbf{k}} \rightarrow \frac{1}{\delta} \frac{s}{(2\pi)^2} \int d^2k_x \frac{1}{(2\pi)^2} 2\pi \int k_1dk_1, \]  

(201)

\( f(k) \) is Fermi-Dirac distribution function. The generic form of Berry curvature is defined by expression \[ 86 \]

\[ \Omega_j(k) = \hat{z} \cdot \nabla_k \times [ \langle v_j(k)|t\nabla_k|v_j(k) \rangle ], \]

(202)

where \( |v_j(k)\) is the periodic part of the Bloch function and \( j \) is the band index. The Berry curvature \[ 86 \] of bulk GaN which are shown to be connected with intraband photontransitions with \( C_{6v} \) point group symmetry is specified like

\[ \Omega_j(k) = \hat{z} \text{det} \begin{pmatrix} e_x & e_y & e_z \\ m_0 \frac{\partial H}{\partial k_x} & m_0 \frac{\partial H}{\partial k_y} & m_0 \frac{\partial H}{\partial k_z} \\ 0 & 0 & \frac{m_0}{\hbar^2} \{ H_{\frac{d\Omega}{d\epsilon}} U - \frac{e}{\hbar} \} \end{pmatrix}. \]

(203)

### 4.5 Rashba spin-orbit splitting in zinc-blende GaN quantum wells

Direct wide band gap group III-nitride semiconductors based on GaN and its alloys have received great attention due to prospective applications in optoelectronic device such as light-emitting diodes and lasers at green-blue and near-ultraviolet wavelengths, solar-blind photodetectors \[ 87, 88, 89, 90, 91 \]. A number of ultraviolet light-emitting diodes \[ 92, 93, 94, 95, 96, 97 \] and laser diodes \[ 98, 99, 100, 101, 102, 103, 104 \] already have been demonstrated. However, nitride structures and devices are still in the developmental stage.

Internal strain effects in heterostructures become increasingly important in modern solid state technology. An important problem in growing GaN on crystalline substrates Si, SiC, GaAs, ZnO and sapphire is an internal strain. Internal strains are related to the large lattice mismatch and the difference in the thermal-expansion coefficients of the epitaxial layer and a substrate. They can cause large biaxial stresses in the epitaxial layers. Biaxial stresses can be compressive or tensile depending on the crystalline substrate material \[ 105, 106, 107 \]. The internal strain effects are studied in this paper. We present studies of the influence of biaxial strain on the valence band spectra of zinc-blende AlGaN/GaN/AlGaN quantum well of width \( w \) perpendicular to the growth direction (001) and located at \( -w/2 < z < w/2 \). Under biaxial strain, the transverse components of strain are proportional to the difference in lattice constants \( a_0 \), also depend on Al content \( x \): \( \epsilon_{xx} = \epsilon_{yy} = x (a_{\text{AlN}}^N - a_{\text{GaN}}^N)/a_{\text{GaN}}^N = -0.029x < 0 \), when as \( \epsilon_{xy} = \epsilon_{yx} = \epsilon_{zz} = 0 \) \[ 108, 109 \]. The longitudinal component of strain can be expressed as \( \epsilon_{xx} = -2(C_{12}/C_{11})\epsilon_{xx} \), where \( C_{12} \) and \( C_{11} \) are the elastic constants. Since \( \epsilon_{xx} < 0 \) then the lattice mismatch causes the compressive strain of the quantum well. Situations under which, the crystalline substrate causes the tensile strain of the quantum well are studied. To compare the role of the compressive and the tensile biaxial strain effects we consider unstrained thin film GaN.

To describe the emission or absorption processes the energies, as well as the wave functions of the lowest conduction band states in the vicinity of Brilloin zone center are spin degenerate and characterize by a single effective mass for cubic symmetry and two effective mass parameters for hexagonal symmetry.

The point group of the zinc-blende structure is \( C_{4v} \). The configuration of nearest neighbors in the wurtzite crystal is also tetrahedral. The configuration of nearest neighbors of the first coordination sphere in the wurtzite lattice coincides with that in zinc-blende structures under a relatively small deformation in the (111) direction \[ 11 \]. For this reason, the physical background for the cubic approximation is based on similarity between the (0001) axis in the wurtzite structure and (111) direction in the cubic crystal \[ 11 \].

The space group of the wurtzite structure is \( C_{4v} \). The cohesige energy of the wurtzite structure is very close to that of the zinc-blende structure \[ 85 \]. For that reason, GaN can crystallize in both zinc-blende and wurtzite polytypes. It is known \[ 110, 11, 85, 56 \], that the valence-band spectrum at the \( \Gamma \) points originates from sixfold degenerate \( \Gamma_{15} \) state. In zinc-blende structures, the \( \Gamma_{15} \) level splits by the spin-orbit interaction, forming the fourfold degenerate \( \Gamma_8 \) heavy (HH) and light (LH) holes levels and double degenerate \( \Gamma_7 \) spin split-off (SH) holes level. Under the action of the hexagonal crystal field and the spin-orbit interaction in wurtzite crystals \( \Gamma_{15} \) splits leading to the formation of three spin degenerate levels: \( \Gamma_9 \), upper \( \Gamma_7 \), and lower \( \Gamma_7 \) levels which are denoted by heavy holes, light holes and split-off holes, respectively. Conduction-band states in the vicinity of Brillouin zone center are spin degenerate and characterize by a single effective mass for cubic symmetry and two effective mass parameters for hexagonal symmetry.

The Hamiltonian for the wurtzite valence band which accounts for the interaction of \( \Gamma_9 \), \( \Gamma_7 \) and \( \Gamma_7 \) levels has been derived within the kp method \[ 110 \]. Later, an derivation of the wurtzite Hamiltonian based the method of invariants with including the effects of strain on the hole spectra has been proposed \[ 111, 11 \]. A transformation of the Hamiltonian written in the basis \( |1, m\rangle |1/2, s\rangle \) to the basis of angular momenta 3/2 and 1/2 with the spin-orbit split-off band included has been performed in papers \[ 112, 56 \]. The basis of angular momenta 3/2 and 1/2 is frequently used for the 6 × 6 Luttinger-Kohn Hamiltonian for zinc-blende structures. Using a unitary transformation, a more convenient block-diagonal form with two 3 × 3 blocks in the framework the envelope function formalism has been proposed \[ 112, 56, 13 \]. Latter approaches \[ 112, 56, 13 \] are used in this work.
Figure 4. (Color online) Unstrained thin film GaN: (a) the valence subband structure; the momentum matrix elements for (b) the x- (or y-) polarization and (c) z-polarization.
Figure 5. (Color online) GaN/AlGaN quantum well with the compressive biaxial strain $\varepsilon_{xx} = -0.72\%$: (a) the valence subband structure; the momentum matrix elements for (b) the x- (or y-) polarization and (c) the z-polarization.
Figure 6. (Color online) GaN/AlGaN quantum well with the tensile biaxial strain $\varepsilon_{xx} = 0.79\%$: (a) the valence subband structure; the momentum matrix elements for (b) the x- (or y-) polarization and (c) the z-polarization.
### 4.5.1 Theory

It is known [113], that the optical material gain can be calculated from Fermi golden rule:

\[
\alpha_0 = \frac{\pi e^2}{\epsilon \sqrt{4\pi e m_0 \omega}} \sum_{\sigma, \pm=1} \sum_{\sigma, \pm=+} \sum_{m, a} \int \frac{dk_1 dk_2}{2\pi} \left| e M^{\sigma m}_a (k_i) \right|^2 (f^{\sigma}_m (k_i) - f^{\sigma}_m (k_i)) \delta (E^{cv}_m, ma (k_i) - \hbar \omega),
\]

(204)

where \(e\) is the magnitude of the electron charge, \(m_0\) is the electron rest mass in free space, \(c\) is the velocity of light in free space, \(\epsilon\) is the permittivity of the host material, \(f^{\sigma}_m\) and \(f^{\sigma}_m\) are the Fermi-Dirac distributions for electrons in the conduction and valence bands, \(\epsilon\) is a unit vector of vector potential of electromagnetic field, \(E^{cv}_m, ma (k_i)\) is the interband energy of the conduction and valence bands, and \(\hbar \omega\) is an optical energy. We have considered the electromagnetic wave, which propagates in plane of quantum well.

Although the carriers within each band are in a strongly nonequilibrium states, however interband relaxation times are much larger than intraband relaxation times. Therefore the Fermi-Dirac statistics may be used in the calculations.

\(M^{\sigma m}_a (k_i) = \langle \Psi^{\sigma c}_{m, \alpha} | p \Psi^{\sigma v}_{m, \kappa} \rangle\) is the momentum matrix elements for transitions between the conduction band state \(\Psi^{\sigma c}_{m, \kappa} (x)\) and the valence band state \(\Psi^{\sigma v}_{m, \alpha} (x)\), and \(p\) is momentum operator.

The initial state, corresponding to the conduction band is described of an orbital Bloch functions \(|S\rangle\) and spinor \(|\sigma_z\rangle = |\uparrow\rangle, |\downarrow\rangle\), corresponding to two directions of electron spin. The wave function of the nth conduction subband can be written as

\[
\Psi^{\sigma c \nu}_{m, \kappa} (r) = e^{ik_m r_i} \sqrt{A} x_m (z) |\sigma_z\rangle,
\]

(205)

where \(A\) is the area of the quantum well in the \(xy\) plane, \(\rho_i\) is the two-dimensional vector in the \(xy\) plane, \(k_i = (k_x, k_y)\) is in-plane wave vector, and \(x_m (z)\) is the \(z\)-dependent part of the envelope function.

To symmetrize the p-like valence band, one can consider the similarity between the p-like states and the atomic p wave functions [85]. It is known that p states are triple degenerate. We define three states with the orbital angular momentum \(l = 1\) and the eigenvalues \(m_i\) of its \(z\) component:

\[
|1, \pm 1\rangle = (\mp |X\rangle - i |Y\rangle)/\sqrt{2},
\]

\[
|1, 0\rangle = |Z\rangle,
\]

which are known as spherical harmonics. The eigenfunctions of the spin-orbit interaction Hamiltonian are eigenstates of the total angular momentum and its \(z\) component. Thus the final electron state belongs to a valence band and can be defined of these eigenfunctions. The latter functions can be expressed as linear combinations of eigenfunctions of the orbital angular momentum and spin, i.e. \(|1, m_l\rangle|1/2, s\rangle\) (the projections \(s = \pm 1/2\) correspond to two possible spin orientations) [114]:

\[
|\Gamma_{\pm} (HH); \pm \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (|X - i Y, + \frac{1}{2}\rangle + \sqrt{2} |Z, \pm \frac{1}{2}\rangle),
\]

(206)

\[
|\Gamma_{\pm} (LS); \pm \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} (|X - i Y, - \frac{1}{2}\rangle - \sqrt{2} |Z, \pm \frac{1}{2}\rangle),
\]

\[
|\Gamma_{s} (SH); \pm \frac{1}{2}\rangle = \frac{1}{2} (|X - i Y, + \frac{1}{2}\rangle \mp |Z, \pm \frac{1}{2}\rangle).
\]

Defining of "(l=1)-like" states in both zinc-blende and wurtzite GaN crystals is based on the Hamiltonian [110, 11, 115]:

\[
-H = \Lambda I + \Xi J^2 - \Delta \sum_{s=\pm} J_s \sigma_s - \sqrt{2} \Delta \sum_{s=\pm} (J_+ \sigma_+ + J_- \sigma_-) + \Xi J_+ + \Xi J_-
\]

(207)

where

\[
\Lambda = \Delta_1 + \Delta_2 + A_1 k_x^2 + A_3 k_y^2 + D_1 \epsilon_{zz} + D_3 \epsilon_i,
\]

\[
\Xi = - \Delta_1 + A_2 k_x^2 + A_4 k_y^2 + D_2 \epsilon_{zz} + D_4 \epsilon_i,
\]

\[
\Pi = A_5 k_x^2 + D_5 \epsilon_{zz},
\]

\[
\Sigma = A_6 k_y k_x + D_6 \epsilon_{zz},
\]

\[
\Gamma = i \frac{\hbar^2 \mathbf{\Omega} k}{2 m_0},
\]

\[
k_\pm = k_x \pm i k_y, k_x^2 = k_x^2 + k_y^2,
\]

\[
J_\pm = \frac{1}{\sqrt{2}} (J_x \pm i J_y), 2 [J_+ J_+] = J_x J_+ + J_- J_-,
\]

\[
\sigma_\pm = \frac{1}{2} (\sigma_x \pm i \sigma_y),
\]

\[
\epsilon_{zz} = \epsilon_{zz} \pm i \epsilon_{zz}, \epsilon_\pm = \epsilon_{xx} - \epsilon_{yy} \pm 2 i \epsilon_{xy}.
\]
The term linear in the wave vector describes the circular loop of valence band maxima in crystals with wurtzite symmetry [11]. For zinc-blende type materials, the term linear in the wave vector does not exist [11].

A transformation of the Hamiltonian written in the basis \( |1, m_1\rangle |1/2, s\) to the basis of angular momenta 3/2 and 1/2 is performed with help of Eq. (78) [56]. By choosing a unitary transformation in manner similar to the cubic case [112, 56]:

\[
\begin{align*}
|1, \pm\rangle &= \frac{1}{\sqrt{2}} \left( \frac{1}{2} \pm \frac{1}{2} i \right) e^{-3i\phi/2} \left[ \frac{1}{2}, \pm \right], \\
|2, \pm\rangle &= \frac{1}{\sqrt{2}} \left( \frac{1}{2} \pm \frac{1}{2} i \right) e^{-i\phi/2} \left[ \frac{1}{2}, \pm \right], \\
|3, \pm\rangle &= \frac{1}{\sqrt{2}} \left[ \pm(1, \frac{1}{2}) \right] e^{-i\phi/2} \left[ \frac{1}{2}, \pm \right],
\end{align*}
\]

(208)

where \( \tan \phi = k_y/k_x \), the full \( 6 \times 6 \) Hamiltonian can be transformed to a block-diagonal form with spin \( \sigma_z \) corresponding to two possible spin orientations as in paper [56]:

\[
H = -\begin{pmatrix} H^+ & 0 \\ 0 & H^- \end{pmatrix},
\]

(209)

and \( H^\pm \) for the specified biaxial strain are defined as

\[
H^\pm = \begin{pmatrix} P + Q & R \mp iS \\ R \pm iS & P - Q \end{pmatrix} = \sqrt{2}R \pm i\sqrt{2}S
\]

(210)

in the basis \( [1, \sigma_z], [2, \sigma_z], [3, \sigma_z] \), where

\[
P = \frac{1}{3} \Delta_{\sigma_z} + \alpha_1 k_z^2 + \alpha_2 k_t^2 + d_1 \varepsilon_{xx} + d_2 (\varepsilon_{xx} + \varepsilon_{yy}),
\]

\[
Q = -\frac{1}{3} \Delta_{\sigma_z} - 2\alpha_3 k_z^2 + \alpha_4 k_t^2 - 2d_3 \varepsilon_{xx} + d_4 (\varepsilon_{xx} + \varepsilon_{yy}),
\]

\[
R = \sqrt{3} \alpha_6 k_z^2,
\]

\[
S = 2\sqrt{3} \alpha_6 k_z k_t,
\]

\[
k_t^2 = k_x^2 + k_y^2.
\]

The relations between the material parameters introduced here and the parameters of the Hamiltonian in the basis \( [1, m_1]|1/2, s\) are written as:

\[
\begin{align*}
\alpha_1 &= A_1 + \frac{2}{3} A_2, \quad \alpha_2 = A_3 + \frac{2}{3} A_4, \quad \alpha_3 = -\frac{1}{6} A_2, \\
\alpha_4 &= \frac{1}{3} A_4, \quad \alpha_5 = -\frac{1}{3} A_5, \quad \alpha_6 = -\frac{1}{3\sqrt{2}} A_6, \\
\Delta_{\sigma_z} &= \Delta_1, \quad \Delta_{\sigma_z} = 3 \Delta_2 = 3 \Delta_3.
\end{align*}
\]

(211)

In a similar way may be expressed the deformation potential parameters:

\[
\begin{align*}
d_1 &= D_1 + \frac{2}{3} D_2, \quad d_2 = D_3 + \frac{2}{3} D_4, \\
d_3 &= -\frac{1}{6} D_2, \quad d_4 = \frac{1}{3} D_4.
\end{align*}
\]

(212)

Parameters \( A_1 - A_6 \) are related with a set of Luttinger-like parameters [56]:

\[
\begin{align*}
-A_1 &= \gamma_{1}\tau_1 + 4 \gamma_{3\tau}, \quad -A_2 = \gamma_{1}\tau_1 - 2 \gamma_{3\tau}, \quad A_3 = 6 \gamma_{3\tau}, \\
-A_4 &= 3 \gamma_{3\tau}, \quad A_5 = 2 \gamma_{3\tau}, \quad A_6 = \sqrt{2} (2 \gamma_{3\tau} + \gamma_{3\tau}).
\end{align*}
\]

(213)

In a similar fashion can be defined expressions for the deformation potentials:

\[
\begin{align*}
-D_1 &= \delta_{1\tau} + 4 \delta_{3\tau}, \quad -D_2 = \delta_{1\tau} - 2 \delta_{3\tau}, \quad D_3 = 6 \delta_{3\tau}, \\
-D_4 &= 3 \delta_{3\tau}, \quad D_5 = 2 \delta_{3\tau}, \quad D_6 = \sqrt{2} (2 \delta_{3\tau} + \delta_{3\tau}).
\end{align*}
\]

(214)
The correspondence between Luttinger-like parameters and Luttinger parameters $\gamma_1, \gamma_2, \gamma_3$ and deformation potentials $a, b, d$ of cubic crystal is simple [56]:

$$\gamma_{1z} = \gamma_{1r} \rightarrow \gamma_1, \gamma_{2z} = \gamma_{2r} \rightarrow \gamma_2, \gamma_{3z} = \gamma_{3r} \rightarrow \gamma_3, \tag{215}$$

$$\delta_{1z} = \delta_{1r} \rightarrow -a_v, \delta_{2z} = \delta_{2r} \rightarrow -b/2, \tag{216}$$

$$\delta_{3z} = \delta_{3r} \rightarrow -d/2\sqrt{3}.$$  

In both cubic and hexagonal materials, upper six valence bands originate from $p^3$ atomic orbitals, corresponding to the vector representation $\Gamma_{15}$ split by the spin-orbit interaction or hexagonal crystal field [11, 85]. We calculate the momentum matrix elements using a vector representation of the Bloch functions. We introduce the Bloch function written as vector in the three-dimensional Bloch space:

$$|a \sigma, k_i\rangle = \left\| \begin{array}{c} \phi_{(1)}^{x}(z, k_i) \\ \phi_{(2)}^{x}(z, k_i) \\ \phi_{(3)}^{x}(z, k_i) \end{array} \right\| |1, \sigma_{v}\rangle, \tag{217}$$

where

$$\phi_{(j)}^{x} = \sum_{i=1}^{n} V_{k_{i}}^{(j)}[i, \alpha] \chi_{x}(z), \tag{218}$$

and $j = 1, 2, 3$. The Bloch vector of $\alpha$-type hole with spin $\sigma_{v} = \pm$ and momentum $k_i$ is specified by its three coordinates $[V_{k_1}^{(1)}[n, \alpha], V_{k_2}^{(2)}[n, \alpha], V_{k_3}^{(3)}[n, \alpha]]$ in the basis $[|1, \sigma_{v}\rangle, |2, \sigma_{v}\rangle, |3, \sigma_{v}\rangle]$. The envelope $z$-dependent part of the quantum well eigenfunctions can be specified from the boundary conditions $\chi_{n}(z = -w/2) = \chi_{n}(z = w/2) = 0$ of an infinitely deep quantum well as

$$\chi_{n}(z) = \sqrt{\frac{2}{w}} \sin\left(\pi n \left(\frac{z}{w} + \frac{1}{2}\right)\right), \tag{219}$$

where $n$ is a natural number. The hole wave function can be written as

$$\Psi_{\alpha,k_i}(r) = \frac{e^{ik_{z}z}}{\sqrt{A}} |a \sigma, k_i\rangle. \tag{220}$$

The valence subband structure $E_{a}^{\sigma_{v}}(k_{i})$ can be determined by solving

$$\sum_{j=1}^{3} (H_{ij}^{\sigma_{v}}(k_{z} = -\frac{\pi}{2}) + \delta_{ij} E_{a}^{\sigma_{v}}(k_{i})) \phi_{a}^{(j)\sigma_{v}}(z, k_{i}) = 0, \tag{221}$$

where $i = 1, 2, 3$.

The only nonzero matrix elements between the basis functions exist [114, 56]:

$$\langle S | \tilde{p}_{+} | 1, 0 \rangle = P_{z}, \tag{222}$$

$$\langle S | \tilde{p}_{-} | 1, -1 \rangle = -\langle S | \tilde{p}_{-} | 1, 1 \rangle = \sqrt{2} P_{\perp},$$

due to symmetry properties of the Bloch functions, where $\tilde{p}_{\pm} = \hat{p}_{x} \pm i \hat{p}_{y}$. Two momentum matrix elements constants can be defined as: $P_{\perp} \equiv \langle S | \tilde{p}_{-} | X \rangle$ and $P_{z} \equiv \langle S | \tilde{p}_{z} | Z \rangle$.

The momentum-matrix elements for the $x$- (or $y$-) polarization ($e \perp z$) can be defined as [58]:

$$|e_{x}M_{m_{x}}^{\pm}(k_{i})|^2 = \frac{1}{4} (|\chi_{m}|^{2})^{2}$$

$$\times (|\langle \chi_{m} | \phi_{a}^{(1)} \rangle|^{2} + \frac{1}{2} |\langle \chi_{m} | \phi_{a}^{(2)} \rangle|^{2})$$

$$+ \frac{1}{2} |\langle \chi_{m} | \phi_{a}^{(3)} \rangle|^{2}$$

$$\times (\cos 2\phi \langle \chi_{m} | \phi_{a}^{(1)} \rangle \langle \chi_{m} | \phi_{a}^{(2)} \rangle + \cos 2\phi \langle \chi_{m} | \phi_{a}^{(1)} \rangle \langle \chi_{m} | \phi_{a}^{(3)} \rangle), \tag{223}$$

The momentum-matrix elements for the $z$-polarization ($e \parallel z$) can be given by

$$|e_{z}M_{m_{z}}^{\pm}(k_{i})|^2 = \frac{1}{3} (|\langle \chi_{m} | \phi_{a}^{(2)} \rangle|^{2}$$

$$+ \frac{1}{3} |\langle \chi_{m} | \phi_{a}^{(3)} \rangle|^{2} - \sqrt{2} \langle \chi_{m} | \phi_{a}^{(2)} \rangle \langle \chi_{m} | \phi_{a}^{(3)} \rangle), \tag{224}$$

It is known, [56] that the values of constants $|P_{z,\perp}|^2$ can be found from kp theory

$$\frac{m_{0}}{m_{z,c}} = 1 + \frac{2}{m_{0}} \sum_{j \neq c} \frac{|c|_{j}^{2}}{E_{e}^{0} - E_{j}^{0}}, \tag{225}$$
and from experimentally measured conduction band effective mass \( m_{\perp}^{(c)} \) can be estimated

\[
\frac{2|P_{\perp}|^2}{m_0} \approx E_g \left( \frac{m_0}{m_{\perp}^{(c)}} - 1 \right)
\]

(226)

Here we use the effective-mass parameters, spin-orbit splitting energy, and deformation potential parameters as in papers [116, 58, 56]. The physical parameters for zincblende GaN are as follows. We take the effective-mass parameters Table 9, 10: \( A_1, A_2, A_3, A_4, A_5, A_6 \), the parameters for deformation potential: \( D_1, D_2, D_3, D_4, D_{c1}, D_{c2} \) in meV, and the energy parameters at 300 K: \( E_g, \Delta_{so}, P_1^2, P_2^2 \) in meV the lattice constants: \( a_{GaN} \) and \( a_{AlN} \) as well as the elastic constants \( C_{13} \) and \( C_{33} \) in GPa.

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4.5.2 Results and discussions

We consider the pseudomorphically strained zinc-blende GaN/Al_{0.3}Ga_{0.7}N quantum well of width 5.2 nm. A rectangular form of potential for the quantum well is assumed.

The results of numerical calculations of the valence band spectra and the k-dependence of the matrix elements as a function of the wave vector \( k_r = (k_x, k_y) \), which lies in plain of the quantum well, are presented in Figs. 4-6. Here for all structures, the two highest hole bands are heavy hole band and light hole band.

To clarify the role of the compressive and the tensile biaxial strain effects we consider unstrained thin film GaN. In Fig. 4, we show the valence-band structure and the k-dependence of the matrix elements. Fig. 4a show that each band consists of a mixture of heavy hole, light hole and spin-orbit split hole states.

It is known that the p-like sixfold degenerated valence band at the \( \Gamma \) point is separated into a fourfold degenerated \( \Gamma_8 \) state and a twofold degenerated \( \Gamma_7 \) state by the spin-orbit coupling. The value of this separation is the spin-orbit splitting energy, which is defined from the matrix element of the spin-orbit interaction Hamiltonian between the atomic orbitals and is usually referred to as the spin-orbit splitting width. The degeneracy is governed by the cubic symmetry. In the case when the quantum well is grown along the (001) direction, the crystal symmetry is changed to the tetragonal [117]. This implies removing of the degeneracy of the \( \Gamma_8 \) state. It is shown in the Fig. 4a.

In Fig. 5, we show the valence-band structure and the k-dependence of the matrix elements of the quantum well under the compressive biaxial strain. Components of strain are equal: \( \varepsilon_{xx} = -0.0072, \varepsilon_{zz} = 0.0039 \). This strain is consistent with the aluminum content 30%. In Fig. 5a one can see that the compressive stress causes a downward shift of the valence bands. Such behavior agrees with the calculations strain effects on valence band structure in wurtzite GaN quantum wells for nitride-based devices, which are fabricated on (0001) sapphire substrates [118].

We consider optical transitions between the initial and final states such as: with angular momentum \( J = 3/2 \) and the magnetic quantum numbers \( m_J = \pm 3/2, m_l = \pm 1/2 \) as well as with \( J = 1/2, m_l = \pm 1/2 \) of the valence band and with \( J = 1/2, m_l = \pm 1/2 \) of the conduction band. Transitions from the valence band states \( m_l = \pm 1/2 \) obey selection rules such as \( \Delta m = 0 \) and \( \Delta m = \pm 1 \), therefore they have both the x (or y) and z light polarizations. Transitions from the valence band states \( m_l = \pm 3/2 \) obey selection rules \( \Delta m = \pm 1 \), therefore they have only the x (or y) polarization [114].

Under the compressive strain, an increase in the aluminum content is accompanied with both an increase of the splitting width between the heavy hole and light hole bands and a decrease of valence-bands mixing effects. Consider transitions from the heavy hole band. Figs. 4, 5 clearly indicate, that the matrix elements have the stricter contribution of x (or y) light polarization as goes from the unstrained thin film to the strained heterostructure in which \( \varepsilon_{xx} = -0.0072 \). Thus in the case of the compressively strained quantum well, the matrix elements have the strict x (or y) light polarization. Such behavior agrees with the calculations [11, 119, 120] of the momentum matrix elements in crystals of wurtzite symmetry and associated quantum well structures, in which the considered transitions are allowed for the x (or y) light polarization, while for the z light polarization are forbidden.

In Fig. 6 we show the valence band structure and the k-dependence of the matrix elements of the quantum well under the tensile biaxial strain. The strain components are equal: \( \varepsilon_{xx} = 0.0079, \varepsilon_{zz} = -0.0042 \). In Fig. 6a one
can see, that the tensile strain causes both the strong transformation of the hole effective mass and a decrease of the splitting width due to an upward shift of the light valence band to the top of heavy hole band. The former leads to arising of the large negative mass at the Brillouin zone center, while the latter results in arising of the casual twofold degeneration of double spin degenerated heavy hole and light hole states at the Brillouin zone center. We show that a fourfold degeneration of the valence band states at the Brillouin zone center may be found in zinc-blende (001) GaN quantum well with the former deriving double spin degeneration of the heavy hole and light hole states and the latter under the action of the tensile strain additionally the casual twofold degeneration. In general arising of the degeneracy causes an increase of the density of states. The light hole band can be shifted upward above of the heavy hole band with the tensile strain increase. This implies removing of a fourfold degeneration of the valence band states. Thus at εxx > 0.0054 the highest quantized hole subband is the light band. It is expected that the density of states is changed by the action of strain.

Such behavior qualitatively agrees with the calculations of internal strain effects on the valence band structure of Si1-xGex [121]. In zinc-blende GaN the states of the light hole band are composed of the |X ± iY⟩ characters as well as the |Z⟩ character. Comparing Figs. 4, 6 show an increase of presence of the |Z⟩ state in the light hole band as one moves from the unstrained thin film to the strained heterostructure, in which εxx = 0.0079. There is more the |Z⟩ state in the light hole band in the strained heterostructure, than in the thin film. Therefore in the strained quantum well with εxx > 0.0072, the states of the highest-lying light hole band are almost composed of the |Z⟩ character, which yields the strong matrix element for the z light polarization.

Although both the compressive and the tensile biaxial stresses were studied, only zinc-blende GaN quantum well under the tensile strain exhibits a region of the spectrum with negative effective mass and the strong modification of the matrix elements for the z light polarization. The density of states, the carrier population inversion, the matrix elements, the light gain spectrum vary notably with arising of the spectrum region with negative effective mass at the Brillouin zone center.

A understanding of the influence of internal strain effects under the lattice mismatch on laser gain properties should help towards improving the laser performance and optimal device configurations.

It is found, that the effective mass is drastically changed under the tensile strain. It can be explained of arising of the circular loop with radius k = 0.7 × nm−1 in valence band structure of zinc-blende GaN quantum well under the tensile strain. The extremum loop effects in the band structure of wurzite symmetry, in which exists the linear term in wave vector, are known from papers [12]. With arising of the spectrum region with negative effective mass at the Brillouin zone center, holes are located on the loop of valence-band maxima. In consequence of which, the optical transitions near band-edge occur with the large light absorption, suppressing the laser effect. Under the tensile strain, the shift of the valence and conduction bands leads to a red shift of the absorption spectra, with respect of the band-edge of unstrained quantum well.

In both zinc-blende and wurzite crystal structures each atom is surrounded by four nearest neighbors forming an ideal tetrahedron. The valence electrons of such crystal structure form hybridized sp2 orbitals [85]. This sp2 hybridization is well known from the bonding of a methane molecule. It is interesting to consider the analogy existing between the dependence of the matrix elements on strain under the lattice mismatch and strain effects on behavior of the bond angles of the tetrahedron. It is known [122], that in the case of tensile biaxial strain the bonding tetrahedra are compressed along the c axis by shrinking the distance between the Ga-N layers toward a planar structure changing the bond angles. This causes dehybridization from sp3 hybrids towards sp2 and pz orbitals. The quantum mechanical problem of dehybridization sp3 hybrids towards sp2 and pz orbitals is consistent with a tendency of an increase of the |Z⟩ state in the light hole band under the tensile biaxial strain, which yields the matrix elements for the z polarization. It is shown in the Fig. 6c.

Our theoretical studies have well agreement with the experimental results [55].

4.5.3 Conclusions

We have investigated the strain effects on the valence band structures, the interband matrix elements, and the light gain spectrum in the pseudomorphically strained zinc-blende nitride quantum well. In this purpose we use a 3 × 3 block Hamiltonian to calculate the valence band spectra in the quantum well heterostructure. A detailed analysis is presented for the dependence of the hole spectra, the matrix elements, and light gain spectra on strain under the lattice mismatch in the heterostructures. A analysis of the band structure of the quantum well under the compressive strain exhibits a downward shift of the valence bands. For the quantum well with the compressive strain εxx = −0.72%, the matrix elements for transitions from the first hole band have the strict x (or y) light polarization, when as with the tensile strain εxx = 0.79%, the considered matrix elements have the strict z light polarization. Under the tensile strain, both the large negative mass and the strong modification of the matrix elements arise at the Brillouin zone center. The casual twofold degeneration of double spin degenerated heavy hole and light hole states arises at the Brillouin zone center. An increase of the |Z⟩ state in the light hole band under the tensile strain is found. It yields the strong matrix element for the z polarization. The circular loop or ring of valence band maxima with the finite
radius in the heterostructure under the tensile strain is found. Under the compressive strain, holes are located on the upper valence subbands, when as under the tensile strain, holes are located on the circular loop or ring of valence band maxima. It is shown, that laser effect is suppressed in GaN quantum well with the tensile strain $\varepsilon_{xx} = 0.79\%$, while at $\varepsilon_{xx} = -0.72\%$ the stimulated emission is pronounced. In the paper, the importance of the extremum loop of the valence band in zinc-blende GaN quantum well under the tensile strain is found. Although the extremum loop or ring effects in wurtzite crystals were studied [12, 47, 48, 49, 50, 51, 52, 53, 54, 55], the both the suppressing of laser effect and Spin Hall effects in bulk GaN as well as in GaN/AlGaN Quantum wells were not found in publications New Years of 1996, 1997 Eve [56, 57, 58, 59, 60]. It should be noted that in 1998 the Science discovery of Quantum Fractional Hall Effects in Quantum Matter was Nobel Prize winner by Kingdom Academy of Sciences of Sweden. Both Rashba spin splitting [123] in zinc-blende GaN quantum wells as well as the concerned geometry of the valence band spectra are shown to be related with the found optical transitions of $\sigma$ light polarization. In the article RSOI (Rashba spin-orbit interaction) effect is found. It is found that the internal strain effects play the significant role on the optical properties in the quantum well heterostructures.

4.6 Quantum Spin Hall effect in intersubband transitions of bulk GaN

Unlike for the transitions between the valence and conduction band, the Bloch function contributions of zeroth order in $k$ vanish due to symmetry properties (except the small part proportional to the spin splitting constant $k_s$). Because

\begin{table}[h]
\centering
\caption{The irreducible representation of $C_{6v}$ [9].}
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
$C_{6v}$ & $\Gamma_1 + \Gamma_5$ & $E$ & $C_2$ & $2C_3$ & $2C_6$ & $3\sigma_v$ & $3\sigma'_v$ \\
\hline
$\chi_0^L(g)$ & 3 & -1 & 0 & 2 & 1 & 1 & \\
$g^2$ & $E$ & $E$ & $C_3$ & $C_3$ & $E$ & $E$ & \\
$\chi_y(g^2)$ & 3 & 3 & 0 & 0 & 3 & 3 & \\
$\frac{1}{2} [+]$ & 6 & 2 & 0 & 2 & 2 & 2 & $\Gamma_1 + \Gamma_5 + \Gamma_6$ \\
$\frac{1}{2} [-]$ & 3 & -1 & 0 & 2 & -1 & -1 & $\Gamma_2 + \Gamma_3$ \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{The irreducible representation of $C_{6v}$ [9].}
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
$C_{6v}$ & $E$ & $C_2$ & $2C_3$ & $2C_6$ & $3\sigma_v$ & $3\sigma'_v$ \\
\hline
$\chi_v$ & 3 & -1 & 0 & 2 & 1 & 1 & $\Gamma_1 + \Gamma_5$ \\
$\frac{1}{2} [+]$ & 6 & 2 & 0 & 2 & 2 & 2 & $2\Gamma_1 + \Gamma_5 + \Gamma_6$ \\
$\frac{1}{2} [-]$ & 3 & -1 & 0 & 2 & -1 & -1 & $\Gamma_2 + \Gamma_3$ \\
\hline
\end{tabular}
\end{table}

Intraband phototransitions integral can write in the generic form [10, 12, 14]

\[
\langle U_{j'\sigma'k}|\hat{p}|U_{j\sigma k}\rangle:
\]

\[
\chi_v(g)\frac{1}{2}\left[\chi_\mu^{(s)}(g) - \chi_\mu^{(s)}(g^2)\right] = (A_1 + E_1) \times (A_2 + E_1) = (E_1 \times E_1).
\]

But we consider intersubband phototransitions because the influence of time inversion operator has been importantly inserted [10]. So

\[
\langle j'\sigma'k|U_{\nu k}\rangle|j\sigma k\rangle:
\]

\[
\chi_\mu^{(s)}(g)\chi_v(g)\chi_\phi(g) = (A_1 + E_1) \times (A_1 + E_1) = (A_1 \times A_1) + (E_1 \times E_1).
\]

As well known vector can be transformable by vector representation $(A_1 \times A_1) + (E_1 \times E_1)$.

In the paper the expressions for momentum matrix elements have presented in the following general form:

\[
0\langle j'\sigma'k|e^{\theta_k} |j\sigma k\rangle_0,
\]

\[
|j\sigma k\rangle_\varphi = U_{\varphi} |j\sigma k\rangle_0.
\]
One can derive the expressions for calculation of momentum matrix elements for interband transitions as well as intraband transitions in stimulated emission by writing

\[
\left[0\left(v_1, \sigma^\prime|v_{jk}\sigma\right) + 0\left(v_2, \sigma^\prime|v_{jk}\sigma\right) + 0\left(v_3, \sigma^\prime|v_{jk}\sigma\right) + 0\left(v_4, \sigma^\prime|v_{jk}\sigma\right)\right] U_{\psi} e^{\frac{i}{\hbar} \hat{H}_{U}} U_{\psi} - \left[v_{jk}\sigma_1^\prime|v_1, \sigma_0\right] + v_{jk}^{(2)}|v_2, \sigma_0\right] + v_{jk}^{(3)}|v_3, \sigma_0\right].
\] (233)

Since

\[
\frac{\partial}{\partial \varepsilon_k}(U_{\psi}\hat{H}U_{\psi}^\dagger) = U_{\psi}\frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + \frac{\partial}{\partial \varepsilon_k}U_{\psi}\hat{H} + U_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + U_{\psi}^\dagger \hat{H}U_{\psi}^\dagger - U_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + U_{\psi}^\dagger \hat{H}U_{\psi}^\dagger = H\frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + U_{\psi}^\dagger \hat{H}U_{\psi}^\dagger - U_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + U_{\psi}^\dagger \hat{H}U_{\psi}^\dagger =
\]

as well as using

\[
U_{\psi}^\dagger U_{\psi} = I \implies \frac{\partial}{\partial \varepsilon_k}(U_{\psi}^\dagger U_{\psi}) = 0 \implies U_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + \frac{\partial}{\partial \varepsilon_k}U_{\psi} = 0,
\] (235)

one can find the following unitary transformation for momentum

\[
\frac{\partial}{\partial \varepsilon_k}(U_{\psi}\hat{H}U_{\psi}^\dagger) = -HU_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + U_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + U_{\psi}^\dagger \hat{H}U_{\psi}^\dagger - U_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger + U_{\psi}^\dagger \hat{H}U_{\psi}^\dagger
\]

In the spherical coordinate system one can find

\[
e U_{\psi}^\dagger \frac{\partial}{\partial \varepsilon_k}U_{\psi}^\dagger = e [\exp(-i\varepsilon_k \cos \theta) + \frac{1}{\exp(-i\varepsilon_k \cos \theta)}] =
\]

\[
e [\frac{i}{\sin \theta} \frac{\partial}{\partial \varepsilon_k} U_{\psi}^\dagger] + e [\frac{\partial}{\partial \varepsilon_k} U_{\psi}^\dagger] + \frac{i}{\sin \theta} \frac{\partial}{\partial \varepsilon_k} U_{\psi}^\dagger - \frac{i}{\sin \theta} \frac{\partial}{\partial \varepsilon_k} U_{\psi}^\dagger =
\]

\[
= \frac{\partial}{\partial \varepsilon_k} (\sin \theta \cos \theta) + \frac{i}{\sin \theta} \frac{\partial}{\partial \varepsilon_k} (\sin \theta \sin \theta) + \frac{\partial}{\partial \varepsilon_k} \cos \theta.
\]

Therefore a formula Eq. (233) can be rewritten as following

\[
\left[0\left(v_1, \sigma^\prime|v_{jk}\sigma\right) + 0\left(v_2, \sigma^\prime|v_{jk}\sigma\right) + 0\left(v_3, \sigma^\prime|v_{jk}\sigma\right) + 0\left(v_4, \sigma^\prime|v_{jk}\sigma\right)\right] U_{\psi} e^{\frac{i}{\hbar} \hat{H}_{U}} U_{\psi} - \left[v_{jk}\sigma_1^\prime|v_1, \sigma_0\right] + v_{jk}^{(2)}|v_2, \sigma_0\right] + v_{jk}^{(3)}|v_3, \sigma_0\right] = \hbar \sum_{i,j=1}^{3} \delta_{\sigma^\prime, \sigma} K_{ijk}^{(i)} (\sin \theta \cos \varphi + \frac{i}{\sin \theta} \frac{\partial}{\partial \varepsilon_k} (\sin \theta \sin \theta) - \frac{\partial}{\partial \varepsilon_k} \cos \theta).
\] (239)

where

\[
K_{ijk}^{(i)} = -\frac{\mu_0}{\hbar^2 \kappa_k} \left[H, \frac{\partial}{\partial \varepsilon_k} U_{\psi}^\dagger \right],
\]

\[
K_{jk}^{(i)} = -\frac{\mu_0}{\hbar^2 \kappa_k} \left[H, \frac{\partial}{\partial \varepsilon_k} U_{\psi}^\dagger \right],
\]

\[
K_{ijk}^{(i)} = \begin{cases} (\gamma_{11} - 2\gamma_{31}) \kappa_k & 0 & \pm \frac{3}{\sqrt{2}} \gamma_2 \kappa_k, \\ 0 & (\gamma_{11} - 2\gamma_{31}) \kappa_k & \pm \frac{3}{\sqrt{2}} \gamma_2 \kappa_k, \\ \pm \frac{3}{\sqrt{2}} \gamma_2 \kappa_k & \pm \frac{3}{\sqrt{2}} \gamma_2 \kappa_k & (\gamma_{11} + 4\gamma_{31}) \kappa_k \end{cases}
\]

\[
K_{ijk}^{(i)} = \begin{cases} (\gamma_{11} + \gamma_{31}) \kappa_k & 3\gamma_1 \kappa_k & \pm k_x \pm \frac{1}{\sqrt{2}} \gamma_2 \kappa_k, \\ 3\gamma_1 \kappa_k & (\gamma_{11} + 3\gamma_{31}) \kappa_k & \pm k_x \pm \frac{1}{\sqrt{2}} \gamma_2 \kappa_k, \\ \pm k_x \pm \frac{3}{\sqrt{2}} \gamma_2 \kappa_k & \pm k_x \pm \frac{3}{\sqrt{2}} \gamma_2 \kappa_k & (\gamma_{11} - 2\gamma_{31}) \kappa_k \end{cases}
\]

In the low-energy limit the Hamiltonian of wurtzite

\[
\hat{H}_0 = \hat{I} (\Delta_+ + \Delta_2) +
\]

\[
+ \Delta_1 J^2 + \Delta_2 J^2 \sigma_z + \sqrt{2} \Delta_3 (J_+ \sigma_- + J_- \sigma_+),
\]

\[
\hat{H}_k = A_1 k_x^2 + A_2 k_y^2 + (A_3 k_x^2 + A_4 k_y^2) J^2 +
\]

\[
+ A_3 k_x (2[J J_z] k_x + 2[J J_z] k_x) +
\]

\[
+ A_6 (J_+^2 k_x^2 + J_-^2 k_x^2) + iA_7 (J_+ k_y - J_- k_y),
\] (244)
In the basis of spherical wave functions with the orbital angular momentum \( l = 1 \) and the eigenvalue \( m_i \) of its \( z \) component:

\[
|1, \xi_1\rangle = \frac{1}{\sqrt{2}}(Y^1_1\psi(1/2)e^{-\text{i}3\pi/2}e^{3\pi i/4} \pm Y^1_{-1}\psi(-1/2)e^{\text{i}3\pi/2}e^{3\pi i/4})
\]

\[
|2, \xi_2\rangle = \frac{1}{\sqrt{2}}(\pm Y^1_{-1}\psi(-1/2)e^{-\text{i}3\pi/2}e^{-3\pi i/4} + Y^1_1\psi(1/2)e^{\text{i}3\pi/2}e^{-3\pi i/4})
\]

\[
|3, \xi_3\rangle = \frac{1}{\sqrt{2}}(\pm Y^1_1\psi(1/2)e^{-\text{i}3\pi/2}e^{-3\pi i/4} + Y^1_{-1}\psi(-1/2)e^{\text{i}3\pi/2}e^{-3\pi i/4})
\]

the Hamiltonian may be transformed to the diagonal form indicating two spin degeneracy [13]:

\[
H_{\pm} = \begin{bmatrix} F & K_t & \mp iH_t \\ K_t & G & \Delta \mp iH_t \\ iH_t & \Delta \mp iH_t & \lambda \end{bmatrix} \begin{bmatrix} 1, \xi_1 \rangle \\ 2, \xi_2 \rangle \\ 3, \xi_3 \rangle \end{bmatrix},
\]

where \( F = \Delta_1 + \Delta_2 + \lambda + \theta, \ G = \Delta_1 - \Delta_2 + \lambda + \theta, \ \lambda = \lambda_k + \lambda_e, \ \theta = \theta_k + \theta_e, \ \lambda_k = \frac{\hbar^2}{2m_0}(A_1k_z^2 + A_2k_y^2), \ \lambda_e = D_1\epsilon_{zz} + D_2(\epsilon_{xx} + \epsilon_{yy}), \ \theta_k = \frac{\hbar^2}{2m_0}(A_3k_z^2 + A_4k_y^2), \ \theta_e = D_3\epsilon_{zz} + D_4(\epsilon_{xx} + \epsilon_{yy}), \ k_t = \frac{\hbar^2}{2m_0}(A_5k_z^2), \ H_t = \frac{\hbar^2}{2m_0}(A_6k_z), \ \Delta = \sqrt{\Delta_3}, \ k_i^2 = k_x^2 + k_y^2\).

Inserting the new basis [56, 57]

\[
|v_1, \pm\rangle = \frac{1}{\sqrt{2}}(|1, 1\rangle \uparrow \mp i|1, -1\rangle \downarrow) \exp^{\text{i}3\pi/2} \exp^{-\text{i}3\pi/2} \\
|v_2, \pm\rangle = \frac{1}{\sqrt{2}}(|1, 1\rangle \uparrow \mp i|1, -1\rangle \downarrow) \exp^{-\text{i}3\pi/2} \exp^{\text{i}3\pi/2} \\
|v_3, \pm\rangle = \frac{1}{\sqrt{2}}(|1, 1\rangle \uparrow \mp i|1, -1\rangle \downarrow) \exp^{\text{i}3\pi/2} \exp^{-\text{i}3\pi/2}
\]

one can find the basis [56, 57] from the derivatives of Hamiltonian built on which have derived a matrix formulas of Eq. (234) and Eq. (235)

\[
|u_1, \pm\rangle = |v_1, \pm\rangle \\
|u_2, \pm\rangle = \frac{1}{\sqrt{2}}|v_2, \pm\rangle - \frac{1}{\sqrt{2}}|v_3, \pm\rangle \\
|u_3, \pm\rangle = \frac{1}{\sqrt{2}}|v_2, \pm\rangle + \frac{1}{\sqrt{2}}|v_3, \pm\rangle
\]

Also keeping in mind the spherical coordinate system and from conditions of inverted bands wave vectors solutions of Schrödinger equations one can find

\[
\nu_{jk} = \begin{bmatrix} \cos \theta_{jk} & \cos \phi_{jk} \\ \sin \theta_{jk} & \sin \phi_{jk} \end{bmatrix},
\]

\[
\theta_{hh} = 0, \\
\theta_{hh, hh} = \frac{\pi}{2}, \\
\phi_{hh} = \phi_{hh} - \frac{\pi}{2},
\]

after the solving the integral Eq. (239) the intrasubband phototransitions have been found as following

\[
\frac{\sum_{\nu_{hh}} |\tilde{p}_{\nu_{hh}}|^2}{\hbar^2} = (9\gamma^2k_z^2 + 2k_y^2)(\cos \phi)^2(\sin \theta)^2,
\]

\[
\frac{\sum_{\nu_{hh}} |\tilde{p}_{\nu_{hh}}|^2}{\hbar^2} = (9\gamma^2k_z^2 + 2k_y^2)(\cos \phi)^2(\sin \theta)^2 + (\gamma_{zz}^2 - 2\gamma_{zz}^2k_z^2 + 3\gamma_{33}^2k_y^2)(\sin \phi)^2(\cos \theta)^2,
\]

\[
E_{hh, hh} = -\gamma_{1z} + 2\gamma_{33}^2k_z^2 + 3\gamma_{33}^2k_y^2,
\]

Quantum Hall effect is connected with intersubband transitions of bulk GaN. Quantum Hall effect is specified as spin Hall effect [27, 28, 29, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41]. The intrinsic Hall conductivity can write as follows [86]

\[
\sigma^{\text{int}} = e^2 \int d^2k f(k)\Omega(k),
\]

where in planar specified space
$$d^2 k = \frac{dk}{(2\pi)^2},$$

(256)

$f(k)$ is Fermi-Dirac distribution function. The generic form of Berry curvature is defined by expression [86]

$$\Omega_j(k) = \hat{z} \cdot \nabla_k \times \{ v_j(k) | t \nabla_k v_j(k) \},$$

(257)

where $|v_j(k)|$ is the periodic part of the Bloch function and $j$ is the band index. The Berry curvature [86] of bulk GaN which are shown to be connected with intraband phototransitions with $C_{6v}$ point group symmetry is specified like

$$\Omega_j(k) = \hat{z} \det \begin{vmatrix} e_x & e_+ & e_3 \\ K^{(e)} & K^{(i)} & K^{(v)} \\ 0 & 0 & 3\gamma_z k_z \sin(\phi) \sin(\theta) \end{vmatrix} = e_+ K^{(i)} 3\gamma_z k_z \sin(\phi) \sin(\theta) - e_- K^{(v)} 3\gamma_z k_z \sin(\phi) \sin(\theta).$$

(258)

Since Theta function of Hévithaide is specified like

$$\theta(x) = \lim_{k \to -\infty} \frac{1}{1 + \exp(-2kx)},$$

(259)

then $f(k) = \frac{1}{\exp(B_\mu - \mu/2)} = \theta(-\frac{x + u}{2})$ is Fermi-Dirac distribution function at the temperature $T = 4.4K$.

$$\sigma^{int} = \frac{e^2}{\pi} \frac{1}{(2\pi)^2} 2\pi \int k_1 dk_1 dk_2 \theta(-\frac{x + u}{2})(e_x K^{(i)} - e_- K^{(v)}) 3\gamma_z k_z \sin(\phi) \sin(\theta),$$

(260)

Table 13. Datasets for the valence band effective mass parameters $A_i$, where $i = 1..6$, for the deformation potentials $D_j$, where $j = 1..4$ in meV and for the energy parameters $\Delta_1 = \Delta_{cr}$ as well as $\Delta_2 = \Delta_3 = \Delta_{cr}/3$ in meV for bulk GaN materials, and elastic constants $C_{ij}$ in GPa.

<table>
<thead>
<tr>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$A_4$</th>
<th>$A_5$</th>
<th>$A_6$</th>
<th>$D_1$</th>
<th>$D_2$</th>
<th>$D_3$</th>
<th>$D_4$</th>
<th>$E_g$</th>
<th>$\Delta_1$</th>
<th>$\Delta_2$</th>
<th>$C_{13}$</th>
<th>$C_{33}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-6.56</td>
<td>-0.91</td>
<td>5.65</td>
<td>-2.83</td>
<td>-3.13</td>
<td>-4.86</td>
<td>700</td>
<td>2100</td>
<td>1400</td>
<td>-700</td>
<td>3507</td>
<td>16</td>
<td>4</td>
<td>106</td>
<td>398</td>
</tr>
</tbody>
</table>

Table 14. Datasets for the concentrations of holes $p$ in $cm^{-3}$, the temperatures $T$ in $K$, the Fermi energies $E_F$ of holes of bulk GaN in $meV$, the Fermi wave vectors $k_F$ of holes in $cm^{-1}$ at the dimensionless wave vector of three dimensional space of bulk GaN $k_0^{2-dim}$ in $cm^{-1}$.

<table>
<thead>
<tr>
<th>$p$</th>
<th>$T$</th>
<th>$E_F$</th>
<th>$k_F$</th>
<th>$k_0^{2-dim}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.5 \times 10^{16}$</td>
<td>4.4</td>
<td>23.01</td>
<td>0.15</td>
<td>1.38 $\times 10^4$</td>
</tr>
<tr>
<td>$10^{16}$</td>
<td>4.4</td>
<td>23.27</td>
<td>0.095</td>
<td>1.38 $\times 10^4$</td>
</tr>
<tr>
<td>$10^{15}$</td>
<td>4.4</td>
<td>24.335</td>
<td>1.38 $\times 10^4$</td>
<td></td>
</tr>
</tbody>
</table>

We have found the upper bound for specify definite integral of wave vectors by solving the following equations $\frac{-x + u}{2} = 0$. In the table 10 the upper bound are shown to be related with the Fermi wave vectors $k_F$ of holes and we have found that for holes of bulk GaN $k_1^{upper bound} = k_2^{upper bound} = k_F$.

4.7 Exciton insulator states in $ZnO/(Zn,Mg)O$ quantum wells: Theoretical study

In the low-energy limit the Hamiltonian of würtzite

$$\hat{H}_0 = I(\Delta_1 + \Delta_2) + \Delta_1 J_z^2 + \Delta_2 J_z \sigma_z + \sqrt{2}\Delta_3 (J_+ \sigma_- + J_- \sigma_+),$$

(261)

$$\begin{align*}
\hat{H}_k &= A_1 \epsilon^2 + A_2 \epsilon^2 + (A_3 \epsilon^2 + A_4 \epsilon^2) J_z^2 + A_5 \epsilon^2 (2[J_+ J_- J_+] + 2[J_+ J_- J_-]) + A_6 (J_z^2 \epsilon^2 + J_z^2 \epsilon^2) + iA_7 (J_+ \epsilon_- J_- - J_- \epsilon_+ J_+), \\
\hat{H}_l &= D_1 \epsilon_{zz} + D_2 \epsilon_{zz}^2 + (D_3 \epsilon_{zz} + D_4 \epsilon_{zz}) J_z^2 + D_5 (2[J_+ J_- \epsilon_{zz}^2]_{+} + 2[J_+ J_- \epsilon_{zz}^2]_{-}) + D_6 (J_z^2 \epsilon_{zz}^2 - J_z^2 \epsilon_{zz}^2). 
\end{align*}$$

(262) (263)

In the basis of spherical wave functions with the orbital angular momentum $l = 1$ and the eigenvalue $m_l$ of its $z$ component:
\[ |1, \zeta_\nu\rangle = \frac{1}{\sqrt{2}}(Y^1_1 \psi(1/2)e^{-3i\pi/2}e^{-3i\pi/4} \pm Y^{-1}_1 \psi(-1/2)e^{3i\pi/2}e^{3i\pi/4}) \]
\[ |2, \zeta_\nu\rangle = \frac{1}{\sqrt{2}}(Y^1_1 \psi(-1/2)e^{3i\pi/2}e^{-3i\pi/4} + Y^{-1}_1 \psi(1/2)e^{-3i\pi/2}e^{3i\pi/4}) \]
\[ |3, \zeta_\nu\rangle = \frac{1}{\sqrt{2}}(Y^1_1 \psi(1/2)e^{-i\pi/2}e^{-i\pi/4} + Y^{-1}_1 \psi(-1/2)e^{i\pi/2}e^{i\pi/4}) \]

(264)

the Hamiltonian may be transformed to the diagonal form indicating two spin degeneracy \[ |1, \zeta_\nu\rangle \]
\[ H_{\pm} = \begin{pmatrix} F & K_t & \mp iH_t \\ K_t & G & \Delta \mp iH_t \\ \pm iH_t & \Delta \pm iH_t & \lambda \end{pmatrix} \]
\[ |1, \zeta_\nu\rangle \]
\[ H_{\pm} = \begin{pmatrix} F & K_t & \mp iH_t \\ K_t & G & \Delta \mp iH_t \\ \pm iH_t & \Delta \pm iH_t & \lambda \end{pmatrix} \]
\[ |2, \zeta_\nu\rangle, |3, \zeta_\nu\rangle \]

where \( F = \Delta_1 + \Delta_2 + \lambda + \theta, \) \( G = \Delta_1 - \Delta_2 + \lambda + \theta, \) \( \lambda = \lambda_2 + \lambda_x, \) \( \theta = \theta_1 + \theta_2, \lambda_k = \frac{\kappa}{2m_0}(A_1 k_z^2 + A_2 k_y^2), \) \( \lambda_\epsilon = D_1 \epsilon_{zz} + D_2(\epsilon_{xx} + \epsilon_{yy}), \) \( \theta_\epsilon = D_3 \epsilon_{zz} + D_4(\epsilon_{xx} + \epsilon_{yy}), \) \( K_t = \frac{\kappa}{2m_0}(A_3 k_z^2), \) \( H_t = \frac{\kappa}{2m_0}(A_6 k_x k_z), \) \( \Delta = \sqrt{\epsilon_3} \lambda_3, k_z^2 = k_x^2 + k_y^2. \)

From Kane model one can define the band-edge parameters such as the crystal-field splitting energy \( \Delta_{\sigma \sigma}, \) the spin-orbit splitting energy \( \Delta_{so}, \) the e\( \perp z \) polarization: \( P_z \equiv \langle S|\hat{p}_z|Z\rangle, \) \( P_z \equiv \langle S|\hat{p}_z|X\rangle \equiv \langle S|\hat{p}_z|Y\rangle. \)

We consider a quantum well of width \( w \) in ZnO under biaxial strain, which is oriented perpendicularly to the growth direction (0001) and localized in the spatial region \(-w/2 < z < w/2. \) In the ZnO/MgZnO quantum well structure, there is a strain-induced electric field. This piezoelectric field, which is perpendicular to the quantum well plane (i.e., in \( z \) direction) may be appreciable because of the large piezoelectric constants in wurtzite structures.

The transverse components of the biaxial strain are proportional to the difference between the lattice constants of materials of the well and the barrier and depend on the Mg content \( x: \) \( \epsilon_{xx} = \epsilon_{xy} = \frac{m_{ZnO} - m_{MgZnO}}{m_{ZnO}}. \)

The physical parameters for ZnO are as follows. We take the effective-mass parameters Table 15, 16: \( A_1, A_2, A_3, A_4, A_5, A_6, m_{\sigma \perp}, m_0, \) where \( m_0 \) is the electron rest mass in the vacuum, the parameters for deformation potential: \( D_1, D_2, D_3, D_4, D_5, D_6, D_7, \) in meV and the energy parameters at 300 K: \( E_g, \Delta_1, \Delta_2/3, \Delta_3/3 \) in meV, the elastic constant: \( C_{13} \) and \( C_{33} \) in GPa, the permittivity of the host materials \( \kappa. \)

\[ \begin{array}{cccccccccc}
| & A_1 & A_2 & A_3 & A_4 & A_5 & A_6 & m_{\sigma \perp} & D_1 & D_2 & D_3 & D_4 & D_5 & D_6 & D_7 & E_g |\\
\hline
| & -2.743 & -0.393 & 2.377 & -2.069 & -2.051 & -2.099 & 0.329m_0 & -3800 & -3800 & -800 & 1400 & -6860 & -6260 & 3400 |
\end{array} \]

\[ \begin{array}{cccccc}
\Delta_1 & \Delta_2/3 & \Delta_3/3 & C_{13} & C_{33} & \kappa |
\hline
36.3 & 0.63 & 2.47 & 90 & 196 & 7.8 |
\end{array} \]

### ZnO/(Zn,Mg)O quantum well

We take the following wave functions written as vectors in the three-dimensional Bloch space:

\[ |\nu, \zeta_\nu, k_z\rangle = \sum_{n=1}^{m} \psi_{n(1)}[\nu, \lambda, \zeta_\nu] \psi_1(Z) \]
\[ |\nu, \zeta_\nu, k_z\rangle = \sum_{n=1}^{m} \psi_{n(2)}[\nu, \lambda, \zeta_\nu] \psi_1(Z) \]
\[ |\nu, \zeta_\nu, k_z\rangle = \sum_{n=1}^{m} \psi_{n(3)}[\nu, \lambda, \zeta_\nu] \psi_1(Z) \]

(266)

The Bloch vector of \( \nu \)-type hole with spin \( \zeta_\nu = \pm 1/2 \) and momentum \( k_z \) is specified by its three coordinates \( [\psi_{k_z}[m, n]] \).

\( \psi_{n(1)}[m, n], \psi_{n(2)}[m, n], \psi_{n(3)}[m, n] \) in the basis \([1, \zeta_\nu], [2, \zeta_\nu], [3, \zeta_\nu] \) \[13\]

known as spherical harmonics with the orbital angular momentum \( l = 1 \) and the eigenvalue \( m_\sigma \) its \( z \) component. The envelope \( Z \)-dependent part of the quantum well eigenfunctions can be specified from the boundary conditions \( \psi_m(Z = 0) = \psi_m(Z = 1) = 0 \) of the infinite quantum well as

\[ \psi_m(Z) = \sqrt{\frac{2}{w}} \sin(\pi m Z), \]

(267)
where \( Z = (\frac{Z}{w} + \frac{1}{2}) \), \( m \) is a natural number. Thus the hole wave function can be written as

\[
\Psi_{\nu \xi, k_z}(r) = \frac{e^{ik_z r}}{\sqrt{A}} \psi_{\nu \xi, k_z}(r).
\]  
\[(268)\]

The valence subband structure \( E_{\nu}^{(j)}(k_z) \) can be determined by solving equations system:

\[
\sum_{j=1}^{m}(H_{ij}^{(j)}(k_z) = -i \frac{\partial}{\partial z} + V(z) + \delta_{ij}E_{\nu}^{(j)}(k_z)) \phi_{\nu}^{(j)}(z, k_z) = 0,
\]  
\[(269)\]

where \( \phi_{\nu}(z, k_z) = \sum_{m=1}^{\infty} \Psi_{k_z}^{(m)}(n, \nu) \psi_{n}(z), j = 1, 2, 3. \)

The wave function of electron of first energy level with accounts QCSE \[125\]:

\[
\Psi(r) = \frac{1}{\sqrt{A}} e^{i(k \cdot \rho)} \Psi(Z, \xi) |S| |\xi|, \quad \Psi(Z, \xi) = \begin{cases} 
\psi_1(Z, \xi) = C_1 e^{i(k_0 - \xi)(w Z)}, Z \in (-\infty, 0), \\
\psi_2(Z, \xi) = C_2 \sin(k_0 w (Z - \frac{1}{2}) + \delta_0)e^{-Z^{-\frac{1}{2}}}, Z \in [0, 1], \\
\psi_3(Z, \xi) = C_3 e^{-i(k_0 + \xi)w(Z - 1)}, Z \in (1, \infty).
\end{cases}
\]  
\[(270)\]

\(|S| = Y_0^0, |\xi| = \pm 1/2.\)

From bond conditions \[125, 114\]:

\[
\psi_1(Z, \xi)|_{Z=0} = \psi_2(Z, \xi)|_{Z=1} = \psi_3(Z, \xi)|_{Z=0} = \psi_3(Z, \xi)|_{Z=1} = 0,
\]

one can find \( C_1 = C \sin(-k \frac{w}{2} + \delta_0)e^{\frac{\xi}{2}}, C_2 = C \sin(k \frac{w}{2} + \delta_0)e^{-\frac{\xi}{2}}, \quad C_3 = \frac{k_0 w}{\sin k_0 w}, \delta_0 = \frac{k_0 w}{2} + \arctan \frac{k_0}{k_0 w}, \) where \( \Lambda \) is the area of the quantum well in the xy plane, \( \rho \) is the two-dimensional vector in the xy plane, \( k_z = (k_x, k_y) \) is in-plane wave vector. The constant multiplier \( C \) is found from normalization condition:

\[
\int_{-\infty}^{\infty} |\Psi(Z, \xi)|^2 w dZ = 1.
\]  
\[(272)\]

One can find the functional, which is built in the form:

\[
J(\xi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle},
\]  
\[(273)\]

where

\[
H = H_c + V(z),
\]  
\[(274)\]

where \( H_c \) is a conduction band kinetic energy including deformation potential:

\[
H_c = E_g + \Delta_1 + \Delta_2 + \frac{h^2}{2m_y^2} k_z^2 - \frac{h^2}{2m_z^2} \frac{\partial^2}{\partial z^2} + D_{cz} e_{zz} + D_{c_{zz}} (e_{xx} + e_{yy}).
\]  
\[(275)\]

Figure 7. (Color online) For the quantum well ZnO/Mg0.27Zn0.73O with a width 6 nm, at a carriers concentration \( 4 \times 10^{12} \text{ cm}^{-2} \), (a) conduction band energy; (b) valence band energy.
Figure 8. (Color online) For the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 6 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300K (Curve 4, Curve 6) Self-satisfied wave functions square; (Curve 1, Curve 3) Non Self-satisfied wave functions square.

Figure 9. (Color online) For the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 6 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300K (Curve 1) Self-satisfied Hartree-Fock screening potential; (Curve 2) Non Self-satisfied Hartree-Fock screening potential.

Figure 10. (Color online) For the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 6 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 300K (l) Self-satisfied charge density; (r) Non Self-satisfied charge density.
The potential energies $V(z)$ can look for as follows:

$$ V(z) = e\Phi^H(z) + \delta U_{c,v}(z) + \Phi_{xc}(z), \quad (276) $$

where $\Phi^H(z)$ is the solution of one-dimensional Poisson’s equation with the strain-induced electric field in the quantum well, $\delta U_{c,v}(z)$ are the conduction and valence band edge discontinuities which can be represented in the form  [126]:

$$ \delta U_{c}(z) = \begin{cases} U_0 - eEz(\frac{z}{w} + 1), & z \in (-\infty, -w/2) \\ eEz, & z \in [-w/2, w/2] \\ U_0 - eEz(\frac{z}{w} - 1), & z \in (w/2, \infty). \end{cases} \quad (277) $$

$\Phi_{xc}(z)$ is exchange-correlation potential energy which is found from the solution of three-dimensional Poisson’s equation includes local exchange-correlation potential for semiconductor of the space region $z$.

Hence we have replaced the Eqs. (98) in the space region $z > 0$ by of the three-dimensional Poisson’s equation includes local exchange-correlation potential for semiconductor of the space region $z > 0$ for moving of carriers in space confined quantum well along Oz axis in consideration of dipoles on interface of ferroelectric thin film in incommensurate phase/semiconductor nanoheterostructures as well as free charges for specifying of charge quantization.

The solution of equations system Eqs. (269), (273), (278) as well as Eqs. (269), (273), (279) does not depend from a temperature.

Solving one-dimensional Poisson’s equation Eq. (279) one can find screening polarization field and Hartree potential energy by substituting her in the Schrödinger equations. From Schrödinger equations wave functions and bandstructure

![Absorption coefficient](Image)

Figure 11. (Color online) Absorption coefficient for the quantum well ZnO/Mg$_{0.27}$Zn$_{0.73}$O with a width 6 nm, at a carriers concentration $4 \times 10^{12}$ cm$^{-2}$, at a temperature 310 K.
are found. The conclusive determination of screening polarization field is determined by iterating Eqs. (269), (273), (278) until the solutions of conduction and valence band energies and wave functions are converged:

\[
\Phi^H(z) = \Phi^H_0(z) + \Phi^H(e_z(z)),
\]

(283)

\[
e^{i\Phi^H_E(z)} = \frac{2\pi}{h} \sum_{\nu, m, l, \nu_1} g_1 \int k_l d k_l (v_1, v_2, \nu_1, \nu_2, [v, m] \Psi_{\nu_1 [v, l]}(v_1, v_2), f_{v, p}(k_1)) \times
\]

\[
\begin{align*}
&\left(\frac{\cos \pi \frac{2l}{m} (m+n)}{\frac{\pi}{2} l (m+n)^2} - \frac{\cos \pi \frac{2l}{m} (m-l)}{\frac{\pi}{2} l (m-l)^2}\right) m \neq l,
&\left(\frac{\cos \pi \frac{2l}{m} (m+n)}{\frac{\pi}{2} l (m+n)^2} + \frac{\cos \pi \frac{2l}{m} (m-l)}{\frac{\pi}{2} l (m-l)^2}\right) m = l,
\end{align*}
\]

(284)

\[
e^{i\Phi^H_E(z)} = \frac{2\pi}{h} g_1 \int k_l d k_l C^2 f_{1m}(k_1) \times
\]

\[
\begin{align*}
&\left\{1 - \cos(-k_0 z + 2 k_m)\right\} e^{-\frac{2k_0^2}{2\pi^2}} \int_{-2w/2}^{2w/2} z e^{-\xi w} e^{-2k_0^2 + \frac{2k_0^2}{2\pi^2}} (\xi^2 - k_0^2) + \sin 2(k_0 z + 2k_m) e^{-2k_0^2}iz^0, z \in (-\infty, -w/2]
&\left\{1 - \cos(k_0 z + 2k_m)\right\} e^{-\frac{2k_0^2}{2\pi^2}} \int_{w/2}^{\infty} z \in (w/2, \infty),
\end{align*}
\]

(285)

where \( z = z + \frac{1}{2}, g_1 \) and \( g_1 \) correspond to the degeneration of the \( v \) hole band and the first quantized conduction band, respectively, \( e \) is the value of electron charge, \( k_0 \) is the permittivity of a host material, and \( f_{v, p}(k_1), f_{1m}(k_1) \) are the Fermi-Dirac distributions for holes and electrons.

Exchange-correlation charge density may be determined as:

\[
\rho^{xc}_{\nu, \nu_1}(k_f, \nu) = \sum_{\nu_1} \int_{-2\xi w}^{2w/2} \rho^{xc}_{\nu, \nu_1}(k_f, \nu) \left| \Psi_{\nu_1 [\nu, l]}(k_f, \nu) \right|^2 Y_{\nu_1 \nu}(\frac{\rho - \rho'}{|\rho - \rho'|}),
\]

(286)

using the expansion of plane wave

\[
\sum_{\nu=0}^{\infty} \int_{-2\xi w}^{2w/2} \rho^{xc}_{\nu, \nu_1}(k_f, \nu) \left| \Psi_{\nu_1 [\nu, l]}(k_f, \nu) \right|^2 Y_{\nu_1 \nu}(\frac{\rho - \rho'}{|\rho - \rho'|}) =
\]

\[
ed^i\xi k \rho = 4 \pi \sum_{\nu=0}^{\infty} \int_{-2\xi w}^{2w/2} i^l j_l(k_f, \rho) Y_{\nu_1 \nu}(k_f, \nu) Y_{\nu_1 \nu}(\frac{\rho - \rho'}{|\rho - \rho'|}).
\]

(287)

At the condition \( [\Psi_{\nu, \nu_1}(k_f, \nu) \sin k_f \rho] << 1 \), the solution Eq. (280) may be found as follows

\[
\Phi_{\nu, \nu_1}(x_c) = \int_{0}^{|\rho - \rho'|} \rho \rho_{00}(\rho) \frac{1}{\rho} d \rho.
\]

(288)

The solution the three-dimensional Poisson’s equation may be presented in the form:

\[
\Phi_{\nu, \nu_1}^{xc}(x_c) = \Phi_{\nu, \nu_1}^{xc}(z) \Phi_{\nu}(x_c).
\]

(289)

The complete potential which describes piezoelectric effects and local exchange-correlation potential in quantum well one can find as follows

\[
\Phi(z) = \Phi_{\nu, \nu_1}^{H}(z) + \Phi_{\nu, \nu_1}^{H}(z) \Phi_{\nu}(x_c) + \Phi_{\nu, \nu_1}^{H}(z) \Phi_{\nu}(x_c).
\]

(290)

### 4.7.2 Uncertainty Heisenberg principle

The excitons in semiconductors have been studied by [46, 128].

The Heisenberg equation for a microscopic dipole \( \hat{p}_{\nu, \nu_1}^{v, y} = (\hat{b}_p \hat{a}_p) \) due to an electron-hole pair with the electron (hole) momentum \( p (\bar{p}) \) and the subband number \( v_e (v_h) \) is written in the form:

\[
\frac{\partial \hat{p}_{\nu, \nu_1}^{v, y}}{\partial t} = i \frac{\hbar}{\hbar} [\hat{H}, \hat{p}_{\nu, \nu_1}^{v, y}].
\]

(291)

We assume a nondegenerate situation described by the Hamiltonian \( \hat{H} = \hat{H}_0 + \hat{V} + \hat{H}_{int} \), which is composed of the kinetic energy of an electron \( e_{\nu, p}^{v} \) and the kinetic energy of a hole \( e_{\nu, p}^{v_h} \) in the electron-hole representation:

\[
\hat{H}_0 = \sum_p e_{\nu, p}^{v} \hat{a}_p^{\dagger} \hat{a}_p + e_{\nu, p}^{v_h} \hat{b}_{-p}^{\dagger} \hat{b}_{-p},
\]

(292)

where \( p \) is the transversal quasimomentum of carriers in the plane of the quantum well, \( \hat{a}_p, \hat{a}_p^{\dagger}, \hat{b}_{-p}, \) and \( \hat{b}_{-p}^{\dagger} \) are the annihilation and creation operators of an electron and a hole. The Coulomb interaction Hamiltonian for particles in the electron-hole representation takes the form:
The transition frequency is the Coulomb potential of the quantum well, \( k \) is the dielectric permittivity of a host material of the quantum well, and \( A \) is the area of the quantum well in the \( xy \) plane. The Hamiltonian of the interaction of a dipole with an electromagnetic field is described as follows:

\[
\hat{H}_{\mathrm{int}} = -\frac{A}{\hbar} \sum_{\nu,\nu',\mu} ((\mu_{p})^{\nu}_{\nu'}E^{e,i\omega t} + (\mu_{p})^{\nu'}_{\nu}E^{e,-i\omega t}),
\]

where \( \mu_{p}^{\nu}_{\nu'} = (\hat{b}_{-p}\hat{a}_{q}) \) is a microscopic dipole due to an electron-hole pair with the electron (hole) momentum \( p \) \((-p)\) and the subband number \( \nu \) \((\nu')\), \( \mu_{k}^{\nu,\nu'} = \int d^{3}r U_{j'}^{\nu'} \epsilon \hat{p} U_{j,\nu}^{\nu} \) is the matrix element of the electric dipole moment, which depends on the wave vector \( k \) and the numbers of subbands, between which the direct interband transitions occur, \( e \) is a unit vector of the vector potential of an electromagnetic wave, \( \hat{p} \) is the momentum operator. Subbands are described by the wave functions \( U_{j,\nu}^{\nu'} \), \( U_{j'}^{\nu'} \), where \( j' \) is the number of a subband from the conduction band, \( \nu' \) is the electron spin, \( j \) is the number of a subband from the valence band, and \( \sigma \) is the hole spin. We consider one lowest conduction subband \( j' = 1 \) and one highest valence subband \( j = 1 \). \( E \) and \( \omega \) are the electric field amplitude and frequency of an optical wave.

The polarization equation for the wurtzite quantum well in the Hartree-Fock approximation with regard for the wave functions for an electron and a hole written in the form [40, 27], where the coefficients of the expansion of the wave function of a hole in the basis of wave functions (known as spherical functions) with the orbital angular momentum \( l = 1 \) and the eigenvalue \( m_{l} \) of its \( z \) component, depend on the wave vector can look for as follows:

\[
\frac{d\rho_{p}^{\nu,\nu'}}{dt} = -i\omega_{p}^{\nu,\nu'}\rho_{p}^{\nu,\nu'} - i\Omega_{p}^{\nu,\nu'}(-1 + \hat{r}_{p}^{\nu} + \hat{n}_{p}^{\nu'}).
\]

The transition frequency \( \omega_{p}^{\nu,\nu'} \) and the Rabi frequency with regard for the wave function [40, 27] are described as

\[
\omega_{p}^{\nu,\nu'} = \frac{-\hbar}{\sum_{q} V^{\nu,\nu',\nu}_{q}} \left( \sum_{q} \frac{1}{E_{q,p}^{e} + \epsilon_{q,p}^{\nu,\nu'}} \right),
\]

\[
\Omega_{p}^{\nu,\nu'} = \frac{1}{\sum_{q} V^{\nu,\nu',\nu}_{q}} \left( \sum_{q} \frac{1}{E_{q,p}^{h} + \epsilon_{q,p}^{\nu,\nu'}} \right),
\]

where \( e_{q,p}^{\nu,\nu'} \) - Hartree-Fock energies for electron and holes,

\[
\frac{1}{2} \sum_{q} \frac{1}{2\pi} \int d\varphi \sum_{g} g_{\alpha} \int d\zeta \times
\]

\[
\times \int d\zeta' \int d\zeta \chi_{n_{1}}(\zeta) \chi_{m_{1}}(\zeta) \chi_{n_{2}}(\zeta' \times \chi_{m_{2}}(\zeta')) \times
\]

\[
\times e^{-i\zeta'z_{1}C_{p}^{i}n_{1,1}V_{p}^{i}m_{1,1}} = n_{1} = n_{2} = m_{2} = 1,
\]

\[
Q_{1} = q + p.
\]
where $\chi_n(z)$ is the envelope of the wave functions of the quantum well, $V^p_j[m_1, 1]$ and $C^j[n_1, 1]$ are coefficients of the expansion of the wave functions of a hole and electron at the envelope part, $\varphi$ is the angle between the vectors $p$ and $q$, and $g_\alpha$ is a degeneracy order of a level.

Numerically solving this integro-differential equation, we can obtain the absorption coefficient of a plane wave in the medium from the Maxwell equations:

$$\alpha(\omega) = \frac{\omega}{\kappa n c E} \mathrm{Im} P,$$

(300)

where $c$ the velocity of light in vacuum, $n$ is a background refractive index of the quantum well material,

$$P = \frac{2}{A} \sum_{\gamma, \nu, \mu} (\mu^p_\gamma)^* \rho^p_\nu e^{-i \omega t}.$$

(301)

The light absorption spectrum presented in the paper in Fig. 11, reflects only the strict TE ($x$ or $y$) light polarization.

From Uncertainty Heisenberg principle:

$$\Delta x \Delta p \geq \frac{\hbar}{2},$$

(302)

can be found the localization range particle-hole pair $\Delta x \geq \frac{n}{4mc}$.

Table 17. The localization range particle-hole pair $\Delta x$ in cm, exciton binding energy $Ry$ in meV, carriers concentration $n = p$ in cm$^{-2}$, Bohr radius $a_B$ in cm.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>Ry</th>
<th>$n = p$</th>
<th>$a_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.95 x 10$^{-10}$</td>
<td>2.16</td>
<td>4 x 10$^{12}$</td>
<td>4.26 x 10$^{-6}$</td>
</tr>
</tbody>
</table>

Hence the exciton Bohr radius is grater than the localization range particle-hole pair, and the excitons may be spontaneously created.

### 4.7.3 Results and discussions

We consider QCSE in strained wurtzite ZnO/Mg$_{0.27}$Zn$_{0.73}$O quantum well with width 6 nm, in which the barrier height is a constant value for electrons and is equal to $U_0 = 536.22$ meV. The theoretical analysis of piezoelectric effects and exchange-correlation effects is based on the self-consistent solution of the Schrödinger equations for electrons and holes in quantum well of width $W$ with including Stark effect and the Poisson equations. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes along the polarization field distribution the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition.

We have calculated carriers population of the lowest conduction band and the both heavy hole and light hole valence band. Solving Eq. (269) for holes in the infinitely deep quantum well and finding the minimum of functional Eq. (278) for electrons in a quantum well with barriers of finite height, we can find the energy and wave functions of electrons and holes with respect to Hartree potential and exchange-correlational potential in a piezoelectric field at a carriers concentration $n = p = 4 \times 10^{12}$ cm$^{-2}$. The screening field is determined by iterating Eqs. (269), (273), (278) until the solution of energy spectrum is converged.

The Hartree-Fock dispersions of the valence bands and the conduction band are presented in Fig. 10. The light absorption spectrum presented in the paper in Fig. 11. It is found that the localization range particle-hole pair $\Delta x \geq \frac{n}{4mc} \sim 9.95 \times 10^{-10}$ cm. Exciton binding energy is equal Ry=2.16 meV at carriers concentration $n = p = 4 \times 10^{12}$ cm$^{-2}$. Bohr radius is equal $a_B = 4.26 \times 10^{-6}$ cm.

If the exciton Bohr is grater than the localization range particle-hole pair, the excitons may be spontaneously created. We consider the pairing between oppositely charged particles with complex dispersion. The Coulomb interaction leads to the electron-hole bound states scrutiny study of which acquire significant attention in the explanations of high-temperature superconductivity. If the exciton Bohr radius is grater than the localization range particle-hole pair, the excitons may be spontaneously created.

It is found that $E_{(\text{Hartree-Fock band gap})} - E_{(1\text{exciton})} = 0.2$ meV If the electron and hole are separated, their energy is higher on 0.2 meV than if they are paired. Hence it can be energetically favorable for them to be paired.

If the Hartree-Fock band gap energy is greater than the exciton energy in ZnO/(Zn,Mg)O quantum wells then excitons may be spontaneously created. It is known in narrow-gap semiconductor or semimetal then at sufficiently low temperature the insulator ground state is instable with respect to the exciton formation [83, 70], leading to a spontaneously creating of excitons. In a system undergo a phase transition into a exciton insulator phase similarly to Bardeen-Cooper-Schrieffer (BCS) superconductor.

An exciton insulator states with a gap 3.4 eV are predicted. The particle-hole pairing leads to the Cooper instability.
4.7.4 Appendix: Matrix elements of interband transitions

\[ J_+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \]  
\[ J_- = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \]  
\[ J_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \]  
\[ J_2^+ = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \]  
\[ J_2^- = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \]  
\[ J_2^z = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \]  
\[ 2[J_z J_+] = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}, \]  
\[ 2[J_z J_-] = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \]  
\[ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]  
\[ \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \]  
\[ \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \]

4.7.5 Conclusions

In this paper a theoretical studies of the space separation of electron and hole wave functions in the quantum well ZnO/Mg_{0.27}Zn_{0.73}O by the 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 local exchange-correlation potential are presented. The exchange-correlation potential energy is found from the solution of three-dimensional Poisson's equation, using both an expression by Gunnarsson and Lundquist [127], and following criterions. The criterion \( k_F > \sqrt{n/4} \) at carrier densities \( 4 \times 10^{12} \text{ cm}^{-2} \), at a temperature \( T=0 \text{ K} \) is carried as \( 1 > 0.1 \). The criterion does not depend from a width of well. The solution of equations system Eqs. (269), (273), (279) as well as Eqs. (269), (273), (278) does not depend from a temperature. The ratio of Coulomb potential energy to the Fermi energy is \( r_s = E_C/E_F = 0.63 < 1 \). The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes along the polarization field distribution the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition. The problem consists of the one-dimensional Poisson's equation solving of which may be found Hartree potential energy and three-dimensional Poisson's equation which is separated on one-dimensional and two-dimensional equations by separated of variables. At the condition that the ratio of wave function localization in the longitudinal z direction on transversal in-plane wave function localization is less 1. It is found that the localization range particle-hole pair \( \Delta x \geq \frac{n}{4mc} \sim 9.95 \times 10^{-10} \text{ cm} \). Exciton binding energy is equal \( Ry=2.16 \text{ meV} \) at carriers concentration \( n = p = 4 \times 10^{12} \text{ cm}^{-2} \). Bohr radius is equal \( a_B = 4.26 \times 10^{-6} \text{ cm} \). It is found that the exciton binding
energy is greater than the localization range particle-hole pair, and the excitons may be spontaneously created. If the electron and hole are separated, their energy is higher on 0.2 meV than if they are paired. Hence it can be energetically favorable for them to be paired. An exciton insulator states with a gap 3.4 eV are predicted. The particle-hole pairing leads to the Cooper instability.

4.8 Rashba spin-orbit splitting in wurtzite GaN nanotubes grown along c axis

It is known that the Hamiltonian for wurtzite GaN nanotubes in which the geometric axis of cylinder has coincided with hexagonal c axis of wurtzite may be transformed to the diagonal form indicating two spin degeneracy [13]:

\[
H_{\pm} = \begin{pmatrix}
F & K_t \\
K_t & G
\end{pmatrix} \pm \i H_t, \\
\Delta \pm \i H_t
\]

where \( F = \Delta_1 + \Delta_2 + \lambda + \theta, \) \( G = \Delta_1 - \Delta_2 + \lambda + \theta, \) \( \lambda = \lambda_1 + \lambda_2, \) \( \theta = \theta_1 + \theta_2, \) \( \lambda_k = \frac{n^2}{2m_0}(A_1k_x^2 + 2k_y^2), \) \( \lambda_1 = D_1\epsilon_{xx} + D_2(\epsilon_{yy} + \epsilon_{yy}), \) \( \theta_k = \frac{n^2}{2m_0}(A_2k_z^2 + 2k_y^2), \) \( \theta_e = D_3\epsilon_{xx} + D_4(\epsilon_{yy} + \epsilon_{yy}), \) \( K_t = \frac{n^2}{2m_0}(A_3k_x^2), \) \( H_t = \frac{n^2}{2m_0}(A_4k_z^2), \) \( \Delta = \sqrt{2}\Delta_3, \) \( k_z^2 = k_x^2 + k_y^2. \)

Hence the Schrödinger equations system are shown to be connected with the symmetry point group of \( C_{6v}. \)

The valence subband structure \( E_V(k_z) \) can be determined by solving equations system:

\[
\sum_{j=1}^{3}(H_{ij}^k(k_\rho) = -\i \frac{\partial}{\partial \rho} + \i \frac{\partial}{\partial \theta} + \frac{1}{2} \left( \i \frac{\partial}{\partial \phi} \right)^2 + V(\rho) + \delta_{ij}E_V(k_z))\phi^{(i)0}(\rho, k_z) = 0,
\]

where \( \phi^{(i)0}(\rho, k_z) = \sum_{n=1}^{m} \psi^{(i)}[n, \nu] \psi^{(i)}(\rho), \) \( j = 1, 2, 3. \) The solutions of Schrödinger equations can be found in the later form by premultiply the equations system Eq. (315) on \( \psi^{(i)}(\rho) \) functions and by integrating the later equations system on weighted orthogonality functions domain. It is known that in cylindrical coordinates the function \( f(x) \) at sufficiently general conditions can expand into series

\[
f(x) = \sum_{k=1}^{\infty} a_k J_m(\mu_k x),
\]

which is known as Fourier-Bessel series. Here \( \mu_1, \mu_2,... \) are specified as the positive zeroes of Bessel \( J_m(x) \) functions in increasing order as well as for the coefficients \( a_k \) the integral expression

\[
a_k = \frac{2}{[J_{m+1}(\mu_k)]^2} \int_0^1 tf(t)f_{m}(\mu_k t)dt.
\]

Weighted orthogonality functions condition can be specified as follows. If the solutions \( \mu_1, \mu_2,... \) were specified as two real zeroes of \( J_m(\rho) \) function then the following weighted orthogonality condition can specify:

\[
\int_0^1 J_m(\mu_1 x)J_m(\mu_k x)dx = \left\| \frac{1}{2} J_m'(\mu_1) \right\|^2 = \left\| \frac{1}{2} J_m'(\mu_k) \right\|^2 = 0, \quad \text{if } i \neq k.
\]

Certain integral formulas which contain the cylindrical functions:

\[
\int_0^x J_m(\alpha x)J_m(\beta x)dx = \frac{x}{\alpha^2 - \beta^2} [\alpha J_m(\beta x)J_{m+1}(\alpha x) - \beta J_m(\alpha x)J_{m+1}(\beta x)] = \frac{x}{\alpha^2 - \beta^2} [\beta J_{m-1}(\beta x)J_m(\alpha x) - \alpha J_{m-1}(\alpha x)J_m(\beta x)],
\]

if \( (\alpha^2 - \beta^2 \neq 0), \)

\[
\int_0^x [J_m(\alpha x)]^2 dx = \frac{x^2}{2} [J_{m}'(\alpha x)]^2 + \frac{1}{2} (x^2 - \frac{m^2}{\alpha^2}) [J_m(\alpha x)]^2,
\]

if \( m > -1 \) which have been known as Lommel integrals as well as

\[
\int_0^x x^{-m+n} J_m(\alpha x)dx = 2^{-m} \alpha^{m-n-1} \Gamma(n+1) \Gamma(m-n+1),
\]

if \( (-1 < n < 2m + 1) \).

The nabla or Hamiltonian operator in cylindrical system of coordinates was specified as

\[
\nabla = \frac{\partial}{\partial \rho} + \frac{1}{\rho} \frac{\partial}{\partial \phi} + \frac{\partial}{\partial z},
\]

as well as the Laplace operator was specified as
Figure 12. (Color online) wurzite GaN nanotubes: (a) Radius of nanotube $R = 5.2$ nm; (b) Radius of nanotube $R = 5$ nm; (c) Radius of nanotube $R = 4.8$ nm.
\[ \Delta = \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\omega^2}{\beta^2}. \]  

(323)

The physical parameters for GaN are as follows. We take the effective-mass parameters Table 18, 19: \( A_1, A_2, A_3, A_4, A_5, A_6, A_7 \), the parameters for deformation potential: \( D_1, D_2, D_3, D_4, D_{c1}, D_{c2} \) in meV, and the energy parameters at 300 K: \( E_g, \Delta_1, \Delta_2, \Delta_3 \) in meV, the lattice constants: \( c_{GaN} \) and \( c_{AlN} \) as well as \( a_{GaN} \) and \( a_{AlN} \) in Å.

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References
